

## Electronic Supplementary Information

### **Oxidative functionalization of yndiamides catalyzed by gold(I) or Brønsted acid systems: Computational study of mechanism, selectivity patterns, and effects of substituents**

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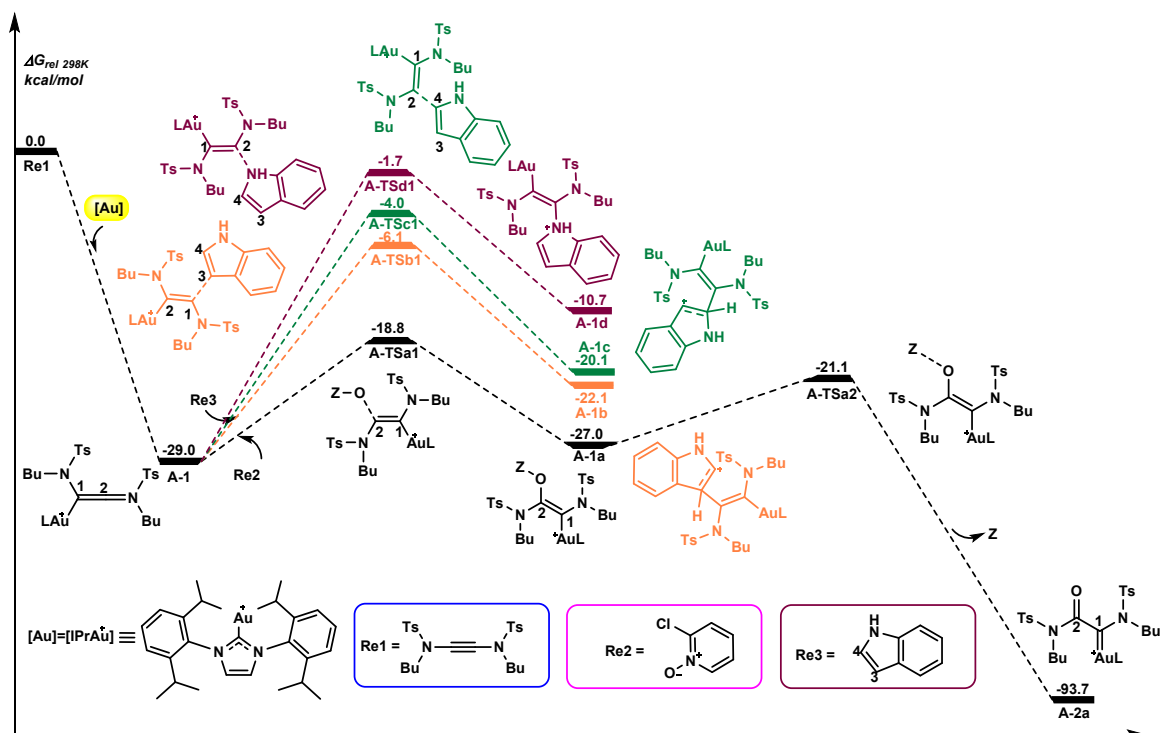


Figure S1 Full energy curves calculated for series A at the M06-D3/SMD/6-311++G(d, p) //B3LYP/6-31G(d, p) level. Relative energies are in kcal/mol.

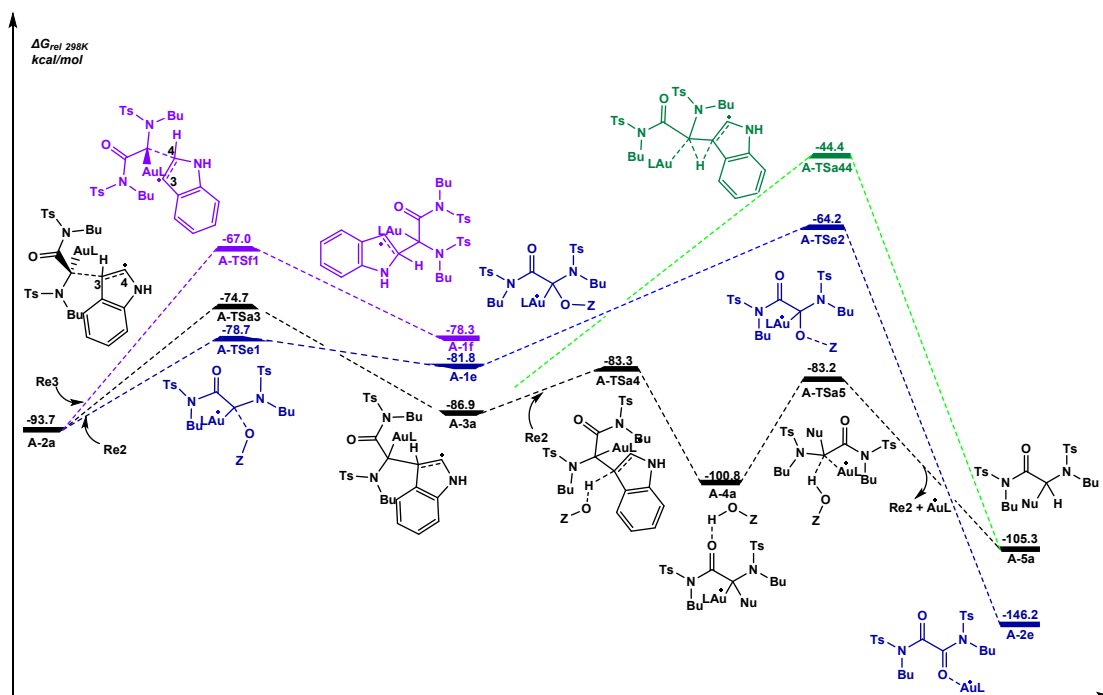


Figure S2 Full energy curves calculated for series A (continuation) at the M06-D3/SMD/6-311++G(d, p) //B3LYP/6-31G(d, p) level. Relative energies are in kcal/mol.



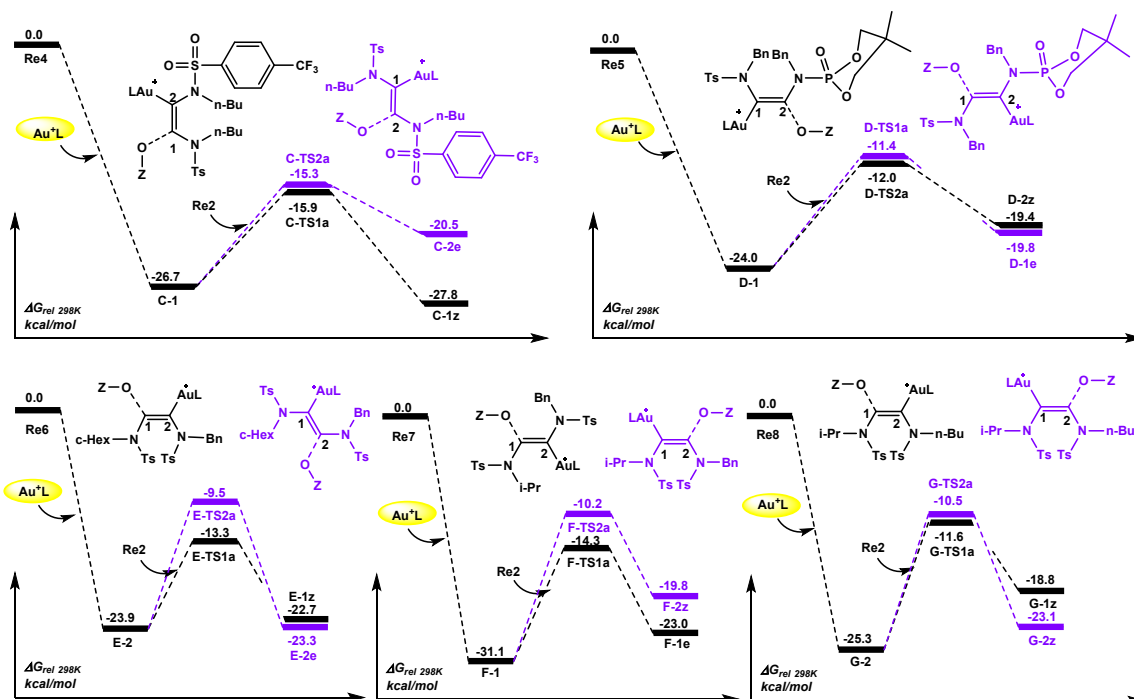


Figure S5. Energy profiles of the first steps of gold-catalyzed oxidative functionalization of asymmetrical yndiamides (Series C–G) at the M06-D3/SMD/6-311++G(d, p) //B3LYP/6-31G(d, p) level. Relative energies are expressed in kcal/mol.

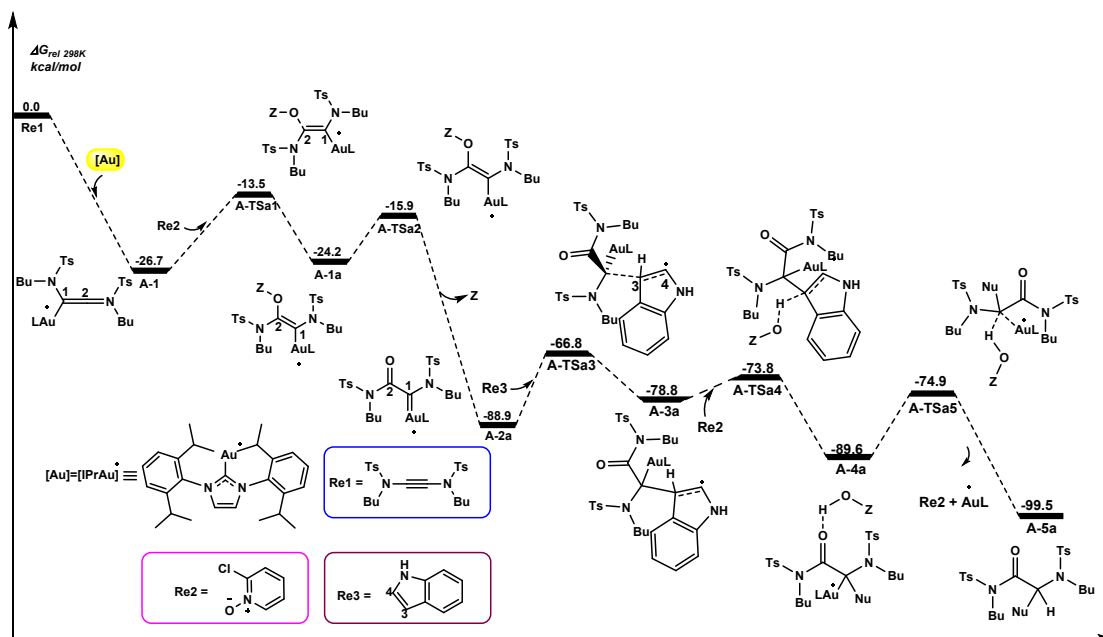


Figure S6 Full energy curves calculated for series A at the M06-D3/SMD/def2-TZVP//B3LYP/def2-SVP level. Relative energies are in kcal/mol.

**Table S1. Energy calculations for key transition states in the series A at two levels. Relative energies are in kcal/mol.**

	<i>M06-D3/6-311++G(d, p) //B3LYP/6-31G(d, p)</i>	<i>M06-D3/6-311++G(d, p) //M06/6-31G(d, p)</i>	<i>M06-D3/6-311++G(d, p)//B3LYP-D3/6-31G(d, p)</i>
A-TSd1	27.3	27.5	26.9
A-TSc1	25	26.7	24.2
A-TSb1	22.8	23.6	22.1
A-TSa1	10.1	12.8	9.9
A-TSe2	29.5	29.7	28.2
A-TSf1	26.7	24.1	24.1
A-TSa3	19	19.6	18.9
A-TSe1	15	16.2	14.9

**Table S2. Energy comparison with and without the dispersion feature added for key transition states in the series A. Relative energies are in kcal/mol.**

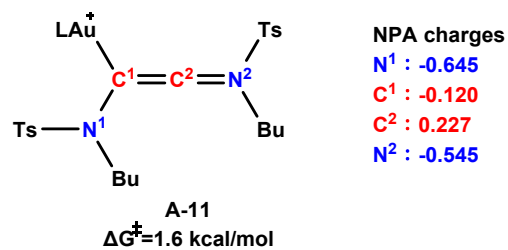
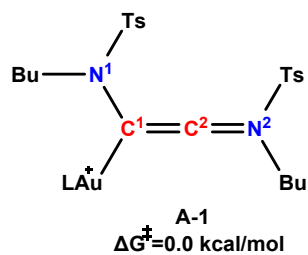
	<i>M06-D3/SMD/6-311++G(d, p) //B3LYP/6-31G(d, p)</i>	<i>M06-D3/SMD/6-311++G(d, p) //B3LYP/6-31+G(d)</i>
A-TSd1	17.2	16.1
A-TSc1	14.9	14.6
A-TSb1	12.7	11.8
A-TSa1	0.0	0.0
A-TSe2	14.5	16.2
A-TSf1	11.7	18.9
A-TSa3	4.0	11.3
A-TSe1	0.0	0.0

**Table S3. Considering solvent effects at the optimisation stage in the series A. Relative energies are in kcal/mol.**

	<i>M06-D3/SMD/6-311++G(d, p) //B3LYP/6-31G(d, p)</i>	<i>M06-D3/SMD/def2-TZVP //B3LYP-D3/SMD/def2-SVP</i>
A-TSa1	0.0	0.0
A-TSb1	12.7	14.4
A-TSc1	14.9	18.9
A-TSd1	17.2	16.5
A-TSe1	0.0	0.0
A-TSa3	4.0	3.2
A-TSf1	11.7	13.0
A-TSe2	14.5	13.8

**Table S4. Considering solvent effects at the optimisation stage in the series B. Relative energies are in kcal/mol.**

	<i>M06-D3/SMD/6-311++G(d, p)</i> <i>//B3LYP/6-31G(d, p)</i>	<i>M06-D3/SMD/def2-TZVP //</i> <i>B3LYP-D3/SMD/def2-SVP</i>
B-TSa1	0.0	0.0
B-TSb1	7.4	7.1
B-TSc1	6.6	10.6
B-TSd1	11.2	12.1
B-TSa3	0.0	0.0
B-TSe1	7.7	4.1
B-Tsg2	13.3	22.1
B-TSf1	16.0	15.6



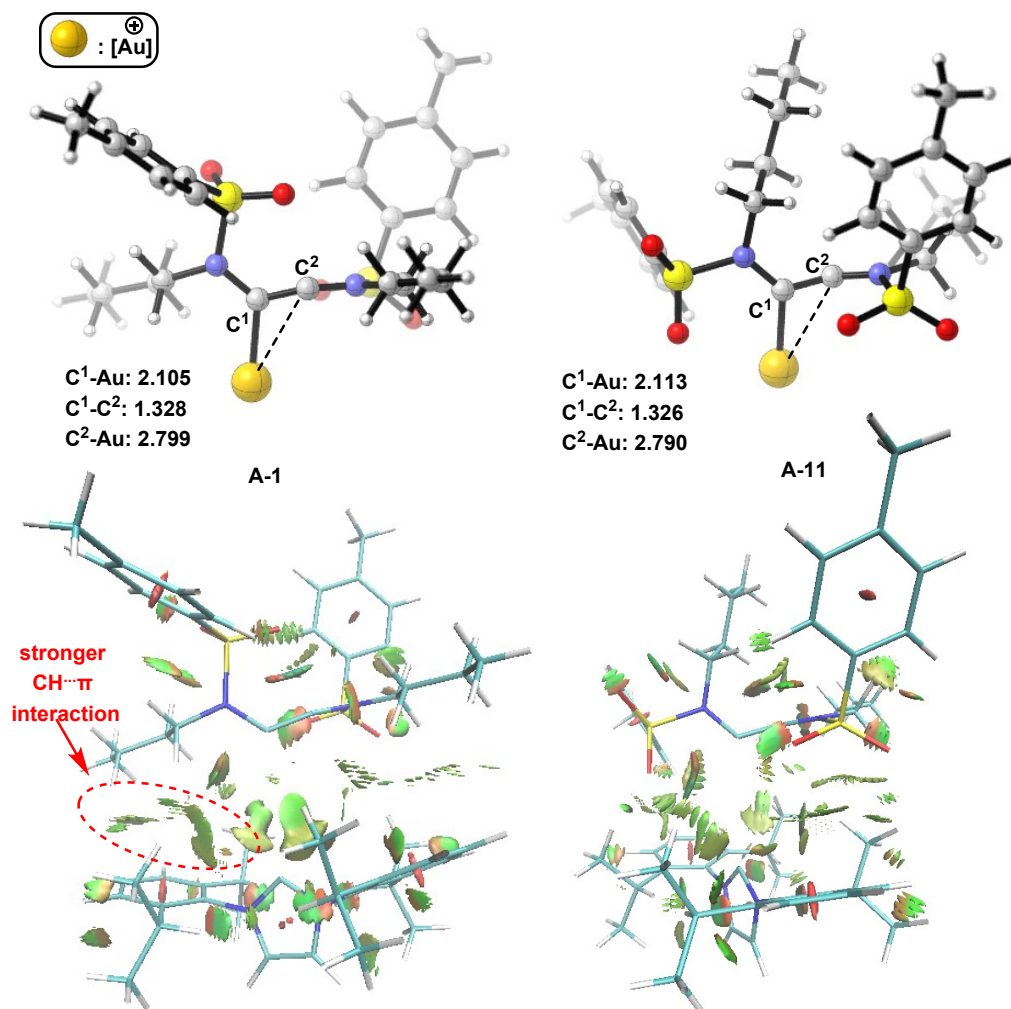


Figure S7. Calculated NBO charges (in e), 3D geometries and NCI analyses for key intermediates in the series A. Blue, green, and red surfaces represent the strong interaction, weak interaction, and steric effect, respectively.



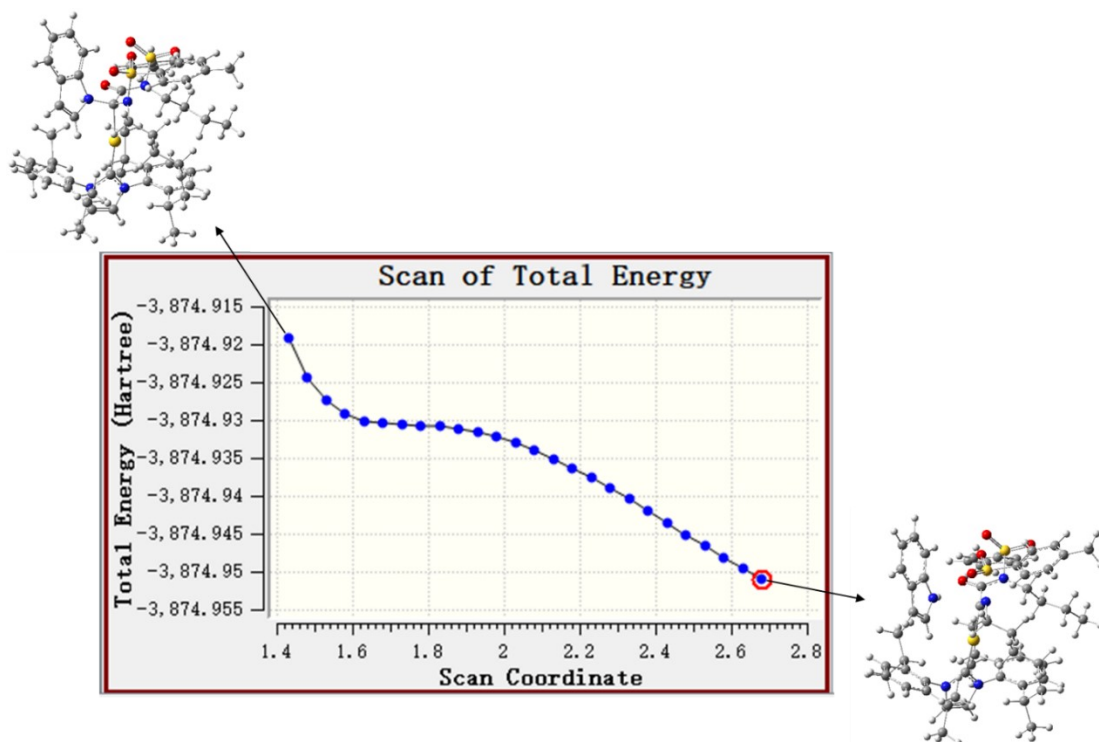


Figure S8. Scanning diagram of the C-N bond in the Re3 (N) attack mode.

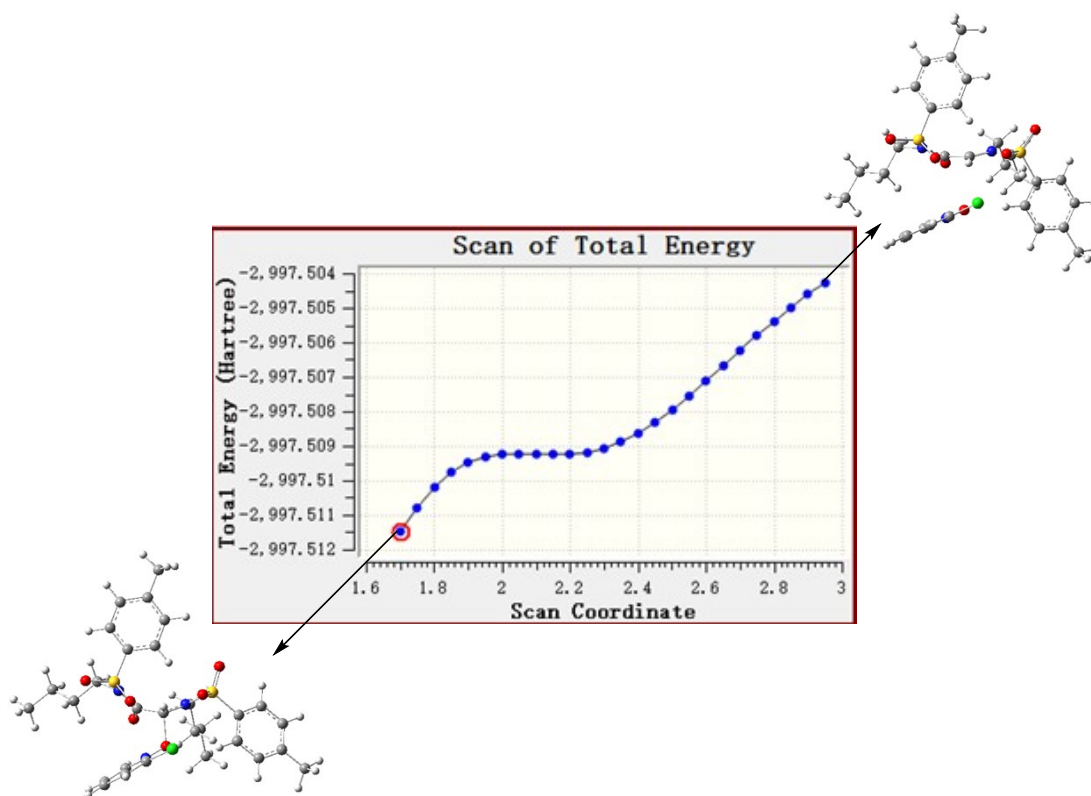


Figure S9. Scanning diagram of the C-O bond in the B-TSg1 at the B3LYP-D3/def2-SVP level. Although B-TSg1 is a no barrier process, B-TSg2 requires an extremely high barrier limiting the reaction pathway.

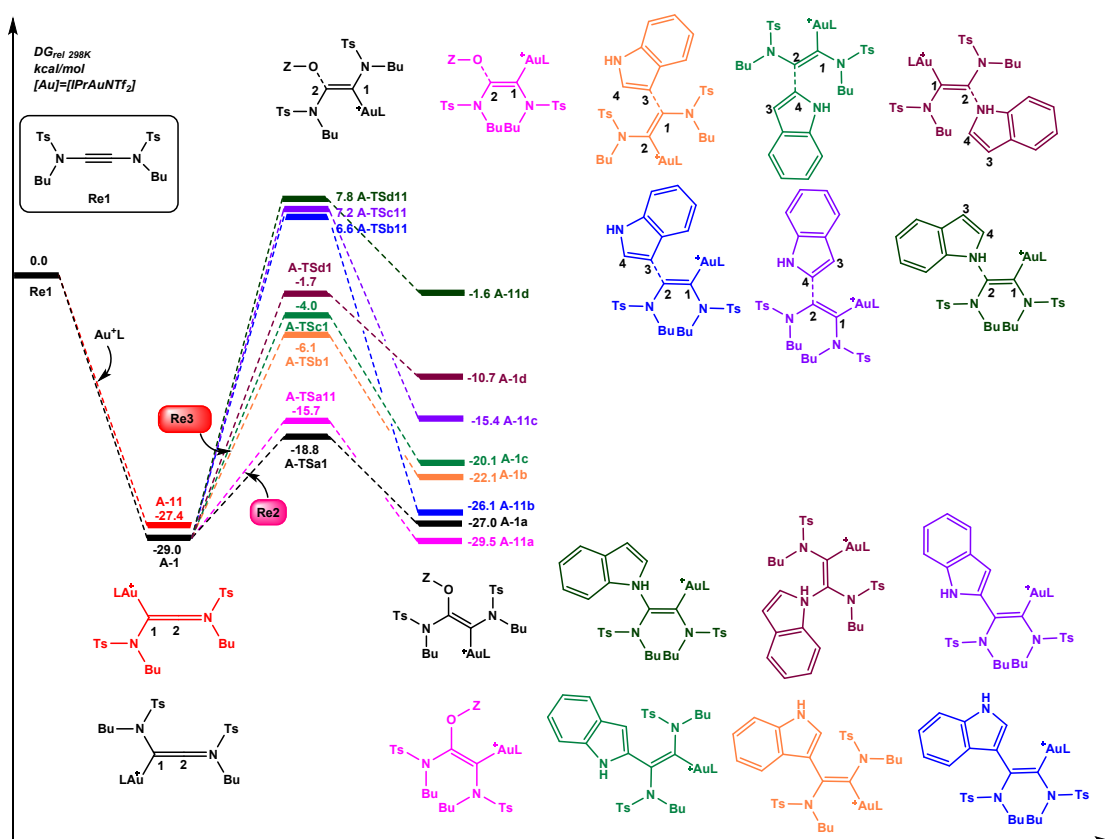


Figure S10. Different conformers and configurations of the transition states for the C-X (X=O, C, N) bond formation (series A). Energy values are in kcal/mol.

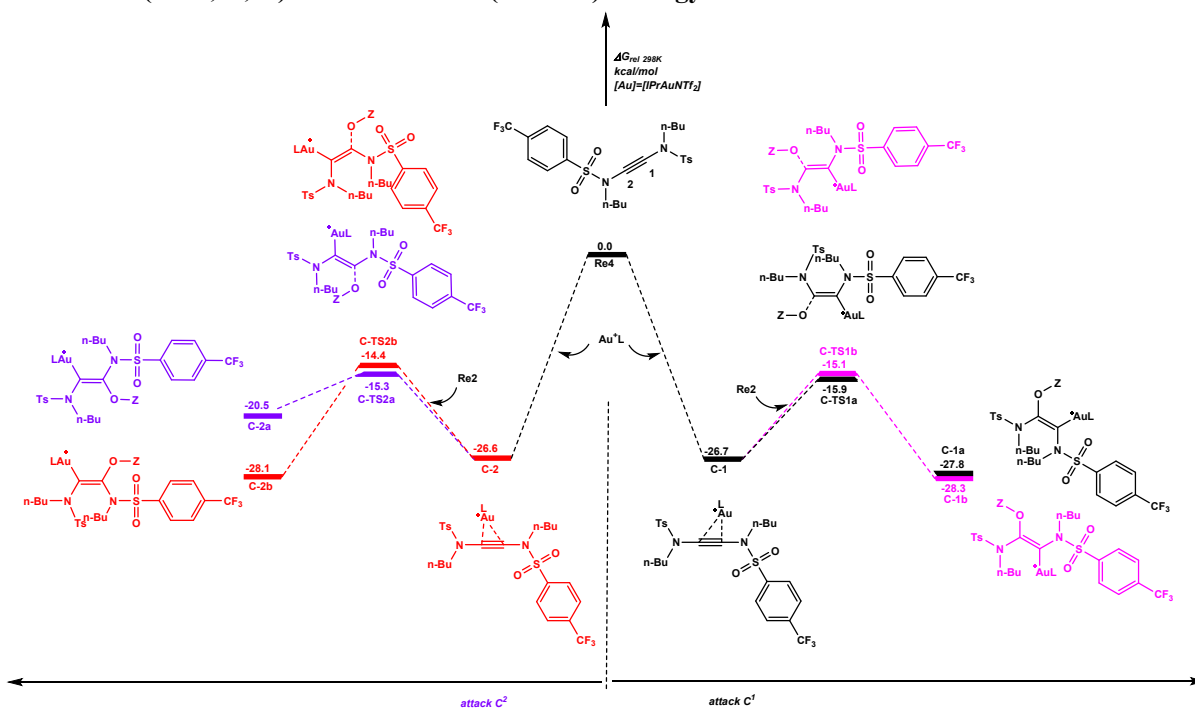


Figure S11. Different conformers and configurations of the transition states for the C-O bond formation (series C). Energy values are in kcal/mol.

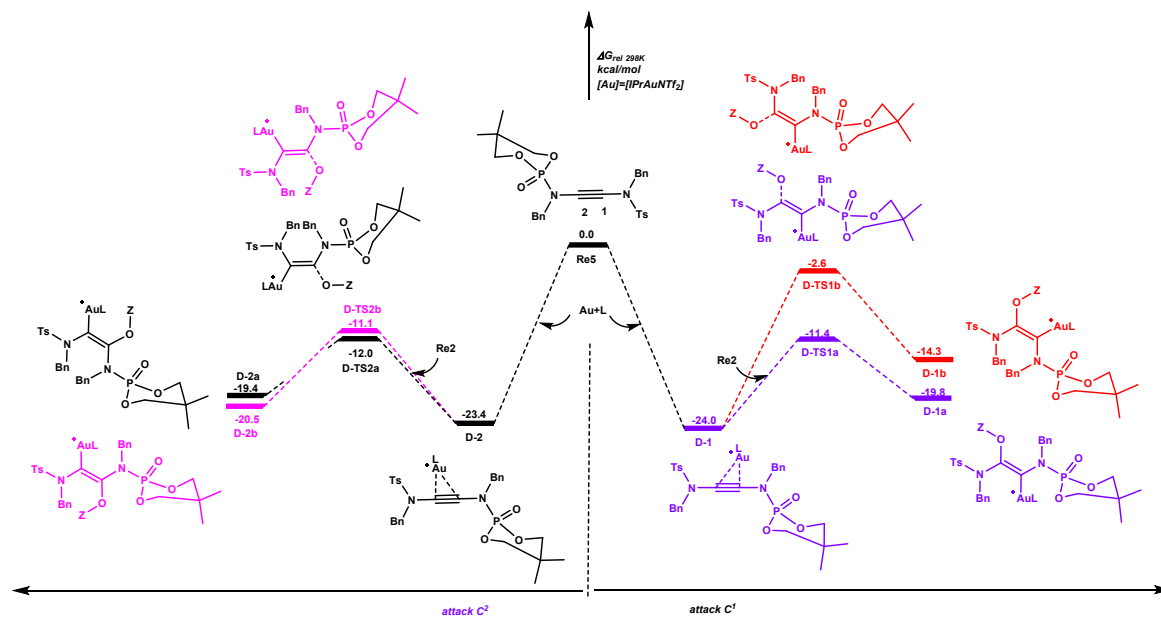


Figure S12. Different conformers and configurations of the transition states for the C-O bond formation (series D). Energy values are in kcal/mol.

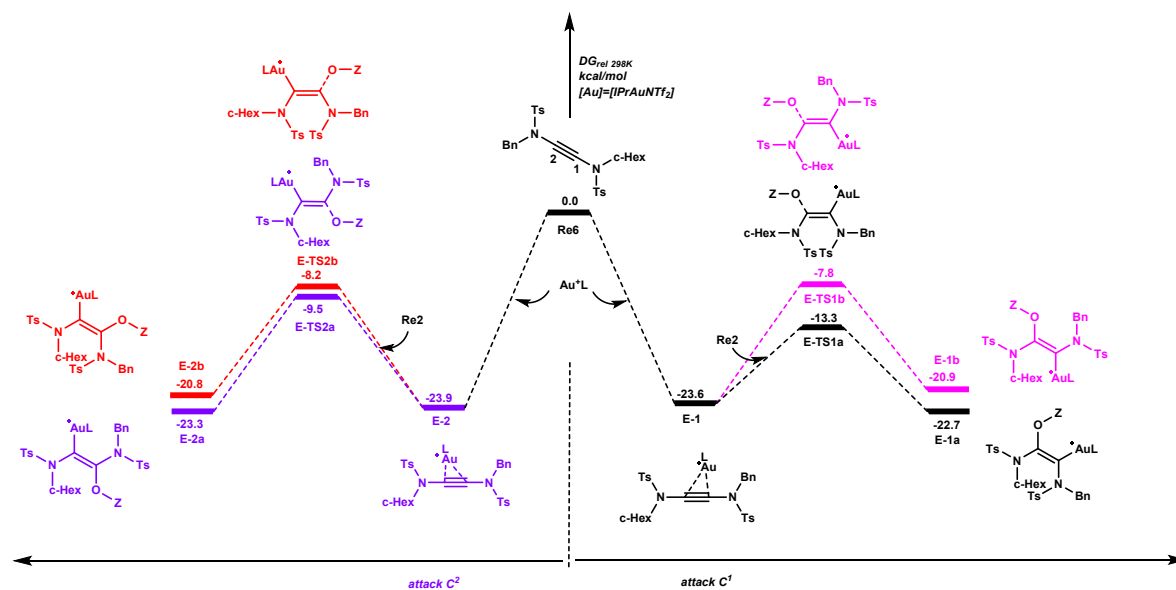


Figure S13. Different conformers and configurations of the transition states for the C-O bond formation (series E). Energy values are in kcal/mol.

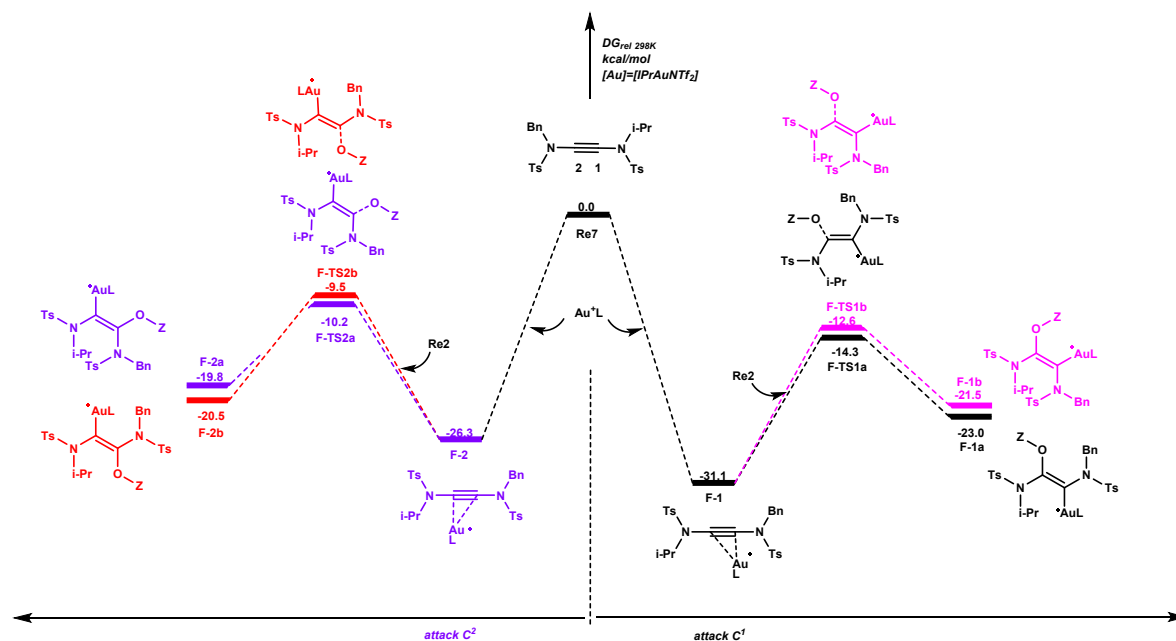


Figure S14. Different conformers and configurations of the transition states for the C-O bond formation (series F). Energy values are in kcal/mol.

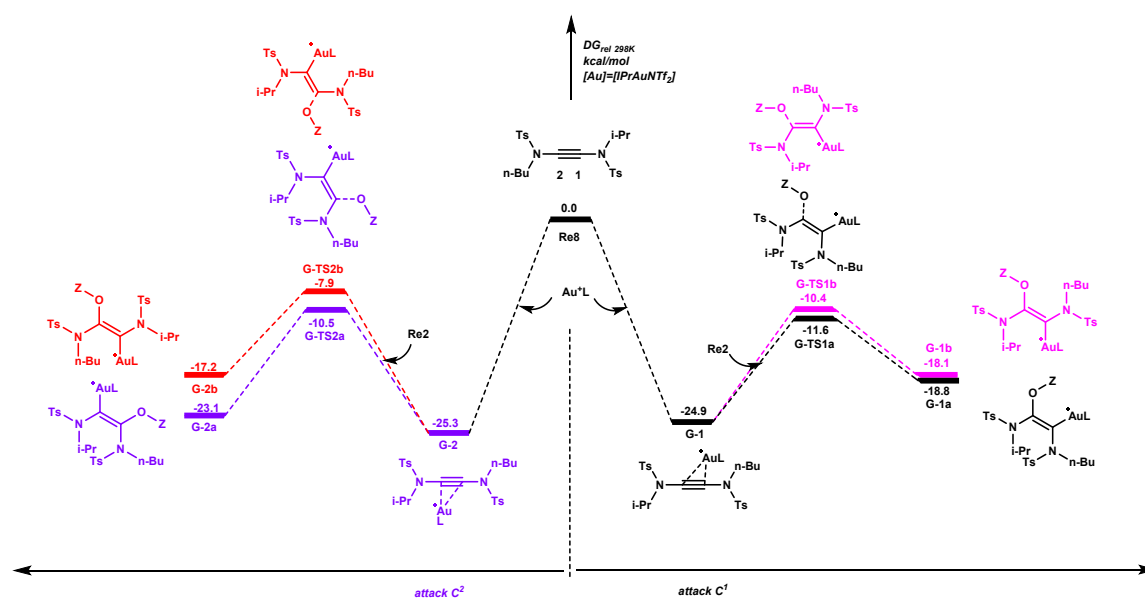


Figure S15. Different conformers and configurations of the transition states for the C-O bond formation (series G). Energy values are in kcal/mol.

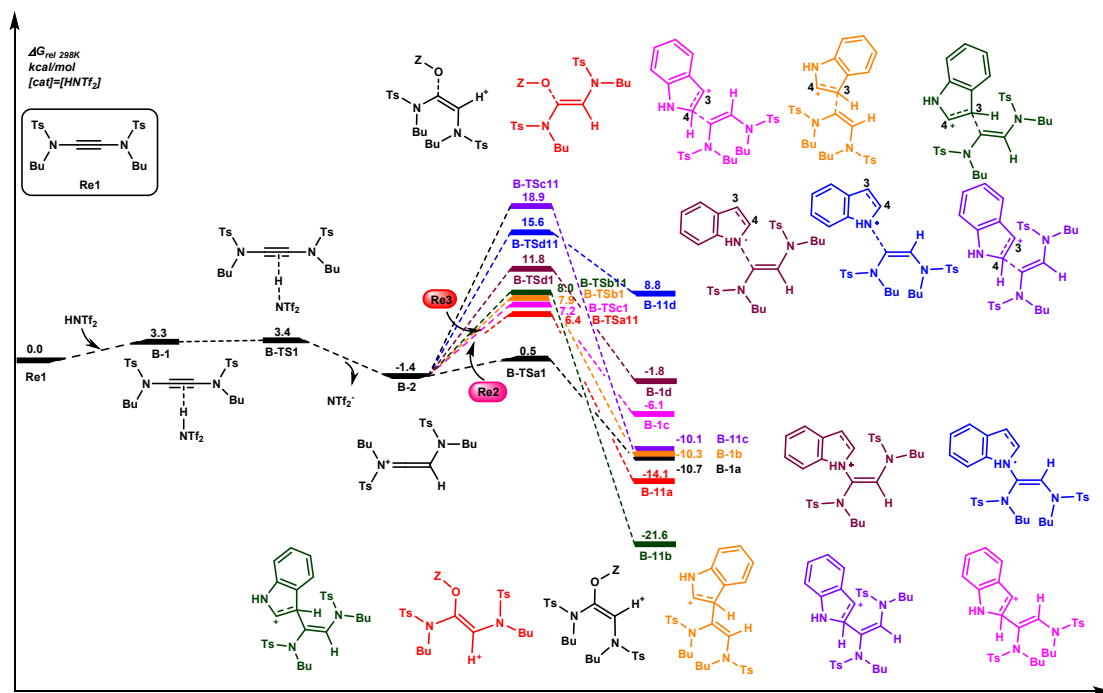


Figure S16. Different conformers and configurations of the transition states for the C-X (X=O, C, N) bond formation (series B). Energy values are in kcal/mol.

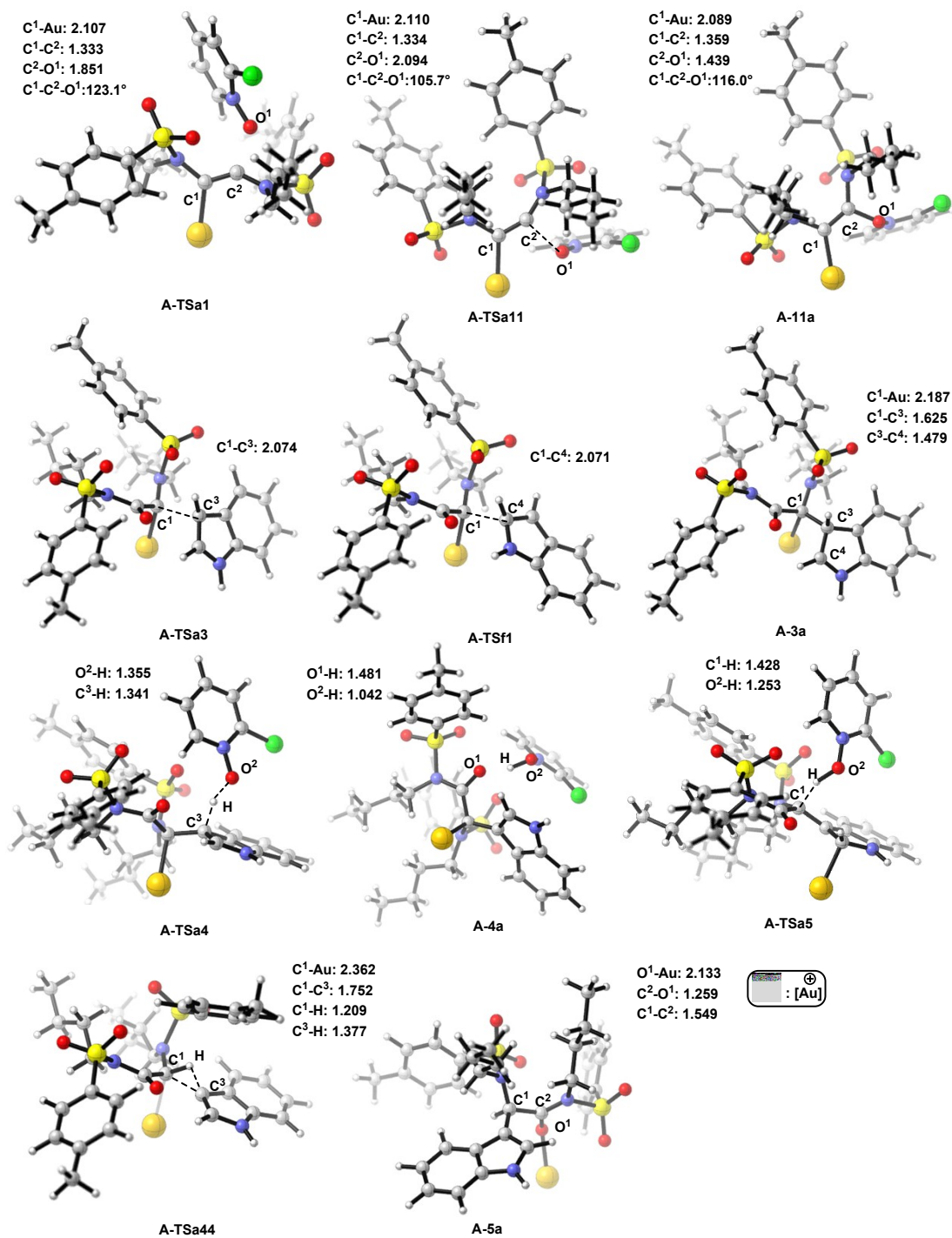
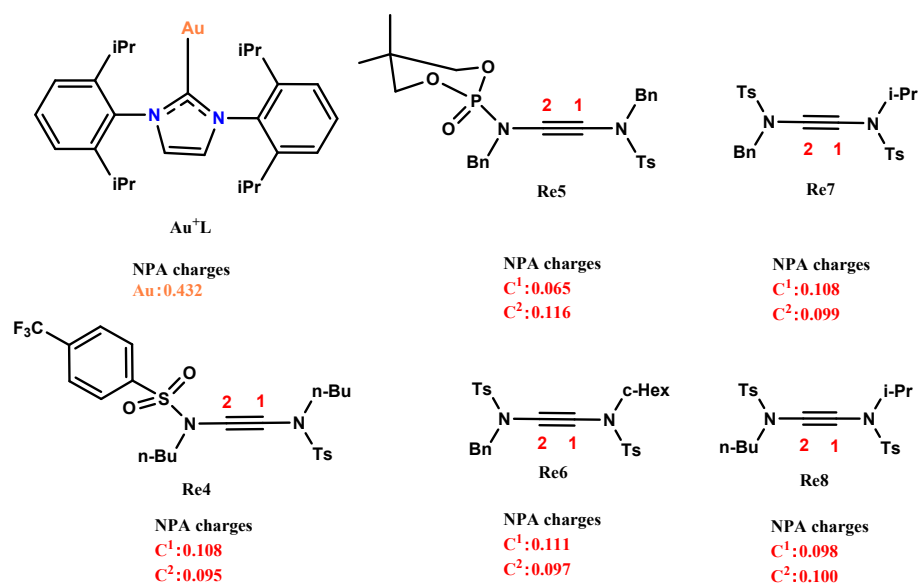


Figure S17. Optimized 3D geometries of series A. Bond lengths are in Å.



**Figure S18. Calculated NPA charges (in e) for Re4-Re8.**

## Cartesian coordinates of the stationary points

Au<sup>+</sup>L

79	-0.000002697	-0.000000376	-0.000001849
6	0.000003672	-0.000006397	0.000000695
6	-0.000007403	0.000009848	-0.000007911
6	0.000006326	-0.00000916	-0.000006296
1	-0.000001846	-0.000000503	0.000002026
1	0.00000221	0.000000582	0.000001623
7	-0.000004219	-0.000003133	0.000006137
7	0.000001664	0.000000445	0.000009086
6	0.000006245	-0.000007552	0.000002945
6	-0.000004924	-0.000001054	-0.000000334
6	-0.000001715	0.000004932	-0.000001784
6	0.000002038	0.000001694	-0.000001238
6	0.000002048	-0.000000574	0.0000009
6	-0.000001874	-0.000000171	-0.000000471
1	0.000000017	0.000000473	-0.00000001
1	0.000000638	0.000000395	-0.000000129
1	0.000000285	0.000000409	0.000000235
6	-0.000007645	-0.000003626	0.00000063
6	0.000002737	0.000005337	-0.000003342
6	0.000005555	-0.000002119	0.000002366
6	-0.000004061	-0.000001795	0.000000247
6	0.000000929	0.000001152	-0.000001196
6	0.000002319	0.000002097	-0.00000079
1	-0.000001176	-0.000000468	0.000000551
1	-0.000000076	0.000000059	0.000000086
1	-0.000000634	0.000000731	0.000000167
6	0.000000509	-0.000006013	-0.000000209
6	-0.000001636	0.000001431	0.000000511
6	0.00000295	0.000004007	0.000002875
1	-0.000002667	0.000002004	0.000000089
1	0.000000232	-0.000000444	-0.000000785
1	0.000000427	-0.000000057	-0.000000954
1	0.000000498	-0.000000288	-0.000000086
1	-0.000000713	0.000000242	-0.000000428
1	-0.00000058	-0.000000435	-0.000000088
1	-0.000000317	-0.000000696	-0.000000094
6	-0.000001737	0.000000183	-0.000004379
6	0.000000814	0.000007395	0.00000712



6	0.000001555	0.000000453	-0.00000181
1	0.000002444	0.000001565	0.000000897
1	0.000001092	0.000000075	-0.000003593
1	-0.000000036	-0.000001711	-0.000000112
1	0.000000562	-0.000001759	-0.000000227
1	0.000000199	0.000000398	0.000000525
1	0.000000274	0.000000361	0.000000827
1	-0.00000106	0.000000223	-0.000000173
6	-0.000000521	-0.000003697	-0.000002252
6	-0.000002237	0.000002302	0.000002812
6	0.000000659	-0.000000168	0.000002139
1	0.000001662	0.000000971	-0.000000639
1	0.000000348	-0.000000035	-0.000000738
1	0.00000013	-0.000000163	-0.000000534
1	0.00000134	-0.000000632	-0.000000566
1	-0.00000008	-0.000000549	-0.000000224
1	-0.000000274	0.000000483	-0.000001001
1	0.000000046	0.000000028	-0.000000651
6	0.000000271	-0.000000015	0.000001548
6	0.000000013	-0.000000687	-0.000001261
6	-0.000000726	0.000003822	0.000002961
1	-0.000001024	0.000000732	-0.000000892
1	-0.000000102	0.000000306	0.000000498
1	0.000000044	-0.000000088	0.000000119
1	-0.000000116	0.000000008	0.000000421
1	-0.000000152	-0.000000595	-0.00000019
1	-0.000000085	-0.000000023	-0.000000729
1	-0.000000092	-0.000000424	0.000000203

Zero-point correction=	0.572657 (Hartree/Particle)
Thermal correction to Energy=	0.605223
Thermal correction to Enthalpy=	0.606167
Thermal correction to Gibbs Free Energy=	0.504559
Sum of electronic and zero-point Energies=	-1294.803490
Sum of electronic and thermal Energies=	-1294.770924
Sum of electronic and thermal Enthalpies=	-1294.769980
Sum of electronic and thermal Free Energies=	-1294.871588

Re1

6	0.000002518	0.000002529	0.0000004
6	0.000002401	-0.000002598	-0.000003818
7	-0.000000723	0.000002911	-0.000005881
7	-0.000005278	-0.000004575	0.000001201
16	0.000004615	0.000003918	0.000001183
8	0.000004288	0.000000522	-0.000003258

8	-0.00000179	-0.00000111	-0.000006423
6	-0.000000108	-0.000000679	0.00000264
6	-0.000000071	0.000002012	-0.000001752
6	-0.000000021	0.000005124	0.000000666
6	-0.000000792	0.000003398	0.000000136
6	-0.000001617	0.000000339	-0.0000007
6	-0.000000835	0.000004066	-0.000001301
1	0.000001433	0.000002771	-0.00000103
1	-0.000000132	0.000003529	-0.000000382
1	-0.000000943	0.000002378	0.000000615
1	0.000000228	0.000000808	-0.00000006
6	-0.000001998	0.000004306	0.000000212
1	-0.000002626	0.000004529	0.000001697
1	-0.000001634	0.000004266	-0.000000696
1	-0.00000086	0.000002908	0.00000157
6	0.000002299	-0.000002104	0.000002869
6	-0.00000025	0.000000912	-0.000002836
1	0.000002274	-0.00000101	-0.000000905
1	0.00000193	0.000001222	-0.000002221
6	0.000000883	-0.000000964	0.000000037
1	0.000000685	-0.000000681	-0.000000586
1	0.000001281	0.000000487	-0.000000236
6	0.000002028	0.000000663	-0.000000498
1	0.000002391	0.000000438	-0.000002283
1	0.000002001	-0.000001255	-0.000001362
1	0.000000794	-0.000000162	-0.000000705
1	0.000000594	-0.000000558	-0.000000905
1	0.000001005	0.000000024	-0.000000443
6	-0.000000205	-0.000000891	0.000001576
6	-0.000004312	-0.000002148	0.000002451
1	-0.00000034	-0.00000134	0.000001575
1	-0.000001531	-0.000001502	0.000000186
6	-0.000003532	-0.000002441	0.000000346
1	-0.000000418	-0.000001462	0.00000055
1	0.000000698	-0.000002938	0.000001774
6	-0.000000939	-0.0000003	0.000004844
1	-0.000001916	-0.000000863	0.000000593
1	-0.000002026	-0.000002403	0.000002149
1	-0.00000459	-0.000001689	0.000003266
1	-0.00000173	-0.000000222	0.000000552
1	-0.00000204	-0.000004436	0.000001443
16	0.000005061	0.00000632	-0.000000011
8	0.000000065	-0.000009255	0.000002715
8	-0.000001067	-0.000005049	-0.000000195

6	0.00000764	0.00002923	-0.00002022
6	0.00000453	-0.00003435	-0.00003382
6	-0.0000147	-0.00003686	0.00005631
6	0.00000959	-0.00001773	0.00001613
1	0.00001421	-0.00000754	-0.00000971
6	0.00000417	-0.00003253	-0.00002188
1	-0.00000049	-0.00002107	0.00000737
6	-0.00002426	0.00004843	-0.00000562
1	0.00002317	0.00000758	-0.00001183
1	0.00000295	-0.00000797	0.00000854
6	0.00003665	0.00001351	-0.00000585
1	-0.00000799	-0.00000935	0.00000705
1	-0.00000425	-0.00001111	-0.00000239
1	-0.00000027	0.00000229	-0.00000077
<b>Zero-point correction=</b>			<b>0.526554 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>0.562200</b>
<b>Thermal correction to Enthalpy=</b>			<b>0.563144</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>0.450013</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-2139.935753</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-2139.900108</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-2139.899163</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-2140.012294</b>

## Re2

6	0.000293054	-0.000124358	0.000000454
6	0.000065234	0.000192653	0.000000163
6	-0.000273087	-0.0000955	-0.000000116
6	0.000280194	-0.000171839	0.000000156
6	-0.00002766	0.000129558	0.000000486
1	0.000026976	0.000048818	0.000000003
1	-0.000077203	-0.000013552	-0.000000023
7	-0.000339847	0.00003199	-0.000001902
8	0.000060784	0.000000854	0.000000767
1	-0.000045604	0.000009179	0.000000027
1	0.000001723	-0.000015665	-0.000000049
17	0.000035436	0.000007862	0.000000033
<b>Zero-point correction=</b>			<b>0.083412 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>0.089604</b>
<b>Thermal correction to Enthalpy=</b>			<b>0.090548</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>0.052545</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-782.958570</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-782.952378</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-782.951434</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-782.989437</b>

Re3

6	-0.000047117	0.000178025	0.000026371
6	-0.000080455	-0.000018268	-0.000112071
6	0.000002223	-0.000129103	-0.00001906
6	0.000101441	0.000097072	0.000015446
6	-0.000113708	0.000078376	0.000026887
6	0.000015328	-0.000161323	-0.000013795
6	-0.00029092	-0.000276189	-0.00005816
6	0.000526845	0.000098413	0.000080975
1	-0.000005093	0.000002713	0.000004403
1	-0.000006001	0.000001427	0.00000564
1	0.000010332	-0.000004363	-0.000013365
1	0.000005286	0.000009973	0.000008291
1	-0.00000772	0.000004374	0.000020401
1	-0.000127499	0.000032375	-0.000060934
7	0.000053859	0.000094466	0.000086032
1	-0.000036799	-0.000007969	0.000002942

Zero-point correction=			0.129871 (Hartree/Particle)
Thermal correction to Energy=			0.136183
Thermal correction to Enthalpy=			0.137127
Thermal correction to Gibbs Free Energy=			0.099550
Sum of electronic and zero-point Energies=			-363.700169
Sum of electronic and thermal Energies=			-363.693857
Sum of electronic and thermal Enthalpies=			-363.692913
Sum of electronic and thermal Free Energies=			-363.730490

A-1

6	0.000005962	0.000003775	-0.000006239
6	-0.0000057	0.00000119	0.000006608
7	-0.000001147	-0.000000677	0.000004832
7	0.000001277	-0.000003275	-0.00000525
16	-0.000004009	-0.00000371	0.000004139
8	0.000003825	0.000001888	-0.00000598
8	0.000002115	-0.000000283	0.000000881
6	0.000002051	-0.000000254	-0.000000351
6	-0.000000458	0.00000068	0.000000019
6	0.000001049	-0.000000143	-0.000003075
6	0.000000269	-0.000001079	0.000000059
6	0.000000944	0.000001703	-0.000000525
6	0.000000035	-0.000000841	-0.000001469
1	0.000001212	-0.000000453	-0.00000101
1	0.000001055	-0.000000276	-0.000001185

1	0.000000481	0.000000381	-0.000000612
1	0.000000582	0.000000095	-0.000000764
6	0.00000139	0.000000778	-0.000001223
1	0.000000628	0.000000496	-0.000001143
1	0.000000835	0.000000446	-0.000001484
1	0.000000652	0.000000651	-0.000001251
6	-0.00000193	0.000000212	-0.000003303
6	-0.000000683	-0.000001131	-0.000000683
1	0.000000772	-0.000000677	-0.000001409
1	0.000000839	0.000000061	0.000001024
6	0.000001769	-0.000000324	-0.000000674
1	0.000001177	-0.000000749	-0.000000029
1	0.00000008	0.000000171	-0.000000198
6	0.000000642	-0.000001656	-0.000001925
1	0.000000728	-0.000000496	-0.000001025
1	0.000000498	-0.000000208	-0.000001018
1	0.000001129	-0.000000068	-0.000001013
1	0.00000082	-0.000000803	-0.000000083
1	0.000000605	-0.000000337	-0.000000575
6	0.000003011	-0.00000135	0.000002457
6	-0.000001423	0.000002077	0.000001253
1	-0.000001504	-0.000000588	0.000000078
1	-0.000001048	-0.000000024	0.000000958
6	-0.000000035	0.000000088	0.000000061
1	-0.000000059	-0.000000003	0.000000155
1	-0.000000164	-0.000000963	0.000000255
6	-0.000000279	0.000000872	0.000001482
1	-0.000000595	-0.000000377	0.000000673
1	-0.000000918	-0.000000407	0.000000855
1	-0.000001313	0.000000426	0.000000844
1	-0.000000442	0.000000494	0.000000113
1	-0.000000059	0.000000746	0.000000791
16	-0.000000743	0.000000487	0.000001252
8	-0.000000886	0.000000904	-0.000000003
8	-0.000002102	-0.000003394	0.000000125
6	0.000001194	-0.000002887	-0.000000288
6	-0.000001128	-0.000000448	0.000000478
6	-0.000000315	-0.000000011	0.000002389
6	0.000000848	-0.000002269	0.000000292
1	0.000000052	-0.000001022	-0.000000016
6	-0.000000417	-0.000002224	0.000000331
1	-0.000000636	-0.000001742	-0.000000102
6	-0.000000699	-0.000000949	0.000000438
1	0.000000033	-0.000001564	-0.000000168

1	-0.00000598	-0.00001648	0.00001264
6	0.00000114	-0.00001754	0.00000638
1	-0.00000317	-0.000002	0.00000858
1	-0.00000255	-0.00002368	0.00000488
1	-0.0000001	-0.00001951	0.00000319
79	-0.00002542	0.00000712	-0.00002539
6	0.00004886	-0.00005413	0.00009746
6	0.00005917	0.00004767	-0.00001523
6	-0.00005672	-0.00000151	-0.00003001
1	0.00000658	0.00000927	0.00001083
1	-0.00000944	0.00000251	0.0000113
7	-0.00001578	0.00003135	-0.00005212
7	-0.00004684	0.0000076	-0.0000205
6	-0.00002679	-0.0000435	0.00002818
6	0.0000032	0.00002896	-0.00001194
6	0.00000146	0.0000201	-0.00001947
6	-0.00000189	-0.00000006	-0.00000607
6	0.00000964	-0.00001097	-0.00000387
6	0.00000484	0.00000036	-0.00000432
1	0.00000896	0.00000476	-0.0000094
1	0.00000171	-0.00000604	-0.00000614
1	0.00000582	-0.00000218	-0.00000951
6	0.00001271	-0.00000802	0.00003296
6	-0.00003664	0.00000718	-0.00000476
6	-0.00000697	0.00002572	0.00002157
6	0.0000053	-0.0000026	0.00001915
6	-0.00000581	0.00001182	0.00000314
6	-0.00001706	0.00000725	0.00000047
1	-0.00000794	0.00000037	0.00000669
1	-0.00000533	0.00000694	0.00000602
1	-0.00000642	0.0000074	0.0000136
6	0.00001543	0.00001601	0.00000121
6	-0.00000373	0.00001404	0.00001726
6	0.00000456	-0.00000496	0.00002541
1	0.00000574	0.00000115	0.00001028
1	-0.00001265	-0.00000508	0.00000697
1	-0.00001178	-0.00000039	0.00000968
1	-0.00000697	0.00000392	0.00001642
1	-0.00001031	0.00000085	-0.00000474
1	-0.00001328	-0.00000969	0.00001045
1	-0.00000826	-0.00000317	0.00001003
6	0.00003927	0.00003459	-0.00001759
6	-0.00003509	0.00000364	0.00000081
6	-0.00002381	-0.00000402	0.00001251

1	0.00000689	0.00001582	0.00000205
1	0.00000437	0.0000066	-0.00000174
1	0.00000047	0.00000538	-0.00000317
1	0.00000267	0.00002384	0.00000428
1	-0.00000305	0.00001605	0.00000305
1	0.00000448	0.00000858	-0.00000106
1	-0.00000429	0.00002009	0.00000261
6	0.00002128	-0.00000615	-0.00000421
6	-0.00001904	0.00000943	0.00000163
6	0.00000174	-0.00000493	0.00000399
1	0.00001423	-0.00000168	0.00000389
1	-0.00000064	-0.00001052	0.00000594
1	-0.00000184	-0.00000913	0.00000229
1	0.00001321	-0.00001856	-0.00000571
1	-0.00000222	0.00000101	0.00000218
1	-0.00000325	0.0000014	0.00000136
1	-0.00000695	-0.00000422	0.00000027
6	0.00002519	0.0000068	-0.00000426
6	-0.00001023	0.00001609	-0.00000329
6	-0.00001165	0.00000199	-0.00001501
1	-0.00000109	0.00001332	-0.00000355
1	0.00000495	0.00001082	-0.0000067
1	0.0000062	0.00001386	-0.00000852
1	0.00000876	0.00001054	-0.00000957
1	0.00000705	0.00000559	-0.00000814
1	0.00000974	0.00000965	-0.00001044
1	0.00000575	0.00001125	-0.00000607

Zero-point correction=	1.101424 (Hartree/Particle)
Thermal correction to Energy=	1.170698
Thermal correction to Enthalpy=	1.171643
Thermal correction to Gibbs Free Energy=	0.984372
Sum of electronic and zero-point Energies=	-3434.798009
Sum of electronic and thermal Energies=	-3434.728735
Sum of electronic and thermal Enthalpies=	-3434.727790
Sum of electronic and thermal Free Energies=	-3434.915061

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6	0.000010646	0.00001845	0.00001116
6	-0.000011031	-0.00000085	0.000003747
7	-0.00000693	0.00003538	0.00002315
7	0.000006653	-0.00000552	0.00001917
16	0.00002547	-0.00005961	-0.00002182
8	-0.00000515	0.00000331	0.00001275
8	-0.00003579	-0.00000217	0.00001016

6	-0.000002573	0.000000287	0.000001521
6	-0.000001807	0.000000877	0.000002795
6	-0.000002799	0.000000566	0.000002544
6	-0.000002687	0.00000111	0.000001484
6	-0.000004286	0.000000673	0.000000992
6	-0.000002042	0.000000806	0.000001701
1	-0.000001967	0.000000313	0.000002127
1	-0.000002872	0.000000489	0.000003021
1	-0.000003517	0.000000539	0.000001319
1	-0.000002486	0.000000033	0.000000288
6	-0.000003849	0.000000226	0.000002582
1	-0.000004556	0.000000992	0.000002289
1	-0.000004038	0.000000846	0.000002936
1	-0.000003944	0.000000881	0.00000304
6	0.000001258	0.000000458	-0.000000119
6	0.000000371	0.000000592	0.000002851
1	-0.000000505	-0.000000098	0.000002466
1	-0.000000788	0.000000562	0.000002093
6	0.000000062	0.000000427	0.000003071
1	0.000000816	-0.000000383	0.000001387
1	-0.000000434	0.000000277	0.000002272
6	0.000001106	0.000000072	0.000002835
1	-0.000000003	0.000000188	0.000003232
1	0.000000866	0.000000026	0.000002925
1	0.000001145	0.000000011	0.000003533
1	0.000001283	0.000000029	0.000002748
1	0.000000767	0.000000062	0.000003018
6	-0.000004152	0.000002184	-0.00000136
6	-0.000000484	-0.000001226	0.000001421
1	-0.000001444	0.000000197	0.000000469
1	-0.000002196	0.000000158	0.000000654
6	-0.000002045	0.000000039	0.000001273
1	-0.000000092	0.000000657	0.000001566
1	-0.000000732	0.000000383	0.000000773
6	-0.000001231	0.000000088	0.000001675
1	-0.000002294	0.000000353	0.000001353
1	-0.000001962	0.000000309	0.000001692
1	-0.000001873	0.000000547	0.000002514
1	-0.000001159	0.000000329	0.00000248
1	-0.000001304	0.000000415	0.000002022
16	-0.000001595	-0.000003731	0.000001776
8	-0.000003076	-0.000000636	-0.000003607
8	-0.000001185	0.00000119	-0.000001404
6	-0.000000906	0.00000129	-0.000000194



6	-0.000000503	-0.000000034	-0.000001146
6	0.000000104	0.000000103	-0.000001038
6	-0.000001218	0.000000388	0.000000172
1	-0.000001228	-0.000000094	-0.000000536
6	0.000001201	-0.000000956	-0.000000302
1	0.000000642	-0.000000334	-0.000000355
6	0.000000398	0.000000235	-0.000001363
1	-0.000000415	0.000000109	-0.000000375
1	0.000001204	0.000000024	-0.000000418
6	0.000001088	0.000000134	-0.000000681
1	0.000000927	-0.000000044	-0.000000176
1	0.000000864	-0.000000532	-0.000000353
1	0.000000903	-0.000000173	-0.000000271
79	-0.000000103	-0.000000535	-0.000002932
6	0.000000154	0.000003403	-0.000000125
6	0.000002226	0.000000602	-0.00000026
6	-0.000000051	-0.000000722	-0.000001148
1	0.000001756	-0.000000291	-0.000001655
1	0.000002129	-0.000000596	-0.000001941
7	0.000003334	-0.000002011	-0.000000133
7	0.000000877	-0.00000015	-0.000000238
6	0.000000647	-0.000001697	-0.000000376
6	0.00000223	0.000001578	-0.000001471
6	0.000002942	-0.000000412	-0.000001153
6	0.000001031	-0.000000952	-0.000002319
6	0.000003293	0.000001192	-0.00000102
6	0.000001309	-0.000000433	-0.000000928
1	0.00000166	-0.000000373	-0.000002411
1	0.000002311	-0.000000702	-0.000000184
1	0.000002634	-0.000000553	-0.000001392
6	0.00000069	-0.000001187	0.000000575
6	0.000000615	0.000000025	-0.000001284
6	-0.000000147	-0.000000977	-0.000002812
6	0.000000111	-0.000000221	-0.000000692
6	-0.000000337	0.000000223	-0.000001072
6	-0.000001614	0.000000571	-0.000000046
1	-0.000000007	0.000000088	0.000000155
1	-0.000001351	0.000000268	-0.000001471
1	-0.000001234	0.000000141	-0.000000311
6	-0.000000542	-0.000000738	0.000000711
6	0.000001845	0.000000383	-0.000000115
6	0.00000162	0.000001067	0.000001125
1	0.000001743	-0.000000179	0.000000065
1	0.000001347	0.000000033	-0.000000016

1	0.000001736	-0.000000126	0.000000558
1	0.000000847	-0.000000127	0.000000051
1	0.000001185	-0.000000071	0.000000578
1	0.000000105	0.000000215	0.000000993
1	0.000001036	-0.000000492	0.000001373
6	-0.000000617	-0.000000029	-0.0000001
6	-0.00000118	0.000000432	-0.000000282
6	-0.000000737	0.000000227	-0.0000003258
1	-0.000000243	-0.000000412	-0.0000002488
1	-0.000001028	0.000000099	-0.000001155
1	-0.000000897	-0.000000009	-0.0000002529
1	-0.000001496	-0.000000032	-0.000001933
1	0.000000225	-0.000000159	-0.0000002766
1	-0.000000637	0.000000000	-0.0000002492
1	-0.000000512	-0.000000184	-0.0000002996
6	0.0000002545	-0.000001182	0.000000498
6	0.000001783	-0.000000138	-0.000000112
6	0.000002721	-0.000000375	-0.000000986
1	0.000002063	-0.000000142	-0.000000215
1	0.000001129	0.000000141	0.000001235
1	0.000002417	-0.000000023	0.000000862
1	0.000002568	-0.000000471	0.000000896
1	0.000003128	-0.000000614	-0.000000367
1	0.000003502	-0.000000307	0.000000041
1	0.000003087	-0.000000448	0.000000506
6	0.000000487	-0.000000767	-0.0000004227
6	0.000002256	-0.000000544	-0.0000002775
6	0.000000435	-0.000000083	-0.000001887
1	0.000000239	0.000000028	-0.0000002787
1	0.000002182	-0.000000443	-0.0000003313
1	0.000001298	-0.000000638	-0.0000003474
1	0.000001784	-0.000000161	-0.0000003406
1	0.000000678	-0.000000064	-0.000001792
1	0.000001067	-0.000000598	-0.0000002891
1	0.000000033	-0.000000276	-0.0000003295

Zero-point correction=	1.100830 (Hartree/Particle)
Thermal correction to Energy=	1.170395
Thermal correction to Enthalpy=	1.171339
Thermal correction to Gibbs Free Energy=	0.981844
Sum of electronic and zero-point Energies=	-3434.789073
Sum of electronic and thermal Energies=	-3434.719507
Sum of electronic and thermal Enthalpies=	-3434.718563
Sum of electronic and thermal Free Energies=	-3434.908058

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6	0.000000198	0.000000038	0.000001115
6	0.000000624	-0.000000579	-0.000001809
7	-0.000000198	-0.000000195	-0.000000823
7	-0.00000112	0.000000568	0.000000783
16	0.000000431	0.000000641	-0.000000424
8	0.000000432	0.000000413	-0.000000485
8	0.00000036	0.000000136	-0.00000028
6	0.00000043	0.000000217	-0.000000679
6	0.000000267	0.000000578	-0.000000727
6	0.000000338	0.000000497	-0.000000797
6	0.000000228	0.000000859	-0.000000759
6	0.000000463	0.000000628	-0.000000723
6	0.000000509	0.000000383	-0.000000423
1	0.000000497	0.000000737	-0.000000764
1	0.00000062	0.000000868	-0.00000101
1	0.000000402	0.000000034	-0.000000611
1	0.000000254	0.000000224	-0.000000275
6	0.000000481	0.000000818	-0.000000892
1	0.000000831	0.000000544	-0.000001018
1	0.000000497	0.000001061	-0.000001161
1	0.00000032	0.000000669	-0.000000701
6	-0.000000217	0.000000674	-0.000000086
6	-0.000000176	0.000000264	-0.000000349
1	-0.000000268	0.000000554	-0.000000497
1	-0.000000216	0.000000457	-0.000000363
6	-0.000000569	0.000000887	-0.000000517
1	-0.000000222	0.000000655	-0.000000475
1	-0.000000357	0.000000328	-0.000000233
6	-0.000000557	0.000000698	-0.000000531
1	-0.000000733	0.00000066	-0.000000339
1	-0.00000037	0.000000883	-0.000000683
1	-0.000000743	0.00000091	-0.000000575
1	-0.000000451	0.000000843	-0.000000553
1	-0.000000696	0.00000066	-0.000000335
6	-0.000000679	0.000000182	0.000000004
6	-0.000000796	0.000000275	-0.000000002
1	-0.000000833	0.000000322	-0.000000011
1	-0.000000788	0.000000254	0.000000275
6	-0.000001024	0.000000207	0.000000167
1	-0.000000774	0.000000398	0.000000078
1	-0.000000666	0.000000143	0.000000171
6	-0.00000115	0.000000293	0.000000216
1	-0.000001193	0.00000014	0.000000371
1	-0.000001214	0.00000039	0.000000121

1	-0.000001347	0.000000305	0.000000244
1	-0.000001074	0.00000039	0.000000024
1	-0.000001031	0.000000103	0.000000307
16	-0.000000044	0.000000083	0.000000076
8	0.000000002	-0.000000045	-0.000000119
8	-0.000000876	0.000000108	0.000000278
6	-0.000000754	0.000000584	-0.000000241
6	-0.000000153	0.000000524	-0.000000295
6	-0.000000739	0.000000387	-0.000000077
6	-0.000000541	0.000000819	-0.000000455
1	-0.000000229	0.000000505	-0.000000423
6	-0.000001091	0.000000555	-0.000000414
1	-0.000000899	0.000000338	0.000000056
6	-0.000000802	0.000000747	-0.000000499
1	-0.000000426	0.000000881	-0.000000659
1	-0.000001081	0.000000692	-0.000000214
6	-0.000000845	0.000000982	-0.000000592
1	-0.000001036	0.000001166	-0.000000498
1	-0.000000777	0.000000908	-0.000000592
1	-0.000000822	0.000001133	-0.000000866
79	0.000000392	-0.000000094	0.000000318
6	0.000000492	-0.000000437	0.000000165
6	0.000000429	-0.000000561	0.000000341
6	0.000000543	-0.000000627	0.000000231
1	0.000000626	-0.000000845	0.000000594
1	0.000000678	-0.000000543	0.000000196
7	0.000000379	-0.000000288	-0.000000086
7	0.000000081	-0.000000712	0.000000421
6	0.000000534	0.00000035	-0.000000473
6	0.000000697	-0.000000476	-0.000000024
6	0.000000614	-0.000000109	-0.000000003
6	0.000000228	0.000000345	-0.000000206
6	0.000000917	0.000000047	-0.000000336
6	0.000000549	0.000000203	-0.000000692
1	0.000000203	0.000000248	-0.00000024
1	0.000000975	0.000000112	-0.000000423
1	0.000000639	0.000000331	-0.000000542
6	0.000000166	-0.000000875	0.000000703
6	0.000000326	-0.000000736	0.000000736
6	-0.000000161	-0.000000767	0.000000555
6	0.000000339	-0.000000858	0.000000697
6	-0.00000007	-0.000000558	0.000000963
6	0.000000117	-0.000000956	0.000000976
1	0.000000426	-0.000000808	0.000000539

1	-0.000000193	-0.000000784	0.000000685
1	-0.000000018	-0.000000097	0.000000891
6	0.000000464	-0.000000577	0.000000231
6	0.000001023	-0.000000914	0.000000312
6	0.000000773	-0.000000584	0.000000287
1	0.000000818	-0.000000731	0.000000309
1	0.000000865	-0.000001003	0.000000607
1	0.000001035	-0.000000918	0.000000506
1	0.000000781	-0.000001084	0.000000783
1	0.000000578	-0.000000508	0.000000135
1	0.000000063	-0.000000705	0.000000349
1	0.000000824	-0.000000621	0.000000213
6	-0.000000079	-0.000000072	0.000000409
6	-0.000000005	-0.000000467	0.000000684
6	-0.000000123	-0.000000789	0.000000796
1	0.000000027	-0.000000514	0.000000726
1	-0.000000135	-0.000000529	0.000000067
1	-0.000000508	-0.000000422	0.000000607
1	-0.000000547	-0.000000424	0.000000827
1	-0.000000007	-0.000000869	0.000000811
1	-0.000000309	-0.000000892	0.000000956
1	-0.000000259	-0.000000741	0.000000811
6	0.000000848	-0.000000369	-0.000000022
6	0.000001057	-0.000000143	-0.000000249
6	0.000001182	-0.000000329	-0.000000016
1	0.000000848	-0.000000356	0.000000014
1	0.000000998	-0.000000032	-0.000000438
1	0.000001173	-0.000000232	-0.000000211
1	0.000001229	-0.000000098	-0.000000487
1	0.000001098	-0.000000306	-0.000000085
1	0.000001299	-0.000000252	-0.000000262
1	0.000001328	-0.000000451	-0.000000007
6	0.000000102	-0.000000023	0.000000214
6	0.000000078	-0.000000117	0.000000001
6	-0.000000069	0.000000041	0.000000166
1	-0.000000013	-0.000000151	-0.000000012
1	0.000000301	-0.000000219	0.000000144
1	-0.000000046	-0.000000158	0.000000199
1	0.000000004	0.000000014	-0.000000113
1	-0.000000346	0.000000193	-0.000000161
1	-0.000000178	0.000000277	-0.000000118
1	-0.000000327	0.000000014	0.000000031
6	-0.000000046	-0.000000239	0.000000361
6	-0.000000087	-0.000000423	0.000000506

6	-0.000000154	-0.000000643	0.000000615
6	-0.000000413	-0.000000463	0.000000846
6	-0.000000432	-0.000000387	0.000000417
1	-0.000000177	-0.000000629	0.000000597
1	0.000000014	-0.000000265	0.000000023
7	-0.00000013	-0.000000343	0.000000584
8	-0.000000888	-0.00000016	0.000000573
1	-0.000000629	-0.000000522	0.000000734
1	0.000000135	-0.000000424	0.000000265
17	-0.000000663	-0.00000045	0.00000058
Zero-point correction=			1.185334 (Hartree/Particle)
Thermal correction to Energy=			1.261707
Thermal correction to Enthalpy=			1.262651
Thermal correction to Gibbs Free Energy=			1.060336
Sum of electronic and zero-point Energies=			-4217.726151
Sum of electronic and thermal Energies=			-4217.649778
Sum of electronic and thermal Enthalpies=			-4217.648834
Sum of electronic and thermal Free Energies=			-4217.851150

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6	0.0000001	-0.000007936	0.000003804
6	-0.000003982	0.000000305	-0.000000939
7	-0.000000607	0.000005234	0.000001156
7	0.00000641	-0.000002369	-0.000002758
16	-0.000000974	-0.00000328	0.000000362
8	0.000001498	-0.000000865	-0.000000656
8	0.0000021	0.000002015	-0.000000121
6	-0.000001826	0.000001514	0.000000139
6	0.000000267	-0.000000225	0.000000936
6	0.000001663	-0.000000262	0.000001056
6	-0.000000239	0.000001295	0.000001201
6	-0.00000091	-0.000000552	-0.000000377
6	0.000001784	-0.000000518	-0.00000119
1	-0.000000563	0.000000395	-0.000000456
1	-0.000000116	0.000000164	0.000000313
1	0.00000062	0.000000357	0.000000928
1	0.000000355	0.000000468	0.000001172
6	0.000000046	0.000001015	0.000000807
1	0.000001021	-0.000001371	0.000000474
1	-0.000000437	0.000000546	0.000000102
1	0.000001116	0.000000056	0.000001938
6	-0.000000513	-0.000000437	0.000000068
6	-0.000000674	0.000000851	0.000000239
1	-0.000000739	0.000000483	0.000000045

1	-0.000000411	0.000000976	0.000000545
6	-0.000000567	0.000000653	-0.000000047
1	-0.000000724	0.000000572	-0.000000004
1	-0.000000703	0.000000323	-0.000000582
6	-0.000001936	0.000001113	0.000000218
1	-0.000001182	0.000000986	0.000000248
1	-0.000000808	0.000000709	0.000000118
1	-0.000001629	0.000000733	-0.000000079
1	-0.00000137	0.000000285	-0.000000622
1	-0.000001362	0.000000826	-0.000000037
6	-0.000000755	0.000001545	-0.000000065
6	-0.000000849	0.000001277	0.000000819
1	0	0.000000564	0.000001623
1	0.000000191	0.000001346	0.000000799
6	-0.000000815	0.000000843	0.000001071
1	-0.000000637	0.000000013	0.000000508
1	-0.000000237	0.000000923	0.000001008
6	-0.000001113	0.000000765	0.00000005
1	-0.000000457	0.000000827	0.000001091
1	-0.000000705	0.000001272	0.000001043
1	-0.000001176	0.000001208	0.000000762
1	-0.000001247	0.000001113	0.000000658
1	-0.000001075	0.000000964	0.000000425
16	-0.000002172	0.000002945	0.000003882
8	0.000000272	-0.000000587	0.000001418
8	0.000000802	0.000000514	0.000001096
6	0.000000076	-0.000000285	0.00000208
6	0.000000339	0.000001186	0.000001425
6	-0.000000072	0.000001124	0.00000143
6	0.000000382	0.000001034	0.000000956
1	-0.00000007	0.000000148	0.000000831
6	-0.00000006	0.000001267	0.000002728
1	0.000000061	0.000000984	0.000001653
6	0.000000243	0.000000511	0.000001998
1	0.000000092	0.000001048	0.000001299
1	0.000000242	0.000001412	0.000002088
6	0.000000229	0.000000811	0.000001844
1	-0.000000055	0.000001306	0.000001902
1	0.000000035	0.000002145	0.000002211
1	-0.000000264	0.000001518	0.000002616
79	0.000000843	0.000001312	-0.000003315
6	-0.000001131	-0.000001763	0.000000437
6	0.000001539	0.000000363	0.000000174
6	-0.000001171	-0.000002758	-0.000000412

1	0.000000549	-0.00000076	-0.000001823
1	-0.000000765	-0.000000736	-0.000001922
7	0.000000274	-0.000001595	-0.000002122
7	0.000001378	0.00000052	-0.000000272
6	-0.000000922	0.000000538	-0.000000488
6	-0.000001887	-0.00000099	-0.000002834
6	-0.000001594	0.000000406	-0.00000068
6	-0.000000901	0.000000294	-0.000000895
6	-0.000000748	-0.000000138	-0.000001727
6	-0.000001008	-0.000000197	-0.000000733
1	-0.000001419	0.000000425	-0.000000876
1	-0.00000051	-0.000000201	-0.000001577
1	-0.000001416	0.000000092	-0.00000114
6	0.000001437	-0.000001131	-0.000001135
6	-0.000000107	-0.000001154	0.000000273
6	-0.000001227	-0.000000189	-0.000001018
6	0.00000126	-0.000001518	-0.000000591
6	0.000001393	-0.000000149	0.00000016
6	0.000001011	-0.000000709	-0.000000435
1	0.000001298	-0.000000958	-0.000000297
1	0.000001474	-0.000000688	-0.000000283
1	0.000001469	-0.000000904	0.000000146
6	0.000001549	-0.000000528	-0.000000873
6	-0.000000268	-0.000001416	-0.000001921
6	0.000001353	-0.000001126	0.000000483
1	0.000001195	-0.000001248	-0.000000788
1	0.000000862	-0.000001177	-0.000001338
1	0.000001077	-0.000001416	-0.000001058
1	0.000002071	-0.000001366	-0.00000077
1	0.000000415	-0.000000072	-0.000001045
1	0.000001176	-0.000000976	-0.000000771
1	0.000000925	-0.000001071	-0.000000724
6	0.000000574	-0.000000314	-0.000001859
6	0.000001126	-0.000000364	-0.000000149
6	0.00000121	-0.000000283	-0.000000613
1	0.00000025	-0.000000251	-0.000000434
1	-0.000000108	-0.000000428	0.000001155
1	-0.000000075	0.000000199	-0.000000369
1	0.000000115	-0.000000348	0.0000001
1	0.00000028	-0.000001091	-0.000000879
1	0.000000458	-0.000000741	-0.000000583
1	-0.000000037	-0.000000655	-0.000000567
6	-0.000000571	-0.000001971	-0.00000202
6	0.000000797	0.000000909	-0.000001115



6	-0.000000756	-0.000000244	-0.000001414
1	0.000000552	-0.000000023	-0.000001259
1	-0.00000134	-0.000000813	-0.000001012
1	-0.000000349	-0.000000095	-0.000001472
1	-0.000000467	-0.000001232	-0.000001188
1	-0.000000254	-0.000000956	-0.000001808
1	-0.000000596	-0.000000976	-0.000001882
1	-0.000000179	-0.00000117	-0.00000179
6	-0.000001187	0.000000021	0.000000039
6	-0.000000926	-0.000000138	-0.000000694
6	-0.000000149	0.000000179	-0.000000363
1	-0.000000862	-0.000000532	-0.000001192
1	-0.000000957	-0.000000231	-0.000001357
1	-0.000000881	-0.000000043	-0.000001102
1	-0.0000014	-0.000000077	-0.000001071
1	-0.000000449	0.000000162	-0.000000136
1	-0.000001443	0.000000537	-0.000000496
1	-0.000000645	0.000000183	-0.00000057
6	0.000001319	-0.000000492	0.000002929
6	0.000001376	-0.000000741	0.000000372
6	0.000001199	0.000000608	-0.000000234
6	0.000001424	0.000000076	0.000002142
6	0.000000975	-0.000000927	0.00000054
1	0.000001783	-0.000000375	0.000000731
1	0.000000823	-0.000000019	0.000000434
7	-0.00000058	0.000000851	-0.000002925
8	0.000001255	0.000003045	0.000001851
1	0.000001037	-0.000000245	0.000000959
1	0.000001272	-0.000000524	0.000000737
17	-0.000000234	-0.000000589	0.000001093

Zero-point correction=

1.187481 (Hartree/Particle)

Thermal correction to Energy=

1.263502

Thermal correction to Enthalpy=

1.264446

Thermal correction to Gibbs Free Energy=

1.062292

Sum of electronic and zero-point Energies=

-4217.745411

Sum of electronic and thermal Energies=

-4217.669390

Sum of electronic and thermal Enthalpies=

-4217.668446

Sum of electronic and thermal Free Energies=

-4217.870600

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6	0.000001235	-0.000000642	-0.000000195
6	-0.000000683	0.000000805	-0.000000165
7	-0.000000217	-0.000000262	-0.000000011
7	0.00000002	0.000000822	0.000000895

16	0.000000241	-0.000000698	-0.000000731
8	-0.000000148	-0.000000223	0.000000038
8	0.000000204	0.000000011	-0.000000044
6	0.000000083	0.000000075	-0.000000103
6	0.000000035	-0.000000346	-0.000000147
6	0.000000218	-0.000000631	-0.000000483
6	-0.000000727	0.000000656	-0.000000681
6	0.000000531	-0.000000134	-0.000000227
6	0.000000729	-0.000000115	-0.000000371
1	0.000000066	-0.000000234	-0.000000466
1	0.000000286	-0.000000382	-0.000000421
1	0.000000374	-0.000000398	-0.000000067
1	0.000000408	-0.000000161	-0.000000011
6	0.000000959	-0.000001408	-0.000000622
1	0.000000461	-0.000000285	0.000000203
1	0.000000277	-0.000000554	0.000000409
1	0.000001012	0.000000429	-0.000000382
6	-0.000000418	0.000000006	-0.000000426
6	-0.000000314	0.000000166	-0.000000344
1	0.000000052	0.000000035	-0.000000562
1	0.000000134	-0.000000134	-0.000000014
6	-0.000000358	0.000000125	-0.000000378
1	-0.000000209	0	-0.000000406
1	-0.000000078	0.000000128	-0.000000189
6	-0.00000005	0.000000177	-0.000000357
1	-0.000000122	0.000000095	-0.000000182
1	-0.000000196	0.000000002	-0.000000546
1	-0.000000519	0.000000186	-0.000000455
1	-0.000000453	0.000000093	-0.000000512
1	-0.000000407	0.000000173	-0.00000038
6	0.000000034	-0.000000001	-0.00000001
6	0.000000165	-0.000000246	0.000000103
1	0.000000228	0.000000001	0.000000038
1	0.000000334	-0.000000021	0.000000014
6	0.000000545	-0.000000322	0.000000121
1	0.000000299	-0.000000009	0.000000068
1	0.000000386	-0.000000404	-0.000000141
6	0.000000525	-0.000000003	0.000000005
1	0.000000481	-0.000000264	0.000000199
1	0.000000455	-0.000000176	0.000000187
1	0.000000665	-0.000000381	0.000000127
1	0.000000557	-0.000000291	-0.000000003
1	0.000000632	-0.000000378	-0.000000056
16	-0.000000444	-0.000000496	-0.000000312

8	-0.000000249	0.000000351	-0.000000015
8	0.000000363	-0.000000074	0.000000116
6	-0.000000003	0.000000333	-0.000000262
6	0.000000017	0.000000068	-0.000000301
6	0.000000314	0.000000286	-0.000000519
6	-0.00000001	-0.000000173	-0.000000894
1	-0.000000501	0.000000307	-0.000000088
6	-0.000000344	0.000000216	0.000000102
1	-0.000000585	-0.000000316	0.000000392
6	0.000000581	-0.000000328	0.000000998
1	-0.000000453	0.000000181	-0.000000049
1	-0.000000378	0.00000001	-0.000000416
6	-0.00000108	0.000000496	-0.000001171
1	-0.000000697	0.000000234	-0.000000359
1	-0.000001091	0.000000658	0.000000122
1	-0.000000668	-0.000000175	-0.000000806
79	-0.000000159	-0.000000111	0.000000122
6	-0.000000087	0.000000091	-0.000000003
6	-0.000000047	0.000000122	0.000000383
6	0.000000007	0.000000205	0.00000042
1	-0.000000006	0.000000144	0.000000591
1	-0.000000199	0.000000229	0.000000413
7	0.00000011	0.000000095	0.000000347
7	0.000000304	-0.000000083	0.000000669
6	-0.000000571	-0.000000095	0.00000024
6	0.00000003	0.000000312	-0.00000016
6	-0.000000539	0.000000034	-0.000000049
6	-0.000000022	0.000000151	0.00000001
6	-0.000000484	0.000000197	-0.000000067
6	-0.000000387	0.000000063	0.000000015
1	-0.000000151	0.000000101	-0.00000014
1	-0.000000466	0.000000264	-0.000000008
1	-0.000000407	0.000000191	-0.000000182
6	0.00000003	0.000000171	0.00000036
6	0.000000074	0.000000125	0.000000406
6	0.000000146	0.000000011	0.00000024
6	0.000000121	0.000000048	0.000000421
6	0.00000007	-0.000000025	0.000000568
6	0.000000198	0.000000142	0.00000005
1	0.000000091	0.000000096	0.000000517
1	0.000000402	-0.000000085	0.000000519
1	0.000000328	0.000000044	0.000000587
6	-0.000000132	0.000000269	0.000000531
6	-0.000000061	0.000000316	0.00000072

6	-0.000000141	0.000000175	0.000000353
1	-0.000000047	0.000000119	0.000000428
1	-0.000000112	0.000000242	0.000000626
1	-0.000000227	0.000000362	0.000000634
1	-0.00000018	0.000000281	0.000000718
1	-0.000000134	0.000000206	0.000000436
1	-0.000000233	0.000000242	0.000000429
1	-0.000000193	0.000000193	0.000000447
6	0.000000324	-0.000000059	0.000000262
6	0.000000403	-0.000000188	0.000000335
6	0.000000402	0.000000002	0.000000586
1	0.000000089	-0.000000049	0.000000344
1	0.000000442	-0.000000123	0.000000159
1	0.000000484	-0.000000244	0.000000189
1	0.000000321	-0.000000211	0.000000277
1	0.000000286	0.000000033	0.000000579
1	0.000000443	-0.000000095	0.000000583
1	0.000000416	-0.000000102	0.000000458
6	-0.000000349	0.000000281	0.000000115
6	-0.0000004	0.000000281	0.0000001
6	-0.000000461	0.000000462	0.000000195
1	-0.000000205	0.000000173	0.000000135
1	-0.000000422	0.000000346	0.000000088
1	-0.000000499	0.000000252	0.000000052
1	-0.000000545	0.000000255	0.000000046
1	-0.000000363	0.000000268	0.000000317
1	-0.000000494	0.000000433	0.000000091
1	-0.000000591	0.000000434	0.000000365
6	-0.000000001	0.000000018	0.000000088
6	-0.000000025	0.000000011	0.000000124
6	0.000000133	-0.000000265	0.000000024
1	0.000000066	0.000000056	0.000000298
1	-0.000000043	0.000000137	0.000000299
1	0.000000134	-0.000000032	0.000000227
1	-0.0000001	0.000000111	0.000000066
1	0.000000066	-0.00000009	-0.000000018
1	-0.00000009	0.00000008	-0.000000068
1	0.000000242	-0.000000098	0.000000015
6	0.000000127	-0.000000108	-0.0000000645
6	-0.000000064	-0.000000065	-0.000000537
6	-0.000000176	-0.00000019	-0.000000904
6	0.000000117	-0.000000402	-0.000000682
6	0.000000212	-0.000000408	-0.000000526
1	-0.000000071	-0.000000178	-0.000000787

1	-0.000000445	0.000000277	-0.000000765
7	0.000001242	0.000000284	-0.000000053
8	-0.000000211	-0.000001877	-0.000000155
1	0.000000025	-0.000000314	-0.000000068
1	-0.000000202	-0.000000015	-0.000000553
17	0.000000366	-0.000000184	-0.000000366
Zero-point correction=			1.186071 (Hartree/Particle)
Thermal correction to Energy=			1.262100
Thermal correction to Enthalpy=			1.263044
Thermal correction to Gibbs Free Energy=			1.063843
Sum of electronic and zero-point Energies=			-4217.721828
Sum of electronic and thermal Energies=			-4217.645799
Sum of electronic and thermal Enthalpies=			-4217.644855
Sum of electronic and thermal Free Energies=			-4217.844056

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6	0.000005125	0.000002087	0.000000437
6	-0.000012891	-0.000000803	0.000001564
7	0.000000742	-0.000008372	0.000008475
7	0.000003976	0.000001532	-0.000008133
16	-0.000004816	0.000011503	-0.000004995
8	0.00000043	-0.000002598	-0.000002814
8	0.000000132	-0.000002342	-0.000000419
6	-0.00000228	-0.000001693	-0.000002122
6	0.000000084	-0.000000837	0.000000824
6	-0.000001274	0.000000226	0.000000437
6	0.000000204	-0.000000399	-0.000001583
6	-0.000000144	0.00000151	0.000000047
6	0.000001327	0.000000402	-0.000001604
1	-0.000001081	0.000000581	-0.000000577
1	-0.000000964	-0.000000175	0.000000063
1	-0.000000205	-0.000000492	0.000000115
1	-0.000000686	-0.000000608	0.000000637
6	-0.00000071	-0.000000559	-0.000000002
1	-0.000000283	0.000000119	0.000000187
1	-0.000000637	0.000000201	0.000000078
1	-0.000000481	0.00000004	0.000000262
6	-0.000001441	0.000001083	-0.000003632
6	-0.000001238	-0.000001143	0.000000747
1	-0.00000105	-0.000000347	0.000000158
1	-0.000000176	-0.000000742	0.000000231
6	-0.000000857	-0.000000219	0.000001149
1	-0.000000498	-0.000000154	0.000000175
1	0.000000014	-0.000000495	-0.000000579

6	-0.000001242	0.000000416	-0.000000841
1	-0.000000189	-0.000000347	-0.000000175
1	-0.000000067	0.000000163	-0.000000166
1	-0.000001107	0.000000218	-0.000000144
1	-0.000001175	-0.000000399	-0.000000021
1	-0.000000913	-0.000000129	0.000000168
6	0.000002058	-0.000000699	0.000004316
6	0.000002272	-0.000001338	-0.000000057
1	0.000000486	0.000000014	0.000000166
1	0.000000585	0.000000037	-0.000000708
6	-0.00000004	0.000000005	-0.000001608
1	0.000000144	-0.000000168	-0.000000079
1	-0.000000239	-0.000000082	-0.000000047
6	0.00000192	-0.000000756	-0.000000253
1	0.000000909	-0.000000672	-0.000000184
1	0.000001375	-0.000000358	-0.000000167
1	0.000001174	-0.000000496	-0.000000549
1	0.000001243	-0.000000679	-0.000000721
1	0.000000737	-0.000000647	-0.000000879
16	-0.000003541	-0.000000709	-0.000002144
8	-0.000001047	0.000002196	0.000000379
8	0.000005841	-0.000001299	0.000001482
6	-0.000000507	0.000000489	-0.000000254
6	-0.000000743	-0.000000973	-0.000003816
6	0.000000706	-0.000000195	0.000001197
6	-0.00000112	-0.000000599	0.000000784
1	-0.00000011	0.000000089	0.000001665
6	-0.000000725	-0.000000657	-0.000001406
1	0.000000159	-0.00000138	-0.000000978
6	0.000001097	0.000000024	-0.000000297
1	0.000000134	-0.000000234	-0.000000214
1	-0.000000146	-0.000000045	-0.000000755
6	-0.000000584	-0.000000611	-0.000000665
1	-0.000000711	-0.000000161	-0.000000469
1	-0.000000525	-0.000000513	-0.000000649
1	-0.000000301	-0.000000311	-0.000000144
79	0.000001306	0.000000118	-0.000000822
6	0.000000029	0.000003778	0.000000074
6	0.000000999	0.000002146	0.000001065
6	0.000000127	-0.000000482	0.000000775
1	0.000000529	0.000000524	0.00000009
1	0.000000093	0.00000168	0.000000192
7	-0.000003439	-0.000004235	0.000002017
7	-0.000000588	0.000001471	-0.000003488

6	0.000003945	0.000007684	-0.000002207
6	-0.000002316	-0.000007935	-0.000001477
6	-0.000000251	0.000001162	0.000005967
6	-0.000000604	0.000001762	0.000005894
6	-0.000001382	-0.000001672	-0.000001071
6	-0.000002325	0.000004244	-0.000002175
1	-0.000000973	0.000000294	-0.000000153
1	-0.000001471	-0.000000295	0.000000225
1	-0.000000918	0.000000497	0.000000509
6	0.000003528	-0.000000835	0.000003267
6	0.000000437	-0.000001072	-0.000000441
6	0.000001482	0.000000266	-0.000001724
6	0.00000151	0.000000406	0.000001359
6	0.000000126	-0.000000605	0.000000166
6	0.000001743	0.000001261	0.000000322
1	0.000000974	-0.000000191	0.000000457
1	0.000001639	0.000000191	0.000000349
1	0.000001354	-0.000000032	0.000000283
6	-0.000000361	-0.000000006	0.000000641
6	-0.000000331	0.000001111	0.000000076
6	0.000002033	0.000001832	0.000002646
1	0.000001201	0.000000156	0.000000515
1	0.000000071	0.000000924	0.000000653
1	0.000001147	0.000000314	0.000000691
1	0.000001409	0.000000471	0.000000582
1	0.000000358	-0.000000878	-0.000001142
1	-0.000000099	-0.000000192	-0.000000547
1	0.00000009	0.000000234	-0.000000665
6	0.000001029	0.000000266	0.00000194
6	0.000000213	0.000000257	-0.000001129
6	-0.000000083	0.000001018	0.000001564
1	-0.000000427	0.000000093	0.000000112
1	0.000000333	0.000000554	0.000000301
1	0.000000671	-0.000000124	0.000000708
1	0.000001022	0.000000028	0.000000593
1	0.000000097	0.000000477	0.000000028
1	0.000001128	0.000000069	0.000000237
1	0.000000825	0.000000469	0.00000004
6	-0.000001825	-0.000000655	-0.000000928
6	0.000000083	0.000002149	0.000000444
6	0.000000508	-0.000000035	0.000000948
1	-0.000002163	0.000000938	0.000001462
1	-0.000000051	-0.000000409	0.00000004
1	0.000000028	-0.000000257	0.000000429

1	-0.000001154	-0.000000832	0.000000507
1	-0.000000213	0.000000662	0.000001192
1	-0.000001593	0.000001713	0.000000814
1	0.000000351	0.000000676	0.000000674
6	0.000004566	0.000002636	0.000000238
6	-0.000003932	-0.000000421	0.000001869
6	-0.000000966	0.000000244	0.000001068
1	-0.000000325	-0.000000478	0.000000087
1	-0.000000358	0.000000594	0.000000748
1	-0.000000425	0.000001065	0.000000535
1	0.000000127	0.000001163	0.000000052
1	-0.000000548	0.000000029	0.000000369
1	-0.000001135	0.000000053	0.000000589
1	-0.000000036	-0.000000253	0.000000441
6	0.000001988	-0.000001467	0.000000073
6	-0.000000115	-0.000000905	-0.000002646
6	-0.000002466	-0.000000042	-0.000001231
6	-0.000000338	-0.000001215	-0.000000412
6	0.000001649	-0.000002118	-0.000001142
1	-0.000000062	-0.000000894	-0.000000748
1	-0.000001358	0.000000056	-0.00000102
7	0.000000788	-0.00000148	-0.000005452
8	0.00000293	-0.000001482	0.00000367
1	-0.000000037	-0.000001306	-0.000002237
1	-0.000000877	-0.00000127	-0.000000372
17	-0.000000236	-0.000001062	-0.00000137

Zero-point correction=

1.188169 (Hartree/Particle)

Thermal correction to Energy=

1.263975

Thermal correction to Enthalpy=

1.264920

Thermal correction to Gibbs Free Energy=

1.066709

Sum of electronic and zero-point Energies=

-4217.726774

Sum of electronic and thermal Energies=

-4217.650968

Sum of electronic and thermal Enthalpies=

-4217.650024

Sum of electronic and thermal Free Energies=

-4217.848234

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6	0.000000037	0.000000389	0.000000324
6	-0.000000485	0.000000354	0.000000659
7	0.000000101	0.000000306	0.000000653
7	-0.00000004	0.000000442	0.000000433
16	-0.000000076	0.000000987	0.000000937
8	0.000000468	0.000001085	0.000001122
8	-0.000000357	0.000000722	0.000000949
6	0.000000083	0.000000729	0.000000168



6	0.00000089	0.000001525	0.00000141
6	0.000000956	0.000000704	0.000001564
6	0.000000229	0.000000531	-0.00000035
6	0.000000464	0.000000942	0.000000902
6	0.000000178	0.000000111	0.000001326
1	0.000000911	0.00000094	0.000001235
1	0.000001058	0.00000101	0.000001162
1	0.000000075	0.000000478	0.000000446
1	-0.000000209	0.000000524	0.000000637
6	0.000001115	0.000000541	0.000000022
1	0.000001418	0.000001119	0.000000974
1	0.000001077	-0.000000065	0.000001717
1	0.000001344	0.000000717	0.000001564
6	0.000000747	0.000000243	0.000000567
6	0.000001042	0.000000424	0.000000512
1	0.000000659	0.000000257	0.000000553
1	0.000000631	0.00000032	0.000000054
6	0.000001512	0.000000271	0.000000423
1	0.000001047	0.00000075	0.000000925
1	0.000000958	0.000000198	0.000000431
6	0.000001778	0.00000043	0.000000549
1	0.000001539	0.000000065	0.000000176
1	0.000001599	0.000000344	0.000000578
1	0.000002152	0.000000293	0.000000485
1	0.000001835	0.000000618	0.000000848
1	0.000001705	0.000000274	0.000000515
6	-0.000001257	0.000000196	0.000000265
6	-0.000001508	0.000000699	0.000000626
1	-0.000001273	0.000000101	0.000000106
1	-0.00000091	0.000000124	0.000000247
6	-0.000001988	0.000000353	0.000000392
1	-0.000001489	0.000000671	0.000000779
1	-0.000001264	0.00000057	0.000000858
6	-0.000001981	0.000000796	0.000000084
1	-0.000001779	0.000000354	0.000000371
1	-0.000001961	0.000000301	0.000000032
1	-0.00000243	0.00000064	0.00000007
1	-0.000002268	0.000000833	0.000000902
1	-0.000002015	0.000000853	0.000000948
16	-0.000001089	0.000000439	0.000000478
8	-0.000000968	0.000000058	0.000000133
8	-0.000000675	0.000000625	0.000000891
6	-0.000000169	0.000000521	0.000000426
6	-0.000000096	0.000000275	0.000000147

6	-0.000000114	0.000000614	0.000000573
6	0.000000203	0.000000329	-0.000000081
1	-0.000000502	-0.000000189	-0.000000273
6	0.000000327	0.000000139	0.000000623
1	-0.000000153	0.000000611	0.000000759
6	0.000001234	-0.000000436	0.000000178
1	0.000000476	-0.000000491	-0.000000374
1	0.000000542	0.000000238	0.000000563
6	0.000000791	-0.000000298	-0.00000004
1	0.000001174	-0.000000129	-0.000000476
1	0.000000944	0.000000042	0.000000453
1	0.000000487	-0.000000182	-0.000000105
79	0.000000164	-0.000000196	-0.000000007
6	-0.000000337	-0.000000082	-0.000000278
6	-0.000000203	-0.000000904	-0.000001152
6	-0.000000136	-0.000000889	-0.000001163
1	-0.000000505	-0.000001237	-0.000001441
1	0.000000285	-0.000001205	-0.000001433
7	0.000000383	-0.000000655	-0.000000834
7	-0.000000045	-0.000000648	-0.000000731
6	0.000001132	-0.000000393	-0.000000785
6	0.000000548	-0.000000667	-0.000001153
6	0.000001191	-0.000000959	-0.000000928
6	0.000001279	-0.000000048	-0.000000678
6	0.000001408	-0.000000688	-0.000000633
6	0.000001414	-0.00000005	-0.000000794
1	0.00000126	-0.000000397	-0.000000529
1	0.00000165	-0.000000532	-0.000000564
1	0.000001878	-0.000000465	-0.000000048
6	-0.000000962	-0.000000689	-0.000000779
6	-0.000001001	-0.000000958	-0.000000584
6	-0.000001147	-0.000000398	-0.000000677
6	-0.000001481	-0.000000489	-0.000000915
6	-0.000001769	-0.000000517	-0.000000696
6	-0.000001741	-0.000000464	-0.000000433
1	-0.000001656	-0.000000465	-0.000000761
1	-0.000001757	-0.000000304	-0.000000534
1	-0.00000211	-0.000000308	-0.000000518
6	-0.000000705	-0.000000804	-0.000000993
6	-0.000000851	-0.00000105	-0.000001281
6	-0.000000871	-0.000000482	-0.000000085
1	-0.000000372	-0.000000609	-0.000000963
1	-0.00000067	-0.00000101	-0.000001479
1	-0.00000059	-0.000001044	-0.000001353

1	-0.000001178	-0.000001061	-0.000001363
1	-0.000000893	-0.000000357	-0.000000413
1	-0.000001224	-0.000000593	-0.000000729
1	-0.000000643	-0.000000534	-0.000000737
6	-0.000001041	-0.000000365	-0.000000836
6	-0.000001015	-0.000000221	-0.000000164
6	-0.000001276	-0.000000652	-0.000000927
1	-0.000000678	-0.000000513	-0.000000712
1	-0.000000741	-0.000000101	-0.000000193
1	-0.000000936	-0.000000232	-0.000000356
1	-0.000001542	-0.000000083	-0.000000361
1	-0.000001215	-0.000000945	-0.000001196
1	-0.000001634	-0.000000736	-0.000000908
1	-0.00000116	-0.000000725	-0.000000968
6	0.000001001	-0.000000717	-0.000000796
6	0.000001229	-0.000000599	-0.000000842
6	0.000001137	-0.000001138	-0.000001362
1	0.000000606	-0.000000797	-0.000000896
1	0.000001088	-0.000000348	-0.000000333
1	0.000001038	-0.000000698	-0.000000788
1	0.000001446	-0.000000638	-0.000000678
1	0.000000843	-0.000001188	-0.000001498
1	0.000001304	-0.000001142	-0.000001466
1	0.000000965	-0.000001181	-0.000001392
6	0.000000526	-0.000000566	-0.000000597
6	0.000000501	-0.000000776	-0.000000847
6	0.000000398	-0.000000269	-0.000000157
1	-0.000000331	-0.000000804	-0.000000521
1	0.000000455	-0.000000935	-0.000001167
1	0.000000226	-0.000000746	-0.000000911
1	0.000000806	-0.00000072	-0.000000765
1	0.000000209	0.000000188	-0.00000019
1	0.000000605	-0.00000019	-0.000000247
1	0.000000085	-0.000000288	-0.000000024
6	0.00000017	0.00000101	0.000001126
6	0.00000051	0.000001047	0.000001252
6	0.000000248	0.000001308	0.000001547
6	-0.000000002	0.000001393	0.000001687
6	-0.000000371	0.000001154	0.000001525
1	0.000000493	0.000001454	0.000001851
1	0.000000323	0.00000047	0.000000802
7	-0.000000174	0.000000934	0.000001185
8	-0.000000384	0.000000896	0.000000595
1	-0.000000178	0.000001625	0.000002014

1	0.00000076	0.000000956	0.000001271
17	-0.000000751	0.000001301	0.000001665
Zero-point correction=			1.186315 (Hartree/Particle)
Thermal correction to Energy=			1.261798
Thermal correction to Enthalpy=			1.262742
Thermal correction to Gibbs Free Energy=			1.064664
Sum of electronic and zero-point Energies=			-4217.729005
Sum of electronic and thermal Energies=			-4217.653522
Sum of electronic and thermal Enthalpies=			-4217.652577
Sum of electronic and thermal Free Energies=			-4217.850656

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6	0.000001452	-0.000003693	-0.000001491
6	-0.000002695	0.000005608	0.000001691
7	-0.000000067	0.000001692	0.000001579
7	0.000000686	-0.000003763	-0.000002018
16	-0.000000717	-0.000000215	0.000000635
8	0.000002146	0.000002288	-0.000000054
8	0.000001074	0.000000296	0.000000565
6	0.000000003	0.000001725	0.000000118
6	0.000000636	0.000001654	-0.000000063
6	0.000000948	0.000000749	-0.000000701
6	0.000000239	0.000000325	0.000000185
6	-0.000000785	0.000000641	-0.000000106
6	0.000000338	-0.000001207	0.000000088
1	0.000000804	0.000001346	-0.000000405
1	0.000001027	0.000000572	-0.000000772
1	-0.000000347	-0.000000431	0.000000268
1	-0.000000364	0.000000484	0.000000851
6	0.000000126	-0.000000181	-0.000000345
1	0.000000103	-0.000000573	-0.000000432
1	0.000000025	-0.000000207	-0.000000285
1	0.000000032	-0.000000337	-0.000000081
6	0.000001042	0.000000786	-0.000000078
6	0.000001333	0.000000774	-0.000000954
1	0.000000387	0.000000806	-0.000000883
1	0.000000507	0.000000463	-0.000000696
6	0.000001536	0.000000954	-0.000002476
1	0.000001254	0.000001211	-0.000000962
1	0.000000981	0.000000852	-0.000001149
6	0.000001636	0.000000952	-0.000001876
1	0.000001409	0.000000063	-0.000001858
1	0.000001589	0.000001081	-0.000001864
1	0.000002147	0.000000901	-0.000002478

1	0.000002176	0.00000164	-0.000001815
1	0.000001829	0.000001314	-0.00000195
6	-0.000001246	0.00000274	0.000002391
6	-0.000001512	-0.000001111	0.000000871
1	-0.000001065	-0.000000703	0.00000157
1	-0.00000067	0.000000452	-0.00000033
6	-0.000000901	-0.000000251	0.000001838
1	-0.000001267	0.000000037	0.000002522
1	-0.000001155	0.000001062	0.000001884
6	-0.00000182	-0.000000599	0.000001876
1	-0.00000095	-0.000000622	0.000000968
1	-0.000001201	-0.000000949	0.000001601
1	-0.000001579	-0.000000952	0.000001994
1	-0.000001734	-0.000000434	0.000002381
1	-0.000001397	-0.000000302	0.000001743
16	-0.000000084	0.000002082	0.000003832
8	-0.000001601	0.000002583	0.000000636
8	-0.000001015	0.000001549	0.00000127
6	0.000000155	0.000000809	0.000001461
6	-0.000001101	0.000001571	0.000002992
6	-0.000000692	0.000001553	0.000001404
6	-0.000000849	0.000001621	0.000002269
1	-0.000000872	0.000000545	0.000002059
6	0.000000096	0.00000267	0.000002408
1	0.000000336	0.000002493	0.000001428
6	-0.000000165	0.000002253	0.000001458
1	-0.000000445	0.000001188	0.000002195
1	0.000000695	0.000002754	0.000001642
6	-0.000000503	0.000003037	0.000002297
1	-0.000000018	0.000001957	0.000001998
1	0.000000324	0.000002442	0.000001306
1	-0.000000173	0.000002514	0.000002149
79	-0.000000585	-0.000003225	0.000000261
6	0.00000255	0.0000043	0.00000022
6	0.000001066	-0.000002208	-0.000000615
6	-0.000000492	-0.000002374	0.000000128
1	-0.000000211	-0.000001266	-0.000001153
1	0.000000171	-0.000000573	-0.000001561
7	0.000001686	-0.000001367	-0.000000219
7	-0.000002447	-0.000001404	-0.000003136
6	-0.000001198	0.000001372	-0.000001043
6	0.000000761	-0.000000441	-0.000002321
6	0.000001823	0.000000124	0.000000026
6	0.000001989	-0.000000487	-0.000001334

6	0.000000927	0.000000599	-0.000001014
6	0.00000145	0.000000979	-0.00000216
1	0.000001566	0.000000393	-0.000002916
1	0.000001352	0.000001805	-0.000001
1	0.000002143	0.000001274	-0.000001887
6	-0.00000078	-0.00000395	0.000003094
6	0.000000668	0.000000891	0.000000655
6	-0.000003064	-0.000003369	-0.000002113
6	-0.000002641	-0.000002169	0.000000398
6	0.00000002	-0.000001097	-0.000000589
6	-0.000002237	-0.000003693	0.000000805
1	-0.000001657	-0.000000978	0.000002186
1	-0.000001129	-0.000001758	0.000000724
1	-0.000001693	-0.000001917	0.000000984
6	-0.000000213	-0.000001767	-0.000001475
6	-0.000002955	-0.000000239	0.000002479
6	0.000000037	0.000000076	0.000002518
1	-0.000000064	-0.000000867	0.000001884
1	-0.000001433	-0.000001436	0.000000401
1	-0.000001361	-0.000001014	0.000000977
1	-0.000001925	-0.000002213	0.000001198
1	-0.000001004	-0.000000249	0.00000013
1	-0.000002285	-0.000000647	0.00000084
1	-0.000001136	0.000000307	0.00000134
6	0.000001322	-0.000001737	-0.000000613
6	-0.000001074	-0.000001424	-0.000000905
6	-0.000001325	-0.000002794	-0.000000417
1	0.000000401	-0.000002291	-0.000000736
1	-0.000000373	-0.000001228	-0.000000943
1	-0.000000089	-0.000001937	-0.000001141
1	-0.000000671	-0.000002439	-0.000000571
1	-0.000000634	-0.000002926	-0.000001071
1	-0.000000836	-0.000002623	-0.000001542
1	-0.000000536	-0.000002735	-0.000001644
6	-0.000000496	0.00000019	-0.000000807
6	0.000000642	0.000001329	0.000000469
6	0.000000458	0.000000588	-0.000000722
1	-0.00000072	0.00000056	0.000000206
1	0.000000596	0.000001335	-0.000000019
1	0.000000627	0.00000161	0.000000096
1	0.000000653	0.000000765	0.000000133
1	0.000000697	0.000000188	-0.000000525
1	0.000000755	0.000001589	-0.000000359
1	0.000000729	0.000000721	0.00000005

6	0.000002104	-0.000001299	-0.000000953
6	0.000000796	-0.000001149	-0.000002953
6	0.000000233	-0.00000103	-0.000002717
1	0.000001319	-0.000001394	-0.000001801
1	0.000001037	-0.000001283	-0.000002605
1	0.000000979	-0.000001741	-0.000002822
1	0.000001976	-0.000000622	-0.000003312
1	0.000001246	-0.000000594	-0.000001605
1	0.000001606	-0.00000078	-0.000002029
1	0.000000855	-0.000001161	-0.000002537
8	0.000000005	0.000002337	0.000003588

Zero-point correction= 1.106537 (Hartree/Particle)

Thermal correction to Energy=	1.176427
Thermal correction to Enthalpy=	1.177371
Thermal correction to Gibbs Free Energy=	0.990379
Sum of electronic and zero-point Energies=	-3510.033891
Sum of electronic and thermal Energies=	-3509.964001
Sum of electronic and thermal Enthalpies=	-3509.963057
Sum of electronic and thermal Free Energies=	-3510.150049

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6	-0.000000352	0.000000418	0.000000027
6	0.000000393	-0.000000293	0.000000501
7	0.000000844	-0.000001337	-0.000000315
7	0.000000158	-0.000000138	0.000001072
16	0.000000288	-0.000000094	0.000000715
8	0.000000037	-0.000000544	0.000000537
8	0.00000067	0.000000305	0.000000435
6	0.00000042	-0.000001046	0.000001059
6	0.000000156	-0.000001384	0.000000835
6	0.000000118	-0.000001693	0.000001218
6	0.000000415	-0.000001612	0.000001715
6	0.000000768	-0.000001283	0.000001727
6	0.00000068	-0.000000676	0.000001541
1	-0.000000175	-0.000001284	0.000000563
1	-0.000000024	-0.000002133	0.000001247
1	0.000001028	-0.00000137	0.000002053
1	0.000000811	-0.000000466	0.000001435
6	0.000000513	-0.000002208	0.000002005
1	0.000000786	-0.000002193	0.000002261
1	0.000000689	-0.000002278	0.000002238
1	0.000000264	-0.000002525	0.000002063
6	-0.000000242	-0.000000296	-0.000000093
6	-0.000000026	-0.000001272	-0.000000061

1	-0.000000827	0.000000002	-0.000000521
1	-0.000000538	-0.000000078	-0.000000118
6	-0.000000842	-0.000001375	-0.000000196
1	-0.000000266	-0.000000962	-0.000000043
1	-0.000000046	-0.000001077	0.000000655
6	-0.000001088	-0.000001967	-0.000000185
1	-0.000001019	-0.00000145	-0.000000313
1	-0.000001264	-0.000001183	-0.000000343
1	-0.000001465	-0.000002176	-0.000000225
1	-0.00000115	-0.000001884	-0.000000015
1	-0.000000903	-0.000002165	0.000000271
6	0.000000759	-0.000000448	0.000000317
6	0.000000272	-0.000001127	0.000001344
1	0.000000067	-0.000000668	0.00000108
1	0.000000085	-0.000000815	0.000001026
6	0.000000242	-0.000001465	0.000000889
1	0.000000508	-0.000001016	0.000001526
1	0.000000363	-0.000001219	0.000000782
6	0.000000036	-0.00000198	0.000001286
1	-0.000000232	-0.000001546	0.000000845
1	0.000000256	-0.000001444	0.000001288
1	-0.000000206	-0.000002295	0.000001302
1	0.000000302	-0.000002033	0.000001616
1	-0.000000138	-0.000002103	0.000001087
16	0.00000114	-0.000000192	0.000001153
8	0.000001203	-0.000000378	0.000001758
8	0.000001436	0.000000124	0.000001704
6	0.000001342	0.000000523	0.000001309
6	0.000001542	0.000000361	0.000001379
6	0.000001626	0.000000887	0.000001403
6	0.000001973	0.000001126	0.000001687
1	0.000001369	0.000000028	0.000001478
6	0.000001742	0.000000955	0.000001514
1	0.000001551	0.000001063	0.000001158
6	0.000001883	0.000001291	0.000001494
1	0.000001749	0.000000721	0.00000154
1	0.000001945	0.000001733	0.000001123
6	0.000002183	0.000001755	0.000001413
1	0.000001957	0.000001503	0.000001356
1	0.000002213	0.000002081	0.000001059
1	0.000002451	0.000001789	0.000001881
79	-0.000000304	0.000000156	0.000000027
6	-0.000000803	0.000000063	0.000000101
6	-0.000000646	0.000000584	-0.00000108



6	-0.00000448	0.00000018	-0.000001001
1	-0.000000991	-0.000000126	-0.000001072
1	-0.000000528	0.000000912	-0.000001255
7	0.000000128	0.000001161	-0.000000795
7	-0.000000486	0.000000166	-0.000000902
6	-0.000000519	0.000000607	-0.000000793
6	-0.000000521	0.000001597	-0.000001541
6	0.000000538	0.000001254	-0.000000326
6	0	0.000001948	-0.000001074
6	0.000000287	0.000001887	-0.000000936
6	-0.000000042	0.000001936	-0.000000475
1	-0.000000035	0.000002444	-0.000001599
1	0.000000912	0.000002191	-0.000000439
1	0.000000611	0.00000263	-0.000001156
6	-0.000001193	-0.000000874	-0.000000412
6	-0.000000909	-0.000000936	-0.000000437
6	-0.00000126	-0.000000289	-0.000000834
6	-0.000000816	-0.00000138	-0.000000132
6	-0.000001341	-0.000001479	-0.000000875
6	-0.00000102	-0.00000163	-0.000000214
1	-0.000000657	-0.000001633	0.000000358
1	-0.000001479	-0.000001478	-0.000000924
1	-0.000001237	-0.000001991	-0.000000103
6	0.000000091	-0.000000624	-0.000000173
6	-0.000000508	-0.00000071	-0.000000082
6	-0.000000161	-0.000000919	0.000000488
1	-0.00000039	-0.000000359	0.000000181
1	-0.000000774	-0.000000546	-0.000000358
1	-0.000000305	-0.000000735	0.000000118
1	-0.000000705	-0.000001196	0.000000062
1	0.000000104	-0.000000846	0.000000692
1	-0.000000128	-0.000001223	0.000000691
1	0.000000273	-0.000000668	0.000000647
6	-0.000001368	-0.000000387	-0.000001182
6	-0.000001397	-0.000000746	-0.000001194
6	-0.000001829	-0.000000455	-0.000001626
1	-0.000000972	-0.000000184	-0.000001328
1	-0.000001074	-0.000000415	-0.000001007
1	-0.000001459	-0.000000282	-0.000001612
1	-0.0000017	-0.000000942	-0.000001337
1	-0.000001612	-0.000000586	-0.000001602
1	-0.00000188	-0.000000919	-0.000001668
1	-0.000001793	-0.000000372	-0.000001876
6	0.000000171	0.000001031	-0.000000053

6	0.000000906	0.000001149	0.000000335
6	0.000000667	0.000001289	-0.000000272
1	0.00000031	0.000000844	-0.000000196
1	0.000001041	0.000001173	-0.000000272
1	0.000001316	0.000001126	0.000000256
1	0.000000943	0.000001731	0.000000253
1	0.000000336	0.000001327	-0.000000419
1	0.000000776	0.000001746	-0.0000002
1	0.000000724	0.000001058	0.000000151
6	-0.00000067	0.00000158	-0.000001733
6	-0.000000915	0.000001443	-0.000002095
6	-0.000000796	0.000001132	-0.000001878
1	-0.000000895	0.000000791	-0.000001569
1	-0.000000931	0.00000141	-0.000001898
1	-0.000001258	0.000001383	-0.000002261
1	-0.000000804	0.000001889	-0.000002125
1	-0.000000746	0.000001123	-0.000001402
1	-0.000000697	0.000001757	-0.000001835
1	-0.00000117	0.000001229	-0.000002072
8	0.000000373	0.000000289	0.000000332
6	0.000000015	0.000001294	-0.00000114
6	0.000000168	0.00000103	-0.000001031
6	0.00000041	0.000001796	-0.000000614
6	0.000000174	0.000002003	-0.000001315
6	-0.000000468	0.000001955	-0.000001501
6	-0.000000447	0.000001336	-0.000001396
6	0.000000268	-0.000000081	0.000000215
6	0.000000251	0.000001508	-0.000000393
1	0.000000919	0.000001908	-0.000001769
1	0.000000082	0.000002415	-0.000001457
1	-0.000000496	0.000001927	-0.000001777
1	-0.000000582	0.000001047	-0.000001391
1	-0.00000013	0.000000256	-0.00000033
1	0.000001041	0.000000462	-0.00000068
7	-0.000000641	0.000001864	0.000000782
1	0.000000719	0.000001363	0.000000024

Zero-point correction=

1.238213 (Hartree/Particle)

Thermal correction to Energy=

1.314318

Thermal correction to Enthalpy=

1.315262

Thermal correction to Gibbs Free Energy=

1.120478

Sum of electronic and zero-point Energies=

-3873.689762

Sum of electronic and thermal Energies=

-3873.613658

Sum of electronic and thermal Enthalpies=

-3873.612713

Sum of electronic and thermal Free Energies=

-3873.807498

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6	-0.000005114	0.000000727	-0.000008657
6	0.000002637	0.000003838	0.000009703
7	0.000006149	-0.000003074	-0.000003082
7	-0.000004701	-0.000002069	0.000003348
16	-0.000002841	0.000002998	0.000002762
8	-0.000002316	0.000004844	-0.000002269
8	-0.000001973	-0.000004765	-0.000001477
6	-0.000001416	-0.000001307	-0.000001343
6	-0.000001361	-0.000001222	-0.000000066
6	0.000001096	-0.000002063	-0.000000303
6	-0.000000695	-0.000001578	-0.000003355
6	-0.000001178	-0.000002495	-0.000004172
6	0.000000462	-0.000002632	-0.000000946
1	0.000000203	-0.000000546	-0.000001101
1	0.000000463	-0.000002397	-0.000001459
1	-0.000000915	-0.000003009	-0.000003972
1	-0.000002372	-0.000001111	-0.000003191
6	0.000000042	-0.000003214	-0.000003388
1	-0.000000199	-0.000003905	-0.0000003
1	-0.000000559	-0.000004523	-0.000003056
1	0.000000515	-0.000004186	-0.000003197
6	-0.000003486	0.000007875	-0.000000155
6	0.000000524	-0.000004312	0.000001386
1	0.000003085	-0.000002677	-0.000001772
1	0.000000494	0.000000668	-0.000000001
6	0.000003176	0.000002201	0.000003066
1	0.000002701	-0.000000433	0.000001447
1	0.000001688	-0.000001114	-0.000000028
6	0.000001912	-0.000001996	0.000001483
1	0.000001685	-0.000000697	0.000001189
1	0.000000584	0.000000603	0.000001964
1	0.000002589	-0.000001333	0.00000156
1	0.000003029	-0.000002018	0.000001183
1	0.000002314	-0.000002075	0.000000831
6	-0.000000383	-0.000007223	-0.000012191
6	0.000002086	-0.000000565	0.000001694
1	0.000000159	-0.000001501	0.000000062
1	-0.000000222	-0.000001435	-0.000000241
6	0.00000435	-0.000001677	-0.000000671
1	0.000000215	-0.00000382	-0.000001769
1	-0.000000021	-0.000002749	-0.000000283
6	0.000000013	-0.000005829	-0.000002329

1	0.000000871	-0.00000262	-0.000000803
1	0.000001548	-0.000004111	-0.000002429
1	0.000002232	-0.00000397	-0.000000583
1	0.000001762	-0.000003969	-0.000001615
1	0.000002331	-0.000003109	-0.000001
16	0.000004844	-0.000005038	-0.000011423
8	-0.000002442	-0.000002989	-0.000007481
8	-0.000004566	0.000002905	0.000006177
6	-0.000000754	0.000004026	-0.000004806
6	-0.000003354	-0.000002641	-0.00000387
6	-0.000003019	-0.000000642	-0.00000261
6	-0.0000026	-0.000001982	-0.000002641
1	-0.000000154	-0.000002926	-0.000002564
6	-0.000002183	-0.0000007	-0.000004023
1	-0.000002876	0.000000292	-0.000003786
6	-0.00000186	-0.000001045	-0.000003219
1	-0.000001527	-0.000002565	-0.000003602
1	-0.000003636	0.000000051	-0.000004015
6	-0.000002992	-0.000001038	-0.000004063
1	-0.000002068	-0.000001561	-0.000003806
1	-0.000003919	-0.000000043	-0.00000394
1	-0.000003458	-0.000001549	-0.000005682
79	-0.000001939	-0.000000135	0.000003235
6	0.000003647	0.00000427	0.000005057
6	-0.000002085	0.000001357	0.000000013
6	0.000003319	0.000001479	0.000001883
1	0.0000031	-0.000000539	0.00000358
1	0.000001756	0.000000213	0.000003325
7	-0.000000321	0.00000235	-0.000002082
7	-0.000000072	-0.000004298	0.000002252
6	-0.000002753	0.000001083	0.000001317
6	-0.000001438	0.00000214	0.000000271
6	-0.000000275	0.000005912	-0.000000828
6	-0.000000056	0.000004774	0.000002817
6	-0.000002059	0.00000064	-0.000002219
6	-0.00000301	0.000001836	0.000001528
1	-0.000000998	0.000004458	0.000001642
1	-0.000003546	0.000002647	0.000000075
1	-0.000002624	0.000003784	0.000000269
6	0.00000297	-0.000006202	0.00000325
6	-0.000002494	-0.000001012	-0.00000069
6	0.000005978	0.00001108	0.000000912
6	0.000004154	0.00000351	0.000001117
6	-0.000001163	-0.000004021	-0.000001046

6	0.000004853	-0.000006507	0.000006024
1	0.000003277	-0.000002992	0.000001829
1	0.000003992	-0.000000492	0.000002906
1	0.000003732	-0.00000195	0.000002416
6	0.000002064	-0.000003359	0.000003765
6	0.000003329	-0.000002909	0.000000122
6	0.000001931	-0.000002386	0.00000006
1	0.000000938	-0.00000051	0.000003037
1	0.000002627	-0.000000656	0.000000899
1	0.000002885	-0.000002149	0.000001194
1	0.000002618	-0.000002967	0.000002338
1	0.000001257	-0.000002836	-0.000001487
1	0.000002694	-0.000003344	-0.000001318
1	0.000002456	-0.000003659	-0.000000368
6	0.0000022	-0.000002823	0.000000962
6	0.000000768	0.000001515	0.000006392
6	0.000000739	0.000001975	0.000005184
1	0.00000361	0.000002063	0.000001724
1	0.000001257	0.000001802	0.000002506
1	0.000001477	0.00000249	0.000003342
1	0.000002366	0.000001947	0.000002128
1	0.000002773	0.000001129	0.000004058
1	0.000005557	0.000000148	0.000004449
1	0.000002504	0.000001779	0.000005294
6	-0.00000387	0.000000074	0.00000066
6	0.000000907	0.000001024	0.000000712
6	0.000001377	-0.000000176	-0.000000605
1	0.000000202	-0.000000319	0.000000822
1	-0.000000921	0.000000117	-0.000000994
1	-0.000001488	-0.00000062	-0.000002796
1	-0.00000267	0.0000008	-0.00000193
1	0.000000277	0.000001139	0.00000026
1	-0.000001618	0.000000479	0.000000238
1	-0.000000373	-0.000000607	-0.000000889
6	0.000004485	0.000000937	0.000000064
6	-0.000003169	0.000003991	0.000005181
6	-0.000001627	0.000004457	0.000005323
1	0.000002593	0.000003137	0.000002458
1	0.00000019	0.000003623	0.000002839
1	0.000000457	0.000004125	0.0000042
1	0.000000715	0.000003394	0.000002821
1	-0.000001387	0.000004738	0.000001431
1	-0.000000941	0.000006025	0.000002265
1	-0.000000265	0.000004142	0.000003211

8	-0.000004004	-0.000006623	-0.000006449
6	0.00000374	0.000003253	0.00000237
6	-0.000000654	0.000001299	0.000003242
6	-0.000006171	0.000003872	-0.000003887
6	-0.00000182	0.000001454	0.00000246
6	0.000000097	0.000006939	0.000001502
6	-0.000007834	0.000005066	0.00000099
6	-0.000005135	0.000009947	-0.000002246
6	-0.000003842	-0.00000523	0.000005254
1	-0.000001993	0.000003773	-0.000000504
1	-0.000003362	0.000005696	0.000001094
1	-0.000002591	0.000005756	0.000001696
1	-0.000001235	0.000003632	0.000000887
1	0.000001002	0.000000926	-0.000000505
1	-0.000002303	0.000000616	-0.000001506
7	-0.000002846	0.00000253	-0.000008286
1	-0.00000001	0.000003	0.00000331

<b>Zero-point correction=</b>	<b>1.239476 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>	<b>1.315602</b>
<b>Thermal correction to Enthalpy=</b>	<b>1.316546</b>
<b>Thermal correction to Gibbs Free Energy=</b>	<b>1.120438</b>
<b>Sum of electronic and zero-point Energies=</b>	<b>-3873.699726</b>
<b>Sum of electronic and thermal Energies=</b>	<b>-3873.623600</b>
<b>Sum of electronic and thermal Enthalpies=</b>	<b>-3873.622656</b>
<b>Sum of electronic and thermal Free Energies=</b>	<b>-3873.818764</b>

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6	-0.000000754	-0.000000949	-0.000000371
6	0.000000389	-0.000000645	-0.000000692
7	0.000000078	-0.000001614	0.000000647
7	0.000001383	-0.000000707	0.000000042
16	0.000000163	-0.000002546	0.000000046
8	-0.000000154	-0.000002628	0.000000979
8	0.000000705	-0.000002012	0.000000001
6	0.000000328	-0.000001799	0.000000426
6	0.000000059	-0.000003014	0.000001316
6	0.000000001	-0.000003323	0.000000497
6	0.000000369	-0.000003869	0.000002097
6	0.000001865	-0.000003061	0.000000277
6	0.000000777	-0.000002775	0.000000106
1	-0.000000052	-0.000002873	0.000001179
1	-0.000000208	-0.000003208	0.000001318
1	0.000001645	-0.000002978	0.000000076
1	0.000001316	-0.000002486	-0.000000045

6	0.000001371	-0.000003668	0.00000003
1	-0.000000971	-0.000003847	-0.000000354
1	0.000001876	-0.000002504	0.00000022
1	0.000002009	-0.000002842	0.000000766
6	-0.00000079	-0.000001332	0.000000982
6	-0.000000888	-0.000001158	0.0000008
1	-0.000001169	-0.000000869	0.00000091
1	-0.000000857	-0.000001704	0.000001067
6	-0.000001484	-0.000001143	0.000001407
1	-0.000000783	-0.000000567	0.000000954
1	-0.000000489	-0.000001281	0.000000849
6	-0.000001633	-0.000001012	0.00000138
1	-0.00000153	-0.000001676	0.000001517
1	-0.000001931	-0.000000924	0.000001364
1	-0.000002155	-0.000001093	0.000001705
1	-0.000001689	-0.000000441	0.000001264
1	-0.000001387	-0.000001308	0.000001309
6	0.00000086	-0.000000499	-0.000000189
6	0.000000617	-0.000000938	0.000000101
1	0.000001024	-0.000000129	-0.000000568
1	0.000000127	-0.000000534	-0.000000101
6	0.000000319	-0.000000559	0.000000012
1	0.000001032	-0.000001295	-0.0000002
1	0.000000435	-0.000001533	0.000000077
6	0.000000226	-0.000001047	0.000000227
1	-0.00000003	-0.000000039	0.000000084
1	0.000000633	-0.000000298	-0.000000332
1	0.000000024	-0.000000777	0.000000255
1	0.000000661	-0.000001374	0.00000003
1	-0.000000041	-0.000001447	0.000000472
16	0.000001967	-0.000000849	-0.000000824
8	0.000001948	-0.000001041	-0.000000753
8	0.000002054	-0.000001783	-0.000000712
6	0.00000232	-0.000000771	-0.000001659
6	0.000002064	0.000000407	-0.000001214
6	0.000002522	-0.000000546	-0.000001192
6	0.000002938	0.000000312	-0.000001644
1	0.000002221	0.000000097	-0.000001344
6	0.000002282	0.000000163	-0.00000156
1	0.000002324	-0.000001066	-0.000001034
6	0.000002941	0.000000135	-0.000002351
1	0.000002741	0.00000079	-0.000001934
1	0.000002988	-0.000000447	-0.000001607
6	0.000003788	0.000000928	-0.000002835

1	0.000004271	-0.000000043	-0.000002335
1	0.000002886	0.000001204	-0.000002387
1	0.000002778	0.000000859	-0.000002206
79	-0.000000148	0.000000133	0.000000285
6	-0.000000832	0.000001304	-0.000000309
6	-0.000000456	0.000002382	-0.000000054
6	-0.000001	0.000002231	-0.000000298
1	-0.000000986	0.000002587	-0.000000186
1	-0.000000569	0.000002637	-0.000000455
7	-0.000000426	0.000001254	-0.000000121
7	-0.000000512	0.000001477	-0.000000083
6	-0.00000008	0.000001881	-0.000000371
6	-0.000000638	0.00000152	0.000000189
6	0.000000101	0.000001168	-0.000000734
6	-0.000000532	0.000001268	-0.000000126
6	0.000000482	0.000001279	-0.000000409
6	0.000000061	0.000001393	-0.000000441
1	-0.000000966	0.00000122	0.000000056
1	0.000000919	0.000000981	-0.000000903
1	0.000000122	0.000001061	-0.000000462
6	-0.000001072	0.000001976	0.000000044
6	-0.000000218	0.000001532	0
6	-0.000001569	0.000001034	0.000000269
6	-0.000000895	0.000001103	-0.000000246
6	-0.000001265	0.000000873	0.000000894
6	-0.000001254	0.000001415	0.000000484
1	-0.000000284	0.000001103	-0.000000167
1	-0.000001905	0.000000705	0.000001038
1	-0.000001238	0.000000819	0.000000495
6	0.000000226	0.000001573	-0.000000565
6	0.000000111	0.000002432	-0.000000809
6	0.000000644	0.00000119	-0.000000774
1	0.000000171	0.000001786	-0.000000717
1	-0.000000356	0.000002709	-0.000000688
1	0.000000398	0.000002639	-0.000001153
1	-0.000000126	0.000002443	-0.000000814
1	0.000000753	0.00000072	-0.000000719
1	0.000000583	0.000001333	-0.000000087
1	0.000001052	0.000001527	-0.000001178
6	-0.0000019	0.000000886	0.000000687
6	-0.000002088	0.000000473	0.000001117
6	-0.00000242	0.000001729	0.000000089
1	-0.000001711	0.000001394	0.000000616
1	-0.000001716	0.000000285	0.000000078



1	-0.000002428	0.000000577	0.000001306
1	-0.000002247	0.00000039	0.000001415
1	-0.000002316	0.000002279	0.000000662
1	-0.000002566	0.000001653	0.000001165
1	-0.000002699	0.000001809	0.000001075
6	0.000000893	0.000001267	-0.000001045
6	0.000001412	0.000001021	-0.000001342
6	0.000000916	0.00000214	-0.000001515
1	0.000000666	0.000001398	-0.000000816
1	0.00000106	0.000000309	-0.000000699
1	0.000001662	0.000000905	-0.000001379
1	0.000001587	0.000000636	-0.000001119
1	0.000000662	0.000002523	-0.000001252
1	0.000001284	0.000002099	-0.000001382
1	0.000001368	0.000002169	-0.000001551
6	-0.000001414	0.000001576	0.000000336
6	-0.000001672	0.000002316	0.000000328
6	-0.000001801	0.000001049	0.000000731
1	-0.000001437	0.000001647	0.000000359
1	-0.000001426	0.000002653	-0.000000001
1	-0.000002133	0.00000242	0.000000529
1	-0.000001679	0.000002272	0.000000241
1	-0.000001517	0.000000582	0.000000738
1	-0.000001795	0.000000986	0.000000736
1	-0.000002202	0.000001192	0.000001002
8	0.000001319	-0.000001145	-0.000000291
6	-0.000000345	-0.000001287	0.000000602
6	-0.000000428	-0.000000628	0.000000649
6	-0.000001167	-0.000000567	0.000000914
6	-0.00000137	-0.000001149	0.000001231
6	-0.000001227	-0.000001561	0.000001341
6	-0.000000898	-0.000001617	0.000001023
6	0.000000103	-0.000001228	0.000000558
6	0.000000152	-0.000000557	-0.000000006
1	-0.000001224	-0.000000229	0.000000809
1	-0.000001846	-0.000001052	0.000001492
1	-0.000001566	-0.000001963	0.000001634
1	-0.000000549	-0.000002052	0.000001139
1	0.000000557	-0.00000159	0.000000103
1	0.000000828	-0.0000004	-0.000000326
7	-0.000000062	-0.000000038	0.000000226
1	-0.000000017	0.000000007	-0.000000036

Zero-point correction=

1.239109 (Hartree/Particle)

Thermal correction to Energy=

1.315007

Thermal correction to Enthalpy=	1.315951
Thermal correction to Gibbs Free Energy=	1.121159
Sum of electronic and zero-point Energies=	-3873.695299
Sum of electronic and thermal Energies=	-3873.619402
Sum of electronic and thermal Enthalpies=	-3873.618458
Sum of electronic and thermal Free Energies=	-3873.813250

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6	0.000001479	0.000006239	0.000011205
6	-0.00000389	-0.000008778	0.000002306
7	-0.000010735	-0.000002855	-0.000008779
7	0.000005411	-0.000000552	0.000000955
16	-0.000007706	-0.000002315	0.000000462
8	0.000002564	-0.000001363	0.000001481
8	0.000004278	0.000003002	0.000001808
6	-0.00000076	-0.00000075	-0.000003048
6	0.000002535	0.000002504	-0.000004816
6	0.000001097	-0.000002914	-0.000002583
6	-0.000000508	-0.000001663	-0.000000382
6	-0.000001118	-0.000002842	-0.000002419
6	0.000001645	0.000000417	0.000001196
1	-0.000001805	-0.000002489	-0.000001235
1	-0.000000091	-0.000001322	-0.000002181
1	-0.000001187	-0.000002196	-0.000001036
1	0.000001029	-0.000003976	-0.000002153
6	0.000000155	-0.000002592	-0.000002038
1	0.000000133	-0.000001547	-0.000001674
1	0.000000057	-0.000001714	-0.000002318
1	-0.000000212	-0.000000509	-0.000002083
6	0.000007813	-0.000006125	0.00000117
6	0.000000899	0.000004773	-0.000004692
1	-0.000000685	-0.000002335	0.000000308
1	-0.00000208	-0.000002382	-0.000004559
6	0.000001087	0.000000287	-0.000001229
1	-0.00000191	-0.000001231	0.000000682
1	0.000001151	0.000000909	0.000000016
6	0.000001436	-0.000000704	-0.000000006
1	0.000000594	-0.000000955	-0.000001813
1	0.000002117	-0.000000625	-0.000000008
1	0.000001404	-0.000000218	-0.000001061
1	0.000000322	0.000000705	-0.000000672
1	0.000000757	-0.000000548	-0.000002101
6	-0.000001904	-0.000001895	-0.000000028
6	0.000001115	-0.000002616	-0.000000377

1	0.00000142	0.000002339	-0.000002913
1	0.000001528	0.000001708	0.000001135
6	0.000001805	0.000001487	0.000000563
1	0.000000071	0.000001218	-0.000001267
1	0.000000509	0.000000325	0.00000022
6	-0.000001108	-0.000003513	-0.000002595
1	0.000000436	-0.000000587	-0.000000964
1	0.000001736	-0.000000439	-0.000000653
1	0.000000055	0.000000303	-0.000001264
1	0.000000518	-0.000000257	-0.000000041
1	0.00000149	0.000001001	-0.000000898
16	-0.000007033	0.000001115	0.000010222
8	0.000002188	-0.00000242	0.000001162
8	-0.000003633	0.000001682	-0.000004061
6	-0.000001451	-0.000005233	-0.00000068
6	-0.000000254	0.000001037	0.000002563
6	-0.000000882	-0.000000087	0.000000611
6	0.000000816	-0.000001076	0.000000094
1	-0.0000007	0.000000091	-0.000000146
6	-0.000002375	0.000000772	0.000000723
1	-0.000000677	-0.000000057	-0.000001675
6	-0.000001398	-0.000000082	0.000000303
1	-0.000000501	0.000000513	0.000001681
1	-0.000001798	-0.000000382	0.000001451
6	-0.000001969	0.000000263	0.000000008
1	-0.000001181	-0.000000059	0.000003462
1	-0.000002243	0.000000875	0.000001754
1	0.000000085	-0.00000004	0.000001729
79	0.00000827	0.000004152	0.000001812
6	-0.00000636	0.000005214	0.000003705
6	0.00000249	-0.000000663	0.000001741
6	-0.000002296	0.000002005	0.000003328
1	0.000001732	0.000001858	0.000000075
1	-0.000000834	0.000002552	-0.000000297
7	-0.000001655	-0.000003609	0.000000913
7	0.000004066	-0.000004158	-0.000001906
6	0.00000266	0.000001706	-0.000000431
6	-0.000003738	0.000002194	-0.000005579
6	0.000000674	0.00000507	0.000006721
6	0.000000089	0.00000414	0.000005122
6	-0.00000267	-0.000000515	-0.000003063
6	-0.000001036	-0.00000587	0.000004961
1	-0.00000051	0.00000144	-0.000000559
1	-0.000001921	0.000001112	0.000001742

1	-0.000001272	0.000000572	0.00000121
6	0.000000772	0.000002683	0.000001026
6	0.0000024	-0.000004783	-0.000010999
6	0.000005836	0.000007046	-0.000001526
6	0.000002248	0.000006062	0.000001998
6	-0.000004074	-0.000002864	-0.000006169
6	0.000004659	-0.000004109	0.000001072
1	0.00000035	-0.000001831	0.000002013
1	0.000001113	0.000002132	-0.000001493
1	0.000000697	0.00000186	-0.00000079
6	-0.000002716	0.000001885	0.000006484
6	0.000001033	0.000000829	-0.000002797
6	0.000001936	0.000002533	-0.000001816
1	0.000000669	0.000004041	0.000001103
1	0.000001167	0.000000773	0.000001844
1	0.00000182	0.000002239	0.000001
1	-0.000000107	0.000002197	0.000001633
1	0.000000097	0.000003219	0.000001168
1	0.000003046	-0.000000077	0.000003122
1	-0.000001932	0.000001166	0.000000582
6	0.000005534	0.000000036	0.000000746
6	-0.000000144	-0.000001885	0.000000479
6	0.000000333	0.000000761	-0.000000589
1	-0.000001309	0.000001435	0.000002583
1	0.000002414	-0.000000383	-0.000000761
1	0.000000516	0.000000826	-0.000000599
1	0.000001413	0.000000924	0.000000831
1	0.000001069	0.000001481	-0.000000033
1	0.000000562	0.00000213	-0.000000555
1	0.00000106	0.000001531	0.000000258
6	-0.000005947	-0.000007188	0.000003996
6	0.000005683	0.000000949	-0.000000917
6	0.000000954	0.000005211	-0.000000457
1	0.000000016	0.000001083	-0.000001018
1	-0.000003748	-0.000002591	0.000000529
1	-0.000002611	0.000002085	-0.000000304
1	-0.000001483	0.000000804	0.000002388
1	-0.000001617	0.000000298	0.000002273
1	-0.000001277	-0.00000028	0.000002192
1	-0.000000184	0.000001299	0.00000183
6	0.000002716	-0.000000681	0.000000818
6	-0.000001726	-0.000000008	0.000001627
6	-0.000000115	-0.000000363	0.000000225
1	-0.000000456	0.000000544	0.000000217

1	-0.000000542	0.000000871	0.000001782
1	0.00000028	0.000001283	0.000000654
1	0.00000042	0.000000598	0.000001523
1	0.000000252	0.000001438	-0.000000088
1	-0.000000413	-0.000000608	-0.000000093
1	-0.000000149	0.000000006	0.000000485
8	0.000002904	0.000000307	0.000000128
6	0.000002143	0.000001489	-0.000001446
6	-0.000002116	0.000000226	0.000002342
6	0.000000141	-0.000000857	0.000002414
6	-0.000000918	-0.000001147	-0.000000674
6	0.000000092	0.00000043	0.000000582
6	0.000001236	-0.000001068	0.000001469
6	-0.00000006	0.00000083	-0.000013478
6	-0.000007812	-0.000007481	0.000005316
1	-0.000001199	-0.000000586	0.000000139
1	-0.000000513	-0.000001209	-0.000001053
1	-0.000000488	-0.000001159	-0.000000915
1	0.000000937	-0.000001844	-0.000000745
1	-0.000006445	-0.000002848	-0.000005352
1	-0.000002557	-0.000000117	-0.000000328
7	0.000006692	-0.000002832	-0.000004456
1	-0.000001198	-0.00000186	-0.00000014

Zero-point correction=	1.240256 (Hartree/Particle)
Thermal correction to Energy=	1.316279
Thermal correction to Enthalpy=	1.317223
Thermal correction to Gibbs Free Energy=	1.121458
Sum of electronic and zero-point Energies=	-3873.702296
Sum of electronic and thermal Energies=	-3873.626273
Sum of electronic and thermal Enthalpies=	-3873.625329
Sum of electronic and thermal Free Energies=	-3873.821095

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6	-0.000001179	-0.000000894	-0.000000423
6	-0.000000195	-0.000001156	0.000000279
7	0.000000105	-0.000000627	0.000000947
7	-0.000000131	-0.000000096	-0.000000788
16	0.000000147	-0.000000979	0.000000203
8	0.000000025	-0.000001214	0.000001056
8	-0.000000877	-0.000001769	0.000000294
6	0.000000014	-0.000001841	0.000000758
6	0.000000079	-0.000001298	0.000001292
6	0.000000654	-0.000000967	0.000001465
6	0.000000131	-0.000001365	0.000001146

6	-0.000000297	-0.000001276	0.000001024
6	-0.000000107	-0.000001126	0.000000657
1	0.000000422	-0.000000832	0.000001501
1	0.000000572	-0.00000106	0.000001745
1	-0.000000164	-0.000001269	0.000000526
1	-0.000000086	-0.000000926	0.000000227
6	0.000000271	-0.000001216	0.000001283
1	0.000000443	-0.000000994	0.000001585
1	0.000000134	-0.000001149	0.000001052
1	0.000000228	-0.000001647	0.000001475
6	0.000000902	-0.000000522	0.000000629
6	0.000000638	-0.000000325	0.000001468
1	-0.000000418	0.000000307	0.000000611
1	0.000000353	-0.000000606	0.000001347
6	0.000000836	-0.00000001	0.000001443
1	0.000000282	-0.000000005	0.000000899
1	0.000000332	-0.000000186	0.000000957
6	0.000001034	0.000000203	0.000001706
1	0.000000765	-0.00000028	0.000001612
1	0.000000548	0.000000026	0.000001495
1	0.000001111	0.000000345	0.000001949
1	0.000000974	0.000000558	0.000001397
1	0.000000964	0.0000001	0.000001758
6	0.000000287	0.000000098	-0.00000006
6	0.000000203	-0.000000245	0.000000613
1	-0.000000282	0.000000251	0.000000085
1	0.000000525	-0.000000151	0.000000023
6	0.000000621	0.000000189	0.000000385
1	0.000000095	-0.000000151	0.000000436
1	0.000000089	-0.000000374	0.000000646
6	0.000000545	0.000000035	0.000001023
1	0.000000582	0.000000593	0.000000651
1	0.000000313	0.000000054	0.000000051
1	0.000000726	0.000000583	0.000001092
1	0.00000005	0.000000096	0.000000878
1	0.000000614	0.000000003	0.000001262
16	-0.000000301	-0.000000628	-0.000000944
8	-0.000000443	-0.000000403	-0.000000064
8	-0.000000553	-0.000000787	-0.000000754
6	-0.000000528	-0.000000762	-0.000000307
6	-0.000000367	0.000000033	-0.000000844
6	-0.000000786	-0.000000495	-0.000001424
6	-0.000001375	0.000001056	-0.000001725
1	-0.000000272	0.000000196	-0.000000898

6	-0.00000024	-0.000000132	-0.00000124
1	-0.00000091	-0.000000733	-0.000001443
6	-0.000000822	0.000000083	-0.000001463
1	-0.000000563	0.000000701	-0.000001563
1	-0.000001078	-0.000000318	-0.000001967
6	-0.000000964	0.000000394	-0.000002286
1	-0.000001309	0.000000209	-0.000001602
1	-0.000000263	0.000000489	-0.000002405
1	-0.000001521	0.000000688	-0.000002802
79	0.000000391	0.000000998	0.0000001
6	0.000000365	0.000000454	0.000001114
6	0.00000023	0.000001435	-0.000000168
6	0.000000176	0.000001424	-0.00000046
1	0.000000507	0.000001882	-0.000000409
1	0.000000122	0.000001438	-0.000000838
7	0.00000038	0.000001173	-0.000000658
7	0.000000592	0.000001602	-0.000000384
6	-0.000001192	0.000000408	-0.000001174
6	-0.000000226	0.000000333	-0.000000227
6	-0.000000203	0.000000576	-0.000001085
6	-0.000000115	0.000000252	-0.000000774
6	-0.000000502	0.000000117	-0.000000991
6	-0.000000662	0.000000395	-0.000001078
1	-0.000000239	0.000000105	-0.000000796
1	-0.000000718	0.00000022	-0.000001605
1	-0.000000703	-0.000000156	-0.000001384
6	0.00000006	0.000000482	-0.000000297
6	0.000000545	0.000001419	0.000000078
6	0.000000776	0.000001302	0.000000707
6	0.000000523	0.000001084	0.000000747
6	0.000001133	0.000001507	0.000000632
6	0.000001114	0.000001081	0.000000506
1	0.000000745	0.000001664	0.000000038
1	0.000001117	0.000001546	0.000001179
1	0.00000105	0.000001522	0.000001051
6	0.000000299	0.000001413	-0.000000366
6	0.00000004	0.000001912	-0.000000664
6	0.000000232	0.00000127	-0.000000341
1	0.000000353	0.00000107	-0.000000513
1	0.00000041	0.000001988	-0.000000554
1	0.000000221	0.000001912	-0.000000831
1	0.000000555	0.000002135	-0.000000239
1	0.000000208	0.000000846	-0.000000124
1	0.000000352	0.000001515	-0.000000182

1	0.000000071	0.000001275	-0.000000729
6	0.000000682	0.000001758	0.000000774
6	0.000000732	0.000000779	0.000000832
6	0.000001	0.000001595	0.000000804
1	0.000000268	0.000000937	0.000000489
1	0.000000917	0.000000279	0.000001342
1	0.000000776	0.000000728	0.000001234
1	0.000001001	0.000000749	0.000001129
1	0.000000971	0.000001748	0.00000062
1	0.000001035	0.000001682	0.000001016
1	0.000000985	0.000001579	0.0000009
6	-0.000000236	0.00000078	-0.00000112
6	-0.000000462	0.000000343	-0.000001219
6	-0.000000544	0.00000094	-0.000001878
1	-0.000000384	0.000000581	-0.000001158
1	-0.000000683	0.000000097	-0.000001017
1	-0.000000645	0.000000441	-0.000001419
1	-0.000000681	0.000000085	-0.00000158
1	-0.000000421	0.000001238	-0.000001602
1	-0.000000826	0.000000744	-0.00000188
1	-0.000000551	0.000001113	-0.000001728
6	0.000000069	0.000000336	-0.000000013
6	0.000000104	0.000000657	-0.00000026
6	-0.00000014	0.000000153	0.000000257
1	0.000000365	0.00000089	-0.000000185
1	0.00000005	0.000001074	-0.000000637
1	0.000000342	0.000001023	0.000000033
1	0.000000108	0.000000576	-0.000000498
1	0.000000186	-0.00000042	-0.000000099
1	-0.000000023	0.000000054	0.000000092
1	0.000000375	0.00000031	0.000000383
8	-0.000000413	-0.00000008	-0.000000718
6	-0.000000505	-0.000001356	0.000000127
6	-0.000001071	-0.000000881	0.000000653
6	-0.000000122	-0.000000448	0.000000031
6	-0.000000163	-0.000001392	0.000000184
6	-0.000000727	-0.000001369	0.000001049
6	-0.000000196	-0.000000266	0.000000083
6	0.000000993	-0.000000765	-0.00000055
6	-0.000000982	-0.000000507	-0.000000642
1	-0.000000252	-0.000000943	-0.000000307
1	0.000000013	-0.000001402	0.000000392
1	0.00000016	-0.000001415	0.000000099
1	0.000000381	-0.000001014	0.000000699



1	-0.000000083	-0.000001232	0.000000107
1	-0.000000626	-0.000000443	-0.000000619
7	-0.000000711	-0.000000567	-0.000000273
1	-0.000000365	-0.000000493	-0.000000777
6	-0.000000834	-0.000001536	-0.000000032
6	-0.000001233	-0.000001937	-0.000000063
6	-0.000000843	-0.000002762	-0.00000007
6	-0.000001043	-0.000002296	0.000000108
6	-0.000001149	-0.000002187	-0.000000561
1	-0.000000869	-0.000002648	-0.000000057
1	-0.000000682	-0.000001276	-0.000000329
7	-0.000000482	-0.000001843	-0.000000677
8	-0.000000366	-0.000001849	-0.000000323
1	-0.000000835	-0.00000272	0.000000331
1	-0.000001005	-0.000001784	-0.000000346
17	-0.000000643	-0.000002328	0.000000415

Zero-point correction=	1.320299 (Hartree/Particle)
Thermal correction to Energy=	1.403820
Thermal correction to Enthalpy=	1.404764
Thermal correction to Gibbs Free Energy=	1.192533
Sum of electronic and zero-point Energies=	-4656.664545
Sum of electronic and thermal Energies=	-4656.581024
Sum of electronic and thermal Enthalpies=	-4656.580079
Sum of electronic and thermal Free Energies=	-4656.792311

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6	-0.000000376	-0.000000073	-0.000001501
6	0.000005057	-0.000008348	0.000010424
7	0.000002176	-0.000004026	0.000002445
7	-0.000005025	0.000000585	-0.000001347
16	-0.00000291	0.000001904	0.000000716
8	0.000000687	-0.000001216	-0.000001199
8	0.000000953	-0.000002052	0.000004251
6	0.000002978	0.000000692	0.000003136
6	0.000001388	-0.00000182	0.000000892
6	0.000002547	-0.00000041	0.000002167
6	0.000000738	-0.000001272	0.000001198
6	0.000000566	-0.00000174	0.000002283
6	0.000000038	-0.000001105	0.00000171
1	0.000001353	-0.000001357	0.000001845
1	0.000001675	-0.000001467	0.000001687
1	0.000000094	-0.000000578	0.000002007
1	0.000000279	-0.000000486	0.000002161
6	0.000000857	-0.000000949	0.000002296

1	0.000002219	-0.000001409	0.000001509
1	0.000001246	-0.000001529	0.000001757
1	0.000001817	-0.000001752	0.000002036
6	-0.000000689	0.000001344	-0.000004784
6	0.000001922	-0.000002646	0.000001903
1	0.000001653	-0.000000781	0.000001023
1	0.000001537	-0.000000826	0.000001315
6	0.000001815	-0.000000178	-0.000001937
1	0.000001336	-0.000000263	-0.000000151
1	0.000001417	-0.000000525	-0.000000272
6	0.000002011	-0.000000832	-0.000000348
1	0.000002198	-0.000001099	0.000000647
1	0.000002131	-0.000000543	-0.000000266
1	0.000003007	-0.000000537	-0.000000594
1	0.000002142	-0.000000859	-0.000000913
1	0.000002473	-0.000000682	-0.000000215
6	0.000001868	-0.000001221	0.000000613
6	0.000001201	-0.000001012	0.000000953
1	-0.000001289	0.000000769	-0.000000008
1	-0.00000003	0.000000595	0.000000651
6	0.000000402	0.000000541	-0.000000154
1	-0.000000112	-0.000000669	0.000000291
1	0.000001166	0.000000031	0.000000322
6	0.000001312	-0.000000684	0.000000096
1	0.000000908	-0.000000347	-0.000000397
1	0.000000476	-0.000000011	-0.000000536
1	0.000001527	-0.000000288	-0.000000345
1	0.000000905	-0.000000592	0.000000035
1	0.000001463	-0.000000062	0.000000229
16	0.000000142	-0.000001774	0.000000217
8	0.000000492	0.000002139	0.000000212
8	0.000001211	-0.00000005	0.000001627
6	-0.000003842	0.000000414	0.000000617
6	-0.000002176	0.000001704	-0.000000373
6	-0.00000108	-0.000000219	-0.000000082
6	-0.000002535	0.000000262	-0.000000233
1	-0.000000716	0.000000368	-0.000000067
6	-0.000003015	0.000000037	0.000001944
1	-0.000001528	0.000000806	0.000000941
6	-0.000001798	0.00000114	-0.000001017
1	-0.000002452	0.000000682	-0.000000268
1	-0.000002916	0.000000755	0.000000988
6	-0.00000403	0.000001097	0.000000175
1	-0.000003152	0.000000966	0.000000212

1	-0.000002849	0.000001528	-0.000000232
1	-0.000003466	0.000001196	0.000000179
79	-0.000001699	-0.000001267	-0.000001631
6	0.000002863	0.000003378	-0.000002265
6	0.000001073	-0.000000663	-0.000000179
6	0.000001269	0.000001617	-0.000003532
1	-0.000000068	0.000000948	-0.00000281
1	-0.000000717	0.000001301	-0.000002291
7	0.000000108	-0.000000064	-0.000000528
7	-0.000004323	0.000000516	-0.000000554
6	-0.000001712	0.000000186	-0.000000149
6	-0.000000272	-0.000001359	-0.000001238
6	-0.000001334	0.000001816	-0.000001841
6	-0.000000882	0.000000192	-0.000001405
6	-0.000002056	0.000000114	-0.000000532
6	-0.000001207	0.000000616	0.000000377
1	-0.000000013	0.000000232	-0.000000145
1	-0.000002151	0.000000685	-0.000000245
1	-0.000001649	0.000000609	-0.000000195
6	0.000001511	0.000000791	-0.000000881
6	0.000000872	0.000000583	-0.000000141
6	0.000000499	0.000000031	-0.000001547
6	0.000000112	-0.000000246	-0.000001287
6	0.000001619	0.000000278	-0.000002003
6	0.000001102	0.000000404	-0.000001953
1	0.000000157	0.000000691	-0.000002167
1	0.000002026	0.000000306	-0.000001927
1	0.000001582	0.000000188	-0.000001922
6	-0.000001107	0.000000715	-0.000002641
6	-0.000000632	0.000000965	-0.000002033
6	-0.000000346	0.000001135	-0.000000817
1	-0.000000547	0.000000906	-0.000001752
1	-0.000000334	0.000001122	-0.000000219
1	-0.000000091	0.000001214	-0.000002234
1	-0.000000241	0.000001156	-0.000000237
1	-0.000000194	0.000000602	-0.000000913
1	-0.000000435	0.000000686	-0.000001608
1	-0.000001033	0.000000692	-0.000001407
6	0.000000335	-0.000000327	-0.000002704
6	0.000000564	0.000000287	-0.000000078
6	0.000000393	0.000000922	-0.000002658
1	0.000001047	0.000000072	-0.000002015
1	0.000001655	-0.000000091	-0.000000603
1	0.000001953	-0.000000022	-0.000001595

1	0.000002698	-0.000000359	-0.000001695
1	0.000001556	0.000000541	-0.000002621
1	0.000002359	0.000000295	-0.000002363
1	0.000001791	0.00000003	-0.00000246
6	-0.000003389	0.000000325	-0.000000647
6	-0.00000094	0.000000466	-0.000000339
6	-0.000001381	0.000001534	-0.000001432
1	-0.000001417	0.000000973	-0.000001108
1	-0.000001663	0.000000738	-0.000000292
1	-0.000002035	0.000001297	-0.000000567
1	-0.000002267	0.000000719	-0.000000403
1	-0.000001794	0.00000139	-0.000001672
1	-0.000002426	0.000001512	-0.000001021
1	-0.000002233	0.000001371	-0.000001429
6	0.000002447	0.000000984	-0.000003125
6	-0.000000842	-0.000000213	-0.000001336
6	-0.000000673	0.000000453	0.000001089
1	0.000001542	0.000000537	-0.000001907
1	0.000000097	0.000001122	-0.000001583
1	0.000000285	0.00000048	-0.000001597
1	0.00000069	0.000000398	-0.000000477
1	0.000000545	0.000000154	0.000000189
1	0.000000773	0.00000016	-0.000001646
1	0.0000009	-0.000000503	-0.000000894
8	-0.000005839	0.000011461	-0.000000896
6	0.000001406	-0.000002135	0.000001953
6	0.00000149	-0.000002575	0.00000385
6	-0.00000141	0.000000664	0.000000459
6	0.000001041	-0.000000537	0.000001717
6	0.000000878	-0.000000502	0.00000138
6	-0.00000052	-0.000000188	-0.000001754
6	0.000000685	0.000001734	-0.000001908
6	-0.000002923	-0.000001527	0.000000984
1	0.000000343	-0.000000629	0.000000615
1	0.000000365	-0.000000764	0.000001265
1	0.0000012	-0.000001242	0.000001064
1	0.000001952	-0.000000391	0.000002226
1	0.000007316	-0.000010073	0.000000794
1	-0.000000935	0.000000172	0.000000621
7	-0.000003242	0.000003094	-0.000000352
1	0.000000703	-0.000000778	0.000000746
6	-0.000001139	0.000000735	0.000002069
6	0.000000039	-0.000001251	0.000002408
6	-0.000000547	0.00000018	0.000004119

6	-0.000002604	-0.000002271	0.000003207
6	0.000002449	0.00000009	0.00000284
1	-0.000000372	-0.000001314	0.000003689
1	-0.000000997	-0.000001066	0.000002503
7	-0.000001771	-0.000001025	0.000003145
8	-0.000007242	0.000004827	-0.000000861
1	-0.000000236	-0.000001099	0.000003405
1	-0.000000882	-0.000000882	0.000003026
17	-0.000001737	-0.000001564	0.000002297

Zero-point correction=	1.324665 (Hartree/Particle)
Thermal correction to Energy=	1.408689
Thermal correction to Enthalpy=	1.409633
Thermal correction to Gibbs Free Energy=	1.195511
Sum of electronic and zero-point Energies=	-4656.688223
Sum of electronic and thermal Energies=	-4656.604199
Sum of electronic and thermal Enthalpies=	-4656.603255
Sum of electronic and thermal Free Energies=	-4656.817377

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6	-0.00000074	-0.000000815	0.000001008
6	0.000001163	0.000000697	-0.000001203
7	0.000000258	0.000000016	0.000000441
7	-0.000000168	0.000000015	-0.000000397
16	-0.000000047	-0.000000087	-0.000000648
8	0.00000014	-0.000001066	-0.000000113
8	0.000000363	-0.000000853	0.000000513
6	-0.000000033	-0.000000071	-0.000000324
6	-0.000000753	-0.000000552	-0.000001044
6	-0.000000182	-0.000000239	-0.000001683
6	-0.000000416	0.000000025	-0.000001493
6	-0.000000518	0.000000464	-0.000001232
6	-0.000000017	0.000000389	-0.000000787
1	-0.000000325	-0.000001019	-0.000001207
1	-0.000000538	-0.000000606	-0.00000192
1	-0.000000318	0.000001046	-0.000001254
1	0.000000063	0.000000655	-0.000000652
6	-0.000000505	0.000000541	-0.000002071
1	-0.000000724	0.000000222	-0.000002349
1	-0.000000515	0.000000763	-0.000002161
1	-0.000000556	0.000000059	-0.000002058
6	-0.000000638	-0.000001201	-0.000000739
6	-0.000000302	-0.000000048	-0.000001077
1	-0.000000264	-0.000000601	-0.000000676
1	0.00000001	-0.000001215	-0.000000332

6	-0.00000564	-0.000001355	-0.000001142
1	-0.000000121	-0.000000609	-0.000001357
1	-0.00000057	-0.00000132	-0.000001016
6	-0.000000431	-0.000001325	-0.000001982
1	-0.000000385	-0.00000164	-0.000001038
1	-0.000000371	-0.000001154	-0.000001322
1	-0.000000603	-0.000001668	-0.000002065
1	-0.000000636	-0.000000999	-0.000002108
1	-0.000000586	-0.000001735	-0.000001808
6	0.000000006	0.000000466	-0.000001116
6	-0.000000134	0.000000648	-0.000001451
1	-0.000000136	0.00000111	-0.000000688
1	-0.000000335	0.000000139	-0.000000805
6	-0.000000764	0.000000576	-0.000001616
1	-0.000000348	0.000000907	-0.000001515
1	-0.000000415	0.000000453	-0.000001365
6	-0.000000691	0.00000051	-0.000002305
1	-0.000000335	-0.000000065	-0.000001932
1	-0.000000519	0.000000771	-0.000002059
1	-0.000000706	0.000000372	-0.00000026
1	-0.000000588	0.000000849	-0.000002589
1	-0.000000694	0.000000126	-0.000002503
16	-0.000000031	0.000002119	-0.000000042
8	-0.000000514	0.000001283	-0.000000892
8	0.000000406	0.000000816	0
6	0.000000069	0.000001867	-0.000000342
6	-0.000000212	0.000002099	-0.000000621
6	0.000000107	0.000001956	0.000000086
6	-0.000000076	0.000002509	-0.000000898
1	-0.000000324	0.000001963	-0.000001076
6	0.000000002	0.000002357	0.000000202
1	0.000000224	0.000001482	0.000000447
6	0.00000008	0.000003167	-0.000000219
1	-0.000000224	0.000002568	-0.000001203
1	0.000000124	0.000002173	0.000000583
6	0.00000005	0.000003116	-0.000000027
1	0.000000088	0.000003421	-0.000000195
1	-0.000000095	0.000003066	-0.000000681
1	0.000000012	0.000002895	-0.000000007
79	0.000000561	-0.000000394	0.000000902
6	0.00000077	0.000000215	-0.000000058
6	-0.00000005	0.000000089	0.000000688
6	0.000000361	-0.00000035	0.000000056
1	-0.000000055	-0.000000427	-0.000000189

1	0.0000001	-0.000000459	0.000000903
7	-0.000000054	-0.000000639	0.000001494
7	-0.000000587	-0.000000076	0.000000005
6	0.000000411	-0.000000152	0.000001408
6	0.000000285	-0.000001144	0.000001108
6	0.000000579	-0.000000062	0.000002141
6	0.000000663	-0.000001087	0.000002358
6	0.00000073	-0.000000051	0.000002024
6	0.000000677	-0.000000135	0.000002613
1	0.000000633	-0.000001141	0.000002444
1	0.000000693	0.000000564	0.000002443
1	0.000000773	-0.000000257	0.000002914
6	-0.000000375	-0.000000623	-0.000000521
6	0.000000059	0.000000062	-0.000000699
6	-0.000000445	-0.000000883	-0.000000525
6	-0.00000025	0.000000024	-0.000001293
6	-0.000000388	-0.000000751	-0.00000123
6	-0.000000332	-0.000000311	-0.000001528
1	-0.000000382	0.000000548	-0.000001464
1	-0.000000472	-0.000001174	-0.000001471
1	-0.000000536	-0.000000297	-0.000001928
6	-0.000000187	0.000000087	-0.000000369
6	-0.000000266	0.000000981	-0.000000777
6	-0.000000157	0.000001373	-0.000000388
1	-0.000000036	0.000000594	-0.000000309
1	-0.000000185	0.000000795	-0.000000851
1	-0.000000104	0.000001397	-0.000000551
1	-0.000000282	0.000001162	-0.000001204
1	0.000000039	0.000000766	-0.000000267
1	-0.000000088	0.000001185	-0.000000897
1	0	0.000001551	-0.00000011
6	-0.000000109	-0.000001557	-0.000000541
6	0.000000082	-0.000001632	-0.000000361
6	-0.000000168	-0.000001355	-0.000000889
1	-0.000000059	-0.000001083	-0.000000434
1	0.000000064	-0.000001254	-0.000000208
1	-0.000000011	-0.000002093	-0.000000075
1	-0.000000026	-0.000001676	-0.000000747
1	-0.000000248	-0.000001247	-0.000000719
1	-0.000000428	-0.000002092	-0.000001333
1	-0.000000382	-0.000002193	-0.000000462
6	0.000000456	0.000000709	0.00000146
6	0.000000221	0.000000953	0.000001544
6	0.000000365	0.000000876	0.000001724

1	0.00000272	0.00000906	0.00000671
1	0.00000584	0.00000987	0.00001158
1	0.00000405	0.00001555	0.00001372
1	0.0000058	0.00001117	0.00001927
1	0.00000362	0.00000838	0.00001557
1	0.00000661	0.0000118	0.00001946
1	0.00000489	0.00001439	0.00001504
6	0.00000259	-0.0000134	0.00001171
6	0.00000438	-0.00001682	0.00001557
6	0.00000295	-0.00001635	0.00001417
1	0.00000128	-0.00001229	0.00001133
1	0.00000383	-0.00001378	0.00001548
1	0.0000029	-0.00002111	0.00001294
1	0.00000466	-0.0000181	0.0000202
1	0.00000362	-0.00001473	0.00001275
1	0.00000504	-0.00001938	0.00001873
1	0.00000277	-0.00002153	0.00001267
8	-0.00000622	0.0000081	0.00000793
6	0.00000214	-0.00000587	0.00000471
6	0.0000017	-0.00000923	0.00000933
6	0.00000598	-0.00001351	0.00001298
6	0.00000501	-0.00001595	0.00001698
6	0.00000064	-0.00001992	0.00001403
6	0.00000316	-0.00001785	0.00000029
6	0.00000298	-0.00000084	0.0000145
6	0.00000236	-0.00000751	0.00000588
1	0.00000488	-0.00001517	0.00002128
1	0.00000421	-0.00002142	0.00001989
1	0.00000078	-0.00002219	0.00001199
1	0.00000014	-0.00001328	0.00000649
1	0.00001102	0.00002753	-0.00000044
1	0.00000382	0.00000161	0.00001333
7	0.00000353	-0.00000049	0.00001792
1	0.00000153	-0.00000625	0.00001875
6	0.00000616	0.00000953	0.00000743
6	0.00000314	0.00000909	0.00000965
6	0.00000338	0.00000604	0.00001481
6	0.00000915	-0.00000066	0.00001499
6	0.00000473	0.00000107	0.00001126
1	0.00000334	0.00000567	0.00001345
1	0.00000072	0.00001103	0.00000523
7	-0.00001503	0.00002574	0.00000969
8	0.00000133	-0.0000289	0.00002363
1	0.00000453	-0.00000299	0.00001706



1	0.00000205	0.000001185	0.000000741
17	0.000000316	-0.000000581	0.000001759
Zero-point correction=			1.319942 (Hartree/Particle)
Thermal correction to Energy=			1.404044
Thermal correction to Enthalpy=			1.404988
Thermal correction to Gibbs Free Energy=			1.188456
Sum of electronic and zero-point Energies=			-4656.677412
Sum of electronic and thermal Energies=			-4656.593310
Sum of electronic and thermal Enthalpies=			-4656.592366
Sum of electronic and thermal Free Energies=			-4656.808898

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6	-0.000001709	0.000003756	-0.000000015
6	0.000004166	0.000002026	0.000001632
7	0.00000115	-0.000002406	-0.000001643
7	-0.000002033	-0.000001988	-0.000003907
16	0.000001116	0.000000681	0.000001506
8	0.000000137	0.000001396	0.000000377
8	-0.000001388	-0.000002231	0.000001426
6	-0.000000368	0.000000054	-0.000000152
6	-0.000000336	-0.0000007	0.000000612
6	0.000000452	-0.000000491	0.000000128
6	-0.000000264	0.000000671	0.000000591
6	-0.000000812	-0.000001021	0.000001775
6	-0.000000478	0.000000053	-0.000000029
1	0.000000138	0.000000221	0.000000286
1	-0.000000298	-0.000000331	0.000000471
1	-0.000000569	-0.000000411	0.000001036
1	-0.000000521	-0.000000178	0.000001246
6	-0.000000711	-0.000000275	0.000000663
1	-0.000000512	-0.000001162	0.000000387
1	-0.000000741	-0.000000449	0.000000626
1	-0.00000008	-0.000000546	0.000000423
6	-0.000000327	0.000001826	-0.000002426
6	-0.000000898	-0.000000244	0.000001456
1	-0.0000007	-0.000000887	0.000001275
1	-0.000000766	-0.000000065	0.000000069
6	-0.000000808	0.000000064	0.000000085
1	-0.000000804	-0.000000276	0.000000433
1	-0.000000302	0.000000327	0.000001856
6	-0.000000292	-0.000000185	0.000001223
1	-0.000000293	0.000000111	0.000001391
1	-0.000000481	-0.000000392	0.000000097
1	-0.000000573	-0.000000029	0.000001353

1	-0.000000565	-0.000000095	0.000000962
1	-0.000000401	0.000000067	0.000001293
6	-0.000000454	0.00000141	0.000001352
6	0.000000289	0.000000583	0.000001861
1	0.000000286	0.000000239	0.000000656
1	0.000000309	0.000000382	0.0000015
6	0.000000339	0.000000709	0.000001396
1	-0.000000539	0.000000956	-0.000000049
1	-0.000000278	0.000000939	0.000001014
6	0.000000343	0.000000391	0.000000834
1	0.000000054	0.000000454	0.000000321
1	-0.000000261	0.000000703	0.000000532
1	-0.000000056	0.000000912	0.000001221
1	0.000000006	0.000000997	0.000000927
1	-0.000000202	0.000000764	0.00000124
16	0.000000684	0.000003788	0.000004275
8	-0.000000088	-0.000001244	-0.000001012
8	0.000000166	-0.000000504	-0.000001907
6	0.000002435	0.00000235	-0.000002137
6	0.000002044	-0.000001634	0.000002032
6	-0.000004226	0.000001807	0.000003177
6	-0.000003387	0.00000043	0.000000974
1	-0.000001065	0.000000704	-0.000000813
6	0.000002945	-0.000003628	0.000002255
1	0.000001412	0.000000739	-0.000000267
6	0.000000868	0.000003317	-0.000003611
1	0.000000764	0.000000773	-0.000000748
1	0.000000266	0.000002042	-0.0000006
6	0.000000428	-0.00000014	0.000001292
1	0.0000013	0.000000501	-0.00000058
1	0.000000954	0.000001583	0.00000042
1	-0.000000312	0.000001919	-0.000000116
79	0.00000271	-0.0000012	-0.000005271
6	-0.000000513	0.000001641	0.000000703
6	-0.000000189	-0.000000106	-0.000001176
6	0.000000458	-0.000000068	-0.000001802
1	0.000000376	-0.000000358	-0.000001251
1	0.000000256	-0.0000006	-0.000000627
7	-0.000000787	0.000000229	-0.000000983
7	-0.000000613	-0.000000913	0.000000402
6	0.000000156	0.000000291	-0.000002005
6	0.000000852	-0.000000328	-0.000000399
6	-0.000000215	-0.000000586	0.000000197
6	0.00000007	-0.00000111	-0.000000022

6	-0.000001008	-0.000000646	0.000000064
6	-0.000000037	-0.000000296	-0.000000589
1	-0.000000016	-0.000000338	-0.000000122
1	-0.000000243	-0.000000799	-0.000000382
1	-0.000000164	-0.000000667	-0.000000321
6	0.000000782	-0.000000212	-0.000000399
6	-0.000000375	0.000000153	-0.000000834
6	0.000000031	0.000000534	-0.000000726
6	0.000000694	-0.000000472	-0.000000864
6	0.000000541	0.000000031	-0.000000617
6	0.000000417	0.000000686	0.000000101
1	0.000000017	0.000000178	-0.000000833
1	0.000000615	0.000000719	-0.000001121
1	0.000000565	0.000000328	-0.000000917
6	0.000000696	0.000000435	-0.000001291
6	0.000000374	-0.000000719	-0.000000776
6	-0.000000011	-0.000000405	-0.000000629
1	-0.000000118	-0.000000596	-0.000000201
1	0.000000153	-0.000000503	-0.000000949
1	0.000000005	-0.000000704	-0.000000833
1	-0.000000107	-0.000000208	-0.000000842
1	-0.000000166	-0.000000021	-0.000000472
1	0.000000003	-0.000000018	-0.000000232
1	-0.000000049	-0.000000202	-0.000000341
6	0.000000404	0.000000893	-0.000000673
6	0.000000727	0.000000746	-0.000000878
6	0.000000646	-0.000000289	-0.000001074
1	0.000000412	0.000000063	-0.000000525
1	0.000000649	0.000000783	-0.000000083
1	0.000000434	0.000000578	-0.000000094
1	0.000000479	0.000000914	-0.000000367
1	0.000000522	0.000000252	-0.000000984
1	0.000000068	0.000000702	-0.000001055
1	0.000000701	0.000000528	-0.000000093
6	0.000000543	-0.000001137	-0.000000476
6	-0.000000078	-0.000001006	0.000000104
6	0.000000052	-0.000000856	-0.000000558
1	-0.000000344	0.000000026	-0.000000085
1	-0.000000105	-0.000000482	-0.000000259
1	-0.000000152	-0.000000845	-0.000000357
1	-0.000000297	-0.000000598	-0.000000261
1	-0.000000231	-0.000000853	-0.000000732
1	-0.000000315	-0.000001013	-0.000000542
1	-0.000000282	-0.000000992	-0.000000621

6	0.000000028	0.000000712	0.000000037
6	0.000000363	0.000000066	-0.000000652
6	0.000001186	-0.000000146	-0.000000461
1	0.000000347	-0.000000485	-0.000000335
1	0.000000373	-0.000000306	-0.000000764
1	0.000000354	0.000000172	-0.000000918
1	0.000000226	-0.000000176	-0.000000767
1	-0.000000229	-0.000000038	-0.000000262
1	-0.000000063	0.000000112	-0.000000255
1	0.000000438	0.000000047	-0.000000273
8	-0.000000003	-0.000001896	0.000001739
6	0.000000504	0.000000667	0.000000163
6	-0.000000064	-0.000002698	0.000000623
6	0.000000203	-0.000000115	0.000000072
6	-0.000000073	-0.000000791	0.000000572
6	-0.00000002	-0.000000838	-0.000000375
6	-0.000000795	0.000000327	0.000001083
6	-0.000002297	-0.000003934	0.000002319
6	0.000000308	0.000001012	-0.000000131
1	-0.000000574	-0.000000601	0.000000154
1	-0.000000555	-0.000000956	0.000000269
1	-0.000000575	-0.000000909	0.000000399
1	-0.000000843	-0.000000721	0.000000664
1	-0.000000887	-0.000000332	0.000000418
1	0.000000075	0.000000045	0.000000638
7	0.000000057	0.000003994	-0.000000085
1	-0.000000442	-0.000002594	0.000000333

Zero-point correction=	1.241175 (Hartree/Particle)
Thermal correction to Energy=	1.318139
Thermal correction to Enthalpy=	1.319083
Thermal correction to Gibbs Free Energy=	1.114818
Sum of electronic and zero-point Energies=	-3873.757320
Sum of electronic and thermal Energies=	-3873.680356
Sum of electronic and thermal Enthalpies=	-3873.679412
Sum of electronic and thermal Free Energies=	-3873.883677

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6	0.000000114	0.000000164	0.000002543
6	-0.000000287	-0.000000637	-0.000000815
7	-0.000001088	0.00000209	0.000001215
7	0.000001347	0.000000391	-0.000000791
16	-0.000000112	-0.000000047	-0.000000362
8	-0.000000467	0.000000672	0.00000009
8	-0.000000059	0.000000115	0.000000917

6	0.000000666	0.000000053	-0.000000354
6	0.000000595	-0.000000617	-0.000000674
6	0.000001927	-0.000000283	-0.000000835
6	0.000000809	-0.000001411	-0.000000813
6	0.000000023	-0.000002363	-0.000000016
6	0.000000256	-0.000001333	-0.000000108
1	0.000001017	0.000000185	-0.000000804
1	0.000001095	-0.000000708	-0.000001715
1	0.000000834	-0.000002106	0.000000017
1	0.000000131	-0.000000982	0.000001057
6	0.000001272	-0.000001953	-0.000000121
1	0.000002022	-0.000002672	-0.000001687
1	0.000001138	-0.000001856	-0.000001426
1	0.000002242	-0.000001927	-0.000000677
6	-0.000000012	0.000000043	0.000000546
6	-0.000001035	0.000001586	0.000000674
1	-0.000000859	0.000000615	0.000000411
1	-0.000001028	0.000000212	0.000001565
6	-0.000001258	0.00000146	0.000001442
1	-0.000001032	0.000001126	0.000000609
1	-0.00000086	0.000000739	0.000000965
6	-0.000001789	0.000002379	0.000001659
1	-0.000001912	0.000000868	0.000001649
1	-0.000001163	0.000001435	0.000000822
1	-0.000002085	0.000002366	0.000001837
1	-0.000001684	0.000002406	0.000000895
1	-0.000001712	0.000001765	0.000001609
6	-0.000000044	0.000000866	-0.000001035
6	-0.000000196	0.000001421	-0.000000944
1	-0.000000404	0.000001912	-0.000001677
1	-0.00000013	0.000001359	-0.000000015
6	-0.000000407	0.000001917	-0.000000639
1	0.000000086	0.000002007	-0.000000746
1	-0.000000578	0.000001879	-0.000001108
6	-0.000000769	0.000002733	-0.000000702
1	-0.000000836	0.000002378	-0.000000229
1	-0.000000596	0.000002552	-0.000001036
1	-0.000001025	0.000003202	-0.000000621
1	-0.000000557	0.000002973	-0.00000101
1	-0.000000925	0.00000269	-0.000000434
16	0.000000655	0.000000923	-0.000001073
8	0.000000802	0.000001728	-0.000002396
8	0.000000746	0.000000162	-0.000002297
6	0.000001407	-0.000000342	-0.000002325

6	0.000001107	0.000001063	-0.00000211
6	0.000001448	0.000000342	-0.000002547
6	0.000001602	0.000000325	-0.000002731
1	0.000000969	0.000001247	-0.000002531
6	0.000001688	0.000000001	-0.000002419
1	0.000001471	-0.000000663	-0.000002295
6	0.000001586	0.000000096	-0.000003
1	0.000001316	0.000000909	-0.000002923
1	0.000001979	-0.000000924	-0.000002693
6	0.000001899	-0.000000252	-0.000003247
1	0.000002292	-0.000000884	-0.000002832
1	0.000002349	-0.000000276	-0.000003919
1	0.000001737	0.000000208	-0.000003174
79	-0.000000694	0.000000941	0.00000032
6	-0.000000121	-0.000001095	0.00000033
6	-0.000000222	-0.000000242	0.000000553
6	-0.000000541	0.000000735	0.000000858
1	-0.000000731	0.000000516	0.000000868
1	-0.000000194	-0.000000679	0.000000672
7	-0.000000099	-0.000000273	0.000000382
7	-0.000000194	-0.000000247	0.000000681
6	0.000000038	-0.000000881	0.000000727
6	-0.000000025	-0.000001587	0.000001191
6	0.000000811	-0.000001602	-0.000000255
6	0.000000105	-0.000002376	0.000001395
6	0.000001237	-0.000002043	-0.000000128
6	0.000000481	-0.000002629	0.000000393
1	0.000000502	-0.000002663	0.000001362
1	0.000001035	-0.000002201	-0.000000456
1	0.000001022	-0.00000309	0.000000426
6	-0.000001003	0.000001474	-0.000000505
6	-0.000000012	0.000000858	0.000000379
6	-0.000001795	0.000000927	0.000001455
6	-0.000000894	0.000002414	-0.000000423
6	-0.000001206	0.000002265	0.000000508
6	-0.000001199	0.000002232	0.00000064
1	-0.000000828	0.000002529	-0.000000419
1	-0.000001772	0.000002111	0.000001722
1	-0.000001424	0.000002819	0.000000449
6	-0.000000368	0.000001559	-0.000001024
6	-0.000000261	0.000001697	-0.000000794
6	-0.000000218	0.00000154	-0.000001055
1	-0.000000091	0.000001028	-0.000000251
1	-0.000000412	0.000001787	-0.000000422

1	-0.00000018	0.000001683	-0.000001196
1	-0.000000508	0.000002346	-0.000000908
1	-0.000000204	0.000001334	-0.000000599
1	0.000000231	0.000002066	-0.000001111
1	0.000000409	0.000001335	-0.000001689
6	-0.000001774	0.000000395	0.000001467
6	-0.00000132	0.000001025	0.000001739
6	-0.000001775	0.000000886	0.000002292
1	-0.000000906	0.000000313	0.000001307
1	-0.000001588	0.000000503	0.000001895
1	-0.000001552	0.000000328	0.000002407
1	-0.00000161	0.000000831	0.000001966
1	-0.000001392	0.000001176	0.00000173
1	-0.000001789	0.00000173	0.000002274
1	-0.000001839	0.000000508	0.000002496
6	0.00000063	-0.00000074	-0.00000057
6	0.000001093	-0.000000919	-0.000000967
6	0.000001024	-0.000001404	-0.000000947
1	0.000000689	-0.000000715	-0.000000922
1	0.000001527	-0.000001316	-0.000001536
1	0.000001305	-0.000000795	-0.000001541
1	0.000001376	-0.000001604	-0.000001233
1	0.000000785	-0.000001137	-0.000000513
1	0.000001466	-0.000001497	-0.000000955
1	0.000001091	-0.000000821	-0.000001409
6	-0.000000398	-0.000001289	0.000001512
6	-0.000000488	-0.000001706	0.000002092
6	-0.000000608	-0.000001428	0.000002231
1	-0.000000335	-0.000000881	0.000001976
1	-0.000000477	-0.000001668	0.000001867
1	-0.000000844	-0.000001658	0.000002404
1	-0.00000019	-0.000002292	0.000002163
1	-0.000000236	-0.00000124	0.00000157
1	-0.000000268	-0.000002404	0.000002053
1	-0.000000944	-0.000001454	0.000002509
8	0.000001489	0.000000069	-0.000001389
6	-0.000000459	-0.000001235	0.000000815
6	-0.000000231	-0.000001864	0.000000725
6	0.000000116	-0.000002157	0.000001441
6	-0.000000044	-0.000002578	0.000001863
6	-0.000000553	-0.000001558	0.000002337
6	-0.000000095	-0.000000523	0.000001563
6	-0.000000192	-0.000001721	-0.000000607
6	0.000000726	-0.000001549	0.000000081

1	0.00000387	-0.00002953	0.00001449
1	-0.00000259	-0.00002693	0.0000233
1	-0.00000744	-0.00001545	0.00002338
1	-0.00000288	-0.00001387	0.00001214
1	0.00001003	-0.00001008	-0.00001671
1	0.00000703	-0.00001444	-0.00000325
7	0.00000848	-0.00002089	0.00000617
1	0.0000091	-0.0000024	0.00000403

Zero-point correction=	1.235264 (Hartree/Particle)
Thermal correction to Energy=	1.311920
Thermal correction to Enthalpy=	1.312864
Thermal correction to Gibbs Free Energy=	1.115818
Sum of electronic and zero-point Energies=	-3873.630827
Sum of electronic and thermal Energies=	-3873.554171
Sum of electronic and thermal Enthalpies=	-3873.553227
Sum of electronic and thermal Free Energies=	-3873.750273

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6	-0.00001709	0.00003756	-0.00000015
6	0.00004166	0.00002026	0.00001632
7	0.0000115	-0.00002406	-0.00001643
7	-0.00002033	-0.00001988	-0.00003907
16	0.00001116	0.00000681	0.00001506
8	0.00000137	0.00001396	0.00000377
8	-0.00001388	-0.00002231	0.00001426
6	-0.00000368	0.00000054	-0.00000152
6	-0.00000336	-0.0000007	0.00000612
6	0.00000452	-0.00000491	0.00000128
6	-0.00000264	0.00000671	0.00000591
6	-0.00000812	-0.00001021	0.00001775
6	-0.00000478	0.00000053	-0.00000029
1	0.00000138	0.00000221	0.00000286
1	-0.00000298	-0.00000331	0.00000471
1	-0.00000569	-0.00000411	0.00001036
1	-0.00000521	-0.00000178	0.00001246
6	-0.00000711	-0.00000275	0.00000663
1	-0.00000512	-0.00001162	0.00000387
1	-0.00000741	-0.00000449	0.00000626
1	-0.00000008	-0.00000546	0.00000423
6	-0.00000327	0.00001826	-0.00002426
6	-0.00000898	-0.00000244	0.00001456
1	-0.0000007	-0.00000887	0.00001275
1	-0.00000766	-0.00000065	0.00000069
6	-0.00000808	0.00000064	0.00000085



1	-0.000000804	-0.000000276	0.000000433
1	-0.000000302	0.000000327	0.000001856
6	-0.000000292	-0.000000185	0.000001223
1	-0.000000293	0.000000111	0.000001391
1	-0.000000481	-0.000000392	0.000000097
1	-0.000000573	-0.000000029	0.000001353
1	-0.000000565	-0.000000095	0.000000962
1	-0.000000401	0.000000067	0.000001293
6	-0.000000454	0.00000141	0.000001352
6	0.000000289	0.000000583	0.000001861
1	0.000000286	0.000000239	0.000000656
1	0.000000309	0.000000382	0.0000015
6	0.000000339	0.000000709	0.000001396
1	-0.000000539	0.000000956	-0.000000049
1	-0.000000278	0.000000939	0.000001014
6	0.000000343	0.000000391	0.000000834
1	0.000000054	0.000000454	0.000000321
1	-0.000000261	0.000000703	0.000000532
1	-0.000000056	0.000000912	0.000001221
1	0.000000006	0.000000997	0.000000927
1	-0.000000202	0.000000764	0.00000124
16	0.000000684	0.000003788	0.000004275
8	-0.000000088	-0.000001244	-0.000001012
8	0.000000166	-0.000000504	-0.000001907
6	0.000002435	0.00000235	-0.000002137
6	0.000002044	-0.000001634	0.000002032
6	-0.000004226	0.000001807	0.000003177
6	-0.000003387	0.00000043	0.000000974
1	-0.000001065	0.000000704	-0.000000813
6	0.000002945	-0.000003628	0.000002255
1	0.000001412	0.000000739	-0.000000267
6	0.000000868	0.000003317	-0.000003611
1	0.000000764	0.000000773	-0.000000748
1	0.000000266	0.000002042	-0.0000006
6	0.000000428	-0.00000014	0.000001292
1	0.0000013	0.000000501	-0.00000058
1	0.000000954	0.000001583	0.00000042
1	-0.000000312	0.000001919	-0.000000116
79	0.00000271	-0.0000012	-0.000005271
6	-0.000000513	0.000001641	0.000000703
6	-0.000000189	-0.000000106	-0.000001176
6	0.000000458	-0.000000068	-0.000001802
1	0.000000376	-0.000000358	-0.000001251
1	0.000000256	-0.0000006	-0.000000627

7	-0.000000787	0.000000229	-0.000000983
7	-0.000000613	-0.000000913	0.000000402
6	0.000000156	0.000000291	-0.000002005
6	0.000000852	-0.000000328	-0.000000399
6	-0.000000215	-0.000000586	0.000000197
6	0.00000007	-0.00000111	-0.000000022
6	-0.000001008	-0.000000646	0.000000064
6	-0.000000037	-0.000000296	-0.000000589
1	-0.000000016	-0.000000338	-0.000000122
1	-0.000000243	-0.000000799	-0.000000382
1	-0.000000164	-0.000000667	-0.000000321
6	0.000000782	-0.000000212	-0.000000399
6	-0.000000375	0.000000153	-0.000000834
6	0.000000031	0.000000534	-0.000000726
6	0.000000694	-0.000000472	-0.000000864
6	0.000000541	0.00000031	-0.000000617
6	0.000000417	0.000000686	0.000000101
1	0.000000017	0.000000178	-0.000000833
1	0.000000615	0.000000719	-0.000001121
1	0.000000565	0.000000328	-0.000000917
6	0.000000696	0.000000435	-0.000001291
6	0.000000374	-0.000000719	-0.000000776
6	-0.000000011	-0.000000405	-0.000000629
1	-0.000000118	-0.000000596	-0.000000201
1	0.000000153	-0.000000503	-0.000000949
1	0.00000005	-0.000000704	-0.000000833
1	-0.000000107	-0.000000208	-0.000000842
1	-0.000000166	-0.000000021	-0.000000472
1	0.00000003	-0.00000018	-0.000000232
1	-0.000000049	-0.000000202	-0.000000341
6	0.000000404	0.000000893	-0.000000673
6	0.000000727	0.000000746	-0.000000878
6	0.000000646	-0.000000289	-0.000001074
1	0.000000412	0.000000063	-0.000000525
1	0.000000649	0.000000783	-0.000000083
1	0.000000434	0.000000578	-0.000000094
1	0.000000479	0.000000914	-0.000000367
1	0.000000522	0.000000252	-0.000000984
1	0.00000068	0.000000702	-0.000001055
1	0.000000701	0.000000528	-0.000000093
6	0.000000543	-0.000001137	-0.000000476
6	-0.000000078	-0.000001006	0.000000104
6	0.000000052	-0.000000856	-0.000000558
1	-0.000000344	0.000000026	-0.000000085

1	-0.000000105	-0.000000482	-0.000000259
1	-0.000000152	-0.000000845	-0.000000357
1	-0.000000297	-0.000000598	-0.000000261
1	-0.000000231	-0.000000853	-0.000000732
1	-0.000000315	-0.000001013	-0.000000542
1	-0.000000282	-0.000000992	-0.000000621
6	0.000000028	0.000000712	0.000000037
6	0.000000363	0.000000066	-0.000000652
6	0.000001186	-0.000000146	-0.000000461
1	0.000000347	-0.000000485	-0.000000335
1	0.000000373	-0.000000306	-0.000000764
1	0.000000354	0.000000172	-0.000000918
1	0.000000226	-0.000000176	-0.000000767
1	-0.000000229	-0.000000038	-0.000000262
1	-0.000000063	0.000000112	-0.000000255
1	0.000000438	0.000000047	-0.000000273
8	-0.000000003	-0.000001896	0.000001739
6	0.000000504	0.000000667	0.000000163
6	-0.000000064	-0.000002698	0.000000623
6	0.000000203	-0.000000115	0.000000072
6	-0.000000073	-0.000000791	0.000000572
6	-0.00000002	-0.000000838	-0.000000375
6	-0.000000795	0.000000327	0.000001083
6	-0.000002297	-0.000003934	0.000002319
6	0.000000308	0.000001012	-0.000000131
1	-0.000000574	-0.000000601	0.000000154
1	-0.000000555	-0.000000956	0.000000269
1	-0.000000575	-0.000000909	0.000000399
1	-0.000000843	-0.000000721	0.000000664
1	-0.000000887	-0.000000332	0.000000418
1	0.000000075	0.000000045	0.000000638
7	0.000000057	0.000003994	-0.000000085
1	-0.000000442	-0.000002594	0.000000333

Zero-point correction=

1.241175 (Hartree/Particle)

Thermal correction to Energy=

1.318139

Thermal correction to Enthalpy=

1.319083

Thermal correction to Gibbs Free Energy=

1.114818

Sum of electronic and zero-point Energies=

-3873.757320

Sum of electronic and thermal Energies=

-3873.680356

Sum of electronic and thermal Enthalpies=

-3873.679412

Sum of electronic and thermal Free Energies=

-3873.883677

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6	-0.000000461	0.000000077	0.000000136
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6	0.000000425	0.000000179	0.000000237
7	0.000000016	-0.000000164	0.000000163
7	0.000000471	0.000000102	0.000000742
16	0.00000027	-0.000000248	0.000000717
8	0.000000452	0.000000096	0.000000653
8	0.000000436	-0.000000121	0.000000448
6	0.000000581	-0.000000623	0.000000886
6	0.000000462	-0.000000423	0.000000745
6	0.000000893	-0.000000552	0.000000918
6	0.000000727	-0.000000989	0.000000613
6	0.00000036	-0.000000915	0.000000278
6	0.00000054	-0.000000607	0.000000594
1	0.000000539	-0.00000018	0.000000755
1	0.000000776	-0.000000593	0.000000843
1	0.000000547	-0.000000946	0.00000023
1	0.000000434	-0.000000374	0.000000201
6	0.000000824	-0.000001105	0.000000545
1	0.000000722	-0.000001149	0.000000553
1	0.000000845	-0.000001051	0.000000785
1	0.000000666	-0.000001104	0.000000562
6	0.000000214	-0.000000121	0.00000042
6	0.000000244	0.000000201	0.000000418
1	0.000000355	-0.000000156	0.000000399
1	0.000000167	-0.000000208	0.000000194
6	0.000000196	0.000000182	0.000000422
1	0.00000027	0.000000331	0.000000568
1	0.000000069	0.000000404	0.000000309
6	0.000000188	0.00000044	0.000000536
1	0.000000114	0.000000137	0.000000241
1	0.00000028	0.000000068	0.000000536
1	0.000000151	0.000000429	0.000000505
1	0.000000214	0.000000514	0.000000675
1	0.000000027	0.000000548	0.000000432
6	0.000000173	0.000000613	0.00000062
6	0.000000126	0.000000707	0.000000508
1	0.000000164	0.000000593	0.000000716
1	0.000000257	0.00000041	0.000000601
6	0.000000006	0.000000906	0.000000646
1	-0.00000007	0.000000754	0.00000052
1	-0.000000036	0.000000668	0.000000351
6	-0.000000063	0.000001085	0.000000551
1	0.000000162	0.000000855	0.000000683
1	0.000000123	0.000000978	0.000000885
1	-0.000000041	0.000001274	0.000000711

1	-0.00000013	0.000001232	0.000000605
1	-0.000000133	0.000001123	0.000000483
16	0.000000438	0.000000505	0.000000899
8	0.000000382	0.000000294	0.000000792
8	-0.000000071	0.000000568	0.00000043
6	0.000000201	-0.000000047	0.000000626
6	0.000000186	-0.000000031	0.000000378
6	0.000000212	0.000000322	0.000000319
6	0.00000033	-0.000000051	0.000000254
1	0.000000218	-0.000000221	0.000000472
6	0.000000033	0.000000196	0.000000264
1	0.000000111	0.000000051	0.00000049
6	0.00000024	-0.000000021	0.000000235
1	0.000000215	-0.00000037	0.000000193
1	0.000000073	0.000000302	0.000000303
6	0.000000115	-0.000000252	0.00000018
1	0.000000138	-0.000000331	-0.000000006
1	0.000000062	-0.00000004	0.000000042
1	0.000000274	-0.000000249	0.00000025
79	-0.000000044	0.00000018	-0.000000036
6	-0.000000382	0.000000097	-0.000000313
6	-0.000000253	-0.000000317	-0.000000687
6	-0.000000336	-0.000000395	-0.000000774
1	-0.000000405	-0.000000401	-0.000000946
1	-0.000000315	-0.000000388	-0.000000806
7	-0.000000183	-0.000000293	-0.000000576
7	-0.000000283	-0.000000248	-0.000000576
6	-0.000000104	-0.000000112	-0.000000401
6	-0.000000025	-0.000000459	-0.000000251
6	-0.000000218	-0.00000001	-0.000000454
6	0.000000061	-0.000000282	-0.000000213
6	-0.000000157	0.000000063	-0.000000204
6	-0.000000069	-0.000000159	-0.000000174
1	0.000000068	-0.000000488	-0.000000147
1	-0.000000202	0.000000218	-0.000000218
1	0.000000001	-0.000000113	-0.000000076
6	-0.000000029	-0.000000196	-0.000000554
6	-0.000000374	-0.000000035	-0.000000617
6	-0.000000158	-0.000000512	-0.000000408
6	-0.000000447	-0.000000016	-0.000000639
6	-0.000000023	-0.000000043	-0.000000623
6	-0.000000248	-0.000000181	-0.000000564
1	-0.000000392	0.00000016	-0.000000688
1	-0.000000103	-0.000000525	-0.000000481

1	-0.000000229	-0.000000157	-0.000000613
6	-0.000000547	0.000000154	-0.000000077
6	-0.000000646	0.000000112	-0.000000975
6	-0.000000535	0.000000374	-0.000000575
1	-0.00000004	0.000000187	-0.000000647
1	-0.000000615	-0.000000004	-0.000001022
1	-0.000000698	0.000000265	-0.000001058
1	-0.000000669	0.000000016	-0.000001022
1	-0.00000038	0.000000322	-0.000000443
1	-0.000000532	0.000000483	-0.000000063
1	-0.000000577	0.000000524	-0.000000688
6	-0.000000053	-0.000000729	-0.000000048
6	0.000000043	-0.000000609	-0.000000226
6	-0.000000007	-0.000000887	-0.000000603
1	-0.000000025	-0.000000687	-0.000000469
1	0.000000154	-0.000000542	-0.000000109
1	0.000000175	-0.000000845	-0.000000216
1	0.000000188	-0.000000609	-0.000000256
1	-0.000000151	-0.000000084	-0.000000764
1	-0.000000049	-0.000000825	-0.000000694
1	0	-0.000001011	-0.000000598
6	-0.000000025	0.000000308	-0.000000442
6	-0.000000251	0.000000374	-0.000000032
6	-0.000000455	0.000000029	-0.000000583
1	-0.000000427	0.000000118	-0.000000053
1	-0.000000239	0.000000309	-0.000000174
1	-0.000000454	0.000000575	-0.000000353
1	-0.000000344	0.000000557	-0.000000228
1	-0.000000494	0.000000013	-0.000000075
1	-0.000000496	0.000000382	-0.000000564
1	-0.000000573	0.000000414	-0.000000721
6	0.000000125	-0.000000643	-0.000000218
6	0.000000048	-0.000000839	-0.000000437
6	0.000000187	-0.000000671	-0.000000006
1	0.000000054	-0.000000636	-0.000000436
1	-0.00000001	-0.000000747	-0.000000062
1	0.000000059	-0.000000954	-0.000000503
1	0.000000102	-0.000000834	-0.000000373
1	0.000000219	-0.000000493	0.000000019
1	0.000000261	-0.000000729	-0.000000008
1	0.000000228	-0.000000845	-0.000000156
6	0.000000075	0.000000523	0.000000051
6	-0.000000615	0.000000321	0.000000027
6	-0.000000031	0.000000774	-0.000000012

6	-0.000000239	0.000000828	0.000000493
6	-0.000000068	0.000000809	0.000000135
6	-0.000000246	0.000000897	-0.000000186
6	-0.000000096	0.000000422	0.000000344
6	-0.000000121	0.000000225	-0.000000133
1	-0.000000136	0.000000689	-0.000000136
1	-0.000000281	0.000001061	0.000000005
1	-0.000000343	0.000001187	0.000000039
1	-0.000000126	0.000000948	-0.000000019
1	-0.000000147	0.000000328	-0.000000054
1	-0.000000226	0.000000021	-0.000000156
7	-0.000000029	0.000000353	-0.000000112
1	-0.000000025	0.000000189	-0.000000199

Zero-point correction=	1.232650 (Hartree/Particle)
Thermal correction to Energy=	1.308661
Thermal correction to Enthalpy=	1.309605
Thermal correction to Gibbs Free Energy=	1.110452
Sum of electronic and zero-point Energies=	-3798.423675
Sum of electronic and thermal Energies=	-3798.347663
Sum of electronic and thermal Enthalpies=	-3798.346719
Sum of electronic and thermal Free Energies=	-3798.545873

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6	0.000001532	-0.000001659	0.000000564
6	-0.000004398	-0.000001249	-0.000001863
7	-0.000000381	0.000002366	0.000011612
7	-0.000001207	-0.000007821	-0.000001447
16	0.000000094	-0.000000662	0.000000126
8	-0.000000377	0.00000232	0.000001424
8	-0.000001355	0.000001095	-0.000002906
6	-0.000000336	0.000001574	0.000000941
6	0.000000061	0.000002467	0.000002362
6	0.000000342	0.00000219	0.000002619
6	0.000000177	0.000002984	0.00000289
6	0.000000096	0.000002777	0.000001559
6	-0.000000344	0.000001747	0.000000476
1	0.000000179	0.000001215	0.000003077
1	0.000000031	0.000002142	0.00000355
1	0.000000756	0.000003137	0.000001453
1	0.000000661	0.000002303	0.000001176
6	0.000000753	0.000003504	0.000003001
1	0.000000766	0.000003745	0.000002481
1	0.000000612	0.000003425	0.000003431
1	0.000000531	0.000003091	0.000002477

6	-0.000001107	-0.000000812	0.000002401
6	0.000000073	-0.000000462	0.000001643
1	0.000001095	-0.00000005	0.000000092
1	0.000000269	-0.000000062	0.000000983
6	-0.00000061	-0.000000685	0.000002286
1	-0.000001197	-0.000001014	0.000001932
1	-0.000000128	-0.000001717	0.000000072
6	-0.000001006	-0.000002301	0.000003177
1	-0.000000411	-0.000001307	0.000002037
1	-0.000000783	-0.000001013	0.000002832
1	-0.000001235	-0.000001827	0.00000266
1	-0.000001286	-0.000002193	0.000002749
1	-0.000000987	-0.000002239	0.000001478
6	0.000000077	0.000001129	-0.000000137
6	-0.000000939	-0.000002971	-0.000000151
1	-0.000001093	-0.000001512	0.000001138
1	0.000000945	-0.000000269	0.000000506
6	-0.000001135	-0.000001883	0.000000688
1	-0.00000048	-0.000001394	-0.000000134
1	-0.000000386	-0.000002775	0.000000642
6	-0.000000916	-0.000003291	0.000000678
1	-0.00000081	-0.000001832	0.000001738
1	-0.000000897	-0.000002192	0.000001193
1	-0.000001285	-0.000003458	0.000001237
1	-0.00000123	-0.000003202	0.000000377
1	-0.000001121	-0.000003115	0.000000704
16	0.000001273	0.000009154	0.000007825
8	0.000003586	-0.000000151	-0.000003966
8	-0.000000083	-0.000004184	-0.000003587
6	-0.000000682	0.000000283	-0.000002568
6	0.00000047	-0.000000772	0.000000435
6	-0.000000105	0.000001075	0.000003421
6	-0.000000608	0.000000346	0.000001373
1	-0.00000044	-0.000000411	0.00000142
6	0.000000117	0.000000572	0.000001479
1	0.000000923	0.000001485	0.000000202
6	0.000000093	-0.000000022	-0.000000136
1	-0.000000461	-0.000000581	0.000000935
1	0.000000178	0.000001426	0.000001543
6	-0.000000587	0.000001248	0.000002107
1	-0.00000039	0.000000778	0.000002629
1	0.000000566	0.000000956	0.00000275
1	0.000000367	0.000001362	0.000002051
79	0.00000222	0.000001698	-0.000001845



6	-0.000002904	-0.000000756	-0.000000288
6	-0.000000792	-0.000000053	-0.000001102
6	0.000000692	0.000000963	-0.000001791
1	0.000000798	0.000000828	-0.000002785
1	0.000000292	-0.000000089	-0.000000566
7	0.000002907	-0.000000165	0.000000822
7	0.000000237	-0.000000231	0.000000096
6	-0.000001975	0.000000804	-0.000001632
6	0.000000383	-0.000001809	0.000001284
6	-0.000000787	-0.000000608	0.000001444
6	-0.000000085	0.000000458	0.000002377
6	-0.000001124	-0.000002257	0.000000858
6	0.000000026	-0.000000255	-0.000000166
1	-0.000000008	0.000000413	0.00000152
1	-0.000000751	-0.00000178	0.000001024
1	-0.000000603	-0.00000119	0.000002344
6	0.000001504	0.00000109	-0.000003161
6	-0.000000222	-0.000002165	-0.00000211
6	0.000000787	0.000002036	-0.000001017
6	0.000001014	0.000001047	-0.00000289
6	0.000000174	0.000000649	-0.000002383
6	0.000000793	0.000001171	-0.000003688
1	0.000000487	0.000000052	-0.000003333
1	0.000001186	0.000002243	-0.000002282
1	0.000001026	0.000001206	-0.000003496
6	-0.000001002	0.000002788	-0.000002047
6	0.00000102	-0.0000028	-0.000003413
6	0.00000172	-0.000002535	-0.000003546
1	-0.000000425	-0.00000042	-0.000002133
1	0.000000424	-0.000000355	-0.000003385
1	0.000000271	-0.000001284	-0.000003494
1	-0.000000174	0.000000005	-0.000004535
1	-0.00000108	-0.000001171	-0.000002325
1	-0.000000435	-0.000000688	-0.000002376
1	-0.00000013	-0.000002095	-0.000002855
6	0.000001205	0.00000108	-0.000001753
6	0.000000691	0.000002099	-0.000001113
6	0.000000978	0.000002909	-0.000001769
1	0.000000738	0.000001517	-0.00000102
1	0.000000908	0.000002033	-0.000000853
1	0.000000983	0.00000276	-0.000000391
1	0.000001222	0.000002583	-0.00000108
1	0.000000956	0.000002331	-0.000001953
1	0.000001262	0.000002713	-0.000002358

1	0.000001158	0.000003021	-0.000001422
6	-0.000002861	0.000000001	-0.000000899
6	0.000000979	-0.000003416	-0.000000366
6	0.000000722	-0.000002995	0.000000252
1	-0.000000779	-0.000000974	-0.000000083
1	-0.000001131	-0.000001496	-0.000000253
1	-0.000000539	-0.000002498	-0.000000596
1	-0.000001517	-0.000002623	0.000000705
1	-0.000000592	-0.000001714	-0.000000942
1	-0.000000844	-0.000001678	-0.000000681
1	-0.000000321	-0.000002777	-0.000001091
6	0.000001145	0.000000595	0.000000329
6	0.000000312	0.00000147	0.000000493
6	-0.000000426	0.000001476	0.000002123
1	0.000000836	0.00000126	0.000000576
1	0.000000181	0.000001029	0.000000763
1	0.000000386	0.000001995	0.000001176
1	0.000000097	0.000001071	0.000001541
1	0.0000004	0.000001435	0.000001927
1	0.000000122	0.000001647	0.000002635
1	0.000000755	0.000001687	0.00000107
6	-0.000000806	-0.000000942	-0.00000125
6	-0.000000303	-0.000000428	-0.000003077
6	0.000000641	-0.00000108	-0.000002532
6	-0.000000048	-0.000001819	-0.000002953
6	-0.000000456	-0.000002336	-0.000001681
6	0.000000699	-0.000000904	-0.000001703
6	0.000003087	0.000000009	-0.000001223
6	-0.000001346	0.000003217	-0.000003755
1	0.000000122	-0.000000937	-0.000003324
1	-0.00000027	-0.000002332	-0.000003192
1	-0.000000665	-0.000002788	-0.000002041
1	-0.000000684	-0.000001138	-0.000001074
1	-0.000001448	0.000001321	0.000000511
1	0.000000994	-0.000000064	-0.000000164
7	0.000002506	-0.000003069	-0.000001872
1	-0.000000542	0.000001599	-0.000002579

Zero-point correction=	1.235200 (Hartree/Particle)
Thermal correction to Energy=	1.310900
Thermal correction to Enthalpy=	1.311844
Thermal correction to Gibbs Free Energy=	1.111746
Sum of electronic and zero-point Energies=	-3798.471962
Sum of electronic and thermal Energies=	-3798.396262
Sum of electronic and thermal Enthalpies=	-3798.395318

Sum of electronic and thermal Free Energies= -3798.595416

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6	-0.000001006	0.000001275	0.000002027
6	-0.000000034	-0.000004645	-0.000001113
7	0.000000069	0.000001076	-0.000000122
7	0.000000648	0.000003128	-0.000000187
16	-0.000002065	0.000002504	0.000001823
8	0.000001004	0.000000201	0.000001829
8	0.000000954	0.000000177	0.000001429
6	0.000000778	0.000001325	0.00000191
6	0.000000261	-0.000000797	0.000001739
6	0.000000435	-0.000000349	-0.000000343
6	-0.000000657	-0.000000292	0.000003554
6	-0.000000886	-0.000000749	0.000000472
6	0.000000172	0.000000652	-0.000000025
1	0.000001385	0.000000179	0.000001655
1	0.00000141	-0.000000274	0.000000058
1	-0.000000611	0.000000069	-0.000000279
1	-0.000000689	0.000000663	0.000000978
6	0.000001547	0.000001423	-0.000002562
1	0.000001503	0.000000871	0.000000107
1	0.000000359	-0.000000885	-0.000000414
1	-0.000000445	0.000000043	-0.000000867
6	0.00000141	-0.00000005	0.000001186
6	0.000001975	-0.000000093	0.000000073
1	0.000001594	-0.000000076	0.000001135
1	0.000000545	0.000000164	0.000000213
6	0.000002556	-0.000000544	0.000000614
1	0.000001925	0.000000015	0.000001136
1	0.000001192	-0.000000217	0.000000385
6	0.000003082	-0.000000043	0.000000213
1	0.000002617	-0.000000345	-0.000000006
1	0.000002744	-0.000000278	0.000000821
1	0.000003682	-0.000000841	0.000000202
1	0.000003193	-0.000000389	0.000001018
1	0.00000281	-0.000000989	-0.000000004
6	-0.000000049	0.000000037	0.000001281
6	-0.000001148	0.000000906	0.000000467
1	-0.00000173	0.000000069	0.000001482
1	-0.000001148	0.000000342	0.000000072
6	-0.000002811	0.000001622	0.000001279
1	-0.000001567	0.000000905	0.000000481
1	-0.000001598	0.000001291	0.000001652

6	-0.000003394	0.00000139	0.000001627
1	-0.000002509	0.000000939	0.000001165
1	-0.000002612	0.000000902	0.000000705
1	-0.000003672	0.000001511	0.000001559
1	-0.000003081	0.000001702	0.000002101
1	-0.000002785	0.000001563	0.000001729
16	-0.000001452	0.000000344	-0.000000872
8	-0.000000831	-0.000000052	-0.000000831
8	-0.000001035	0.000000504	0.000002035
6	-0.000000174	0.000001366	0.000000769
6	0.000000458	0.000000868	0.000001629
6	0.000000843	0.000000943	0.000001185
6	0.000001959	0.000000811	0.000000595
1	0.000001058	-0.000000249	0.000001158
6	0.000000161	0.000000656	0.000002011
1	-0.000000494	0.000000859	0.00000164
6	0.000001139	-0.000001698	0.000001758
1	0.000002425	-0.000000231	0.000001442
1	0.000001008	0.000000358	0.000002263
6	0.000002417	-0.00000133	0.000001747
1	0.000001956	0.000001706	0.000002346
1	0.000002183	0.000001049	0.000001377
1	0.000002071	0.000000903	0.000003279
79	-0.000000611	-0.000001736	-0.000002188
6	-0.000000596	-0.000001098	0.000001764
6	-0.000000079	-0.000001392	-0.000002387
6	-0.000001078	-0.000001322	-0.000002337
1	-0.000001418	-0.000000503	-0.000002796
1	0.000000191	-0.000001202	-0.000002992
7	-0.000000123	0.000000927	-0.000002024
7	-0.000000681	-0.000000082	-0.000002473
6	0.000000781	-0.000001821	-0.000002427
6	0.000002035	-0.0000009	-0.000001637
6	0.000000539	-0.000001125	-0.000001513
6	0.000002032	-0.000001304	-0.00000179
6	0.000002011	-0.000001147	-0.0000023
6	0.000002464	-0.000001416	-0.000001767
1	0.000002196	-0.000001323	-0.000001101
1	0.000002358	-0.000001019	-0.00000114
1	0.000002926	-0.000001418	-0.000001523
6	-0.000001691	-0.000001385	-0.000001463
6	-0.000001035	-0.000000601	-0.000001198
6	-0.000002375	0.000000581	-0.000001154
6	-0.000002887	-0.000000153	-0.000000913

6	-0.0000029	-0.00000017	-0.000001143
6	-0.000003053	0.000000363	-0.000000973
1	-0.000002852	0.000000474	-0.000001328
1	-0.000003137	0.000000746	-0.000000861
1	-0.00000351	0.000000616	-0.000000717
6	-0.000002265	-0.000000601	-0.000002022
6	-0.000001586	-0.000000685	-0.000002602
6	-0.000002587	-0.000000145	-0.000001803
1	-0.000000363	0.000000373	-0.000001673
1	-0.000002031	-0.000000909	-0.000002801
1	-0.000001513	-0.000000057	-0.000002929
1	-0.000002356	-0.000000778	-0.000002358
1	0.000000326	-0.000000243	-0.000001287
1	-0.000001572	0	-0.000001344
1	-0.000001054	-0.000000693	-0.000001655
6	-0.000002037	-0.000000273	-0.000001431
6	-0.000001798	0.000000289	-0.000000476
6	-0.000001909	-0.000000272	-0.000001539
1	-0.00000115	-0.000000125	-0.000001393
1	-0.000001878	0.000000388	-0.000000036
1	-0.000001891	0.000000437	-0.000000674
1	-0.000002523	0.000000476	-0.000000499
1	-0.000002114	-0.000000302	-0.00000233
1	-0.000002741	-0.000000026	-0.000001971
1	-0.000001891	-0.000000028	-0.00000182
6	0.000001239	-0.000001463	-0.000001323
6	0.000001434	-0.000000083	-0.000001265
6	0.000001192	-0.000001176	-0.00000236
1	0.000000728	-0.000000672	-0.00000245
1	0.000001306	-0.000000407	-0.000000577
1	0.000001004	-0.000000823	-0.00000131
1	0.000001735	-0.000001013	-0.000001169
1	0.000001054	-0.000001655	-0.000002962
1	0.000001804	-0.000001334	-0.000002735
1	0.000000819	-0.000001261	-0.000002512
6	0.000000688	-0.000000607	-0.000001685
6	0.00000008	-0.000001245	-0.000002552
6	0.000001219	-0.000001275	-0.000000798
1	0.000000281	-0.000000058	-0.000001819
1	0.000000528	-0.000001414	-0.000002827
1	0.000000478	-0.000001165	-0.000002388
1	0.00000137	-0.000001429	-0.000002512
1	0.000000911	-0.000000484	-0.000000744
1	0.000001497	-0.000000659	-0.000001527

1	0.00000054	-0.000000158	-0.000001403
6	-0.000004151	0.000002828	0.000000854
6	0.000000907	0.000000548	0.000002381
6	0.000000903	0.000001336	0.000003752
6	0.000000185	0.000001289	0.000003012
6	-0.000000534	0.00000144	0.00000312
6	-0.000000476	0.000001761	0.000002577
6	-0.000000308	0.000001608	0.000007003
6	0.000000285	0.000001465	0.00000207
1	0.000001082	0.000001137	0.000003509
1	0.00000023	0.000001483	0.000003759
1	-0.000000994	0.000001668	0.00000337
1	-0.000001395	0.000001294	0.000003932
1	0.00000426	-0.0000021	0.000003362
1	0.00000139	0.000001764	0.000001885
7	0.00000252	0.000000659	0.00000339
1	0.000001852	0.000000676	0.000003086

Zero-point correction=	1.232608 (Hartree/Particle)
Thermal correction to Energy=	1.308615
Thermal correction to Enthalpy=	1.309559
Thermal correction to Gibbs Free Energy=	1.110468
Sum of electronic and zero-point Energies=	-3798.443083
Sum of electronic and thermal Energies=	-3798.367076
Sum of electronic and thermal Enthalpies=	-3798.366132
Sum of electronic and thermal Free Energies=	-3798.565224

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6	-0.000004673	-0.000012836	0.000000449
6	-0.000000444	0.000006979	-0.000000612
7	0.00000186	0.00000536	0.00000076
7	0.000004443	0.000005993	0.000000262
16	-0.000004224	0.000003948	-0.000002384
8	-0.000001827	-0.000001937	-0.000000061
8	0.000001795	-0.000002418	0.000001075
6	-0.000000216	0.000001947	0.000001116
6	-0.000002895	-0.000002596	-0.000001975
6	0.000001232	0.000001491	-0.000001433
6	-0.000001089	-0.000004292	0.000001319
6	-0.000003013	0.00000154	0.000000062
6	-0.00000088	-0.000000044	-0.000001104
1	-0.000001977	0.000001577	0.00000019
1	-0.000001721	-0.000000422	-0.00000042
1	0.000000143	-0.000000882	-0.000000159
1	0.000001459	0.000001214	-0.000000588

6	-0.000001273	-0.000001029	-0.000000216
1	-0.000001025	-0.000000004	-0.000000744
1	-0.000001536	-0.000001041	-0.000000561
1	-0.000000367	-0.000000842	-0.000000056
6	-0.000002775	0.000000018	0.000002023
6	-0.000001591	-0.000002503	-0.000000821
1	-0.000000125	-0.000000295	-0.000001711
1	-0.000001887	0.000000013	-0.000000734
6	-0.000000177	0.000001582	-0.000001441
1	-0.000000393	-0.000000563	-0.000001475
1	0.000000016	0.000000644	-0.000000747
6	-0.000002471	-0.000001902	-0.000001371
1	-0.000002855	-0.000001072	-0.000000357
1	-0.000001478	-0.000000531	-0.000000262
1	-0.00000138	-0.000000364	-0.000000321
1	-0.000001076	0.000000048	-0.000000395
1	-0.000000595	-0.000000005	-0.000000109
6	-0.000001735	-0.000003062	0.000000776
6	0.000002239	0.000000241	-0.000001646
1	-0.000001127	0.000001086	0.000000031
1	0.000001377	0.000000634	-0.000000607
6	0.00000129	0.000000738	0.000002518
1	0.000000631	0.000002057	-0.000000811
1	-0.000001167	0.000001571	-0.000000022
6	0.000000838	0.000001561	-0.000000017
1	0.000001085	0.00000107	-0.000000047
1	0.000001578	0.000001269	0.000000242
1	0.000001212	0.000001375	0.000000076
1	0.000001378	0.000001767	0.000000338
1	0.000000924	0.000001826	0.000000111
16	-0.000001189	-0.000001094	-0.000000345
8	0.000002584	-0.000000534	0.000002993
8	-0.00000101	0.000003254	-0.000000253
6	0.000001924	-0.000001078	0.000000764
6	-0.000002211	-0.000000107	0.000000885
6	0.000000335	0.000003341	-0.000001751
6	0.000001246	0.000001496	-0.000000701
1	0.000000761	-0.000000213	-0.000000225
6	-0.000000062	-0.000000565	0.000001148
1	0.000000578	0.000001265	0.000000575
6	-0.000001889	0.000002659	-0.000001122
1	-0.000000668	0.000000853	-0.000000821
1	0.000000026	0.000001799	-0.000000435
6	-0.000000318	0.000001081	-0.000000701

1	-0.000000296	0.000001863	-0.000000489
1	0.000000023	0.000001226	-0.000000407
1	-0.000000856	0.000001292	-0.000001086
79	0.000001161	0.000000829	-0.000001105
6	-0.000003427	0.000006305	0.000000104
6	-0.000000231	0.000002411	0.000001054
6	0.000000481	-0.000004245	0.000001216
1	0.00000184	-0.000001683	0.000001005
1	-0.000000074	-0.000000639	0.000001534
7	0.000002582	-0.000008416	-0.000000265
7	0.000003786	0.000002673	0.000002583
6	0.000000023	-0.000000949	0.000000498
6	-0.000001585	-0.000000771	-0.000000399
6	0.000000218	-0.000001045	-0.000000166
6	-0.000000988	-0.000002565	0.000000904
6	-0.000000092	-0.000000368	-0.000000351
6	0.000000247	-0.000002156	-0.000000029
1	-0.000000487	-0.00000151	-0.000000272
1	-0.000001027	-0.000001234	-0.000000541
1	-0.000001044	-0.000001407	-0.000000194
6	0.00000185	-0.000003932	-0.000001286
6	0.000001061	0.00000032	-0.000000499
6	0.000000799	-0.000001089	0.000000318
6	0.000001755	-0.000000032	0.000001818
6	-0.000000189	0.000000717	-0.000000048
6	0.000001608	-0.000000085	-0.000000057
1	0.000001186	0.000000074	0.000001396
1	0.000001337	0.000000244	0.000000936
1	0.000001977	0.000000569	0.000000654
6	-0.00000175	-0.000001882	0.000000265
6	0.000000889	-0.000000113	0.000001898
6	0.000001134	-0.000001807	-0.000000333
1	0.000001422	0.000000498	0.000000812
1	0.000001474	-0.000001061	0.000000032
1	0.000001918	-0.000000404	0.000000087
1	0.000002233	-0.000000055	0.000001043
1	0.000002137	0.000000683	0.000000252
1	0.000001606	0.000000028	0.000000788
1	0.000001417	0.000000396	0.000001173
6	0.000002527	0.000000009	-0.000001236
6	0.000000031	0.000000162	0.000001064
6	0.000000054	-0.000000813	0.000000598
1	0.000000382	-0.000001204	0.000000937
1	0.000000216	0.000000194	0.000000075



1	0.000000556	-0.000000128	0.000000408
1	0.000000396	-0.000000488	-0.000000118
1	0.000000314	-0.000001682	0.000000121
1	0.000001533	-0.000000741	0.000000589
1	0.000000668	-0.000000892	0.000000552
6	-0.000000483	-0.000001907	0.000000387
6	-0.000000695	-0.000001431	0.000000106
6	0.000001164	-0.000000972	0.000000891
1	0.000000123	-0.00000005	-0.000000737
1	-0.000000558	0.000000264	-0.000000646
1	-0.000000199	-0.000000369	0.000000142
1	-0.000000039	-0.000000112	0.000000029
1	0.000000058	-0.000001954	0.000000189
1	-0.00000001	-0.000001361	0.000000409
1	0.000000502	-0.000000111	0.000000054
6	0.000000827	-0.000000899	0.000000622
6	-0.000000862	-0.000002457	-0.000000177
6	-0.000001616	-0.000001745	-0.000000512
1	0.000000351	-0.000001027	0.000000357
1	-0.000000124	-0.000001721	0.000000025
1	-0.000000677	-0.000002139	0.000000113
1	-0.000000633	-0.000002078	0.000000204
1	-0.000000412	-0.000000143	-0.000000168
1	-0.000000676	-0.000001445	0.000000581
1	-0.000000579	-0.000001163	0.000000006
6	-0.000001293	0.000004047	-0.000000686
6	-0.000004147	0.000004388	-0.000002692
6	0.000000421	0.000001933	-0.000001612
6	-0.000000366	0.000001986	-0.000000344
6	0.000001149	0.000002749	-0.000001105
6	-0.000003273	0.000000074	0.000000561
6	0.000004227	0.000003253	-0.000001927
6	0.000001338	-0.000000028	-0.000000029
1	-0.000000044	0.000000229	-0.000000177
1	-0.000000021	0.000002395	-0.000000735
1	0.000000644	0.000000192	-0.000000505
1	0.000001018	0.000001908	0.000000451
1	-0.000002089	0.000000005	0.000000812
1	-0.000001446	-0.000000138	0.000001335
7	0.000001469	-0.000001597	0.000001773
1	-0.000000332	0.000000092	-0.000001256

Zero-point correction=

1.234933 (Hartree/Particle)

Thermal correction to Energy=

1.310397

Thermal correction to Enthalpy=

1.311342

Thermal correction to Gibbs Free Energy=	1.114830
Sum of electronic and zero-point Energies=	-3798.458343
Sum of electronic and thermal Energies=	-3798.382879
Sum of electronic and thermal Enthalpies=	-3798.381934
Sum of electronic and thermal Free Energies=	-3798.578446

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6	0.000000686	0.000000606	-0.000002289
6	0.000001747	0.000001049	0.000001632
7	-0.000000852	0.000000765	-0.000001837
7	0.000000165	-0.000000231	-0.000000295
16	0.000000234	-0.000000316	-0.000001591
8	0.000000035	0.000000021	-0.000001607
8	-0.000000003	-0.0000000892	-0.000001303
6	-0.000000243	-0.000000012	-0.000002701
6	-0.000000735	0.000000049	-0.000002068
6	-0.000001155	-0.000001058	-0.000002432
6	-0.000002351	0.000000896	-0.000000171
6	0.000000865	0.000001113	-0.000001699
6	0.000000403	-0.000000601	-0.000000766
1	-0.000000626	0.000000022	-0.000002369
1	-0.000000605	0.000000189	-0.000003107
1	0.000000247	-0.000000665	-0.000001927
1	0.000000245	-0.000000472	-0.000001306
6	0.000000797	-0.000000593	-0.000004128
1	-0.000000669	-0.000001899	-0.00000324
1	0.000000934	0.000001456	-0.000002937
1	0.000000347	-0.000000579	-0.00000033
6	-0.000001233	0.000000447	-0.000000478
6	-0.000001031	0.000001008	-0.000000082
1	-0.000000232	0.000000582	-0.000001238
1	-0.000000519	0.000000132	-0.000000391
6	-0.000001162	0.000001519	-0.000000803
1	-0.000000854	0.000000071	-0.00000124
1	-0.000000684	0.000000912	-0.000000402
6	-0.000001494	0.000001741	-0.000000819
1	-0.000001254	0.000001213	-0.000000413
1	-0.000001145	0.000001411	-0.000001158
1	-0.000001758	0.000002139	-0.000000789
1	-0.000001499	0.000001664	-0.000001231
1	-0.000001339	0.000001766	-0.000000041
6	-0.000000154	0.000000138	-0.000001031
6	-0.000000347	0.000000093	-0.000000496
1	0.000000029	0.00000003	-0.000000959

1	0.000000044	-0.000000045	-0.000000874
6	-0.000000686	0.000000629	-0.000000507
1	-0.000000154	0.000000295	-0.000000416
1	-0.000000467	0.000000065	0.000000004
6	-0.000000394	0.000001045	-0.000000011
1	-0.000000839	0.00000118	-0.00000102
1	-0.00000064	0.000000206	-0.000000854
1	-0.000001122	0.000001116	-0.000000389
1	-0.000000284	0.000000618	-0.00000002
1	-0.000000829	0.000001123	0.000000496
16	0.000000896	-0.000000691	-0.000000587
8	0.000000723	-0.000001016	-0.000000616
8	0.000000848	-0.000001384	-0.000000439
6	0.000000457	-0.000001127	-0.000001643
6	0.000000569	-0.000000807	-0.000001629
6	0.000000578	-0.000001019	-0.000001597
6	0.000000743	-0.000000891	-0.000001843
1	0.000000371	-0.000000748	-0.000001585
6	0.000000418	-0.000001441	-0.000002919
1	0.000000685	-0.000001249	-0.000001726
6	-0.000000071	-0.000001947	-0.000003602
1	0.00000038	-0.000000942	-0.000002769
1	0.000000759	-0.000001441	-0.000002912
6	0.000001003	-0.000000792	-0.00000304
1	0.000001091	-0.000001141	-0.00000332
1	0.000000882	-0.000001481	-0.000003797
1	-0.000000205	-0.000001017	-0.000003449
79	-0.000000148	-0.000000234	-0.00000012
6	0.000000446	-0.000000177	0.000000512
6	0.000000033	0.000000368	0.000001482
6	0.000000418	0.000000188	0.0000013
1	0.000000485	-0.000000719	0.00000203
1	-0.000000121	0.000000491	0.00000169
7	-0.000001148	-0.000001355	0.000002834
7	0.000001086	0.000000725	0.000001461
6	0.000000324	0.000000741	0.000000977
6	-0.000000737	0.000000741	-0.00000004
6	-0.000001574	0.000001414	0.000000969
6	-0.000000687	0.000000947	0.000000105
6	-0.000000836	0.000001593	0.000000889
6	-0.000001416	0.000001643	0.000000273
1	-0.000000845	0.000001264	-0.000000108
1	-0.000001462	0.000001899	0.000000807
1	-0.000001387	0.000001886	0.000000085

6	0.000000261	0.000000551	0.000001313
6	0.000001061	-0.000000727	0.000001888
6	0.000001236	-0.000001192	0.000000975
6	0.000000603	-0.000001393	0.000002117
6	0.000002229	-0.00000153	0.000001153
6	0.000001361	-0.000001261	0.000001508
1	0.000001176	-0.000001294	0.000002205
1	0.000001337	-0.000001799	0.000000903
1	0.00000167	-0.000001799	0.000001586
6	0.000000261	-0.000000574	0.000002767
6	0.000000702	-0.000000092	0.000002911
6	0.000000463	-0.000000212	0.000002579
1	-0.000000095	0.000000206	0.000002134
1	0.000001017	-0.00000027	0.000003238
1	0.000000297	-0.000000301	0.000003132
1	0.000000871	-0.000000452	0.000002936
1	0.000000611	0.000000099	0.000002415
1	0.000000823	-0.000000597	0.00000265
1	0.00000013	0.000000434	0.000002774
6	0.000000244	-0.000001116	0.000000861
6	0.000000942	-0.00000124	0.000000792
6	0.000000696	-0.000001651	0.000000264
1	0.000001497	-0.000000432	0.000000063
1	0.000000755	-0.000001415	-0.000000466
1	0.000000889	-0.000001305	-0.000000084
1	0.000001377	-0.000001335	-0.000000196
1	0.000001178	-0.000001233	0.000001213
1	0.000001459	-0.000001781	0.000000888
1	0.000001152	-0.000001359	0.000000488
6	-0.000000548	0.000001018	0.000001541
6	-0.000000848	0.000001129	0.000001157
6	-0.000001044	0.000001615	0.000002339
1	0.000000148	0.000000987	0.000001891
1	-0.000000724	0.000001299	0.000001058
1	-0.000000805	0.00000147	0.000001643
1	-0.000000941	0.000001553	0.000001308
1	-0.000000802	0.000000981	0.000001864
1	-0.000000848	0.000002312	0.000001799
1	-0.00000117	0.000001481	0.000002812
6	-0.00000032	0.000000565	0.000000299
6	-0.000000447	0.000000494	0.000000426
6	-0.000000287	0.000000225	-0.000000524
1	0.000000206	0.000000113	0.000000603
1	-0.000000326	0.00000051	0.00000066

1	-0.000000132	0.000000206	0.000000231
1	-0.000000556	0.000000506	0.00000006
1	-0.000000342	0.000000014	-0.000000072
1	-0.000000375	0.000000541	-0.000000865
1	-0.000000071	-0.000000319	-0.000000653
6	0.000000036	-0.000000045	0.000001448
6	-0.000000459	-0.000000128	0.000001325
6	0.000000267	0.000000046	0.000000983
6	0.000000357	0.000000064	0.000001308
6	0.000000424	-0.000000417	0.000001663
6	0.000000609	-0.000000024	0.000000706
6	0.000000829	0.000000774	-0.000000026
6	-0.000002515	-0.000004887	0.000001711
1	-0.000000145	0.000000655	0.000001218
1	-0.000000012	0.000000432	0.000001639
1	0.000000236	-0.000000266	0.000001446
1	0.000000593	-0.00000008	0.000000853
1	0.000001283	-0.000001342	0.000000118
1	0.000000131	0.000000326	0.000001222
7	-0.000000435	0.000000035	-0.000000457
1	0.000000629	-0.000000103	0.00000003

Zero-point correction=

1.231624 (Hartree/Particle)

Thermal correction to Energy=

1.307930

Thermal correction to Enthalpy=

1.308874

Thermal correction to Gibbs Free Energy=

1.106486

Sum of electronic and zero-point Energies=

-3798.434860

Sum of electronic and thermal Energies=

-3798.358553

Sum of electronic and thermal Enthalpies=

-3798.357609

Sum of electronic and thermal Free Energies=

-3798.559997

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6	-0.000000588	0.000000437	0.000000208
6	-0.000007139	0.000001356	0.000000093
7	0.000000731	0.000002795	-0.000000646
7	0.000001591	0.000001947	-0.000000543
16	0.000001672	-0.000000018	-0.000000766
8	-0.000004756	-0.000000816	0.000001447
8	-0.000001483	-0.000003243	-0.000005016
6	0.000002053	0.000002147	-0.000002503
6	0.000000477	-0.000000484	-0.000000964
6	0.000001867	-0.000000262	-0.00000223
6	0.000000104	0.000000078	-0.000000543
6	0.000000846	-0.000000251	-0.000001608
6	-0.000000059	-0.000000275	0.000000373

1	-0.00000037	0.000000704	-0.000002042
1	0.00000036	0.000000037	-0.000001842
1	0.000001245	-0.000000662	-0.000000933
1	0.000000667	-0.000000526	-0.000000904
6	0.000000872	-0.000000212	-0.00000014
1	0.000000756	-0.000000216	-0.000001886
1	0.000001669	-0.000000353	-0.000000085
1	0.000002041	-0.000000812	-0.000002029
6	-0.000001098	0.000001524	0.000002782
6	-0.000002128	0.000000951	-0.00000173
1	0.000000991	0.000001041	-0.000001878
1	-0.000001722	-0.000000811	-0.000000503
6	-0.00000089	0.000000679	-0.000000983
1	-0.000000813	0.000000206	-0.000000661
1	-0.000000544	0.000000123	-0.000000253
6	-0.000001696	0.000000929	-0.000000324
1	-0.000001091	0.000000726	-0.000000209
1	-0.000000761	0.000000921	-0.000000904
1	-0.000001588	0.000000885	-0.000000572
1	-0.000001542	0.000001066	-0.000001084
1	-0.000001584	0.000000997	-0.000000126
6	-0.000001349	0.00000062	0.000001155
6	-0.000001441	-0.000001227	0.000000698
1	-0.000000527	0.0000015	-0.000001553
1	-0.000000025	0.000000194	-0.000001548
6	-0.000001276	0.000001355	-0.000001241
1	-0.000000417	0.000001069	-0.000000512
1	0.000000003	0.000001125	-0.000000038
6	-0.000001966	0.000000873	-0.000000182
1	-0.000001635	0.000001295	-0.000000744
1	-0.000000947	0.00000072	-0.000001224
1	-0.000001905	0.000001312	-0.000000512
1	-0.00000177	0.000000949	-0.000000271
1	-0.000001526	0.000000962	-0.000000073
16	0.000002849	-0.000001663	-0.000004417
8	-0.000000611	0.00000195	-0.000001221
8	-0.000000398	-0.000000763	0.000000643
6	-0.00000111	0.000001209	-0.00000145
6	-0.000001056	0.000000487	-0.000002046
6	0.000000735	0.00000058	-0.000001198
6	0.000000133	-0.000000062	-0.000002525
1	-0.000000127	0.000000347	-0.000001316
6	0.000000051	0.000000448	-0.000001707
1	0.000001582	0.000000036	-0.000001313

6	0.000000617	0.000000951	-0.000003092
1	-0.000000249	0.000000721	-0.000002342
1	0.000000731	0.000000113	-0.000002536
6	0.000000172	0.000000363	-0.000003212
1	0.000000494	0.000000307	-0.000003186
1	0.000000092	0.000000829	-0.000002946
1	0.000000085	0.000000089	-0.000003272
79	0.000000513	-0.000001962	-0.000000354
6	-0.000003673	0.000004843	-0.000000266
6	-0.000000752	-0.000000289	0.000002542
6	-0.000001225	-0.000002404	0.000002092
1	0.000000059	-0.000000424	0.000001394
1	-0.000000032	0.000000273	0.000001374
7	0.000004142	-0.000000689	0.000001438
7	0.000002224	-0.000001472	-0.000000246
6	-0.000000659	0.000000472	-0.000000298
6	-0.000002226	0.000000432	-0.000000107
6	-0.000000794	-0.000000286	0.000003519
6	0.000000342	0.000000313	0.000002225
6	-0.000001013	-0.000000672	0.000000452
6	-0.000001035	0.000000074	-0.000000392
1	-0.000000387	-0.000000188	0.000000007
1	-0.000001105	0.000000774	0.000000993
1	-0.000000546	0.000000745	0.000000031
6	0.000001417	-0.000000178	0.000000995
6	0.000000561	0.000000154	0.000001138
6	-0.000000395	-0.000000946	0.000002787
6	0.000000805	-0.000000899	0.000000912
6	0.000000971	-0.000000156	0.000001123
6	0.000000793	-0.000001602	0.000001564
1	0.000000643	-0.000000771	0.000001572
1	0.000001912	-0.000001141	0.000000949
1	0.000001203	-0.000000794	0.000001133
6	0.00000307	-0.000001134	0.000000097
6	-0.000001501	0.000000061	0.000002757
6	-0.000002622	-0.000000882	0.000003257
1	0.000000824	-0.000000063	0.000001297
1	0.000000039	-0.000000626	0.000002328
1	-0.000000604	-0.000000471	0.000002578
1	0.000000912	-0.000000887	0.000002473
1	-0.000000105	0.000000082	0.000000845
1	0.000000227	0.000000121	0.000000721
1	-0.000000612	0.000000168	0.000001433
6	0.00000259	-0.000002108	0.000000026

6	0.000000037	0.000000316	0.000000086
6	0.000001156	-0.000001398	0.000001165
1	0.000001542	-0.000000962	0.000000805
1	0.000001389	-0.000000558	-0.000000715
1	0.000001469	-0.000001088	0.000000335
1	0.000002158	-0.000001317	0.000000192
1	0.000001562	-0.000001065	0.000001327
1	0.000002047	-0.000001023	0.000000706
1	0.000001475	-0.000000893	0.000000985
6	-0.000001348	-0.000001112	0.00000141
6	0.000000033	0.000002506	0.00000117
6	-0.000000246	-0.000000257	0.000002546
1	-0.000001805	-0.00000001	0.000001644
1	-0.000001196	0.000000154	0.000000144
1	-0.000001216	0.000000002	0.000001257
1	-0.000002405	-0.000000563	0.000000834
1	-0.000001067	0.000000285	0.000001568
1	-0.000001886	0.000000938	0.000001296
1	-0.000001203	0.000000825	0.000001623
6	0.000001175	-0.000000898	0.000000484
6	0.000000095	-0.000001201	0.000000901
6	0.000000075	-0.000000316	-0.000000168
1	0.000001214	-0.000000661	0.000000708
1	0.000000165	-0.000000681	0.000001343
1	0.000000551	-0.000000453	0.000000687
1	0.000000843	0.000000278	0.000000748
1	0.000000932	-0.000000172	0.000000175
1	0.000000298	-0.000000362	-0.000000275
1	0.000000464	-0.000000444	0.000000273
6	-0.000000009	0.000001325	0.000000107
6	-0.000004042	-0.000002541	-0.000000408
6	0.000001468	0.000001115	0.000001443
6	-0.000000014	-0.000000044	0.000000268
6	0.000000346	-0.000000083	0.000000019
6	0.000001156	-0.000000769	0.000000645
6	-0.000002445	-0.000002863	-0.000007312
6	0.000002439	-0.000004367	0.00000926
1	-0.000001072	0.000000015	0.000000657
1	-0.000000095	-0.000000248	0.000000682
1	0.000000757	-0.000000648	0.000000632
1	0.000000906	-0.000000388	0.000000396
1	0.000000795	-0.000000033	-0.000000037
1	0.000000388	-0.000000355	-0.000000272
7	0.000010779	0.00000411	-0.000002034



1	-0.000006847	0.0000006	0.000000461
Zero-point correction=			1.234051 (Hartree/Particle)
Thermal correction to Energy=			1.309936
Thermal correction to Enthalpy=			1.310880
Thermal correction to Gibbs Free Energy=			1.111430
Sum of electronic and zero-point Energies=			-3798.463959
Sum of electronic and thermal Energies=			-3798.388074
Sum of electronic and thermal Enthalpies=			-3798.387130
Sum of electronic and thermal Free Energies=			-3798.586579

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6	0.000000747	-0.000000124	-0.000000008
6	-0.000002003	-0.000000779	0.000000941
7	0.000000942	0.000000039	-0.000000345
7	-0.000000229	0.000001129	-0.000001085
16	0.000001715	0.000000681	-0.000000327
8	0.000001298	0.000001611	0.000000729
8	0.000000889	0.000000905	0.000000108
6	0.000001733	0.000000453	0.000000736
6	0.000002256	0.000000269	0.000000656
6	0.000002977	0.000000416	0.000000529
6	0.000002473	-0.000000595	0.000000363
6	0.000001981	-0.000000311	0.000000555
6	0.000002037	0.000000028	0.000000298
1	0.000002417	0.000000072	0.000000758
1	0.000003087	0.000000106	0.000000812
1	0.00000203	-0.000000482	0.000000558
1	0.000001291	0.000000116	0.000000436
6	0.00000315	-0.000000438	0.000000834
1	0.000003657	-0.000000058	0.000000866
1	0.000002897	-0.000000905	0.000001019
1	0.000002489	-0.000000795	0.000001023
6	0.000000753	0.000000172	0.000000724
6	0.000001029	0.000000116	0.000000297
1	0.000001492	0.000000379	0.000000366
1	0.000001379	-0.000000248	0.000000203
6	0.000001002	-0.000000376	0.000000375
1	0.000000828	0.000000458	0.000000305
1	0.000000475	0.000000006	0.000000096
6	0.000000876	-0.000000352	0.000000151
1	0.000001092	-0.000000742	0.000000037
1	0.000001564	-0.000000194	0.000000394
1	0.00000104	-0.000000702	0.000000319
1	0.000000083	-0.000000015	0.000000287

1	0.000000395	-0.00000053	0.00000012
6	-0.000000945	0.000000863	0.000000395
6	-0.000001075	0.000001408	-0.00000025
1	-0.000000784	0.000000627	-0.000000306
1	-0.000000264	0.000001257	-0.000000173
6	-0.000001295	0.000001642	-0.000000432
1	-0.00000146	0.000001308	-0.000000532
1	-0.000001242	0.000001878	-0.000000114
6	-0.000001795	0.000001939	-0.000000497
1	-0.000000808	0.000001817	-0.000000329
1	-0.000001327	0.000001196	-0.000000344
1	-0.000001829	0.000002127	-0.000000542
1	-0.000002085	0.000001839	-0.000000653
1	-0.000001672	0.00000023	-0.000000586
16	-0.000000351	0.000000695	-0.000000859
8	-0.000000536	-0.000000493	0.000000004
8	-0.000001449	0.000000143	-0.000000477
6	-0.00000158	0.00000124	0.000000316
6	-0.000000757	0.000000997	-0.000000796
6	-0.000001655	0.00000116	-0.000000698
6	-0.000001341	0.000001227	-0.000000233
1	-0.000000615	0.000000688	-0.00000006
6	-0.000001721	0.000001567	-0.000000885
1	-0.00000188	0.000001609	-0.000000366
6	-0.000001362	0.000001762	-0.000000283
1	-0.000000902	0.000001206	-0.000000227
1	-0.000002081	0.000001731	-0.00000053
6	-0.000001621	0.000001381	-0.000000343
1	-0.00000166	0.000002144	-0.000000509
1	-0.000002301	0.000002302	-0.000000765
1	-0.000002195	0.000001755	-0.000000926
79	0.000000496	0.000000272	-0.000000013
6	-0.000000528	-0.000001041	-0.000000186
6	0.000000001	-0.000001916	-0.000000007
6	-0.000000214	-0.000001519	-0.000000011
1	-0.000000455	-0.000001762	-0.000000076
1	-0.000000017	-0.000002337	0.000000101
7	0.000000094	-0.000001491	0.000000101
7	-0.000000285	-0.000001435	0.000000124
6	0.000000463	-0.000001907	0.000000276
6	0.000000772	-0.000001617	0.000000073
6	-0.000000067	-0.000001635	0.000000269
6	0.00000106	-0.000001841	0.000000515
6	0.000000227	-0.000001953	0.000000006

6	0.000000711	-0.000002108	0.000000311
1	0.000001477	-0.00000019	0.000000448
1	0.000000007	-0.000001894	0.000000036
1	0.000000907	-0.000002064	0.000000312
6	-0.000000773	-0.000000141	-0.000000062
6	-0.000001205	-0.000000663	-0.000000261
6	-0.000000091	-0.000000437	-0.000000021
6	-0.000000145	-0.000000151	-0.000000355
6	0.000000009	-0.000000136	-0.000000293
6	-0.000000927	0.000000229	-0.000000031
1	-0.000001686	-0.000000161	-0.000000478
1	-0.000000215	0.000000017	-0.000000001
1	-0.000001122	0.000000429	-0.000000274
6	-0.000001352	-0.000000943	-0.000000282
6	-0.000001644	-0.000001435	-0.000000399
6	-0.000001754	-0.000000754	-0.000000567
1	-0.000001225	-0.000001154	-0.000000215
1	-0.000001431	-0.000001636	-0.000000346
1	-0.000001978	-0.000001617	-0.000000467
1	-0.000001911	-0.000001193	-0.000000462
1	-0.000001706	0.000000004	-0.000000267
1	-0.000002083	-0.000000419	-0.000000524
1	-0.000001981	-0.000000856	-0.000000494
6	0.000000094	-0.000000505	0.000000149
6	0.000000546	0.000000007	0.000000324
6	0.000000344	-0.000000854	0.000000006
1	0.000000541	-0.000000085	0.000000171
1	0.000000899	0.000000635	0.000000235
1	0.000001205	0.000000102	0.000000246
1	0.000000749	0.000000013	0.000000177
1	0.000000323	-0.000001376	0.000000073
1	0.000000422	-0.000000066	0.000000198
1	0.000000979	-0.000000999	0.000000329
6	-0.00000055	-0.000001476	-0.000000143
6	-0.00000058	-0.000001537	-0.000000292
6	-0.00000009	-0.000002232	-0.000000137
1	-0.000000778	-0.000001555	-0.000000021
1	-0.000000758	-0.000000726	-0.000000224
1	-0.000001264	-0.000001225	-0.000000305
1	-0.000000928	-0.00000144	-0.000000113
1	-0.000000788	-0.00000242	-0.000000082
1	-0.000000848	-0.000002442	-0.000000146
1	-0.000001293	-0.000002147	-0.000000298
6	0.000001467	-0.000001656	0.000000383

6	0.000001276	-0.000002342	0.000000422
6	0.000001772	-0.000001342	0.000000575
1	0.00000103	-0.000001555	0.000000221
1	0.000000961	-0.000002577	0.000000367
1	0.000001552	-0.00000023	0.000000511
1	0.000001586	-0.000002549	0.000000538
1	0.000001736	-0.000001161	0.000000494
1	0.000002052	-0.00000161	0.000000725
1	0.000001924	-0.000001497	0.000000557
6	-0.00000038	0.000001894	-0.000000132
6	-0.000000411	0.000001703	-0.000000444
6	-0.000000593	0.00000025	-0.000000441
6	-0.000001033	0.000002915	-0.000000308
6	-0.00000053	0.000003056	-0.000000377
6	-0.00000015	0.000002668	0.00000004
6	0.000000958	0.000002281	-0.000000177
6	0.000000276	0.000001734	0.000000123
1	-0.000000802	0.000002294	-0.000000182
1	-0.000001275	0.000003165	-0.000000439
1	-0.000000761	0.000003248	-0.000000324
1	-0.000000072	0.000002669	-0.000000034
1	0.000000414	0.000001723	-0.000000177
1	0.000000443	0.00000019	0.000000167
7	0.000001373	0.000002781	-0.000000652
1	-0.000000354	0.000000606	0.000000075

Zero-point correction=	1.232654 (Hartree/Particle)
Thermal correction to Energy=	1.308742
Thermal correction to Enthalpy=	1.309687
Thermal correction to Gibbs Free Energy=	1.109458
Sum of electronic and zero-point Energies=	-3798.448894
Sum of electronic and thermal Energies=	-3798.372805
Sum of electronic and thermal Enthalpies=	-3798.371861
Sum of electronic and thermal Free Energies=	-3798.572090

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6	-0.000000762	0.00000097	-0.000000791
6	0.000002365	-0.00000474	0.000002184
7	-0.000000411	0.000000889	-0.000000976
7	-0.000001828	0.000004012	0.000003246
16	0.000000636	-0.000000532	0.000002313
8	0.000001113	0.000000313	0.00000139
8	0.000000349	-0.000001078	0.000002309
6	0.000001087	0.000001152	0.000000112
6	-0.000000286	-0.000001397	0.000002502

6	0.000001074	-0.000001546	0.000005227
6	0.000003215	0.000002403	-0.000003016
6	0.000000333	-0.000003255	0.000001498
6	0.000001382	-0.000001207	0.000002712
1	0.000001719	-0.000000308	0.000001978
1	0.000001686	-0.000002339	0.000001204
1	0.000000318	-0.000002996	0.000000553
1	0.000000017	-0.000001433	0.000000703
6	0.000001128	-0.000005851	-0.000003179
1	0.000000574	-0.000001824	0.000003526
1	0.000000079	-0.000002047	0.00000042
1	0.000000903	-0.000000817	0.000004318
6	0.000001501	-0.000000637	0.00000124
6	-0.000000218	0.000001713	0.000000976
1	0.000001081	-0.000000173	0.000000669
1	0.000000582	0.000000861	0.00000107
6	0.000001576	0.000000495	0.000000814
1	0.000001067	0.000000921	0.000001396
1	0.000000578	0.000000657	0.000000866
6	0.000000969	0.000002149	0.000001196
1	0.000000362	0.000001262	0.000000924
1	0.00000143	0.000001167	0.000001217
1	0.000001165	0.000001648	0.000001055
1	0.000001342	0.000001735	0.000001281
1	0.000000742	0.000001788	0.000000549
6	0.000000131	-0.000000338	-0.000000361
6	-0.000000436	0.000000001	-0.000000047
1	-0.000000152	0.000000245	-0.000000045
1	-0.000000379	0.000000007	-0.000000277
6	-0.000000216	-0.000000061	-0.000000401
1	0.000000361	0.000000238	0.000000185
1	0.000000165	-0.000000226	0.000000229
6	-0.000000042	-0.000000074	-0.000000035
1	-0.000000407	-0.000000897	-0.000000296
1	-0.000000048	-0.000000049	-0.00000005
1	-0.000000286	-0.000001153	-0.000000124
1	-0.000000014	-0.000000591	0.000000079
1	0.000000073	-0.000001014	0.000000336
16	0.000000636	-0.000000373	-0.000001811
8	0.000000016	0.000000505	-0.000000781
8	-0.000000919	0.000000101	-0.000001296
6	-0.000000774	0.000002946	-0.000000281
6	-0.000001309	0.000000457	-0.00000164
6	0.000000765	0.000001735	-0.000000685

6	0.000001007	0.000000735	-0.000000067
1	-0.000000534	0.000001196	-0.000001195
6	-0.000001227	0.000000978	-0.000003423
1	0.00000012	0.000001237	-0.000000276
6	-0.000001546	0.00000445	-0.000000125
1	-0.000000873	0.000001693	-0.00000159
1	-0.000000049	0.000001545	-0.000000511
6	-0.000001089	0.000002976	0.000000065
1	-0.00000171	0.000002864	-0.000003522
1	-0.000000191	0.000002403	-0.000000233
1	-0.000000159	-0.000000214	-0.000002971
79	0.000000392	-0.000000622	0.000000655
6	0.00000008	-0.000000487	-0.000000868
6	-0.000002466	-0.000002378	-0.00000205
6	0.000000885	0.00000063	0.00000077
1	-0.000000852	-0.000000799	-0.000000933
1	-0.000000741	-0.000000798	-0.00000098
7	0.000000286	0.000000593	-0.000000091
7	-0.000000541	-0.000001555	-0.0000012
6	0.000000754	-0.000000112	0.000000164
6	-0.000000748	0.0000003	0.000000993
6	0.000000455	0.000000202	-0.000000118
6	0.000000447	-0.000000241	0.000000516
6	0.000000397	0.00000139	-0.00000045
6	0.000000493	-0.000000002	0.000000018
1	0.000000489	-0.000000437	0.000000665
1	0.000000237	0.000001315	-0.000000038
1	0.00000041	0.000000708	0.000000504
6	0.000000001	0.000000842	-0.000000512
6	-0.000001891	-0.000002247	-0.000000816
6	-0.000000582	-0.000000591	-0.000001762
6	-0.000001394	-0.000000885	-0.000001087
6	-0.000000488	-0.000002135	-0.000000788
6	-0.000001037	-0.000001269	-0.000001376
1	-0.000001624	-0.000000879	-0.000001672
1	-0.000000829	-0.000001793	-0.000000623
1	-0.000001269	-0.000001531	-0.000001267
6	-0.000001201	0.000000188	-0.000002127
6	-0.000001569	-0.000000674	-0.000001849
6	-0.000000754	0.000000138	-0.000001173
1	-0.000001779	-0.000000557	-0.00000117
1	-0.00000175	-0.00000075	-0.000001841
1	-0.00000168	-0.000000078	-0.00000208
1	-0.000001722	-0.000000548	-0.000002056

1	-0.00000098	0.000000525	-0.000001514
1	-0.000001452	0.000000146	-0.000001671
1	-0.000001237	0.000000703	-0.000001823
6	-0.000000477	-0.000002198	-0.000000538
6	-0.000000604	-0.000001346	0.00000055
6	-0.000000792	-0.000002192	-0.000000306
1	-0.000000354	-0.000001286	-0.000000163
1	-0.000000209	-0.000001878	0.000000222
1	0.000000208	-0.00000227	0.000000122
1	-0.000000403	-0.000002135	0.000000021
1	-0.000000812	-0.00000235	-0.000001017
1	-0.000000789	-0.000002404	-0.000000594
1	-0.000000534	-0.000002315	-0.000000121
6	-0.000000296	0.000000566	-0.000000544
6	-0.000000644	0.000001182	-0.000000719
6	-0.000000726	0.00000071	-0.000001251
1	-0.000000448	0.000000433	-0.00000071
1	0.000000013	0.000001748	-0.00000013
1	-0.000000564	0.000001122	-0.000001103
1	-0.000000517	0.00000136	-0.000000253
1	-0.000000885	0.000000431	-0.000001082
1	-0.000000605	0.000001203	-0.000000844
1	-0.000000833	0.000000962	-0.000001334
6	0.00000049	-0.000000969	-0.000000361
6	0.000000037	-0.000001416	0.000000325
6	0.000000578	-0.000000835	0.000001234
1	-0.00000005	-0.000001385	0.0000001
1	-0.000000387	-0.000001422	-0.000000093
1	-0.000000089	-0.000001681	0.000000307
1	0.000000231	-0.000001125	0.000000543
1	0.000000472	-0.00000081	0.000000978
1	0.000000377	-0.000001026	0.000001273
1	0.000000015	-0.000001291	0.000000754
6	0.000000199	0.000000579	0.000001325
6	0.000000818	0.000000837	0.00000135
6	0.000001034	0.00000195	0.000000477
6	0.000000958	0.000002087	0.000000768
6	0.000000969	0.000001529	0.000000973
6	0.000000948	0.000000626	0.00000125
6	0.000001469	-0.000000738	0.000001766
6	-0.000000566	0.000007464	-0.000002951
1	0.000000764	0.000002326	0.000000532
1	0.000000965	0.000002355	0.000000699
1	0.000001105	0.000001652	0.000001036

1	0.000000985	0.00000077	0.000001146
1	0.000000944	0.000000443	0.000001213
1	0.00000167	-0.000001334	0.000001119
7	0.000001858	0.000003241	0.000000527
1	0.00000062	0.000000906	-0.000000109
Zero-point correction=			1.234888 (Hartree/Particle)
Thermal correction to Energy=			1.310503
Thermal correction to Enthalpy=			1.311447
Thermal correction to Gibbs Free Energy=			1.113363
Sum of electronic and zero-point Energies=			-3798.477961
Sum of electronic and thermal Energies=			-3798.402345
Sum of electronic and thermal Enthalpies=			-3798.401401
Sum of electronic and thermal Free Energies=			-3798.599485

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6	-0.000000325	0.000000621	-0.000000833
6	-0.000000261	0.000000476	0.000001833
7	0.000001685	-0.000000435	0.000000051
7	-0.000000132	0.000000657	0.000000179
16	0.000000144	-0.000000036	-0.000000732
8	0.000000617	0.000000312	-0.000000399
8	0.000001396	0.000000426	-0.000000261
6	0.000000963	0.000000255	-0.000001678
6	0.000000555	-0.000001315	-0.000001869
6	0.000000805	-0.000001554	-0.000001515
6	0.000001239	0.000000312	-0.0000005122
6	0.000000988	-0.000000075	-0.000001534
6	0.000002013	-0.000000103	-0.000000639
1	0.000000702	-0.000000036	-0.000001284
1	0.000000967	-0.000000077	-0.000001787
1	0.000001429	-0.000000128	-0.000000963
1	0.000001378	0.000000088	-0.000000966
6	0.000000372	-0.000000753	-0.000000774
1	0.000001172	-0.000001728	-0.000002237
1	0.00000038	0.000000067	-0.000001801
1	0.000002121	-0.0000001	-0.000002416
6	-0.000000388	-0.000000539	-0.000000541
6	-0.000000778	-0.000000521	-0.000000029
1	0.000000015	-0.000000524	-0.000000057
1	-0.000000037	-0.000001129	-0.000000069
6	-0.000000919	-0.000001182	-0.000000644
1	-0.000000557	-0.000000448	-0.000000105
1	-0.000000755	-0.000000629	-0.000000002
6	-0.000001442	-0.000001316	-0.000000423



1	-0.00000815	-0.000001216	-0.000000762
1	-0.00000823	-0.000001125	-0.000000867
1	-0.000001676	-0.00000152	-0.000000546
1	-0.000001469	-0.000001101	-0.000000156
1	-0.000001592	-0.000001115	-0.000000129
6	-0.000000337	0.000000397	0.000000905
6	-0.000000869	0.000000396	0.000001582
1	-0.000000535	0.000000095	0.000000483
1	-0.00000064	-0.000000014	0.000000962
6	-0.000001459	0.000000263	0.000001305
1	-0.000000777	0.000000474	0.000001748
1	-0.000000058	0.000000131	0.000001123
6	-0.000001692	0.000000165	0.000001876
1	-0.000001567	-0.000000065	0.00000012
1	-0.000001364	0.000000176	0.000001386
1	-0.000001988	0.000000038	0.000001998
1	-0.000001568	0.000000582	0.000002139
1	-0.000001803	0.000000361	0.00000202
16	0.000000075	0.000000867	0.000000594
8	0.000000046	0.00000012	0.000000222
8	-0.000000349	0.000000589	0.000001232
6	0.000000836	0.000000908	0.000001013
6	0.000002399	0.000000446	0.000001847
6	0.000000741	0.000000617	0.000001442
6	0.000001859	0.000000855	0.000000764
1	0.000001053	0.000001202	0.000000236
6	0.000001581	0.000001503	0.000002299
1	0.000000021	0.000001665	0.000001556
6	-0.000000888	0.000003749	0.000000748
1	0.000001317	0.000002233	0.000000552
1	0.000000474	0.000002717	0.000001879
6	0.000000323	0.000004316	0.000001304
1	0.000002568	0.000000993	0.000001534
1	0.000002351	0.000001619	0.000002056
1	0.000002932	0.00000124	0.000001572
79	-0.000000044	-0.000000486	-0.000000246
6	0.000000016	0.000001747	-0.000000612
6	-0.000000035	-0.000000173	-0.000000696
6	0.000000355	-0.000000289	-0.000000673
1	0.000000269	-0.000000366	-0.00000049
1	-0.00000031	-0.000001013	-0.000001117
7	-0.000000529	-0.000002163	-0.00000011
7	-0.000000122	-0.00000181	-0.000000794
6	-0.000000174	-0.000000735	-0.000000479

6	-0.000000919	-0.000000929	-0.000001196
6	-0.000000795	-0.000001573	-0.000000977
6	-0.000000615	-0.000001294	-0.000001727
6	-0.000001066	-0.000001443	-0.000000783
6	-0.000001253	-0.000001829	-0.000001415
1	-0.00000051	-0.000001569	-0.000001922
1	-0.000001594	-0.000001414	-0.000000472
1	-0.000001295	-0.000001856	-0.000001343
6	0.00000057	0.000000764	0.000000113
6	0.00000027	0.000000344	0.000000702
6	0.000000795	0.000000982	-0.000000102
6	0.000000494	0.000000904	0.000000702
6	0.000001005	0.000000604	0.000000383
6	0.000000954	0.000000875	0.000000465
1	0.000000255	0.000001013	0.000001058
1	0.000001433	0.000001074	0.000000169
1	0.000001166	0.000001349	0.000000854
6	-0.000000348	0.000000074	0.000000664
6	-0.00000045	0.000000288	0.000000567
6	-0.000000595	0.000000012	0.000001095
1	-0.000000515	0.000000022	0.000000013
1	-0.000000056	0.000000088	0.000000216
1	-0.000000688	-0.000000024	0.000000667
1	-0.000000118	0.000000489	0.000000847
1	-0.000000457	0.000000155	0.000001003
1	-0.000000401	0.000000629	0.000001282
1	-0.000001028	0.000000174	0.000000982
6	0.000001114	0.000000568	-0.000000037
6	0.000001478	0.000000636	-0.000000634
6	0.00000149	0.000000328	-0.000000683
1	0.00000103	0.000000061	-0.000000833
1	0.00000138	0.000000739	-0.000000113
1	0.000001835	0.000000453	-0.000001036
1	0.000001912	0.000000083	-0.000000547
1	0.00000106	0.000000031	-0.000000986
1	0.000001725	0.000000487	-0.000000775
1	0.000001555	0.000000198	-0.000001302
6	-0.000000595	-0.00000045	-0.000000212
6	-0.000001909	-0.000001072	0.00000001
6	-0.000001384	-0.000001097	-0.000000447
1	-0.000000932	-0.000000475	0.000000343
1	-0.000001628	-0.000000836	0.00000002
1	-0.000001534	-0.000000833	0.000000401
1	-0.000001894	-0.000001068	0.000000011

1	-0.00000111	-0.000000937	-0.000000467
1	-0.000001757	-0.00000136	-0.000000292
1	-0.000001554	-0.000000954	0.000000203
6	0.000000344	-0.000000923	-0.000001527
6	0.000000153	-0.000001184	-0.000001985
6	0.000000769	-0.000001156	-0.000002195
1	0.000000575	-0.000000411	-0.000001413
1	0.000000057	-0.000001514	-0.000001964
1	0.000000508	-0.000001276	-0.000002128
1	0.000000313	-0.000001691	-0.000002241
1	-0.000000168	-0.00000051	-0.000001875
1	0.000000371	-0.000001292	-0.000001932
1	0.000001235	-0.000001343	-0.000002341
6	-0.000000712	0.000000594	0.000001356
6	-0.000000314	0.000000442	0.000000901
6	-0.000001029	-0.000000048	0.000001166
6	-0.000001462	0.000000172	0.000001493
6	-0.000001109	0.000000532	0.000001845
6	-0.00000089	0.000000383	0.000001686
6	-0.000000544	0.000000639	0.000001712
6	0.000000331	0.000001642	0.000001201
1	-0.000001803	-0.000000092	0.000000274
1	-0.000001793	-0.000000197	0.000001321
1	-0.000001718	0.000000364	0.000002118
1	-0.000001068	0.000000963	0.000002285
1	-0.000000081	0.00000135	0.000001936
1	0.000000618	0.000001385	0.000001314
7	-0.000000017	0.000000252	0.000000351
1	0.000000196	0.000000602	0.000000779

Zero-point correction=

1.233127 (Hartree/Particle)

Thermal correction to Energy=

1.308678

Thermal correction to Enthalpy=

1.309622

Thermal correction to Gibbs Free Energy=

1.112747

Sum of electronic and zero-point Energies=

-3798.422401

Sum of electronic and thermal Energies=

-3798.346850

Sum of electronic and thermal Enthalpies=

-3798.345906

Sum of electronic and thermal Free Energies=

-3798.542781

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6	0.000001874	0.000010125	-0.000005885
6	0.000005481	-0.000010708	0.000002495
7	-0.000005966	-0.000014895	-0.000005116
7	-0.000002155	0.000011289	0.000002405
16	0.00000553	0.000011144	0.000003691

8	-0.000001601	-0.000003957	0.000001231
8	-0.000000841	0.000001251	-0.000004264
6	0.000003238	0.000000312	-0.00000315
6	0.000001657	0.000000094	-0.000001721
6	0.000000268	-0.000000483	-0.000001715
6	0.000000807	0.000001442	-0.000003482
6	0.000002733	-0.000000037	-0.000000345
6	-0.000000214	0.000000665	0.000000228
1	0.000001153	-0.00000075	-0.000001918
1	0.000001244	0.000000442	-0.000001881
1	0.000001049	0.000001345	-0.000000572
1	0.000000926	0.000000049	-0.000001044
6	0.000000914	0.000001795	-0.00000193
1	0.000001988	0.000001763	-0.000001459
1	0.00000116	0.000001743	-0.000001347
1	0.000001771	0.000001289	-0.000000805
6	0.000004609	-0.000000658	0.000001607
6	-0.000001163	-0.000001441	-0.000001936
1	-0.000000812	-0.000000161	-0.000000791
1	0.000000025	-0.000000536	0.000000195
6	0.000000562	-0.000001976	-0.000001158
1	0.000000044	-0.000001443	-0.000000266
1	-0.000000546	-0.000001009	0.000000713
6	-0.000000498	-0.000002015	-0.000000285
1	-0.000000706	-0.000001073	-0.000000111
1	-0.000000084	-0.000001277	-0.000000712
1	-0.000000612	-0.000002002	-0.000000191
1	-0.00000055	-0.000002151	-0.000000325
1	-0.000000915	-0.00000169	0.000000031
6	0.000000291	-0.00000545	-0.00000167
6	0.000000091	-0.000002957	-0.00000106
1	0.000000917	-0.000002271	0.000000671
1	-0.000001101	-0.000002013	-0.000000059
6	-0.000000698	-0.000002146	-0.000000158
1	-0.000000069	-0.000001661	-0.000000529
1	-0.000000357	-0.000000437	-0.000001184
6	-0.000000942	-0.000003057	-0.000000946
1	-0.000000707	-0.000002576	-0.000000327
1	-0.00000057	-0.000002782	-0.000000631
1	-0.000000831	-0.000003358	-0.000000411
1	-0.000000833	-0.000003164	-0.000000604
1	-0.000001265	-0.000002681	0.000000113
16	-0.000006552	-0.000009446	-0.000004412
8	0.00000004	-0.000000896	-0.000000812

8	0.00000221	-0.000002662	-0.000002025
6	0.000000771	0.000001491	0.000000131
6	0.000001312	-0.000001849	-0.000001676
6	0.000000958	-0.00000174	-0.000001225
6	0.000000902	0.000000354	-0.000001216
1	0.000000992	0.000000317	-0.000001364
6	-0.000000419	-0.000000124	-0.000001541
1	-0.000000045	-0.000001085	-0.000001135
6	0.000001	-0.000000193	-0.000001286
1	0.000001207	0.000000063	-0.000001596
1	0.000000531	-0.000000651	-0.000001081
6	0.000001274	0.000001126	-0.000001041
1	0.000000834	0.000000639	-0.000001301
1	0.000000817	0.000000407	-0.000001051
1	0.000000919	0.000000396	-0.000001403
79	-0.000002716	-0.000001069	0.000000388
6	0.000001415	0.000001006	-0.000004147
6	0.000000362	-0.00000175	-0.000000955
6	-0.000000173	0.000005362	0.000002491
1	-0.000000762	0.000002144	0.0000013
1	-0.000000805	0.000001142	0.000001786
7	-0.000000795	0.000003246	0.000004081
7	-0.000001369	-0.000001901	0.000003653
6	-0.000000944	-0.000000312	0.000000262
6	0.000000408	0.000001395	0.000000206
6	0.000000163	0.000000469	0.000001413
6	-0.000000703	0.000000396	0.000000563
6	-0.000001082	0.000000186	0.000000898
6	-0.000000028	-0.000000475	0.000000484
1	0.000000151	0.000000552	0.000000151
1	-0.000001795	-0.000000036	0.000001542
1	-0.000000718	-0.000000053	0.000000701
6	-0.000001525	0.000001548	0.000000286
6	-0.000002789	-0.000000051	0.000004558
6	0.000001058	0.00000141	0.000002871
6	0.000001443	0.000001034	-0.000000286
6	0.000000174	0.00000214	-0.000001503
6	-0.000000037	0.000001688	0.000001216
1	0.000000256	0.000001383	0.00000105
1	0.000000635	0.000001961	-0.000000017
1	0.000000246	0.00000185	0.000000693
6	0.000002217	0.000001518	-0.000001807
6	-0.000002173	-0.000000298	0.00000349
6	-0.000002079	0.000000607	0.000002439

1	0.00000054	0.000000329	0.000001372
1	-0.000000045	0.000001286	0.000001968
1	-0.000001043	0.00000122	0.000002376
1	-0.000000364	0.000001909	0.000002179
1	-0.000000655	0.000000212	0.000001917
1	-0.00000064	-0.000000013	0.00000149
1	-0.000001434	-0.000000082	0.000002127
6	0.000000766	0.000001069	-0.000000194
6	0.000000593	0.000002003	-0.000000365
6	-0.000000028	0.000002485	0.000000333
1	0.000000217	0.000002023	-0.000000477
1	0.000000944	0.000001402	-0.000000904
1	0.000001047	0.000001983	-0.000000902
1	0.000001127	0.000002062	-0.000000262
1	0.000000507	0.000002891	0.000001109
1	0.00000095	0.00000281	0.000000499
1	0.000000982	0.000002326	0.000000194
6	-0.00000345	-0.000001292	0.000001543
6	0.000000185	-0.000001497	0.000000368
6	-0.000000026	0.000000586	0.000002532
1	-0.000000831	0.000001077	0.000000616
1	-0.00000041	-0.000000878	0.000000263
1	-0.000001349	-0.000000703	0.000001604
1	-0.000000748	-0.00000174	0.000002234
1	-0.000001317	-0.000000041	0.000001973
1	-0.000001248	-0.000000066	0.000001788
1	-0.000001413	-0.000000024	0.000002373
6	0.000001431	0.000001036	0.000000103
6	-0.000000701	0.000000986	-0.000000058
6	-0.000001308	0.000000732	0.000000804
1	0.000000932	0.00000109	0.000000473
1	0.000000472	0.00000143	0.00000104
1	0.000000657	0.000001842	0.000000662
1	0.000000256	0.00000124	0.000000577
1	0.000001391	0.000001119	-0.000000428
1	0.000000507	0.000000679	-0.000000661
1	0.000001201	0.000001009	-0.000001047
6	-0.000000079	-0.000001417	0.000001152
6	-0.000000248	-0.000002491	-0.000003424
6	0.000000166	-0.00000102	0.000000338
6	-0.000000706	-0.000000773	0.00000135
6	-0.000001394	-0.000001459	0.00000069
6	-0.00000069	-0.000001712	0.000001198
6	0.000002803	0.000000637	-0.000000884

6	-0.000000844	-0.000001098	-0.00000101
1	-0.000000617	-0.000000555	0.00000077
1	-0.000001413	-0.000001514	0.00000125
1	-0.000001162	-0.000001419	0.000001309
1	-0.000000882	-0.000001137	0.000000881
1	-0.000000426	-0.000000977	0.000000601
1	0.000000633	0.000000227	-0.00000046
7	-0.000004225	0.000008152	0.000001751
1	0.000001911	0.000001463	-0.000001896

Zero-point correction=	1.235113 (Hartree/Particle)
Thermal correction to Energy=	1.310547
Thermal correction to Enthalpy=	1.311491
Thermal correction to Gibbs Free Energy=	1.114432
Sum of electronic and zero-point Energies=	-3798.427545
Sum of electronic and thermal Energies=	-3798.352112
Sum of electronic and thermal Enthalpies=	-3798.351167
Sum of electronic and thermal Free Energies=	-3798.548226

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6	-0.000000239	0.000000523	0.000000135
6	0.000000362	0.000001446	-0.000002279
7	0.000000231	-0.000000109	0.000000025
7	-0.000001282	-0.000001041	0.000002668
16	0.000001403	0.000000536	0.000000841
8	0.000000599	-0.000000157	-0.000000199
8	-0.000000098	-0.000000334	-0.000001277
6	0.000000697	-0.000000179	0.000000173
6	0.000000568	-0.000000057	-0.00000046
6	0.000000739	-0.000000223	0.00000002
6	0.00000113	-0.00000077	0.00000094
6	0.00000043	-0.000000285	-0.000000063
6	0.000000126	0.000000238	0.000000175
1	0.000000901	-0.000000332	0.000000252
1	0.000000995	-0.000000678	0.000000545
1	0.000000645	-0.00000066	0.000000421
1	0.000000486	-0.000000322	0.000000315
6	0.000001331	-0.000001102	0.000000848
1	0.000000429	-0.000000301	0.000000254
1	0.000000322	-0.000000552	0.000000196
1	0.000000807	-0.00000033	-0.000000139
6	0.000000274	-0.000000058	0.000000157
6	0.000000168	-0.000000166	0.000000054
1	0.000000393	-0.000000214	0.000000129
1	0.000000774	-0.000000054	0.000000429

6	0.00000039	-0.00000019	0.000000158
1	0.000000484	0.000000182	0.000000036
1	0.000000075	0.000000023	-0.000000166
6	0.000000177	-0.000000054	0.000000095
1	0.000000149	-0.000000267	0.000000096
1	0.000000464	-0.000000021	0.000000126
1	0.000000203	-0.000000125	0.000000067
1	0.000000352	0.000000074	-0.000000018
1	0.000000098	0.000000093	-0.000000044
6	0.000000063	0.000001038	-0.000000451
6	0.000000823	0.000002725	-0.000000906
1	-0.000000795	0.000000137	-0.000000165
1	0.000000168	0.000000922	-0.000000124
6	-0.000000004	-0.000000083	0.000000265
1	0.000001735	-0.000000482	-0.000000653
1	-0.000000201	0.000000169	-0.000000156
6	-0.000000251	0.000000843	-0.000000426
1	0.000000172	0.000000567	0.000000091
1	-0.000000213	0.000000318	-0.000000185
1	-0.000000062	0.000000557	-0.000000255
1	-0.000000189	0.000000596	-0.000000346
1	-0.000000099	0.000000755	-0.000000455
16	0.000000704	-0.000000276	-0.000001859
8	-0.000000768	0.000000869	-0.000000421
8	-0.000000866	-0.000000106	-0.000000977
6	0.000000591	-0.00000171	0.000000491
6	-0.000000783	0.000000594	-0.000000007
6	-0.000000414	0.000001415	-0.000000103
6	0.000000141	0.000001157	-0.000000522
1	-0.000000118	0.000000449	-0.000000179
6	-0.000001144	0.00000103	-0.000000369
1	-0.000002016	0.000000837	0.000000528
6	-0.000000191	-0.000000034	-0.000000636
1	-0.000000139	0.000000848	-0.000000292
1	-0.000000554	0.000000836	-0.000000361
6	0.000000287	0.000001544	0.000000066
1	-0.000000507	0.000000966	-0.000000794
1	0.000000245	0.000001168	-0.000000999
1	-0.000001119	0.000000772	-0.000000571
79	-0.000000106	-0.000000471	0.000000058
6	-0.000000373	-0.000000502	0.000000552
6	-0.000000358	-0.000000465	0.000000341
6	-0.000000514	-0.000000497	0.000000296
1	-0.000000479	-0.000000532	0.000000207



1	-0.000000367	-0.000000662	0.000000267
7	-0.000000145	-0.000000169	-0.000000212
7	0.000000006	-0.000000176	-0.000000331
6	0.000000018	-0.000000934	0.000000535
6	0.000000016	-0.000000271	0.000000387
6	-0.000000595	-0.000000241	0.000000148
6	0.000000134	-0.000000606	0.000000367
6	-0.000000498	-0.000000408	-0.000000016
6	-0.000000015	-0.000000522	0.000000352
1	0.000000177	-0.000000071	0.000000277
1	-0.000000213	-0.000000389	0.000000144
1	0.000000065	-0.000000603	0.000000299
6	-0.000000487	-0.000000418	0.000000034
6	-0.000000495	-0.000000214	0.000000086
6	-0.000000092	-0.000000219	0.000000012
6	-0.000000551	0.000000039	-0.000000006
6	-0.000000431	0.000000106	-0.000000005
6	-0.000000412	-0.000000022	-0.000000037
1	-0.000000753	0.000000106	-0.000000141
1	-0.000000264	-0.000000019	-0.000000001
1	-0.000000435	0.000000075	-0.000000098
6	-0.000000789	-0.000000098	0.000000107
6	-0.000000809	-0.000000204	0.000000105
6	-0.000000702	0.000000056	-0.000000068
1	-0.000000609	-0.000000148	0.000000083
1	-0.000000718	-0.000000392	0.000000121
1	-0.000000923	-0.000000245	0.000000055
1	-0.000000891	-0.000000155	0.000000018
1	-0.000000488	-0.000000012	-0.000000012
1	-0.000000837	0.000000136	-0.000000137
1	-0.000000784	-0.000000086	-0.000000038
6	0.000000073	-0.000000487	0.000000078
6	0.000000194	-0.000000205	0.000000149
6	-0.000000045	-0.000000387	0.000000325
1	-0.000000004	-0.000000048	0.000000015
1	0.000000257	0.000000124	-0.000000162
1	0.000000278	-0.000000034	0.00000001
1	0.000000163	-0.000000205	0.000000052
1	-0.000000277	-0.000000469	0.000000026
1	-0.000000158	-0.000000343	0.000000173
1	0.000000031	-0.000000504	0.000000028
6	-0.000000067	-0.000000278	-0.000000013
6	-0.000000305	-0.000000306	0.000000064
6	-0.000000451	-0.000000412	0.000000086

1	-0.000000589	-0.000000408	0.000000187
1	-0.000000009	0.000000046	0.000000086
1	-0.000000529	-0.000000041	-0.000000048
1	-0.000000368	-0.000000237	0.000000151
1	-0.000000622	-0.000000061	0.000000268
1	-0.000000048	-0.000000445	0.000000164
1	-0.000000707	-0.000000291	0.000000014
6	0.000000057	-0.000000073	0.000000484
6	-0.000000003	-0.000000859	0.000000046
6	0.000000386	-0.000000652	0.000000224
1	-0.000000003	-0.000000671	0.000000417
1	-0.000000038	-0.000000896	0.000000392
1	0.000000177	-0.000000854	0.000000466
1	0.000000152	-0.000000911	0.000000529
1	0.000000228	-0.000000489	0.000000121
1	0.000000348	-0.000000065	0.000000469
1	0.000000474	-0.000000696	0.000000541
6	0.000000311	0.000000742	-0.000000044
6	0.000000294	0.000000045	0.000000183
6	0.000000309	0.000000754	-0.000000163
6	0.000000333	0.000000667	-0.000000564
6	0.000000164	0.000001079	-0.000000263
6	0.000000078	0.000000826	-0.000000312
6	0.000000607	0.000000655	-0.000000803
6	-0.000000168	0.000000977	-0.000000026
1	0.000000684	0.000000427	-0.000000439
1	0.000000479	0.000000077	-0.000000455
1	0.000000368	0.000001028	-0.000000514
1	0.000000393	0.000000859	-0.000000587
1	0.000000293	0.000000817	-0.000000445
1	0.000000496	0.000000358	-0.000000178
7	0.000000819	-0.000001038	-0.000000348
1	0.000001213	0.000001834	0.000001003

Zero-point correction=

1.233259 (Hartree/Particle)

Thermal correction to Energy=

1.309047

Thermal correction to Enthalpy=

1.309992

Thermal correction to Gibbs Free Energy=

1.111127

Sum of electronic and zero-point Energies=

-3798.449145

Sum of electronic and thermal Energies=

-3798.373356

Sum of electronic and thermal Enthalpies=

-3798.372412

Sum of electronic and thermal Free Energies=

-3798.571277

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6	-0.000002306	-0.000000595	0.000000606
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6	-0.000001072	0.000006899	-0.000000789
7	0.000002486	0.000001741	-0.000001859
7	-0.000000388	-0.000004697	-0.000001073
16	-0.000001886	-0.000000985	0.000000017
8	-0.00000124	-0.000000268	-0.000002029
8	0.000000296	0.000000688	-0.000002925
6	0.00000169	0.000000772	-0.000003984
6	-0.000002864	0.00000093	-0.000002521
6	0.000000379	0.00000222	-0.000004029
6	-0.000000033	0.000003124	-0.000000154
6	-0.000000273	0.000001911	-0.000002433
6	0.000000629	0.000002263	-0.000000094
1	-0.000000366	0.000000034	-0.000002432
1	-0.000000814	0.000000468	-0.000002777
1	0.000000361	0.000001292	-0.000001098
1	0.000000384	0.000000311	-0.000002891
6	-0.000000125	-0.000000834	-0.000003392
1	0.000001186	0.000003145	-0.000000302
1	-0.000000707	0.000003357	-0.000002531
1	-0.000001376	0.00000265	-0.000003734
6	-0.000001806	-0.000001163	-0.000000126
6	-0.00000088	-0.000001864	-0.000001032
1	-0.000000992	0.00000004	-0.000001421
1	-0.000000563	-0.000000063	-0.000001061
6	-0.000000885	-0.000001343	-0.000001494
1	-0.00000106	-0.000000942	-0.000001552
1	-0.000000838	-0.000000915	-0.000000844
6	-0.000001102	-0.000002157	-0.000001251
1	-0.000000813	-0.000001433	-0.000001161
1	-0.000001261	-0.000001394	-0.000001749
1	-0.00000146	-0.000002248	-0.000001392
1	-0.000001453	-0.000002207	-0.000001583
1	-0.000001249	-0.000002136	-0.000000832
6	0.000000033	0.000000057	0.000000845
6	0.000001368	-0.000000104	0.000001411
1	0.00000063	-0.000000193	0.000000928
1	-0.00000005	0.000000821	-0.000000267
6	0.000000491	0.000000692	0.000000795
1	0.000000149	-0.000000108	0.0000014
1	-0.00000006	0.000000076	0.000000592
6	0.000000754	0.000000694	0.000001446
1	0.00000076	0.00000105	0.000000793
1	0.000000714	0.000000735	0.000001289
1	0.000001028	0.000001057	0.000001639

1	0.000000831	0.00000035	0.000001813
1	0.000000708	0.000000633	0.0000013
16	0.000001537	0.000001158	0.000003327
8	-0.000001859	-0.000001368	-0.000001469
8	-0.000001936	-0.00000126	0.000001134
6	-0.000000334	-0.000000882	-0.000000059
6	0.000000968	-0.000001661	0.000000121
6	-0.000000465	-0.000002297	0.000000219
6	-0.000001235	-0.000002392	0.000001288
1	-0.000000661	-0.000001604	0.000000684
6	0.000001668	-0.000001742	0.000003253
1	0.000000694	-0.000001013	0.000002183
6	-0.000002378	-0.000001945	0.000004037
1	-0.000000182	-0.000001667	0.000000969
1	0.000000146	-0.000001338	0.000002051
6	0.000002495	-0.000001682	-0.000000754
1	-0.000001291	-0.000002258	0.000002219
1	0.00000062	-0.000001297	0.000002931
1	-0.000000008	-0.000002294	0.000002933
79	-0.000001215	-0.000000339	0.00000078
6	0.000001927	0.00000187	-0.000002478
6	-0.000001516	-0.000000535	-0.000000026
6	0.000002001	0.000001475	0.000001823
1	0.000000925	0.000000762	0.000001355
1	-0.000000199	-0.00000021	-0.000000047
7	0.000001355	-0.000001343	0.000001172
7	-0.000001455	0.000000298	0.000000717
6	-0.000001853	0.000001094	0.00000076
6	0.000000456	0.000000407	-0.000000908
6	0.000000159	-0.000001146	0.000000136
6	-0.000000485	-0.000000578	-0.000000665
6	-0.000000649	-0.000001102	-0.000000392
6	-0.00000115	-0.000000706	-0.000000957
1	-0.000000746	-0.000000322	-0.000001582
1	-0.000001154	-0.000001688	-0.00000068
1	-0.000000913	-0.000001262	-0.000001302
6	0.000000532	-0.000000433	0.000000179
6	0.000001156	0.000001423	0.000001538
6	-0.000000109	0.000002331	0.000000939
6	0.000001284	0.00000075	0.000001849
6	0.000001481	0.000001655	0.000001102
6	0.000000894	0.000000941	0.000001232
1	0.000001339	0.000000661	0.000002081
1	0.000000919	0.000001752	0.00000088

1	0.000001263	0.000001699	0.00000181
6	0.000000235	-0.000000556	0.000001869
6	0.000001141	0.000000931	0.000002225
6	0.000000734	0.000000359	0.00000162
1	0.000000875	-0.000000244	0.000001612
1	0.000001462	0.000000637	0.000002363
1	0.000000761	-0.000000156	0.000002436
1	0.000001266	0.00000032	0.000002472
1	0.00000015	-0.000000595	0.000001837
1	0.000000658	-0.000000085	0.000002447
1	0.000000542	-0.000000903	0.00000227
6	0.000000746	0.000001773	0.000000352
6	0.000000693	0.000001676	-0.000000491
6	0.000000989	0.000002166	0.000000242
1	0.000000553	0.000001353	0.000000344
1	0.000000348	0.000001098	-0.000000379
1	0.000000753	0.000002314	-0.000000333
1	0.00000092	0.000002369	-0.000000144
1	0.000000985	0.000002031	0.000000487
1	0.000001126	0.000002437	0.000000387
1	0.000000931	0.000002373	-0.000000164
6	-0.000000663	-0.000001285	0.00000067
6	-0.000000068	-0.000001004	0.000000505
6	0.000000045	-0.000001149	0.000000949
1	0.00000021	-0.000000911	0.000000659
1	-0.000000219	-0.000001448	0.000000037
1	-0.000000263	-0.000001646	0.000001084
1	-0.000000073	-0.000001407	0.000000204
1	-0.000000074	-0.000000884	0.000000949
1	-0.000000451	-0.000001893	0.000000535
1	-0.000000109	-0.000001377	0.000001207
6	0.000000253	-0.000000102	-0.000001332
6	-0.000000159	0.000001171	-0.000000827
6	-0.00000025	0.000001177	-0.000001639
1	0.000000615	0.000000915	-0.000000608
1	-0.000000108	0.000000755	-0.000000621
1	0.000000058	0.000001345	-0.000001333
1	-0.000000125	0.000000473	-0.000001026
1	0.00000019	0.000000491	-0.000001902
1	-0.000000478	0.000000412	-0.000001767
1	-0.000000094	0.000001505	-0.000001496
6	-0.000000235	-0.00000113	-0.000000946
6	-0.00000154	0.000000038	-0.000000244
6	0.000000219	0.000000883	-0.000000125

6	-0.00000003	0.000000312	-0.000000309
6	-0.000000222	0.000000066	-0.000000486
6	-0.00000005	-0.000000547	-0.000000437
6	0.000000095	-0.000000802	-0.000000195
6	-0.000002177	-0.00000046	-0.000002614
1	0.000000027	0.000000606	-0.000000593
1	0.000000165	0.000000791	-0.000000258
1	-0.000000202	0.000000104	-0.000000218
1	-0.000000589	-0.000000947	-0.000000371
1	-0.000000096	-0.000001753	-0.000000668
1	-0.000000597	-0.000001414	-0.000000463
7	0.00000545	-0.000002726	0.0000016
1	-0.000001986	-0.000001726	-0.000001816

Zero-point correction=	1.235089 (Hartree/Particle)
Thermal correction to Energy=	1.310680
Thermal correction to Enthalpy=	1.311624
Thermal correction to Gibbs Free Energy=	1.113201
Sum of electronic and zero-point Energies=	-3798.460625
Sum of electronic and thermal Energies=	-3798.385033
Sum of electronic and thermal Enthalpies=	-3798.384089
Sum of electronic and thermal Free Energies=	-3798.582512

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6	-0.00000329	-0.000004829	0.000000108
6	-0.000000754	-0.000001428	-0.00000171
7	0.000003491	0.000002968	0.000001409
7	0.000000144	-0.00000027	-0.000001358
16	0.000000394	-0.000001663	-0.000000333
8	0.00000011	-0.000001977	0.000000863
8	-0.000000251	-0.000002105	-0.000000404
6	0.000000389	-0.000001673	0.000000362
6	-0.000000015	-0.000001387	0.000000567
6	-0.000000079	-0.000001692	0.000001057
6	0.000000976	0.000001359	0.000002264
6	0.000000817	-0.000000993	-0.000000605
6	0.000000005	-0.00000139	-0.000000414
1	0.000000286	-0.000001869	0.000001142
1	0.000000446	-0.000001952	0.000001362
1	-0.000000232	-0.000001357	-0.000000547
1	-0.000000075	-0.000001379	-0.000000813
6	-0.000000548	-0.000003735	-0.000000407
1	0.000003049	-0.000001149	-0.000001206
1	-0.000000536	-0.000002652	0.000000412
1	-0.000002663	-0.000002153	0.000001581

6	0.000000597	-0.000001055	0.000000444
6	0.000000282	-0.000000361	0.000001292
1	0.000000423	-0.000000899	0.000001147
1	0.000000346	-0.000001533	0.000001115
6	0.000000756	-0.000000747	0.000001796
1	0.000000236	0.000000184	0.000000914
1	0.000000312	-0.000000845	0.000001107
6	0.000000694	-0.000000302	0.000002165
1	0.000000669	-0.000001214	0.000001978
1	0.000000691	-0.000000349	0.000002047
1	0.000000861	-0.000000344	0.000002706
1	0.000000626	0.000000176	0.000002098
1	0.000000708	-0.000000386	0.000002128
6	-0.000000021	0.000000162	-0.000000244
6	0.000000004	0.000000394	-0.000000319
1	0.000000027	0.000000539	-0.000000712
1	0.000000409	0.000000303	-0.000000015
6	-0.000000057	0.000000489	0.000000037
1	-0.000000148	-0.000000026	-0.000000388
1	0.000000061	-0.000000429	0.000000267
6	0.000000249	0.000000048	0.000000065
1	0.000000299	0.000000782	0.000000636
1	-0.000000012	0.000001074	0.000000008
1	0.000000275	0.000000962	0.000000924
1	0.000000137	0.000000489	0.000000244
1	0.000000349	0.000000118	0.000001002
16	-0.000000478	-0.000000692	-0.000000491
8	-0.000000402	0.000000194	-0.000001893
8	-0.000000761	-0.000000922	-0.000001989
6	-0.000000697	-0.000000243	-0.000001986
6	-0.000000749	0.000000469	-0.000002336
6	-0.000000683	-0.000000299	-0.000002396
6	-0.000000831	0.000000058	-0.000002986
1	-0.000000662	0.000001042	-0.000002135
6	-0.000001072	0.000000015	-0.000002959
1	-0.000000842	-0.000001007	-0.000002559
6	-0.000001121	0.000000486	-0.000002868
1	-0.000000962	0.000001357	-0.000002966
1	-0.00000114	-0.000000525	-0.000003301
6	-0.000001435	0.000000792	-0.000003776
1	-0.000001182	0.000000596	-0.000004345
1	-0.000001284	0.00000109	-0.000003607
1	-0.000001005	0.000000349	-0.00000378
79	-0.000000195	-0.000000294	0.000000346

6	0.000000161	0.000000308	0.000000777
6	0.000000155	0.000001286	0.000000158
6	0.000000435	0.00000153	0.000000364
1	0.000000615	0.000001663	0.000000658
1	-0.000000011	0.000001508	0.000000001
7	-0.000000022	0.000001	-0.000000004
7	-0.00000001	0.000001503	0.000000983
6	0.000000127	0.000000554	-0.000000452
6	-0.000000072	0.000000136	-0.000000243
6	-0.000000434	0.00000039	-0.000001332
6	-0.000000122	-0.000000307	-0.000000674
6	-0.000000622	0.000000088	-0.000001502
6	-0.000000467	-0.00000014	-0.000001257
1	-0.000000176	-0.000000484	-0.000000626
1	-0.000000069	0.000000196	-0.000002062
1	-0.000000554	-0.000000415	-0.000001668
6	0.000000322	0.0000011	0.000000619
6	0.000000357	0.000001352	0.000001107
6	0.000000444	0.00000082	0.000001384
6	0.000000142	0.000001884	0.000000912
6	0.000000862	0.000000782	0.000002167
6	0.000000682	0.000001127	0.000001841
1	0.00000009	0.000001889	0.000000973
1	0.000000837	0.000000536	0.000002649
1	0.000000079	0.000001415	0.000002216
6	0.000000294	0.000001145	0.000000463
6	0.000000278	0.000002625	0.000000551
6	0.000000489	0.000002512	-0.000000068
1	-0.000000491	0.000002215	-0.000000621
1	-0.000000223	0.000003081	0.000000807
1	0.000000043	0.000002871	0.000000054
1	0.000000768	0.00000346	0.000000829
1	-0.000000829	0.000001165	0.000000017
1	0.000000083	0.000001805	0.000000619
1	-0.000000305	0.000002156	-0.000000754
6	0.000000697	0.000000621	0.000001815
6	0.000000609	-0.000000019	0.000002027
6	0.000000687	0.000000816	0.000002158
1	0.000000474	0.000000371	0.000001545
1	0.000000236	-0.000000875	0.00000139
1	0.000000709	-0.000000455	0.000002166
1	0.000000711	-0.000000107	0.000002432
1	0.000000668	0.000001392	0.000002063
1	0.000000858	0.000000945	0.000002731



1	0.00000074	0.000000609	0.000002384
6	-0.00000022	0.000000828	-0.000001148
6	-0.000000485	0.000000393	-0.000001727
6	-0.00000056	0.00000147	-0.00000155
1	-0.000000211	0.000000949	-0.000000977
1	-0.000000581	0.00000001	-0.000001709
1	-0.000000622	0.000000715	-0.000001829
1	-0.000000652	0.000000394	-0.000002162
1	-0.000000491	0.000001788	-0.000001328
1	-0.000000596	0.000001385	-0.000001918
1	-0.00000058	0.000001788	-0.000001811
6	-0.00000004	0.000000083	0.000000369
6	0.000000138	0.000000396	0.000000457
6	0.000000185	-0.000000589	0.000000554
1	0.000000203	0.000000271	0.000000581
1	0.000000147	0.000000944	0.000000329
1	0.000000315	0.000000465	0.000000096
1	0.000000092	0.000000234	0.000000205
1	0.000000096	-0.000000521	0.000000769
1	0.000000097	-0.000000909	0.000000401
1	0.000000378	-0.000000567	0.000001096
8	-0.000000297	-0.000000434	-0.000000097
6	0.000000114	-0.00000193	0.000000486
6	0.000000233	-0.000002587	0.000000716
6	0.000000138	-0.000002073	0.000000667
6	0.000000032	-0.000001915	-0.000000184
6	-0.00000008	-0.00000214	-0.000000033
1	0.00000023	-0.000002552	0.000000739
1	0.000000465	-0.000002254	0.000000554
7	-0.000001339	-0.000000061	0.000000173
8	0.000000145	-0.000002936	-0.000001665
1	-0.000000074	-0.000001914	-0.000000185
1	0.000000035	-0.000002739	0.000001072
17	-0.000000554	-0.000001267	-0.000001195
<b>Zero-point correction=</b>			<b>1.191755 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>1.267875</b>
<b>Thermal correction to Enthalpy=</b>			<b>1.268820</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>1.072668</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-4292.957142</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-4292.881022</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-4292.880078</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-4293.076229</b>

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6	-0.000002109	-0.000009532	0.000006456
6	0.000019873	0.000007581	-0.000011766
7	-0.000009526	0.00001292	0.00000448
7	-0.00000205	-0.000004142	0.000004852
16	0.00000196	-0.000007123	-0.000007531
8	0.000001826	0.00000045	0.000001457
8	0.000003178	0.000007788	0.000003157
6	-0.00000147	0.000004151	0.00000024
6	-0.000000443	-0.000001643	0.000002616
6	-0.000002511	0.000002083	-0.000001503
6	0.00000082	-0.000004293	0.000003491
6	0.00000148	0.000002048	0.00000309
6	-0.000000997	-0.000000213	-0.000000059
1	0.000001151	0.000001987	0.000001472
1	-0.000000197	0.00000102	0.000002098
1	-0.000000334	0.000000168	0.000000662
1	-0.000000221	0.000000369	0.000002447
6	0.000000624	0.000000231	0.000001585
1	-0.000000226	0.000000324	0.000001034
1	-0.000000033	0.000001884	0.000001368
1	-0.000000359	0.000000573	0.00000255
6	0.000010504	-0.00000785	0.000004197
6	0.000002212	0.00000988	-0.000001516
1	-0.000003063	0.000001432	-0.000001567
1	0.000000697	0.000001547	0.000000491
6	-0.00000132	-0.00000525	0.000002535
1	-0.000001073	-0.000000803	0.000002536
1	-0.000001321	0.000000302	0.000000264
6	0.000001083	0.000001045	0.000001162
1	0.000000004	0.00000135	0.000000858
1	0.000000092	0.000001644	0.000000074
1	-0.000000951	0.000000416	0.000002988
1	0.000000145	0.000000131	0.000000713
1	-0.000000977	-0.000000563	0.000001734
6	-0.000002373	0.000001048	0.000006189
6	0.000002182	-0.000004414	-0.000000478
1	-0.000001326	0.000001487	0.000001838
1	-0.000001141	-0.00000193	-0.000001314
6	-0.00000486	-0.000000235	-0.000000247
1	0.000000437	0.000001754	-0.000000324
1	0.000000244	-0.00000046	0.000001199
6	0.000000099	0.000000405	0.000000777
1	-0.00000018	-0.000000943	0.000000222
1	-0.000000894	-0.00000116	0.000001483

1	-0.000001158	-0.000000399	0.000000614
1	-0.000001074	-0.000000644	0.000001202
1	-0.000000269	-0.000000362	0.000000853
16	0.000005639	-0.000000661	-0.000010327
8	0.000001136	-0.000000931	0.000001268
8	0.000000463	0.000003047	0.000004362
6	-0.000000969	0.000002779	0.000002327
6	-0.000001046	0.000001909	-0.000002093
6	-0.000001567	0.000000871	-0.000002523
6	-0.000002276	-0.000000664	-0.000001237
1	0.000000171	-0.000001208	-0.000000068
6	0.000000775	-0.000001011	-0.000001638
1	0.000001384	0.000000391	0.000000256
6	0.000001027	-0.000000496	0.000000394
1	0.000000001	-0.000001065	-0.000001265
1	0.000000933	-0.000000032	-0.000001278
6	0.000000301	-0.000000035	-0.000000527
1	0.000000131	-0.000000236	-0.000003671
1	0.000001151	-0.000000944	-0.000001539
1	-0.000001025	0.000000056	-0.000001698
79	-0.000001718	0.000000467	-0.000008934
6	0.000007241	-0.000004374	0.000001183
6	-0.000002997	0.000002997	-0.000001705
6	0.000002056	-0.000005931	0.000000994
1	-0.00000119	-0.000000024	-0.000000529
1	-0.000001394	-0.000000078	-0.00000139
7	0.000002574	-0.000002672	-0.000002078
7	-0.000004497	0.000006726	0.000000562
6	-0.000001604	-0.000000053	-0.000005079
6	0.000002989	0.000000564	0.000001828
6	-0.000001471	0.000004434	0.000001776
6	-0.000000406	0.000000566	0.000000234
6	0.000001247	-0.000000891	-0.000002722
6	0.000000439	-0.000001315	-0.00000188
1	0.00000103	0.000000336	-0.000001634
1	0.000000037	-0.000000466	-0.00000133
1	0.000001093	0.000000216	-0.000001792
6	-0.000002287	0.000001701	-0.000002753
6	0.000001771	-0.000000445	0.000002573
6	-0.000001129	-0.000003869	0.000002402
6	-0.000000483	-0.000001918	-0.000000023
6	0.000000016	-0.000000026	0.000000982
6	-0.000001025	-0.000000236	0.000000653
1	-0.000000568	-0.000000779	0.000000832

1	-0.000000854	-0.000000183	0.000000263
1	-0.000001542	-0.000000895	0.000001627
6	-0.000000389	-0.000000741	-0.000002551
6	-0.000001768	-0.000001203	0.000001977
6	-0.000000615	0.000000158	-0.000000278
1	-0.000000405	-0.000000778	-0.000000012
1	-0.000000085	-0.000001503	-0.000000344
1	-0.000001091	-0.00000108	-0.000000698
1	-0.000000206	-0.000001036	-0.000000441
1	0.000001009	-0.000000826	-0.000000047
1	-0.000000717	-0.000000097	0.000001139
1	-0.000000969	-0.000001109	0.000000064
6	0.000000456	0.000000598	0.00000128
6	0.000000273	-0.000000448	0.000000513
6	-0.000000714	0.000000053	-0.000000508
1	-0.000001299	-0.000001312	0.000000489
1	0.000000323	0.000000127	-0.000000029
1	0.000000109	0.000000017	0.000000418
1	0.000000296	-0.000000114	0.000001643
1	-0.000000042	-0.000001127	0.000000023
1	-0.000000802	-0.000000184	0.000000493
1	0.000000031	-0.000000253	0.000000265
6	-0.000000841	-0.000001885	-0.000002231
6	0.000002385	0.000000079	0.000000992
6	0.000001091	-0.000000656	-0.000002763
1	-0.000000189	-0.000000202	-0.000000529
1	-0.000000664	-0.000000218	-0.000001224
1	-0.000000002	-0.000000571	-0.000001633
1	-0.000000277	0.000000225	-0.000002179
1	-0.000000266	-0.000000448	-0.000001444
1	-0.000000321	-0.000000627	-0.000000083
1	-0.000000024	-0.000001002	-0.000001433
6	-0.000000201	-0.000000693	-0.000002038
6	0.000000078	-0.000000409	0.000001123
6	0.000001618	0.000000784	-0.000002377
1	0.000000252	-0.00000002	0.000000723
1	0.000000103	-0.000000937	-0.000000417
1	0.000000394	-0.000000181	-0.000000937
1	0.000000016	0.000000763	-0.000000824
1	0.000003238	-0.000000282	-0.000002773
1	0.000000737	0.000000508	-0.000000558
1	0.000000033	0.000000176	-0.000000425
8	-0.000008644	-0.000005924	0.000007764
6	-0.000000648	0.000005379	0.000003989

6	0.000005794	-0.000001104	0.000002496
6	-0.000002317	-0.000000178	-0.000002076
6	-0.000001481	0.000000059	0.000001634
6	0.000007499	0.000003638	-0.000002696
1	0.000002384	0.000002387	-0.000000064
1	0.000001565	0.000000096	-0.000002149
7	-0.000005414	0.000003163	-0.000009593
8	-0.000007341	0.000000171	0.000000709
1	0.000000481	-0.000000356	0.000001819
1	0.000001373	0.000001368	0.000000982
17	-0.000001889	-0.000002011	0.000002513
<b>Zero-point correction=</b>			<b>1.192350 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>1.268908</b>
<b>Thermal correction to Enthalpy=</b>			<b>1.269852</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>1.072585</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-4292.956921</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-4292.880363</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-4292.879418</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-4293.076686</b>

#### A-TSe2

6	-0.00000005	-0.000000365	-0.00000038
6	0.000000092	-0.00000021	0.000000291
7	0.000000215	0.000000172	0.000000089
7	0.000000067	-0.00000006	-0.000000032
16	-0.000000708	-0.000000524	0.000000926
8	-0.0000006	-0.00000053	0.000000975
8	-0.000000429	-0.000000344	0.000000282
6	-0.000000596	-0.000000046	0.000000096
6	-0.000000653	-0.000000076	0.000000869
6	-0.000000536	0.000000026	0.000001135
6	0.000000026	0.000000023	0.000001699
6	-0.000000338	-0.000000075	0.00000101
6	0.000000112	-0.000000135	0.000000639
1	-0.00000038	-0.000000439	0.000001209
1	-0.000000475	-0.000000177	0.000001636
1	0.000000014	0.000000065	0.000001092
1	-0.000000376	-0.000000043	0.000000067
6	-0.000000206	0.000000191	0.000001938
1	-0.000000093	0.000000031	0.000001391
1	-0.000000498	0.000000056	0.00000148
1	-0.000000208	0.000000115	0.000001699
6	-0.000000499	-0.000000025	0.000000075
6	-0.000000249	-0.000000117	0.000000711

1	-0.000000383	-0.000000334	0.000000372
1	0.000000015	0.000000041	0.000000617
6	-0.000000186	0.000000045	0.000001139
1	-0.000000318	0.000000285	0.000000561
1	-0.000000658	-0.000000308	0.000001084
6	-0.000000231	0.000000076	0.000001375
1	-0.000000388	-0.000000094	0.000000864
1	-0.000000038	0.000000008	0.000000792
1	-0.000000015	0.000000108	0.000001409
1	-0.000000013	0.000000024	0.000001276
1	-0.000000333	-0.000000014	0.000001384
6	0.000000084	0.000000213	0.000000198
6	0.000000341	0.000000114	0.000000594
1	0.000000211	0.000000498	0.000000194
1	0.000000154	0.000000216	0.000000438
6	0.000000279	0.000000561	0.000000625
1	0.000000194	0.000000031	0.000000612
1	0.000000188	0.000000291	0.000000073
6	0.000000036	0.000000618	0.000001075
1	0.000000177	0.000000275	0.000000693
1	0.000000074	0.000000496	0.000000566
1	0.000000533	0.000000641	0.000001108
1	0.000000469	0.000000546	0.000001031
1	0.000000269	0.000000039	0.000001118
16	0.000000344	0.000000241	0.000000058
8	0.000000369	0.000000425	0.000000102
8	0.000000047	-0.000000008	0.000000099
6	0.000000139	0.000000151	-0.000000036
6	0.000000919	0.000000111	-0.000000436
6	0.000000166	0.000000081	-0.000000434
6	0.000000555	0.000000135	-0.000000697
1	0.000000588	0.000000445	-0.000000308
6	0.000000746	-0.000000179	-0.000000844
1	-0.000000004	-0.000000103	-0.000000466
6	-0.000000812	0.000001398	-0.00000104
1	0.000000582	0.000000058	-0.000000741
1	-0.000000031	-0.000000008	-0.000000967
6	0.000000702	-0.000000266	-0.000001559
1	0.000000698	0.000000359	-0.000001309
1	0.000000075	-0.000000795	-0.000001128
1	0.000001433	0.000000554	-0.000001203
79	0.000000308	0.000000316	0.000000153
6	0.000000186	-0.000000421	-0.000000644
6	0.000000288	0.000000089	-0.000000712

6	0.000000247	0.000000196	-0.000000431
1	0.000000046	0.000000303	-0.000000489
1	0.000000313	0.000000032	-0.000000947
7	0.000000211	-0.000000233	-0.000000778
7	0.000000108	0.000000558	-0.000000157
6	-0.000000154	-0.000000261	-0.000000849
6	-0.000000265	-0.000000281	-0.000000889
6	0.000000053	-0.000000128	-0.000000954
6	-0.000000358	-0.000000051	-0.000001014
6	-0.000000199	-0.000000326	-0.000001178
6	-0.000000279	-0.000000503	-0.000001218
1	-0.000000545	-0.000000582	-0.000001119
1	-0.000000039	-0.00000003	-0.000001403
1	-0.000000448	-0.000000627	-0.000001405
6	0.000000385	0.000000266	0.000000231
6	0.000000568	0.000000283	0.000000186
6	-0.000000033	0.000000278	-0.000000085
6	0.000000764	0.000000478	0.000000471
6	0.000000101	0.000000398	0.000000415
6	0.000000409	0.000000493	0.000000643
1	0.000000758	0.000000681	0.000000384
1	0.000000188	0.000000257	0.000000615
1	0.000000492	0.000000572	0.000000741
6	0.000000773	0.000000353	0.000000049
6	0.000000836	0.000000747	-0.000000181
6	0.000000852	0.000000548	-0.000000275
1	0.000000587	0.000000446	-0.000000484
1	0.000000637	0.000000556	-0.000000333
1	0.000001005	0.000000726	-0.000000508
1	0.000000998	0.000000867	-0.000000072
1	0.000000073	0.000000694	-0.000000008
1	0.000000731	0.000000718	0.000000022
1	0.000000867	0.000000643	-0.000000097
6	0.000000174	-0.000000109	0.000000268
6	-0.000000235	-0.000000218	0.000000305
6	0.000000136	0.000000012	0.000000014
1	-0.000000198	0.000000068	0.000000008
1	-0.000000287	-0.000000125	0.000000312
1	-0.000000355	-0.000000329	0.000000318
1	-0.000000246	-0.000000018	0.000000628
1	0.000000212	0.000000016	-0.000000053
1	0.000000079	0.000000012	0.000000417
1	-0.000000014	-0.000000108	0.000000061
6	0.000000249	-0.000000006	-0.000000983

6	0.00000021	0.000000119	-0.000000874
6	0.000000349	0.000000169	-0.00000123
1	0.000000197	0.000000085	-0.000000581
1	-0.000000417	-0.000000426	-0.00000093
1	0.000000151	0.000000208	-0.000000935
1	0.000000083	-0.000000162	-0.000001092
1	0.000000377	0.000000105	-0.000001295
1	0.000000302	0.000000005	-0.00000144
1	0.000000552	0.000000251	-0.000001208
6	-0.000000386	-0.000000049	-0.000000605
6	-0.00000028	-0.000000226	-0.000000977
6	-0.00000072	-0.000000564	-0.000000323
1	-0.000000066	-0.000000432	-0.000000515
1	-0.000000185	-0.000000323	-0.000000965
1	-0.000000375	-0.000000445	-0.000000751
1	-0.000000496	-0.000000056	-0.000000995
1	-0.000000136	-0.000000371	-0.000000569
1	-0.000000546	-0.000000868	-0.000000715
1	-0.00000078	-0.000000058	-0.000000024
8	-0.000000001	-0.000000126	-0.000000192
6	-0.000000974	-0.000000459	0.000000118
6	-0.000000922	-0.000000854	0.000000013
6	-0.000001018	-0.000000885	-0.000000024
6	-0.000001001	-0.000000744	-0.000000515
6	-0.000000558	-0.000000622	-0.000000345
1	-0.00000116	-0.00000102	-0.000000289
1	-0.000000736	-0.000000057	0.000000417
7	-0.000000485	-0.000000621	-0.000000443
8	-0.00000067	-0.000000096	0.000000139
1	-0.000000929	-0.000000898	-0.000000691
1	-0.000001067	-0.000000837	0.000000205
17	-0.00000067	-0.000000503	-0.000000887

Zero-point correction=

1.189375 (Hartree/Particle)

Thermal correction to Energy=

1.266189

Thermal correction to Enthalpy=

1.267134

Thermal correction to Gibbs Free Energy=

1.067703

Sum of electronic and zero-point Energies=

-4292.932490

Sum of electronic and thermal Energies=

-4292.855676

Sum of electronic and thermal Enthalpies=

-4292.854731

Sum of electronic and thermal Free Energies=

-4293.054162

A-2e

6	-0.000003836	0.000003993	-0.000000419
6	0.000001212	-0.000000473	-0.000000517



7	-0.000003048	0.000002758	-0.00000327
7	-0.000001424	0.000006786	0.000000835
16	0.000001953	-0.000001353	0.000003437
8	0.000000749	0.000002629	0.000000501
8	0.000001165	0.000002425	0.000001611
6	-0.000000354	0.000002431	0.000001024
6	-0.000000856	0.000002834	0.000000433
6	-0.000000107	0.000002954	-0.000000581
6	0.000000285	0.000004336	0.000001644
6	-0.000000428	0.000001455	0.000001481
6	0.000000525	0.000000929	0.000002201
1	-0.000000569	0.000003038	0.00000013
1	-0.000000955	0.000003509	-0.000000182
1	0.000000377	0.000002364	0.000001541
1	-0.000000455	0.000002706	0.000000684
6	-0.000000567	0.000003502	-0.000000268
1	-0.000000253	0.000002732	0.00000103
1	-0.000000131	0.000002854	0.000001252
1	-0.000000327	0.000002654	0.000001184
6	-0.000000855	0.000003693	0.000002084
6	-0.000000518	0.000000872	-0.000001555
1	-0.000000616	0.000001044	-0.000001491
1	-0.000000658	0.000002015	-0.000000942
6	-0.000001223	0.000002628	-0.000001791
1	-0.000000987	0.000001048	-0.000001324
1	-0.000001099	0.000001935	-0.000001037
6	-0.00000164	0.000000856	-0.000001939
1	-0.000001234	0.000002473	-0.000001495
1	-0.000001337	0.000001795	-0.000001822
1	-0.000001891	0.00000216	-0.000002599
1	-0.000001044	0.000001237	-0.000002275
1	-0.000001338	0.000002191	-0.000001682
6	-0.000000873	-0.000001982	0.000001034
6	0.000000896	0.000004244	-0.000000303
1	0.000000125	-0.000000736	0.000000725
1	0.000000164	0.000000527	0.000000391
6	0.00000043	-0.000000702	0.000000149
1	-0.000000019	0.00000009	0.000000532
1	-0.000000374	0.000001119	0.000000348
6	-0.000001076	0.000000848	-0.000000528
1	-0.000000683	0.000000889	-0.000000326
1	-0.000000018	0.000000208	0.000000011
1	-0.000000416	0.000000489	-0.000000943
1	0.000000222	0.000001107	0.00000002

1	-0.000000701	0.000001128	-0.000000381
16	0.000001458	-0.000005755	0.000000271
8	0.000000048	-0.000000292	0.000002841
8	0.000001441	0.000001305	0.000001894
6	0.000002799	0.000000561	0.000000919
6	-0.000000464	-0.000000992	0.000001959
6	0.000002408	0.000001768	0.000003609
6	0.000004198	-0.000000974	0.000001312
1	0.000001347	-0.000001414	0.000001358
6	-0.000001359	0.000000003	0.000001011
1	0.000001245	0.000000045	0.000001729
6	0.000000884	-0.000002323	0.000006164
1	0.000001348	-0.000001893	0.000002073
1	0.000001724	-0.000000224	0.000002617
6	0.000000923	-0.000001528	0.000003643
1	0.000002727	-0.000001138	0.00000147
1	0.000000873	-0.000001564	0.000002791
1	0.000002942	-0.000002434	0.00000312
79	-0.000001272	-0.000001817	-0.000000943
6	0.000002356	-0.000000087	-0.000000456
6	0.000001843	-0.000000735	0.000002803
6	0.000002862	-0.000000811	-0.000002905
1	-0.000000876	-0.00000246	-0.00000075
1	-0.000000054	-0.000001906	-0.000001709
7	-0.000005518	-0.000004631	-0.00000206
7	-0.00000091	0.000000055	0.000002223
6	0.000001452	-0.000001014	-0.00000089
6	-0.000001142	0.000000139	-0.00000123
6	0.000000523	0.000000469	0.00000224
6	0.000000474	0.000000365	-0.000000106
6	0.000000604	-0.000000059	-0.000001427
6	-0.000000366	0.00000125	0.000000823
1	-0.000000789	0.000001186	-0.000000308
1	0.000000029	0.000000934	0.00000169
1	0.000000114	0.000001151	0.000000534
6	0.000000092	-0.000005031	-0.000002826
6	0.00000117	-0.000002421	0.000000779
6	-0.000000526	-0.000002	-0.000002255
6	-0.000000393	-0.000002462	-0.000000057
6	-0.000000505	-0.000000546	-0.000001163
6	0.000000154	-0.000002668	-0.000001701
1	0.000000281	-0.000002267	-0.000001224
1	-0.000000371	-0.000002281	-0.000001605
1	-0.000000333	-0.000002966	-0.00000191

6	-0.00000607	-0.000001357	-0.000001724
6	0.000000854	-0.000003164	0.000000954
6	0.000000926	-0.00000127	0.000000567
1	-0.000000563	-0.000001834	-0.000000116
1	0.000000996	-0.000003286	0.000000151
1	0.000001393	-0.000003244	0.000000569
1	0.0000007	-0.000003806	-0.000000108
1	0.000001183	-0.000001622	0.000001057
1	0.000000338	-0.000001377	0.000000635
1	0.000001005	-0.00000209	0.000001519
6	0.000000076	-0.000001401	-0.00000143
6	-0.000000177	-0.000000958	-0.000002455
6	-0.000000593	-0.000002131	-0.000001921
1	-0.00000026	-0.00000129	-0.000001623
1	-0.000001191	-0.000000326	-0.000001919
1	-0.000001477	-0.000000515	-0.000002615
1	-0.000001024	-0.000000953	-0.000002398
1	-0.000001101	-0.000001924	-0.000002802
1	-0.000000934	-0.000001969	-0.000003104
1	-0.000001335	-0.000001457	-0.000003064
6	0.000001899	-0.000001062	0.000001112
6	-0.000001138	-0.000000004	0.000000311
6	0.00000028	-0.000001229	0.00000129
1	-0.000000387	-0.000000741	0.000000307
1	0.000001219	-0.000000625	0.000001878
1	0.000001344	-0.000000458	0.000001644
1	0.000001242	0.000000117	0.000002143
1	0.000000948	-0.000001154	0.000000815
1	0.000000874	-0.000000878	0.000001394
1	0.000001294	-0.000001545	0.000001485
6	-0.000000252	0.000001032	-0.000001307
6	-0.000000974	0.000000382	-0.000001196
6	-0.000001383	0.000000867	-0.000001279
1	0.000000083	-0.000000192	-0.000000954
1	-0.000000581	-0.000000667	-0.000001267
1	-0.000001152	-0.000000219	-0.000002324
1	-0.000000626	-0.000000248	-0.000001706
1	-0.000000626	0.000000164	-0.000001369
1	-0.000000495	0.000001467	-0.000001244
1	-0.000001493	0.000000047	-0.000002058
8	0.00000016	-0.000000321	0.000002168
8	0.000001823	0.000001967	-0.000001155

Zero-point correction=

1.111259 (Hartree/Particle)

Thermal correction to Energy=

1.182440

Thermal correction to Enthalpy=	1.183384
Thermal correction to Gibbs Free Energy=	0.990603
Sum of electronic and zero-point Energies=	-3585.279817
Sum of electronic and thermal Energies=	-3585.208636
Sum of electronic and thermal Enthalpies=	-3585.207692
Sum of electronic and thermal Free Energies=	-3585.400472

HNTf<sub>2</sub>

7	0.000006035	0.000006153	0.000009464
1	0.000001078	-0.000003234	0.000002408
16	-0.000023355	-0.000003274	-0.000010518
8	0.000003047	-0.000002746	0.000001695
8	0.000011116	-0.000000192	0.000005127
16	0.000000846	0.000003006	0.000004231
8	-0.000002621	-0.000000726	-0.000000908
8	-0.000006461	-0.000000104	-0.000007446
6	0.000038286	-0.000002456	0.000028743
6	0.000015208	0.000019855	-0.000043537
9	-0.000012606	-0.000008051	0.00000801
9	0.000003287	-0.0000003	0.000001155
9	-0.000008211	-0.000001752	-0.000002211
9	-0.000016378	-0.000008054	0.000011479
9	-0.000007118	0.000006519	-0.000002401
9	-0.000002153	-0.000004643	-0.000005291

Zero-point correction=	0.065377 (Hartree/Particle)
Thermal correction to Energy=	0.080488
Thermal correction to Enthalpy=	0.081432
Thermal correction to Gibbs Free Energy=	0.020644
Sum of electronic and zero-point Energies=	-1827.637224
Sum of electronic and thermal Energies=	-1827.622113
Sum of electronic and thermal Enthalpies=	-1827.621169
Sum of electronic and thermal Free Energies=	-1827.681958

NTf<sub>2</sub><sup>-</sup>

7	0.000000039	-0.000000162	0.000074364
16	-0.000027153	0.000039554	-0.000054279
8	0.000000326	-0.00000597	-0.000022698
8	-0.000020815	-0.00002219	0.000036765
16	0.000027134	-0.000039407	-0.000054264
8	-0.000000335	0.000005953	-0.000022722
8	0.000020831	0.000022223	0.00003683
6	0.000021946	-0.000021148	0.00001131
6	-0.000021893	0.000021203	0.000011417

9	-0.00003851	0.000015353	0.00000449
9	-0.00003214	0.000011087	-0.000003153
9	0.000007389	0.000030193	-0.000009656
9	-0.000007397	-0.000030227	-0.000009717
9	0.000003831	-0.000015356	0.000004447
9	0.000003162	-0.000011105	-0.000003134
Zero-point correction=			0.053382 (Hartree/Particle)
Thermal correction to Energy=			0.067855
Thermal correction to Enthalpy=			0.068799
Thermal correction to Gibbs Free Energy=			0.009216
Sum of electronic and zero-point Energies=			-1827.151939
Sum of electronic and thermal Energies=			-1827.137466
Sum of electronic and thermal Enthalpies=			-1827.136522
Sum of electronic and thermal Free Energies=			-1827.196105

## Z

6	-0.000387838	-0.000249468	-0.000000171
6	0.000140512	0.000232751	0.000000041
6	0.000104199	-0.000133738	-0.000000007
6	-0.000081243	0.00001012	-0.000000092
6	-0.000124566	0.000007488	0.000000376
1	-0.000003528	0.000020037	0.000000008
1	0.000069919	0.000031794	0.000000003
7	0.000254713	0.000078032	-0.000000065
1	0.000044026	-0.000004796	-0.000000022
1	-0.000014998	-0.000015903	0.000000013
17	-0.000001197	0.000023685	-0.000000112
Zero-point correction=			0.079241 (Hartree/Particle)
Thermal correction to Energy=			0.084604
Thermal correction to Enthalpy=			0.085548
Thermal correction to Gibbs Free Energy=			0.049523
Sum of electronic and zero-point Energies=			-707.810087
Sum of electronic and thermal Energies=			-707.804724
Sum of electronic and thermal Enthalpies=			-707.803780
Sum of electronic and thermal Free Energies=			-707.839805

## B-1

6	0.000008409	-0.000007879	-0.000001692
6	-0.000001477	0.000004222	-0.000000838
7	-0.000003135	0.000001361	0.000009967
7	-0.000001848	0.000001334	-0.000000844
16	-0.000000859	-0.000000995	-0.000002024
8	-0.000000584	0.000001217	-0.000001528

8	0.00000268	-0.00000145	-0.000002154
6	0.000002206	-0.00000046	0.000002816
6	-0.000000396	-0.000000591	-0.000000124
6	-0.000000993	0.000000181	-0.000000438
6	-0.000001002	0.000000384	-0.000000625
6	-0.000001265	-0.000000177	0.000000067
6	-0.000001834	0.000000985	-0.000002184
1	-0.00000034	-0.000000155	-0.000000549
1	-0.000000995	-0.000000323	-0.000000695
1	-0.000000773	-0.000000138	-0.000000287
1	0.000000446	0.000000308	0.000000101
6	-0.000001322	0.000000036	-0.000000935
1	-0.000001261	-0.000000085	-0.000000555
1	-0.000001712	-0.000000294	-0.000000601
1	-0.00000018	-0.000000131	-0.000000007
6	0.000004161	-0.000002386	-0.000003323
6	-0.000001051	-0.000000829	0.000000763
1	-0.000000431	0.000002035	0.000000249
1	-0.000000751	0.000000266	0.000000743
6	0.000001961	-0.000002368	0.000001411
1	0.000000947	0.000000452	0.000000969
1	0.000000846	0.000000031	0.000000292
6	0.000000481	-0.000000213	0.000001375
1	0.000000389	-0.000000151	0.000001038
1	-0.000001184	0.000001165	0.000000926
1	0.000000527	-0.000000508	0.00000158
1	0.000000879	-0.000000209	0.000001246
1	0.000000988	-0.000000178	0.000000944
6	0.000001237	-0.000000894	0.000001539
6	0.000000803	0.000001358	0.000000991
1	0.000001361	0.000000199	-0.000000124
1	-0.000000028	0.000000368	-0.000000982
6	0.000000648	0.000000013	-0.000000033
1	0.000001094	-0.000000336	-0.000000016
1	0.000000238	0.000000014	-0.000000064
6	0.000000774	-0.000000221	0.000000141
1	0.000000955	0.000000012	-0.000000153
1	0.000001144	0.000000269	-0.000000176
1	0.000001198	0.000000213	0.000000212
1	0.000001123	0.000000018	0.000000312
1	0.000000807	0.000000091	0.000000032
16	-0.000001335	-0.000001105	0.000000264
8	0.000000388	0.000000216	-0.000001503
8	0.000000091	0.000001496	0.000000015

6	-0.000000709	0.000000427	-0.000001272
6	-0.000000728	-0.000000146	-0.000001044
6	-0.000000201	0.000000909	-0.000001643
6	0.00000014	0.000000744	-0.000001588
1	0.00000007	0.000000675	-0.000000792
6	-0.000000375	-0.000000096	-0.000001289
1	-0.000000115	0.000000083	-0.000000897
6	0.000000304	0.0000004	-0.000001618
1	-0.000000058	0.000000716	-0.000001401
1	-0.000000187	0.000000606	-0.000001543
6	0.000000107	0.000000616	-0.000002341
1	-0.000000074	0.000000847	-0.000002229
1	-0.000000381	0.000000988	-0.000001822
1	0.000000227	0.000000583	-0.000001787
7	0.0000009303	-0.0000004498	0.0000005363
1	-0.00001309	0.000002848	-0.000003599
16	-0.00000308	-0.000001811	-0.000001741
8	0.000000302	0.000000369	0.000002808
8	-0.000000351	-0.000000096	0.000000384
16	0.000001442	-0.000001874	0.000001526
8	0.00000121	0.000000095	0.000001101
8	-0.000002616	-0.000000225	-0.000001224
6	-0.000003542	-0.000003218	0.000002815
6	0.00000532	0.000004907	0.00000497
9	0.000001788	0.000000507	0.000001015
9	-0.000000767	0.000000359	-0.000000556
9	-0.000000414	0.000001795	0.000000955
9	0.000000206	-0.000001808	0.000001621
9	-0.000001625	-0.000001071	-0.00000019
9	-0.000000665	-0.000001777	0.000000193

Zero-point correction= 0.592886 (Hartree/Particle)

Thermal correction to Energy= 0.645014

Thermal correction to Enthalpy= 0.645958

Thermal correction to Gibbs Free Energy= 0.495457

Sum of electronic and zero-point Energies= -3967.588321

Sum of electronic and thermal Energies= -3967.536194

Sum of electronic and thermal Enthalpies= -3967.535249

Sum of electronic and thermal Free Energies= -3967.685750

#### B-TS1

6	-0.000000376	0.000000938	-0.000000149
6	0.000000761	0.000001498	-0.000000065
7	0.000000307	-0.000000053	0.000000974
7	-0.000000603	-0.000000852	-0.000000679

16	0.000000428	0.000000838	0.000001041
8	0.000000025	0.000000828	0.000000576
8	0.000000018	0.000001018	0.000001723
6	0.000000224	0.000001043	0.00000081
6	-0.000000071	-0.00000028	0.000002427
6	0.000000675	-0.000001868	0.000001828
6	0.000000115	0.000001109	0.000000766
6	0.00000007	-0.000000542	0.000003332
6	0.000000806	-0.000000961	0.000001765
1	0.000000054	-0.000000567	0.000000898
1	0.000000192	-0.000001542	0.000001763
1	0.000000366	-0.000000304	0.000003306
1	0.000000208	0.000000589	0.000002549
6	0.000000228	-0.000001256	0.000002936
1	0.000000889	-0.000001541	0.00000347
1	0.000000575	-0.000001623	0.000003053
1	0.000000422	-0.000001994	0.000003445
6	-0.000000121	0.000000063	0.000001434
6	0.000000119	0.000000642	0.000001057
1	0.000000071	-0.000000236	0.000000864
1	0.000000294	-0.000000003	0.000001631
6	0.000000133	0.000000605	0.000001557
1	0.000000032	0.000000912	0.000000616
1	0.000000141	0.000001122	0.000001352
6	0.000000126	0.000001123	0.00000146
1	0.000000244	0.000000428	0.000001974
1	0.000000164	0.000000146	0.000001247
1	0.000000163	0.000000995	0.000001734
1	0.000000046	0.000001226	0.000000954
1	0.000000145	0.000001576	0.000001667
6	-0.000000059	0.000000342	-0.000001439
6	-0.000000283	0.000000293	-0.000001981
1	-0.0000002	0.000001181	-0.000001358
1	-0.000000425	0.000000572	-0.000001566
6	-0.000000393	0.000000875	-0.000002445
1	-0.000000134	0.000000369	-0.00000173
1	-0.00000028	-0.000000153	-0.000002003
6	-0.000000412	0.000000608	-0.000003023
1	-0.00000045	0.000000857	-0.000002686
1	-0.000000375	0.00000137	-0.000002357
1	-0.000000503	0.000000975	-0.000003417
1	-0.00000038	0.000000641	-0.000002822
1	-0.000000432	0.000000153	-0.000003178
16	-0.000000161	0.000000339	-0.000000459



8	0.000000105	-0.000000898	-0.000000319
8	-0.000000024	-0.000001403	-0.000001317
6	-0.000000007	-0.000000669	-0.000000727
6	-0.000000161	0.000000576	-0.000000866
6	-0.000000307	-0.000000325	-0.00000185
6	0.000000235	0.000000884	-0.000000877
1	0.000000034	0.000000444	0.000000066
6	-0.000000715	0.000000139	-0.000001724
1	-0.000000178	-0.000000463	-0.00000177
6	-0.000000678	-0.000000126	-0.000000004
1	-0.000000225	0.000001153	0.000000119
1	-0.000000234	0.000000299	-0.000001835
6	-0.000000252	0.000000601	-0.000000006
1	-0.000000052	0.000000396	-0.000001791
1	0.000000322	0.000001016	-0.000000699
1	-0.000000051	0.000001202	-0.000001556
7	0.000000139	-0.000000501	-0.000000224
1	-0.000000097	-0.000000465	-0.000000139
16	-0.000000306	-0.000001145	-0.000000129
8	0.000000093	-0.000001697	-0.000000072
8	0.000000398	-0.000001646	0.000000059
16	-0.000000112	-0.000000287	-0.000000604
8	-0.000000117	-0.000000842	-0.000001332
8	-0.000000205	0.000000285	-0.000001222
6	-0.000000063	-0.000001902	-0.000000774
6	0.000000085	0.000000014	-0.000000148
9	0.000000137	-0.000001588	-0.000000513
9	0.000000105	-0.000002418	-0.000000253
9	0.000000012	-0.000001818	-0.000001142
9	-0.000000006	-0.000000556	0.000000003
9	-0.000000126	0.000000584	-0.000000268
9	-0.000000081	0.000000007	-0.000000828

Zero-point correction=	0.588837 (Hartree/Particle)
Thermal correction to Energy=	0.640333
Thermal correction to Enthalpy=	0.641278
Thermal correction to Gibbs Free Energy=	0.493126
Sum of electronic and zero-point Energies=	-3967.588785
Sum of electronic and thermal Energies=	-3967.537288
Sum of electronic and thermal Enthalpies=	-3967.536344
Sum of electronic and thermal Free Energies=	-3967.684496

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6	-0.000010747	-0.000009718	-0.000013049
6	0.000011402	0.000016089	0.000004305

7	-0.000001734	-0.000000426	0.000017991
7	0.000000319	-0.000004251	-0.000005749
16	-0.000002832	0.00000222	-0.000007956
8	0.000000975	-0.000001527	-0.000001107
8	-0.00000381	-0.000000763	-0.000002319
6	0.00000503	-0.000001688	0.000006217
6	0.000001545	0.000002287	-0.000000567
6	0.000002101	0.000000368	0.000004381
6	0.000002184	-0.000001734	0.000003184
6	-0.000000425	-0.000001658	0.000001454
6	-0.00000303	0.000000852	0.000002242
1	0.00000119	-0.000000429	-0.000000265
1	0.000002664	-0.000001265	0.00000249
1	0.000000716	0.000000199	0.000003975
1	-0.000000006	0.000000477	0.000002653
6	0.000004035	-0.000001032	0.000004221
1	0.000002441	-0.000000648	0.000004705
1	0.000000865	-0.000000071	0.000003318
1	0.000001343	-0.000002732	0.000003731
6	0.000004592	0.000002821	-0.000006439
6	-0.000002865	-0.000000165	-0.000001327
1	-0.000000469	-0.000001219	-0.000001694
1	-0.000000264	0.000000121	0.000001004
6	0.000000392	0.000000088	-0.000001905
1	-0.000000601	0.000000987	-0.000002217
1	0.000000012	0.000000686	-0.000001383
6	-0.000002104	0.000000728	-0.000001952
1	-0.000000861	0.000000327	-0.000001189
1	-0.000000132	-0.000000311	-0.000002321
1	-0.000001333	0.000000922	-0.000002806
1	-0.000001576	0.000000804	-0.000003246
1	-0.00000204	0.00000124	-0.000002635
6	-0.000002115	-0.000002441	-0.000001872
6	-0.000000172	0.000002021	-0.00000101
1	0.000000457	0.000000885	-0.000000844
1	-0.000002754	-0.000000393	-0.000001558
6	-0.000002225	0.000000961	-0.000003401
1	-0.000000611	0.000000099	-0.000002517
1	0.000000804	-0.000000127	-0.000003602
6	-0.00000138	0.000000012	-0.000004299
1	-0.00000142	0.000000288	-0.000002826
1	-0.000001713	0.000001332	-0.000002868
1	-0.000001816	0.000001014	-0.000004777
1	-0.000001061	0.000000528	-0.000004229

1	-0.00000485	0.00000457	-0.000004357
16	0.000001641	0.000004309	0.000013052
8	0.000000788	-0.00000473	-0.000003764
8	0.000002368	-0.000003463	-0.00000066
6	-0.000004209	-0.00000006	-0.000004125
6	0.000000164	-0.000002585	0.000002124
6	0.000002983	-0.000000095	0.000003396
6	-0.000000315	0.000001185	0.000000443
1	0.000000452	0.00000003	0.00000154
6	-0.000001738	0.000002497	0.000001285
1	0.000001052	-0.000000942	-0.000001595
6	0.000001148	-0.000002505	0.000004722
1	0.00000004	0.000000131	0.000002343
1	0.000000327	-0.000000284	0.000001474
6	-0.000000068	-0.000000948	0.000001332
1	0.000000278	-0.000000137	0.000002546
1	-0.000000497	0.000000393	0.000005445
1	-0.00000015	0.000002443	0.000003292
1	0.000004651	-0.000001605	-0.000000437

Zero-point correction=

0.538577 (Hartree/Particle)

Thermal correction to Energy=

0.573353

Thermal correction to Enthalpy=

0.574298

Thermal correction to Gibbs Free Energy=

0.466981

Sum of electronic and zero-point Energies=

-2140.330383

Sum of electronic and thermal Energies=

-2140.295607

Sum of electronic and thermal Enthalpies=

-2140.294663

Sum of electronic and thermal Free Energies=

-2140.401979

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6	-0.000000346	0.000003602	0.000000444
6	-0.000003313	-0.000001408	-0.000001773
7	0.00000161	-0.000000026	-0.000001049
7	0.000003327	0.000000091	0.000000359
16	-0.000001728	-0.000000137	0.000000194
8	-0.000000781	0.000000842	0.000001357
8	-0.00000112	0.000000557	0.00000158
6	-0.000000335	-0.000000226	0.000001616
6	-0.000000365	-0.000000422	0.000001509
6	-0.000000257	-0.000000649	0.000001725
6	-0.000000369	-0.000000642	0.000001669
6	-0.000000205	0.000000689	0.000002609
6	0.000000011	0.000000679	0.000001445
1	0.00000006	-0.000000483	0.000001273
1	-0.000000117	-0.000000723	0.000002051

1	-0.000000674	0.000000257	0.000002372
1	-0.000000784	0.000000551	0.000001552
6	-0.000000724	0.000000257	0.000001673
1	-0.00000022	-0.000000323	0.000003195
1	-0.000000639	-0.000000236	0.000003346
1	-0.000000122	-0.000000671	0.00000282
6	0.000000403	0.000000562	0.000001119
6	-0.000001023	0.000000018	0.000000755
1	-0.00000007	0.000000053	0.00000071
1	-0.00000021	-0.000000042	0.000000704
6	-0.000000316	0.000000448	0.000000358
1	-0.000000619	0.000000246	-0.000000023
1	-0.000001087	0.000001183	0.000000354
6	-0.000000524	0.000000623	0.000000333
1	-0.000000326	0.000000335	0.000000558
1	-0.000000265	0.000000433	0.000000566
1	-0.000000485	0.000000715	0.000000274
1	-0.000000373	0.000000602	-0.000000132
1	-0.000000747	0.000000902	0.000000024
6	0.000000585	0.000000334	-0.000000238
6	-0.00000007	-0.000000942	-0.000000752
1	0.000000382	-0.000000267	0.00000012
1	0.000000489	-0.00000041	-0.000000733
6	0.000000271	0.000000242	0.000000317
1	0.000000103	-0.000000127	-0.000000225
1	-0.000000112	-0.000000279	-0.00000077
6	0.000000031	-0.000000272	-0.000000161
1	0.000000523	-0.000000588	-0.000000546
1	0.000000336	-0.000000633	0.000000246
1	0.00000019	-0.00000025	-0.000000084
1	-0.000000179	0.000000235	0.000000062
1	-0.000000006	-0.000000034	-0.000000416
16	-0.000000343	0.000000179	-0.000001958
8	-0.000000282	0.000000085	-0.000000766
8	0.000000031	0.000000442	-0.000001141
6	0.000001594	-0.00000095	-0.00000115
6	0.00000068	-0.000000438	-0.000000886
6	0.00000042	-0.000000234	-0.00000156
6	0.000000602	-0.000001058	-0.000001188
1	0.000000587	-0.000000821	-0.000001276
6	0.000000904	-0.000000904	-0.000001678
1	0.000000352	-0.000000273	-0.000001436
6	0.000001954	-0.000004359	-0.000002827
1	0.000001192	-0.00000143	-0.000001468

1	0.000000968	-0.000000971	-0.000001829
6	0.000001767	0.000000966	-0.000001222
1	0.000001309	-0.000001971	-0.000000714
1	0.000001484	-0.000001469	-0.000001058
1	0.000000531	-0.000000494	-0.000004229
1	0.000000127	-0.000000352	0.000000418
6	-0.000000371	0.000000668	-0.000000768
6	-0.000000056	0.000001138	-0.000000022
6	-0.000000853	0.000000652	-0.000001011
6	-0.000000265	0.000001696	-0.000000901
6	0.000000038	0.000000915	-0.000000548
1	-0.000000922	0.000001629	-0.000000892
1	-0.000000826	0.000000991	0.000000044
7	-0.000000586	-0.000000517	-0.000002327
8	0.000001158	-0.000003199	0.000003357
1	-0.000000762	0.000001682	-0.000001119
1	-0.000000631	0.000001356	-0.000000366
17	0.000000089	0.000002376	-0.000002063

Zero-point correction=	0.622978 (Hartree/Particle)
Thermal correction to Energy=	0.665825
Thermal correction to Enthalpy=	0.666769
Thermal correction to Gibbs Free Energy=	0.539500
Sum of electronic and zero-point Energies=	-2923.289936
Sum of electronic and thermal Energies=	-2923.247089
Sum of electronic and thermal Enthalpies=	-2923.246145
Sum of electronic and thermal Free Energies=	-2923.373414

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6	-0.000001362	0.000000101	-0.000000208
6	-0.000001033	0.000000504	-0.000000613
7	0.000001846	-0.000000481	-0.000000843
7	0.000002258	-0.000001603	-0.000000136
16	-0.000000267	0.000001251	0.000002642
8	0.000000018	0.000000345	0.000000304
8	-0.000000025	0.000000451	0.000002359
6	0.000000912	0.000000262	0.000002058
6	0.000000103	0.000000482	0.000000752
6	0.000000195	0.000000028	0.000000345
6	0.000000774	0.000000265	0.000001894
6	-0.000000125	0.000000051	0.000001821
6	-0.000000682	0.000000162	0.000002081
1	0.000000544	0.000000567	0.000000393
1	0.000000233	0.000000286	0.000000822
1	-0.000000535	-0.000000089	0.000000311

1	-0.00000448	0.00000172	0.000002686
6	-0.00000404	-0.00000812	0.00000376
1	0.00000217	0.00000246	0.000000782
1	-0.00000432	0.00000111	0.000001793
1	0.00000269	0.000000875	0.000001141
6	-0.00000762	-0.00000125	0.000001224
6	-0.00001268	-0.000000861	0.000000626
1	-0.00001077	-0.000000902	0.000000195
1	-0.00000725	-0.000000641	0.000001198
6	-0.00000169	-0.000001571	0.000001822
1	-0.000001018	-0.000000981	0.000000944
1	-0.000000987	-0.000000804	0.000001875
6	-0.000002085	-0.000002023	0.000001738
1	-0.000001781	-0.000001479	0.000001716
1	-0.000001934	-0.000001833	0.000000089
1	-0.000002486	-0.000002277	0.000001941
1	-0.000002027	-0.000001968	0.000001376
1	-0.000001948	-0.000001533	0.000002351
6	0.000000667	0.000000752	-0.00000209
6	0.000000981	0.000000721	-0.00000228
1	0.000000774	0.000000313	-0.000001211
1	0.000000488	0.000000106	-0.00000178
6	0.000001597	0.000001264	-0.000002141
1	0.000001584	0.000001183	-0.000001152
1	0.000001223	0.000001075	-0.000001852
6	0.000002097	0.000001669	-0.000002806
1	0.000001277	0.000000698	-0.000002898
1	0.000001461	0.000001066	-0.000002303
1	0.000002229	0.000001716	-0.000003218
1	0.000002392	0.000002058	-0.000002341
1	0.00000217	0.000001697	-0.000002936
16	0.000001675	0.000001308	-0.000000006
8	-0.000000332	0.000000635	-0.000000733
8	-0.000001267	-0.00000014	-0.000002479
6	-0.000000224	-0.000000299	-0.000001085
6	-0.00000094	-0.000001222	-0.000000812
6	-0.000000732	-0.000001411	-0.000001567
6	-0.000001381	-0.000001795	-0.000000541
1	-0.000000696	-0.00000076	0.000000009
6	-0.000001088	-0.000001519	-0.000002604
1	-0.000000069	-0.000000593	-0.000002617
6	-0.000001256	-0.000001408	-0.000001386
1	-0.000001728	-0.000001868	-0.000000387
1	-0.000001083	-0.000001724	-0.000002697

6	-0.000002023	-0.000002548	-0.000001712
1	-0.000002322	-0.000002685	-0.000001209
1	-0.000002031	-0.000002646	-0.000002184
1	-0.000002169	-0.00000273	-0.00000195
1	-0.00000013	-0.000000489	-0.000000333
6	0.000001254	0.00000139	0.000000059
6	0.000001597	0.000002859	-0.000000204
6	0.00000223	0.000001694	0.000000835
6	0.000000937	0.000001483	0.000001583
6	0.000000759	0.000002685	0.000000077
1	0.000002103	0.000002504	0.000000983
1	0.000001476	0.000001196	0.000000584
7	0.00000098	0.000000196	0.000001273
8	0.000001296	0.000000605	-0.000000016
1	0.000001478	0.000001589	0.00000132
1	0.000002215	0.000002306	0.000000178
17	0.000000266	0.000000509	0.000001786

Zero-point correction=	0.626065 (Hartree/Particle)
Thermal correction to Energy=	0.668338
Thermal correction to Enthalpy=	0.669283
Thermal correction to Gibbs Free Energy=	0.543130
Sum of electronic and zero-point Energies=	-2923.316577
Sum of electronic and thermal Energies=	-2923.274304
Sum of electronic and thermal Enthalpies=	-2923.273360
Sum of electronic and thermal Free Energies=	-2923.399512

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6	0.000000908	0.000001947	0.000001111
6	0.000000648	-0.000002875	-0.000000727
7	0.00000071	0.000000383	0.000000024
7	-0.000002797	0.000000985	-0.000000254
16	0.000000125	-0.000000434	0.000000356
8	-0.000001265	0.000000605	0.000000069
8	-0.000001313	-0.000000227	0.00000105
6	-0.000001397	-0.000001127	0.000001471
6	-0.000000531	-0.000000868	0.000001281
6	-0.000000485	-0.000001136	0.000001765
6	-0.000000642	-0.00000115	0.000001874
6	-0.000000763	-0.000001446	0.000002391
6	-0.000000524	-0.000000714	0.000002428
1	-0.000000236	0.000000144	0.000000786
1	-0.000000013	-0.000001243	0.00000191
1	-0.000000932	-0.000001213	0.000003128
1	-0.000000088	-0.000000457	0.000002114

6	-0.00000694	-0.000002053	0.000002945
1	-0.000001143	-0.00000137	0.000003466
1	-0.000000978	-0.000001408	0.000002702
1	-0.000000327	-0.000001906	0.000003125
6	0.000000415	-0.000001402	0.000001057
6	0.00000052	-0.000000845	0.000000556
1	0.000000953	-0.000001246	0.000000576
1	0.000000072	-0.000000944	0.000001105
6	0.000000736	-0.00000114	0.000000644
1	0.000000798	-0.000000609	0.000000023
1	0.000000169	-0.000000195	0.000000457
6	0.00000091	-0.000000793	0.000000533
1	0.000000687	-0.000001385	0.000001176
1	0.000001118	-0.000001552	0.000000643
1	0.000000992	-0.000001526	0.000000628
1	0.000001024	-0.000001057	-0.000000048
1	0.00000045	-0.00000067	0.000000507
6	0.000001072	0.000000208	-0.000000942
6	0.000000097	0.000000894	-0.000001074
1	0.000000007	0.00000071	-0.000001092
1	-0.000000467	0.000001398	-0.00000131
6	0.000000102	0.000001058	-0.00000248
1	0.000000388	0.000000454	-0.000001358
1	0.000000265	0.000001733	-0.000001934
6	0.00000044	0.000001454	-0.000002265
1	-0.000000148	0.000001793	-0.000002001
1	-0.000000093	0.000001329	-0.000001685
1	0.00000028	0.000001947	-0.000002876
1	0.000000875	0.0000012	-0.000002636
1	0.000000616	0.000001706	-0.000002881
16	-0.000000203	-0.000000297	0.000000039
8	0.000000297	0.000000024	0.000000092
8	0.000000574	0.000000885	-0.000000975
6	-0.000000683	0.000000326	-0.000000226
6	-0.000001402	0.000002323	0.000000784
6	-0.000000252	0.0000023	-0.000000549
6	-0.000001555	0.000001361	0.000000805
1	-0.000000412	0.000000135	0.000000597
6	-0.000001198	0.000002007	-0.000000628
1	-0.000000663	0.000001203	-0.000001064
6	-0.000001102	-0.000000023	-0.000000788
1	-0.000002365	0.000000744	0.000000297
1	-0.00000209	0.000001697	-0.000001208
6	-0.000004376	-0.000000388	-0.000002883



1	-0.000002381	0.00000225	0.000002493
1	-0.000001844	0.000002526	0.000001359
1	-0.000002094	0.000003647	0.000000491
1	0.000000718	-0.000000859	-0.000001074
6	0.000001909	-0.000000022	-0.000001002
6	0.000001841	-0.000000631	-0.000001943
6	0.000002065	-0.000000491	-0.000000998
6	0.000002224	-0.000000742	-0.000000059
6	0.000001119	-0.000001159	-0.000001528
1	0.000002117	-0.000000661	-0.000001526
1	0.000001277	0.000000137	-0.000001921
7	0.000000444	-0.000000049	-0.000000295
8	0.000002361	-0.000000061	-0.000000281
1	0.000001954	-0.000001188	-0.000000533
1	0.000001845	0.000000104	-0.000002191
17	0.000002128	-0.000001609	0.000000945
Zero-point correction=			0.623801 (Hartree/Particle)
Thermal correction to Energy=			0.666481
Thermal correction to Enthalpy=			0.667425
Thermal correction to Gibbs Free Energy=			0.540157
Sum of electronic and zero-point Energies=			-2923.300659
Sum of electronic and thermal Energies=			-2923.257979
Sum of electronic and thermal Enthalpies=			-2923.257035
Sum of electronic and thermal Free Energies=			-2923.384303

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6	-0.000007087	-0.000003679	0.000010545
6	-0.000009493	0.000001805	-0.000011028
7	0.000008945	0.000014501	-0.000008346
7	0.00001506	-0.000004558	0.000001564
16	0.000000192	-0.000008013	0.000006107
8	-0.000003852	0.000000951	-0.000000392
8	0.000001224	-0.000001581	-0.000001845
6	0.000000803	-0.000000981	0.000003261
6	0.000001465	-0.000000037	0.000001848
6	-0.000002075	-0.000002408	0.000001289
6	0.000001704	-0.000000479	-0.000000468
6	-0.000000729	0.000001067	0.000002805
6	-0.000001823	-0.000000888	0.000000023
1	-0.000000253	0.000000086	-0.000000815
1	-0.000000965	0.000000005	0.000000889
1	-0.000000231	-0.000001256	0.000002071
1	0.000000826	-0.000001901	0.000001953
6	-0.000000243	-0.000000509	0.000000835

1	-0.00000371	-0.000002362	0.000001883
1	-0.000000957	0.000000977	0.00000092
1	-0.00000328	-0.000000761	0.000003157
6	-0.000001962	-0.000005983	0.00000408
6	0.000000752	-0.000001449	0.000003496
1	-0.000000059	-0.000000272	0.000002914
1	-0.000001483	-0.000000424	-0.000001049
6	-0.000000907	-0.000001889	0.000001506
1	-0.00000025	-0.000001352	0.000000259
1	0.000000147	-0.000000718	0.000000771
6	0.000000328	-0.000001134	0.000002895
1	0.000000257	-0.000001828	0.000002561
1	-0.000000618	-0.000001113	0.00000237
1	-0.000000016	-0.000002245	0.000002657
1	-0.00000011	-0.00000169	0.000001732
1	0.000000841	-0.000001947	0.000001986
6	-0.000001564	-0.000000515	-0.000001698
6	0.000000808	0.000001456	0.000000871
1	0.000000639	0.000000391	0.000000468
1	-0.000000454	-0.00000019	-0.000000888
6	0.00000093	-0.000000262	-0.000002624
1	-0.000000642	0.000000309	-0.00000135
1	-0.000000175	0.000000756	-0.000001679
6	0.000000877	0.000001097	-0.000000885
1	0.000001395	0.000000466	-0.000001134
1	0.00000096	-0.000000226	-0.000000355
1	0.000001228	0.000000342	-0.00000127
1	0.000000376	0.000000385	-0.000000912
1	0.000000577	0.000000833	-0.000001758
16	-0.000001717	0.0000045	0.00000678
8	-0.000003359	0.000000279	-0.000004899
8	0.000000426	-0.000000399	-0.000000797
6	0.000002334	0.000000673	-0.000000379
6	0.000001222	-0.000002076	-0.000002465
6	-0.000000367	0.000001024	-0.000002528
6	0.00000184	0.000000313	-0.000002647
1	0.000000737	0.000000844	-0.000000373
6	0.000000145	0.000001057	-0.000000724
1	0.000001881	0.000000658	-0.000001652
6	0.000003052	0.000000526	-0.000000434
1	0.000001489	0.000000065	-0.000001492
1	0.000002045	0.000000994	-0.000002465
6	0.000004244	0.000000091	-0.000002758
1	0.000000568	0.000000263	-0.000002561

1	0.00000199	0.00000022	-0.000000168
1	0.00000309	0.000000141	-0.00000271
1	-0.000000042	0.000001	0.000002336
6	0.000001028	0.000002337	-0.000002021
6	-0.000002039	0.000001765	-0.000001218
6	-0.000002539	0.000001751	-0.000001097
6	-0.000002094	0.000002046	-0.000000231
6	0.00000012	-0.000001293	-0.00000097
1	-0.000002291	0.000002202	-0.000001314
1	-0.000001442	0.000000884	-0.000000736
7	-0.000010001	0.000004241	0.000005939
8	0.000005317	-0.000001816	-0.000004622
1	-0.000002674	0.000001403	-0.000000283
1	-0.000001509	0.00000217	-0.000001968
17	-0.000002189	0.000001361	-0.000000767

Zero-point correction=	0.626088 (Hartree/Particle)
Thermal correction to Energy=	0.668279
Thermal correction to Enthalpy=	0.669223
Thermal correction to Gibbs Free Energy=	0.544209
Sum of electronic and zero-point Energies=	-2923.308987
Sum of electronic and thermal Energies=	-2923.266796
Sum of electronic and thermal Enthalpies=	-2923.265852
Sum of electronic and thermal Free Energies=	-2923.390866

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6	-0.000005265	0.00000125	-0.000000869
6	0.000004752	-0.000000137	0.000000583
7	0.000000905	-0.000000928	-0.000001492
7	0.000001314	0.000000178	-0.000000136
16	-0.000000849	0.000000121	0.000001223
8	-0.00000035	0.000000311	0.000000104
8	0.00000005	-0.000000328	-0.000000359
6	0.000000553	0.000000182	0.00000015
6	0.000000723	-0.00000062	0.000000204
6	0.000000793	-0.000001545	0.000000301
6	0.00000109	-0.000002742	0.000000795
6	0.000000338	-0.000001074	0.000000423
6	-0.000000137	-0.00000089	-0.000000028
1	0.000001057	-0.000000929	0.000000453
1	0.000000845	-0.000001592	0.000001092
1	0.000000632	-0.000001457	0.000000653
1	0.000000167	-0.000000556	0.000000155
6	0.00000044	-0.000000813	0.000001642
1	0.000000768	-0.000002408	0.000000671

1	0.000001638	-0.000001588	0.000001731
1	0.000001069	-0.000001983	0.000001077
6	-0.000000707	-0.000000382	-0.000001191
6	-0.000000423	-0.000000552	-0.000001568
1	-0.000000344	-0.000001155	-0.000001168
1	-0.00000023	-0.000000568	-0.000000909
6	-0.000000706	-0.000000802	-0.000001736
1	-0.000000746	-0.000000316	-0.000001666
1	-0.000000723	0.000000072	-0.000001357
6	-0.000001122	-0.000000353	-0.000002296
1	-0.000000662	-0.000000855	-0.00000183
1	-0.000000738	-0.000001044	-0.000002053
1	-0.000001086	-0.000000644	-0.000002694
1	-0.000001127	-0.000000284	-0.000002507
1	-0.000001133	-0.000000021	-0.000002325
6	-0.000000505	0.000001019	0.000000015
6	-0.000000663	0.000001809	-0.000000496
1	-0.000000451	0.000000944	-0.00000037
1	-0.000000197	0.000000843	0.000000316
6	-0.000000499	0.000001782	-0.000000249
1	-0.000000665	0.000000094	-0.000001411
1	0.00000004	0.000000978	-0.000000022
6	-0.000000982	0.000001977	-0.000000857
1	-0.000000502	0.000001966	-0.000000079
1	-0.000000739	0.000001793	-0.000000768
1	-0.000000954	0.000002352	-0.000000839
1	-0.000000915	0.000001703	-0.000001111
1	-0.000000566	0.000001967	-0.000000571
16	-0.000002866	-0.00000117	-0.000000633
8	-0.000000074	0.000000024	0.000001137
8	0.000002056	-0.000000341	0.000000581
6	0.000000999	0.000001224	0.000001155
6	0.000000022	-0.000000781	0.000000984
6	0.000000105	0.000000883	0.000001349
6	0.000000915	0.000001237	0.000000651
1	0.000000763	0.000000018	0.000001116
6	0.000000004	0.000000019	0.000002616
1	0.000000489	0.000001355	0.000001223
6	-0.000002287	0.000001134	0.000002311
1	0.000000849	0.000000803	0.00000183
1	0.000000619	0.000001929	0.000001954
6	0.000001501	0.000001957	0.000001146
1	0.000001556	0.000002732	0.000001795
1	0.000001581	0.000000108	0.000004115

1	0.00000167	0.000002496	0.000001776
1	-0.00000046	-0.000000915	-0.000001186
6	-0.00000011	-0.000000301	0.000000338
6	0.000000207	-0.00000038	-0.000000539
6	0.000000143	-0.000001004	-0.000000103
6	-0.000000176	-0.000001316	-0.00000014
6	-0.000000025	-0.000001371	-0.000001208
1	0.000000372	-0.000001136	0.000000188
1	0.000000008	0.000000469	0.000000425
7	-0.00000197	-0.000000349	0.000000252
8	-0.000000254	-0.000000413	-0.000001529
1	0.000000462	-0.000001604	0.000000044
1	0.00000002	-0.000000182	0.000000124
17	0.000000511	-0.000000966	-0.000000406

Zero-point correction=	0.624391 (Hartree/Particle)
Thermal correction to Energy=	0.666504
Thermal correction to Enthalpy=	0.667448
Thermal correction to Gibbs Free Energy=	0.541962
Sum of electronic and zero-point Energies=	-2923.304973
Sum of electronic and thermal Energies=	-2923.262860
Sum of electronic and thermal Enthalpies=	-2923.261915
Sum of electronic and thermal Free Energies=	-2923.387402

B-2a

6	0.000000699	0.000001948	0.000000368
6	-0.000000326	-0.000002106	0.000002082
7	-0.000002351	-0.000004331	0.000002744
7	0.000000648	0.000000339	0.000004199
16	0.000002043	-0.000000097	-0.000002154
8	-0.000000789	-0.000001488	-0.000001585
8	-0.00000174	-0.00000231	-0.000000627
6	0.000000193	-0.000001213	-0.000002906
6	0.000001275	0.00000103	-0.000001758
6	0.000001772	0.000001593	-0.000002936
6	0.0000019	0.000001228	-0.000003663
6	0.000001188	-0.000000595	-0.000003561
6	0.000000923	-0.000000557	-0.000002364
1	0.000000963	0.000001002	-0.000001518
1	0.000002283	0.000002389	-0.000003039
1	0.000001163	-0.000000649	-0.000003942
1	0.00000001	-0.000002162	-0.000002617
6	0.000002745	0.000001726	-0.000004636
1	0.000002457	0.00000169	-0.000004683
1	0.000002717	0.000001682	-0.000005461

1	0.000002952	0.000002808	-0.000004063
6	-0.000000731	0.000000361	0.000001577
6	-0.000001252	-0.000001926	0.000001669
1	-0.000000485	0.00000045	0.000001681
1	-0.000000352	-0.000000194	0.000000312
6	-0.000001655	-0.000000754	0.000002638
1	-0.000001836	-0.000001285	0.000002936
1	-0.000001628	-0.000002452	0.000001424
6	-0.000002198	-0.000002324	0.000003204
1	-0.000001124	-0.000001106	0.000001683
1	-0.000001272	-0.000000151	0.000003145
1	-0.000002333	-0.000001877	0.000003781
1	-0.000002648	-0.000002143	0.000004315
1	-0.000002529	-0.000003121	0.000002824
6	-0.000003728	-0.000000897	0.000000139
6	0.000000023	-0.000000325	0.000004427
1	-0.000001017	-0.00000021	0.000001355
1	-0.000000214	0.000000027	0.000000823
6	-0.000002674	-0.000001121	0.000002307
1	-0.00000183	-0.000001198	0.000003296
1	-0.000001287	0.000000363	0.000002993
6	-0.000002215	-0.000001115	0.000004682
1	-0.000001242	-0.000000779	0.000002808
1	-0.000002047	-0.000002348	0.000002727
1	-0.000002594	-0.000001542	0.000004801
1	-0.000002781	-0.000001614	0.00000052
1	-0.00000202	-0.000000081	0.000005158
16	0.000000297	-0.000001088	0.000001481
8	-0.000000687	0.000001776	-0.000000242
8	0.000001233	0.000003394	0.000001013
6	0.000001955	0.000002641	-0.000000898
6	0.000000133	0.000000343	-0.00000017
6	0.000001132	0.000002547	-0.000001121
6	0.000001084	0.00000103	-0.000003058
1	0.000000653	0.000000085	-0.000001779
6	0.000001702	0.000002371	-0.000001591
1	0.000001152	0.000003147	0.000000623
6	0.00000272	0.000001823	-0.000002266
1	0.000001603	0.000000108	-0.000003776
1	0.000002227	0.000003378	-0.000001482
6	0.000002395	0.000002188	-0.000003799
1	0.000002039	0.000001164	-0.000004471
1	0.000003087	0.000002861	-0.000004342
1	0.000002597	0.000001491	-0.000005388

1	-0.00000102	0.000000193	0.000002402
8	-0.000001358	-0.000002124	0.000000611
Zero-point correction=			0.544417 (Hartree/Particle)
Thermal correction to Energy=			0.580545
Thermal correction to Enthalpy=			0.581489
Thermal correction to Gibbs Free Energy=			0.471194
Sum of electronic and zero-point Energies=			-2215.583659
Sum of electronic and thermal Energies=			-2215.547531
Sum of electronic and thermal Enthalpies=			-2215.546586
Sum of electronic and thermal Free Energies=			-2215.656881

#### B-TSe1

6	-0.000001895	0.000003482	-0.000000011
6	-0.000001969	0.000000368	-0.00000006
7	0.000002385	-0.000001016	-0.000000794
7	0.000000024	0.000000302	-0.000000129
16	0.000000409	0.000000423	-0.000000338
8	-0.000000486	0.000000537	0.000001322
8	0.000000521	0.000000035	0.000000725
6	-0.000000224	-0.000000459	0.000000833
6	0.000000118	-0.000000056	0.00000107
6	-0.000001398	-0.000001491	0.000001105
6	-0.000000847	-0.000000933	0.000001082
6	0.000000057	0.000000424	0.000001057
6	0.000000136	-0.000000566	0.000001049
1	-0.000000566	-0.000000343	0.000000948
1	-0.000001102	-0.000000718	0.000001144
1	-0.000000045	-0.000000406	0.000001245
1	0.000000112	-0.00000002	0.000000963
6	-0.000001371	-0.000000831	0.000001234
1	-0.000001617	-0.000000911	0.000001546
1	-0.000000416	-0.000001348	0.000000079
1	-0.000000605	0.00000001	0.000001413
6	0.000000642	0.000000239	0.000000136
6	0.000000008	0.000000006	-0.000000116
1	0.000000796	0.000000136	0.000000691
1	0.000000527	0.000000568	-0.000000578
6	0.000000535	0.000000028	-0.000000069
1	0.000000298	0.000000177	0.000000373
1	0.000000062	-0.000000004	-0.000000092
6	0.000000216	0.000000195	-0.000000259
1	0.000000814	0.000000479	-0.000000228
1	0.000000717	0.000000016	0.000000338
1	0.000000477	0.000000287	-0.000000254

1	0.000000119	0.000000082	-0.000000008
1	0.000000166	0.000000201	-0.000000462
6	-0.000000455	0.000000556	-0.000000863
6	-0.000000634	-0.000000355	0.000000047
1	-0.000000431	-0.000000406	-0.000000402
1	-0.000000641	-0.000000276	-0.000000103
6	-0.000000901	-0.000000103	-0.000000057
1	0.000000027	-0.000000275	0.000000058
1	-0.000000067	0.000000128	-0.000000037
6	-0.000000725	-0.000000517	0.000000269
1	-0.000000843	-0.000000397	-0.000000264
1	-0.000000892	-0.000000476	0.000000087
1	-0.000000873	-0.000000465	0.000000275
1	-0.000000431	-0.000000027	0.000000513
1	-0.000000466	-0.000000243	0.000000114
16	0.000000186	-0.000000483	-0.000000479
8	0.000000454	0.000000528	-0.000000851
8	-0.000000161	0.000000171	-0.000000447
6	-0.000000157	0.000000154	-0.000001036
6	-0.000000385	0.000000144	-0.000001065
6	-0.000000044	0.000000007	-0.000001138
6	-0.000000435	0.000000119	-0.000000986
1	-0.000000315	-0.000000008	-0.000001024
6	-0.000000991	-0.000000142	-0.000002138
1	-0.000000266	0.000000165	-0.000001118
6	-0.000000098	0.000000226	-0.000001652
1	-0.000000852	-0.000000118	-0.000001518
1	-0.000000704	0.000000034	-0.000001761
6	-0.000001218	-0.000000032	-0.00000209
1	-0.000001082	-0.000000062	-0.000001956
1	-0.000000899	0.000000256	-0.000001801
1	-0.000001416	0.000000014	-0.000002388
1	-0.000000705	-0.000000008	0.000000469
8	-0.000000151	-0.000000126	0.000001533
6	0.000001168	0.000000066	-0.000000073
6	0.000001664	0.000000763	-0.000000305
6	0.000001057	0.000000145	0.000000953
6	0.000001285	0.000000481	0.000000834
6	0.000002088	0.000000089	0.000000472
6	0.000001288	0.000000828	0.000000136
6	0.000000453	-0.000001554	-0.000000051
6	0.000001223	-0.000001656	0.000000878
1	0.000001195	0.000000297	0.000001118
1	0.000001572	0.000000528	0.000001172



1	0.00000194	0.000000837	0.000000544
1	0.000001546	0.000000732	-0.000000109
1	0.000000717	0.000000808	-0.000000763
1	0.000000378	0.000000541	-0.000000152
7	0.000002414	0.000001434	0.000001359
1	0.000001153	0.000000088	0.000000784
Zero-point correction=			0.676109 (Hartree/Particle)
Thermal correction to Energy=			0.719227
Thermal correction to Enthalpy=			0.720171
Thermal correction to Gibbs Free Energy=			0.592469
Sum of electronic and zero-point Energies=			-2579.279416
Sum of electronic and thermal Energies=			-2579.236298
Sum of electronic and thermal Enthalpies=			-2579.235353
Sum of electronic and thermal Free Energies=			-2579.363056

#### B-1e

6	-0.000004932	-0.000001055	-0.000001374
6	0.000002839	0.000005045	0.000000288
7	0.000001122	0.000000529	0.000000692
7	0.000003901	0.000005733	-0.000004397
16	0.000001676	-0.000007945	-0.000003612
8	-0.000000723	0.00000024	0.000000287
8	-0.000000289	0.000003436	0.000002907
6	0.000002684	-0.000002629	0.000001316
6	-0.000001759	0.000002577	0.000000819
6	-0.000000121	0.000000444	0.000000007
6	0.000000639	0.000002985	-0.00000013
6	0.000000659	-0.000000062	0.00000018
6	-0.000001954	0.000000362	0.000001775
1	0.000001053	-0.000000507	0.000001104
1	-0.000000155	0.000000965	0.000000476
1	-0.000000522	0.000000545	0.000000821
1	0.000000049	-0.000000001	0.000000029
6	0.000000551	0.000001659	0.000000227
1	-0.000000761	0.000000175	0.000000918
1	-0.000000149	0.000000489	0.000001808
1	-0.000000721	0.000000206	0.000001561
6	0.00000172	-0.000000002	-0.000001349
6	-0.000001984	0.000000556	0.000003984
1	-0.00000011	-0.000000315	0.000000149
1	0.000000091	-0.000000843	0.000000921
6	0.000001133	-0.000001185	-0.00000126
1	0.00000036	-0.000000408	-0.00000038
1	0.000000155	0.000000143	-0.000000717

6	-0.000000144	-0.000000049	-0.000000058
1	-0.000000138	-0.000000347	0.000000269
1	-0.000000006	-0.000000414	0.000000035
1	0.000000425	-0.000000342	-0.000000228
1	0.000000028	-0.000000341	-0.000000178
1	0.000000494	-0.000000476	-0.000000456
6	0.000001136	-0.00000143	0.000001354
6	-0.000000171	0.000000591	-0.000002456
1	-0.000000209	0.000000203	-0.000000741
1	0.000000442	0.000000409	-0.000000296
6	0.000000129	0.000000655	0.000000833
1	-0.000000347	0.000000103	0.000000439
1	0.000000062	0.000000019	-0.000000013
6	-0.000000956	-0.000000197	0.000000019
1	-0.000000211	0.000000368	-0.000000732
1	-0.000000422	0.000000767	-0.000000345
1	-0.000000337	0.000000648	-0.000000315
1	-0.000000229	0.000000719	-0.000000092
1	-0.000000076	0.000000481	-0.000000022
16	-0.000010127	-0.000002287	0.000012504
8	0.00000182	0.000001668	-0.000005469
8	0.000004737	0.000000116	-0.000002273
6	0.000000024	0.000002104	-0.000002569
6	-0.000000288	-0.000000099	-0.00000206
6	-0.000001223	-0.000000187	-0.000000695
6	-0.000000246	0.000000623	-0.000000085
1	0.000000114	-0.000000548	-0.000000355
6	-0.000000445	-0.000000861	-0.000001897
1	0.000000061	-0.000000021	-0.000001086
6	0.000000686	-0.000001175	0.000000098
1	-0.000000328	-0.000000065	-0.000000586
1	-0.000000196	-0.000000301	-0.000000902
6	-0.000001693	0.000001317	-0.000000396
1	-0.000000299	0.000000007	-0.000001755
1	0.000000044	-0.000000102	-0.00000195
1	0.000000026	-0.000000221	-0.000002319
1	0.000000075	-0.000000231	-0.000000958
8	-0.000005753	-0.000000243	0.000000565
6	0.000000852	-0.000000541	0.000001888
6	0.000002785	0.000000288	0.000002193
6	-0.000002339	-0.000000083	-0.000000699
6	0.000000869	0.000000648	-0.000000024
6	0.000001813	-0.000000724	0.000000686
6	-0.00000117	-0.000001278	-0.000000005

6	0.000002295	-0.000002252	0.00000211
6	0.00000259	-0.000003331	-0.000003435
1	0.000000927	-0.000000497	0.000000595
1	0.000000508	-0.000000999	-0.000000106
1	0.000000216	-0.000000251	0.000000254
1	0.000000132	0.000000029	0.000000825
1	-0.000000281	-0.000000485	0.000000056
1	-0.000000063	0.000002739	-0.000000496
7	-0.000003864	-0.000004362	-0.000000143
1	0.000003084	0.000000396	-0.000003252
Zero-point correction=			0.677978 (Hartree/Particle)
Thermal correction to Energy=			0.721060
Thermal correction to Enthalpy=			0.722004
Thermal correction to Gibbs Free Energy=			0.593403
Sum of electronic and zero-point Energies=			-2579.286857
Sum of electronic and thermal Energies=			-2579.243775
Sum of electronic and thermal Enthalpies=			-2579.242830
Sum of electronic and thermal Free Energies=			-2579.371432

#### B-TSf1

6	-0.000000079	-0.000002119	-0.000000272
6	0.000003984	0.000000009	0.000002182
7	-0.000002693	0.000001944	0.000001342
7	-0.000001514	-0.000000062	0.000000664
16	-0.000000748	0.000000227	-0.000000295
8	0.000000172	0.000000155	-0.000001782
8	0.000000115	-0.000000406	-0.000000647
6	-0.000000193	0.000000199	-0.000001338
6	-0.000000786	0.000000729	-0.000001486
6	-0.000001097	0.000000328	-0.000001755
6	-0.000001433	0.000000963	-0.000001763
6	-0.000000973	0.000000921	-0.000000708
6	-0.000000831	0.000000575	-0.000000991
1	-0.000000148	0.000000404	-0.000001881
1	-0.000000971	0.000000081	-0.000002247
1	-0.000001584	0.000000883	-0.000000937
1	-0.000000851	0.000000304	-0.000000419
6	-0.000001834	0.000001019	-0.000001744
1	-0.000002131	0.000000976	-0.000001703
1	-0.000001837	0.000001446	-0.000002091
1	-0.000001588	0.000001209	-0.00000183
6	-0.000000117	0.000000262	-0.000002056
6	0.000000385	0.000000337	-0.000000677
1	-0.000000324	0.000000208	-0.000000905

1	-0.00000011	-0.000000031	0.000000313
6	0.00000012	0.000000416	-0.00000149
1	0.000000523	-0.000000019	-0.000001382
1	0.000000443	0.000000167	-0.000001082
6	0.000000658	-0.000000108	-0.000001551
1	-0.000000106	0.000000071	-0.000001006
1	-0.000000403	0.000000046	-0.000001664
1	0.000000223	0.000000313	-0.000001907
1	0.000000581	0.000000251	-0.000002147
1	0.000000765	0.000000101	-0.000001627
6	0.000000914	-0.000000615	0.000000759
6	0.000001224	-0.000000868	0.000001019
1	0.000001274	-0.000000791	0.000000022
1	0.000000697	-0.000000588	0.000000832
6	0.000001717	-0.000000877	0.000001376
1	0.000001392	-0.000000065	0.000000785
1	0.000000903	-0.000000704	0.000001257
6	0.000002012	-0.000001238	0.000001494
1	0.000001514	-0.000000904	0.000001387
1	0.000001949	-0.000001013	0.00000008
1	0.00000226	-0.000001283	0.00000171
1	0.000002101	-0.000001137	0.000001389
1	0.000001737	-0.00000109	0.000001943
16	0.000000445	-0.000000228	0.000000335
8	-0.000000088	-0.000000199	0.000000166
8	-0.00000015	-0.000000158	0.000001446
6	-0.000000124	-0.000000022	0.000000536
6	0.000000289	-0.000000578	0.000000044
6	-0.00000032	-0.00000022	0.000000995
6	-0.000000223	-0.000000402	0.000000898
1	0.000000154	0.000000209	-0.000000051
6	0.000000117	-0.000000167	0.000000161
1	-0.000000021	-0.000000182	0.000001478
6	0.000000028	-0.000000091	0.000000555
1	0.000000031	0.000000147	-0.000000239
1	-0.000000008	-0.000000287	0.000001382
6	0.000000085	0.000000131	0.000000496
1	0.000001013	-0.000000406	0.000000216
1	-0.000000405	-0.000000193	0.000001439
1	-0.000000697	0.000000249	-0.000000248
1	0.000001081	-0.000000973	0.000000384
8	0.000000485	-0.000000564	-0.000000838
6	-0.000000638	-0.000000337	0.000001121
6	-0.000000557	-0.000000395	0.000001047

6	-0.00000719	0.00000018	0.000000367
6	-0.000001121	0.000000357	0.000000737
6	-0.000001439	0.000000469	0.000001205
6	-0.000000856	0.000000087	0.000001599
6	-0.000000214	-0.000000206	0.000000984
6	0.000001223	-0.000000134	0.000001532
1	-0.000001009	0.0000000892	0.000000158
1	-0.000001644	0.0000000572	0.0000000547
1	-0.000001669	0.000000037	0.000001468
1	-0.000000865	-0.000000005	0.000001946
1	0.000000023	-0.0000000314	0.000001737
1	0.000000653	-0.0000000591	0.000000732
7	0.000002273	0.000002275	-0.000002356
1	-0.000000576	0.000000701	-0.000000066

Zero-point correction=	0.677288 (Hartree/Particle)
Thermal correction to Energy=	0.720024
Thermal correction to Enthalpy=	0.720968
Thermal correction to Gibbs Free Energy=	0.595157
Sum of electronic and zero-point Energies=	-2579.250591
Sum of electronic and thermal Energies=	-2579.207855
Sum of electronic and thermal Enthalpies=	-2579.206911
Sum of electronic and thermal Free Energies=	-2579.332721

#### B-1f

6	0.000002172	0.000004432	0.000000056
6	-0.000002487	-0.000000687	-0.000007387
7	-0.000002972	-0.000001579	-0.000005717
7	-0.000000536	-0.000000757	0.000011171
16	-0.000002698	-0.000001339	0.000002974
8	0.000001803	-0.000001509	-0.000001049
8	0.000001986	-0.000000125	-0.000001703
6	0.000001261	-0.000000677	-0.000001821
6	0.000001237	-0.000003594	-0.000000646
6	-0.000001162	-0.000000333	-0.000001604
6	0.000000434	-0.000001833	-0.000001543
6	0.000001835	-0.000003381	-0.000002074
6	-0.000000066	-0.000001109	-0.000000121
1	-0.000000529	-0.000002847	0.000000187
1	-0.000000238	-0.000000387	-0.000000369
1	0.000000864	-0.000002189	-0.000000311
1	0.000000949	-0.000001568	-0.000001487
6	-0.000000029	-0.000003241	-0.000002274
1	0.000000537	-0.000003446	-0.000002601
1	0.000000612	-0.000005582	-0.000002495

1	0.00000677	-0.00004653	-0.00000773
6	-0.00001721	0.00000268	0.00001808
6	0.00002855	0.00000356	-0.00003995
1	0.00001563	0.00001918	-0.00003306
1	0.00001966	0.00002928	-0.0000008
6	0.00000612	0.00001692	-0.00000269
1	0.00000219	0.00002075	-0.00002033
1	0.00000836	0.00001403	-0.0000117
6	0.00001331	0.00002811	-0.00003631
1	0.00001506	0.00002971	-0.00002214
1	0.00001324	0.00002745	-0.00002748
1	0.00001649	0.00003233	-0.00003528
1	0.0000187	0.00001976	-0.00003595
1	0.00001361	0.00002275	-0.00002818
6	0.00000484	-0.00003046	0.00000518
6	-0.00001823	-0.00000443	0.00002656
1	-0.00000894	-0.00001331	0.00001599
1	-0.00000074	-0.00001178	0.00001144
6	-0.00001406	-0.00001603	0.00003529
1	-0.00000948	-0.00001111	0.00002588
1	-0.00000938	0.00000232	0.00003373
6	-0.0000231	-0.00002067	0.00004118
1	-0.00001601	-0.00001672	0.00003016
1	-0.00001365	-0.00002607	0.00002842
1	-0.00002171	-0.00002447	0.00004645
1	-0.00001967	-0.00001788	0.00004425
1	-0.00002064	-0.00000969	0.00004636
16	0.00002022	0.00002239	-0.00006705
8	-0.00000312	0.00001748	0.00001815
8	-0.00001161	0.00000276	0.00002886
6	-0.00000222	0.00001875	-0.00000045
6	-0.00001209	-0.00001359	0.00001202
6	0.00001581	0.00001723	0.00001598
6	0.00002529	-0.00000012	0.00000535
1	0.00001058	-0.00000129	-0.00001199
6	0.00000112	-0.00001527	-0.00000672
1	-0.00000625	0.00001312	0.0000129
6	-0.00000828	0.00002104	-0.0000022
1	0.00000458	-0.00000717	-0.00002313
1	0.00000228	0.00000709	0.0000006
6	0.00000848	-0.00000187	-0.00002205
1	0.00000816	-0.00001786	-0.00000596
1	0.00000357	0.00000051	-0.00000627
1	0.00000995	-0.00000424	-0.00002649

1	-0.000000101	-0.000000394	-0.000000327
8	0.000000308	0.000001258	0.000000315
6	-0.000001526	0.000004225	0.000001109
6	0.000004565	-0.000001004	-0.000005346
6	-0.000002375	0.000000132	0.000003771
6	0.000001786	0.000001619	-0.000001017
6	-0.000001061	0.000002093	0.000001197
6	0.000000032	0.000002527	0.000002551
6	-0.000002513	0.000000128	0.000003023
6	0.000000212	0.000000786	0.000001376
1	0.000000082	0.000001348	-0.000001592
1	0.000000959	0.000000245	-0.000000093
1	0.000000256	0.000003807	0.000000446
1	-0.000000121	0.000002619	0.000001525
1	-0.000001423	0.000001897	0.000002329
1	-0.00000185	-0.000000333	0.000004176
7	-0.000005815	0.000005831	0.000007662
1	0.000000228	-0.000002683	-0.000000692
<b>Zero-point correction=</b>			<b>0.678956 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>0.721744</b>
<b>Thermal correction to Enthalpy=</b>			<b>0.722689</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>0.596990</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-2579.278739</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-2579.235951</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-2579.235007</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-2579.360706</b>
<b>B-TSa3</b>			
6	0.00000134	-0.000001703	0.000000071
6	0.000001321	0.000000437	0.000002894
7	-0.000000869	0.000000799	0.000000043
7	-0.000000606	-0.000000273	-0.000000162
16	0.000001578	0.000000849	-0.000001121
8	0.000001283	0.000002405	-0.000000163
8	0.000000978	0.000000722	-0.000002339
6	0.000001062	0.000002342	-0.00000148
6	0.000001583	0.000002109	-0.00000158
6	0.00000191	0.000002357	-0.000001288
6	0.000001568	0.000002252	-0.00000271
6	0.000001487	0.000001391	-0.000003247
6	0.000001239	0.000000948	-0.000002496
1	0.000001821	0.00000028	-0.000000038
1	0.000002123	0.000003453	-0.000001182
1	0.000001164	0.000001038	-0.000003867
1	0.000000662	0.000000295	-0.000002917

6	0.000002176	0.000002807	-0.000002932
1	0.000001717	0.000002085	-0.000003572
1	0.000002552	0.00000322	-0.000003728
1	0.000002114	0.000002943	-0.000002328
6	-0.000002171	-0.000000403	-0.000003947
6	-0.000000705	-0.000001322	-0.000002148
1	0.000000696	0.000000067	-0.000001524
1	0.000000601	-0.000002435	0.000003098
6	-0.000000901	-0.000002236	-0.000002322
1	-0.000000419	-0.000000899	-0.000002438
1	-0.000000774	-0.000001638	-0.000001852
6	-0.000001192	-0.000003054	-0.000003193
1	-0.000001453	-0.00000289	-0.000001663
1	-0.000000841	-0.000002059	-0.000002763
1	-0.000001508	-0.000003605	-0.000003563
1	-0.000000922	-0.000002509	-0.000004078
1	-0.000001441	-0.000003208	-0.000003184
6	-0.000000101	-0.000000012	0.000001875
6	0.000000158	0.000000878	0.000003163
1	0.000000665	0.000001364	0.000001448
1	-0.000000064	0.000000646	0.000001422
6	0.000000543	0.000001721	0.000003592
1	0.000000263	0.000001412	0.000003166
1	-0.000000392	0.000000201	0.000003435
6	0.000000258	0.000001743	0.0000049
1	0.000000139	0.000001328	0.000003568
1	0.000000846	0.000002283	0.00000336
1	0.000000479	0.00000229	0.000005368
1	0.000000462	0.000002165	0.000005048
1	-0.00000023	0.000001145	0.000005357
16	-0.000001346	-0.000001536	0.000000321
8	-0.000000968	-0.00000073	-0.000000003
8	-0.000001222	-0.000001278	0.000001633
6	-0.000000539	-0.000001469	0.000000437
6	-0.000000116	0.000000377	-0.000001514
6	-0.000001311	-0.000002076	0.000001075
6	-0.000002132	-0.000001245	0.000002173
1	0.00000036	-0.000000674	-0.000001117
6	0.000001086	-0.00000048	-0.000004051
1	-0.000001198	-0.000001641	0.000001317
6	-0.000000039	-0.000000646	-0.000000468
1	-0.000000087	-0.000000847	-0.000002478
1	-0.000001318	-0.000001654	0.000000335
6	-0.000000466	-0.000001183	-0.000002224



1	0.000003014	0.000001212	-0.000000524
1	-0.00000312	-0.0000026	0.000000688
1	-0.000000716	-0.000001836	-0.0000006094
1	0.000000173	-0.000000737	0.000000409
8	0.00000079	0.000002134	0.00000067
6	-0.000001131	0.000000238	0.000002198
6	0.000000184	-0.000000264	0.000001802
6	-0.000000829	-0.000000515	0.000001109
6	-0.000000989	-0.000001412	0.000001935
6	-0.00000106	-0.000002117	0.000001878
6	-0.000002103	-0.000001671	0.000002493
6	-0.000001063	0.000000859	0.00000315
6	0.000000325	0.000000526	0.000002
1	-0.000000422	-0.000000042	0.000000849
1	-0.000001464	-0.000001825	0.000001203
1	-0.00000204	-0.000002816	0.000001737
1	-0.000001448	-0.000001767	0.000000155
1	-0.000000469	-0.000000606	0.000002434
1	0.000000839	0.000001663	0.000001512
7	0.000000082	0.000000744	0.000001366
1	0.000000549	0.000001668	0.000000932

Zero-point correction=	0.676675 (Hartree/Particle)
Thermal correction to Energy=	0.718933
Thermal correction to Enthalpy=	0.719877
Thermal correction to Gibbs Free Energy=	0.593023
Sum of electronic and zero-point Energies=	-2579.280925
Sum of electronic and thermal Energies=	-2579.238667
Sum of electronic and thermal Enthalpies=	-2579.237723
Sum of electronic and thermal Free Energies=	-2579.364577

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6	0.000009053	0.000034112	-0.000012854
6	-0.000010217	0.000000185	0.000023
7	-0.000004087	-0.000022834	0.000005497
7	0.000004554	0.000006082	-0.000018058
16	-0.000004835	0.000004122	-0.000005646
8	0.000001979	-0.00000119	-0.000001041
8	0.000002955	0.000000721	0.000001708
6	0.000005853	-0.000006298	0.000008548
6	-0.00000293	0.000002273	-0.000005856
6	0.000004109	0.000001981	-0.000001483
6	0.000003095	-0.000004026	-0.000000422
6	-0.000001157	0.000000331	-0.000000918
6	0.000000838	0.00000286	0.00000147

1	0.000000175	-0.000000214	0.000001844
1	0.000002045	-0.000002359	-0.000001046
1	0.000003042	-0.000001518	-0.000000913
1	0.000001596	0.000000121	0.000000061
6	0.000002804	-0.00000246	-0.000002856
1	0.000001903	-0.000001413	0.000000053
1	0.000001745	-0.000001148	0.000000975
1	0.000001333	-0.000001299	0.000000052
6	0.000002075	-0.000003093	0.000002829
6	-0.000000962	0.000002416	-0.000001441
1	0.000002659	0.00000147	0.00000275
1	-0.000001307	0.000002331	-0.000001239
6	0.000000008	0.000000064	0.000001384
1	0.000000747	0.000000413	0.000001689
1	-0.000000845	0.000000374	0.000001037
6	0.000000679	0.000000936	-0.000000034
1	-0.000000411	0.000001253	0.000000584
1	0.000000165	0.000001068	0.000000079
1	0.000000023	0.000001228	0.000000564
1	0.000000604	0.000000634	0.000000555
1	-0.000000325	-0.000000059	0.000000302
6	0.000002838	-0.000006867	0.000004436
6	-0.000001539	-0.000000094	-0.000001138
1	-0.000000338	-0.000000664	-0.000000933
1	-0.000000092	-0.000000402	-0.000000954
6	-0.000000556	-0.000000248	-0.000000712
1	-0.000000407	-0.000000496	-0.000000536
1	-0.000001343	-0.000000282	-0.000000456
6	-0.000001452	-0.000001532	-0.0000012
1	-0.000001123	-0.000001501	-0.000001153
1	-0.000000621	-0.000001252	-0.000001011
1	-0.000001393	-0.000001311	-0.000001353
1	-0.000001252	-0.000000593	-0.000000799
1	-0.000001905	-0.000000855	-0.000001104
16	0.000002742	-0.000005305	0.000001169
8	-0.000006994	0.00000339	-0.000003437
8	-0.000001219	-0.000005282	-0.000002358
6	-0.000004015	0.00000481	0.00000335
6	0.000000009	-0.000004213	-0.000001341
6	0.000001063	-0.00000175	-0.000003661
6	0.000001262	-0.000000852	-0.000003386
1	0.000000626	0.000000378	0.00000003
6	-0.00000141	-0.000004296	0.000000358
1	-0.000001157	-0.000000995	-0.000000475

6	-0.00000108	0.0000018	-0.000000112
1	0.000000965	-0.000000774	-0.000000313
1	-0.000001173	-0.000001671	-0.000001849
6	-0.000000488	-0.00000099	-0.000001529
1	0.000001171	-0.000003802	-0.000001936
1	-0.000000807	-0.000001754	-0.000002453
1	0.000000676	-0.000002181	0.000000259
1	0.000000264	-0.000004626	0.000000875
8	0.000005227	-0.000000982	-0.000012337
6	-0.000006159	0.000001824	0.000003147
6	0.000003063	0.00000298	0.000004983
6	-0.000000903	0.000003656	0.000000107
6	-0.000000321	0.000002974	0.000002739
6	-0.000001031	0.000002631	0.000001698
6	0.000000742	0.000001783	0.000001559
6	0.000002672	-0.000003092	0.000000995
6	-0.000008276	0.00000281	0.000001832
1	0.00000011	0.000002383	0.000002157
1	-0.000000421	0.00000264	0.000002253
1	-0.000000983	0.000002303	0.000001589
1	-0.000000904	0.000001596	0.000001237
1	-0.000003732	-0.00000043	-0.000002589
1	0.000001974	0.000006085	0.000000703
7	0.000001822	-0.000002926	-0.000001742
1	-0.000000342	0.000000335	0.000002002

Zero-point correction=	0.679683 (Hartree/Particle)
Thermal correction to Energy=	0.722233
Thermal correction to Enthalpy=	0.723178
Thermal correction to Gibbs Free Energy=	0.598555
Sum of electronic and zero-point Energies=	-2579.294753
Sum of electronic and thermal Energies=	-2579.252202
Sum of electronic and thermal Enthalpies=	-2579.251258
Sum of electronic and thermal Free Energies=	-2579.375880

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6	-0.000000611	0.000000079	0.000000644
6	0.000004486	-0.000000864	-0.000000512
7	0.000001778	0.000009148	-0.000003632
7	-0.000005742	0.000001107	-0.000001128
16	0.000001263	-0.000005747	0.000007651
8	-0.000000719	-0.00000003	0.000000899
8	-0.000000689	0.000000252	0.000002681
6	-0.000001139	0.00000215	0.000001253
6	0.000000831	0.000001947	0.000001066

6	-0.000001835	0.000002256	-0.000000094
6	0.000000894	-0.000003385	0.000000398
6	-0.000000378	0.000002067	0.000002736
6	-0.000002911	-0.000000428	0.000001105
1	-0.000000744	0.000000063	0.000000599
1	-0.000001182	0.000000076	0.000001794
1	-0.000000502	-0.000000821	0.000002916
1	0.000000036	0.000000019	0.000000214
6	0.000001307	-0.000002257	0.000002302
1	-0.000001503	0.000002154	0.000001486
1	-0.000001447	0.000003185	0.000001483
1	-0.000001863	0.000002308	0.000001304
6	-0.000002547	-0.000003332	-0.000001061
6	0.000001486	-0.000001175	0.000001697
1	0.000000497	-0.000000217	0.000000708
1	0.000001167	-0.000000638	0.000000524
6	0.000000976	-0.000001427	0.000000962
1	-0.000000049	-0.000000388	0.000001136
1	0.000000007	-0.000000626	0.000000708
6	0.000000995	-0.00000182	0.000001761
1	0.000000849	-0.000001564	0.000001068
1	0.000000885	-0.000001406	0.000001612
1	0.000001121	-0.000002028	0.0000018
1	0.000000645	-0.000001459	0.00000208
1	0.000000842	-0.000001665	0.000001452
6	0.000002341	0.000000399	-0.000001603
6	-0.000000757	0.000000407	-0.000000293
1	-0.000000082	0.000001119	0.000000014
1	-0.000000063	0.000000015	-0.000000642
6	-0.000000675	0.000000578	-0.000001909
1	-0.000000733	0.000000501	-0.000001407
1	-0.000000369	0.000000142	-0.000001989
6	0.000000083	0.000001745	-0.00000249
1	-0.000000456	0.000000084	-0.000002035
1	-0.000000448	0.000001079	-0.000001578
1	-0.000000638	0.000001202	-0.0000027
1	-0.000000517	0.000000788	-0.000001855
1	0.000000002	0.00000104	-0.000002561
16	0.00000371	-0.000002455	-0.000002253
8	-0.000000545	-0.000000508	0.000001393
8	0.000000328	-0.000000474	-0.000001026
6	0.000001085	-0.000002109	0.000000064
6	0.000000311	0.000000578	-0.000000182
6	0.000000187	-0.000000336	-0.000000994

6	0.000000216	-0.000000165	0.000000485
1	0.000000498	-0.000000295	0.000000858
6	0.000000393	-0.000000813	-0.000000456
1	0.000000851	-0.000000975	-0.000000834
6	0.000000198	-0.000000815	0.000000095
1	0.000000042	-0.000000167	0.000000705
1	0.000000691	-0.000000794	-0.000000463
6	0.000000507	-0.000000257	0.000000806
1	0.00000003	-0.000000265	0.000000449
1	0.000000031	-0.000000898	0.000000315
1	0.000000036	-0.000000736	0.000000813
1	0.000000004	0.000000256	-0.000001067
8	-0.000001038	0.000000703	0.000000036
6	0.000000444	0.000002079	0.000000053
6	-0.00000109	-0.000000312	0.000001049
6	-0.000000124	0.000000546	0.000000557
6	0.000000029	-0.000000278	0.000000351
6	0.000000152	-0.000000587	0.000000508
6	0.00000009	-0.000001113	0.000000177
6	0.000003906	-0.000005004	0.000000249
6	-0.000001903	0.000001718	-0.000000867
1	-0.000000561	0.000000046	0.000000058
1	0.000000218	-0.000000035	0.000000091
1	0.000000652	-0.000000868	0.000000617
1	0.000000257	-0.000001031	0.000000013
1	-0.000003783	0.000003228	-0.000001158
1	0.000000054	0.000000966	0.000000199
7	-0.000000001	-0.000000229	0.000000342
1	-0.000000885	0.000001035	0.000000088
7	0.000003575	0.000000207	-0.000002197
16	0.000001392	-0.00000101	-0.000002689
8	-0.000001154	0.000000222	-0.000001597
8	-0.000000247	0.000000285	-0.000001314
16	-0.000002038	0.000007856	0.000000139
8	0.000000271	-0.00000359	-0.000002836
8	-0.000000655	-0.000000021	0.000000136
6	0.000000151	-0.000002541	0.000002877
6	-0.000002385	-0.000000026	-0.000003189
9	-0.000000015	-0.000000026	-0.000001348
9	0.000000599	-0.000000506	-0.000005166
9	0.000001497	-0.000000654	-0.000003394
9	0.000000786	0.000000422	-0.000001257
9	0.000000179	0.000001153	-0.000001015
9	-0.000000234	0.000001916	-0.000000815

Zero-point correction=	0.733597 (Hartree/Particle)
Thermal correction to Energy=	0.792710
Thermal correction to Enthalpy=	0.793654
Thermal correction to Gibbs Free Energy=	0.629011
Sum of electronic and zero-point Energies=	-4406.554442
Sum of electronic and thermal Energies=	-4406.495329
Sum of electronic and thermal Enthalpies=	-4406.494385
Sum of electronic and thermal Free Energies=	-4406.659028

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6	-0.000000416	-0.000000277	0.00000081
6	-0.000000041	-0.000000726	-0.000000375
7	0.000000434	0.000001015	0.000001431
7	0.000000002	-0.000000303	-0.000000955
16	-0.000000005	-0.000001045	0.000002062
8	0.000000018	-0.000001372	0.000002137
8	-0.000000006	-0.000000071	0.000003298
6	0.000000506	-0.000001225	0.000002408
6	0.000000545	-0.000001047	0.000000573
6	-0.000001185	-0.000002152	0.00000042
6	0.000001214	-0.000003407	0.000001486
6	0.000000193	-0.000000789	0.00000059
6	-0.000001241	-0.000001065	0.000001943
1	-0.000000198	-0.000002442	0.000000479
1	-0.000000293	-0.000003152	-0.00000041
1	-0.000000118	-0.000000994	0.000001249
1	0.000000083	-0.000000212	0.000002346
6	0.000000161	-0.000003344	-0.000000662
1	-0.000000596	-0.000001758	0.000000869
1	-0.000000446	-0.000002919	0.000000283
1	-0.000000272	-0.000001676	-0.000000826
6	0.000000349	0.000001352	0.000001687
6	0.000000154	0.000001819	0.000001528
1	0.000000118	0.000001444	0.000002721
1	0.000000252	0.000002033	0.000001336
6	0.000000399	0.000002977	0.00000207
1	0.000000171	0.000001487	0.000001951
1	0.000000204	0.000001845	0.000000837
6	0.000000321	0.00000035	0.000001812
1	0.000000299	0.000003452	0.000001541
1	0.0000004	0.000003066	0.000002782
1	0.000000394	0.000004374	0.000002075
1	0.00000032	0.000003105	0.000002316
1	0.00000031	0.00000352	0.00000097

6	-0.00000053	-0.000001137	-0.000001992
6	-0.000000227	-0.000001287	-0.000002563
1	-0.000000107	-0.000001515	-0.000001659
1	-0.000000237	-0.000000606	-0.000002554
6	-0.000000286	-0.000002313	-0.000003444
1	-0.000000268	-0.000001702	-0.000001785
1	0.000000049	-0.000000581	-0.000002954
6	-0.000000383	-0.000002556	-0.000003933
1	-0.00000032	-0.000001769	-0.000004004
1	-0.000000313	-0.000002828	-0.000003009
1	-0.000000396	-0.000003064	-0.000004463
1	-0.000000274	-0.000002775	-0.000003375
1	-0.000000327	-0.000001886	-0.000004253
16	0.00000027	0.000000892	-0.000001633
8	-0.000000124	0.000001649	-0.000000683
8	0.000000091	0.000001216	-0.000002458
6	-0.000000008	0.000001133	-0.000001811
6	-0.000000121	0.000000776	-0.00000116
6	-0.000000169	0.000001199	-0.000002814
6	0.000000026	-0.000000047	-0.000000357
1	0.000000092	0.000000397	-0.00000013
6	-0.000000138	0.000001922	-0.000004143
1	0.000000026	0.000001676	-0.000003307
6	-0.000000035	0.000001087	-0.000001922
1	-0.000000014	0.000000609	-0.000000815
1	0.000000007	0.000001694	-0.000003674
6	0.000000066	0.000000092	-0.000002435
1	-0.000000164	0.000001201	-0.000002545
1	0.000000062	0.000000964	-0.00000249
1	0	0.000000975	-0.000002827
1	0.000000214	0.000001032	0.00000046
8	-0.000000245	-0.00000174	-0.000000043
6	0.000000402	0.00000038	0.00000204
6	0.000000126	-0.0000006	0.000002507
6	0.000000105	-0.000000223	0.000003742
6	0.000000183	0.000000756	0.000003875
6	0.000000219	0.000001538	0.000003327
6	0.000000228	0.00000116	0.000002614
6	0.000001468	-0.000002383	-0.000000228
6	0.000000145	-0.000001233	0.000002102
1	0.000000126	-0.00000083	0.000004147
1	0.000000259	0.000001054	0.000004609
1	0.000000361	0.000002364	0.000003522
1	0.000000279	0.000001853	0.00000195

1	-0.000000027	0.000000336	0.000000674
1	0.000000195	-0.000002458	0.00000109
7	-0.000000398	-0.000001379	0.000002424
1	0.000000154	-0.000002289	0.000002683
7	-0.000002302	-0.000000526	0.000000552
16	0.000000621	0.000002348	-0.000000271
8	-0.000000187	0.000001516	-0.000000811
8	-0.000000156	0.000001953	0.000000474
16	0.000000373	-0.000000153	-0.000000977
8	0.000000474	-0.000000832	-0.000000667
8	-0.000000467	-0.000001374	-0.000000034
6	-0.000000157	0.000001415	-0.000001894
6	-0.000000005	-0.000001337	0.000000452
9	-0.000001584	0.000000469	-0.000000379
9	0.000000658	0.000002282	-0.000002053
9	0.000000331	0.000001145	-0.00000148
9	-0.000000191	-0.000000139	-0.000000098
9	-0.000000013	-0.000000966	0.00000171
9	0.000000015	-0.000002395	0.000000107

Zero-point correction=

0.728810 (Hartree/Particle)

Thermal correction to Energy=

0.787702

Thermal correction to Enthalpy=

0.788646

Thermal correction to Gibbs Free Energy=

0.623381

Sum of electronic and zero-point Energies=

-4406.552228

Sum of electronic and thermal Energies=

-4406.493336

Sum of electronic and thermal Enthalpies=

-4406.492392

Sum of electronic and thermal Free Energies=

-4406.657656

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6	-0.000013308	0.000001096	0.000009265
6	0.000006527	-0.000004579	-0.000015051
7	0.000006303	0.000020822	-0.000017725
7	-0.000005546	0.000002365	-0.000006771
16	0.000004584	-0.000012067	0.000018085
8	-0.000001304	0.00000046	-0.000000069
8	-0.000000762	0.000000054	-0.000000824
6	-0.000000485	-0.000000088	-0.000001397
6	-0.000000518	-0.000000729	0.000000062
6	-0.000001597	-0.000001603	0.000000119
6	0.00000141	-0.000000368	0.000000062
6	-0.000000218	0.000000212	0.000001562
6	-0.000002046	-0.000003125	0.000000943
1	0.000000622	0.000000485	0.000000893
1	-0.000000246	-0.000000838	0.000000723



1	-0.00000681	-0.000002018	0.000001247
1	-0.000001328	0.000000051	0.000001197
6	-0.0000002	-0.000001558	0.000001387
1	-0.000000398	-0.000001867	0.000001616
1	-0.000000152	-0.000001956	0.000001649
1	-0.000000682	-0.000001816	0.000001527
6	-0.000004827	-0.000009021	-0.000004706
6	0.000001992	0.000000218	0.000004355
1	-0.000000883	0.000000573	-0.000000638
1	0.000002218	0.000000995	-0.00000018
6	-0.000000352	-0.000000785	-0.00000204
1	-0.000000632	-0.000000663	-0.000000699
1	-0.000001333	0.000000069	-0.000000595
6	0.00000104	-0.000000141	0.000000546
1	0.000000498	0.000000542	0.000000015
1	-0.000000015	0.000000015	0.000000366
1	0.000000229	-0.000000004	0.000000016
1	-0.000000173	-0.000000802	0.000000759
1	0.000000778	-0.000000085	0.000000132
6	0.000002913	0.000002574	0.000002512
6	0.00000068	0.000002773	0.000000541
1	-0.000001124	0.000000259	-0.000001212
1	0.000001351	-0.000001094	-0.000000036
6	0.000000018	-0.000001614	0.000000536
1	0.00000061	-0.000000608	0.000000239
1	0.000001142	0.000000719	-0.000000078
6	0.000002074	-0.000006017	-0.000005969
1	0.000001653	0.000000843	0.000001116
1	0.000000364	0.000000095	-0.000000956
1	0.000000997	0.00000141	-0.000000972
1	-0.000001175	0.000000391	0.0000007319
1	0.00000123	0.000001075	-0.000000033
16	0.000006592	0.000000916	0.000000411
8	-0.00000307	-0.00000246	-0.000000079
8	-0.000000701	0.000000536	0.000002027
6	0.000003954	-0.00000979	0.00000468
6	0.000000052	0.000003335	-0.000000034
6	0.000000756	0.000003932	-0.000001969
6	0.000002468	-0.000000105	-0.000000087
1	0.000000846	0.000000182	0.000001595
6	0.000000545	-0.000000762	0.000002266
1	0.000002549	-0.000000345	0.000001302
6	0.000001277	-0.000002209	0.000001133
1	0.000000641	-0.000001271	0.000002154

1	0.000001971	-0.00000033	0.000001221
6	0.000001744	-0.00000242	0.000001164
1	0.000001366	-0.00000024	0.000001685
1	0.000001799	-0.000001307	0.000001358
1	0.000000809	-0.000001532	0.000002537
1	0.000000549	-0.000000177	-0.000002378
8	-0.000003333	-0.000000337	0.000011986
6	-0.00000259	0.000000156	-0.000002568
6	-0.000000362	0.000004611	-0.000004135
6	-0.000000099	0.000000325	-0.000001401
6	0.000000091	0.000002483	-0.000001941
6	-0.000000166	0.000001073	-0.000000772
6	-0.000000182	0.000002401	-0.000000137
6	0.000004019	0.000003952	-0.000005096
6	-0.000005683	0.000000465	0.000003267
1	-0.000000341	0.000001762	-0.000001582
1	0.000000285	0.000001899	-0.000002004
1	0.000000771	0.000001772	-0.000001198
1	-0.000000028	0.000000279	-0.000000431
1	0.000005566	-0.000006579	-0.000007557
1	-0.000003023	0.000000416	-0.000002664
7	0.000006537	-0.000008623	-0.000001848
1	-0.00000303	0.000006901	0.000000781
7	-0.000015792	0.000012395	0.000005242
16	-0.000007654	0.00000216	-0.000000058
8	-0.000001254	0.000005738	-0.000002741
8	-0.000000428	-0.000000813	0.000001035
16	0.000013568	0.00000549	0.000000064
8	-0.000003169	-0.000002381	0.000000272
8	-0.000003314	-0.000003003	-0.000003416
6	0.00000165	0.00000412	0.000006571
6	0.000015032	0.000009334	0.000000987
9	0.000002247	-0.000004517	-0.000000513
9	-0.000008288	-0.000007452	-0.000004044
9	0.0000033	-0.000003844	-0.000000064
9	-0.000005988	-0.000005274	-0.00000354
9	-0.000001865	0.000000813	-0.000002633
9	-0.000009737	0.000000155	-0.000000091
<b>Zero-point correction=</b>			<b>0.733773 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>0.793345</b>
<b>Thermal correction to Enthalpy=</b>			<b>0.794290</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>0.627505</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-4406.581735</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-4406.522163</b>

Sum of electronic and thermal Enthalpies= -4406.521219  
Sum of electronic and thermal Free Energies= -4406.688004

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6	-0.00001899	0.00000415	0.000003268
6	-0.00000774	-0.000010838	-0.000006916
7	-0.00002418	0.000002169	0.000004149
7	-0.00001131	0.00001293	0.000000342
16	-0.00000621	0.000003009	0.000001085
8	0.00001859	0.000000455	0.000001206
8	0.00000585	0.000001782	0.00000144
6	0.000001	0.000000847	0.000001029
6	0.00000466	0.000000612	0.000001169
6	-0.00000006	0.000000259	0.00000193
6	-0.00000456	0.000003413	0.000000823
6	0.000001121	0.000001578	0.000001316
6	-0.00000117	0.000002052	0.000001293
1	0.000001128	0.000000546	0.000001404
1	0.000001017	0.000001028	0.000001573
1	0.000000333	0.000003504	0.000002213
1	0.000000155	0.000002903	0.00000177
6	0.000001403	0.00000175	0.000002564
1	0.000000196	0.000000717	0.000002213
1	0.000001235	0.000002401	0.000001646
1	0.000001446	0.000001715	0.000002966
6	-0.000000545	0.000001036	-0.000000156
6	-0.000001254	0.000001811	-0.000000264
1	-0.000001037	0.00000168	-0.000000279
1	-0.000000743	0.000002746	0.000000495
6	-0.00000202	0.000002311	-0.000000589
1	-0.000001603	0.00000158	-0.000000866
1	-0.000001775	0.000002234	-0.000000465
6	-0.000002534	0.000002708	-0.000001204
1	-0.000001831	0.000003236	-0.000000363
1	-0.00000221	0.000002423	-0.000000934
1	-0.000002975	0.000003112	-0.000001333
1	-0.000002621	0.000002296	-0.00000172
1	-0.000002685	0.000002922	-0.000001144
6	0.000000888	-0.000004658	0.000001505
6	0.000001775	0.000003019	0.000001794
1	0.000000251	-0.000001783	0.000000049
1	0.000001164	-0.000002024	-0.000000446
6	0.000001879	-0.000002618	0.000000671
1	0.00000024	-0.000000793	0.000000321

1	0.000001512	-0.000006325	0.00000078
6	0.000002265	-0.000001724	0.000001346
1	0.000001833	-0.000001912	0.000000944
1	0.000001776	-0.000002513	0.000000315
1	0.000002691	-0.000002288	0.000001593
1	0.000002003	-0.00000171	0.0000012
1	0.000002153	-0.000001342	0.000001856
16	-0.000000268	-0.000001172	-0.000003376
8	-0.000000549	-0.000000475	-0.000001145
8	0.00000037	-0.000001491	-0.000000973
6	-0.000000979	-0.000001751	-0.000001645
6	-0.000000945	-0.000001664	-0.000001975
6	-0.000000465	-0.000002152	-0.000001926
6	-0.000001155	-0.000001722	-0.000002283
1	-0.000001228	-0.000000623	-0.000001885
6	-0.000000577	-0.000002893	-0.000002045
1	-0.000000057	-0.000002562	-0.00000185
6	-0.000000801	-0.000002681	-0.000002668
1	-0.000001233	-0.000001553	-0.00000258
1	-0.000000169	-0.000003544	-0.000002452
6	-0.000001392	-0.000003194	-0.000002907
1	-0.00000123	-0.000003157	-0.000003581
1	-0.000000921	-0.000002831	-0.000002691
1	-0.00000043	-0.00000363	-0.000003011
1	-0.000000405	-0.000000051	-0.000001035
6	0.000000296	-0.000001023	0.000000777
6	0.000000209	0.000000491	-0.000001137
6	0.000000402	-0.000001417	0.00000045
6	0.000001068	-0.000001362	0.000001203
6	0.00000137	-0.000001268	0.000002066
6	-0.000000003	0.000000521	0.000001604
6	0.000003325	-0.000002183	-0.000000899
6	-0.000000691	0.000003852	-0.000002932
1	0.000000648	-0.000001292	-0.000000235
1	0.000001695	-0.000001574	0.000000865
1	0.000002207	-0.000000507	0.000001305
1	0.000001145	0.000003035	0.000000836
1	0.000001155	0.000000366	0.000003025
1	-0.000000807	0.000000937	-0.000000191
7	-0.000000426	-0.000002647	0.000003877
1	-0.000000219	0.000000811	-0.000002177
Zero-point correction=			0.669157 (Hartree/Particle)
Thermal correction to Energy=			0.712137
Thermal correction to Enthalpy=			0.713081

Thermal correction to Gibbs Free Energy=	0.586630
Sum of electronic and zero-point Energies=	-2504.017908
Sum of electronic and thermal Energies=	-2503.974928
Sum of electronic and thermal Enthalpies=	-2503.973984
Sum of electronic and thermal Free Energies=	-2504.100435

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6	-0.000003265	0.000000477	0.000000419
6	0.000003028	0.000006753	0.000001513
7	0.000001824	-0.000003942	0.000005313
7	0.000000415	-0.000016778	0.000000213
16	-0.000005024	-0.000003502	-0.000000197
8	0.000000736	0.000000091	-0.000001127
8	-0.000001649	-0.000001747	0.000001006
6	0.000002742	-0.000001179	0.000000467
6	-0.000001143	-0.000003063	-0.000000455
6	0.000000911	-0.000000008	0.000000864
6	0.00000117	0.000001665	0.00000122
6	0.000000195	-0.000001292	0.000001717
6	-0.000003325	0.000001754	0.000000061
1	-0.000000782	-0.000001563	0.000001919
1	0.000000892	-0.000003391	0.000000981
1	0.000000692	-0.000004222	0.000002071
1	0.00000095	-0.000004046	0.000001527
6	0.000003453	-0.000009028	0.000003107
1	0.000000299	-0.000000909	0.000000731
1	0.000000272	-0.0000003	0.000001326
1	-0.000001524	-0.000000344	0.000002839
6	-0.000000337	0.000003969	0.000001941
6	-0.000000735	-0.000002307	-0.000003569
1	0.00000075	-0.00000192	0.000001065
1	-0.000002183	-0.00000212	0.000000441
6	0.000000561	0.000001103	0.000003545
1	0.000002447	-0.000001128	-0.000000075
1	0.000000057	-0.000000286	0.0000017
6	0.0000007	-0.000001581	-0.000000086
1	-0.00000039	-0.000001476	0.000000637
1	0.000000432	-0.000001165	0.000000663
1	0.000000521	-0.000001063	0.000000929
1	0.000000527	-0.000000645	0.000000657
1	-0.000000533	-0.000000389	0.000001214
6	-0.000000526	0.000003003	-0.000003157
6	-0.000002471	-0.000002223	-0.000005704
1	0.000002553	0.000000923	-0.000001174

1	0.000001449	-0.00000055	-0.000000537
6	-0.000000857	0.00000243	0.000002245
1	-0.000000567	0.000002737	-0.000001004
1	0.000004038	0.000000142	0.000007832
6	-0.00000032	-0.000001112	0.000000078
1	-0.000000055	0.000000865	-0.000001127
1	0.000000475	-0.000000099	-0.000000221
1	0.000000223	0.000000715	-0.000000359
1	-0.000000994	0.000000731	-0.000000889
1	-0.000001524	0.000001176	-0.000000964
16	-0.000006026	0.000012103	0.000001815
8	0.000002905	-0.000000659	-0.000001168
8	0.00000018	0.000001598	-0.00000183
6	0.000001292	0.000000596	0.000003906
6	0.000000426	0.000002054	-0.000000007
6	0.000004297	0.000000253	-0.000001288
6	0.000001937	0.000002492	-0.000002285
1	0.000000007	0.000000185	-0.000000849
6	0.000000206	-0.000000921	-0.000000913
1	0.000000029	0.000004079	-0.000002205
6	0.000002942	0.000001816	0.000002227
1	0.000002045	0.000000501	0.000000235
1	0.000002961	0.000001411	-0.000000589
6	0.000003885	0.000000616	-0.000000898
1	0.000003144	0.000000667	0.000000558
1	0.000003069	0.000000584	0.000000455
1	0.000003426	0.000001	0.000000222
1	-0.000000416	-0.000002901	-0.000001239
6	-0.000000084	0.000000555	-0.000004507
6	-0.00000056	0.000000343	-0.000000358
6	-0.000002541	-0.00000042	-0.000001719
6	-0.000003381	0.00000078	-0.000001314
6	-0.000001719	0.000001969	-0.000001821
6	-0.000003617	0.000003073	-0.00000167
6	-0.000001785	0.000002652	-0.000006178
6	-0.0000003	-0.000000399	0.000005209
1	-0.000002308	0.00000239	-0.000001673
1	-0.000002861	0.000001449	-0.000001726
1	-0.000002502	0.000000811	-0.00000142
1	-0.000001789	0.000000666	-0.00000367
1	-0.000003707	0.000001848	0.000001229
1	-0.000000157	0.000000928	-0.000001993
7	-0.000002232	0.000002045	-0.00000398
1	-0.000000874	0.000000681	-0.000000155

Zero-point correction=	0.673707 (Hartree/Particle)
Thermal correction to Energy=	0.715633
Thermal correction to Enthalpy=	0.716577
Thermal correction to Gibbs Free Energy=	0.591814
Sum of electronic and zero-point Energies=	-2504.056666
Sum of electronic and thermal Energies=	-2504.014740
Sum of electronic and thermal Enthalpies=	-2504.013796
Sum of electronic and thermal Free Energies=	-2504.138558

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6	-0.000000579	-0.000000702	-0.000000733
6	-0.000000387	0.000001993	0.000003381
7	0.000000919	0.000000429	-0.000000679
7	-0.000000424	-0.000000808	-0.000001526
16	-0.000000267	-0.000000193	0.000000171
8	-0.000000003	0.000001244	0.000000842
8	-0.000000385	0.000000156	0.000000272
6	0.000000733	-0.000001082	-0.000000553
6	0.000000017	-0.000000385	0.000000274
6	0.000000366	-0.000000861	0.000000444
6	0.000000811	-0.000000088	-0.000000282
6	0.000000125	-0.000000703	-0.000000131
6	-0.000000016	-0.000000517	0.000000003
1	0.000000703	-0.000000748	0.000000502
1	0.000000535	-0.000000912	0.000000402
1	0.000000276	-0.000000044	0.000000184
1	0.000000151	-0.000000047	0.000000144
6	0.000000588	-0.000001196	0.000000275
1	0.000000452	-0.000000985	0.000000547
1	0.000000068	-0.000001213	0.000000564
1	0.000000591	-0.000001337	0.000000163
6	-0.000000529	0.000000053	0.000000131
6	-0.000000404	-0.000000299	-0.000001269
1	-0.000000145	-0.000000743	-0.000000869
1	-0.000000047	-0.000000036	-0.000000052
6	-0.000000512	-0.000000151	-0.000000862
1	-0.000000506	0.000000033	-0.000000944
1	-0.000000389	-0.000000336	-0.000000915
6	-0.000000397	-0.000000019	-0.000001544
1	-0.000000438	-0.000000218	-0.000001067
1	-0.000000505	-0.000000411	-0.000001198
1	-0.000000784	-0.000000113	-0.000001632
1	-0.000000881	0.000000157	-0.000001557
1	-0.000000795	0.000000329	-0.000001297

6	0.000000113	0.000000338	0.000000807
6	-0.000000477	0.000000884	-0.000000611
1	0.000000259	0.000000406	0.000000501
1	-0.000000114	0.000000258	0.000000757
6	-0.000000297	0.000000086	0.000000387
1	-0.000000813	0.000000257	-0.000000015
1	-0.000000256	0.000000729	-0.000000063
6	-0.000000391	0.000001269	-0.000000254
1	-0.000000354	0.000000928	0.000000023
1	-0.000000163	0.000001077	0.000000345
1	-0.000000491	0.000001507	0.000000088
1	-0.000000537	0.000001266	0.000000056
1	-0.000000549	0.000001249	-0.000000027
16	0.000001488	-0.000000306	0.000001227
8	-0.000000893	-0.000001301	0.000000079
8	0.000000329	0.000000421	-0.000000084
6	0.000000079	-0.000000168	0.000000395
6	0.000000326	-0.000000625	0.000000414
6	0.000001024	-0.000000187	0.000001241
6	0.000000244	0.000000503	0.000000734
1	-0.000000092	0.000000002	0.000000028
6	0.000000161	0.000000325	0.000000925
1	0.000000037	-0.000000057	0.000000366
6	0.000001562	-0.000000095	0.000002099
1	0.000000281	0.000000212	0.000001234
1	0.000000615	0.000000439	0.000001395
6	0.000001283	0.000000784	0.000001871
1	0.000000701	0.000000139	0.000001691
1	0.000000531	-0.000000537	0.000001658
1	-0.000000012	0.000000937	0.000001094
1	-0.000000459	-0.000000063	-0.000000802
6	0.000000159	0.000000156	-0.000000688
6	-0.000000069	-0.000000517	-0.000001359
6	-0.000000014	0.000000083	0.000000269
6	-0.000000677	0.000000047	-0.000000009
6	-0.000000206	0.000000505	-0.000000087
6	0.000000575	0.000000096	-0.000000007
6	-0.000001436	-0.000000058	-0.000002237
6	0.000001206	-0.000000056	-0.000001975
1	0.000000172	0.000000093	0.000000114
1	-0.000000141	0.000000552	0.000000022
1	-0.000000399	0.000000703	-0.000000327
1	-0.000000338	0.000000557	-0.000000032
1	-0.000000092	0.000000078	-0.000000626



1	0.00000071	-0.00000488	-0.00000684
7	0.00000491	-0.00000153	0.000001
1	-0.00000404	-0.000000803	0.000000133
Zero-point correction=			0.671310 (Hartree/Particle)
Thermal correction to Energy=			0.713610
Thermal correction to Enthalpy=			0.714554
Thermal correction to Gibbs Free Energy=			0.590612
Sum of electronic and zero-point Energies=			-2504.023180
Sum of electronic and thermal Energies=			-2503.980881
Sum of electronic and thermal Enthalpies=			-2503.979937
Sum of electronic and thermal Free Energies=			-2504.103878

#### B-1b

6	0.000002732	0.000004776	0.00000201
6	0.000001104	-0.000013732	0.000007185
7	-0.000000991	0.000000367	-0.00000036
7	-0.000000123	0.000010602	-0.000004856
16	-0.000007762	-0.000006293	-0.000001149
8	0.000003134	-0.000005264	0.000000284
8	0.000001123	-0.000001435	-0.000000451
6	0.000002704	-0.000000626	-0.000001393
6	0.000001648	-0.000002282	-0.000000034
6	0.000000236	-0.000002118	-0.000000838
6	0.000000908	-0.000002913	-0.000001124
6	0.000000251	-0.000003676	0.000000175
6	-0.00000048	-0.000003086	0.000000255
1	0.000001614	-0.000001682	-0.000000663
1	0.00000155	-0.000001846	-0.000000805
1	-0.00000041	-0.000004139	-0.000000034
1	-0.000000943	-0.000003094	-0.000000591
6	0.000000828	-0.000003409	-0.000000888
1	0.000000546	-0.000004118	-0.000000093
1	0.000001553	-0.000003201	-0.000001179
1	0.00000036	-0.00000291	-0.000000712
6	-0.000003323	-0.000001844	-0.000001127
6	-0.00000264	0.000000258	0.000000014
1	-0.000002876	-0.000000901	0.000000634
1	-0.000001478	-0.000002068	0.000003411
6	-0.000002938	-0.000002414	0.000001797
1	-0.000002534	-0.000000139	0.000002181
1	-0.000002087	-0.00000219	0.000001364
6	-0.000004292	-0.000001437	0.000001794
1	-0.000003604	-0.000002266	0.000001395
1	-0.00000393	-0.000001019	0.000001654

1	-0.000004859	-0.000001738	0.000002077
1	-0.000004251	-0.000000781	0.000002071
1	-0.000004152	-0.000001723	0.000001816
6	-0.000002036	-0.000000678	-0.000000943
6	-0.000000633	0.000000104	0.000000619
1	0.000001041	0.000001598	-0.00000018
1	0.000000456	0.000003692	0.000000882
6	-0.00000028	0.000001	0.000000015
1	-0.000000192	-0.000000704	-0.000000664
1	-0.000000628	0.000000406	-0.000000027
6	-0.000001498	0.000000489	0.000000905
1	-0.000000658	0.000001611	0.000000855
1	0.000000264	0.000000792	0.000000043
1	-0.000001424	0.000000327	0.000000746
1	-0.000001012	-0.000000656	0.000000317
1	-0.000001939	0.000000079	0.00000112
16	0.000005803	0.000000054	-0.000002471
8	0.000000083	0.000001933	-0.000002454
8	-0.000000794	0.000004259	-0.000000045
6	-0.00000011	-0.000000061	0.000001927
6	0.000004101	0.000000507	-0.000001136
6	0.000002649	0.000001548	-0.000003404
6	0.000002011	0.000000231	-0.000003032
1	0.00000231	-0.000000345	-0.000000732
6	0.000001773	-0.000000401	-0.000000072
1	0.000002531	0.000002243	-0.000000042
6	0.000006132	-0.000000772	-0.000001053
1	0.00000347	-0.000001693	-0.000001669
1	0.000004399	0.000000952	-0.000001977
6	0.000004054	0.000001346	-0.000002166
1	0.000004826	-0.000001112	-0.000002216
1	0.000004521	-0.000002156	-0.000002722
1	0.000004169	-0.000001047	-0.00000261
1	0.000000231	0.000000672	0.000001
6	0.000000137	0.000002422	0.00000216
6	0.000000205	0.000006191	0.000001113
6	0.000000392	0.00000414	0.000000906
6	-0.000000792	0.000003993	0.000001375
6	-0.000002497	0.00000318	0.000001443
6	-0.000000683	0.00000246	0.000001222
6	-0.000005509	0.000004529	-0.000004579
6	0.000003048	0.000006637	0.000000121
1	0.000000072	0.000005175	0.000000477
1	-0.000001249	0.000005212	0.000001608

1	-0.000002032	0.000003538	0.0000015
1	-0.000001226	0.000001854	0.000001026
1	-0.000001747	0.000000275	-0.00000048
1	0.000000328	0.000001068	0.000000166
7	0.000000312	-0.000001039	0.000002418
1	0.000001004	0.000004486	-0.000001049
Zero-point correction=			0.673549 (Hartree/Particle)
Thermal correction to Energy=			0.715478
Thermal correction to Enthalpy=			0.716422
Thermal correction to Gibbs Free Energy=			0.591922
Sum of electronic and zero-point Energies=			-2504.041948
Sum of electronic and thermal Energies=			-2504.000019
Sum of electronic and thermal Enthalpies=			-2503.999075
Sum of electronic and thermal Free Energies=			-2504.123575

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6	0.000001013	-0.000002058	-0.000000789
6	0.000005946	0.000004202	0.000003522
7	-0.000002269	0.000003133	-0.000001915
7	-0.000002105	-0.000002084	-0.000001328
16	0.000001479	-0.000003516	0.000002171
8	-0.000000625	0.000001018	-0.000000974
8	-0.000000417	0.000001201	-0.000001189
6	-0.000000295	0.000001412	0.000000282
6	-0.000000152	0.000001984	0.000000812
6	0.000000129	0.000002723	0.00000112
6	-0.000000108	0.000001692	0.000000369
6	-0.000000258	0.000001633	0.000000305
6	-0.000000285	0.00000114	-0.000000091
1	-0.000000142	0.000001691	0.000000364
1	0.000000067	0.000002426	0.000000933
1	-0.000000206	0.000001665	0.000000323
1	-0.000000392	0.000000907	-0.000000191
6	0.000000201	0.000003055	0.000001067
1	0.000000378	0.000002912	0.000001388
1	-0.000000362	0.000003027	0.00000131
1	0.000000544	0.000002718	0.000001491
6	0.000000787	-0.000001221	0.000000949
6	0.000000282	-0.000001177	0.000000586
1	0.000001123	0.000000273	0.000000466
1	-0.000000301	0.000000441	-0.000000004
6	0.000000829	-0.00000155	0.000000866
1	0.000000391	-0.000000651	0.000000406
1	0.000000686	-0.000000959	-0.000000274

6	0.000001087	-0.000001983	0.000000695
1	0.000000662	-0.000000976	0.000000377
1	0.000001255	-0.000000806	0.000001123
1	0.000001381	-0.000002004	0.000000889
1	0.000001309	-0.000002054	0.000000779
1	0.000000812	-0.00000217	0.00000032
6	0.000000237	0.000001017	-0.000000247
6	-0.000001012	0.000000217	-0.000001378
1	-0.000000376	0.000000442	0.00000017
1	-0.000000401	0.000000841	0.000000064
6	-0.000001126	0.000001213	-0.000000754
1	-0.000000938	0.000001004	-0.000000375
1	-0.000000679	0.000000994	0.000001378
6	-0.000001526	0.000001586	-0.000001344
1	-0.000000946	0.000001438	-0.000000599
1	-0.000000964	0.000001742	-0.000000443
1	-0.000001633	0.000002026	-0.000001312
1	-0.000001725	0.000001592	-0.000001487
1	-0.000001645	0.000001168	-0.000001502
16	-0.000000743	-0.000000649	0.000000019
8	0.00000072	-0.000001644	-0.000000069
8	-0.000000571	-0.000000066	-0.000000953
6	0.000000622	-0.000000304	0.000000638
6	0.000000581	-0.000000601	0.000000721
6	0.000000683	-0.000000071	0.000000058
6	0.000001112	-0.000000276	0.000001285
1	0.000001037	-0.000000069	0.000000936
6	0.000000775	0.000000029	0.000000815
1	-0.000000091	-0.000000134	-0.000000134
6	0.000000827	0.000000007	0.000001332
1	0.000001455	-0.000000359	0.000001652
1	0.000000494	0.000000255	0.000000679
6	0.000001489	0.000000089	0.000001543
1	0.000001664	0.000000381	0.000002215
1	0.00000121	0.000000057	0.00000175
1	0.000001574	-0.000000022	0.000001813
1	0.000000751	0.000000288	0.00000102
6	-0.000000207	-0.00000189	0.000000213
6	0.00000005	-0.000003439	-0.000000172
6	-0.000000791	-0.000000918	-0.000001444
6	-0.000000022	-0.000002477	-0.000001233
6	-0.000000052	-0.000002922	-0.000001012
6	-0.000000341	-0.000002681	-0.000001705
6	-0.000001818	-0.000001583	-0.000004759

6	-0.000003361	0.000000202	-0.000000308
1	-0.000000495	-0.000001836	-0.000001295
1	-0.000000232	-0.000002921	-0.000001332
1	-0.000000147	-0.000003208	-0.000001293
1	-0.00000003	-0.000002417	-0.000001251
1	-0.000001873	0.000000488	-0.000002408
1	-0.000000024	-0.00000401	-0.000001474
7	-0.000004721	0.000006793	-0.000002397
1	0.000001054	-0.000004512	-0.000002262
Zero-point correction=			0.669256 (Hartree/Particle)
Thermal correction to Energy=			0.712087
Thermal correction to Enthalpy=			0.713031
Thermal correction to Gibbs Free Energy=			0.585582
Sum of electronic and zero-point Energies=			-2504.012172
Sum of electronic and thermal Energies=			-2503.969341
Sum of electronic and thermal Enthalpies=			-2503.968397
Sum of electronic and thermal Free Energies=			-2504.095846

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6	-0.000002752	0.000000222	-0.000004088
6	0.000004748	0.000004548	0.000003601
7	0.000002443	-0.000001625	0.00000327
7	-0.00000025	0.000005068	-0.000000162
16	-0.000000859	0.00000057	-0.000001718
8	0.000002358	-0.000001274	-0.000001394
8	-0.000003992	-0.000002875	0.000001217
6	0.000000298	0.000002053	0.000002823
6	-0.000000304	-0.000000315	0.000001
6	0.000002329	-0.000001194	0.000000221
6	-0.000002579	-0.000001401	0.000001213
6	0.000000114	0.000003276	-0.000001384
6	-0.000000721	-0.000002922	-0.000000792
1	-0.000000257	0.000001469	-0.000000367
1	-0.000000661	-0.000000224	0.000000514
1	-0.000000424	-0.000000799	0.000000472
1	0.000001002	-0.000000562	0.000000858
6	0.000001515	-0.000000024	-0.000000034
1	-0.000000005	-0.000000006	0.000001095
1	-0.000001773	-0.000001031	0.000000087
1	-0.000000848	-0.000000401	-0.000000825
6	0.000000387	-0.000000586	0.000000258
6	0.000000483	0.000001161	0.000001117
1	-0.000000343	0.000000375	0.000000005
1	-0.000000764	-0.000000284	-0.000001432

6	0.000000936	-0.000000543	0.000000283
1	0.000000559	-0.000000583	0.000000034
1	0.000000165	-0.000000156	0.000000373
6	0.000000146	0.000000202	-0.00000034
1	0.000000273	0.000000016	0.000000628
1	0.00000068	0.000000023	0.000000046
1	0.000000749	-0.000000032	0.000000406
1	0.000000746	0.00000003	-0.000000052
1	0.000000586	-0.000000184	0.000000472
6	-0.000001477	-0.000002514	-0.000000488
6	0.000000449	0.000000789	0.000001086
1	-0.000000217	0.000000999	-0.000000717
1	0.000000183	-0.000000073	0.000000229
6	-0.000000821	-0.00000012	-0.000000846
1	-0.00000002	-0.000000671	-0.000000921
1	-0.000000658	-0.000000513	-0.000000771
6	-0.000000358	-0.000000213	0.000000879
1	-0.000000413	0.000000024	-0.000000446
1	-0.000000775	0.000000069	-0.000000034
1	-0.000000711	0.000000044	-0.000000105
1	-0.000000622	-0.000000133	-0.000000277
1	-0.000000692	-0.000000015	-0.000000364
16	-0.000000119	-0.000011289	0.000002466
8	0.000001992	0.000006141	-0.000002686
8	-0.000000487	0.000001836	0.000000214
6	-0.000000319	0.000001324	-0.000000123
6	0.000000021	-0.000000235	-0.000000158
6	0.000000764	0.000000493	0.00000008
6	-0.000000237	0.000001559	-0.000000204
1	0.000000192	0.000000334	-0.000000071
6	0.000000849	-0.000000687	-0.000000856
1	-0.000000668	0.000000206	-0.000000512
6	-0.000000128	-0.000000193	0.000000385
1	0.000000143	0.000000057	-0.000000036
1	-0.000000259	0.000000606	-0.000000781
6	-0.000000941	0.000000804	-0.000000402
1	0.000000649	-0.000000225	-0.000000162
1	-0.000000203	0.000001033	-0.000000624
1	0.000001109	0.000000563	-0.000000156
1	-0.000000102	0.000000551	-0.000000553
6	0.000004105	0.000001991	-0.000001219
6	-0.000003046	0.000000411	-0.000000259
6	0.000000294	-0.000000399	0.000000589
6	-0.000000622	0.000000268	0.000000543

6	0.000000903	0.000000983	-0.000000737
6	0.000000165	-0.000001664	0.000000726
6	-0.00000286	0.000000614	-0.00000031
6	-0.000001804	-0.000005748	-0.000004415
1	0.000000192	-0.000000397	0.000000382
1	0.000000415	-0.000000031	0.000000299
1	0.000000339	0.000000073	-0.000000002
1	-0.000000054	-0.000000026	-0.000000135
1	0.000001619	-0.000000015	0.000001877
1	-0.000003061	0.000000494	0.000000263
7	0.000006005	-0.000001462	0.000004748
1	-0.00000289	0.000001693	-0.00000233
<b>Zero-point correction=</b>			<b>0.672044 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>0.714411</b>
<b>Thermal correction to Enthalpy=</b>			<b>0.715356</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>0.588414</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-2504.049831</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-2504.007463</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-2504.006519</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-2504.133461</b>

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6	-0.000000528	0.000000063	-0.000000753
6	-0.000000798	-0.000000359	-0.000000019
7	0.000000208	-0.000000051	-0.000000167
7	-0.000000013	0.000000412	0.000000506
16	0.000000349	-0.000000152	-0.000000903
8	0.000000577	-0.000000061	0.000000016
8	0.000001629	-0.000000252	-0.000001179
6	-0.000000003	-0.000000137	-0.000001327
6	-0.000001115	-0.000000187	-0.000001101
6	-0.000001632	0.000000005	-0.000001016
6	-0.000000972	-0.000000288	-0.000002214
6	-0.000000145	-0.000000502	-0.000002152
6	0.000000204	-0.000000549	-0.000001611
1	-0.000001298	-0.000000001	-0.000000524
1	-0.000002111	-0.000000048	-0.000001032
1	0.000000323	-0.000000389	-0.000002466
1	0.000001172	-0.000000355	-0.000001925
6	-0.000000097	-0.000000087	-0.000001851
1	-0.000001873	-0.000000187	-0.000001335
1	-0.000002433	-0.000000454	-0.000002219
1	-0.000001472	-0.000000628	-0.000002618
6	0.000000282	-0.000000028	-0.000002392

6	0.000000987	-0.000000461	-0.000002746
1	-0.00000038	-0.000000561	-0.000002716
1	0.0000003	-0.000000493	-0.000002521
6	0.000001054	-0.000000594	-0.000003772
1	0.00000072	-0.000000456	-0.000002364
1	0.000001671	-0.000000468	-0.000002332
6	0.000001811	-0.000000759	-0.000003997
1	0.000001232	-0.000000769	-0.000004003
1	0.000000423	-0.000000701	-0.00000403
1	0.00000189	-0.000000865	-0.000004768
1	0.00000164	-0.000000701	-0.000003742
1	0.000002517	-0.000000731	-0.000003714
6	0.000000267	0.000000064	0.000001197
6	0.000000934	0.000000232	0.000000471
1	0.000000857	0.000000238	0.000001591
1	0.000000196	0.000000247	0.000001872
6	0.000001803	0.000000264	0.000001134
1	0.000001261	0.00000002	0.000000234
1	0.000001337	-0.000000171	0.000000107
6	0.000002649	0.000000034	0.000000642
1	0.000001705	0.000000252	0.000001795
1	0.000002284	0.000000216	0.000001586
1	0.000003254	0.000000144	0.000001017
1	0.00000291	-0.000000068	0.000000159
1	0.00000242	-0.000000035	0.000000274
16	-0.000001757	0.000000623	0.000001551
8	-0.000001793	0.000000121	0.000000931
8	-0.000001151	0.000000328	0.000002109
6	-0.000000514	0.000000285	0.000001956
6	-0.000000609	0.000000359	0.000001459
6	-0.000000097	0.000000465	0.000002812
6	0.000000111	0.000000467	0.000001974
1	-0.000000638	0.000000212	0.000001077
6	-0.000000016	0.000000056	0.000000338
1	-0.000000548	0.000000488	0.000003247
6	0.000000525	0.000000719	0.000003658
1	0.000000239	0.000000385	0.000002013
1	0.000000457	0.000000791	0.000004255
6	0.000001099	0.000000677	0.000003745
1	0.000000286	0.000000668	0.000003916
1	0.000001197	0.000000359	0.000003182
1	0.000001301	0.000000692	0.000003902
1	-0.00000078	-0.000000251	-0.000001433
6	-0.000001135	0.000000053	0.000000271



6	-0.00000168	0.000000202	0.000001069
6	-0.00000179	0.000000373	0.000001938
6	-0.000001235	0.000000037	0.000002191
6	-0.000000664	0.000000305	0.000001555
6	-0.00000056	0.000000115	0.000000733
6	-0.00000127	0.000000026	-0.000000568
6	-0.000002029	-0.000000109	0.000000072
1	-0.000002216	0.000000543	0.000002472
1	-0.00000125	0.000000539	0.000002869
1	-0.000000175	0.000000314	0.000001755
1	-0.000000016	0.000000057	0.000000182
1	-0.000001198	-0.000000164	-0.000000708
1	-0.00000226	0.000000056	-0.000000794
7	-0.000002349	0.000000311	0.000000338
1	-0.000002585	0.000000139	0.000001301
<b>Zero-point correction=</b>			<b>0.670881 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>0.713426</b>
<b>Thermal correction to Enthalpy=</b>			<b>0.714370</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>0.588294</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-2504.021641</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-2503.979097</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-2503.978153</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-2504.104229</b>

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6	0.000002217	0.000003361	-0.000000675
6	-0.000001822	-0.000003269	-0.000002512
7	-0.000002139	-0.000002794	-0.000002154
7	0.000002633	0.00000056	0.000004195
16	0.000000956	0.000001231	0.000001037
8	-0.000000783	0.000000539	0.000002296
8	0.000001351	0.000001235	0.000000764
6	0.000000011	0.000000488	0.000001172
6	-0.000002285	0.000003412	-0.000000023
6	0.000000493	0.000003662	0.000001899
6	-0.000001797	0.000001342	0.000001476
6	-0.000000993	0.000002511	-0.000000857
6	0.000000329	0.000003525	0.000001467
1	-0.000000225	0.000001642	0.000000766
1	-0.000001232	0.000002876	0.000000899
1	-0.000000712	0.000002509	0.000001471
1	-0.000000447	0.0000019	0.000000996
6	-0.000001639	0.00000035	0.000000769
1	-0.000001359	0.000004154	0.000001383

1	-0.000001031	0.000004541	0.000000897
1	-0.000001757	0.000004456	0.000001049
6	0.000000437	0.000003201	0.000001054
6	-0.000001069	-0.000001407	-0.000000315
1	-0.000001122	0.000001037	-0.000000455
1	-0.000000302	0.000000349	0.000000052
6	-0.00000003	0.000001217	-0.000001187
1	-0.000001295	0.000000046	-0.000000823
1	0.000000189	-0.000000021	-0.000000522
6	-0.000001095	-0.000000744	-0.000001466
1	-0.000000821	0.000000001	-0.000000786
1	-0.000001726	0.000000565	-0.000001361
1	-0.000001358	-0.000000451	-0.000001797
1	-0.000001413	-0.000000429	-0.000001817
1	-0.000000803	-0.000001013	-0.000001495
6	0.000000679	0.000001456	-0.000000122
6	0.000000172	-0.000001745	-0.000000896
1	0.000000042	-0.000001092	-0.000000252
1	-0.000000071	-0.000001437	0.000000509
6	0.000000275	-0.00000198	-0.000000503
1	-0.000000051	-0.000000868	-0.00000166
1	0.000000062	-0.000001662	-0.000000813
6	-0.000000022	-0.00000247	-0.000001576
1	0.000000764	-0.000002371	-0.000000314
1	0.000000185	-0.000001546	-0.00000143
1	0.000000192	-0.000002803	-0.000001606
1	-0.000000214	-0.00000217	-0.000001934
1	0.000000263	-0.000002717	-0.000001524
16	0.000000384	-0.000001668	-0.000004605
8	0.000002049	0.000000071	0.000004517
8	-0.00000035	-0.000001659	0.000000368
6	0.000001534	0.000000765	0.000000964
6	0.00000058	0.000000079	0.000000478
6	0.000001006	-0.000001558	0.000001018
6	0.000002198	-0.000000085	0.000001974
1	0.000001735	-0.000000385	0.000001733
6	0.000002603	-0.000001058	0.000000716
1	0.00000165	-0.000001589	0.000000588
6	0.000002359	-0.000002534	0.000002972
1	0.000001839	-0.000000401	0.000002424
1	0.000002044	-0.000002409	0.000001662
6	0.000002944	-0.000001724	0.000002649
1	0.000002931	-0.00000106	0.000002676
1	0.000002508	-0.000000714	0.000002104

1	0.000003086	-0.000001455	0.000001868
1	-0.00000049	0.00000073	-0.000000321
6	-0.000003215	-0.00000204	-0.000000619
6	-0.000002489	0.000001691	-0.000002109
6	-0.00000058	-0.000000025	0.000000016
6	-0.000000789	-0.000000824	-0.000001047
6	-0.000000538	-0.000000879	-0.000002175
6	-0.000000526	-0.000001189	-0.000001458
6	0.000002416	-0.000001423	-0.000002206
6	-0.000003877	0.000003427	-0.000000971
1	0.000000148	-0.000000309	-0.000000038
1	-0.000000395	-0.000000963	-0.000001045
1	-0.00000088	-0.000001505	-0.000001881
1	-0.000001113	-0.000001324	-0.000002087
1	-0.000001195	-0.000000123	-0.000000828
1	0.000000064	0.000000375	-0.000001244
7	0.000000951	0.000000296	0.000002403
1	0.000000038	-0.000000669	-0.00000123

Zero-point correction=

0.672668 (Hartree/Particle)

Thermal correction to Energy=

0.714725

Thermal correction to Enthalpy=

0.715670

Thermal correction to Gibbs Free Energy=

0.591168

Sum of electronic and zero-point Energies=

-2504.039911

Sum of electronic and thermal Energies=

-2503.997853

Sum of electronic and thermal Enthalpies=

-2503.996909

Sum of electronic and thermal Free Energies=

-2504.121410

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6	-0.000000017	-0.000000745	-0.000000654
6	0.000001775	-0.000000634	-0.000000934
7	-0.000000365	-0.000000642	-0.000001727
7	-0.000000249	0.000000524	-0.000001528
16	-0.000001169	0.000000241	-0.00000124
8	-0.000000242	0.000000358	-0.00000217
8	-0.000000821	-0.000001938	-0.000002679
6	0.000000013	0.00000037	-0.000002227
6	0.000000483	0.000000937	-0.00000173
6	0.000000972	0.000001174	-0.000001962
6	0.000000409	0.000001013	-0.000002036
6	0.000000001	0.000000533	-0.000002307
6	-0.000000077	0.000000066	-0.000002252
1	0.000000567	0.000001168	-0.000001628
1	0.000001192	0.000001923	-0.000001873
1	-0.000000135	0.000000314	-0.000002649

1	-0.00000077	-0.000000475	-0.00000249
6	0.000000745	0.000001777	-0.000002728
1	0.000000708	0.000001378	-0.000002226
1	0.000001122	0.000001809	-0.000002997
1	0.000001088	0.000002298	-0.000002009
6	-0.00000074	-0.000001011	-0.00000016
6	-0.000000978	-0.000001425	0.000000047
1	-0.000000462	-0.000000708	-0.000000447
1	-0.000001117	-0.000001174	-0.000001212
6	-0.000001395	-0.000001953	0.000000415
1	-0.000000968	-0.000001356	0.000000721
1	-0.000001392	-0.000001879	-0.000000115
6	-0.000001669	-0.000002382	0.000001111
1	-0.000001638	-0.000002068	-0.000000084
1	-0.000001128	-0.000001521	0.000000601
1	-0.000001872	-0.000002689	0.000001304
1	-0.000001471	-0.000002295	0.000001619
1	-0.000002001	-0.000002833	0.000000868
6	0.000000471	0.000001081	0.000000561
6	0.000000841	0.000001254	-0.000000647
1	0.000000836	0.000000709	0.000000065
1	0.000000267	0.000000427	-0.000000108
6	0.000001127	0.000001638	-0.000000864
1	0.000001036	0.000001326	-0.000000307
1	0.000000488	0.000000909	-0.000001107
6	0.000001411	0.000002149	-0.000001632
1	0.000000876	0.00000138	-0.000001123
1	0.000001379	0.000001907	-0.000000034
1	0.000001645	0.000002511	-0.000001781
1	0.000001665	0.000002429	-0.000001352
1	0.000001112	0.000001935	-0.000000214
16	-0.000000071	-0.000001034	0.000000678
8	-0.000000221	-0.000000646	0.000001958
8	0.000000069	-0.000000201	0.000001432
6	0.000000944	0.000000437	0.000002115
6	0.000000717	0.000000355	0.000002554
6	0.000000964	0.000000898	0.000002301
6	0.000001193	0.000001039	0.000002699
1	0.00000038	0.000000318	0.000002206
6	0.000001497	0.000001343	0.000003349
1	0.000000633	0.000000692	0.000002237
6	0.00000201	0.000000954	0.000002829
1	0.000001206	0.000001248	0.000002956
1	0.000001518	0.00000151	0.000003174

6	0.000001816	0.000002367	0.000003812
1	0.000002123	0.000001526	0.000004314
1	0.000002249	0.000002445	0.000003438
1	0.000002215	0.000002247	0.000003586
1	0.000000502	0.000000437	0.000000471
6	-0.000001198	-0.000001267	-0.000000249
6	-0.00000111	-0.000001887	0.000000357
6	-0.000001721	-0.000002347	0.000000432
6	-0.000001479	-0.000002299	0.000001002
6	-0.000001532	-0.000001987	0.000000942
6	-0.00000133	-0.000001844	0.000000031
6	-0.0000011	-0.000000554	-0.000000889
6	-0.00000046	-0.000000057	-0.00000132
1	-0.000001479	-0.000001934	0.000000668
1	-0.000001783	-0.000002648	0.000001466
1	-0.000001637	-0.000002463	0.000001271
1	-0.000001182	-0.000001635	0.000000161
1	-0.000000699	-0.000000705	-0.00000128
1	-0.00000035	-0.000000326	-0.000001679
7	-0.000002751	0.000001533	-0.000002501
1	-0.000001484	-0.000003327	0.000003046

Zero-point correction=

0.669069 (Hartree/Particle)

Thermal correction to Energy=

0.712048

Thermal correction to Enthalpy=

0.712992

Thermal correction to Gibbs Free Energy=

0.585671

Sum of electronic and zero-point Energies=

-2504.013312

Sum of electronic and thermal Energies=

-2503.970333

Sum of electronic and thermal Enthalpies=

-2503.969389

Sum of electronic and thermal Free Energies=

-2504.096710

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6	0.000003169	-0.000003992	-0.000000669
6	-0.000005174	0.000001748	-0.00000288
7	0.000004877	-0.000002545	-0.000003411
7	-0.000000955	0.000012438	0.000001392
16	-0.000001198	0.00000051	0.000005109
8	-0.000003126	-0.000003421	-0.000005297
8	-0.000000359	-0.00000213	-0.000001749
6	-0.000001463	-0.000002968	-0.00000086
6	-0.000000347	-0.000001188	0.000000978
6	-0.000000802	-0.000001999	0.000001298
6	-0.000000131	-0.000001803	0.000001132
6	-0.00000051	-0.000001247	0.000000459
6	0.000000368	-0.000003155	0.000000066

1	-0.00000799	-0.000001977	0.000001063
1	-0.000001479	-0.000002239	0.00000174
1	-0.000000299	-0.000001919	0.000000103
1	0.000000615	-0.000001892	-0.000000986
6	-0.000000845	-0.000001796	0.000001665
1	-0.000001243	-0.000001599	0.000001842
1	-0.000001903	-0.000003239	0.000002034
1	-0.00000226	-0.000001929	0.00000285
6	0.000002442	0.000000312	-0.000000698
6	0.000001736	-0.000000007	-0.000001121
1	0.00000058	0.000000279	-0.000001386
1	0.000000129	-0.000000246	-0.000001617
6	0.000000916	0.000002149	-0.000001824
1	0.000000794	0.000002551	-0.000001185
1	0.000001068	0.00000113	-0.000002893
6	0.000001862	0.000002956	-0.000002008
1	0.000001853	0.00000157	-0.000002339
1	0.000001128	0.000002153	-0.000001509
1	0.000001754	0.000003462	-0.000002314
1	0.000001503	0.000003562	-0.000001997
1	0.000002261	0.00000261	-0.000003092
6	-0.000000002	-0.000003092	-0.000001133
6	-0.000000385	-0.00000146	0.00000138
1	-0.000000727	-0.000000672	-0.000000716
1	0.000000371	-0.000000268	0.000001124
6	-0.000001498	-0.000002233	0.00000078
1	-0.000000871	-0.00000043	0.000000931
1	-0.000001765	-0.000003054	0.000000282
6	-0.000000704	-0.000003347	0.000001656
1	-0.000000646	-0.000002169	0.000000818
1	-0.000001143	-0.000001407	0.000001726
1	-0.000001873	-0.000003353	0.000002
1	-0.000002047	-0.000002124	0.000002453
1	-0.000001265	-0.000003549	0.000001525
16	0.000002333	0.000002768	0.000003182
8	-0.000001421	-0.000000471	-0.000002845
8	0.000004134	-0.000000711	0.000000216
6	-0.000001641	0.000002739	0.00000281
6	-0.000001	0.000002257	0.000001786
6	0.000000403	0.000000852	-0.000000698
6	-0.000001609	0.000000908	0.000001803
1	-0.000001469	0.000002394	0.000002339
6	-0.000001731	0.000002833	0.000002423
1	-0.000001334	0.000001992	0.000002666

6	-0.000001593	0.000002911	0.000004388
1	-0.000001927	0.000002243	0.000003328
1	-0.000001868	0.000002387	0.000003348
6	-0.000002681	0.000002603	0.000005513
1	-0.00000241	0.000003577	0.000003458
1	-0.00000231	0.000002222	0.000004043
1	-0.000002543	0.000002175	0.000003873
1	0.000000281	0.00000182	0.000002512
6	-0.000000873	-0.000000132	-0.000002021
6	0.000000562	-0.000004203	-0.000002815
6	0.000002551	0.000001379	-0.000002103
6	0.000000458	0.000002278	-0.000002535
6	0.000002235	0.000000764	-0.000002468
6	0.00000224	-0.000000225	-0.000003521
6	0.000003649	-0.000002566	0.000000025
6	0.000001261	-0.000000437	-0.000011653
1	0.00000148	0.000001088	-0.000001264
1	0.000002182	0.000002352	-0.000002748
1	0.000002391	0.000001379	-0.000003465
1	0.000002164	-0.000000529	-0.000003009
1	0.000001078	-0.000001824	-0.000002192
1	0.000001815	-0.00000252	0.000000331
7	0.00000078	-0.000000865	0.000002281
1	0.000002809	-0.000000421	-0.00000171

Zero-point correction=

0.672927 (Hartree/Particle)

Thermal correction to Energy=

0.715087

Thermal correction to Enthalpy=

0.716031

Thermal correction to Gibbs Free Energy=

0.590548

Sum of electronic and zero-point Energies=

-2504.035441

Sum of electronic and thermal Energies=

-2503.993281

Sum of electronic and thermal Enthalpies=

-2503.992337

Sum of electronic and thermal Free Energies=

-2504.117820

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6	-0.000000422	-0.000000707	-0.00000018
6	-0.000000743	0.000000511	-0.000001686
7	-0.000000188	0.000000352	-0.000000194
7	0.00000047	0.000000166	0.000000418
16	0.000000822	0.000000286	0.000000246
8	0.000000552	0.000000814	0.000001273
8	-0.000000114	0.000000051	-0.000000083
6	-0.000000496	0.000000051	0.000001072
6	0.000000001	-0.00000003	0.000000851
6	-0.000000893	-0.000001047	0.000001429

6	-0.000001433	-0.000000753	0.00000059
6	-0.00000028	-0.000000377	0.00000122
6	-0.000000358	-0.000000181	0.000000922
1	-0.000000279	-0.000000492	0.000000712
1	-0.000000733	-0.000001064	0.000001517
1	-0.000000439	-0.000000189	0.000001812
1	-0.000000242	0.000000363	0.000001008
6	-0.000001867	-0.00000057	0.000003822
1	-0.000000267	-0.000000935	0.000002382
1	-0.000000748	0.000000246	0.000002678
1	-0.000000285	-0.000000702	0.000001695
6	-0.000000107	-0.00000048	0.000000179
6	0.000000126	0.000000103	-0.000000655
1	-0.000000142	-0.000000679	-0.000000377
1	-0.000000105	-0.000000347	0.000000022
6	0.000000015	-0.00000044	-0.000000885
1	0.000000212	-0.000000272	-0.000000991
1	0.000000375	0.000000244	-0.000000577
6	0.000000412	0.00000007	-0.000001321
1	0.000000097	-0.000000236	-0.000000594
1	0.000000057	-0.000000641	-0.000000908
1	0.000000433	-0.000000202	-0.000001338
1	0.000000433	-0.000000081	-0.000001652
1	0.000000485	0.000000353	-0.00000123
6	0.000000632	0.000000357	-0.000000668
6	0.000000581	0.000001699	-0.000000575
1	0.000000408	0.000000574	-0.000000146
1	0.00000021	0.000000609	-0.000000977
6	0.000000826	0.000000948	-0.00000093
1	0.000000196	0.000000147	-0.000000718
1	0.000000695	0.000000743	-0.000000642
6	0.000000778	0.00000173	-0.000001364
1	0.000000596	0.000001346	-0.000001173
1	0.000000579	0.000001617	-0.000000643
1	0.00000091	0.000001953	-0.00000135
1	0.000000749	0.000001738	-0.000000824
1	0.000000856	0.000001369	-0.000001479
16	-0.000000387	0.000000261	0.000000234
8	-0.000000034	-0.000000563	-0.000000193
8	-0.000000049	-0.000000804	0.000000236
6	-0.000000463	-0.00000005	0.000000068
6	-0.000000203	-0.00000011	0.000000419
6	-0.000000424	0.00000019	0.000000074
6	-0.000000421	0.000000769	0.000000087



1	-0.000000394	0.000000658	0.000000805
6	-0.000000038	0.000000948	0.000000822
1	0.000000275	0.000000346	0.000000314
6	0.000000374	0.000002672	0.000002294
1	-0.000000227	0.000000982	0.00000205
1	0.000000177	0.000001078	0.000001254
6	0.000000217	0.000001162	0.000002644
1	-0.000000651	0.00000078	0.000001644
1	-0.000000522	0.000001509	0.000001381
1	0.00000014	0.000001672	0.000000957
1	0.000000008	-0.000000713	-0.00000074
6	-0.000000013	-0.000001284	-0.000000949
6	0.000000068	-0.00000116	-0.000000482
6	-0.000000088	-0.00000137	-0.000000586
6	-0.000000453	-0.000001929	-0.00000073
6	-0.000000357	-0.000001746	-0.00000055
6	0.000000013	-0.000001292	-0.000000937
6	0.000000273	-0.000000382	-0.000001488
6	0.000000496	-0.000000301	-0.000001489
1	-0.000000151	-0.000001511	-0.000000432
1	-0.000000425	-0.000002147	-0.000000351
1	-0.000000371	-0.000002183	-0.000000603
1	0.000000002	-0.000001559	-0.000001109
1	0.000000434	-0.000000542	-0.000001564
1	0.000000084	0.000000377	-0.000001902
7	0.000000863	-0.000001591	-0.000000871
1	-0.000000252	-0.000000372	-0.000001388

Zero-point correction=

0.671058 (Hartree/Particle)

Thermal correction to Energy=

0.713386

Thermal correction to Enthalpy=

0.714330

Thermal correction to Gibbs Free Energy=

0.589369

Sum of electronic and zero-point Energies=

-2504.008083

Sum of electronic and thermal Energies=

-2503.965755

Sum of electronic and thermal Enthalpies=

-2503.964811

Sum of electronic and thermal Free Energies=

-2504.089772

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6	-0.000007896	0.00000729	0.000002745
6	-0.000000043	-0.00000486	0.000001999
7	0.000009215	-0.000015362	-0.000009281
7	0.000001971	0.00000084	0.000006262
16	-0.000004366	0.00000784	0.000006545
8	-0.000002457	-0.000001085	-0.000001885
8	0.000003238	0.000001733	-0.000002487

6	-0.000002969	-0.000002293	0.000003705
6	0.00000189	0.000000179	-0.000001612
6	-0.000000407	-0.000003322	-0.000000242
6	-0.00000194	-0.000003051	-0.000000085
6	-0.000001549	-0.000003193	-0.000000831
6	-0.000000787	-0.000004082	-0.000002988
1	-0.000000854	-0.000002512	0.00000002
1	-0.000001232	-0.000002057	-0.000001296
1	-0.000001038	-0.000003762	-0.0000013
1	-0.000000404	-0.00000118	-0.000000094
6	-0.00000156	-0.000003488	-0.000001748
1	-0.000001826	-0.000004127	-0.000001503
1	-0.000001834	-0.000004376	-0.000001846
1	-0.000001879	-0.000004661	-0.000000912
6	0.000003143	0.000001725	0.000004406
6	-0.000000138	-0.000002792	0.000001002
1	0.00000156	-0.000001591	0.000000821
1	0.000000156	-0.000001984	-0.000000664
6	0.000002946	-0.000001181	0.000001794
1	0.000002147	-0.000000694	0.000001346
1	0.000001378	-0.000001064	0.000000772
6	0.000002312	-0.000001571	0.000002231
1	0.000001483	-0.000002333	0.000001246
1	0.000001999	-0.000002165	0.000001754
1	0.000002734	-0.000001851	0.000002314
1	0.000002788	-0.000000788	0.000002246
1	0.000002221	-0.000000967	0.000001721
6	-0.000000011	0.000003333	-0.000003823
6	0.000000014	0.000001806	-0.000000521
1	-0.0000004	0.000001479	-0.000000628
1	0.000000905	0.000002287	0.000001134
6	0.000000143	0.000002605	0.000000022
1	-0.000000589	0.000001185	0.000000698
1	0.000000582	0.000001566	0.000000321
6	0.000000351	0.000002974	0.000000493
1	0.000000639	0.000003229	0.00000042
1	0.000000173	0.000003261	-0.000000029
1	0.000000709	0.000003461	0.000000404
1	0.000000511	0.000002269	0.000000247
1	0.000000989	0.000002542	0.000001038
16	0.000004862	0.000006042	0.000003199
8	-0.000002321	-0.000001232	-0.000002325
8	-0.000000237	0.000000096	-0.000001194
6	-0.000006603	-0.000004448	-0.000004995

6	0.00000695	0.00005636	0.000001502
6	0.000001509	0.000003842	-0.000000208
6	-0.000003568	-0.000000552	-0.000004074
1	-0.000002134	-0.000000651	-0.000001561
6	-0.000004072	0.000002428	-0.000001053
1	-0.000001884	0.00000202	-0.000000858
6	-0.000000185	0.00000224	-0.00000093
1	-0.000002626	0.000000439	-0.000002047
1	-0.000002087	0.00000274	-0.000002091
6	-0.000002837	0.000001628	-0.000002585
1	-0.000004396	0.000001884	-0.00000302
1	-0.000003343	0.000001572	-0.000002409
1	-0.00000317	0.000002475	-0.000003224
1	0.000002473	-0.000001905	-0.000000586
6	0.000001606	-0.000002962	-0.000001226
6	0.000001587	-0.00000197	0.000004613
6	0.000000619	0.000000734	-0.000001197
6	0.000000497	-0.000000169	0.00000137
6	0.000002305	-0.000000355	0.000001846
6	0.000000133	0.000001486	0.000000979
6	0.000003316	0.000008287	0.000001642
6	0.000001633	-0.000005709	0.000001939
1	0.000000305	-0.000001632	0.0000012
1	0.000000832	-0.000001116	0.000000353
1	0.000001027	0.000000353	0.000001139
1	0.000001097	0.000001343	0.000001013
1	0.000001003	0.000000353	0.000001788
1	0.000002374	0.000004196	0.0000017
7	-0.000003147	0.000005673	-0.000004646
1	0.000002719	-0.000001972	0.000002012

Zero-point correction=

0.673026 (Hartree/Particle)

Thermal correction to Energy=

0.715224

Thermal correction to Enthalpy=

0.716168

Thermal correction to Gibbs Free Energy=

0.592052

Sum of electronic and zero-point Energies=

-2504.010773

Sum of electronic and thermal Energies=

-2503.968575

Sum of electronic and thermal Enthalpies=

-2503.967631

Sum of electronic and thermal Free Energies=

-2504.091747

B-Tsg1

6	-0.000002539	0.000001157	0.000001276
6	-0.000000392	-0.000000679	-0.000000875
7	0.000001727	-0.000001422	-0.000000897
7	-0.000000143	0.000000146	0.000000209

16	0.000000545	0.000000209	-0.000000582
8	0.000000352	-0.000000114	0.000000374
8	0.000000361	0.000000158	0.000000373
6	0.000000485	-0.000000208	0.000000342
6	-0.000000003	0.000000235	0.000000233
6	-0.000000009	0.000000506	0.000000764
6	0.000000251	0.000000231	0.000000644
6	0.000000442	0.000000433	0.000000628
6	0.000000392	0.000000246	0.000000689
1	0.000000037	0.000000245	0.000000522
1	0.000000056	0.000000519	0.000000737
1	0.000000604	0.000000405	0.000000818
1	0.000000622	0.000000238	0.000000506
6	0.000000355	0.000000486	0.000000092
1	0.000000278	0.000000559	0.000001122
1	0.000000032	0.000000535	0.000000985
1	0.000000099	0.000000733	0.000001053
6	0.000001013	-0.000000187	0.000000706
6	-0.000000307	0.000000002	0.000000137
1	0.000000356	0.000000231	0.000000014
1	-0.000000069	0.000000347	0.000000008
6	-0.000000079	0.000000078	0.000000432
1	0.000000129	0.000000212	0.000000181
1	-0.000000263	0.000000243	0.000000011
6	-0.000000425	0.000000217	0.000000292
1	-0.000000125	0.000000158	0.000000185
1	0.000000012	0.000000227	0.000000348
1	-0.000000347	0.000000281	0.000000443
1	-0.000000342	0.000000413	0.000000431
1	-0.000000496	0.000000245	0.000000027
6	-0.000000109	-0.000000248	-0.000000508
6	-0.000000187	-0.000000335	-0.000000544
1	0.000000019	-0.000000236	-0.000000349
1	-0.000000158	-0.000000124	-0.000000275
6	-0.000000019	-0.000000296	-0.000000722
1	-0.000000154	-0.000000337	-0.000000682
1	-0.000000347	-0.000000326	-0.000000508
6	-0.000000391	-0.000000493	-0.000000854
1	-0.000000344	-0.000000387	-0.000000624
1	-0.000000041	-0.000000424	-0.000000701
1	-0.000000031	-0.000000557	-0.000000976
1	-0.000000241	-0.000000517	-0.000000981
1	-0.000000489	-0.000000473	-0.000000881
16	-0.000000312	0.000000004	0.000000005

8	-0.000000242	0.000000079	-0.000000031
8	-0.000000046	-0.000000057	-0.000000193
6	-0.000000444	-0.000000039	0.000000139
6	-0.000000042	-0.000000059	0.000000071
6	-0.000000441	0.000000437	-0.000000067
6	0.000000021	0.000000363	0.000000174
1	0.000000134	-0.000000009	0.000000116
6	-0.000000043	0.000000033	-0.000000012
1	-0.000000643	0.000000049	-0.000000016
6	-0.000000039	0.000000342	0.000000392
1	0.000000029	0.000000108	0.000000026
1	-0.000000655	0.000000084	0.000000093
6	-0.000000359	0.000000014	0.000000339
1	-0.000000419	0.000000255	0.000000314
1	-0.000000014	0.000000322	0.000000047
1	-0.000000207	0.000000135	0.000000207
1	-0.000000276	-0.000000335	-0.000000166
8	0.000000427	0.000000215	-0.000000382
6	0.000000345	-0.000000247	-0.000000381
6	0.000000065	-0.000000036	-0.000000402
6	0.000000324	-0.000000331	-0.000000055
6	0.000000566	-0.000000444	-0.000000637
6	0.000000367	-0.000000736	-0.000000911
1	0.000000795	-0.000000532	-0.000000674
1	0.000000718	-0.000000095	-0.000000306
7	-0.000000699	-0.000000314	-0.000000082
8	0.000000633	-0.000000079	-0.000000068
1	0.000000047	-0.000000612	-0.000000889
1	0.000000008	-0.000000359	-0.000000396
17	-0.000000045	-0.000000311	-0.000000721

Zero-point correction=

0.630190 (Hartree/Particle)

Thermal correction to Energy=

0.673048

Thermal correction to Enthalpy=

0.673992

Thermal correction to Gibbs Free Energy=

0.548567

Sum of electronic and zero-point Energies=

-2998.560912

Sum of electronic and thermal Energies=

-2998.518055

Sum of electronic and thermal Enthalpies=

-2998.517110

Sum of electronic and thermal Free Energies=

-2998.642536

B-1g

6	0.000001553	-0.000002634	-0.000001288
6	-0.000000013	-0.000000874	0.000001187
7	0.000001796	0.000002443	0.000000052
7	0.000001575	0.000000644	-0.000001861
16	0.000001633	0.000000095	0.000002456

8	-0.000001844	-0.000003194	0.000001333
8	-0.000000592	-0.00000135	0.000001838
6	-0.000000248	-0.00000136	0.000000717
6	0.000000131	0.000000716	0.000001967
6	-0.000000271	0.000000495	0.000003237
6	-0.000000139	0.000000382	0.000004768
6	-0.000000491	-0.00000109	0.000004216
6	-0.000000371	-0.000001658	0.000004725
1	-0.000000307	-0.000000077	0.000001414
1	0.000000024	0.000000944	0.000002916
1	-0.000000436	-0.000001342	0.000005215
1	-0.000000419	-0.000001514	0.000003538
6	-0.000000149	0.000000163	0.000004992
1	-0.000000389	-0.000000051	0.000005933
1	-0.000000324	-0.000000147	0.000005024
1	-0.000000146	0.000001153	0.000005188
6	-0.000002641	-0.000000424	0.000001379
6	0.000000597	0.000001005	0.000003078
1	0.000000312	0.000000615	0.000002986
1	0.000000513	0.000000644	0.000001711
6	0.000000455	0.000002858	0.000002313
1	0.000000196	0.000002119	0.000001514
1	-0.000000172	0.000002239	0.000000975
6	0.000000373	0.000003725	0.000002959
1	0.000000125	0.000002398	0.000002688
1	0.000000053	0.000002156	0.000003644
1	0.000000302	0.00000415	0.000003494
1	0.000000259	0.000003753	0.000003051
1	0.000000409	0.000004109	0.000002123
6	-0.000000661	-0.000001623	-0.000002657
6	0.000000467	0.000000232	-0.00000359
1	-0.000000038	-0.000001271	-0.000002569
1	0.000000098	-0.000000227	-0.000003033
6	0.000000238	-0.000000872	-0.000004639
1	0.000000035	-0.000000552	-0.000003404
1	0.000000218	0.000000704	-0.000003794
6	0.000000126	-0.000000339	-0.000005821
1	0.000000219	-0.000000537	-0.000004897
1	0.00000007	-0.000001621	-0.000004681
1	0.000000339	-0.000000775	-0.000006423
1	0.000000029	-0.000000644	-0.000005637
1	0.000000396	0.000000484	-0.000005802
16	-0.000001191	0.000000168	-0.000001557
8	0.00000012	0.000002504	-0.000000145

8	0.000000379	0.000001944	-0.000001995
6	0.000000047	0.00000185	-0.000000337
6	0.000002631	-0.000001152	-0.000002834
6	-0.000002641	0.000000365	-0.000002231
6	-0.000003367	-0.00000093	-0.000000797
1	-0.000000288	-0.00000058	0.000000233
6	0.00000222	0.000000065	-0.000003302
1	0.000000836	0.000002238	-0.000002327
6	0.000001424	0.000000514	0.000000945
1	0.00000035	-0.000001256	0.000000006
1	0.000000051	0.000001261	-0.000001943
6	-0.000000513	-0.000000991	-0.00000062
1	0.000000092	0.000000417	-0.000001628
1	-0.000000167	-0.000000652	-0.000000769
1	0.000000128	-0.000000968	-0.000002139
1	-0.000000572	0.000001468	0.000000017
8	-0.00000061	-0.000000612	-0.000002212
6	-0.000000083	-0.000001337	0.000001307
6	-0.000000745	-0.000002215	-0.000000397
6	-0.00000007	-0.000003557	-0.00000135
6	-0.000000011	-0.000001481	-0.000000841
6	-0.000000395	-0.0000002	-0.000001854
1	-0.000000498	-0.000003384	-0.000001106
1	-0.000000208	-0.000001273	0.000001119
7	-0.000000125	-0.000002457	-0.000002032
8	0.00000055	0.000001067	0.000000613
1	-0.000000016	-0.000001873	-0.000002682
1	-0.00000037	-0.000003284	0.000000768
17	-0.000000111	0.00000029	-0.000002444

Zero-point correction=

0.631587 (Hartree/Particle)

Thermal correction to Energy=

0.674613

Thermal correction to Enthalpy=

0.675557

Thermal correction to Gibbs Free Energy=

0.549829

Sum of electronic and zero-point Energies=

-2998.561487

Sum of electronic and thermal Energies=

-2998.518461

Sum of electronic and thermal Enthalpies=

-2998.517516

Sum of electronic and thermal Free Energies=

-2998.643245

B-Tsg2

6	-0.000000694	-0.000001869	0.000002823
6	-0.000000209	0.000001011	-0.000001736
7	-0.000001203	-0.000000444	0.000000997
7	0.000000657	0.000000591	-0.000000527
16	-0.000002173	0.000000611	0.00000197

8	-0.000001968	0.000000923	0.000000456
8	-0.000002727	0.000000982	0.000001285
6	-0.000001647	0.000000012	0.000002438
6	-0.000000726	-0.000000489	0.00000284
6	-0.000000659	-0.000001195	0.000003992
6	-0.000001486	-0.000001389	0.000004175
6	-0.000002616	-0.000000553	0.000004626
6	-0.000002536	0.000000045	0.000003512
1	-0.000000005	-0.000000582	0.000002256
1	0.000000235	-0.000001699	0.000003892
1	-0.000003369	-0.000000631	0.00000508
1	-0.000003453	0.000000228	0.000003144
6	-0.00000143	-0.000001899	0.00000585
1	-0.000001216	-0.000001727	0.000006496
1	-0.000002279	-0.000001231	0.000006429
1	-0.000000882	-0.000001596	0.000005964
6	-0.000001211	-0.000000661	0.000000434
6	-0.000000643	-0.000000275	0.000002047
1	-0.00000083	-0.00000001	0.000001288
1	-0.000000332	0.000000468	0.000000787
6	-0.000000367	-0.000001009	0.000002914
1	-0.000001607	-0.000000665	0.000003039
1	0.000000144	-0.00000111	0.000002801
6	-0.000000554	-0.000001291	0.000004287
1	0.000000531	-0.000001185	0.000002641
1	-0.000000916	-0.00000059	0.000002755
1	-0.000000186	-0.000001636	0.000004609
1	-0.000001153	-0.000001233	0.00000475
1	0.000000287	-0.000001844	0.000004485
6	0.000000231	0.000000971	-0.000002587
6	0.000001121	0.000000771	-0.000003701
1	-0.000000731	0.000001707	-0.000002637
1	0.000000579	0.00000052	-0.000002698
6	0.000000456	0.000001516	-0.000004732
1	0.000000788	0.00000093	-0.000004002
1	0.00000174	0.000000828	-0.000003606
6	0.000001595	0.000001611	-0.000005974
1	0.000001132	0.000001155	-0.000004438
1	-0.000000362	0.00000185	-0.000004919
1	0.000001421	0.000001805	-0.000006588
1	0.000001229	0.000001741	-0.000006185
1	0.000002444	0.000001135	-0.00000582
16	0.000000811	0.000000226	-0.00000066
8	0.000000942	-0.000001381	-0.000000498



8	0.000002268	-0.000000549	-0.000001375
6	0.000000981	-0.000000487	-0.000000357
6	-0.000000794	-0.000000179	0.000000258
6	0.000001813	-0.000000388	-0.000000313
6	-0.000000849	-0.000000044	0.000000428
1	-0.000000968	-0.000000057	0.000000203
6	0.000001007	-0.000000228	-0.000000034
1	0.00000256	-0.000000601	-0.000000943
6	0.000000918	-0.000000825	0.000000338
1	-0.000001296	0.000000233	0.000000836
1	0.00000215	-0.000000723	-0.000000434
6	-0.00000022	-0.000000158	0.000000638
1	-0.00000121	0.000000429	0.000000655
1	0.000000398	-0.000000148	0.000000163
1	-0.000000254	-0.000000559	0.000001734
1	0.000005378	0.000005696	-0.000003322
8	-0.000001322	0.000000985	-0.000002616
6	-0.000003247	0.00000122	0.000000319
6	-0.000003811	0.00000219	-0.000001157
6	-0.000003367	0.000002403	-0.000002621
6	-0.000002537	0.00000236	-0.000003377
6	-0.000002742	0.000000872	-0.000000524
1	-0.000004248	0.000002895	-0.000003048
1	-0.000002968	0.000000709	-0.000000063
7	-0.000006172	-0.000001541	0.000002907
8	0.000006408	0.000003398	-0.00000855
1	-0.000002359	0.000002453	-0.000004169
1	-0.000004476	0.000002143	-0.000000901
17	-0.000000172	0.000001421	-0.000003947
7	0.000000161	-0.000003809	-0.000002249
16	0.000003511	-0.000002029	0.000000489
8	0.000003692	-0.000000986	0.000000245
8	0.000001808	-0.000001815	0.000001201
16	0.000001717	0.000000051	-0.000001921
8	0.000004542	-0.000000564	-0.000002211
8	0.000001974	0.000000568	-0.000002778
6	0.000003259	-0.000001692	0.000000257
6	0.000002498	-0.000000283	-0.000002491
9	0.000003071	-0.000001198	0.000002065
9	0.000004598	-0.000002198	0.000001233
9	0.000004239	-0.000001852	-0.000000293
9	0.000003507	-0.000000602	-0.000002115
9	0.00000176	-0.000000138	-0.000001843
9	0.000002623	0.000000185	-0.00000035

Zero-point correction=	0.679827 (Hartree/Particle)
Thermal correction to Energy=	0.738753
Thermal correction to Enthalpy=	0.739697
Thermal correction to Gibbs Free Energy=	0.578169
Sum of electronic and zero-point Energies=	-4825.774035
Sum of electronic and thermal Energies=	-4825.715109
Sum of electronic and thermal Enthalpies=	-4825.714165
Sum of electronic and thermal Free Energies=	-4825.875693

B-2g

6	-0.00000504	0.00000934	-0.00001426
6	0.00000818	0.00002214	-0.00004051
7	0.00001258	-0.00004034	-0.00003236
7	-0.00002578	-0.00005038	0.00003822
16	0.00000434	-0.00000949	0.00002048
8	-0.00000518	-0.00002923	-0.0000156
8	-0.0000048	-0.00001027	-0.0000408
6	-0.00000311	-0.00000153	0.00000601
6	-0.00000579	0.00001157	0.00000613
6	0.00001767	0.00001236	0.00001105
6	0.00000312	0.00002525	-0.00000847
6	-0.00000547	0.00000124	0.00000353
6	0.00001524	-0.00000954	-0.00002156
1	0.00000412	0.00000051	0.00000052
1	0.00000746	0.00002603	0.00001746
1	0.0000078	0.00000532	-0.00000639
1	0.00000151	-0.00000662	-0.00001286
6	0.00001053	0.00002685	0.00001729
1	0.00001011	0.00002309	0.00000909
1	0.00000288	0.00002368	0.00001833
1	0.00001402	0.00002949	0.00001232
6	0.00002859	0.00003081	-0.00002485
6	0.00001717	0.00001493	-0.00001835
1	0.00002024	-0.0000114	-0.00003055
1	0.00001479	-0.00000747	-0.0000036
6	0.00002746	0.00000609	-0.00003661
1	0.00002194	0.00001339	-0.00001857
1	0.00002802	0.00001593	-0.00002541
6	0.00004326	0.0000305	-0.0000292
1	0.00003777	0.00001366	-0.00004107
1	0.00003312	0.00001386	-0.00003695
1	0.00004482	0.00003269	-0.00003965
1	0.0000366	0.00003048	-0.00002324
1	0.00004161	0.00003478	-0.00002879

6	-0.00000063	-0.000000735	-0.000001398
6	-0.000001186	-0.00000188	-0.000000853
1	-0.00000118	-0.000002838	-0.000000316
1	-0.000001826	-0.000001536	0.000001352
6	-0.000000787	-0.000002564	-0.000000438
1	-0.000000309	-0.000002057	-0.00000161
1	-0.000000134	-0.00000068	-0.000000244
6	-0.000001108	-0.00000251	-0.000001334
1	-0.000001839	-0.000002193	0.000000432
1	-0.000001898	-0.000003172	-0.000000665
1	-0.000001361	-0.000002979	-0.000001062
1	-0.00000043	-0.000002715	-0.000002128
1	-0.000000425	-0.000001565	-0.000000991
16	0.000001823	0.000001341	-0.000000165
8	-0.000000892	0.000001548	-0.000000261
8	0.000000663	-0.000000307	0.000000336
6	-0.000000997	0.000000428	0.000003452
6	-0.000002104	-0.000001005	0.000000738
6	-0.000000601	0.000000994	0.000003015
6	-0.000001784	0.000000291	0.000003085
1	-0.000001645	-0.000000751	0.000001409
6	-0.000003345	0.000000581	0.00000378
1	-0.000001043	0.000001131	0.000003159
6	-0.000002614	-0.000000576	0.000004735
1	-0.000002905	-0.000001158	0.00000348
1	-0.000002465	0.000000923	0.000004913
6	-0.000003406	-0.000000493	0.000005521
1	-0.000003364	0.000000203	0.000005942
1	-0.000004176	-0.000000409	0.000005819
1	-0.000004519	-0.000000732	0.000004954
8	-0.000001707	-0.000002169	-0.000000477
8	0.000002214	-0.000000645	-0.000002486

Zero-point correction=

0.537348 (Hartree/Particle)

Thermal correction to Energy=

0.574114

Thermal correction to Enthalpy=

0.575058

Thermal correction to Gibbs Free Energy=

0.462917

Sum of electronic and zero-point Energies=

-2290.458926

Sum of electronic and thermal Energies=

-2290.422161

Sum of electronic and thermal Enthalpies=

-2290.421217

Sum of electronic and thermal Free Energies=

-2290.533358

Re4

6	-0.000000574	-0.000000706	-0.000000637
6	-0.00000095	-0.00000261	0.000002822

7	0.000000834	-0.000002877	0.000009431
7	0.000007247	0.000003465	-0.000009774
16	0.000000666	-0.000000274	-0.000005622
8	-0.000000081	0.000000843	0.000001986
8	0.000002175	0.000001009	0.000000086
6	0.000000218	-0.000000756	0.000001377
6	-0.000000043	0.000001835	-0.000000092
6	-0.000001058	0.000000409	-0.000000988
6	-0.000001602	-0.000000175	-0.000001649
6	-0.000001153	-0.000000172	-0.000001086
6	-0.000000099	0.000001223	-0.000001788
1	-0.000000304	0.000000564	0.000000225
1	-0.000001643	0.000000897	-0.000000456
1	-0.000001103	-0.000000259	-0.000001877
1	-0.000000197	-0.000001429	-0.000001441
6	-0.0000002	0.000001222	-0.000001649
1	-0.000002619	0.000000421	-0.000002807
1	-0.000002484	0.000001008	-0.000002245
1	-0.000002656	0.00000015	-0.000002244
6	-0.000001736	0.000002168	-0.000001015
6	0.000000507	0.000000539	0.000002408
1	0.000001631	0.00000002	0.000002552
1	0.000001185	0.000000302	0.000001991
6	-0.000000836	0.000002749	0.000003046
1	-0.000000022	0.000001471	0.000001785
1	-0.000000849	0.000002023	0.000001357
6	-0.000000292	0.000002785	0.000003207
1	0.000000328	0.000002042	0.000003222
1	0.000000414	0.000001601	0.00000297
1	-0.000000706	0.000003116	0.000003539
1	-0.000000101	0.000002728	0.000002469
1	-0.000001166	0.000002744	0.000002233
6	-0.000001141	-0.000003457	0.000007898
6	-0.000000884	0.000002083	-0.000004048
1	-0.000001099	0.00000005	-0.00000019
1	-0.000000118	0.000000065	-0.000000128
6	-0.000003104	0.000001553	-0.000000221
1	-0.000001436	0.000000642	0.000000752
1	0.00000009	0.000000653	0.000002064
6	-0.000001194	0.000001874	0.000001348
1	-0.000000764	0.000000987	-0.000000484
1	-0.000000951	0.000000695	-0.000000844
1	-0.000002017	0.000001911	-0.000000035
1	-0.000001968	0.000002122	0.000000072

1	-0.000001612	0.000001881	0.000000439
16	0.000001384	-0.000001099	0.000001788
8	0.000001658	-0.000001548	0.000002145
8	0.000002036	-0.000001134	0.000001634
6	0.000004026	-0.000000302	0.000000105
6	-0.000001146	-0.000003287	0.000002683
6	0.000000743	-0.000001847	-0.000001385
6	-0.000000133	-0.000000321	-0.000003057
1	0.000002957	-0.00000204	-0.000000248
6	0.000000117	-0.00000348	-0.000000534
1	0.000001465	-0.000001647	-0.000001442
6	0.000002608	-0.000002953	-0.000001394
1	0.00000212	-0.000003003	-0.000001508
1	0.000001886	-0.000003097	-0.000002297
6	0.000001687	-0.000003936	-0.000001829
9	0.00000225	-0.000005256	-0.000004213
9	0.000001841	-0.00000326	-0.00000278
9	0.000001767	-0.000002275	-0.000001623
Zero-point correction=			0.504061 (Hartree/Particle)
Thermal correction to Energy=			0.541383
Thermal correction to Enthalpy=			0.542327
Thermal correction to Gibbs Free Energy=			0.425195
Sum of electronic and zero-point Energies=			-2437.670864
Sum of electronic and thermal Energies=			-2437.633541
Sum of electronic and thermal Enthalpies=			-2437.632597
Sum of electronic and thermal Free Energies=			-2437.749730

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6	0.000000658	-0.000000624	0.000005761
6	0.000000863	-0.000001945	-0.000000222
7	0.000006994	0.000003627	0.00000206
7	-0.000004196	0.000000382	-0.000006633
16	-0.000002672	0.00000029	-0.000006745
8	-0.000001413	-0.000004312	0.000002956
8	-0.000000715	0.000002739	0.000000894
6	-0.000005186	0.000000771	-0.000001759
6	-0.000001438	-0.000008039	-0.000007478
6	-0.000003339	-0.000002161	0.000005405
6	-0.000003852	0.000004355	-0.000002712
6	-0.000002253	-0.000003819	-0.000002644
6	-0.000001971	-0.00000118	0.00000446
1	-0.000000116	0.00000656	0.000000666
1	-0.000001643	-0.000000336	-0.000001143
1	-0.000003296	-0.000000308	0.000000272

1	-0.000002512	-0.000000317	-0.000000495
6	-0.000001944	-0.000000738	0.000000121
1	-0.000003483	-0.000001077	-0.000000614
1	-0.000003315	-0.000001113	-0.000000011
1	-0.000002842	-0.000000773	-0.000000577
6	-0.000014316	-0.000006866	0.000002341
6	0.000001417	0.000001614	-0.000003204
1	0.000001915	0.000002223	-0.00000003
1	-0.000000654	0.000001389	-0.000000469
6	-0.000001372	0.000000108	-0.000000173
1	-0.000000838	0.000000695	-0.000001138
1	-0.000000871	0.000000111	-0.000000989
6	-0.000001021	0.000001803	-0.000002627
1	-0.00000158	0.000000798	-0.000001848
1	-0.000002061	0.000000726	-0.000002184
1	-0.000001355	0.000000975	-0.000002688
1	-0.000000799	0.00000119	-0.000002321
1	-0.000000841	0.000001243	-0.000002171
6	0.000004069	0.000000423	0.000003205
6	0.000001104	0.00000035	-0.00000149
1	0.000000296	0.000000795	-0.000000201
1	-0.000002125	-0.000001136	-0.000000477
6	0.000001085	0.000000447	-0.000000882
1	0.000001205	0.000000669	-0.000000604
1	0.000001127	0.000000901	-0.000000349
6	0.000002938	0.000001066	-0.000000787
1	0.000002331	0.000000893	0.000000545
1	0.000002794	0.000000602	-0.000000246
1	0.000002985	0.000001179	-0.000000818
1	0.000002066	0.000000984	-0.000001205
1	0.000002439	0.000001306	-0.000001193
16	0.000003921	0.000004313	-0.000005504
8	0.00000069	-0.000004336	0.000003595
8	0.000001805	-0.000001411	-0.000000518
6	0.000000779	0.000001085	0.000002157
6	0.000003479	0.000005105	0.000000416
6	-0.00000284	-0.00000214	-0.000001551
6	-0.000000303	-0.000001718	-0.000000182
1	0.000002323	-0.000001977	0.000000054
6	0.000000735	0.000000517	0.000002429
1	0.000000354	0.000000283	0.000001316
6	0.000001252	-0.000002494	0.000002421
1	0.000001502	-0.000000093	0.000001477
1	-0.000000204	-0.000000745	0.000001564

6	-0.000002729	-0.000000775	0.000003784
9	0.000002439	0.000000634	0.000001555
9	0.000001945	-0.000000318	0.000000822
9	0.000003367	-0.000001903	0.000002304
79	0.000005429	-0.000002206	0.000003483
6	0.000001342	0.000006231	-0.000000155
6	-0.000000971	0.000002474	-0.000002693
6	-0.000000857	-0.000001877	0.000003568
1	0.00000147	-0.000001003	0.000001247
1	-0.000000143	-0.000000103	0.000000202
7	0.000001919	-0.000006055	0.000001406
7	-0.000005486	0.00000184	-0.000005045
6	0.000001124	-0.000000591	0.000000654
6	0.000000715	-0.000001989	0.000000046
6	0.000001338	0.000000981	0.000003566
6	0.000002104	0.000000523	0.000001914
6	-0.000000497	-0.000001996	0.000002001
6	0.000000621	-0.000000474	0.000000274
1	0.000002388	-0.000000805	0.000001603
1	-0.000000168	0.000000208	0.000001267
1	0.000001582	-0.00000121	0.00000261
6	0.000000677	-0.000004087	-0.00000481
6	-0.000002406	0.000000969	0.000001751
6	0.000000053	0.000002324	-0.000000824
6	-0.000000504	0.0000012	-0.00000089
6	-0.000000381	-0.000000307	-0.000000799
6	0.000000033	0.000000179	-0.000002451
1	-0.000001558	0.000000458	-0.000001557
1	0.000000753	0.000000504	-0.000001888
1	-0.000000933	0.000001143	-0.000002232
6	0.000000088	0.000002465	0.00000247
6	-0.000001547	-0.000002562	-0.000002025
6	-0.000001679	-0.000003066	-0.000003479
1	-0.000001932	0.000002459	0.000000958
1	-0.000000639	0.000000058	-0.000000821
1	-0.000000968	-0.000000802	-0.000000932
1	-0.000003127	0.000001561	-0.000001137
1	-0.000001336	-0.000000099	-0.000001076
1	-0.00000043	0.000000529	0.000001405
1	-0.000002065	-0.000000847	-0.000000504
6	0.00000106	0.000001325	0.000001241
6	0.00000206	0.000001105	-0.00000158
6	0.000001481	0.000001459	-0.000002282
1	0.00000126	0.000000793	0.000000229

1	0.000001193	0.000001225	-0.000001064
1	0.000001398	0.000000994	-0.000000989
1	0.00000096	0.000001955	-0.000002422
1	0.000000965	0.000000793	-0.000001386
1	0.000000814	0.000001121	-0.000000732
1	0.000001849	0.000000903	-0.000001307
6	-0.000004416	0.000001589	0.000002665
6	0.000000632	-0.000000841	0.00000114
6	0.000003042	-0.000003057	0.000001365
1	-0.000000672	-0.000000466	0.000003035
1	-0.000002386	0.000000329	0.000001253
1	-0.000001098	-0.00000136	0.000001191
1	-0.000001327	-0.000002603	0.000002768
1	-0.000000524	-0.000000792	0.000001775
1	-0.000001157	-0.000000853	0.000001928
1	-0.000001223	-0.000001569	0.000001289
6	0.000004371	-0.000003146	0.000001493
6	0.000000699	0.000000999	0.000001727
6	0.00000126	0.00000245	0.000000789
1	0.000000806	-0.00000034	0.000000632
1	0.000001704	0.000000055	0.00000118
1	0.00000243	0.000000224	0.00000103
1	0.000002652	-0.000000246	0.000001162
1	0.000002036	0.000000987	0.000000596
1	0.000002433	0.000000117	0.00000133
1	0.000002609	0.000000321	0.000000473

Zero-point correction=

1.078529 (Hartree/Particle)

Thermal correction to Energy=

1.149775

Thermal correction to Enthalpy=

1.150719

Thermal correction to Gibbs Free Energy=

0.958959

Sum of electronic and zero-point Energies=

-3732.527398

Sum of electronic and thermal Energies=

-3732.456153

Sum of electronic and thermal Enthalpies=

-3732.455208

Sum of electronic and thermal Free Energies=

-3732.646968

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6	0.000004427	0.000000801	0.000001476
6	-0.000000785	-0.000000612	-0.000000449
7	-0.000006379	-0.000001982	-0.000002824
7	0.000007112	-0.000001594	0.000013672
16	0.000000909	-0.000001963	-0.000002955
8	0.000000775	0.00000234	-0.000001415
8	0.000001296	-0.000001482	-0.000003333
6	-0.000002317	0.000002838	0.000000534



6	-0.000001488	-0.000002092	-0.000001763
6	-0.000000183	0.000000595	-0.000005241
6	-0.000002924	-0.000000527	-0.000003501
6	-0.000002569	-0.000001075	-0.000001982
6	0.000000024	-0.000001266	-0.000004847
1	-0.000001611	0.000002267	-0.000002724
1	-0.000003404	0.000000271	-0.000000914
1	-0.00000254	0.00000001	-0.000004345
1	-0.000000742	0.000000381	-0.000004026
6	-0.000003328	-0.000001415	-0.000003503
1	-0.000003947	0.000000261	-0.000003331
1	-0.000003738	0.000000323	-0.000003861
1	-0.000004137	0.000000416	-0.000002541
6	-0.000003374	-0.000004314	0.000000094
6	-0.000003969	0.000000834	-0.000003093
1	0.000002367	0.000001187	-0.000003523
1	0.000000256	0.000000936	-0.000002094
6	-0.000001572	0.000000129	-0.000002126
1	-0.000000608	-0.000000044	-0.000003134
1	-0.000002445	0.000000032	-0.000001594
6	-0.000003632	0.000000152	-0.000002893
1	-0.00000133	-0.00000035	-0.00000179
1	-0.000001724	-0.000000315	-0.000002885
1	-0.000002952	-0.000000069	-0.000002643
1	-0.000002906	-0.000000066	-0.000002754
1	-0.000003215	0.000000246	-0.00000136
6	-0.000001281	0.000000313	-0.000001523
6	0.000001733	0.000000526	0.000000937
1	0.000000627	0.000000859	0.000001332
1	0.000001463	-0.000000388	0.000003179
6	0.000002397	0.000000027	0.00000131
1	0.000001812	-0.000000495	0.000000297
1	0.000001084	-0.000000264	-0.000000017
6	0.000002792	-0.000000217	0.000000387
1	0.000001568	-0.000000065	0.000000966
1	0.000001801	0.000000116	0.000001709
1	0.000003109	0.000000025	0.000000904
1	0.000003232	-0.000000097	0.000000331
1	0.000002749	-0.000000055	-0.000000089
16	-0.000007671	-0.000003784	-0.000009297
8	-0.00000253	0.000000962	0.000002035
8	0.000001527	0.000001831	-0.000000695
6	-0.000002675	0.000001642	0.000002508
6	-0.000002403	0.000001321	-0.000002167

6	-0.00000817	-0.00000529	0.000001533
6	-0.000003096	-0.00000393	0.00000558
1	-0.00000933	0.00000085	0.000001099
6	-0.000002959	0.000000619	0.00000222
1	-0.000001416	0.000000082	0.000002203
6	-0.000001897	-0.000000047	-0.000000046
1	-0.000002907	0.000000169	-0.000000417
1	-0.000002037	0.00000003	0.000002457
6	-0.000002175	-0.000000784	0.000001747
9	-0.000002401	0.000000458	0.000000917
9	-0.000003793	0.000000243	0.00000208
9	-0.00000385	0.000000311	0.00000023
79	-0.000005353	0.000000881	-0.00000362
6	0.00000508	-0.000000336	0.000001892
6	0.000002968	-0.000000371	0.000001433
6	0.000002554	0.000001205	0.000001798
1	0.000000696	-0.000000225	0.000000949
1	0.000002347	0.00000045	0.000001768
7	0.000000316	0.000000408	0.000000098
7	0.00000024	-0.000002095	0.000001351
6	0.000003234	-0.000001053	0.000001347
6	0.000004156	0.000001314	-0.000000587
6	0.000000056	-0.000000042	0.000001944
6	0.000003776	0.000000042	0.00000115
6	0.000002897	0.000001075	0.000000858
6	0.000004102	0.000000527	0.00000066
1	0.000004225	-0.000000256	0.000000466
1	0.000003172	-0.000000781	0.000002819
1	0.000004004	-0.000000004	0.000001274
6	-0.000003592	-0.000001317	-0.00000063
6	-0.000000164	-0.0000012	0.000002607
6	0.000001873	0.000001678	-0.000001199
6	-0.000001501	0.000000585	-0.000000453
6	-0.000001374	0.000000003	0.000000851
6	-0.000003189	-0.000001304	-0.000000903
1	-0.000002546	0.000000151	0.00000102
1	-0.000000544	-0.000000347	-0.000001422
1	-0.000002506	0.000000543	-0.00000044
6	-0.000001555	0.000001924	0.000002548
6	-0.000001127	-0.000000646	0.000003042
6	-0.000001026	-0.000001417	0.000000124
1	-0.000000465	0.000000059	0.000000948
1	-0.000000844	0.000000625	0.000002861
1	-0.000000075	0.000000233	0.000003144

1	-0.000001904	0.000000064	0.000002595
1	-0.000001593	0.000000537	0.000001628
1	-0.000002368	0.000000725	0.000002145
1	-0.00000156	0.000000501	0.000002825
6	-0.000000769	0.000000609	-0.000000983
6	0.000000807	0.000000035	-0.000001835
6	0.000000563	-0.000000215	-0.000000815
1	0.000001045	-0.00000021	-0.000000497
1	0.0000001	-0.00000032	-0.000001396
1	0.000001513	-0.000000394	-0.000002143
1	0.00000012	-0.000000092	-0.000001851
1	0.000000882	0.000000007	0.000000059
1	0.000000531	0.000000117	-0.000000758
1	0.000001401	-0.000000269	-0.000000836
6	0.000002656	-0.000001197	0.00000068
6	0.000002347	0.000002416	0.000002684
6	0.000002039	0.000000402	0.000004178
1	0.000001206	0.000000331	0.000003257
1	-0.000000611	-0.00000041	0.000002561
1	0.000000336	-0.000000155	0.00000314
1	0.000001313	-0.000000104	0.000003262
1	0.00000276	0.000000128	0.000003408
1	0.00000231	-0.000000012	0.000003455
1	0.000001779	-0.000000011	0.000004019
6	0.000001148	0.000001037	0.00000159
6	0.000004118	-0.000000786	-0.000000963
6	0.000004461	-0.00000155	-0.000002435
1	0.000002355	0.000000428	-0.00000013
1	0.000004014	0.000000234	0.000000707
1	0.000003898	0.000000062	-0.000000765
1	0.000004661	0.000000216	-0.00000032
1	0.000002527	-0.000000434	-0.000001449
1	0.000003166	-0.000000071	-0.000001045
1	0.000003029	0.000000183	-0.000001535
<b>Zero-point correction=</b>			<b>1.077946 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>1.149372</b>
<b>Thermal correction to Enthalpy=</b>			<b>1.150316</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>0.956771</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-3732.516739</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-3732.445312</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-3732.444368</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-3732.637914</b>

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6	-0.000000455	0.000000296	0.00000016
6	-0.000000204	-0.000000394	0.000000578
7	0.000000472	-0.000000393	0.000001042
7	-0.000000309	-0.000000457	0.000001043
16	0.000000659	0.000000158	0.000000121
8	0.000000763	-0.000000153	0.000000225
8	0.000000517	0.00000019	-0.000000578
6	0.000001166	-0.000000159	0.000000086
6	0.000001208	-0.000000321	0.000000921
6	0.000001663	-0.000000482	0.000001162
6	0.000001574	-0.000000708	0.000001413
6	0.000001486	-0.000000525	0.000001078
6	0.000001163	-0.000000487	0.000000794
1	0.000001263	-0.000000292	0.000000637
1	0.00000182	-0.000000569	0.000001304
1	0.000001538	-0.000000543	0.000001288
1	0.000001068	-0.000000268	0.000000568
6	0.000001941	-0.000000641	0.000001678
6	0.000000158	-0.000000428	0.000000815
6	-0.000000511	-0.000000257	0.000000753
1	0.000000096	-0.000000381	0.000000755
1	-0.000000149	-0.000000293	0.000001017
6	-0.000000421	-0.000000316	0.000000845
1	-0.000000407	-0.000000245	0.000000189
1	-0.000000319	-0.000000005	0.000000661
6	-0.000000846	-0.000000242	0.000000838
1	-0.000000585	-0.000000418	0.000001236
1	-0.000000344	-0.000000544	0.00000111
1	-0.000001009	-0.000000439	0.000001114
1	-0.000000686	-0.000000231	0.000000644
1	-0.000001147	-0.000000252	0.000000684
6	-0.000000726	-0.000000274	0.000000471
6	-0.000001256	-0.000000212	0.000001239
1	-0.000000881	-0.000000508	0.000001322
1	-0.000001061	-0.00000004	0.000000826
6	-0.000001581	-0.000000419	0.000000639
1	-0.000000987	-0.000000076	0.000000921
1	-0.000001373	-0.000000049	0.000000384
6	-0.000001917	-0.000000376	0.000000677
1	-0.000001771	-0.000000231	0.000000736
1	-0.00000173	-0.000000394	0.000001243
1	-0.000002288	-0.000000235	0.000000736
1	-0.0000018	-0.000000177	0.000000763
1	-0.000001929	-0.000000054	0.000000286

16	-0.000000026	-0.000000035	0.000001097
8	0.000000404	-0.000000413	0.000000962
8	-0.000000578	-0.000000544	0.000001103
6	0.000000024	-0.000000755	0.000001435
6	0.000000465	-0.000000512	0.00000017
6	-0.000000143	-0.000000865	0.000002041
6	0.000000136	-0.000000754	0.000002118
1	0.000000303	-0.000000605	0.000001421
6	-0.00000006	-0.000000089	0.000002382
1	-0.000000607	-0.000000675	0.000001805
6	-0.000000264	-0.000001015	0.000002503
1	0.000000481	-0.000000854	0.000002204
1	-0.000000548	-0.000000948	0.000002568
6	0	-0.000001143	0.000002851
1	-0.000000345	-0.000001192	0.000000301
1	0.000000023	-0.000001205	0.0000003
1	0.000000072	-0.000001122	0.000002851
79	0.000000331	0.000001076	-0.000000724
6	-0.000000349	-0.000000356	-0.000001471
6	-0.000000331	0.000000734	-0.000001987
6	0.000000294	0.000000387	-0.000001415
1	0.000000226	0.000000868	-0.000001976
1	-0.000000028	0.000000619	-0.000002016
7	0.000000034	0.000000892	-0.000001146
7	0.000000033	0.000000689	-0.000001155
6	-0.000000181	0.000000008	-0.000001487
6	-0.000000415	0.000000427	-0.000001217
6	0.000000176	0.000000523	-0.000001315
6	-0.000001008	0.000000514	-0.000000917
6	-0.000000088	0.000000464	-0.000001094
6	-0.000000474	0.000000034	-0.000001028
1	-0.000001023	0.000000541	-0.000000671
1	0.000000247	0.000000382	-0.000000931
1	-0.000000633	0.000000381	-0.000000852
6	0.000000641	0.000000682	-0.000000766
6	0.000000722	0.000000307	-0.000001027
6	0.000000166	0.000000865	-0.000001287
6	0.000001151	0.000000061	-0.000000764
6	0.00000002	0.000000414	-0.00000105
6	0.000000674	0.00000043	-0.000001106
1	0.000001318	0.000000435	-0.000000936
1	-0.000000024	0.000000418	-0.000001093
1	0.000000715	0.000000352	-0.000000858
6	0.000001074	0.000000171	-0.000000842

6	0.000001454	0.000000554	-0.000001486
6	0.000001496	0.000000026	-0.000000746
1	0.000000867	0.000000555	-0.000001453
1	0.000001375	0.000000058	-0.000001663
1	0.000001776	0.000000543	-0.000001499
1	0.000001657	0.000000382	-0.000001357
1	0.00000138	0.000000085	-0.000000171
1	0.000001558	0.000000199	-0.000000058
1	0.000001598	0.000000254	-0.000000674
6	-0.000000073	0.000000289	-0.000001173
6	-0.000001102	0.000000625	-0.000001055
6	-0.000000522	0.000000843	-0.000001589
1	-0.000000743	0.000000685	-0.000001114
1	-0.000000535	0.000000033	-0.000000507
1	-0.000001146	0.000000045	-0.000001075
1	-0.000000642	0.000000197	-0.000000773
1	-0.000000331	0.000000806	-0.000001939
1	-0.000000645	0.000000501	-0.000001706
1	-0.000000853	0.000000717	-0.000001759
6	0.000000689	0.000000466	-0.000001026
6	0.000001035	0.000000382	-0.000000865
6	0.000000073	0.000000696	-0.00000017
1	0.000000438	0.000000452	-0.000001383
1	0.000000739	0.000000036	-0.000000597
1	0.000001268	0.000000352	-0.000000941
1	0.000000819	0.000000265	-0.000000097
1	0.000000535	0.000000793	-0.000001921
1	0.000000509	0.000000601	-0.000001814
1	0.000001056	0.000000583	-0.000001735
6	-0.000000975	0.000000549	-0.000000934
6	-0.00000129	0.000000561	-0.000001554
6	-0.000001254	0.000000034	-0.000000081
1	-0.000000712	0.000000304	-0.000000988
1	-0.000001079	0.000000079	-0.000001805
1	-0.000001473	0.000000688	-0.000001527
1	-0.00000152	0.000000613	-0.000001446
1	-0.000000826	0.000000237	-0.000000335
1	-0.000001543	0.000000125	-0.000000892
1	-0.000001484	0.000000346	-0.000000799
6	-0.000000158	-0.000000015	0.000000201
6	0.000000483	-0.000000138	0.000000158
6	-0.000000191	-0.000000215	0.000000203
6	-0.000000464	-0.000000078	0.000000275
6	-0.000000055	0.000000033	0.000000359

1	-0.000000029	-0.000000102	0.000000284
1	0.000000018	0.000000168	0.000000031
7	-0.000000446	-0.000000009	0.000000083
8	-0.000000683	-0.000000706	-0.000000239
1	-0.000000806	-0.000000118	0.000000311
1	0.000000501	-0.000000059	0.000000084
17	-0.000001394	0.000000005	0.000000017
9	0.000002425	-0.000000817	0.000001549
9	0.000002183	-0.000000774	0.000001712
9	0.000001796	-0.000000748	0.000002065
Zero-point correction=			1.162752 (Hartree/Particle)
Thermal correction to Energy=			1.240973
Thermal correction to Enthalpy=			1.241918
Thermal correction to Gibbs Free Energy=			1.033869
Sum of electronic and zero-point Energies=			-4515.456819
Sum of electronic and thermal Energies=			-4515.378598
Sum of electronic and thermal Enthalpies=			-4515.377654
Sum of electronic and thermal Free Energies=			-4515.585702

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6	-0.000016957	-0.000006779	0.000002233
6	-0.000006727	0.000000828	-0.000007532
7	0.000024407	0.000005589	-0.000004649
7	0.000009785	-0.000007601	-0.000003593
16	0.000002587	0.000001659	0.000004448
8	0.000000947	0.000001417	-0.000001728
8	-0.000000398	-0.000001653	-0.000002555
6	-0.000000064	0.000000664	0.000002036
6	0.000001188	-0.000001344	-0.000000357
6	0.000001031	-0.00000302	0.000001474
6	0.000001672	0.000003016	0.000004356
6	0.00000395	-0.000002066	0.000001302
6	-0.000001395	-0.000002462	-0.000001062
1	0.000000712	-0.000000147	0.000000388
1	0.000001836	-0.000000106	0.000000882
1	-0.000000054	-0.000000494	0.000000659
1	0.000001492	0.000000204	0.00000119
6	0.000001557	-0.000001909	0.000002081
6	-0.00000091	-0.000000433	0.000003244
6	0.000000287	0.000000411	-0.000001703
1	0.000001335	0.000000561	-0.00000109
1	-0.000000078	-0.000000667	0.000000183
6	-0.000000487	0.000000031	0.000000093
1	-0.000000424	0.000000274	0.000000436

1	-0.00000848	0.00000542	0.00000463
6	-0.00000255	0.00000031	0.00000418
1	-0.00000858	-0.00000107	0.00000607
1	-0.00000556	-0.00000047	0.00000213
1	-0.00000773	0.00000111	0.00000087
1	-0.00000514	0.00000301	-0.0000001
1	-0.00001259	0.00000499	-0.00000157
6	-0.00001674	-0.00001776	0.000004108
6	-0.00000839	-0.00001047	0.000001239
1	-0.00002104	0.00000379	0.000001089
1	-0.00000207	0.00000437	0.000001259
6	-0.00002094	0.00000423	0.000000705
1	-0.00000876	-0.00000721	0.000000992
1	-0.00000321	-0.00000124	0.000001017
6	-0.00001762	0.00000002	0.000000852
1	-0.00001724	0.000000193	0.000000675
1	-0.00001903	0.000000039	0.000001045
1	-0.00002195	0.000000392	0.000000901
1	-0.00001756	0.000000227	0.000000681
1	-0.00001961	0.000000475	0.000000175
16	-0.00005009	0.000005205	0.000007246
8	-0.00002104	-0.00002809	0.000002085
8	-0.00001096	-0.00000709	0.00000065
6	0.00000128	-0.000000054	0.000000473
6	-0.00002079	-0.00002675	-0.000001528
6	0.00001751	-0.00001107	0.000003448
6	0.00003514	-0.0000037	0.000003577
1	-0.00000112	-0.00001439	0.00000208
6	-0.00002339	-0.00004076	0.000002178
1	-0.00000521	-0.00000128	0.000001072
6	-0.00002661	0.00000515	0.000002958
1	-0.00000433	-0.00001228	0.000002095
1	-0.00000097	-0.00001099	0.000002425
6	0.000000657	-0.000000796	0.000000532
1	-0.00000609	-0.00001771	0.00000308
1	0.00000047	-0.00002176	0.000003151
1	-0.000000938	-0.00002161	0.000002931
79	0.00002857	0.000004781	0.000006919
6	-0.00001276	-0.00005837	-0.000002513
6	0.00000184	0.000003049	-0.000002256
6	0.00001001	-0.00003008	0.000000358
1	0.0000005	0.000000702	-0.000001295
1	0.00000029	0.000001388	-0.000001853
7	-0.000000099	0.00000565	-0.000002816



7	-0.000005121	-0.000000978	-0.000002217
6	0.000001309	0.000001731	-0.000002205
6	-0.000000013	0.000000817	0.000001378
6	-0.000000289	-0.000003048	-0.000002438
6	-0.000001236	-0.00000106	-0.000001554
6	0.000000956	0.000001086	0.000001198
6	-0.000000572	0.000002409	-0.000001613
1	-0.000001122	0.000000761	-0.000000662
1	-0.000000128	0.00000016	-0.00000074
1	-0.000000762	0.0000005	-0.000000915
6	0.000005439	0.000002617	-0.000002998
6	0.000000389	0.000000279	0.00000194
6	0.000000915	0.000000903	-0.000000263
6	-0.000000426	-0.000000738	-0.000002168
6	0.000000366	0.00000082	0.000000002
6	0.000000838	0.000000707	-0.000001568
1	0.000001399	0.000000025	-0.000000846
1	0.000000555	0.000000264	-0.000000919
1	0.000001014	0.000000052	-0.000000541
6	-0.000000162	0.000000864	-0.000004064
6	0.000002597	0.000000782	-0.000000996
6	0.000004481	0.000000548	0.000001238
1	-0.000001249	0.000000389	-0.000001476
1	0.000001322	0.00000031	-0.000001532
1	0.00000198	0.000000111	-0.000001627
1	0.000001394	0.000000696	-0.000001242
1	0.000001506	-0.000000554	-0.000002947
1	0.000001009	-0.000001137	0.00000035
1	0.000001431	0.000000321	-0.000001235
6	0.000001303	0.000001018	-0.000000223
6	-0.000002432	0.000000162	-0.000001369
6	-0.000001732	0.00000047	-0.000001608
1	0.000000931	0.00000073	-0.000000998
1	-0.00000155	0.000001365	0.000000139
1	-0.000000679	0.00000099	-0.000000906
1	-0.000000909	0.000000727	0.000000642
1	0.000000313	0.000000942	-0.000001636
1	0.000000252	0.000001459	-0.000001493
1	-0.000001171	0.000001146	-0.000001261
6	0.000000683	0.000001293	-0.000000082
6	0.000000724	0.000000629	-0.000001626
6	0.000000511	0.000000436	-0.000002312
1	0.000000781	-0.000000262	-0.000001472
1	0.000000206	0.000000036	-0.000001552

1	0.000001935	-0.000000169	-0.000000782
1	0.000000803	0.000001062	-0.000001555
1	0.000000333	0.000000721	-0.00000208
1	0.000000757	0.000000817	-0.000001762
1	0.000000851	0.000000787	-0.000001597
6	-0.000001349	0.000000448	-0.000000702
6	-0.000000717	0.000001209	-0.000001392
6	-0.000000604	0.000000783	-0.000001049
1	-0.000001355	0.000001151	-0.000000587
1	-0.000000796	0.000001308	-0.000001728
1	-0.000001092	0.00000131	-0.000001279
1	-0.000001158	0.000001037	-0.000001369
1	-0.000001094	0.000000285	0.000000092
1	-0.000001151	0.000001504	0.000000021
1	-0.000001242	0.000000762	-0.000000595
6	0.000000152	-0.000000411	-0.000000156
6	0.000001238	-0.000001136	0.000000365
6	0.000000023	0.000000166	-0.000000194
6	0.000000005	0.000001277	0.000001705
6	-0.000000582	-0.000005395	0.000000818
1	-0.000000041	-0.000000614	0.000000593
1	0.000001272	0.000000104	-0.000000614
7	0.000001335	0.000009635	0.000009514
8	0.000001633	-0.000008559	-0.000005663
1	-0.000000381	-0.000000131	0.000000352
1	0.000000053	-0.00000004	0.000000442
17	-0.000001035	0.000000314	-0.000000721
9	0.00000175	-0.00000171	-0.000001421
9	-0.000000052	-0.000002445	0.000001563
9	0.000000286	-0.000001063	0.000003361

Zero-point correction=

1.165616 (Hartree/Particle)

Thermal correction to Energy=

1.243041

Thermal correction to Enthalpy=

1.243986

Thermal correction to Gibbs Free Energy=

1.041365

Sum of electronic and zero-point Energies=

-4515.476284

Sum of electronic and thermal Energies=

-4515.398858

Sum of electronic and thermal Enthalpies=

-4515.397914

Sum of electronic and thermal Free Energies=

-4515.600534

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6	0.000000243	0.000000892	-0.0000001
6	-0.000001349	0.000000019	0.000000948
7	-0.000000258	-0.000001083	0.000000689
7	0.000001434	-0.000000487	-0.000000999

16	-0.000000056	-0.000000265	0.00000013
8	-0.000000036	-0.000001544	0.000000627
8	-0.000000724	-0.000001263	0.000000884
6	-0.000000718	-0.000002085	0.000000902
6	-0.000000206	-0.000001553	0.000000471
6	-0.000000113	-0.000002068	0.000001219
6	-0.000001211	-0.000002833	0.000001654
6	-0.000000099	-0.000001668	0.000001447
6	-0.000000087	-0.000001839	0.000001853
1	-0.000000147	-0.000001282	0.000000437
1	-0.000000195	-0.000002073	0.000000881
1	-0.000001324	-0.000001861	0.000002317
1	-0.000001046	-0.000001326	0.00000162
6	-0.000000956	-0.00000263	0.00000167
6	-0.000000668	-0.000000105	0.000001233
6	-0.000000636	0.00000086	0.000001104
1	-0.00000086	-0.000000426	0.000001363
1	-0.00000088	0.000000433	0.000000748
6	-0.000001089	0.000000347	0.000001372
1	-0.000000773	0.000000266	0.00000117
1	-0.000000539	0.000000359	0.00000107
6	-0.000001246	0.000001356	0.000001376
1	-0.000001207	0.000001109	0.000001299
1	-0.000001376	0.00000034	0.000001775
1	-0.000001386	0.000001451	0.000001778
1	-0.000001104	0.000001213	0.000001379
1	-0.000001036	0.000001514	0.000001108
6	0.000000621	-0.00000035	-0.000000527
6	0.000000946	-0.000001069	-0.000000906
1	0.000000939	-0.000000402	-0.000000936
1	0.000001026	-0.000000316	-0.000000804
6	0.00000091	-0.000001624	-0.00000139
1	0.000001021	-0.00000125	-0.000001682
1	0.000000475	-0.000001462	-0.000000374
6	0.000001224	-0.00000199	-0.000001145
1	0.00000089	-0.000001317	-0.000001042
1	0.00000106	-0.000001467	-0.000001469
1	0.000001279	-0.000002481	-0.00000139
1	0.000001263	-0.000002198	-0.000001433
1	0.000000921	-0.000002358	-0.000000826
16	0.000000584	0.000000383	-0.000002029
8	0.000000614	0.000000309	-0.000000612
8	0.000000818	0.000000412	-0.000000938
6	0.000001097	0.000000062	-0.000001445

6	0.00000769	-0.00000917	-0.00001205
6	0.00001873	0.00000762	-0.00001684
6	0.00000741	-0.00000304	-0.00004935
1	0.00000981	-0.00001543	-0.00001188
6	0.00002201	0.00000208	0.00001333
1	0.00001689	0.00000609	-0.00002203
6	0.0000165	-0.00000823	-0.00003658
1	0.00001592	-0.00001206	-0.00002057
1	0.00002019	0.00000005	-0.00003008
6	0.00001888	-0.00001157	-0.00004347
1	0.0000198	0.00000045	0.00000549
1	0.00004283	-0.00003117	-0.00002788
1	0.00000528	0.00000322	-0.0000449
79	-0.00000566	0.00000456	0.00001212
6	-0.00000343	0.00000724	-0.00000941
6	-0.00000505	0.00001021	0.00000088
6	-0.00000068	0.00001193	0.00000042
1	0.00000166	0.00000879	-0.00000289
1	-0.00000553	0.00001493	0.00000715
7	-0.00001175	0.00001835	0.00001901
7	0.00000175	0.00000389	-0.0000068
6	0.00000658	0.00000744	-0.00000236
6	-0.00001976	0.00000841	0.00001958
6	-0.00000436	0.00001879	0.00001143
6	-0.00001776	0.00001168	0.00001761
6	-0.00001278	0.00001692	0.00001616
6	-0.00001362	0.00001209	0.00001568
1	-0.00001685	0.00000874	0.00002242
1	-0.00001059	0.00002308	0.00001255
1	-0.00001708	0.0000164	0.00002081
6	0.00000545	0.00000412	-0.00000421
6	0.00000624	0.00000669	-0.00001318
6	0.00000254	-0.00000066	-0.00000031
6	0.00001108	0.0000003	-0.00001356
6	0.00001061	-0.00000577	-0.00000878
6	0.00001218	-0.00000161	-0.00001358
1	0.00001169	0.00000055	-0.0000018
1	0.00000836	-0.00000111	-0.00000694
1	0.00001229	-0.00000462	-0.00000174
6	0.00000084	0.00000898	-0.00001078
6	0.00000567	0.00001772	-0.00001343
6	0.00000628	0.0000157	-0.00001212
1	0.00000113	0.00001559	-0.00000862
1	0.00000405	0.00001606	-0.00000704

1	0.00000685	0.000002324	-0.000001267
1	0.000000999	0.000001467	-0.000001798
1	0.000000916	0.000001069	-0.000001535
1	0.000000873	0.000001436	-0.000001606
1	0.00000099	0.000001752	-0.000001355
6	-0.000000011	-0.000000836	0.000000368
6	-0.000000103	-0.000000998	-0.000000047
6	-0.000000249	-0.000000387	-0.000000642
1	-0.000000027	-0.000000244	0.000000302
1	0.000000888	-0.000000267	-0.000000835
1	-0.000000051	-0.000001564	0.000000726
1	0.000000078	-0.000002154	-0.000000543
1	0.000000151	-0.000000448	-0.000000315
1	0.000000711	-0.000001059	-0.000000255
1	-0.000000025	-0.000000895	0.000000396
6	-0.000000537	0.000001708	0.000000645
6	-0.000000055	0.000002588	-0.000000201
6	-0.000000534	0.000002656	0.000000725
1	-0.000000067	0.000001707	-0.000000226
1	-0.000000653	0.000002205	-0.000000273
1	-0.000000234	0.000002256	-0.000000022
1	-0.000000575	0.000002412	0.000000714
1	-0.000000745	0.000003024	0.000000048
1	-0.000001152	0.000002798	0.000000491
1	-0.000000386	0.000002934	0.000000246
6	-0.000000498	0.000000691	0.000001478
6	-0.000001189	0.000000384	0.000001579
6	-0.000000669	-0.000000482	0.000001997
1	-0.000001121	-0.000000148	0.000000926
1	-0.000001172	0.000000465	0.000001933
1	-0.000001654	0.000000502	0.00000171
1	-0.000001262	0.000000288	0.000001414
1	-0.000001085	-0.000000065	0.000001318
1	-0.000001593	0.000000272	0.000002283
1	-0.000001148	-0.000000959	0.000001625
6	0.000000282	0.000000121	0.000000841
6	0.000000201	0.000000035	0.00000003
6	-0.000000267	-0.000000096	-0.000000025
6	0.000000006	-0.000000804	0.000000375
6	0.000000483	-0.000000271	-0.000000794
1	-0.000000131	0.000000143	0.000000047
1	-0.000000703	-0.000000322	-0.000000051
7	-0.000000941	-0.000000028	-0.000000115
8	0.000001421	-0.00000178	-0.000001224

1	0.00000302	-0.00000812	-0.00000258
1	-0.00000247	0.00000756	0.00000156
17	0.00000575	-0.00001509	-0.00000466
9	-0.00000742	-0.00002734	0.00001388
9	-0.00001251	-0.00002335	0.00002465
9	-0.00001056	-0.00001994	0.00001849
Zero-point correction=			1.163128 (Hartree/Particle)
Thermal correction to Energy=			1.240363
Thermal correction to Enthalpy=			1.241307
Thermal correction to Gibbs Free Energy=			1.035852
Sum of electronic and zero-point Energies=			-4515.460431
Sum of electronic and thermal Energies=			-4515.383196
Sum of electronic and thermal Enthalpies=			-4515.382252
Sum of electronic and thermal Free Energies=			-4515.587707

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6	-0.00001547	0.00000228	0.00000266
6	0.00000379	-0.00002362	-0.00000412
7	0.00001356	-0.000007419	-0.000006786
7	0.00000294	0.000005201	-0.000003311
16	0.00000185	0.000006541	-0.000001675
8	-0.000001522	-0.000002669	-0.000001679
8	0.000000855	0.000000378	-0.000003194
6	0.000001471	-0.000000024	-0.00000176
6	0.0000009	-0.000001383	-0.000002575
6	0.00000095	-0.00000104	-0.000002533
6	0.000001812	0.000002126	-0.00000199
6	0.000000721	0.000001174	-0.000001287
6	0.000000827	0.000000359	-0.000001948
1	0.000000005	-0.000000531	-0.000002885
1	0.000000636	-0.000000251	-0.000002341
1	0.000001996	0.000001491	-0.000000827
1	0.000001598	0.000000922	-0.000001403
6	0.000003767	0.000006207	-0.000000431
6	-0.00000036	0.000000376	-0.00000049
6	-0.000000859	-0.000001978	-0.000001145
1	-0.000000617	-0.000001544	-0.000002012
1	-0.000000184	-0.000001045	-0.000001129
6	-0.00000175	-0.000002438	-0.000001103
1	-0.000001295	-0.000002546	-0.000001421
1	-0.000001077	-0.000001409	0.000000074
6	-0.0000027	-0.000002704	0.000000163
1	-0.000001753	-0.000002231	-0.00000032
1	-0.000001373	-0.00000247	-0.000000948

1	-0.000002518	-0.000003335	-0.00000034
1	-0.000002115	-0.000003416	-0.000000937
1	-0.000002217	-0.000003072	-0.000000176
6	0.000004001	0.00000033	-0.000000493
6	0.0000017	0.000001404	-0.000001212
1	0.000000937	0.000001235	0.000000657
1	0.000000886	0.000000666	-0.000001282
6	0.000001839	0.000001588	-0.000002337
1	0.00000135	0.00000144	-0.000001994
1	0.00000145	0.000001306	-0.000001697
6	0.000003246	0.000002686	-0.000001532
1	0.000002205	0.00000263	-0.000000954
1	0.000002483	0.000002645	-0.000000746
1	0.000003031	0.000003125	-0.000002366
1	0.000002736	0.0000023	-0.000002543
1	0.000002927	0.000002199	-0.000002961
16	-0.000002343	-0.00000361	-0.000000404
8	0.000002178	0.000001997	-0.000000138
8	0.000000935	0.00000136	-0.000001456
6	0.000002887	-0.000000885	0.000000054
6	-0.000002166	-0.000001699	-0.000001826
6	-0.000001865	-0.000001373	0.000000505
6	-0.000002887	-0.000002995	0.000001519
1	-0.000000927	-0.000000249	0.000000118
6	-0.000002359	-0.000001009	-0.000003183
1	-0.000000548	-0.00000059	-0.000001576
6	0.000001706	-0.000001404	0.000000327
1	-0.000001592	-0.000002067	0.000000568
1	-0.000001464	-0.000002664	-0.000001514
6	-0.000001368	-0.000003395	-0.000000414
1	-0.000002479	-0.00000208	-0.000000573
1	-0.00000194	-0.000004019	-0.000000404
1	-0.000003876	-0.000002949	-0.000000173
79	-0.000000142	-0.000002677	-0.000002649
6	-0.000004117	0.000000091	0.000006084
6	0.000000481	-0.000003707	0.000003093
6	-0.000001554	0.000003357	0.000001682
1	0.000000634	0.000002751	0.000003045
1	-0.000001103	0.000000857	0.000003177
7	-0.000000875	0.000005271	0.000001393
7	0.000000858	-0.000001343	0.00000051
6	-0.00000185	0.000003657	0.000002981
6	0.000001374	-0.000003213	0.000002702
6	-0.000000405	-0.0000028	-0.000000118

6	-0.000001529	-0.000002297	-0.000001164
6	-0.000001294	-0.000002587	0.000003134
6	-0.000003122	0.000001317	0.000002189
1	-0.00000177	-0.000001535	0.000001529
1	-0.000002476	-0.000002263	0.000001978
1	-0.000002259	-0.00000267	0.000001403
6	0.000003022	0.000001754	0.000002593
6	-0.000002188	0.000006266	-0.000000628
6	0.000001437	0.000002517	0.000001886
6	0.000001342	0.000002261	0.000004134
6	-0.000000591	0.000003324	-0.000001783
6	0.000003004	0.000000088	0.000001441
1	0.000000871	0.00000243	0.0000016
1	0.000002165	0.000003565	0.000001215
1	0.000001706	0.000003677	0.000001364
6	-0.000000788	-0.000000579	0.000003344
6	0.000001381	0.000002752	0.000003018
6	0.000001397	0.000000677	0.000001957
1	-0.000000568	0.000000607	0.000002429
1	-0.000000516	0.000001045	0.000003896
1	-0.00000069	0.000001145	0.000003731
1	-0.000000011	0.000001897	0.000003719
1	-0.000000463	-0.000000315	0.000001513
1	-0.000000382	0.000001273	0.000002403
1	-0.000000763	0.000000366	0.000002426
6	0.000004287	0.000001341	-0.000001258
6	0.000001922	0.000002666	0.000000105
6	-0.000000246	0.000003584	0.00000288
1	0.000001398	0.000001279	0.000002906
1	0.000003209	0.000003885	-0.000000782
1	0.000001548	0.000002799	-0.000000563
1	0.000002099	0.000002351	-0.000000122
1	0.000001571	0.000002612	0.000002806
1	0.000003078	0.000003076	0.000002127
1	0.00000181	0.000003116	0.000001618
6	-0.000001045	0.000000298	0.000002578
6	-0.000003335	-0.000002347	0.000002044
6	-0.0000023	-0.000001378	0.000003565
1	-0.000000627	-0.000000066	0.000002009
1	-0.000001526	-0.000001525	0.00000159
1	-0.000002056	-0.000001164	0.000002453
1	-0.000001909	-0.000002213	0.000001701
1	-0.000001889	-0.000000674	0.000003716
1	-0.00000233	-0.000000892	0.000003221



1	-0.000002369	-0.000001163	0.000003703
6	-0.000003028	-0.00000213	0.000000361
6	0.000001637	0.000001443	0.000002078
6	0.000001257	0.000002211	0.000000383
1	-0.000000584	0.000000074	0.000001394
1	-0.000000635	0.000000138	0.000002338
1	-0.000000251	0.000001047	0.000001488
1	-0.000001131	0.000000013	0.000002145
1	-0.000000039	-0.000000422	-0.000000489
1	-0.000000047	-0.000001464	-0.000000048
1	0.000000671	-0.000000412	-0.000000251
6	-0.000001603	0.000000347	-0.000000471
6	0.000002185	0.000000094	-0.000003585
6	-0.000001466	-0.000004017	-0.000006096
6	0.000000325	-0.000001405	-0.000001544
6	0.000001525	0.000000317	-0.000007826
1	-0.000000765	-0.00000286	-0.000004209
1	0.000000341	-0.000003074	-0.000002031
7	-0.000000047	-0.000004098	-0.000003843
8	-0.000002844	-0.000000032	-0.000000004
1	0.000000069	-0.000001954	-0.000004667
1	-0.000001513	-0.000002684	-0.000002728
17	0.000001262	-0.000000373	-0.000002071
9	0.000001936	-0.00000111	-0.000000807
9	0.000002069	0.000000199	-0.000002819
9	-0.000002298	-0.000001499	-0.000001993

Zero-point correction=

1.165641 (Hartree/Particle)

Thermal correction to Energy=

1.243245

Thermal correction to Enthalpy=

1.244189

Thermal correction to Gibbs Free Energy=

1.041051

Sum of electronic and zero-point Energies=

-4515.458189

Sum of electronic and thermal Energies=

-4515.380586

Sum of electronic and thermal Enthalpies=

-4515.379641

Sum of electronic and thermal Free Energies=

-4515.582779

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6	0.000000474	0.000001912	0.000000586
6	0.000000018	-0.000000781	-0.000000061
7	-0.000000016	0.000000387	-0.000001718
7	0.000000534	0.000000698	0.000000362
16	0.000000155	-0.000000872	-0.000000091
8	-0.000000028	0.000000144	-0.000001628
8	-0.000000712	-0.000000367	-0.000000887
6	-0.000000067	-0.000000326	-0.000000198

6	-0.000000598	-0.000000442	-0.000002551
6	-0.000000045	-0.000000671	-0.000002623
6	-0.000001066	-0.000000962	-0.000003093
6	-0.000001215	-0.000000825	-0.000002263
6	-0.000000495	-0.000000718	-0.000001617
1	-0.000000106	-0.000000041	-0.000002662
1	-0.000000463	-0.000000322	-0.000003433
1	-0.000001297	-0.000001071	-0.000001888
1	-0.000000795	-0.000000077	-0.000001183
6	-0.000001239	-0.000000954	-0.000003126
6	0.000000203	0.000000369	-0.000001658
6	0.000000083	0.000000932	-0.000001366
1	0.000000243	0.000000289	-0.000001718
1	0.000000446	0.000000524	-0.000001311
6	0.000001172	0.000001286	-0.000001584
1	0.000000855	0.000000847	-0.000000146
1	0.000001138	0.000000951	-0.000000704
6	0.000001681	0.000001786	-0.000001442
1	0.000001279	0.000001408	-0.000001371
1	0.000000116	0.000001217	-0.000002032
1	0.000001948	0.000002041	-0.000000177
1	0.000001667	0.000000171	-0.000001677
1	0.000001843	0.000001856	-0.000001019
6	0.000000029	0.000000685	-0.000000234
6	0.000001202	0.000001108	0.000000254
1	0.000000743	0.000000784	-0.000000245
1	0.000000696	0.000000535	0.000000747
6	0.000001501	0.000001539	0.000000046
1	0.000001131	0.000001089	-0.000000106
1	0.000001027	0.000001058	0.000000596
6	0.000001895	0.000001917	0.000000501
1	0.000001405	0.000001406	0.000000846
1	0.000001572	0.000001514	0.000000119
1	0.000002229	0.000002219	0.000000685
1	0.000001938	0.000002002	0.000000086
1	0.000001852	0.000001801	0.000000835
16	-0.000000809	0.000000399	-0.000000077
8	-0.000000337	-0.000000796	-0.000000236
8	-0.000000354	-0.000000257	0.000000265
6	0	0.000000206	-0.000000809
6	0.000000217	-0.000000087	-0.000001424
6	-0.000000525	0.000000236	-0.000001169
6	-0.000000747	0.000000285	-0.000002073
1	-0.000000313	-0.000000553	-0.000001175

6	0.000000868	0.000000384	-0.000001321
1	0.000000212	-0.00000002	-0.000000286
6	0.000000232	-0.00000026	-0.000001277
1	-0.000000276	-0.000000237	-0.000000245
1	0.000000486	0.000000342	-0.000001216
6	0.000000021	0.000001139	-0.000002583
1	0.000000104	-0.000000051	-0.000002591
1	0.000000399	-0.000000107	-0.000000288
1	0.000000127	0.000000567	-0.000002992
79	-0.000000075	-0.000001072	0.000000209
6	0.00000047	0.000000557	0.000001398
6	0.000000076	-0.000000015	0.00000101
6	-0.000000691	-0.000000764	0.000001685
1	-0.000000792	-0.00000078	0.000001679
1	0.000000052	-0.000000138	0.000001198
7	-0.00000016	0.000000465	0.000000654
7	-0.000000902	-0.00000082	0.000001232
6	0.000000455	-0.00000053	0.000000682
6	0.000000662	0.000001407	0.00000105
6	0.000000405	0.00000035	-0.000000554
6	0.000000784	0.000001233	0.000000104
6	0.000000763	0.000001053	-0.000000085
6	0.000001121	0.000000585	0.000000067
1	0.000001754	0.000001539	0.000000433
1	0.000000869	0.000000991	-0.000000859
1	0.000001496	0.000001591	-0.000000504
6	-0.000001392	-0.000000861	0.000001375
6	-0.000001351	-0.000001474	0.000000659
6	-0.000000586	-0.000001537	0.000002056
6	-0.000001625	-0.000001836	0.000001034
6	-0.000001031	-0.000001277	0.000002174
6	-0.000001569	-0.000001591	0.000001708
1	-0.000001813	-0.000001978	0.000000956
1	-0.000000882	-0.000001119	0.000002388
1	-0.000001828	-0.000001855	0.000001909
6	-0.000001112	-0.000001364	0.00000048
6	-0.000001587	-0.000001606	0.000000488
6	-0.000001611	-0.000001396	-0.000000231
1	-0.000001115	-0.000001161	0.000000408
1	-0.000001592	-0.000001641	0.000000961
1	-0.000001725	-0.000001711	0.000000123
1	-0.000002001	-0.000002058	0.00000068
1	-0.000001136	-0.00000133	0.000000013
1	-0.000001758	-0.000001947	0.00000004

1	-0.000001649	-0.000001526	-0.000000689
6	-0.000000714	-0.000000643	0.000001688
6	-0.000000398	-0.000000399	0.000002353
6	-0.000000549	-0.000000165	0.000003278
1	0.000000035	0.000000062	0.000002467
1	0.000000406	0.000000138	0.000002048
1	0.000000082	0.000000018	0.000002553
1	-0.000000065	-0.000000578	0.000002687
1	-0.000000738	-0.000000857	0.00000307
1	-0.000000943	-0.000000858	0.000003604
1	-0.000000183	-0.000000363	0.000003345
6	-0.000000233	-0.000000112	-0.000000288
6	-0.00000007	-0.000000004	-0.000001191
6	-0.000000004	-0.000000138	-0.000000464
1	-0.000000314	-0.000000046	-0.000000248
1	0.000000087	-0.000000312	-0.000001369
1	-0.000000406	-0.000000349	-0.000001242
1	0.000000154	0.000000075	-0.000001308
1	-0.00000004	-0.000000078	0.000000119
1	-0.000000031	0.000000214	-0.00000042
1	-0.000000366	-0.000000359	-0.000000407
6	0.000001223	0.000000719	0.00000121
6	0.000001195	0.000001215	0.000002006
6	0.000001168	0.000001215	0.000001274
1	-0.000000082	0.000000569	0.000001724
1	0.000001021	0.000000946	0.000002014
1	0.000001042	0.000001053	0.000002212
1	0.000001468	0.00000126	0.000001573
1	0.000000628	0.000000381	0.000000992
1	0.000001243	0.000001255	0.000000992
1	0.00000108	0.00000098	0.000001753
6	-0.000000833	-0.000000435	0.000000971
6	-0.000000727	-0.000001435	0.00000133
6	-0.000000836	-0.00000082	0.000002008
6	-0.00000037	-0.000000155	0.000002072
6	-0.000000013	-0.000000068	0.000001407
1	-0.000001015	-0.000001021	0.000002094
1	-0.000000625	-0.000000414	0.000000652
7	-0.000000861	-0.000001063	0.000001136
8	0.000001591	0.000000668	0.000000552
1	-0.000000194	-0.000000164	0.000002309
1	-0.000001188	-0.000001249	0.000001222
17	0.000000474	0.000000474	0.000001898
9	-0.000001426	-0.000001581	-0.000002919

9	-0.000001177	-0.000001097	-0.000004016
9	-0.000000613	-0.000000533	-0.000003133
Zero-point correction=			1.163146 (Hartree/Particle)
Thermal correction to Energy=			1.241148
Thermal correction to Enthalpy=			1.242092
Thermal correction to Gibbs Free Energy=			1.036363
Sum of electronic and zero-point Energies=			-4515.457701
Sum of electronic and thermal Energies=			-4515.379698
Sum of electronic and thermal Enthalpies=			-4515.378754
Sum of electronic and thermal Free Energies=			-4515.584484

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6	0.000002433	0.000006909	0.000005221
6	-0.000002349	-0.000002116	-0.000000278
7	-0.000006548	-0.000005977	-0.000002408
7	0.000013649	-0.000004717	0.000001362
16	-0.000000451	0.000010328	0.000001852
8	-0.00000092	-0.000003915	0.000001363
8	-0.000002615	-0.000001011	-0.00000082
6	-0.000001066	0.000000542	-0.000001043
6	0.000000678	0.000001684	0.000001399
6	-0.000002892	0.000000966	0.000001029
6	-0.000001292	0.000001284	0.000001487
6	0.000000134	0.00000257	0.000000914
6	-0.000003086	0.000001631	0.000000481
1	-0.00000087	-0.000000013	0.00000003
1	-0.000000844	0.000001366	0.000000858
1	-0.000001415	0.000001403	0.000001239
1	-0.000000109	0.000000955	0.000000102
6	-0.000001413	0.000001076	0.000002103
6	0.000001303	0.000000457	0.000000317
6	-0.000001013	-0.000000771	0.000003166
1	-0.000000021	0.000000668	0.000001088
1	0.000000294	0.000000506	0.000000719
6	0.000001539	0.000001743	-0.000002352
1	0.000000175	-0.000000928	-0.000000161
1	0.000000528	0.000000785	-0.000000151
6	0.000000532	-0.000000839	0.000000939
1	0.000000803	-0.000000026	0.000000858
1	-0.00000004	-0.000000217	0.000000469
1	0.000001081	0.000000257	0.000000166
1	0.000000264	-0.000000229	-0.000000421
1	0.000001214	-0.000000512	-0.000000004
6	0.000000759	0.000000178	0.000003595

6	0.000000096	0.000000224	-0.000001291
1	0.000002328	0.000000072	0.000001186
1	0.000001938	0.000000737	-0.000000297
6	0.000002024	0.000000617	0.000001157
1	0.000000941	-0.000000764	0.000001205
1	0.000001745	-0.000000004	0.000000181
6	0.000002131	-0.000000016	0.000000897
1	0.000001538	-0.000000099	0.000000724
1	0.000001688	0.000000098	0.00000114
1	0.00000235	-0.000000284	0.000000578
1	0.000001806	-0.000000055	0.000000454
1	0.000001635	-0.000000396	0.00000049
16	-0.000005379	0.000000794	-0.000003139
8	0.000000574	-0.000002495	0.000000251
8	0.000000653	-0.000000924	0.00000198
6	0.000003899	0.000000889	0.000000156
6	-0.000001818	0.000000274	-0.000001527
6	-0.000000276	0.000000242	0.000000281
6	0.000000773	0.000001399	0.000001325
1	0.000000655	0.000001313	0.000001868
6	0.000000752	0.000001275	0.000002296
1	0.000000598	0.000000875	0.000001231
6	0.000000024	0.000002417	0.000002032
1	-0.000000344	0.000001058	0.00000167
1	0.000001007	0.000001728	0.000002237
6	0.000000942	0.000002098	0.000002112
1	0.000000598	0.000002187	0.000002329
1	0.000000027	0.000002034	0.000002267
1	0.000001114	0.000001899	0.000002076
79	0.000002382	0.000003232	0.000000348
6	-0.000003932	0.000001705	-0.000009229
6	-0.000003789	-0.00000106	-0.000000473
6	-0.000001159	-0.000001252	-0.000000889
1	-0.000000366	0.000000195	-0.000001001
1	-0.000000194	-0.000002317	-0.000002536
7	0.000003648	-0.000001916	0.000005363
7	0.000005773	-0.000002237	0.00000037
6	0.000001617	0.000002591	-0.000002717
6	0.000000087	-0.000001096	-0.00000202
6	-0.000000319	-0.00000247	0.000001034
6	-0.000000249	-0.000002705	0.000000231
6	-0.000000892	-0.00000294	-0.000002967
6	0.000000728	0.000001026	-0.000000039
1	0.000001259	-0.00000135	-0.000001267

1	-0.000000745	-0.000000732	-0.000001757
1	0.000001034	-0.00000108	-0.000000658
6	-0.000002405	-0.000000265	-0.000001885
6	0.000001211	-0.000000561	0.000000443
6	-0.000001354	0.000000724	-0.000000033
6	-0.00000135	0.000000821	-0.000001622
6	-0.000000717	-0.000000103	0.000000057
6	-0.000001456	-0.000001438	-0.000001071
1	-0.000001835	-0.000000319	-0.000000081
1	0.000000983	-0.000000923	-0.000000605
1	-0.000000616	0.000000544	-0.000000194
6	-0.00000361	-0.000000511	-0.000000796
6	-0.000000409	-0.000000891	-0.000001875
6	0.000000372	-0.000000317	-0.000000185
1	-0.000002215	-0.000000626	-0.000000545
1	-0.000001718	-0.000000647	-0.000001487
1	-0.000001809	-0.000000469	-0.000001368
1	-0.000002205	-0.000000275	-0.000000917
1	-0.000001385	0.000000805	-0.000000965
1	-0.000002881	0.000000249	-0.000001019
1	-0.000001755	-0.000000332	-0.000000859
6	0.000000697	-0.000003214	-0.000001344
6	-0.000000118	-0.000001323	-0.000000617
6	0.000000857	0.000000385	-0.000000603
1	-0.000000047	-0.000001295	-0.000001083
1	0.000001321	-0.000000188	-0.000000634
1	0.000000463	-0.000000746	-0.000000729
1	-0.000000023	-0.000000406	-0.000000343
1	0.000000026	-0.000001518	-0.000000938
1	-0.000000593	-0.00000142	-0.000001549
1	0.000000535	-0.000001816	-0.000001216
6	-0.000003696	0.000000812	-0.0000011
6	-0.000000366	-0.000001146	-0.000002902
6	0.000001488	-0.000002669	-0.000001614
1	-0.00000101	-0.000000594	-0.000001212
1	-0.000000698	0.000000635	0.000000069
1	-0.000001129	-0.000000258	0.000000022
1	-0.000000913	-0.000000945	0.000000244
1	-0.000000821	-0.000001468	-0.000001929
1	-0.000001466	-0.000000898	-0.000001353
1	-0.000001696	-0.000000659	-0.000001531
6	0.000000762	-0.000002915	-0.000000965
6	0.000000738	-0.000001151	-0.000001508
6	0.00000048	-0.000000354	-0.000001133

1	0.000000274	-0.000001413	-0.000000813
1	0.000000933	-0.000001502	-0.000001193
1	0.00000097	-0.000001475	-0.000001153
1	0.000001229	-0.000001714	-0.000000505
1	0.000000722	-0.000000622	0.000000015
1	0.00000151	-0.000000754	-0.000000456
1	0.000001203	-0.000001581	-0.000000483
6	-0.000002346	-0.000001688	-0.0000007088
6	-0.00000048	-0.00000214	0.000004843
6	0.000001037	0.000003913	0.000002059
6	0.000000543	0.000000023	-0.000003294
6	-0.000002284	-0.000004307	0.000003992
1	-0.000000667	0.000000066	0.000000239
1	-0.000000961	-0.000000056	0.000000493
7	0.000003555	0.000006961	-0.000002164
8	-0.000002327	-0.000002756	0.000005728
1	0.000001315	-0.000000165	0.000000732
1	0.000000039	0.000000798	-0.000000759
17	0.000000565	-0.000000056	0.000000511
9	-0.000000817	0.000002666	0.000000063
9	-0.000000686	0.000001985	0.000001637
9	-0.000000303	0.000002704	0.000002345

Zero-point correction=

1.165550 (Hartree/Particle)

Thermal correction to Energy=

1.243015

Thermal correction to Enthalpy=

1.243959

Thermal correction to Gibbs Free Energy=

1.040926

Sum of electronic and zero-point Energies=

-4515.476360

Sum of electronic and thermal Energies=

-4515.398895

Sum of electronic and thermal Enthalpies=

-4515.397950

Sum of electronic and thermal Free Energies=

-4515.600984

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6	-0.000001362	-0.00000006	-0.000000535
6	0.000001456	-0.000000299	0.000000049
7	0.000000762	0.000000176	-0.000001943
7	-0.000001679	-0.000000942	0.000000415
16	0.000000974	-0.000000986	-0.000000819
8	0.000001239	-0.00000159	0.000000021
8	0.000001341	-0.000001398	-0.000000932
6	0.00000143	-0.000000969	-0.000001273
6	0.000000907	-0.000000366	-0.000000962
6	0.000000882	-0.000000517	-0.000001775
6	0.000001934	-0.000000678	-0.000002762
6	0.000001136	-0.000000867	-0.000002133



6	0.00000141	-0.000001123	-0.000001763
1	0.000000614	-0.000000283	-0.000000999
1	0.000000891	-0.000000001	-0.000001766
1	0.000002213	-0.000001328	-0.000002607
1	0.000001863	-0.000001402	-0.000001949
6	0.000001279	-0.000000603	-0.000002687
1	0.00000156	-0.000000968	-0.000003149
1	0.000001541	-0.000000914	-0.000001992
1	0.000000877	0.000000182	-0.00000256
6	0.000001542	-0.000000325	-0.000001587
6	0.00000058	0.000000436	-0.000002135
1	0.000001198	-0.000000521	-0.000002116
1	0.000000202	0.000000243	-0.000001766
6	0.000000714	0.000000465	-0.000002639
1	0.000000322	0.000000188	-0.00000169
1	0.00000013	0.000000071	-0.00000172
6	0.000000346	0.000001074	-0.000003055
1	0.000000571	0.000000443	-0.000002686
1	0.000000999	0.000000117	-0.000002997
1	0.000000384	0.000001112	-0.000003498
1	0.00000032	0.000001137	-0.000002957
1	0.000000037	0.00000128	-0.000002728
6	-0.00000018	-0.000000025	0.000000028
6	0.000000022	-0.00000041	0.000000722
1	-0.00000032	0.000000785	0.000000596
1	-0.000000234	0.000000028	0.000000252
6	0.000000085	-0.000000719	0.000001161
1	0.000000197	-0.000000709	0.000000749
1	0.000000229	-0.000000435	0.000000071
6	0.000000328	-0.000001147	0.000001434
1	-0.000000141	-0.00000038	0.000000988
1	-0.000000319	-0.00000023	0.000001497
1	0.000000189	-0.000001224	0.000001812
1	0.000000374	-0.000001371	0.000001562
1	0.00000066	-0.000001329	0.000001079
16	-0.000000216	0.000000463	-0.000000882
8	-0.000001209	0.000001537	-0.000000007
8	-0.000000308	0.000001462	-0.000000915
6	-0.00000083	0.000000994	-0.000001069
6	-0.000000632	0.000001341	-0.000001461
6	-0.000001129	0.000001659	-0.000000075
6	-0.000000808	0.000001497	-0.000001592
1	-0.000000142	0.000001401	-0.000001713
6	-0.000000906	0.000001911	-0.000000701

1	-0.000001365	0.000001735	0.000000021
6	-0.000001001	0.000001612	-0.000001503
1	-0.000000514	0.000001769	-0.000002263
1	-0.000001329	0.00000202	-0.000000456
6	-0.000000859	0.000001694	-0.000001711
9	-0.000000585	0.000001908	-0.00000153
9	-0.000001386	0.000002701	-0.000001369
9	-0.000000978	0.000002428	-0.000002107
79	-0.000000085	-0.000000168	0.000000132
6	-0.00000005	-0.000000386	0.000001126
6	-0.000000748	-0.000000084	0.000001984
6	-0.000000623	0.00000007	0.000001485
1	-0.000000873	0.000000263	0.000001631
1	-0.000000755	-0.000000205	0.000002514
7	-0.000000695	-0.000000033	0.000001456
7	0.000000141	0.000000166	0.000000684
6	-0.000000517	-0.000000452	0.000001949
6	-0.000000066	-0.000001098	0.000002226
6	-0.000000621	0.000000019	0.000002257
6	0.000000248	-0.000001308	0.000002362
6	-0.000000681	-0.000000311	0.000002511
6	-0.000000236	-0.000000899	0.00000259
1	0.000000035	-0.000001682	0.000002391
1	-0.000000947	-0.000000096	0.000002718
1	-0.000000224	-0.000001064	0.000002824
6	-0.00000002	0.00000012	0.000000907
6	-0.000000883	0.000000985	-0.000000107
6	0.000000282	0.000000122	0.000000186
6	-0.000000545	0.00000102	-0.000000319
6	-0.000000312	0.000000329	-0.000000438
6	-0.000000298	0.000000614	-0.000000747
1	-0.000000814	0.000001364	-0.000000781
1	0.000000239	-0.000000215	-0.000000433
1	-0.00000002	0.000000787	-0.000001047
6	-0.000001091	0.000001341	0.000000344
6	-0.000001458	0.000001582	0.000000722
6	-0.000000971	0.000001447	-0.000000232
1	-0.000001114	0.000000802	0.000000532
1	-0.000001318	0.000001274	0.00000109
1	-0.000001715	0.000001824	0.000000798
1	-0.000001523	0.000001811	0.000000445
1	-0.000000919	0.000001442	-0.000000053
1	-0.000001348	0.000001841	-0.000000491
1	-0.000001401	0.0000019	-0.000000088

6	0.00000307	-0.00000764	0.00000773
6	0.00000879	-0.00000917	0.00000371
6	0.00000172	-0.00000844	0.00000988
1	-0.00000115	-0.00000805	0.00000961
1	0.00000041	-0.00000079	0.0000001
1	0.00000896	-0.00001484	0.00000543
1	0.00000858	-0.00000963	-0.00000203
1	-0.00000119	-0.00000267	0.00001248
1	0.00000218	-0.00000626	0.00000564
1	0.00000362	-0.00001125	0.00001292
6	-0.00001007	0.00000426	0.00002162
6	-0.00001516	0.00000841	0.00001834
6	-0.00001413	0.00000631	0.00002913
1	-0.00001184	0.00000638	0.00001758
1	-0.00000091	0.00000709	0.00001651
1	-0.00001613	0.00001115	0.00001853
1	-0.00001405	0.00000814	0.00002036
1	-0.00001423	0.00000277	0.00003039
1	-0.00001532	0.00000554	0.00003215
1	-0.00001798	0.00001054	0.00002796
6	0.00000337	-0.0000134	0.00001624
6	0.00000401	-0.00001762	0.00002312
6	0.00000772	-0.00001809	0.00001458
1	0.00000039	-0.00001338	0.00001503
1	0.00000148	-0.00001473	0.00002651
1	0.00000696	-0.00001989	0.00002178
1	0.00000557	-0.00002017	0.00002705
1	0.00000834	-0.00001458	0.00000907
1	0.00000988	-0.00002043	0.00001678
1	0.00001042	-0.00002003	0.00001223
6	0.00000351	0.00000044	-0.00000871
6	0.00000382	-0.00000154	-0.00001057
6	0.00000816	-0.00000783	-0.0000063
6	0.00001102	-0.00001235	-0.00000768
6	0.00000923	-0.00000741	-0.0000114
1	0.00000979	-0.00000913	-0.00000624
1	0.0000015	0.00000371	-0.00000809
7	0.00000911	-0.00000483	-0.00001087
8	0.00001995	0.00000038	-0.00000927
1	0.0000143	-0.00001549	-0.00000699
1	0.00000299	0.00000068	-0.00000868
17	0.00001543	-0.00001362	-0.0000086

Zero-point correction=

1.163684 (Hartree/Particle)

Thermal correction to Energy=

1.241353

Thermal correction to Enthalpy=	1.242297
Thermal correction to Gibbs Free Energy=	1.038161
Sum of electronic and zero-point Energies=	-4515.451107
Sum of electronic and thermal Energies=	-4515.373438
Sum of electronic and thermal Enthalpies=	-4515.372494
Sum of electronic and thermal Free Energies=	-4515.576630

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6	-0.000001421	-0.00000142	0.000002326
6	0.000006784	0.000003818	-0.000001496
7	-0.000004641	0.000003009	-0.000004199
7	0.000001375	0.00000411	0.000004936
16	0.0000034	-0.000002803	0.000007319
8	-0.000001308	0.000002587	0.000001378
8	-0.000001906	0.000003351	-0.000001532
6	-0.000002738	0.000002384	-0.00000275
6	-0.000000397	-0.000002069	0.000000609
6	-0.000001103	-0.000001494	0.000002093
6	-0.00000064	0.000000815	0.000000911
6	-0.000000061	0.000000644	0.000003467
6	-0.000000448	0.00000083	0.000003497
1	0.000000236	-0.000000134	0.000000777
1	-0.00000015	-0.000001201	0.000001406
1	-0.000000831	0.000000383	0.000002575
1	-0.000001129	0.000000307	0.000001364
6	-0.000000936	-0.000000523	0.000002293
1	-0.000001458	-0.000000806	0.000002446
1	-0.000001109	-0.000001087	0.000003654
1	-0.000000147	-0.000000598	0.00000264
6	0.000001144	-0.000002343	0.000002577
6	-0.000001327	0.000001658	0.000000515
1	0.000000344	0.000000711	0.00000227
1	-0.000001831	0.000000971	0.000001636
6	-0.000000955	-0.000000008	0.000001773
1	-0.00000066	-0.000000668	0.000001209
1	-0.00000022	0.000000219	0.000000938
6	-0.000000317	-0.000000931	0.000001993
1	-0.000000227	0.000000615	0.000001978
1	-0.000001061	-0.000000265	0.000001901
1	-0.000000465	-0.00000055	0.000001922
1	-0.000000587	-0.00000083	0.000001828
1	-0.000000348	-0.000000199	0.000001282
6	0.000000884	-0.000001663	-0.000002474
6	-0.00000043	0.000004791	0.000000951

1	0.000001051	0.000000784	-0.000001133
1	0.000001391	0.000000859	-0.000001004
6	0.000000073	0.000000318	-0.000000084
1	0.000000712	0.000000683	0.000000095
1	-0.000000216	-0.00000182	-0.000002757
6	-0.00000078	0.000001298	-0.00000192
1	-0.000000395	0.000000739	-0.000001226
1	0.000001297	0.000001199	-0.000001359
1	0.000000389	0.000001781	-0.000001725
1	0.000000733	0.000001826	-0.000001815
1	-0.000000196	0.000002649	-0.000001455
16	-0.000002412	0.00000017	-0.000007119
8	0.000000606	-0.000003535	0.000000488
8	0.000000357	-0.00000047	-0.000000538
6	-0.000001854	-0.000002291	-0.000001296
6	0.000001432	0.000001828	-0.00000014
6	-0.000001125	0.00000007	-0.000001092
6	-0.000001243	-0.000000188	-0.000001344
1	-0.000000044	-0.000000025	0.000001336
6	0.000001845	0.000001389	-0.00000105
1	-0.000000004	-0.000000281	0.000000015
6	0.000000749	-0.000000239	-0.000000158
1	0	0.000000299	0.000000876
1	0.000000128	0.000000742	-0.000000834
6	0.000001229	0.000000332	-0.00000176
9	-0.000000691	0.00000166	0.000000326
9	-0.000000294	0.000001186	-0.000000096
9	-0.000000238	0.000000115	-0.000000144
79	0.000001341	0.000002688	0.000002702
6	0.000001689	-0.000009397	-0.000010446
6	-0.000001823	-0.000000546	0.000000813
6	-0.000000767	-0.000001167	-0.000004148
1	0.000000954	-0.000001433	0.000000084
1	0.00000046	-0.000000543	-0.000001469
7	-0.000001548	0.000000746	0.000004857
7	0.000001002	0.000002482	0.000003613
6	0.000000806	0.000004049	-0.00000558
6	0.000002192	0.000002519	0.000000275
6	0.00000187	-0.000003885	-0.000002165
6	0.000000356	-0.000000037	-0.000000252
6	0.000000512	0.000000323	-0.000001322
6	-0.000000715	0.000000531	-0.000001936
1	0.000000679	0.000000461	-0.000000773
1	0.000001319	0.000000719	-0.000002367

1	0.000000187	0.000000767	-0.000002046
6	-0.000003208	-0.000000995	0.000000187
6	0.00000142	-0.000000219	0.000000316
6	0.000001633	-0.000003682	0.00000255
6	-0.000000353	-0.000001504	0.000000308
6	-0.000000497	-0.000000639	0.000001508
6	-0.000000787	-0.000001065	0.000000786
1	0.000000607	-0.000002621	0.000000843
1	0.000000311	-0.000002098	0.000000638
1	0.000000121	-0.000002052	0.000001893
6	0.000001119	-0.000000745	-0.000000714
6	0.000000488	-0.000002654	0.000000409
6	-0.00000187	-0.000002437	0.000000758
1	0.000000473	-0.000000434	0.000000545
1	0.000000706	-0.000002182	0.000000047
1	0.000000454	-0.000002066	-0.000000795
1	0.000000205	-0.00000247	-0.000000238
1	0.000000584	-0.000001259	0.000000734
1	0.000000328	-0.000001465	0.000000556
1	0.000001016	-0.000001656	-0.000000898
6	0.000001029	0.000000244	-0.000000542
6	0.000000933	0.00000007	0.000000314
6	-0.000000749	-0.000000803	0.000000183
1	0.000000335	-0.000000202	0.000000248
1	-0.000000727	-0.000000527	0.000000835
1	-0.000000626	-0.000000418	0.000000681
1	-0.000000919	-0.000000909	0.000000735
1	-0.000000184	-0.000001877	0.000000322
1	0.000000703	-0.000001252	0.000001016
1	-0.000000446	-0.000001534	0.000000094
6	0.000000246	0.000000502	0.000000744
6	0.00000074	-0.000001964	-0.00000286
6	0.000000383	0.000000397	-0.000002865
1	0.000002621	-0.000000975	-0.000002167
1	0.000001034	0.000001232	-0.00000053
1	0.000001275	-0.000001238	-0.000000668
1	0.000000092	0.000000637	-0.000001624
1	0.000000956	-0.000002289	-0.000001997
1	0.000001078	0.000000025	-0.000002611
1	0.00000107	-0.000001107	-0.000001751
6	-0.000002632	-0.000003363	-0.000000034
6	0.000001186	0.000002065	-0.000000813
6	-0.000000797	0.000003089	-0.000002803
1	0.000000033	0.000000319	-0.000000354

1	0.000000458	-0.000000062	-0.000000728
1	0.000000291	0.000000461	-0.000000558
1	-0.000000186	0.000000501	-0.000001128
1	0.000000584	0.000001572	0.000000221
1	-0.000000308	0.000001715	-0.000000135
1	0.000000431	0.000001073	0.000000225
6	0.000000044	-0.000000285	-0.000001868
6	-0.000000845	0.000001915	0.000000555
6	-0.000000216	0.000001928	-0.000001239
6	-0.000000001	0.000001847	0.000000714
6	-0.000003027	0.00000301	-0.000001924
1	-0.000000153	0.000002379	0.000000136
1	0.00000068	0.000001167	0.000000405
7	0.000003067	0.000000721	0.000001215
8	-0.000006938	-0.000001254	0.000002059
1	-0.000000935	0.000002556	0.000000041
1	-0.000000342	0.000001138	-0.000000005
17	0.000001694	0.000000774	0.000001736

Zero-point correction=

1.165665 (Hartree/Particle)

Thermal correction to Energy=

1.243012

Thermal correction to Enthalpy=

1.243957

Thermal correction to Gibbs Free Energy=

1.042464

Sum of electronic and zero-point Energies=

-4515.457073

Sum of electronic and thermal Energies=

-4515.379725

Sum of electronic and thermal Enthalpies=

-4515.378781

Sum of electronic and thermal Free Energies=

-4515.580273

Re5

6	-0.000000796	-0.000001653	0.000000445
6	0.000003023	0.000000643	-0.000002529
7	0.000003684	0.000003402	0.000001025
7	-0.00000557	-0.000004744	0.000001128
16	-0.000000139	0.000001141	0.000000137
8	-0.000002232	0.000002154	0.000000007
8	-0.00000068	0.000001796	-0.000000274
6	-0.000000303	-0.000000077	-0.000000027
6	-0.000001621	0.000001272	0.000000287
6	-0.000001466	0.000000796	0.000000625
6	-0.000002126	0.000000249	0.000001023
6	-0.00000183	0.000000091	0.000001467
6	-0.00000192	0.000000905	0.000000166
1	-0.000000578	0.000001294	-0.000000463
1	-0.000001677	0.000000968	0.000000631
1	-0.00000182	-0.000000327	0.000001514

1	-0.000001355	0.000000551	0.000000094
6	-0.000002095	0.000000211	0.000001531
1	-0.000002712	-0.000000198	0.000001998
1	-0.000002614	0.000000041	0.000001673
1	-0.000002046	-0.000000451	0.000001681
6	-0.000003849	0.000001113	-0.000004667
1	0.000001177	0.000000895	-0.000000597
1	0.000000098	0.000001165	-0.000001067
6	0.000000969	-0.000001003	0.000001529
1	-0.000000151	-0.000001287	0.000000098
1	0.000000449	-0.000002249	0.000000441
8	-0.000000016	-0.000000095	0.000000092
6	0.00000253	0.000002514	-0.000000203
6	-0.000000804	0.000001403	-0.000001611
6	0.000000438	0.000000092	-0.000000916
6	0.000000299	0.000000997	-0.000000436
1	-0.000000008	0.000002144	-0.000001228
6	0.000000244	-0.000000278	-0.000001036
1	0.000001127	0.000000018	-0.000000627
6	0.000000858	0.000001042	-0.000000691
1	-0.000000049	0.000001744	-0.000001119
1	0.000000907	-0.000000031	-0.000000057
1	0.000000477	0.000000611	-0.000000753
6	0.000001407	-0.000001946	0.000000779
6	0.000000229	-0.000001864	-0.000000329
6	0.000001754	-0.000002043	0.000000388
6	0.000001276	-0.000002005	0.000000639
1	0.000000271	-0.000001116	0.000000552
6	0.00000177	-0.000002495	-0.000000349
1	0.000001684	-0.000002023	0.000000488
6	0.000002163	-0.00000168	-0.000000029
1	0.000001243	-0.000001686	0.000000217
1	0.000002704	-0.000002651	-0.000000105
1	0.000002383	-0.000002466	-0.000000264
8	-0.000001202	0.000003209	-0.0000010286
8	-0.000001365	-0.000002547	-0.000000987
6	-0.000000084	-0.000000698	0.000000339
6	0.00000068	0.000000698	-0.000001036
1	-0.000000123	0.000001379	-0.000001022
1	-0.000000638	0.000001382	-0.000000453
1	-0.000000582	0.00000012	-0.000000056
6	0.000000059	-0.000000106	-0.000000702
1	0.000000608	0.000000127	-0.000000602
1	-0.000000073	0.000000125	0.000000106



1	0.000000672	-0.000000611	0.000000215
15	0.000007364	-0.000002739	0.000008616
6	-0.00000002	0.000002616	-0.000001085
1	0.000001628	0.000000337	-0.000000911
1	0.000000532	0.000000172	-0.000000718
6	-0.000001324	0.000000802	0.000004541
1	-0.000000512	0.000000369	-0.000000495
1	-0.00000114	0.000000004	0.00000063
Zero-point correction=			0.547382 (Hartree/Particle)
Thermal correction to Energy=			0.583431
Thermal correction to Enthalpy=			0.584376
Thermal correction to Gibbs Free Energy=			0.472343
Sum of electronic and zero-point Energies=			-2310.248909
Sum of electronic and thermal Energies=			-2310.212859
Sum of electronic and thermal Enthalpies=			-2310.211915
Sum of electronic and thermal Free Energies=			-2310.323948

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6	-0.000008399	-0.000004343	-0.000007445
6	-0.00001295	0.000006922	0.000016742
7	0.00001275	-0.000008486	-0.000009307
7	0.000018232	-0.00000648	0.000001968
16	-0.000005453	0.00000932	-0.000001752
8	-0.000001175	0.000001137	-0.000002643
8	0.000003449	-0.00000055	0.000001518
6	-0.000002625	-0.000000297	0.00000216
6	-0.000002215	0.000000691	-0.000000052
6	-0.000000723	0.000000082	-0.000000462
6	-0.000003446	-0.000000143	-0.000000753
6	-0.000000991	-0.000000274	0.000000531
6	-0.000001801	0.000000967	-0.00000282
1	-0.000002342	-0.000000986	0.000000592
1	-0.000002154	0.000000939	0.000000653
1	-0.000002014	-0.000000854	-0.000000374
1	-0.000000937	-0.000001691	-0.000000796
6	-0.000001138	0.000000685	-0.000000557
1	-0.000002592	0.000000077	-0.000000254
1	-0.000002976	0.000000112	0.000000157
1	-0.000002952	0.000000066	-0.000000024
6	-0.000008283	0.000000155	0.000005751
1	0.000000185	0.000000976	0.000000443
1	0.000001545	0.000001151	-0.000000789
6	-0.000005303	-0.000000847	-0.000001174
1	-0.00000046	0.000001352	-0.000000692

1	0.000000834	0.000001936	0.000000935
8	0.000002288	-0.00000062	0.000002103
6	0.000002273	-0.000003311	-0.00000715
6	-0.000000027	0.000001474	0.000001079
6	-0.00000113	0.000000326	0.000003318
6	0.000000746	0.000000704	0.000002876
1	-0.000000351	-0.000000901	-0.000000436
6	-0.000000967	0.000002672	0.000000275
1	-0.000001374	-0.000000807	-0.000000835
6	-0.000000463	-0.000001179	-0.000001253
1	-0.000000277	0.000001303	0.000000748
1	-0.000000854	-0.000000207	-0.000000091
1	-0.000000412	0.00000009	0.000000447
6	0.000002361	-0.000000026	-0.000000732
6	0.000003014	0.000000917	-0.000003591
6	0.000000323	-0.000000803	0.000004989
6	0.000002411	-0.000002882	0.000000965
1	0.000000938	-0.00000043	-0.000001796
6	0.000002181	0.000001358	-0.000000265
1	0.000002033	-0.000000115	-0.000000725
6	-0.000001066	0.000000371	-0.000003027
1	0.000001262	-0.000000661	-0.000000088
1	0.000001335	0.000000396	0.000000513
1	0.000001168	0.000000221	0.000000085
8	0.00000296	0.000007249	0.000004461
8	-0.000001055	0.000000358	0.000003306
6	0.00000022	0.000005038	0.000003493
6	-0.000000457	0.000001204	-0.000000911
1	-0.000001239	0.000001326	0.000001265
1	-0.000002055	0.000000995	0.000000941
1	-0.000001325	0.000001063	0.000001271
6	0.000001294	0.000000504	-0.00000055
1	-0.000000485	0.000001463	0.000001628
1	-0.000001306	0.00000174	0.000001893
1	-0.000001436	0.000001891	0.000001195
15	-0.000008521	0.00000275	-0.000004838
6	-0.000002762	-0.00000163	-0.00000007
1	0.000000093	0.000000817	-0.000000336
1	-0.000001635	0.000001047	0.000000191
6	-0.000002084	-0.000008114	-0.000004413
1	-0.000001722	0.000002667	0.000000926
1	-0.00000169	0.000001646	0.000001365
79	0.000001875	0.00000231	0.000002527
6	0.000005812	0.00000312	-0.000002885

6	0.000001694	-0.000002777	-0.000001419
6	0.000000426	-0.000002248	0.000002622
1	0.000001653	0.000000959	-0.000001402
1	0.000000695	-0.000000361	-0.00000004
7	0.00000017	0.000003271	0.000002463
7	-0.000004854	0.000000613	-0.000002206
6	0.000002248	-0.000000151	-0.000001109
6	0.000002626	-0.000000886	0.000002423
6	0.000002004	0.000000223	0.000001412
6	0.000000126	0.000000053	0.000000151
6	0.000000468	0.000000165	0.00000105
6	0.000001101	0.000001035	0.000000764
1	0.000002849	0.000000814	0.000000351
1	0.00000121	0.000000002	-0.000000135
1	0.000001591	0.0000011	0.000000427
6	0.000002926	0.000001608	-0.000000592
6	0.000001252	-0.000004264	-0.000001021
6	0.000001115	-0.000002724	-0.000001544
6	-0.000000626	-0.000002084	0.000001677
6	-0.000001166	-0.000000077	0.000000531
6	-0.000000198	-0.000001164	-0.000000559
1	-0.000001686	-0.000001096	-0.00000228
1	0.000000388	-0.00000253	-0.000001705
1	-0.00000009	-0.000001164	-0.000000991
6	0.000002295	0.00000033	0.000004819
6	-0.000001375	-0.00000017	-0.000001823
6	-0.00000083	0.000002167	-0.000003618
1	-0.000001496	-0.000001177	-0.000002587
1	-0.000000262	-0.000001749	-0.000000551
1	-0.000000165	-0.000000339	-0.000000052
1	-0.000000924	-0.000000116	-0.000002508
1	-0.000001173	-0.000001115	0.000000882
1	-0.00000026	-0.000002355	0.000000515
1	-0.000000665	-0.000001905	0.000000371
6	-0.000000459	0.000000145	0.000000201
6	0.000001788	0.000000248	-0.000001421
6	0.000000722	-0.000001458	0.000000033
1	-0.0000007	-0.000000685	-0.000001631
1	0.00000051	-0.000001405	-0.000000418
1	0.000000547	-0.000001337	-0.000000587
1	-0.000000966	-0.000000412	0.000000145
1	0.000001429	-0.000001133	-0.000000796
1	-0.000000215	-0.000002143	-0.000001669
1	0.000001196	-0.000001391	-0.000000576

6	0.000000268	0.000000848	0.00000066
6	-0.000001954	0.000000102	-0.000000336
6	0.000000888	0.000001462	-0.000000476
1	0.000000099	-0.00000032	-0.000000098
1	-0.000000091	0.000000924	-0.000000618
1	0.000000022	0.000000095	0.000000635
1	0.000000232	0.000000904	0.000000581
1	0.000000596	0.000000037	0.000000208
1	0.000000623	0.000000408	0.000000624
1	0.000000224	0.00000023	0.000000629
6	0.000001364	0.000001936	-0.00000267
6	0.00000184	0.000000041	0.000001348
6	0.000002775	-0.000003136	0.00000062
1	0.00000125	0.000000061	-0.000000369
1	0.000001555	-0.000000967	-0.000000602
1	0.000001833	-0.000000799	-0.000000244
1	0.00000216	-0.00000042	0.000000021
1	0.000001515	-0.000000984	0.000003288
1	0.000001117	0.000000532	-0.000000088
1	0.000001915	-0.000000223	0.000000222

Zero-point correction=

1.121270 (Hartree/Particle)

Thermal correction to Energy=

1.191468

Thermal correction to Enthalpy=

1.192412

Thermal correction to Gibbs Free Energy=

1.002985

Sum of electronic and zero-point Energies=

-3605.086685

Sum of electronic and thermal Energies=

-3605.016487

Sum of electronic and thermal Enthalpies=

-3605.015543

Sum of electronic and thermal Free Energies=

-3605.204970

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6	0.000007804	-0.000003128	0.000005771
6	-0.00001743	0.000005075	-0.000000584
7	0.000009562	0.000010822	-0.000005867
7	0.000007918	-0.000003371	0.00000164
16	-0.000006658	-0.000002543	-0.000001724
8	-0.000000609	0.000000361	0.000000326
8	-0.000001869	0.000002	0.00000002
6	0.000004586	0.000004177	0.000000874
6	0.00000039	0.000000501	0.000001074
6	0.000001123	0.000002891	-0.000001728
6	0.000000437	0.000001918	0.000000329
6	0.000002118	0.000004375	0.000001481
6	-0.000001696	0.000002055	-0.000000408
1	0.000001489	0.000002161	0.000000449

1	0.000002269	0.000002183	-0.000000123
1	0.000000166	0.000003245	0.000000411
1	0.000000378	0.000003117	0.000000429
6	0.000001567	0.000004032	-0.000000872
1	0.000001137	0.000004007	0.000000129
1	0.000003361	0.000003336	-0.000000022
1	0.000001852	0.000001962	0.000000559
6	-0.000000479	-0.000003386	0.000007175
1	-0.000001413	0.000002815	0.000000677
1	-0.000002257	0.000000683	0.000000359
6	-0.000002141	-0.000000155	0.000001914
1	-0.000001716	-0.000000673	0.000000178
1	-0.000002102	-0.000002074	-0.000000915
8	-0.000001215	-0.000001785	0.000000605
6	-0.000000506	-0.000003017	-0.000004597
6	-0.000001397	0.000001117	0.000000424
6	0.000000015	0.000000509	0.000000653
6	-0.000000418	-0.000000987	0.000000158
1	-0.000001372	-0.000001199	0.000000908
6	0.000000287	-0.000000233	-0.000000329
1	-0.000000009	0.000000733	0.000000101
6	0.000000349	-0.000001044	-0.000000013
1	-0.000000863	-0.000001554	-0.000000086
1	0.000000857	-0.000000174	-0.000000014
1	0.000000242	-0.000001179	-0.000000362
6	-0.000000544	-0.000000555	0.000000968
6	-0.000004013	0.000000209	-0.000000904
6	-0.000004701	-0.000002101	0.000001416
6	-0.000001988	-0.000001502	0.000001725
1	-0.000002818	0.000000128	0.000000151
6	-0.000001944	-0.000000971	0.000000686
1	-0.000002185	-0.000002549	0.000000176
6	-0.000005211	-0.000000404	0.000000552
1	-0.000003608	0.000000272	0.000001001
1	-0.00000037	-0.000002302	0.000000873
1	-0.000003595	-0.000000819	0.000001118
8	-0.000000374	-0.000002186	0.000000005
8	-0.000001747	-0.000000612	0.000001805
6	0.000001363	-0.000001184	-0.000000955
6	0.000002786	-0.000002046	-0.000001798
1	0.000001832	-0.000002228	-0.000000891
1	0.000001338	-0.000001218	-0.000000771
1	0.00000217	-0.000002323	-0.000001007
6	0.000001456	-0.000003416	-0.000000815

1	0.000001048	-0.000003445	-0.000000893
1	0.000001503	-0.000003505	-0.00000109
1	0.000000391	-0.000003346	-0.000000729
15	-0.000001654	-0.000005271	-0.000003365
6	0.000001891	-0.000004247	-0.000002131
1	-0.00000009	-0.000002697	-0.000000107
1	0.000000141	-0.000000844	-0.000001094
6	0.000001489	-0.000002404	-0.000000023
1	0.000001016	-0.000001016	-0.000000625
1	0.000001319	-0.000002053	-0.000000781
79	-0.000002189	-0.000006722	0.000001306
6	-0.000000972	0.000011074	-0.00000141
6	0.000000075	0.000000401	0.0000019
6	0.000000412	-0.00000122	-0.00000271
1	0.000000545	0.000000878	0.000000603
1	-0.000000135	0.000000292	-0.000000105
7	-0.000001038	-0.00000523	-0.000000838
7	0.000002763	-0.000001074	-0.000000125
6	-0.000001635	0.000001145	-0.000001874
6	-0.000001732	0.000000502	-0.000000964
6	0.000001262	-0.000002156	-0.000001542
6	-0.00000302	-0.000000707	0.000001253
6	-0.000001936	-0.000001098	0.00000072
6	-0.000002308	-0.00000156	0.000000298
1	-0.000002668	-0.000000395	0.000000536
1	-0.00000118	-0.000002769	0.00000076
1	-0.000002749	-0.000001838	0.000000708
6	0.000003174	0.000001603	0.000002229
6	0.000003125	-0.000000808	0.000000048
6	0.000000574	0.000001463	-0.00000002
6	0.000002067	0.000001622	-0.000000044
6	0.000001902	0.000002514	-0.000001297
6	0.00000278	0.000002354	-0.00000092
1	0.000002903	0.000001156	-0.000001207
1	0.000001874	0.000002889	0.000000229
1	0.0000033	0.000002293	-0.000000612
6	0.000000923	0.000000623	-0.000002081
6	0.000003236	-0.000001126	-0.000000478
6	0.000002145	-0.000000527	0.000000396
1	0.000001528	-0.000000408	-0.00000112
1	0.000002662	0.000000196	-0.000000961
1	0.000003078	-0.000001199	-0.000000785
1	0.000003415	0.000000471	-0.000001206
1	0.000002453	-0.000000103	-0.000000739

1	0.000002477	-0.000000261	-0.000001718
1	0.000002469	-0.00000144	-0.00000076
6	-0.000000695	0.000001739	0.00000022
6	0.000000519	0.000002431	-0.000000225
6	0.000001683	0.000002589	0.000000809
1	0.000000013	0.000002342	-0.000000628
1	0.000000464	0.000003643	0.000000766
1	-0.000000424	0.000003206	0.000000281
1	0.000001303	0.000003838	0.000000919
1	0.000001214	0.000002959	-0.000000185
1	0.000000905	0.00000349	-0.000000321
1	0.000000197	0.00000312	0.000000513
6	-0.000001947	-0.000002263	0.000001415
6	0.000002418	-0.000001207	-0.000000144
6	0.000000006	-0.000002496	-0.000000911
1	0.000001103	-0.000001835	-0.00000012
1	-0.000000007	-0.000002292	-0.00000058
1	0.000000139	-0.000002939	-0.00000108
1	-0.000000873	-0.00000323	-0.000000595
1	-0.000000234	-0.000001785	-0.000000501
1	-0.000000793	-0.000002984	0.000000024
1	0.000000217	-0.000002397	-0.000000462
6	-0.000000692	0.000001054	0.000003604
6	-0.000002912	0.000000116	-0.000000317
6	-0.000001796	0.00000088	-0.000000213
1	-0.000001208	0.000001499	0.000000979
1	-0.000001952	0.000000697	0.000000737
1	-0.00000225	0.000001724	0.000001029
1	-0.000002466	0.000000901	0.000001245
1	-0.000001505	0.000000657	0.000002487
1	-0.00000312	0.00000092	0.000001288
1	-0.000002212	0.000001845	0.000001142

Zero-point correction=

1.122147 (Hartree/Particle)

Thermal correction to Energy=

1.192056

Thermal correction to Enthalpy=

1.193000

Thermal correction to Gibbs Free Energy=

1.005869

Sum of electronic and zero-point Energies=

-3605.091132

Sum of electronic and thermal Energies=

-3605.021223

Sum of electronic and thermal Enthalpies=

-3605.020279

Sum of electronic and thermal Free Energies=

-3605.207410

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6	0.000001443	-0.000001849	0.000002668
6	-0.000000108	0.000000721	-0.000000852

7	-0.00000208	-0.000000511	-0.000000092
7	-0.000001686	-0.000000457	-0.000000012
16	0.000000189	-0.000000862	0.000001747
8	-0.000000805	-0.000000605	0.000001051
8	-0.000001025	-0.000000423	0.000001296
6	0.000000027	-0.000001292	0.000001676
6	-0.000000056	-0.000001358	0.000001587
6	-0.000001084	-0.000000748	0.000001463
6	0.000000343	-0.000001369	0.000002273
6	0.000001048	-0.000001777	0.000002819
6	-0.000000037	-0.000001364	0.000002351
1	-0.000000506	-0.000000566	0.000001486
1	-0.000000164	-0.000001018	0.000001993
1	0.000000651	-0.00000131	0.000002639
1	0.000000058	-0.000000971	0.000002059
6	0.000000542	-0.0000013	0.000002676
1	0.000000536	-0.000001795	0.000002147
1	0.000000622	-0.000001546	0.000003238
1	0.000000024	-0.000000826	0.000002681
6	0.000000216	-0.000000548	0.000000795
1	-0.000000333	-0.000000807	0.000001189
1	0.000000557	-0.000000635	0.000000549
6	-0.000000744	-0.000000119	-0.000000061
1	-0.00000102	-0.000000969	0.000000201
1	-0.000000761	0.000000178	0.000000063
8	-0.000001015	-0.000000688	0.000000964
6	0.000000361	-0.000000317	0.000001663
6	0.000001239	-0.000001157	0.000002383
6	-0.000000299	-0.000000528	0.000001476
6	0.000000993	-0.000000959	0.000002039
1	0.000001153	-0.000000194	0.000000796
6	0.000000484	-0.000001222	0.000002087
1	0.000000099	-0.000001217	0.00000149
6	0.000001368	-0.000000966	0.000001862
1	0.000001498	-0.000000653	0.00000169
1	0.000000555	-0.000001192	0.000002439
1	0.000001362	-0.000001029	0.000002344
6	-0.000001422	-0.000000088	-0.000000566
6	-0.000002101	-0.00000003	0.000000396
6	-0.000001414	-0.000000479	-0.00000107
6	-0.000002182	0.0000001	-0.000000649
1	-0.000001976	-0.000000433	0.000000307
6	-0.00000201	0.000000278	-0.000001115
1	-0.000001664	0.000000011	0.000000028



6	-0.000001918	0.00000013	-0.000000689
1	-0.000002693	-0.00000025	-0.000000466
1	-0.000001809	0.00000041	-0.000001397
1	-0.000002518	0.000000156	-0.000001136
8	-0.000001204	0.000000369	0.000000185
8	-0.000000644	-0.000000319	0.000000758
6	-0.000000272	0.000000236	-0.000000282
6	-0.000000546	0.00000021	-0.000001092
1	0.000000197	0.000000597	-0.000000798
1	-0.000000286	0.000000741	-0.000001023
1	-0.000000744	0.00000053	-0.000001142
6	-0.000000768	0.000000158	-0.000000374
1	-0.000000228	0.000000098	-0.000000208
1	-0.000000738	0.000000069	-0.000000386
1	-0.000000712	-0.000000336	-0.000000019
15	-0.000000126	0.00000003	-0.000000204
6	0.000000001	0.000000184	-0.000000818
1	0.00000017	0.000000216	-0.000000185
1	-0.000000535	0.000000075	-0.000000502
6	-0.000000713	0.000000033	-0.000000495
1	-0.000001134	0.000000254	-0.000000788
1	-0.00000121	0.000000043	-0.000000805
79	0.000001045	-0.000000075	0.000000148
6	0.000000746	0.000000232	-0.000001898
6	0.000000688	0.000000753	-0.000001295
6	0.000000488	0.000000761	-0.000001207
1	0.000000368	0.000000871	-0.00000124
1	0.00000073	0.000000929	-0.000001458
7	-0.000000026	0.000000817	-0.000001153
7	0.000000268	0.000000306	-0.000001077
6	0.000000277	0.00000078	-0.000001353
6	-0.000000113	0.000001467	-0.000001255
6	0.000001458	0.000000932	-0.00000058
6	0.000000125	0.000000652	-0.000001412
6	0.000001139	0.000000627	-0.000001068
6	0.000001088	0.000001128	-0.000001413
1	0.000000063	0.000000827	-0.000001701
1	0.000001465	0.000000923	-0.000000983
1	0.000000854	0.00000081	-0.000001328
6	-0.000000015	0.000001472	-0.000000767
6	-0.000000099	0.000000049	-0.000000057
6	-0.000000472	-0.000000024	-0.000000751
6	-0.000000065	0.000000284	-0.000000195
6	-0.000000432	0.000000171	-0.000000227

6	-0.000000189	0.000000152	-0.000000012
1	0.000000454	-0.000000027	0.000000042
1	-0.000000949	-0.000000016	-0.000000277
1	-0.000000334	-0.000000119	0.000000102
6	0.000002023	-0.000000048	-0.000000791
6	0.000001062	0.000000462	-0.000000641
6	0.000001177	0.000000039	0.000000377
1	0.000001111	0.000000462	-0.000000034
1	0.000000787	0.000000928	-0.000000903
1	0.000001384	0.000000066	-0.000000574
1	0.000001033	0.000000454	-0.000000469
1	0.000000693	0.000000088	0.000000653
1	0.000001134	-0.000000024	0.000000229
1	0.000001341	0.000000544	-0.000000061
6	-0.000000482	0.000000195	-0.000000741
6	-0.000001423	0.000000162	-0.000000644
6	-0.000000977	0.000000573	-0.000000138
1	-0.000000914	0.000000712	-0.000000566
1	-0.000000934	-0.000000023	-0.000000032
1	-0.000001448	0.000000044	-0.000000667
1	-0.000001342	0.000000242	-0.000000573
1	-0.000000474	0.000000077	-0.000001664
1	-0.000001076	0.000000482	-0.000001185
1	-0.000001064	0.000000538	-0.000001429
6	0.000001234	0.000000127	-0.000000044
6	0.000001329	0.000000299	-0.000000252
6	0.000001822	0.000000926	-0.000000071
1	0.000000885	0.000000774	-0.000000694
1	0.000000628	-0.000000141	-0.000000925
1	0.000001439	0.000000317	-0.000000074
1	0.000000014	0.000000199	-0.000000006
1	0.000001712	0.000000918	-0.000001218
1	0.000001969	0.000000701	-0.000000807
1	0.000001935	0.000000736	-0.000000575
6	0.000000538	0.000000319	-0.000001131
6	-0.000000397	0.000001304	-0.000001815
6	-0.000000552	0.000001143	-0.000002333
1	-0.000000277	0.000000929	-0.000001557
1	0.000000217	0.000001271	-0.000002234
1	-0.000000363	0.000000013	-0.000002458
1	0	0.000001104	-0.000002227
1	0.000000129	0.000000715	-0.000001408
1	-0.000000602	0.000000959	-0.000001642
1	-0.000000084	0.000000521	-0.000001419

6	0.000000188	-0.000000425	0.000000916
6	-0.000000002	-0.000000668	0.000000666
6	0.000000631	-0.000000464	0.000001204
6	0.000000909	-0.000000628	0.000000995
6	0.000000699	-0.000000727	0.000000999
1	0.000000518	-0.000000455	0.000001212
1	-0.000000702	-0.000000192	0.000000288
7	-0.000000304	-0.000001318	0.000000286
8	0.000001246	0.00000144	0.000001972
1	0.000001332	-0.000000374	0.00000126
1	-0.00000007	-0.000000438	0.000000788
17	0.000001562	-0.000000505	0.00000108

Zero-point correction=	1.206315 (Hartree/Particle)
Thermal correction to Energy=	1.282772
Thermal correction to Enthalpy=	1.283716
Thermal correction to Gibbs Free Energy=	1.085791
Sum of electronic and zero-point Energies=	-4388.010588
Sum of electronic and thermal Energies=	-4387.934131
Sum of electronic and thermal Enthalpies=	-4387.933187
Sum of electronic and thermal Free Energies=	-4388.131113

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6	-0.000010367	0.000013148	0.000015766
6	0.000004462	0.000000115	-0.000009451
7	0.000001815	-0.000008701	0.000005057
7	-0.000002132	0.000006268	0.000005879
16	0.000000784	0.000002113	-0.00000738
8	-0.000002199	0.000000604	0.00000165
8	-0.000003824	0.000004846	0.000001033
6	-0.00000099	0.000003283	-0.000000901
6	-0.000000388	0.000001206	0.000000559
6	-0.000001606	0.000004361	0.000002228
6	0.000000835	0.000004423	-0.000001259
6	0.000001224	0.00000226	0.00000144
6	-0.000000427	0.000004362	0.000001478
1	0.000001088	0.000003514	0.000000038
1	0.000001173	0.000004218	0.000000897
1	0.000000555	0.000003943	0.000000832
1	0.000000343	0.000002291	0.000001296
6	0.000001466	0.000004469	0.00000204
1	0.000001153	0.000004906	0.000001356
1	0.000001509	0.000004763	0.000002007
1	0.000001603	0.000004414	0.00000142
6	-0.000000846	0.000007577	-0.000003113

1	-0.000002205	0.000002548	-0.000002679
1	-0.000000989	0.000000236	0.000000341
6	0.000004032	-0.000000319	-0.000002578
1	-0.000003424	0.000000001	0.000000305
1	-0.000001657	-0.000000579	-0.000000728
8	-0.000003052	0.000001841	0.000002918
6	-0.000000904	0.000000095	0.000002395
6	-0.00000035	0.000001898	-0.000000661
6	-0.000001041	0.000004623	-0.000001488
6	-0.000000067	0.00000178	-0.000000172
1	-0.000000943	0.000000764	-0.000000348
6	-0.000001533	0.00000351	0.000000351
1	-0.000001623	0.000002532	-0.000001119
6	-0.00000104	0.000002263	-0.000000058
1	-0.000000309	0.000002089	0.00000035
1	-0.000001358	0.000003737	-0.000000408
1	-0.000000441	0.000003797	0.000000378
6	-0.000003262	0.000001455	-0.000001051
6	-0.000001444	0.000001237	-0.000000737
6	-0.000001924	-0.000000687	-0.000000397
6	-0.000003292	0.000000037	-0.000001999
1	-0.000002397	0.000000826	-0.00000134
6	-0.0000021	-0.000000851	-0.000001281
1	-0.000000907	-0.000001661	-0.000000856
6	-0.000001985	-0.000000437	-0.000002048
1	-0.000003404	0.000000593	-0.000001566
1	-0.000002	-0.000001606	-0.000001347
1	-0.000002724	-0.000000578	-0.00000154
8	-0.00000301	0.000008185	-0.000002163
8	-0.000002872	0.000002701	-0.000001324
6	-0.000002279	-0.000000352	-0.000000524
6	-0.000002411	-0.000002429	-0.000001097
1	-0.000001864	-0.000002044	-0.000001491
1	-0.000001989	-0.000002305	-0.000001131
1	-0.000002755	-0.000002066	-0.000001915
6	-0.000003597	-0.000001685	-0.00000016
1	-0.00000285	-0.00000101	-0.00000172
1	-0.00000323	-0.00000074	-0.000001965
1	-0.000002917	-0.000000111	-0.000001469
15	-0.000001479	-0.000006935	-0.000004354
6	0.000000642	-0.000002296	-0.000000498
1	-0.000001826	-0.000000743	-0.000001206
1	-0.000001569	-0.000000877	-0.000001046
6	-0.000004083	-0.000003526	-0.000003895

1	-0.00000218	-0.000001385	-0.000001151
1	-0.000002536	-0.000001051	-0.000001382
79	0.000004926	-0.000003985	0.000003732
6	0.000001635	0.000002543	0.00000241
6	0.00000266	0.000001162	0.000001693
6	0.000002645	-0.000000475	0.000001138
1	0.000001992	-0.000002292	-0.000000019
1	0.000001053	-0.000003909	0.000000498
7	-0.000005669	-0.000003205	-0.000001036
7	0.000000625	-0.000005884	-0.000002391
6	0.000005134	-0.000003868	-0.000000165
6	-0.000002133	-0.000002422	-0.000000721
6	0.000000281	-0.000001626	0.000001193
6	-0.00000059	-0.000003081	-0.000000462
6	0.000000296	-0.000003299	-0.000000732
6	0.000000695	-0.000002833	-0.000000878
1	-0.00000051	-0.000003053	-0.000000738
1	0.000000198	-0.000002829	-0.000000346
1	-0.00000078	-0.000003443	-0.000000958
6	0.000001232	0.000000289	-0.000001115
6	0.000000649	-0.000003115	0.000002297
6	0.00000077	0.000000884	0.00000247
6	0.000003344	0.000001611	0.00000066
6	0.000000828	0.000001022	0.000000885
6	0.000001956	0.000000249	0.000000582
1	0.000003041	0.00000055	0.000001921
1	0.000001428	0.000000719	0.000000662
1	0.000002297	0.000001326	0.000001387
6	0.0000049	0.000002795	0.000000918
6	0.000002678	-0.000002085	0.000001631
6	0.000000991	-0.000000784	0.000001263
1	0.000002584	-0.000001244	0.000001089
1	0.000003291	-0.00000149	0.000001517
1	0.000003411	-0.000001258	0.00000187
1	0.000003474	-0.000000425	0.000001714
1	0.000001998	0.000000212	0.00000065
1	0.000002988	0.000000274	0.000001786
1	0.000003007	-0.000000372	0.000001621
6	0.000000772	-0.000000866	-0.000000449
6	-0.000000152	-0.000000886	0.000001193
6	0.000000329	-0.000001631	0.000000074
1	0.000000921	-0.000000863	-0.000000227
1	-0.000000099	0.000001058	0.000000541
1	-0.000000194	0.000000007	-0.000000559

1	0.000000064	0.000000166	0.000000067
1	0.000000059	-0.000001378	0.00000118
1	0.000001639	-0.000000652	0.000000836
1	0.000000541	-0.000001286	-0.000000223
6	-0.000000095	-0.000002548	-0.000001603
6	0.000001888	-0.000001981	0.000000862
6	0.000002172	-0.00000255	0.000000886
1	0.000000334	-0.000003064	-0.000000031
1	0.000000343	-0.000000557	-0.000000787
1	0.000001643	-0.00000113	0.000000477
1	-0.000000212	-0.000000676	0.000000149
1	0.00000221	-0.000002728	0.000000758
1	0.000001874	-0.000004016	0.000000069
1	0.000002336	-0.000001912	0.000000638
6	0.000001571	-0.000002253	-0.000000447
6	-0.00000088	-0.000004202	-0.000000764
6	-0.000002122	-0.000002681	-0.000000006
1	-0.00000022	-0.000002021	-0.000000715
1	0.000000443	-0.000004065	-0.000000069
1	-0.0000001	-0.000003813	-0.000000747
1	-0.000000021	-0.000004126	-0.000000827
1	-0.00000038	-0.000001759	-0.000001192
1	-0.000000841	-0.000002958	-0.000001615
1	-0.000000768	-0.000002584	-0.000000987
6	0.000000633	0.000006477	-0.000002795
6	0.000002425	-0.000001763	0.000000918
6	0.000001154	0.000002364	0.000003382
6	0.000001925	0.00000286	0.000000699
6	0.000002413	0.000000671	-0.00000035
1	0.000002236	0.000002212	0.000001391
1	0.000000422	0.000000274	0.000001265
7	-0.000003941	0.000012628	0.000005628
8	0.000008041	-0.000019198	-0.00000785
1	0.000001756	0.000001407	0.000001306
1	0.000001136	0.000002921	0.000001023
17	0.000000801	0.000001586	0.000001065

Zero-point correction=

1.208012 (Hartree/Particle)

Thermal correction to Energy=

1.284323

Thermal correction to Enthalpy=

1.285268

Thermal correction to Gibbs Free Energy=

1.088199

Sum of electronic and zero-point Energies=

-4388.022297

Sum of electronic and thermal Energies=

-4387.945985

Sum of electronic and thermal Enthalpies=

-4387.945041

Sum of electronic and thermal Free Energies=

-4388.142110

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6	-0.000000589	-0.000000061	-0.000000083
6	0.000000062	0.000000359	-0.000000629
7	0.000000213	0.000000446	-0.000000315
7	0.000000387	-0.000000007	0.000000307
16	-0.000000155	-0.000000744	-0.000001074
8	-0.000000061	0.000000112	-0.000000397
8	-0.000000577	0.000000149	-0.000001044
6	-0.000000045	0.000000022	-0.000000131
6	-0.000000571	0.000000204	-0.000001477
6	-0.000000576	0.000000092	-0.000001504
6	-0.000000525	0.000000255	-0.000002055
6	-0.000000623	0.000000232	-0.000002324
6	-0.000000047	-0.000000028	-0.000000165
1	-0.000000368	0.000000124	-0.000001262
1	-0.000000521	0.000000172	-0.000001847
1	-0.000000533	0.000000205	-0.000002222
1	-0.000000496	0.000000095	-0.000001555
6	-0.000000557	0.000000226	-0.000002446
1	-0.000000439	0.000000215	-0.000002704
1	-0.000000429	0.000000171	-0.000002455
1	-0.000000831	0.000000407	-0.000002511
6	0.000000062	0.000000337	-0.000001042
1	-0.000000028	0.000000134	-0.000000481
1	0.000000679	-0.000000267	-0.000000683
6	0.000000774	0.000000144	-0.000000301
1	0.000001127	0.000000126	0.000000059
1	0.000000529	0.000000782	-0.000000647
8	-0.000000015	0.000000064	0.000000103
6	0.000000555	0.000000023	-0.000001312
6	0.000000025	0.000000343	-0.000000931
6	0.000000509	0.000000362	-0.000001702
6	0.000000386	0.000000457	-0.000001722
1	0.000000463	0.000000005	-0.000001208
6	0.000000618	0.000000465	-0.000001751
1	0.000000034	0.000000378	-0.000000132
6	0.000000664	0.000000377	-0.000001944
1	0.000000626	0.000000536	-0.000001739
1	0.000000064	0.000000549	-0.000001873
1	0.000000767	0.000000594	-0.000002099
6	0.000000819	0.000000054	-0.000000172
6	0.000001175	0.000000587	-0.000000256
6	0.000001031	0.000000211	-0.000000029

6	0.000001154	0.000000337	0.00000045
1	0.000000336	0.000000024	0.000000897
6	0.000001294	0.000000292	-0.000000525
1	0.000000928	0.000000416	-0.000000756
6	0.000001498	0.000000565	-0.000000406
1	0.00000094	0.000000484	0.000000321
1	0.000001344	0.000000519	-0.000000771
1	0.000001561	0.000000471	-0.000000231
8	0.000000164	-0.000000024	-0.000000025
8	0.000000428	0.000000132	0.000000545
6	0.000000526	0.000000125	0.000000992
6	0.000000679	-0.000000029	0.000001194
1	0.000000725	-0.000000075	0.000001517
1	0.000000973	0.000000183	0.000001187
1	0.000000701	-0.000000033	0.000001255
6	0.000000142	-0.000000226	0.00000118
1	0.000000044	-0.000000042	0.000001564
1	0.000000045	-0.000000172	0.000000974
1	-0.000000205	-0.000000243	0.000000948
15	-0.000000092	-0.000000065	0.000000847
6	0.000000823	-0.000000034	0.000000866
1	0.000000146	-0.000000038	0.000001234
1	0.000000867	-0.000000027	0.000001205
6	0.000000427	0.000000094	0.000000886
1	0.000000884	0.000000069	0.000000578
1	0.000000056	-0.000000032	0.000000057
79	-0.000000027	-0.000000807	0.000000224
6	-0.000000055	-0.000000106	0.000000254
6	-0.000000455	-0.000000305	0.000000741
6	-0.000000179	-0.000000171	0.000000782
1	-0.000000134	-0.000000181	0.000000977
1	-0.000000078	-0.00000004	0.000001014
7	-0.000000734	-0.000000488	0.000000764
7	-0.000000262	-0.000000032	0.000000676
6	-0.000000634	-0.000000268	0.000000447
6	-0.000000789	-0.000000254	0.000000887
6	-0.000000946	-0.000000432	0.000000274
6	-0.000001079	-0.000000584	0.000000878
6	-0.000001459	-0.000000042	0.000000287
6	-0.000001404	-0.000000475	0.000000593
1	-0.000001234	-0.000000499	0.000001158
1	-0.000001549	-0.000000042	0.000000217
1	-0.000001614	-0.000000575	0.000000587
6	0.000000021	0.000000192	0.000000709



6	0.000000601	0.000000327	0.000000201
6	0.000000429	-0.000000167	0.000000725
6	0.000000527	0.000000571	0.000000206
6	0.000001036	0.000000005	0.000000829
6	0.000001075	0.000000037	0.000000394
1	0.000000746	0.000000297	-0.000000092
1	0.000001133	0.000000187	0.000000903
1	0.000001273	0.000000314	0.000000397
6	0.000000422	-0.000000165	-0.000000102
6	0.000000292	0.000000233	0.000000337
6	0.000000095	0.000000056	-0.000000777
1	-0.000000002	-0.000000188	0.000000141
1	-0.000000162	-0.000000192	0.000000327
1	-0.000000252	-0.000000053	-0.000000201
1	0.000000187	0.000000125	0.000000114
1	0.000000391	0.000000481	-0.000000633
1	0.000000053	0.000000062	-0.000000191
1	-0.000000029	0.000000126	-0.000000459
6	0.000000522	-0.000000117	0.000001144
6	0.000000592	0.000000037	0.000001178
6	0.000000617	-0.000000009	0.000001454
1	0.000000374	-0.000000141	0.000001099
1	0.000001002	0.000000443	0.000000766
1	0.000000061	-0.000000025	0.000001143
1	0.000000094	0.000000035	0.000001118
1	0.000000043	-0.000000096	0.000001445
1	0.000000886	0.000000077	0.000001527
1	0.000000052	-0.000000016	0.000001751
6	-0.000001126	-0.000000222	0.000000146
6	-0.000001122	-0.000000387	-0.000000328
6	-0.00000123	-0.000000393	0.000000123
1	-0.000000814	-0.000000279	-0.000000041
1	-0.000000996	-0.000000246	-0.000000393
1	-0.000001113	-0.000000201	-0.000000532
1	-0.000001429	-0.000000418	-0.000000364
1	-0.000001121	-0.000000415	0.000000467
1	-0.000001521	-0.000000473	0.000000209
1	-0.000001204	-0.000000342	-0.000000071
6	-0.000000615	-0.000000378	0.000001122
6	-0.000000712	-0.000000408	0.000001594
6	-0.000000042	-0.000000003	0.000001177
1	-0.000000336	-0.000000341	0.000001218
1	-0.000000785	-0.000000485	0.000001497
1	-0.000000562	-0.000000046	0.000001179

1	-0.000000994	-0.000000571	0.000001611
1	-0.000000422	-0.000000241	0.000001228
1	-0.000000675	-0.000000481	0.000001343
1	-0.000000028	-0.000000339	0.000001469
6	-0.000000643	0.000000018	-0.000000324
6	-0.000000835	-0.000000046	-0.000000157
6	-0.000000537	-0.000000003	-0.000000028
6	-0.000000276	0.000000038	-0.000000295
6	0.000000061	0.000000218	-0.000000452
1	-0.000000662	-0.000000215	-0.000000076
1	-0.000000618	-0.000000231	-0.000000186
7	-0.000000925	0.000000606	-0.000000368
8	0.000000622	-0.000000429	-0.000000066
1	-0.000000111	0.000000003	-0.000000409
1	-0.000000842	-0.000000245	-0.000000057
17	0.000000334	0.000000225	-0.000000804

Zero-point correction=	1.206620 (Hartree/Particle)
Thermal correction to Energy=	1.283246
Thermal correction to Enthalpy=	1.284190
Thermal correction to Gibbs Free Energy=	1.082982
Sum of electronic and zero-point Energies=	-4388.036967
Sum of electronic and thermal Energies=	-4387.960341
Sum of electronic and thermal Enthalpies=	-4387.959396
Sum of electronic and thermal Free Energies=	-4388.160605

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6	0.000007265	0.00001065	0.000006787
6	-0.000001393	-0.00000667	-0.000002582
7	-0.00000349	-0.000003508	-0.000011542
7	0.000009863	0.00000311	0.000002274
16	-0.000001777	0.000001817	0.000003591
8	0.000000758	-0.000000422	0.000002047
8	-0.000001398	-0.000000549	-0.000000539
6	-0.000000237	-0.000001039	-0.000003407
6	0.000001491	-0.000000813	0.000002965
6	-0.00000134	0.000000108	-0.000001035
6	0.000001082	-0.0000009225	-0.000000964
6	-0.000000151	-0.000001381	-0.000001302
6	-0.000002754	-0.000001246	0.000000241
1	0.000000787	-0.000000503	-0.000001091
1	0.000000125	-0.000001188	-0.000001729
1	-0.000000764	-0.000002239	-0.000003206
1	-0.0000014	-0.000001146	-0.000002872
6	-0.000000975	-0.000003174	-0.000004419

1	-0.000001022	-0.000001363	-0.000000297
1	-0.000001198	-0.000000237	-0.000000902
1	0.000001573	-0.000001238	0.000000005
6	0.000000355	-0.000002347	0.000002399
1	-0.000000705	-0.000000196	-0.000001323
1	-0.000000039	-0.000000492	-0.000001422
6	-0.00000353	-0.000000883	-0.000003225
1	0.000001821	-0.000002102	0.000001588
1	0.000001693	-0.000002285	0.000000284
8	0.000002281	-0.000000184	0.000002606
6	-0.000000942	-0.000002914	-0.000001816
6	0.000000465	-0.00000292	-0.000000461
6	-0.000000874	-0.000001245	-0.000002345
6	-0.000001053	-0.000002057	-0.000002049
1	0.000000215	-0.000002702	-0.000000489
6	-0.000000317	-0.000002732	-0.000002004
1	-0.000001409	-0.000001909	-0.000002184
6	-0.000000759	-0.000004723	-0.000002615
1	0.000000054	-0.00000387	-0.000001163
1	-0.000001398	-0.000003025	-0.000002908
1	-0.000000413	-0.000003657	-0.000002178
6	0.000002086	-0.000003587	0.000002159
6	0.000002271	-0.000000288	0.000000382
6	-0.000000386	-0.000003445	0.000000831
6	0.00000141	-0.000004009	0.000002299
1	0.000001773	-0.000001471	0.000001235
6	0.000002175	-0.000002168	-0.000001169
1	0.000000853	-0.000002016	-0.00000004
6	-0.000000052	-0.000000644	0.000000608
1	0.000001798	-0.000001401	0.000001144
1	0.000000315	-0.000002426	-0.000000701
1	0.000001122	-0.000002602	-0.000000047
8	0.000000674	0.000002098	0.000002116
8	0.000000543	0.000003502	0.000003845
6	0.000002301	0.000003426	0.000003622
6	0.000000947	0.000001728	0.000001973
1	0.000001642	0.000002125	0.000002829
1	0.000000993	0.000002503	0.000002385
1	0.000001315	0.000002499	0.000002853
6	0.000002557	0.000000478	0.000001923
1	0.000002512	0.000000958	0.000003093
1	0.000002002	0.000001336	0.000003188
1	0.000001943	0.000000452	0.000003189
15	-0.000000501	-0.00000136	0.000001036

6	0.000001962	-0.000002971	0.000002294
1	0.000002261	0.000000902	0.000002282
1	0.000000996	0.000001294	0.000001597
6	0.000000504	-0.000000609	-0.000000405
1	0.000000884	0.000001521	0.00000134
1	0.000001232	0.000001311	0.000002222
79	0.000000021	-0.000001849	-0.000002263
6	-0.000001144	0.000002688	0.000001516
6	-0.00000049	0.000002799	-0.000000313
6	-0.000002526	0.000000829	0.000000375
1	-0.000001844	0.000001385	-0.000002226
1	-0.000000968	0.000001823	0.000000297
7	-0.000001108	0.000001163	-0.000000394
7	0.000000295	0.000001687	-0.000001383
6	0.000000033	0.000002809	-0.000000853
6	0.000000639	0.000003385	0.000001682
6	0.000002763	0.000000953	0.00000328
6	0.000002001	0.000000055	0.00000278
6	-0.000001306	0.000003862	0.000001823
6	0.000000615	0.000002812	-0.000000536
1	0.000000814	0.000001865	0.000001886
1	-0.000000083	0.000003037	0.000001894
1	0.000001001	0.000003005	0.000002667
6	-0.000000955	0.000000819	-0.000003825
6	-0.000002503	0.000000328	0.000003587
6	0.000000604	-0.000000524	0.000000336
6	-0.000001275	-0.000000334	-0.000002727
6	-0.000002961	0.000000026	-0.000001706
6	-0.000001293	0.000000225	-0.00000406
1	-0.00000206	0.000000394	-0.000001993
1	-0.000001598	-0.000001054	-0.000002767
1	-0.000002349	-0.000000765	-0.000002398
6	-0.000002317	0.000000936	-0.000005857
6	-0.000001452	0.00000463	0.000000905
6	-0.000002157	-0.000000506	-0.000001941
1	-0.000002748	0.000001556	0.000000344
1	-0.000002456	0.000001867	-0.000002223
1	-0.000002158	0.00000258	-0.000001866
1	-0.000002557	0.000001535	-0.000003242
1	0.000000562	0.00000187	-0.000001619
1	-0.000002056	0.00000168	0.000000258
1	-0.00000116	0.000003173	-0.000000613
6	-0.000001597	-0.000000903	-0.000002607
6	-0.000000275	-0.000000926	-0.000000518

6	-0.000001194	-0.000000666	-0.000001616
1	-0.000000932	0.000000148	-0.000001273
1	-0.000000903	-0.000001704	-0.000001103
1	-0.000000355	-0.000001428	-0.000001629
1	-0.000001216	-0.000001909	-0.000001847
1	-0.000001911	0.000000271	-0.000001866
1	-0.000001583	-0.000000534	-0.000002466
1	-0.000001279	-0.000000324	-0.000001814
6	-0.000003935	0.000001161	-0.000000764
6	0.000001673	0.000004916	0.000000756
6	0.000000852	0.000004502	0.000001748
1	-0.000001787	0.000001271	0.000000016
1	-0.000000347	0.000001852	0.000001547
1	-0.000000606	0.000003245	0.000000708
1	-0.000000812	0.000002912	0.000002005
1	-0.000001025	0.000003738	0.000000644
1	-0.000000925	0.000002771	0.000000257
1	-0.000001019	0.000004365	0.000000078
6	-0.000000424	-0.000000476	0.000000303
6	0.000001461	0.000001796	-0.000000059
6	0.000002111	0.000000764	0.000002406
1	-0.000000124	0.000000504	0.000000412
1	-0.000000468	0.000001249	0.000000216
1	0.000000099	0.000000395	0.000000457
1	-0.000000196	0.000000995	0.000001193
1	0.000000714	-0.000000109	0.000001075
1	0.000000584	0.000000281	0.000001317
1	0.000000654	-0.000000299	0.000000451
6	0.000001417	-0.000000541	0.000000167
6	0.000000604	-0.00000139	0.000001122
6	0.000002007	-0.000000154	0.000002521
6	0.00000208	-0.000000869	0.000000781
6	0.00000019	-0.000002832	0.000001877
1	0.000002015	-0.00000002	0.000002081
1	0.000000156	-0.000000379	0.000000292
7	0.000001065	0.000000956	0.000002711
8	-0.00000541	-0.000007676	-0.000001918
1	0.000002154	-0.000001497	0.000001849
1	0.000001141	0.000000626	0.000001382
17	0.000002417	-0.000001518	-0.000000162

Zero-point correction=

1.209171 (Hartree/Particle)

Thermal correction to Energy=

1.285496

Thermal correction to Enthalpy=

1.286440

Thermal correction to Gibbs Free Energy=

1.087549

Sum of electronic and zero-point Energies=	-4388.032598
Sum of electronic and thermal Energies=	-4387.956273
Sum of electronic and thermal Enthalpies=	-4387.955329
Sum of electronic and thermal Free Energies=	-4388.154220

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6	0.000000163	-0.000000947	-0.000000561
6	0.000001631	-0.000000291	-0.000000803
7	-0.000000479	0.000000106	0.000000012
7	-0.000001106	0.000000173	-0.000000607
16	0.000000023	0.000000026	-0.000000313
8	0.000000224	0.000000004	-0.000000106
8	-0.000000546	0.000000173	0.000000134
6	-0.000000531	-0.000000017	-0.000000054
6	-0.000000266	-0.000000066	-0.000000689
6	-0.000000427	-0.000000004	-0.000000779
6	-0.000000621	0	-0.000000922
6	-0.000001134	-0.000000012	-0.000000073
6	-0.000000896	0.000000045	-0.000000292
1	0.000000143	-0.000000007	-0.000000672
1	-0.000000095	-0.000000057	-0.000001044
1	-0.000001254	-0.000000088	-0.000000671
1	-0.000000977	-0.000000106	-0.000000225
6	-0.000000817	0.000000001	-0.000001115
1	-0.000001185	-0.000000165	-0.000001027
1	-0.000000715	-0.000000015	-0.000001139
1	-0.000000976	-0.000000174	-0.000001409
6	-0.000000039	0.000000047	-0.000000559
1	-0.000000424	-0.000000349	-0.000000862
1	-0.000000653	-0.000000072	-0.000000987
6	0.000000079	0.000000022	-0.000001249
1	-0.000000148	-0.000000014	-0.000000943
1	0.000000002	-0.000000022	-0.000001282
8	0.000000721	-0.000000014	-0.000001019
6	-0.000001349	0.000000263	-0.000001075
6	-0.000001339	-0.000000053	-0.000000442
6	-0.000000674	-0.000000447	-0.000000377
6	-0.000001339	-0.000000224	-0.000000838
1	-0.000001105	-0.000000144	-0.000001341
6	-0.000001537	-0.000000089	0.000000033
1	-0.000000707	-0.000000025	-0.000000518
6	-0.000001927	0.000000068	-0.000000578
1	-0.000001675	-0.000000186	-0.000001285
1	-0.000001437	-0.000000113	-0.000000101

1	-0.000001962	-0.000000104	-0.000000709
6	-0.000000168	-0.000000149	-0.000001592
6	-0.000000715	-0.000000118	-0.000001066
6	-0.000000347	0.000000108	-0.000001863
6	-0.000001186	-0.000000063	-0.00000183
1	-0.000000659	-0.000000063	-0.000001109
6	-0.000000113	-0.000000022	-0.000001893
1	0.000000266	-0.000000161	-0.000001848
6	-0.000000518	-0.000000176	-0.000002215
1	-0.000001061	-0.00000017	-0.000001816
1	0.000000045	-0.000000149	-0.000002384
1	-0.000000634	-0.000000189	-0.000002427
8	0.00000065	-0.000000216	-0.000001272
8	0.000000125	-0.000000426	-0.000002392
6	0.000001055	0.000000352	-0.000000509
6	0.000001027	0.000000096	-0.000000654
1	0.000000951	-0.000000022	-0.000000916
1	0.000000713	-0.000000035	-0.000000574
1	0.000001306	0.000000008	-0.000000456
6	0.000001322	-0.00000016	-0.000001188
1	0.000001333	0.000000092	-0.00000127
1	0.000001588	0.00000006	-0.000001034
1	0.000001292	-0.000000093	-0.000001285
15	0.000001062	-0.000000274	-0.000000761
6	0.000000518	0.000000041	-0.000000641
1	0.000000635	-0.000000009	-0.00000125
1	0.000000581	-0.000000096	-0.000001044
6	0.000001159	0.000000158	-0.000000055
1	0.000000713	0.000000245	-0.000000235
1	0.000001212	0.000000015	-0.000000036
79	0.000000091	0.000000523	0.000000239
6	-0.000000031	-0.000000215	0.000000779
6	0.000000066	0.000000048	0.000001316
6	0.000000397	0.000000019	0.000001573
1	0.000000131	0.000000166	0.000001871
1	0.000000031	0.000000156	0.000001711
7	0.00000012	0.00000016	0.000001798
7	-0.00000018	-0.000000039	0.000000913
6	0.000000189	0.000000143	0.000000626
6	0.000000224	0.000000054	0.000001017
6	0.000000758	-0.00000006	0.000000979
6	0.000000322	-0.000000085	0.000000602
6	0.000000056	0.00000015	0.000000064
6	0.000000395	0.000000118	0.000000617

1	-0.000000103	0.000000012	0.000000571
1	0.000000987	-0.000000031	0.000000757
1	0.000000689	-0.000000002	0.000000537
6	-0.000000363	-0.000000027	0.000001011
6	0.000000006	0.000000091	0.000000935
6	-0.000000246	-0.000000059	0.000001232
6	0.000000019	0.000000232	0.000001169
6	-0.000000053	0.000000165	0.000001072
6	-0.000000433	-0.000000011	0.000000978
1	0.000000233	0.000000075	0.000001003
1	-0.000000962	0.000000009	0.000001112
1	-0.000000441	-0.000000008	0.000001023
6	0.000000704	0.000000071	0.000000955
6	0.000000724	0.000000009	0.000001512
6	0.000000848	0.000000073	0.000000677
1	0.000000686	-0.000000004	0.000000978
1	0.000000647	0.000000012	0.000001693
1	0.000001159	0.000000123	0.000001392
1	0.000000742	0.000000127	0.000001479
1	0.000000697	0.000000076	0.000000433
1	0.000000814	0.000000046	0.000000705
1	0.000001048	0.000000007	0.000000684
6	-0.000000805	-0.000000048	0.000001263
6	-0.000001105	0.000000006	0.000000898
6	-0.000000952	-0.000000012	0.000001643
1	-0.000000835	-0.000000226	0.000001233
1	-0.000000096	-0.000000087	0.000000789
1	-0.000001282	0.000000023	0.000000972
1	-0.000001354	0.000000026	0.000000869
1	-0.000000748	0.000000072	0.000001809
1	-0.000001098	0.000000044	0.000001693
1	-0.000001185	0.000000051	0.000001609
6	0.000001103	0.000000063	0.000000921
6	0.000001161	0.000000166	0.000000589
6	0.000001305	0.000000144	0.000001127
1	0.000000921	0.000000153	0.000001007
1	0.000001012	0.000000142	0.000000384
1	0.000001373	0.000000052	0.000000505
1	0.000001285	0.000000253	0.000000433
1	0.000001306	0.000000176	0.000001478
1	0.00000145	0.000000121	0.000001105
1	0.000001567	0.000000109	0.000001197
6	-0.000000272	0.000000014	0.000000829
6	-0.000000623	0.000000044	0.000001447



6	-0.000000654	0.000000183	0.000000708
1	-0.000000288	0.000000032	0.000000898
1	-0.000000476	0.000000003	0.000001169
1	-0.000000702	0.000000076	0.000001407
1	-0.000000567	-0.000000086	0.000001327
1	-0.000000248	-0.000000049	0.000000655
1	-0.000000073	0.000000197	0.000000769
1	-0.000000097	-0.000000127	0.000000787
6	0.000000982	-0.000000018	-0.000000297
6	0.000001188	0.000000076	-0.000000008
6	0.000000612	-0.000000248	-0.000000055
6	0.000000536	0.000000252	-0.000000179
6	0.000000054	0.000000011	-0.000000575
1	0.000000959	-0.000000048	-0.000000707
1	0.000000552	-0.000000055	-0.000000245
7	-0.000000014	0.000000193	-0.000000152
8	0.000000333	0.000000844	-0.000000192
1	0.000000254	-0.000000006	-0.000000548
1	0.000001366	0.000000004	-0.000000629
17	-0.000000532	-0.000000057	-0.000000003

Zero-point correction=

1.206562 (Hartree/Particle)

Thermal correction to Energy=

1.283257

Thermal correction to Enthalpy=

1.284201

Thermal correction to Gibbs Free Energy=

1.084134

Sum of electronic and zero-point Energies=

-4388.023739

Sum of electronic and thermal Energies=

-4387.947044

Sum of electronic and thermal Enthalpies=

-4387.946100

Sum of electronic and thermal Free Energies=

-4388.146167

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6	-0.000001429	0.000002411	-0.000000614
6	-0.000000047	-0.000001831	0.000000991
7	0.000002582	0.000000364	-0.000006528
7	0.000001143	-0.000000137	0.000002611
16	0.000000248	-0.000000754	0.000001739
8	-0.000000387	0.000001463	-0.000000745
8	-0.000000504	0.000000089	-0.000000049
6	-0.000001284	0.000000673	-0.000001199
6	-0.000000846	0.000000549	-0.000000193
6	0.000000107	0.000001857	-0.000001618
6	-0.000000579	0.000000813	0.000000561
6	-0.000001887	0.000000423	-0.000002128
6	-0.000000046	0.000000487	-0.000000958
1	-0.000000547	0.000000994	-0.000000394

1	-0.00000779	0.00001553	-0.00000084
1	-0.00001071	0.00000748	-0.00000102
1	-0.00000589	0.00000673	-0.00000929
6	-0.00001686	0.00002004	-0.00001313
1	-0.00001009	0.00001041	-0.00001424
1	-0.00000848	0.0000016	-0.00001378
1	-0.00000766	0.00001254	-0.00001242
6	-0.00002553	0.00000971	0.00004332
1	0.00000676	0.00001125	-0.00000014
1	0.00000696	0.00000913	-0.00000378
6	0.00001738	0.00000012	-0.00001149
1	0.00000621	0.00000402	0.00000679
1	0.00000775	0.00000563	0.00000944
8	-0.00000209	0.00001202	0.00000697
6	-0.00002169	-0.00000426	-0.00001169
6	0.00000221	0.00000478	-0.00000737
6	0.00000111	-0.00000282	0.00000901
6	-0.00000059	-0.00000117	0.00000272
1	-0.00000034	0.00000531	-0.00000373
6	0.00000006	-0.00000048	-0.00001157
1	-0.00000091	-0.00000487	0.00000027
6	-0.00001705	-0.00000607	-0.00000451
1	-0.00000569	0.00000177	-0.00000637
1	-0.00000295	-0.00000789	-0.00000071
1	-0.00000542	-0.00000588	-0.00000463
6	0.00000329	0.00000238	0.00000724
6	0.00000214	0.00000024	0.00000271
6	0.00000958	0.00000574	0.00000173
6	0.00000151	0.00000036	0.00000048
1	0.00000448	0.00000051	0.00000193
6	0.00000496	0.00001068	0.00000306
1	0.00000792	0.00001361	0.00000054
6	0.00000486	0.00000758	0.00000314
1	0.00000161	0.00000024	0.00000085
1	0.00000646	0.00001191	0.00000298
1	0.00000037	0.00000835	0.00000071
8	0.00001375	0.00003055	0.00004393
8	0.00000099	0.00000402	-0.00000211
6	-0.00000097	0.00001271	0.00000864
6	0.0000008	0.00000992	-0.00000842
1	0.00000273	0.00001966	-0.00000148
1	0.00000036	0.0000152	-0.00000553
1	0.00000322	0.00001653	-0.00000104
6	0.00000605	0.00001872	0.00000051

1	0.000000702	0.000001887	0.00000025
1	0.00000072	0.000001648	0.00000031
1	0.000000837	0.000001554	0.000000334
15	0.000001076	-0.000002213	-0.000002214
6	0.000000795	0.000001202	0.000000043
1	0.000000665	0.00000202	0.000000431
1	-0.000000096	0.000001258	-0.000000613
6	-0.000001342	-0.000001247	-0.000003472
1	-0.000000038	0.000001456	0.000000364
1	0.000000121	0.000001638	0.000000333
79	-0.000001292	-0.000000191	-0.000000181
6	0.000000557	-0.000003113	0.000000171
6	0.000000746	-0.000002153	0.000000552
6	-0.000000194	-0.000000137	0.000000017
1	-0.000000689	-0.000001539	-0.000000051
1	-0.000000435	-0.000001023	0.000000413
7	-0.000002202	0.000000193	0.000001146
7	0.000001404	-0.000001113	-0.000001729
6	0.00000016	-0.000001122	-0.000000493
6	-0.000000775	0.000000119	0.000001182
6	0.000000021	-0.000000712	0.000001855
6	0.000000826	-0.000002212	0.000001151
6	0.000000741	0.000000403	0.000000959
6	0.000001119	-0.000001254	0.000000465
1	0.000000775	-0.000001097	0.000000098
1	0.000001045	-0.000000949	0.000001251
1	0.000001011	-0.000001014	0.000001285
6	-0.000001034	0.000000806	-0.000000896
6	-0.000000198	-0.000000661	-0.000000422
6	-0.000001146	-0.000001928	0.000000725
6	-0.000001182	-0.000000079	-0.000000333
6	-0.000000067	-0.000000167	-0.000000575
6	-0.000000951	-0.000000132	-0.000001628
1	-0.000000956	0.000000142	-0.000000897
1	-0.00000123	-0.000000644	-0.000000891
1	-0.000001242	-0.000000167	-0.000001039
6	-0.000001261	0.000000228	-0.000000252
6	-0.000000154	-0.000000721	-0.000000061
6	-0.000000204	0.000000072	-0.000000239
1	-0.000000342	-0.000000102	-0.000000081
1	-0.000000674	-0.000000672	-0.000000243
1	-0.000000421	-0.000000312	-0.000000193
1	-0.000000827	-0.000000298	-0.000000525
1	-0.00000003	0.000000073	-0.000000017

1	-0.000000564	0.000000376	-0.000000659
1	-0.000000042	0.000000208	-0.000000253
6	-0.000000856	-0.000000944	-0.000000782
6	-0.000000706	-0.000001457	-0.000000416
6	-0.000000733	-0.000001406	-0.000000347
1	-0.000000827	-0.000001058	-0.000000134
1	-0.000000834	-0.000000342	-0.000000728
1	-0.000000664	-0.000001001	-0.000000364
1	-0.000001167	-0.000000919	-0.000000748
1	-0.000000895	-0.000001547	-0.000000485
1	-0.000001369	-0.000001379	-0.000000906
1	-0.000000958	-0.000001548	-0.000000522
6	0.000001242	-0.000001459	-0.000001185
6	0.000000116	-0.000000232	0.000000685
6	-0.000000301	-0.000000449	0.000000099
1	0.000000245	-0.000000679	0.000000023
1	0.000000978	0.000000011	0.000000723
1	0.000000332	0.000000064	0.000000354
1	0.000000081	-0.000000554	0.000000392
1	0.000000291	-0.000001304	0.000000525
1	0.000000811	-0.000000902	0.000000858
1	0.000000586	-0.000000925	0.000000484
6	0.000000651	-0.000001439	0.000000421
6	0.000000034	-0.000001602	0.000000041
6	-0.000000093	-0.000000955	0.000000654
1	0.000000044	-0.000001152	0.000000163
1	0.000000167	-0.000001783	0.000000539
1	0.000000073	-0.000001863	0.000000495
1	0.000000388	-0.000001809	0.000000783
1	0.000000331	-0.000000878	0.000000606
1	0.000000516	-0.000001282	0.000000577
1	0.000000095	-0.000001294	0.000000435
6	0.000001323	-0.000000248	0.000000069
6	0.000000822	0.000000435	0.000000834
6	0.000001087	0.000000353	0.000001117
6	0.000001217	-0.000000055	0.000000999
6	0.000000818	0.000000467	0.000000442
1	0.000001347	0.000000019	0.000001149
1	0.000000393	0.000000626	0.000000502
7	0.000000806	-0.000000084	0.000001213
8	0.000000349	0.000000792	0.000000814
1	0.000001392	-0.000000116	0.000001289
1	0.000000853	0.000000448	0.000000717
17	0.000001206	-0.000000216	0.000001064

Zero-point correction=	1.207937 (Hartree/Particle)
Thermal correction to Energy=	1.284530
Thermal correction to Enthalpy=	1.285474
Thermal correction to Gibbs Free Energy=	1.085771
Sum of electronic and zero-point Energies=	-4388.036471
Sum of electronic and thermal Energies=	-4387.959878
Sum of electronic and thermal Enthalpies=	-4387.958934
Sum of electronic and thermal Free Energies=	-4388.158637

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6	0.000001001	-0.000000173	-0.000000663
6	0.000000684	0.000000444	0.000002278
7	0.000000125	0.000000389	-0.000000194
7	-0.000001721	0.000000784	-0.000001617
16	0.00000103	0.000000791	0.000000936
8	0.000001152	0.000000328	-0.000000252
8	0.000000895	-0.000000029	0.000000075
6	0.000001018	0.000000787	0.000000341
6	0.000001494	0.000001487	-0.000000121
6	0.000001498	0.000000163	0.000000424
6	0.000001824	0.000001753	0.000000267
6	0.000001932	0.000001537	0.000000223
6	0.000001173	0.000000936	0.000000596
1	0.00000158	0.000001426	0.000000042
1	0.000001987	0.000002028	-0.000000154
1	0.000001851	0.000001109	0.000000563
1	0.000001314	0.000000474	0.000000681
6	0.000002227	0.000002112	0.000000022
1	0.000002194	0.000001825	0.000000716
1	0.00000269	0.000002674	0.000000132
1	0.000002003	0.000002027	-0.000000474
6	-0.000000026	0.000000293	-0.000000168
1	-0.000000086	0.000001323	-0.000000923
1	0.000000896	0.000000778	-0.000000004
6	0.000000535	0.000001074	-0.000000634
1	-0.000000459	0.000000393	-0.000001021
1	-0.000000411	0.000000188	-0.000000848
8	-0.000001605	-0.000000384	-0.000001799
6	-0.000000027	-0.000000286	-0.000000321
6	-0.000000421	-0.00000006	-0.000000778
6	-0.000000387	-0.000000059	0.000000034
6	-0.000001053	-0.000000552	-0.000000232
1	-0.000000519	0.000000162	-0.000000626
6	-0.000000277	-0.000000733	0.000000164

1	0.00000026	-0.000000658	0.000000347
6	-0.000000494	-0.000000802	0.00000004
1	-0.000001122	-0.000000565	-0.000000309
1	-0.000000424	-0.000001316	0.000000716
1	-0.000000996	-0.000001324	0.000000338
6	-0.000000256	0.000001062	-0.000001106
6	-0.000000664	0.000001328	-0.000001638
6	0.000000137	0.000001446	-0.000001518
6	-0.000000892	0.000001392	-0.000002149
1	-0.000001084	0.000000092	-0.000001512
6	0.000000061	0.000001729	-0.000001523
1	0.000000356	0.000001514	-0.000000918
6	-0.000000408	0.00000219	-0.000002085
1	-0.00000109	0.000001496	-0.000002237
1	0.000000043	0.000002232	-0.000001578
1	-0.000000337	0.000002296	-0.000002255
8	-0.000000933	0.000000136	-0.000001665
8	-0.000001111	-0.00000186	-0.000001429
6	-0.000001012	-0.000000922	-0.000001439
6	-0.000001545	-0.000000927	-0.000000694
1	-0.000002059	-0.000001353	-0.000000711
1	-0.000001503	-0.000000786	-0.000000967
1	-0.000002142	-0.000000785	-0.000001343
6	-0.000002219	-0.000000498	-0.000001414
1	-0.000002253	-0.000001083	-0.000001145
1	-0.00000235	-0.000000636	-0.000001596
1	-0.000002063	-0.000000056	-0.000001388
15	-0.000001157	0.000001789	0.000000083
6	-0.000001924	-0.000000319	-0.000000839
1	-0.000001512	-0.000000685	0.000000063
1	-0.000001436	-0.000001002	0.000000329
6	-0.000001452	0.000000365	-0.000001501
1	-0.000001135	0.000000328	-0.000000933
1	-0.000001725	0.000000079	-0.000001453
79	-0.00000002	-0.000000484	0.000000191
6	0.000000284	-0.000001063	0.000000423
6	0.000000262	-0.00000102	0.00000012
6	0.000000444	-0.000001221	0.000000128
1	0.000000342	-0.000001512	0.000001719
1	0.000000243	-0.000000931	0.000001147
7	0.000000216	-0.000000189	0.000000046
7	0.000000512	-0.000001132	0.000001155
6	0.000000054	-0.000000013	0.000000441
6	-0.000000013	-0.000000622	0.000000005

6	-0.000000283	0.000000188	0.000000076
6	-0.000000051	-0.000000004	-0.000000386
6	-0.000000329	0.000000827	0.000000348
6	0.000000054	0.000000333	-0.000000034
1	-0.000000795	-0.000000074	-0.000000059
1	0.000000714	0.000000914	-0.000000202
1	-0.000000125	0.000000676	-0.000000689
6	0.000000116	-0.000001204	0.000001397
6	0.000000799	-0.000000833	0.000001325
6	-0.000000051	-0.000001293	0.000000982
6	0.000000966	-0.000001313	0.000001825
6	0.000000007	-0.000001716	0.00000144
6	0.000000429	-0.000001628	0.000001834
1	0.000001138	-0.000001139	0.000002059
1	-0.000000292	-0.000002046	0.000001447
1	0.000000424	-0.00000177	0.000001883
6	0.000001403	-0.000000745	0.000001643
6	0.000001503	-0.000000922	0.00000204
6	0.000001507	-0.000000485	0.000001843
1	0.000001029	-0.000000469	0.000001457
1	0.000001207	-0.000001147	0.000002213
1	0.000001763	-0.000000764	0.00000214
1	0.000001477	-0.000001172	0.000002349
1	0.000001401	-0.000000146	0.000001369
1	0.000001687	-0.000000521	0.000002091
1	0.000001893	-0.000000049	0.000001722
6	-0.000000066	-0.000001861	0.000001133
6	-0.000000918	-0.000001641	0.000000629
6	-0.000000604	-0.000002405	0.000001329
1	-0.000000477	-0.000001491	0.000000773
1	-0.000000684	-0.000001449	0.000000352
1	-0.000001098	-0.000001774	0.000000601
1	-0.000001153	-0.000001863	0.000000075
1	-0.000000416	-0.000002158	0.000001565
1	-0.000000713	-0.000002472	0.000001565
1	-0.000001008	-0.000002339	0.000001078
6	0.00000139	0.000000075	0.000000741
6	0.000001421	0.000000062	-0.000000035
6	0.000001557	0.000000045	0.000001099
1	0.000000099	0.000000047	0.000000439
1	0.000001067	0.000000609	0.000000913
1	0.000001427	0.000001132	0.00000134
1	0.000001396	0.000001546	-0.000000417
1	0.000001174	0.000000368	0.000001057

1	0.000001524	0.000000476	0.000000685
1	0.00000146	0.000000367	0.000000913
6	-0.000000795	-0.000000895	0.000000324
6	-0.000000716	-0.000001276	0.000000273
6	-0.000001188	-0.000000583	-0.00000015
1	-0.000000498	-0.000000918	-0.000000075
1	-0.000000473	-0.000001249	0.000000686
1	-0.000001084	-0.000001594	0.00000037
1	-0.000001024	-0.00000089	-0.000000021
1	-0.000001123	-0.000000772	-0.000000039
1	-0.00000142	-0.000000732	-0.000000596
1	-0.000001382	-0.000001297	-0.000000023
6	-0.000000134	0.000001194	-0.000002037
6	-0.000000789	0.000001658	-0.000002211
6	-0.000000259	0.000002228	-0.000001964
6	0.000000113	0.000001789	-0.000001586
6	-0.000000214	0.000001579	-0.000001389
1	-0.000000021	0.000002542	-0.000002294
1	-0.000001849	0.000000756	-0.000001323
7	-0.000001419	0.00000163	-0.000001493
8	0.000000385	-0.000000769	-0.000001074
1	0.000000487	0.000002445	-0.000001658
1	-0.000001001	0.000001765	-0.000002353
17	0.000000636	0.000001666	-0.000000828

Zero-point correction=	1.206909 (Hartree/Particle)
Thermal correction to Energy=	1.283576
Thermal correction to Enthalpy=	1.284520
Thermal correction to Gibbs Free Energy=	1.084321
Sum of electronic and zero-point Energies=	-4388.030737
Sum of electronic and thermal Energies=	-4387.954070
Sum of electronic and thermal Enthalpies=	-4387.953126
Sum of electronic and thermal Free Energies=	-4388.153324

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6	-0.000009947	-0.000021613	0.000001771
6	0.00000736	0.000007119	0.000002814
7	0.000010545	-0.000000669	-0.000003905
7	-0.000005521	0.000014771	0.000001279
16	-0.00001015	-0.000003484	-0.000004425
8	-0.00000032	0.000006045	0.000002685
8	-0.000000273	0.000004759	0.000001335
6	-0.000002101	0.000001749	-0.000004789
6	-0.000004327	0.000002905	0.000002261
6	-0.000004988	-0.000007977	-0.000003013



6	-0.000002801	0.000002394	-0.000008174
6	-0.000005943	0.000001517	0.00000274
6	0.000001505	-0.000004047	0.000000704
1	-0.000002148	-0.00000058	-0.000000863
1	-0.00000461	-0.000001579	-0.000002312
1	-0.000004286	-0.000001837	-0.000002476
1	-0.000003652	-0.000001192	-0.000001542
6	-0.0000036	-0.000000874	-0.000003395
1	-0.000007041	-0.000002906	-0.000004895
1	-0.000003829	-0.000000446	-0.00000181
1	-0.000006099	-0.000005114	-0.000000278
6	-0.000005851	0.000001059	-0.000002166
1	-0.000000977	-0.000003045	-0.000001341
1	-0.000001687	-0.000003274	0.000000642
6	0.000001651	-0.000001161	-0.00000166
1	0.000002766	-0.000000348	0.000002097
1	0.000000522	-0.000000809	-0.000000237
8	-0.000001682	-0.000001129	-0.000001489
6	0.000005083	-0.000003898	0.000002948
6	-0.000001039	-0.000003597	-0.000003905
6	-0.000004334	0.000000907	-0.000000082
6	-0.000002827	-0.000001421	0.000000899
1	-0.000000048	-0.000002106	-0.000001431
6	-0.000000865	-0.00000131	-0.000002919
1	-0.000000325	-0.000000763	0.000000738
6	0.000002589	-0.00000052	0.000000631
1	0.000000377	-0.000002288	-0.000001323
1	-0.00000035	0.000000739	0.000000406
1	0.000000148	-0.00000134	-0.000000432
6	0.00000241	-0.000000808	-0.000000105
6	-0.00000038	-0.000001843	-0.000000389
6	0.000001133	-0.000001771	-0.000001345
6	0.000003679	-0.000002016	-0.000001275
1	0.000002938	-0.00000151	0.000000221
6	-0.000000966	-0.000002605	-0.000000671
1	-0.000000141	-0.000000745	-0.00000073
6	0.000001667	-0.000001848	0.00000024
1	0.000002567	-0.000002803	0.00000024
1	0.000000361	-0.00000203	-0.000001022
1	0.000001584	-0.00000302	-0.000000755
8	-0.000001039	-0.000000927	-0.000002808
8	-0.000005844	-0.000006064	-0.000001065
6	0.000003823	-0.000001648	0.000004458
6	0.000001336	-0.000002877	-0.000001828

1	0.000003553	-0.000000719	0.000000179
1	0.000002814	-0.000001593	-0.000000046
1	0.000003041	-0.000002507	0.000000151
6	0.000004679	-0.000002417	-0.000000719
1	0.000003398	-0.000001216	0.000000067
1	0.000003388	-0.000002461	0.000000747
1	0.000002562	-0.00000134	0.000000613
15	0.000013412	-0.000003389	0.000000965
6	-0.000000481	0.000000944	-0.000000372
1	0.000003184	0.000000201	0.000000733
1	0.000003003	-0.000001121	0.000000546
6	0.000003833	-0.000004763	-0.000003361
1	0.000001073	-0.000001466	0.000001079
1	0.000002355	-0.000003064	0.000000199
79	-0.000000866	0.000000545	-0.000001295
6	0.000000562	0.000007895	0.000000739
6	0.000000626	-0.000005608	-0.000007691
6	-0.000002012	0.000008234	0.000011326
1	-0.000000214	0.000004689	0.000002367
1	0.000001694	0.00000058	-0.000000169
7	0.00000098	0.00000433	0.000007857
7	-0.000000204	-0.00000374	-0.000006559
6	0.000000071	0.000001348	-0.000001907
6	0.000004014	0.000004503	0.000001445
6	-0.000001702	0.00000082	0.000002889
6	0.000001403	0.000001202	0.000002744
6	0.000001328	0.000003011	0.000000342
6	0.00000199	-0.000001559	-0.000000393
1	0.000003238	0.000000261	0.000000605
1	0.00000035	0.000000483	0.000000264
1	0.000001678	0.000000949	0.000001191
6	-0.000004934	-0.000002055	-0.00000311
6	0.000001014	0.000009912	-0.00000004
6	-0.000000785	0.000001335	0.000005888
6	-0.000003902	0.000000091	0.000003784
6	0.000000401	0.000006133	-0.000000763
6	-0.000001913	-0.000000454	-0.000002845
1	-0.000003536	0.000002286	-0.000000316
1	-0.000000131	0.000001519	0.000000033
1	-0.000001508	0.000002536	0.000000781
6	-0.000005258	0.000001902	-0.000000669
6	0.000000312	0.000003825	0.000001354
6	-0.000002307	0.000002364	0.000000018
1	-0.000002925	0.000002355	0.000000037

1	-0.000002281	0.000005077	0.000001699
1	-0.000002767	0.000003561	0.000000876
1	-0.000003113	0.000004518	0.000000053
1	-0.000002114	0.000000633	-0.000001801
1	-0.000003456	0.000002416	0.000000163
1	-0.000002636	0.000002185	-0.000000065
6	0.000006468	0.000001166	0.000001842
6	-0.000001719	0.000002157	0.000000998
6	-0.000002031	0.000003084	0.000001168
1	0.000002586	0.000001226	0.000001458
1	0.000000097	0.000001061	0.000000545
1	0.000001804	0.000001308	0.000001735
1	0.000002073	0.000003233	0.00000107
1	0.000000424	0.000003702	0.00000023
1	0.000002151	0.000001333	0.000001444
1	0.000001593	0.000002928	0.000001443
6	-0.000003255	0.000002996	-0.000001927
6	0.000000521	-0.000000429	0.000002006
6	-0.000000047	0.00000229	0.000003156
1	-0.000002218	0.000003334	0.000001201
1	-0.000001106	0.000000655	-0.000002226
1	-0.000001936	0.000001823	0.000000081
1	-0.000001298	0.000003037	-0.000000514
1	-0.00000103	0.000003192	0.000000441
1	-0.000001065	0.000001689	-0.000000225
1	-0.00000127	0.000002977	0.000000747
6	0.000004573	0.00000124	0.000003549
6	0.000002788	0.000003913	0.000001259
6	0.00000231	0.000001048	0.000000207
1	0.00000224	0.000001218	0.000001867
1	0.000002555	0.000004515	0.000003824
1	0.000002426	0.000002545	0.000002208
1	0.000003026	0.000002685	0.000002411
1	0.000002542	-0.000000496	0.000001583
1	0.000002195	0.000001601	0.000001718
1	0.000003113	0.000000815	0.000001723
6	0.000000662	-0.000000284	0.000001052
6	0.000000447	-0.000004381	0.000000594
6	0.000000196	-0.000004303	-0.000001789
6	-0.00000152	-0.000002251	-0.000001173
6	-0.000002861	-0.000003134	0.000000055
1	0.000000258	-0.00000411	-0.000002002
1	0.000000844	-0.00000305	-0.000001484
7	0.000009738	-0.000003817	-0.000005177

8	-0.000001625	-0.000010477	-0.000002526
1	-0.000001011	-0.000003548	-0.000002111
1	0.000002146	-0.000003968	-0.000000794
17	-0.00000162	-0.000003818	-0.000001813
Zero-point correction=			1.209009 (Hartree/Particle)
Thermal correction to Energy=			1.285232
Thermal correction to Enthalpy=			1.286177
Thermal correction to Gibbs Free Energy=			1.088554
Sum of electronic and zero-point Energies=			-4388.038197
Sum of electronic and thermal Energies=			-4387.961973
Sum of electronic and thermal Enthalpies=			-4387.961029
Sum of electronic and thermal Free Energies=			-4388.158652

Re6

6	0.000001087	-0.000000606	0.000000003
6	0.000002498	0.000000111	-0.000002324
7	-0.000001771	-0.000000158	-0.00000005
7	-0.000001414	0.000002668	0.000003046
16	0.00000075	-0.000000879	-0.000003635
8	-0.000000774	0.000001247	-0.000000924
8	-0.00000001	0.000000161	0.000000398
6	0.000000827	0.000001058	-0.000002776
6	-0.000001317	0.000001076	0.000002788
6	-0.000003621	-0.000002671	-0.000003892
6	-0.000000463	0.000000812	-0.000001819
6	-0.000000295	0.000000896	0.000004143
6	-0.000003604	-0.000002397	-0.000003131
1	-0.000001152	-0.000000176	-0.000002205
1	-0.000001554	0.000000439	-0.000000944
1	-0.000001012	-0.000000097	-0.000001193
1	0.000000027	0.000000558	-0.000000128
6	-0.000002829	-0.000000919	0.000001069
1	-0.000000909	0.000000082	-0.000000893
1	-0.000002045	-0.000000443	-0.000000892
1	-0.000001627	0.000000246	-0.000000897
6	0.000000449	0.000000686	-0.000001435
1	-0.000000186	-0.000000061	-0.000001205
1	-0.000000399	-0.000000189	-0.00000158
16	0.000001021	0.000000363	-0.000001033
8	0.000000181	-0.000000875	-0.000000062
8	-0.000000667	-0.000001068	0.000002312
6	0.000001653	-0.00000002	-0.000000096
6	0.000000324	-0.000000427	0.00000151
6	-0.000001193	0.000001709	0.000002581

6	-0.000001825	0.000000733	0.000001481
1	-0.000000381	-0.000000109	0.000000307
6	0.000000273	-0.000001388	0.000002459
1	0.000000087	-0.000000326	0.000001413
6	0.000000606	-0.000000573	-0.000001202
1	-0.000000554	-0.000000441	0.000000925
1	0.000000252	0.000000047	0.000001755
6	-0.000000299	-0.000000126	0.000002463
1	-0.000000364	-0.000000117	0.00000182
1	-0.000000482	-0.000000419	0.000002124
1	-0.000000325	-0.000000082	0.000001212
6	0.000002607	-0.000001462	-0.000001214
6	0.000001826	0.000000533	0.000000234
6	0.000000667	0.000000036	0.000000739
1	0.000000855	0.000000692	0.000000102
6	0.000002382	0.000000588	-0.000000047
1	0.000001153	0.000000233	0.000000321
1	0.000001213	-0.000000003	-0.000000093
6	0.000001697	-0.000000154	0.000000665
1	0.000001346	0.000000229	0.000000717
1	0.000000098	0.000000171	0.000000404
6	0.00000184	0.000000286	0.000000688
1	0.000001947	0.000000227	-0.000000153
1	0.000001794	0.000000192	-0.000000323
1	0.000002348	0.000000554	0.000000911
1	0.000002082	0.000000277	0.000000126
1	0.000002634	0.000000214	0.000000282
1	0.00000225	0.000000118	0.000000784
6	-0.000000241	0.000001796	-0.000000091
6	-0.000000475	-0.000000955	-0.000000741
6	-0.00000125	-0.000000298	-0.000001072
6	-0.000001105	-0.000000237	-0.000000054
1	-0.000000206	0.000000035	-0.000000877
6	-0.000000848	-0.000000594	-0.000000097
1	-0.000000798	-0.000000002	-0.000000905
6	-0.000001019	-0.000000144	-0.000000032
1	-0.000000691	-0.000000007	-0.000000304
1	-0.000001516	-0.000000178	-0.000000108
1	-0.000001461	-0.000000185	0.000000014

Zero-point correction=

0.559901 (Hartree/Particle)

Thermal correction to Energy=

0.596038

Thermal correction to Enthalpy=

0.596982

Thermal correction to Gibbs Free Energy=

0.484477

Sum of electronic and zero-point Energies=

-2330.431474

Sum of electronic and thermal Energies=	-2330.395337
Sum of electronic and thermal Enthalpies=	-2330.394393
Sum of electronic and thermal Free Energies=	-2330.506898

E-1

6	-0.000009192	-0.0000083	0.000005906
6	0.000017358	0.0000069	-0.000006068
7	0.000004742	0.000012683	-0.000004761
7	-0.000005821	-0.000006029	0.000011936
16	-0.000010479	-0.00000839	0.000007496
8	0.000000741	-0.000000036	0.000000887
8	0.000002732	-0.00000004	-0.000000948
6	-0.000002832	0.000000569	-0.000002476
6	0.000001361	-0.000003052	0.000000832
6	0.000000019	-0.000001587	-0.00000296
6	-0.000004098	-0.00000234	0.000003027
6	-0.00000331	-0.000002753	-0.000000686
6	0.000000258	-0.000001033	-0.000001283
1	-0.000000769	-0.000000872	-0.000000811
1	-0.00000028	-0.000001289	-0.000000833
1	-0.000000916	-0.00000181	-0.000000464
1	-0.000001351	-0.000001613	-0.000000199
6	0.000005793	0.000002877	-0.000003842
1	-0.00000449	-0.000003546	-0.000000802
1	-0.00000396	-0.00000401	0.00000006
1	-0.000003165	-0.000003405	-0.000000125
6	-0.000004607	-0.0000123	-0.000001262
1	-0.000001315	0.000001311	0.000000061
1	-0.000003833	0.000000092	0.000000799
16	0.000001339	0.000004961	-0.000007081
8	-0.000003071	-0.000000544	0.000002546
8	0.00000177	0.000000646	0.000000383
6	-0.000003585	0.000002182	0.000004006
6	0.000003053	-0.000001366	0.00000135
6	0.00000367	0.000001334	0.000001238
6	0.000000351	0.000001627	0.000002117
1	-0.000001192	-0.000000142	0.000001049
6	-0.000000089	-0.000000669	0.000001868
1	-0.000000247	0.000001481	0.000001662
6	-0.00000344	0.000002808	0.000002827
1	0.000000154	-0.000000289	0.000002474
1	0.000000666	0.000001184	0.000002994
6	0.000002132	-0.000001888	0.000007881
1	-0.000000398	0.000001302	0.000002524
1	-0.000000115	0.000000624	0.000001123

1	-0.000001654	0.000000977	0.000001969
6	0.000001847	0.000001525	0.000000398
6	-0.000000259	-0.000000403	0.000000401
6	-0.000001091	-0.000000357	0.000001877
1	-0.000000005	0.000000083	0.000000446
6	-0.000000166	-0.000000186	0.000000891
1	0.000000626	0.000000721	0.000001277
1	0.000000722	0.000000915	0.000000724
6	0.000000458	-0.000000715	0.000002182
1	0.000000026	0.000000675	0.000001824
1	-0.000000876	0.000000494	0.000001901
6	-0.000001068	0.000000968	0.000001899
1	0.000000417	0.000000753	0.000000886
1	-0.000000096	-0.000000014	0.000000809
1	-0.000000299	0.000000444	0.000002068
1	-0.000000402	-0.000000008	0.000001761
1	-0.000000027	0.000000262	0.000001446
1	0.000000194	0.000000877	0.000001435
6	0.000005869	0.00000528	0.000003263
6	-0.000000654	-0.000003981	0.000001455
6	-0.000000244	0.000000991	0.000000551
6	0.000000306	0.000001923	-0.000000182
1	-0.000000395	-0.000000069	0.000000013
6	-0.000000819	-0.000000162	0.000003828
1	-0.000000016	-0.0000001432	0.000000151
6	-0.000003096	-0.000000202	0.000000621
1	-0.000000536	-0.000000488	0.000001397
1	-0.000001252	-0.000000292	0.000001619
1	-0.000000246	0.000000121	0.000002341
79	0.000002188	0.000002536	0.000000433
6	0.000001488	-0.000002851	-0.000000468
6	-0.000002691	-0.000000299	-0.000003307
6	0.000002629	0.000000082	-0.000001182
1	0.000000463	0.000000029	-0.000000962
1	0.000001449	0.000001036	-0.000000046
7	-0.000001942	0.000004655	0.000001174
7	-0.000001479	0.000000428	-0.000002642
6	0.000002873	-0.000003388	-0.000000456
6	0.00000003	0.000003363	0.000000877
6	0.000000168	0.000003115	-0.000001202
6	0.000000149	0.000001378	0.00000001
6	0.000000135	-0.000000066	-0.000000099
6	0.000000483	-0.000000681	-0.000000225
1	0.000001036	0.000000844	0.000000037

1	-0.000000153	-0.000000019	-0.000000597
1	0.000000514	0.000001203	0.000000039
6	0.00000113	-0.000002422	-0.000001155
6	0.000000624	0.000001105	-0.000001654
6	-0.00000041	0.000001347	-0.000001721
6	0.000000881	-0.000000327	-0.000001834
6	-0.000001291	0.000000456	-0.000001035
6	0.000000541	-0.000001037	-0.000002027
1	0.00000026	-0.00000094	-0.000001895
1	0.00000009	-0.000000042	-0.000001159
1	0.000000158	-0.000000339	-0.000001278
6	-0.000000207	-0.000002494	-0.00000106
6	0.000000407	0.000000955	-0.000003421
6	-0.000000072	-0.000000376	-0.000002945
1	-0.000000274	-0.000001132	-0.000002277
1	0.000000734	0.000000065	-0.000002761
1	0.00000003	-0.000000565	-0.000002021
1	0.000000437	-0.000001008	-0.000002811
1	-0.000001046	-0.000002288	-0.000001827
1	-0.000001003	-0.000000789	-0.000002223
1	-0.000000017	-0.000000868	-0.000001779
6	0.000000718	0.000003086	-0.00000064
6	0.000001601	-0.000001192	-0.000000803
6	0.000001916	0.000001151	-0.000000678
1	-0.000000106	-0.000000044	-0.000001392
1	0.000000091	0.00000023	-0.000000529
1	0.000000559	0.000000717	0.000000177
1	0.00000023	0.000000555	-0.000000621
1	0.000001192	0.000001	-0.000001385
1	0.000000852	0.000000889	-0.000001306
1	0.000001125	0.000001696	-0.000001301
6	-0.000000253	-0.000004126	-0.000003669
6	-0.000000682	0.000001164	0.000002629
6	0.000000301	0.000002785	-0.000001475
1	0.000000543	-0.000000331	-0.000001988
1	-0.000000701	-0.000001326	-0.000000472
1	0.000000059	-0.000000543	-0.000001436
1	-0.000000434	-0.000000778	-0.000002149
1	0.000000254	-0.00000035	-0.000001812
1	0.00000037	-0.000000855	-0.000000987
1	0.000000298	-0.000000084	-0.000001582
6	0.000002917	-0.000000053	-0.000002122
6	0.000001957	0.000001977	0.000000887
6	0.000001736	0.00000205	-0.000000703



1	0.000001189	0.000002309	0.000000115
1	0.000001547	0.000001833	-0.000001794
1	0.000001262	0.000001638	-0.000000946
1	0.000001535	0.000001532	-0.000000438
1	-0.000000732	0.000000853	0.000000032
1	0.000000159	0.000001641	-0.000000069
1	0.000001119	0.000001883	-0.000000004
Zero-point correction=			1.134300 (Hartree/Particle)
Thermal correction to Energy=			1.204312
Thermal correction to Enthalpy=			1.205256
Thermal correction to Gibbs Free Energy=			1.017996
Sum of electronic and zero-point Energies=			-3625.279058
Sum of electronic and thermal Energies=			-3625.209046
Sum of electronic and thermal Enthalpies=			-3625.208102
Sum of electronic and thermal Free Energies=			-3625.395362

E-2

6	0.000002393	0.000006976	-0.00000191
6	0.000007172	-0.000002558	-0.000000022
7	-0.000002371	-0.000017177	0.000000972
7	-0.000009601	0.000004784	0.000012455
16	0.00000301	0.000007494	-0.00000421
8	0.000000192	0.000001703	0.000001444
8	-0.000002707	-0.000000395	-0.000000664
6	-0.000001013	-0.000001347	0.000002119
6	-0.000000609	0.000000349	-0.00000173
6	-0.000001561	0.000000364	0.000002411
6	-0.00000112	0.000000195	-0.000000339
6	-0.00000123	0.000000681	-0.000000429
6	-0.000001109	0.000001503	-0.000000606
1	-0.000001172	0.000000142	0.000000882
1	-0.000001341	0.000000619	0.000000081
1	-0.000001417	-0.000000099	-0.000000387
1	-0.000000738	-0.000000653	-0.000000256
6	-0.00000192	-0.000000165	0.000000272
1	-0.000001305	0.000001054	-0.000000034
1	-0.000002074	0.000001274	-0.000000114
1	-0.000001656	0.000000338	-0.000000115
6	0.000000658	0.000007682	0.000002033
1	-0.000000659	-0.000001132	-0.000000447
1	-0.000000963	0.000000098	-0.000000607
16	0.000004307	-0.000005219	-0.000006072
8	0.000003134	0.000004549	0.000002297
8	-0.000002435	0.000001017	0.000001133

6	0.000002633	0.000001881	0.000000503
6	-0.000001103	-0.000001725	0.000000606
6	-0.000001891	0.000000363	0.000000783
6	0.000000649	0.000000803	-0.00000009
1	0.00000017	0.000000839	-0.000000524
6	0.000000214	0.00000083	0.000001194
1	-0.000000064	0.00000091	0.000000266
6	-0.000001241	-0.000000048	0.000000109
1	-0.000000553	-0.000000354	-0.000000074
1	-0.000000487	0.000000745	0.000000561
6	0.000000347	0.000000169	-0.000000198
1	-0.000000401	0.000000205	-0.000000012
1	-0.000000781	0.000000204	0.000000212
1	-0.000000558	0.000000371	0.000000272
6	-0.000002418	-0.000000942	-0.000006169
6	-0.000001009	0.000001126	0.000001804
6	-0.000000374	0.000000741	0.000001682
1	-0.000001987	0.000001105	0.000000489
6	-0.00000107	0.00000123	-0.000000156
1	0.000000037	0.000000583	-0.000000182
1	-0.000000009	0.00000126	-0.000000169
6	-0.000002228	0.000000642	-0.000000708
1	-0.000000527	0.00000036	0.000000339
1	-0.000000862	0.000000653	0.000000207
6	-0.000000883	0.000000321	0.000001386
1	-0.000000737	0.000001926	0.00000129
1	-0.000000953	0.000000127	0.000000127
1	-0.000001074	0.000000771	0.000000518
1	-0.000001152	0.000000474	0.000000212
1	-0.000001611	0.000001593	0.000000424
1	-0.000001133	0.000001098	0.000000745
6	-0.000000463	-0.000001726	-0.000000629
6	-0.000000988	0.000000892	-0.000000959
6	-0.000000932	-0.000000249	-0.000000888
6	-0.00000179	0.000000439	-0.000001174
1	-0.000001521	0.000000097	-0.000000158
6	-0.000001922	-0.00000106	-0.000000659
1	-0.000000689	-0.000000679	-0.000000718
6	-0.000001229	-0.000000338	0.000000673
1	-0.000001566	-0.000000246	-0.000000356
1	-0.000001081	-0.000000162	-0.000000021
1	-0.000001721	-0.000000296	-0.000001095
79	0.000000028	-0.000004022	-0.000001591
6	-0.000008948	0.00000162	0.000001424

6	0.00000834	0.00001917	-0.00002836
6	-0.00000695	-0.00003264	0.00001287
1	0.00001474	-0.00001459	-0.00000026
1	0.00001481	-0.00000141	-0.00000568
7	0.00006947	0.00000433	0.00000813
7	0.00006862	-0.00000543	0.00001855
6	0.00000881	0.00000046	-0.00001466
6	-0.00001597	0.00001624	0.00001095
6	0.00003091	-0.00002039	0.00002089
6	0.00003245	-0.00000992	0.00001457
6	-0.00002111	-0.00000119	0.00001893
6	0.00001086	0.00002254	-0.00001207
1	0.00001591	-0.00000154	0.00000096
1	0.00002208	0.00000053	0.0000009
1	0.0000146	0.00000731	0.00001415
6	-0.0000071	0.00001862	-0.00000761
6	0.00001058	-0.00000977	0.00000691
6	0.00001253	-0.00002933	-0.00000382
6	0.0000033	-0.00001463	-0.00001775
6	-0.00000177	-0.00001326	-0.00001701
6	0.00000154	-0.00000317	-0.00001513
1	0.00000166	-0.00000741	-0.00000088
1	0.00000286	-0.00000142	-0.00001244
1	-0.00000272	-0.00001148	-0.00001516
6	-0.00002476	-0.00002191	-0.0000537
6	0.00003736	0.00000093	0.00000899
6	0.00000591	-0.00000177	0.00002643
1	0.00000943	-0.00000053	-0.00000164
1	0.00000301	-0.00001689	-0.00000652
1	0.00001253	-0.00000896	-0.00000588
1	0.00000209	-0.00001491	-0.00001186
1	-0.00000245	-0.00000611	-0.0000016
1	0.00000324	-0.00001389	-0.00000979
1	0.00000532	-0.00000823	-0.0000006
6	-0.00000015	-0.00001541	-0.00001514
6	0.00001239	-0.00000663	0.00000608
6	0.00000522	0.00000186	-0.00000805
1	-0.00000227	-0.00000393	-0.00001163
1	0.00000099	-0.00000147	-0.00000406
1	0.00000469	-0.00000059	-0.00000745
1	-0.00001365	-0.00001047	-0.00000066
1	0.00001352	-0.00001097	-0.00000183
1	0.00000869	-0.00001305	-0.00001212
1	0.00000898	-0.00000727	-0.00000238

6	0.000000365	0.000000265	0.000000033
6	0.000000227	0.000000408	0.000001306
6	0.000001999	0.000000489	-0.000000164
1	0.000001118	0.000000093	0.000000108
1	0.000000604	-0.000000525	0.000000132
1	0.000000799	-0.000000277	0.000000384
1	0.000000728	0.000000562	0.000000523
1	0.00000166	-0.00000015	0.000000368
1	0.000001175	-0.000000057	0.000000611
1	0.000001207	-0.000000082	0.000000558
6	0.000002098	-0.000000566	0.000000704
6	0.000001882	-0.000000123	0.000000713
6	0.000000391	-0.000000092	0.000000013
1	0.000000528	-0.000000076	0.000000402
1	0.0000017	-0.000000468	0.000000224
1	0.000001458	-0.000000263	0.000000209
1	0.000001439	-0.000000094	0.000000351
1	0.000000761	0.000000479	0.000000753
1	0.000000969	0.000000658	0.000000745
1	0.000001049	0.000000076	0.000000032

Zero-point correction= 1.134541 (Hartree/Particle)

Thermal correction to Energy= 1.204529

Thermal correction to Enthalpy= 1.205474

Thermal correction to Gibbs Free Energy= 1.017707

Sum of electronic and zero-point Energies= -3625.278676

Sum of electronic and thermal Energies= -3625.208688

Sum of electronic and thermal Enthalpies= -3625.207744

Sum of electronic and thermal Free Energies= -3625.395511

E-TS1a

6	-0.000001696	-0.000000243	0.000000953
6	0.000002127	-0.000002315	-0.000000357
7	0.00000006	0.000000228	-0.000000555
7	-0.000000119	0.000001353	-0.000000291
16	-0.000000181	-0.000000026	-0.000000207
8	-0.000000003	0.000000127	-0.000000017
8	-0.000000197	-0.000000142	-0.000000008
6	-0.00000053	0.000000648	-0.000000352
6	-0.00000015	0.00000052	-0.000001383
6	-0.00000007	0.000000141	-0.000001998
6	-0.000001373	0.000005448	-0.000000226
6	-0.000001415	-0.00000041	0.000001073
6	-0.000001218	0.000000099	0.000000606
1	-0.000000059	0.000000368	-0.000001032

1	-0.000000642	0.000000117	-0.000000788
1	-0.000000874	-0.000000059	-0.000000268
1	-0.000000459	0.000000224	0.000000001
6	-0.000000989	-0.0000003518	-0.000000092
1	-0.000000268	0.000000427	-0.0000002623
1	-0.000001705	0.000000077	-0.000000374
1	-0.000002003	-0.000000187	0.000000234
6	-0.000000217	-0.000000059	0.000000079
1	-0.000000287	-0.000000189	0.000000445
1	0.000000026	-0.000000272	0.000000426
16	0.000000254	0.000000191	0.000001485
8	0.000000528	-0.000000006	0.000000655
8	0.000000304	-0.000001025	0.000001405
6	0.000000026	-0.000000085	0.000000776
6	0.000000044	-0.000000678	0.000001021
6	-0.000000138	-0.000000307	0.000001483
6	-0.000001262	0.000001053	0.000001801
1	0.000000298	-0.000000286	0.000001048
6	0.000001549	-0.000001471	0.000000599
1	0.000000214	-0.000000465	0.000001621
6	-0.000002126	-0.000000368	0.000001606
1	0.000000615	-0.000000252	0.00000165
1	0.000000518	-0.000000411	0.000002152
6	0.000002136	0.000002774	0.00000038
1	0.000001379	-0.000000426	0.000002621
1	-0.000000723	0.000000605	0.000003066
1	0.00000222	-0.000001446	0.000002173
6	-0.000000886	-0.000000723	0.000001155
6	-0.00000024	-0.000000299	0.000000776
6	-0.000000184	-0.000000011	0.000001171
1	-0.000000776	-0.000000213	0.000000537
6	-0.000001076	0.000000103	0.000000829
1	-0.000000189	-0.000000137	0.000000663
1	-0.000000322	0.00000002	0.000000697
6	-0.000000823	-0.000000079	0.000001224
1	-0.000000343	-0.000000401	0.000001523
1	-0.000000707	-0.000000188	0.00000104
6	-0.000000669	0.000000027	0.000001586
1	-0.000000769	-0.000000134	0.000001329
1	-0.000000922	-0.000000052	0.000000964
1	-0.000000786	-0.000000104	0.000001402
1	-0.000000936	-0.000000002	0.000001154
1	-0.000000992	-0.000000011	0.000001515
1	-0.000000753	-0.000000015	0.000001506

6	-0.00000067	-0.00000055	0.00000049
6	-0.000000851	0.000000203	0.000000151
6	-0.000000405	0.000000011	0.000000783
6	-0.000000961	-0.000000164	0.000000737
1	-0.000000439	0.000000216	0.000000428
6	-0.000000853	0.000000087	0.000000393
1	-0.000000402	0.000000055	0.000000758
6	-0.00000104	0.000000013	0.000000539
1	-0.000001219	0.000000185	0.000000491
1	-0.000000922	0.000000082	0.000000081
1	-0.000001311	0.000000013	0.000000664
79	-0.000000105	-0.000000355	-0.00000106
6	0.000000275	-0.000000162	-0.000001049
6	0.000000678	0.000000109	-0.000000977
6	0.000000864	0.000000014	-0.000001057
1	0.000000099	0.000000147	-0.000001242
1	0.000000634	0.000000012	-0.000001171
7	0.000000237	-0.000000172	-0.000000487
7	0.000001141	0.000000418	-0.000001339
6	0.000000578	0.000000957	-0.000001065
6	0.000000426	0.000000099	-0.000000376
6	-0.000000594	-0.000000177	-0.000000766
6	-0.000000056	-0.000000151	-0.000000658
6	-0.000000273	0.000000465	-0.000000273
6	0.000000004	0.000000299	-0.000000734
1	-0.000000066	-0.000000079	0.000000001
1	-0.000000496	0.000000303	-0.000000071
1	-0.000000326	0.000000123	-0.000000337
6	0.000000378	-0.000000033	-0.000000586
6	0.000000895	0.000000087	-0.000000928
6	0.000001252	-0.000000187	-0.000000503
6	0.000000071	-0.000000001	-0.000000857
6	0.000001136	-0.000000176	-0.000000084
6	0.000001022	0.000000016	-0.000000765
1	0.000000646	0.000000015	-0.000000974
1	0.00000133	-0.000000292	-0.000000518
1	0.000001117	-0.000000083	-0.000000675
6	0.000000135	0.000000209	-0.000000944
6	0.000000613	0.000000266	-0.000001507
6	0.000000232	0.000000019	-0.000001368
1	0.000000221	0.000000021	-0.000001055
1	0.000000788	0.000000148	-0.000001602
1	0.000000447	0.000000309	-0.000001624
1	0.000000575	0.000000028	-0.000001512

1	0.00000019	0.000000192	-0.000000853
1	0.000000381	0.000000133	-0.000001417
1	-0.000000117	0.000000273	-0.000001457
6	0.000000864	-0.00000004	-0.000000439
6	0.000000763	-0.000000216	-0.000000176
6	0.000001305	0.000000074	-0.000000329
1	0.000001306	-0.000000182	-0.000000019
1	0.000000667	-0.000000248	0.000000395
1	0.000001136	-0.000000251	0.000000065
1	0.000001296	-0.000000211	0.000000052
1	0.000001308	-0.000000187	-0.000000655
1	0.00000162	-0.00000008	-0.000000414
1	0.000001476	-0.000000168	-0.000000285
6	-0.000000383	0.000000324	-0.000001007
6	-0.000000565	0.000000333	-0.000000998
6	-0.000000279	0.000000213	-0.000001414
1	0.000000132	0.000000165	-0.000001158
1	-0.000000435	0.00000029	-0.000000785
1	-0.000000624	0.00000038	-0.000001071
1	-0.000000639	0.000000318	-0.000000807
1	-0.000000026	0.000000344	-0.00000138
1	-0.000000299	0.000000328	-0.000001235
1	-0.000000313	0.000000344	-0.00000158
6	0.000000255	0.000000121	-0.000000201
6	0.000000841	-0.00000016	-0.000000509
6	0.000000626	-0.000000049	-0.000000031
1	0.000000716	-0.000000173	-0.000000249
1	0.000000894	-0.000000051	-0.000000738
1	0.000001056	-0.00000008	-0.000000367
1	0.000000672	-0.00000013	-0.000000366
1	0.000000248	-0.000000346	0.000000026
1	0.000000453	-0.000000145	-0.000000093
1	0.00000089	-0.000000001	0.000000119
6	0.000000374	0.000000234	0.000000874
6	-0.000000369	-0.000000292	0.000000717
6	-0.000000473	0.000000046	0.000000217
6	-0.00000072	0.000000246	0.000000029
6	-0.000000371	0.000000076	0.000000462
1	-0.000000779	-0.000000004	0.000000434
1	-0.000000109	0.000000062	0.000000019
7	-0.000000499	0.000000159	-0.000000167
8	0.00000018	0.000001108	0.000000974
1	-0.000000979	0.000000138	0.000000198
1	-0.000000268	-0.000000159	0.000000651

17	-0.0000008	0.000000048	-0.000000003
Zero-point correction=			1.218901 (Hartree/Particle)
Thermal correction to Energy=			1.295502
Thermal correction to Enthalpy=			1.296447
Thermal correction to Gibbs Free Energy=			1.095754
Sum of electronic and zero-point Energies=			-4408.200434
Sum of electronic and thermal Energies=			-4408.123833
Sum of electronic and thermal Enthalpies=			-4408.122889
Sum of electronic and thermal Free Energies=			-4408.323581

E-1a

6	-0.00003955	0.00001238	-0.00000879
6	0.00001145	-0.00002775	0.00000349
7	0.00001987	-0.0000068	0.00000886
7	-0.00001375	0.000009595	0.00000497
16	-0.00000612	0.00000228	-0.0000069
8	0.00000269	-0.00000594	-0.00000181
8	0.00000792	0.0000065	0.000002017
6	0.00001254	0.00000455	0.00000581
6	0.00000585	-0.00001305	-0.0000084
6	0.00000837	0.00000722	0.000002034
6	-0.00002614	-0.00002527	0.000001617
6	-0.00000041	0.00000385	-0.00000642
6	-0.00000005	0.00000771	0.000003449
1	-0.00000072	0.00000558	0.00000128
1	-0.00000105	-0.00000724	0.00000468
1	-0.00000216	-0.00000164	0.000001463
1	0.00000613	-0.00000559	0.000001146
6	-0.00000618	-0.00001161	0.00000977
1	-0.00001485	-0.00000392	0.00000122
1	-0.00000015	-0.00001554	0.000002211
1	0.00001172	0.00000427	0.00000626
6	-0.00001334	0.00000384	0.00000082
1	0.00000253	0.00000857	0.000000139
1	0.00000207	-0.00000992	0.000000034
16	0.000006726	-0.000006686	-0.000007263
8	0.000004784	0.00000143	0.000001941
8	-0.000007431	-0.00000221	0.000000419
6	-0.00001855	0.00000377	0.000001939
6	-0.00001463	0.000002501	0.000000463
6	-0.00000647	0.000001063	0.000000915
6	0.000002963	0.00000762	0.000002258
1	0.00001253	0.00000139	0.000000892
6	0.0000166	-0.00000893	-0.000000282



1	0.000001206	0.000000303	0.000001811
6	-0.000000795	0.000001648	0.000000378
1	0.00000116	0.000000597	0.000000368
1	0.000001126	0.000000098	0.000001916
6	0.000000454	0.000001742	0.000003304
1	0.000002428	0.000000572	0.000000682
1	0.000001225	0.000000061	0.000000512
1	0.000001196	0.000000874	0.000002111
6	0.000003248	-0.000001755	-0.000000267
6	-0.000001119	-0.000001545	-0.000002162
6	-0.000001986	-0.000002522	0.000000136
1	-0.000002999	0.000002033	0.000003553
6	0.000000096	0.000000821	0.000000928
1	0.000001165	-0.000001488	0.000001192
1	-0.000002194	-0.000001323	0.000001587
6	0.000000055	-0.000001428	-0.000000025
1	0.000001598	-0.000000348	0.000001552
1	0.00000023	-0.000000615	0.000000769
6	-0.000000585	-0.000000091	0.000001872
1	-0.000001667	-0.000001525	-0.000000251
1	-0.00000042	-0.000001495	0.000000762
1	-0.000000307	-0.000000494	0.000001787
1	-0.000000184	-0.000001235	0.000001895
1	-0.000000463	-0.000001395	0.000001387
1	-0.000000573	-0.000001268	0.000000095
6	-0.000005053	-0.000004406	0.000003907
6	-0.000000297	0.000000214	-0.000002788
6	0.000002778	0.000001689	0.000002455
6	0.000001601	0.000001701	0.000002841
1	0.000000059	-0.000000675	0.000001144
6	-0.000000026	-0.000001179	-0.000000713
1	0.00000007	-0.000000473	0.000001701
6	-0.00000237	-0.000002644	0.000003011
1	-0.000000959	-0.000001198	0.000000826
1	-0.000000049	-0.000000763	0.000002517
1	-0.000000367	-0.000000976	0.000001463
79	-0.000003817	-0.000000408	-0.000002377
6	0.000006156	-0.000004465	0.000003853
6	0.000000021	-0.000002696	0.000000824
6	0.000002762	0.000003174	-0.000003605
1	0.000000372	0.000000704	-0.000000551
1	-0.000000239	0.000000336	-0.000001467
7	-0.000001473	0.000000394	-0.000005545
7	-0.000001549	0.000005308	0.000000307

6	0.000001128	0.000000159	0.000000373
6	-0.00000145	0.000000892	-0.000002642
6	-0.000000504	0.000000078	-0.000000093
6	-0.000000938	0.000000974	-0.000001156
6	-0.000002332	-0.000001313	-0.000000231
6	0.000000046	-0.000000792	-0.000001469
1	-0.000000282	-0.000000589	-0.00000129
1	-0.000001036	-0.000000584	-0.000001429
1	-0.000001566	-0.000001044	-0.000001337
6	-0.000003556	-0.000001437	-0.00000193
6	0.000001441	0.000002865	-0.000001603
6	0.000001413	0.000000568	-0.000002755
6	0.000002016	0.000000444	-0.000001496
6	0.000000311	0.00000106	0.000000596
6	0.000000226	0.000001546	0.000001165
1	0.000001412	0.000000729	-0.000000457
1	0.000001868	0.00000126	-0.000000079
1	0.000001539	0.000001697	0.000000205
6	-0.000000564	0.000000023	-0.000000183
6	0.000000559	0.000000299	-0.000001637
6	0.000001212	0.000001878	0.000000143
1	0.000000807	-0.00000006	-0.000000055
1	0.00000044	0.000001515	-0.000000651
1	0.000000767	0.000000558	-0.000000561
1	0.000000535	0.000001156	-0.000000512
1	-0.000000417	-0.000000022	0.000000174
1	0.000000086	0.00000046	0.000000762
1	0.000000512	0.000000709	-0.000000105
6	-0.000000855	-0.000001784	-0.000001999
6	0.000002713	0.000003001	0.000000036
6	0.000001063	0.000002687	-0.000000528
1	0.000001082	0.000001003	0.000000084
1	0.000000617	0.00000073	-0.000000709
1	0.000000128	0.000000125	-0.000001199
1	0.000001123	0.000000672	-0.000000166
1	0.000000789	0.000001211	-0.00000162
1	0.000000951	0.000001206	-0.000000804
1	0.000000428	0.000001482	-0.000001405
6	-0.000000276	-0.000000778	-0.000001102
6	-0.000001033	-0.000002568	-0.000000469
6	-0.000001559	-0.000000201	-0.000001211
1	-0.000000172	0.000000392	-0.000000825
1	0.000000621	-0.000000325	-0.00000006
1	-0.000000076	0.000000173	-0.000000425

1	-0.000000849	-0.000000181	-0.000000841
1	-0.000000447	-0.000000071	-0.000001563
1	-0.000000837	-0.000000503	-0.000001038
1	-0.000000682	-0.000000041	-0.00000107
6	0.00000148	0.00000032	-0.00000113
6	-0.000001307	-0.000001156	-0.000001569
6	-0.000001318	0.000000705	0.00000036
1	0.00000014	0.000001024	-0.000001117
1	-0.00000037	0.00000076	-0.000002083
1	-0.000000153	0.00000006	-0.000001964
1	-0.000000547	0.000000641	-0.000002502
1	0.000000149	0.000000478	-0.000001053
1	-0.00000067	-0.000000134	-0.000001724
1	-0.000000422	0.000000271	-0.000002142
6	0.000000056	-0.000000533	0.000001343
6	-0.000000288	-0.000000114	-0.000002034
6	-0.000000392	-0.000001705	-0.000000889
6	-0.000001131	0.000000975	-0.000001232
6	0.000000152	-0.000003791	0.000002885
1	-0.000001525	-0.000001359	-0.00000069
1	-0.000000996	0.000000601	0.000001075
7	-0.000002928	-0.000000189	-0.000004314
8	0.000003572	-0.000001262	0.000000315
1	-0.000000911	-0.000000255	-0.000000952
1	-0.000000655	-0.000000381	-0.000000907
17	-0.000001683	-0.000000321	0.000000436

Zero-point correction=

1.221580 (Hartree/Particle)

Thermal correction to Energy=

1.297773

Thermal correction to Enthalpy=

1.298717

Thermal correction to Gibbs Free Energy=

1.100082

Sum of electronic and zero-point Energies=

-4408.207202

Sum of electronic and thermal Energies=

-4408.131009

Sum of electronic and thermal Enthalpies=

-4408.130065

Sum of electronic and thermal Free Energies=

-4408.328700

E-TS1b

6	0.00000034	-0.000001202	-0.000000066
6	0.000002195	0.000001232	0.000000324
7	0.000001237	0.000001228	0.000000919
7	-0.000001645	-0.000000587	-0.000000935
16	0.000000817	0.000001282	-0.000000335
8	0.000001114	0.000001977	0.000000198
8	0.00000111	0.000002065	-0.000001026
6	0.000001046	0.000001339	-0.000000059

6	0.00000827	0.00000466	-0.0000062
6	0.00001478	0.00000428	-0.00000329
6	0.00001997	0.00002145	-0.00000251
6	0.0000236	0.0000171	-0.00000682
6	0.00001952	0.00001486	-0.00000412
1	0.00000828	0.00000441	-0.00000226
1	0.00001542	0.00000494	-0.00000219
1	0.00002755	0.00002255	-0.00000884
1	0.00002072	0.00002234	-0.00000877
6	0.00002923	0.00001376	-0.00000748
1	0.00002847	0.0000113	-0.0000054
1	0.00002033	0.00001245	-0.00000847
1	0.00002351	0.00000485	-0.00000633
6	0.00002302	0.00001047	-0.000008
1	0.00002252	0.00001136	-0.00000388
1	0.00002052	0.00000551	-0.00000425
16	0.0000066	-0.00001789	-0.00000115
8	-0.00000267	-0.00001858	0.00000987
8	0.00000154	-0.00001102	0.0000016
6	0.00000906	-0.00002583	0.00000321
6	0.00000673	-0.00002089	-0.0000061
6	0.00000802	-0.00002893	0.00000803
6	0.00002308	-0.00003283	0.00000928
1	0.00000546	-0.00002404	0.00000595
6	0.00000642	-0.0000338	0.00000782
1	0.00001486	-0.00001902	0.00000539
6	0.00000338	-0.00002447	-0.00001324
1	0.00001049	-0.00003894	0.00001067
1	0.00001918	-0.00003125	0.00000735
6	0.00002941	-0.00005339	0.00002773
1	0.00002448	-0.00004495	0.00000883
1	0.00001718	-0.0000435	0.00001119
1	0.00001696	-0.00004568	0.00001058
6	0.00000674	-0.00000677	0.0000021
6	0.0000032	-0.00001382	0.00000426
6	-0.00000093	-0.00000518	-0.00000097
1	0.00000861	-0.00000444	-0.00000084
6	0.00000593	-0.00001274	0.00000316
1	0.00000057	-0.00002271	0.00000258
1	0.00001169	-0.00001613	0.00000224
6	-0.00000237	0.00000216	0.00000154
1	-0.00000646	-0.00000538	0.00000259
1	-0.0000034	0.00000229	0.00000099
6	-0.00000083	-0.0000116	0.00000278

1	0.00000695	-0.00001838	0.00000415
1	0.00001203	-0.00000977	0.00000091
1	-0.00001107	-0.00000442	0.00000033
1	0.00000301	0.00000119	-0.00000008
1	-0.00000112	-0.00000815	0.000000178
1	-0.00000665	-0.00001274	0.000000364
6	0.00002618	-0.00000075	-0.00000018
6	0.00001882	-0.00000361	-0.000000223
6	0.00003128	-0.00000011	-0.000000205
6	0.00002236	-0.00000896	-0.000000324
1	0.0000155	-0.00000528	0.00000023
6	0.00003568	-0.00000642	-0.000000167
1	0.00003423	0.00000032	-0.000000489
6	0.00003231	-0.00001268	0.000000007
1	0.00002166	-0.00001417	0.000000185
1	0.00004123	-0.0000007	-0.000000285
1	0.00003461	-0.00001585	-0.000000037
79	-0.00001168	0.00000733	-0.00001867
6	-0.00001357	0.00000934	0.000000318
6	-0.00002734	0.00000836	0.000000073
6	-0.00002518	0.00001448	-0.000000012
1	-0.00002959	0.00001949	-0.000000153
1	-0.00003287	0.00000603	0.000000217
7	-0.00001915	0.00000409	0.000000686
7	-0.00001842	0.00001186	-0.000000154
6	-0.00002182	-0.00000026	0.000000089
6	-0.00002313	-0.00000933	0.000000446
6	-0.00002011	-0.00000723	0.000000356
6	-0.00002185	-0.00001612	0.000000727
6	-0.000019	-0.00001299	0.000000686
6	-0.00002184	-0.00001788	0.000000627
1	-0.00002422	-0.00001956	0.000000754
1	-0.00001645	-0.00001443	0.00000051
1	-0.00002082	-0.00002343	0.00000083
6	-0.00001809	0.00001983	-0.000000374
6	-0.00000906	0.00002681	-0.000000742
6	-0.00001648	0.00002186	-0.000000368
6	-0.00001028	0.00003554	-0.000000713
6	-0.00001228	0.00002842	-0.000000657
6	-0.00000809	0.00003374	-0.000000661
1	-0.00000773	0.00003676	-0.000000904
1	-0.00001132	0.00002969	-0.000000658
1	-0.00000687	0.00003848	-0.000000912
6	-0.00001207	0.00002389	-0.000000417

6	-0.000002052	0.000002691	-0.000000476
6	-0.000000958	0.00000277	-0.000000656
1	-0.000001611	0.000002105	-0.000000215
1	-0.000002558	0.000002478	-0.000000369
1	-0.000002151	0.000002767	-0.000000407
1	-0.000002265	0.000003471	-0.00000062
1	-0.00000044	0.000002728	-0.000000465
1	-0.000000794	0.000003295	-0.000000915
1	-0.000000613	0.000002858	-0.00000057
6	-0.000001719	0.000001786	-0.00000018
6	-0.000001133	0.000001636	-0.000000029
6	-0.000002596	0.000001783	-0.000000138
1	-0.000001719	0.00000114	0.000000052
1	-0.000000589	0.000001455	-0.000000451
1	-0.000001419	0.000001319	-0.000000133
1	-0.000001201	0.000001985	-0.00000039
1	-0.000002994	0.000001893	-0.000000106
1	-0.000002537	0.000002548	-0.000000396
1	-0.000002797	0.000001513	-0.000000084
6	-0.000001431	-0.000000015	0.000000212
6	-0.000000942	-0.000000011	0.000000204
6	-0.000002185	0.000000306	0.0000001
1	-0.000001595	0.000000478	-0.000000003
1	-0.000000456	-0.000000112	-0.000000002
1	-0.000000669	0.000000346	-0.000000003
1	-0.000000845	-0.000000611	0.000000248
1	-0.000002709	0.000000393	0.000000178
1	-0.000002336	-0.000000363	0.000000456
1	-0.000002036	0.000000615	0.000000078
6	-0.000002307	-0.000000557	0.000000799
6	-0.000003439	-0.000000615	0.000000665
6	-0.000002404	-0.000001211	0.000000444
1	-0.000002547	-0.000000103	0.000000134
1	-0.000003698	-0.000000289	0.000000568
1	-0.000003574	-0.00000053	0.000000573
1	-0.000003645	-0.000001229	0.000000637
1	-0.000001724	-0.000001345	0.000000723
1	-0.000002469	-0.000001719	0.000000696
1	-0.000002401	-0.000001089	0.000000551
6	0.000001803	-0.000001271	0.000000159
6	0.000002831	-0.000001551	0.000000135
6	0.000002977	-0.000001794	-0.00000001
6	0.000002807	-0.000001106	0.000000019
6	0.00000273	-0.000000924	0.000000000

1	0.000003369	-0.000002239	0.000000191
1	0.000001962	-0.000000906	0.000000037
7	0.000001507	-0.000000876	-0.000000248
8	0.000002218	0.000001406	-0.000000067
1	0.000003217	-0.000001078	-0.000000115
1	0.000002709	-0.000002284	0.000000278
17	0.000002581	0.000000184	-0.000000343
Zero-point correction=			1.220037 (Hartree/Particle)
Thermal correction to Energy=			1.296027
Thermal correction to Enthalpy=			1.296971
Thermal correction to Gibbs Free Energy=			1.099294
Sum of electronic and zero-point Energies=			-4408.199278
Sum of electronic and thermal Energies=			-4408.123288
Sum of electronic and thermal Enthalpies=			-4408.122344
Sum of electronic and thermal Free Energies=			-4408.320021

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6	-0.000151581	-0.000137885	0.000016026
6	0.000118624	0.000088276	0.000020144
7	0.000132959	0.000028897	-0.000066953
7	0.000041987	0.000051991	0.000138898
16	-0.000089461	0.000071478	0.000071554
8	-0.000011114	-0.000051818	-0.000049154
8	0.000025079	-0.00004326	-0.000018193
6	0.000024742	0.000019636	0.000010896
6	-0.000026313	-0.000008038	-0.000003555
6	-0.000002308	-0.000005731	0.000006552
6	0.000003069	-0.000000851	-0.000010084
6	0.000013964	-0.000001254	0.000001975
6	-0.000001543	-0.000012274	0.00001223
1	-0.000013947	0.000007667	0.000000079
1	-0.000027045	0.000000641	-0.000015451
1	-0.000002554	0.000004626	-0.000000512
1	0.000004152	0.000012758	-0.000006792
6	-0.000003658	0.000001534	-0.000002274
1	-0.000004692	-0.000001416	0.000000995
1	-0.00001082	0.000000246	-0.000008631
1	0.000004853	0.000010197	-0.000002742
6	0.000039571	-0.000024023	-0.000027229
1	-0.000000733	0.000014311	0.000037216
1	-0.000008796	0.000006549	-0.000048496
16	0.000059186	0.000011925	-0.000078715
8	-0.0000442	0.00000624	0.000025365
8	0.000000795	0.000003939	0.000035443

6	-0.000058605	0.000018406	-0.000006192
6	0.000026928	-0.000031205	0.000023342
6	0.000039907	-0.000017677	0.000015525
6	-0.0000031	0.000008763	0.000009498
1	-0.000009193	0.000001027	0.00000138
6	-0.000017174	0.000021657	-0.000000856
1	-0.000010318	0.000011469	-0.000012901
6	0.000005855	-0.00001286	-0.000002892
1	-0.000001114	-0.000000027	-0.000001358
1	0.000004315	-0.000002534	0.000001561
6	0.000000344	0.00000367	0.000006316
1	-0.000003901	0.00000045	-0.000001527
1	-0.000001447	-0.000002154	0.000000328
1	0.000001946	0.000001527	-0.000001583
6	-0.000002729	-0.000024225	-0.00004861
6	0.000014277	0.000027048	0.000007003
6	-0.000012166	-0.000038609	0.000021071
1	0.000001774	0.000019754	0.000014838
6	-0.000003138	-0.000030164	0.000013497
1	-0.000010861	-0.000008067	-0.000017131
1	0.000007341	-0.000001749	0.000000734
6	-0.000048786	0.000021152	0.000003995
1	0.000008401	-0.000003764	0.000014508
1	-0.000010327	0.000004892	0.000012107
6	0.000010942	0.000000724	-0.000040306
1	-0.000001541	0.000001189	-0.000005122
1	0.000000878	0.000005406	0.000003246
1	0.000017719	0.0000112	0.000015165
1	0.000010539	-0.000008961	-0.000002193
1	0.000008313	-0.000007382	0.000004443
1	0.000000159	0.000001918	0.000010098
6	-0.000089047	-0.000054008	-0.000016539
6	0.000036439	0.000033644	0.000029504
6	0.000009384	0.000030693	-0.000025161
6	0.000020089	0.000020486	-0.000017862
1	0.000010044	-0.000027811	-0.00002864
6	0.000016106	-0.00000662	0.000034839
1	0.000007448	0.000000635	0.000000015
6	-0.000025614	-0.000015628	-0.000017453
1	-0.000001794	0.000008707	0.000001577
1	-0.000002131	-0.00000092	-0.000000507
1	-0.000004095	0.000000549	0.000004292
79	0.00011514	-0.000045182	-0.000049005
6	-0.000074683	-0.000014646	0.000055387



6	0.00000103	-0.000012842	-0.000002187
6	-0.000029121	0.000017881	-0.000036373
1	-0.00001085	0.000011461	0.000004192
1	0.000005836	-0.000001769	-0.000015452
7	-0.000038582	0.000067091	0.000061
7	0.000022276	0.000004849	-0.000007437
6	0.000018988	0.000007865	-0.00006542
6	0.000001791	-0.000013608	-0.000042073
6	-0.0000268	0.000005088	0.000074447
6	-0.000028999	-0.000034809	0.000045369
6	0.000010666	0.000025447	0.000018288
6	0.000041604	0.000007437	-0.000046088
1	0.000010782	0.000001059	0.000004947
1	-0.000002585	0.000007654	0.000002905
1	-0.000012229	-0.000004321	-0.000007924
6	-0.000057211	0.000066288	0.000048211
6	0.000030089	-0.000052497	-0.000013057
6	-0.000013307	-0.000008861	-0.000022228
6	0.000023628	0.000003191	0.000052485
6	-0.000014225	0.000010338	0.000011364
6	0.000031377	-0.000032055	-0.000035155
1	-0.000009919	-0.000005413	-0.000006907
1	0.000009508	0.000008388	-0.000014673
1	0.000009325	0.000000667	-0.000002519
6	0.000008078	0.000022177	-0.000009302
6	-0.000008276	-0.00003739	-0.000009567
6	-0.000007684	0.000009659	-0.000024464
1	-0.000008883	-0.000001267	-0.000006737
1	0.000022982	0.000006555	0.000005499
1	-0.000002783	0.000000883	-0.000001144
1	0.000002803	0.000001364	0.000001744
1	0.00001328	0.000016091	0.000033671
1	0.000012194	-0.00000961	-0.000016463
1	0.000004339	0.000015879	0.000005527
6	0.00004705	0.000013828	-0.000000226
6	0.000008383	-0.000027112	-0.000028937
6	-0.000025279	-0.000018428	0.000011809
1	-0.000004107	0.000003572	-0.000024348
1	-0.000011913	0.000019762	0.000001861
1	-0.000007184	0.000000343	0.000017202
1	-0.000000486	0.000012702	-0.000007875
1	0.000015978	0.000011265	0.000000033
1	0.000005616	-0.000002425	-0.000009193
1	-0.000001849	-0.000002459	0.000003637

6	-0.000052307	0.000001764	-0.000051641
6	0.000004135	-0.000000199	0.00000896
6	-0.000007637	-0.000036945	0.000033345
1	0.000018051	-0.000001463	0.00003393
1	0.00000603	-0.000007166	0.000020264
1	0.00001796	-0.000006473	-0.0000099
1	0.000004386	-0.000003407	-0.00001201
1	0.000013805	-0.000002557	-0.000012132
1	0.000009866	0.000016073	0.000003348
1	-0.00000417	-0.000000638	0.000002759
6	-0.000016634	-0.000041934	0.000025934
6	0.00000868	0.00001945	-0.000004896
6	0.000048019	0.000000576	-0.000010482
1	0.000011326	-0.00000886	0.000013125
1	0.00000883	-0.000020056	-0.000005447
1	-0.000000798	-0.000003905	0.000000156
1	-0.000004728	0.000003645	0.000010904
1	-0.000016094	0.000012407	-0.000001854
1	-0.000006793	-0.000000122	0.000015593
1	0.000001098	0.000000285	0.000016797
6	-0.000016946	0.000033566	-0.000030837
6	-0.00002693	0.000002592	0.000022163
6	-0.000000197	-0.000014804	-0.000009986
6	0.000014186	0.000022075	0.000000488
6	-0.000041326	-0.0000411	-0.000029282
1	0.000001184	-0.000005094	-0.000003284
1	0.000022394	-0.000018317	-0.000050388
7	0.000069285	-0.000035358	0.000099926
8	-0.000183935	0.000044693	-0.000071715
1	-0.000000707	0.000000302	-0.000003165
1	0.000019504	-0.000002888	-0.000001249
17	0.00001239	0.00002481	0.000005108

Zero-point correction=

1.221162 (Hartree/Particle)

Thermal correction to Energy=

1.297491

Thermal correction to Enthalpy=

1.298435

Thermal correction to Gibbs Free Energy=

1.098671

Sum of electronic and zero-point Energies=

-4408.214268

Sum of electronic and thermal Energies=

-4408.137940

Sum of electronic and thermal Enthalpies=

-4408.136996

Sum of electronic and thermal Free Energies=

-4408.336760

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6	-0.00000094	-0.00000026	0.000000012
6	0.000000357	-0.000000719	-0.000000774

7	-0.000000295	-0.000000702	-0.00000171
7	0.000000327	-0.000000442	0.00000027
16	-0.000000709	-0.000002599	-0.000001777
8	-0.000000741	-0.000001197	-0.000002037
8	0.000000177	-0.000001438	-0.00000233
6	0.000000059	-0.000001534	-0.000001653
6	0.000000627	-0.000001717	-0.000001275
6	0.000000881	-0.00000185	-0.000001366
6	0.00000129	-0.000002347	-0.000001265
6	0.000001555	-0.000001901	-0.000001682
6	0.000001053	-0.000002166	-0.00000191
1	-0.000000235	-0.000001165	-0.000001714
1	0.000000682	-0.000001208	-0.000001189
1	0.000001813	-0.000002314	-0.000001964
1	0.00000111	-0.00000211	-0.00000215
6	0.000001634	-0.000001795	-0.000001909
1	0.00000209	-0.000001471	-0.000001274
1	0.000002366	-0.000001939	-0.000000247
1	0.000002301	-0.000002163	-0.000002877
6	-0.000000059	-0.000001197	-0.000001598
1	-0.000000866	-0.000000587	-0.000001015
1	-0.000000237	-0.000001127	-0.000001477
16	0.000000389	-0.000000076	-0.000000282
8	-0.000000051	-0.00000008	-0.000000055
8	0.000000782	0.000000497	0.000000828
6	0.000001662	-0.000000722	0.000000046
6	0.000000516	-0.000001642	0.000000006
6	0.000001825	0.000001339	0.000001071
6	0.000001206	-0.000000104	-0.000000006
1	0.000000687	-0.000000989	-0.000000089
6	0.000001612	-0.000000639	0.000000997
1	0.000001765	0.000000264	0.000000827
6	0.000003377	-0.000001447	-0.000001385
1	0.000001156	-0.00000111	-0.000001139
1	0.000002279	-0.000000058	0.000000713
6	0.000002147	-0.000000894	-0.000001301
1	0.000001592	-0.000000809	0.000000619
1	0.000002773	-0.000001152	-0.000000068
1	0.000003141	-0.000000566	0.000000937
6	0.000001477	-0.000000556	-0.000000047
6	0.000001405	-0.000000157	0.000000894
6	0.000001358	-0.000001333	-0.000000756
1	0.000000087	-0.000000098	-0.000000037
6	0.000002655	-0.000000373	0.000000678

1	0.000001662	-0.000000021	0.000000624
1	0.000001578	0.000000253	0.000000494
6	0.000002707	-0.000001196	-0.000000962
1	0.000001975	-0.000000934	-0.000000495
1	0.000001506	-0.000001335	-0.000000957
6	0.000002741	-0.000000919	0.000000043
1	0.000002706	-0.000000258	0.000000686
1	0.00000219	-0.000000568	0.000000205
1	0.000002752	-0.000001556	-0.000000692
1	0.000002312	-0.000001452	-0.000000765
1	0.000003191	-0.000001092	0.000000047
1	0.000002983	-0.00000082	0.000000244
6	-0.000001447	-0.0000008	-0.000001456
6	-0.000002004	-0.000000561	-0.000001433
6	-0.000001601	-0.000001309	-0.000002201
6	-0.000002477	-0.000000507	-0.000001523
1	-0.000001556	0.000000019	-0.000000839
6	-0.000002416	-0.000001239	-0.00000237
1	-0.000001383	-0.00000164	-0.000002404
6	-0.000002891	-0.000000802	-0.000001984
1	-0.000002845	-0.000000057	-0.000001209
1	-0.000002655	-0.000001547	-0.000002744
1	-0.000003346	-0.000000756	-0.000002159
79	-0.000000425	0.00000005	0.000000149
6	-0.000000443	0.000001323	0.000001066
6	-0.000000096	0.000001524	0.000001597
6	-0.000000818	0.000001808	0.000001617
1	-0.000001214	0.000001961	0.000001778
1	0.000000152	0.000001618	0.000001908
7	0.000000197	0.000000886	0.000001092
7	-0.000000625	0.000001222	0.000001234
6	0.000000837	0.000001206	0.000001095
6	0.00000143	0.000000901	0.000001735
6	0.000000945	0.000000431	0.000000626
6	0.000002013	0.00000071	0.000001427
6	0.00000166	0.000000206	0.000001216
6	0.000002136	0.000000569	0.000001226
1	0.000002392	0.000000756	0.000001967
1	0.000001904	-0.000000073	0.000000717
1	0.000002749	0.000000207	0.000001345
6	-0.000001946	0.000001299	0.000000057
6	-0.000002072	0.000001341	0.000000705
6	-0.000001611	0.000001536	0.000000955
6	-0.000002444	0.000001323	0.000000433

6	-0.000002211	0.000001671	0.000001033
6	-0.000002895	0.000001516	0.000000505
1	-0.000003003	0.000001147	0.000000098
1	-0.000002476	0.000001704	0.00000109
1	-0.000003378	0.000001486	0.000000399
6	-0.000001966	0.000000966	0.000000359
6	-0.000002477	0.000001289	0.000000577
6	-0.000001861	0.000000424	-0.000000345
1	-0.000001298	0.000001002	0.000000591
1	-0.000002403	0.000001618	0.000000888
1	-0.000002278	0.000001118	0.000000376
1	-0.000002971	0.000001199	0.000000271
1	-0.000001627	0.000000011	-0.000000411
1	-0.000002519	0.000000358	-0.000000494
1	-0.000001809	0.000000291	-0.000000415
6	-0.000001222	0.00000159	0.000001576
6	-0.000001002	0.000001449	0.000001223
6	-0.000001456	0.000002277	0.000002087
1	-0.000000569	0.000001577	0.000001462
1	-0.000000982	0.000001123	0.000000844
1	-0.000000662	0.000001546	0.000001468
1	-0.000001469	0.000001553	0.000001196
1	-0.000001472	0.000002505	0.000002199
1	-0.000001875	0.000002354	0.000001999
1	-0.000000975	0.000002362	0.000002273
6	0.000000517	0.000000251	0.000000471
6	0.00000059	-0.000000307	-0.000000231
6	0.000000546	0.000000473	0.000000822
1	-0.00000007	0.00000029	0.000000714
1	0.000000461	0.000000002	0.000000164
1	0.000000094	-0.000000263	-0.000000455
1	0.000000916	-0.000000658	0.000000004
1	0.0000005	0.000000828	0.000001128
1	0.000001	0.000000285	0.000000693
1	0.000000167	0.000000407	0.000000452
6	0.000001278	0.000001244	0.000001948
6	0.000001408	0.000001803	0.000002621
6	0.000001474	0.000001247	0.00000189
1	0.000000529	0.000001546	0.000002112
1	0.000001123	0.000002026	0.000002554
1	0.000001232	0.000002174	0.000002945
1	0.00000189	0.000001672	0.00000275
1	0.000001278	0.000000957	0.000001635
1	0.000001851	0.000001123	0.000001908

1	0.00000142	0.000001451	0.000002171
6	-0.000002125	-0.000000781	-0.000001591
6	-0.000002614	-0.000000724	-0.000001667
6	-0.0000029	-0.000000525	-0.000001674
6	-0.000002765	-0.000000143	-0.000001354
6	-0.000002269	-0.000000042	-0.000000969
1	-0.000003553	-0.000000493	-0.00000195
1	-0.000001491	-0.000000638	-0.00000155
7	-0.000001475	-0.000000262	-0.000000669
8	-0.000001085	-0.000000597	-0.00000099
1	-0.0000031	0.000000108	-0.000001186
1	-0.000002772	-0.000001004	-0.000002269
17	-0.000001936	0.000000244	-0.000000241
<b>Zero-point correction=</b>			<b>1.219324 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>1.295787</b>
<b>Thermal correction to Enthalpy=</b>			<b>1.296731</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>1.098116</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-4408.199496</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-4408.123033</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-4408.122089</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-4408.320704</b>

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6	-0.000001103	-0.000000001	-0.000000792
6	0.000000949	-0.000000068	0.000000605
7	-0.000000104	-0.000000075	0.000000087
7	0.000000699	0.000001355	0.000000185
16	0.000000964	0.000000997	-0.00000246
8	0.000000079	0.000001417	-0.00000003
8	-0.000000854	0.000001505	-0.000000244
6	-0.000000225	0.00000287	0.000001402
6	0.000000083	0.000002305	0.00000014
6	0.000001022	0.000002184	0.000001255
6	-0.000000407	0.000001401	0.000001083
6	0.000000278	0.000001863	-0.000000507
6	0.000000812	0.00000124	0.00000058
1	0.000000471	0.000001893	0.000000328
1	0.000000892	0.000001897	0.000000672
1	0.000000707	0.000001997	0.000000111
1	0.000000219	0.000001816	-0.000000288
6	0.000000814	0.000003093	0.000002458
1	0.000001501	0.000002009	0.000000505
1	0.000001524	0.000002382	0.000001787
1	0.000000189	0.000002875	0.000001155

6	-0.00000062	-0.00000079	-0.000000499
1	0.000000135	0.000000493	-0.000000214
1	-0.000000305	0.000000958	-0.000000128
16	0.00000068	0.000000876	0.00000035
8	0.000000525	-0.000001252	-0.00000116
8	0.000000094	-0.000001153	-0.00000031
6	-0.000000003	-0.000000192	0.000000923
6	0.000000214	-0.000000396	0.000000767
6	0.000000362	-0.000000671	0.000000816
6	0.000000428	0.000000081	0.000000489
1	0.000000324	-0.000000063	0.000000388
6	0.000000641	-0.000000721	0.000001827
1	0.000000633	-0.000000832	0.000001314
6	0.000000706	-0.000000285	0.000000619
1	0.000000362	-0.000000082	0.000000731
1	0.000000733	-0.000000086	0.000001712
6	0.000000828	-0.000000359	0.000001625
1	0.000000496	-0.000000787	0.00000149
1	0.000000774	-0.000000162	0.000001425
1	0.000000894	-0.000000682	0.000001635
6	-0.000000033	0.000000851	0.000001218
6	0.000000512	0.000000036	0.00000117
6	0.000000457	0.000000627	0.000000894
1	0.000000271	0.000000559	0.000000737
6	0.000000678	0.000000801	0.000000817
1	0.000000662	-0.000000321	0.000001173
1	0.000000465	0.000000141	0.000000719
6	0.000000939	0.000001193	0.000000977
1	0.000000557	0.000000402	0.000000922
1	0.000000714	0.000000834	0.000000423
6	0.000001002	0.000000537	0.000001785
1	0.000000485	0.000000013	0.000001567
1	0.000000686	0.000000573	0.000001225
1	0.000000871	0.000000948	0.000001358
1	0.000000099	0.000001385	0.000001956
1	0.000001091	0.000000906	0.00000181
1	0.000001065	0.000000252	0.0000017
6	0.000000032	0.000000515	-0.000001059
6	-0.000000668	-0.000000093	-0.000000628
6	-0.000000037	0.000001318	-0.000001341
6	-0.000000064	0.000000219	-0.000001337
1	-0.000000781	0.000000091	-0.000000527
6	-0.000001043	0.000000409	-0.000001444
1	-0.000000728	0.000001459	-0.000001017

6	-0.000000746	0.000000231	-0.000001783
1	-0.000000783	-0.000000455	-0.00000126
1	-0.000000915	0.000001068	-0.00000166
1	-0.000001076	0.000000236	-0.000001729
79	-0.000001023	-0.000001277	0.000000634
6	-0.000000137	-0.000000067	0.000000592
6	0.000000173	-0.000001171	0.000000219
6	-0.000000818	-0.000001026	-0.000000047
1	-0.000000441	-0.000001361	-0.000000648
1	0.000000095	-0.00000126	-0.000000009
7	0.000000262	-0.000000541	0.000000272
7	-0.000000083	-0.000000623	-0.000001632
6	-0.00000032	-0.000000621	0.000000159
6	0.000000201	-0.000000734	0.000001214
6	0.000000239	0.00000029	0.000000245
6	0.00000067	-0.000000435	0.000000967
6	0.000000991	-0.000000145	0.00000091
6	0.000000628	-0.000000052	0.000001082
1	0.00000089	-0.000000591	0.000001506
1	0.000000496	0.000000435	0.000000989
1	0.000000982	0.000000096	0.000001582
6	-0.00000157	-0.000001055	-0.000001213
6	0.000000309	-0.000000552	-0.000000914
6	-0.000000029	-0.000001892	-0.000000371
6	-0.000001221	-0.000001133	-0.000001297
6	-0.000000857	-0.000000819	-0.000001356
6	-0.000001269	-0.000001397	-0.000002077
1	-0.000001231	-0.000000691	-0.000001921
1	-0.000000856	-0.00000166	-0.000001161
1	-0.000001111	-0.000001387	-0.000001873
6	-0.000000738	-0.000000595	-0.000001153
6	-0.000000897	-0.00000046	-0.000001481
6	-0.000000986	0.000000285	-0.000001587
1	-0.000000432	-0.000000627	-0.000000891
1	-0.000000893	-0.000000977	-0.000001523
1	-0.000000929	-0.000000352	-0.000001533
1	-0.00000102	-0.000000686	-0.000002042
1	-0.000000742	0.000000057	-0.000001143
1	-0.000000822	0.000000107	-0.000001561
1	-0.00000078	0.000000243	-0.000001407
6	-0.000000324	-0.000001341	-0.000000901
6	-0.000000301	-0.000002034	-0.000000162
6	-0.000000355	-0.000002405	-0.000000274
1	-0.00000014	-0.000001496	-0.000000107



1	-0.0000004	-0.000001313	-0.000000319
1	-0.000000223	-0.000001691	0.000000036
1	-0.000000495	-0.00000194	-0.000000777
1	-0.000000584	-0.000002182	-0.000000524
1	-0.000000525	-0.000002268	-0.000000703
1	-0.000000303	-0.000002439	-0.000000195
6	0.000000237	0.000000289	0.000000286
6	0.000000025	0.000000755	0.000000036
6	0.000000079	0.000000315	-0.000000026
1	-0.000000182	-0.000000163	-0.000000536
1	0.000000213	0.000000498	0.000000032
1	0.000000031	0.000000959	-0.000000222
1	0.000000114	0.00000085	0.000000208
1	0.000000088	-0.000000074	0.000000125
1	-0.000000031	0.000000582	0.000000472
1	0.000000059	0.000000411	-0.000000019
6	0.000000652	-0.000001174	0.000000789
6	0.000000479	-0.00000181	0.000001302
6	0.000000252	-0.000001243	0.000001168
1	0.000000112	-0.000001428	0.000000527
1	0.000000485	-0.000001664	0.000000889
1	0.000000417	-0.000001971	0.00000108
1	0.000000544	-0.000001507	0.000001249
1	0.000000596	-0.000001099	0.00000098
1	0.000000816	-0.000001388	0.000001656
1	0.000000499	-0.000001687	0.000001156
6	-0.000000723	0.000001268	-0.000000556
6	-0.000000599	0.000001554	-0.000001614
6	-0.000001155	0.000000842	-0.000001975
6	-0.000000582	0.000000234	-0.000001908
6	-0.000001298	0.000000404	-0.000000866
1	-0.000001103	0.000000921	-0.000002136
1	-0.000000282	0.000001438	-0.000001471
7	-0.00000062	0.000000637	-0.000001391
8	-0.00000119	0.000001314	-0.000001223
1	-0.00000095	0.000000014	-0.000001968
1	-0.000000781	0.000001605	-0.00000185
17	0.000000071	-0.000000862	-0.000000913

Zero-point correction=

1.221536 (Hartree/Particle)

Thermal correction to Energy=

1.296970

Thermal correction to Enthalpy=

1.297915

Thermal correction to Gibbs Free Energy=

1.101270

Sum of electronic and zero-point Energies=

-4408.219677

Sum of electronic and thermal Energies=

-4408.144243

Sum of electronic and thermal Enthalpies= -4408.143298  
 Sum of electronic and thermal Free Energies= -4408.339943

E-TS2a

6	0.000001047	0.00000175	0.000001519
6	-0.000000424	0.000000024	-0.000000141
7	-0.000000283	0.000001263	0.000000056
7	0.000003121	0.00000078	0.000001436
16	-0.000002873	-0.000000987	-0.000000585
8	0.00000038	0.000001766	0.000000641
8	-0.000000834	0.000001216	0.000000182
6	-0.000000405	0.000001124	0.000000064
6	-0.000000784	0.000001761	0.000000572
6	-0.000001399	0.000002179	0.000000725
6	-0.000000979	0.000002327	0.000000123
6	-0.000000894	0.00000217	0.000001143
6	-0.000000187	0.000001726	0.000000979
1	-0.000001392	0.000001827	-0.000000175
1	-0.000001392	0.000002159	0.000000839
1	-0.00000083	0.00000231	0.000001057
1	-0.000001118	0.000001051	0.000001217
6	-0.000001027	0.000002752	0.000000148
1	-0.000001101	0.000002957	0.000001318
1	-0.000001686	0.000002909	0.000001086
1	-0.000001204	0.000002816	0.000000136
6	0.000000417	0.000000913	-0.000000154
1	0.000000333	0.000000126	0.000000065
1	-0.000000129	0.00000043	-0.000000397
16	-0.000000106	-0.000000102	0.000000307
8	0.000000224	0.000000107	-0.000000189
8	0.000001438	-0.000000123	-0.000000998
6	0.000001908	-0.000000058	0.000000847
6	-0.000000175	0.000000392	0.000000334
6	0.000000674	0.000001357	0.000000128
6	0.000000087	0.000000973	0.000001216
1	-0.000000244	0.000000941	-0.000000225
6	0.000000645	0.000000923	0.000000522
1	0.000000829	0.000000873	0.000000532
6	-0.000000134	0.000001564	0.000000888
1	-0.000000452	0.000001251	0.000000635
1	0.000000823	0.000001366	0.000001004
6	0.000000683	0.000001522	0.000001161
1	0.000000265	0.000002126	0.000001243
1	0.000000131	0.000001638	0.000001098

1	-0.000000192	0.000001851	0.000001101
6	0.000000078	-0.000000664	-0.000000282
6	0.000001475	0.000000667	-0.000000056
6	0.000000075	-0.000000313	-0.000001431
1	0.000001185	0.000000132	0.000000547
6	0.000002621	0.00000002	0.000001935
1	0.000001069	-0.000000026	-0.000000087
1	0.000001725	0.000000788	0.000001248
6	0.000001977	-0.000000913	0.000001356
1	0.00000153	-0.000001005	0.000000511
1	-0.000000081	0.000000133	0.000000054
6	0.000002284	-0.000000792	-0.000000203
1	0.000002085	0.000000264	0.000000713
1	0.000002367	0.000000222	0.000000469
1	0.000002843	-0.00000111	0.000000311
1	0.00000235	-0.000000365	0.000000531
1	0.000002324	-0.000000512	0.000000235
1	0.000001951	-0.00000047	0.000000224
6	-0.000001075	0.000000085	0.000001922
6	-0.000000172	0.000001179	0.000000599
6	-0.000000793	0.000000514	0.00000007
6	-0.000000288	0.000001359	0.00000049
1	-0.000000009	0.000001065	0.000000349
6	-0.000000874	0.00000077	0.000000503
1	-0.000000716	0.000000646	-0.000000623
6	-0.000000844	0.000001459	0.00000032
1	-0.000000218	0.000001497	0.000000894
1	-0.000001388	0.000000786	0.000000083
1	-0.000001027	0.000001338	0.000000501
79	-0.000000879	-0.000001377	0.000000234
6	0.000000086	-0.00000426	-0.000001043
6	-0.000000573	-0.000000875	-0.000001516
6	-0.000000163	-0.000001578	-0.000000829
1	-0.000000258	-0.000002184	-0.000000987
1	-0.000001018	-0.000001758	-0.000001141
7	-0.000002134	-0.000000679	-0.000000659
7	0.000000292	-0.000001723	-0.000000984
6	-0.000000515	0.000000532	-0.000000492
6	-0.000001599	-0.000001387	-0.000000365
6	-0.000000995	-0.000001165	0.000000642
6	-0.00000128	-0.000000098	-0.000001061
6	-0.000001971	0.000000414	-0.000000535
6	-0.000001998	-0.000000738	-0.000001224
1	-0.000001788	-0.000000791	-0.000000671

1	-0.000002101	0.000000144	-0.00000054
1	-0.000002229	0.000000126	-0.000000523
6	0.000000826	-0.000002226	-0.000001626
6	0.000000581	-0.000001527	0.00000063
6	0.000000331	-0.000000541	-0.00000019
6	0.000001078	-0.000002369	-0.000001424
6	0.000000666	-0.000001635	-0.000000772
6	0.000001083	-0.000001483	-0.00000098
1	0.000001304	-0.000001607	-0.00000065
1	0.00000186	-0.000002121	-0.000000599
1	0.000001794	-0.000001912	-0.000000626
6	-0.000000247	-0.00000077	-0.000000509
6	-0.000000408	-0.000001705	-0.000000935
6	0.000000655	-0.000001548	-0.000000562
1	-0.000000247	-0.000001263	-0.000001393
1	0.000000199	-0.000002188	-0.000001443
1	0.000000014	-0.000001902	-0.00000112
1	0.000000358	-0.000002208	-0.000001102
1	0.000000207	-0.000001265	-0.000000082
1	0.000000743	-0.000001315	-0.000000499
1	0.000000345	-0.000001123	-0.000000484
6	0.000000822	-0.000002038	0.000000204
6	0.000000541	-0.000001215	-0.000000918
6	0.000000653	-0.000001912	-0.000000612
1	-0.000000222	-0.000000318	-0.000001072
1	0.000000941	-0.000001151	-0.000000526
1	0.000000754	-0.000001305	-0.00000054
1	0.000001228	-0.000001521	-0.000000284
1	0.000000467	-0.000002443	-0.000001153
1	0.000000772	-0.000001975	-0.000001299
1	0.000000642	-0.000002095	-0.000001155
6	-0.000002291	-0.000000963	-0.000001069
6	-0.000000782	-0.000000285	0.000000181
6	-0.000001854	-0.000000692	-0.000001002
1	0.000000387	0.000000072	-0.000000955
1	-0.000001105	-0.000000115	-0.000000703
1	-0.000001121	-0.000000105	-0.000000651
1	-0.000002077	-0.000000137	-0.00000049
1	-0.000001339	-0.000001103	-0.000001168
1	-0.000001683	-0.000000736	-0.000001016
1	-0.000001675	-0.00000104	-0.000000698
6	0.00000018	-0.000001402	-0.000000977
6	-0.000000868	-0.00000181	-0.000000695
6	-0.000000992	-0.000000663	-0.00000122

1	-0.00000591	-0.00001185	-0.00000975
1	-0.00001769	-0.00001412	-0.00001236
1	-0.00001195	-0.00001176	-0.00001366
1	-0.00001692	-0.00000827	-0.00000963
1	-0.00001089	0.00000709	0.00000012
1	-0.00000877	-0.00000676	-0.00000745
1	-0.00000548	-0.00000711	-0.00000501
6	0.00000859	0.00001914	0.00001063
6	0.00001282	0.00001041	0.00001448
6	0.00000741	0.00002094	0.00001874
6	0.00001057	0.00002013	0.00001008
6	0.00000433	0.00001824	0.00000431
1	0.00000963	0.00002228	0.00001526
1	0.00000938	0.00000118	0.00000049
7	0.00000491	0.00000752	0.00000862
8	0.00001156	0.00000109	-0.00000401
1	0.00000701	0.00002252	0.00001514
1	0.00001026	0.00001526	0.00001089
17	0.00000729	0.00001806	0.0000152

Zero-point correction=

1.218813 (Hartree/Particle)

Thermal correction to Energy=

1.295566

Thermal correction to Enthalpy=

1.296510

Thermal correction to Gibbs Free Energy=

1.095172

Sum of electronic and zero-point Energies=

-4408.201058

Sum of electronic and thermal Energies=

-4408.124305

Sum of electronic and thermal Enthalpies=

-4408.123361

Sum of electronic and thermal Free Energies=

-4408.324699

E-2a

6	0.00000107	-0.00001552	0.000004349
6	-0.00000825	0.00000767	-0.00001779
7	-0.00002247	0.00000117	-0.000003195
7	-0.00000535	-0.00002719	0.00001229
16	-0.00002655	-0.00000538	0.000003928
8	-0.00000093	-0.00000529	0.000002677
8	-0.00001491	-0.00001106	0.00001328
6	-0.00002427	-0.00001608	0.00001573
6	-0.00000531	0.00000561	0.000000796
6	-0.0000339	-0.00001011	0.00001454
6	-0.00001354	-0.00001306	-0.00000303
6	-0.00002845	-0.00000219	-0.00000138
6	-0.00001935	-0.00000013	-0.000000403
1	-0.00002027	-0.00000788	0.00001533
1	-0.00002288	-0.00000839	0.000000954

1	-0.000002388	-0.000000665	-0.000000683
1	-0.000001835	-0.000000502	-0.000000183
6	-0.000002767	-0.000000749	-0.000000554
1	-0.00000291	-0.000000837	-0.000000061
1	-0.000002973	-0.000001008	-0.000000692
1	-0.000002704	-0.000000235	-0.000000946
6	-0.000000036	-0.000000965	0.000001536
1	0.000000556	-0.000000007	0.000001114
1	-0.000000723	0.000000728	0.000001169
16	0.000000726	0.000001296	-0.000003296
8	-0.000001273	-0.000000096	0.000001084
8	0.000001565	0.000001032	0.000001042
6	0.000000235	0.000000193	0.000001557
6	-0.000002563	0.000000283	0.000000306
6	0.000000905	-0.000001549	0.000000409
6	-0.000000044	-0.000002328	0.000001362
1	-0.000000341	-0.000000114	0.000001267
6	-0.000001814	0.000000501	-0.000000248
1	0.000000125	0.000000271	-0.000000405
6	0.000000402	0.000001148	0.000002085
1	-0.000001354	-0.000000262	0.000002122
1	0.000000005	-0.000000139	0.000000431
6	-0.000001362	-0.000000073	0.000001673
1	-0.000000052	-0.000000253	0.000001413
1	-0.000001357	-0.000000542	0.000001238
1	-0.000001017	-0.000000466	0.000002095
6	0.00000236	0.000000446	0.000000695
6	0.000001424	0.000000743	-0.000000468
6	0.00000036	0.000000728	0.000002247
1	0.000001061	0.000000034	0.000001759
6	0.00000186	0.000000822	0.000001463
1	0.0000017	0.000000384	0.000000371
1	0.000001687	0.000000534	0.000000303
6	0.000002492	0.000000625	0.000000415
1	0.000001547	0.000000549	0.000000598
1	0.000001043	0.000000252	0.000001168
6	0.00000272	0.000000652	0.000001424
1	0.000002827	0.000000787	0.000000301
1	0.000002388	0.000000511	0.000001143
1	0.00000214	0.000000476	0.000001734
1	0.000002039	0.000000362	0.000002261
1	0.0000032	0.000000773	0.000001266
1	0.000002607	0.000000073	0.000000563
6	-0.000000645	0.000000863	0.000000485

6	0.00000606	0.00000646	0.00002007
6	-0.00001525	-0.00001526	0.00003096
6	0.00000184	-0.00000506	0.00002626
1	0.00001271	-0.00000173	0.00001665
6	0.00000321	0.00000447	0.00002752
1	-0.00000487	-0.00000378	0.0000203
6	0.00000637	-0.00000321	0.0000424
1	0.00001632	0.00000367	0.00002731
1	-0.00000932	-0.00000591	0.00003407
1	0.00000181	-0.00000086	0.00003176
79	0.00002227	-0.00000116	-0.00000434
6	-0.00000599	0.00001502	0.00001785
6	0.00002204	0.00000222	-0.00003656
6	0.00000912	0.00001005	-0.00001195
1	-0.00000696	-0.00000031	-0.00002881
1	0.00001036	0.00001012	-0.00002249
7	0.00000181	0.00000371	-0.00003528
7	-0.00002753	-0.00000903	-0.00003622
6	0.00001857	0.00002582	-0.00000672
6	0.00001863	-0.00001501	-0.00003836
6	0.00000898	-0.00000354	0.00000052
6	0.0000229	0.00000389	-0.00000426
6	0.00002442	0.00000266	-0.00001505
6	0.00003505	0.00002511	-0.00001062
1	0.00002795	0.00000688	-0.00001952
1	0.00002745	0.00000847	-0.00000043
1	0.00003288	0.00000872	-0.00001111
6	-0.00001509	0.00001028	-0.00002362
6	-0.0000063	0.00000052	-0.00001072
6	-0.00001972	-0.00001227	-0.00000052
6	-0.00002485	-0.0000017	-0.00000229
6	-0.00002483	-0.00001156	-0.00003154
6	-0.00001984	0.00000355	-0.00001893
1	-0.00002346	-0.00000569	-0.00001173
1	-0.00002494	-0.00000462	-0.00002393
1	-0.00003509	-0.00000759	-0.00001725
6	-0.00002347	-0.00000032	-0.00001558
6	-0.00000628	-0.00000013	-0.00001677
6	-0.00001286	-0.00000847	0.00000736
1	-0.00000256	-0.00000332	-0.00000723
1	-0.00000059	0.00000178	-0.00002071
1	-0.00000038	-0.00000072	-0.00001282
1	-0.00001253	-0.00000222	-0.00001733
1	-0.00001228	-0.00000223	-0.00000377

1	-0.000002059	-0.000000369	-0.000000612
1	-0.000000719	-0.000000117	-0.000000019
6	-0.000000051	-0.000000415	-0.0000003399
6	-0.000002276	0.000000169	-0.000000148
6	-0.000002469	-0.000000571	-0.0000003223
1	0.000000276	-0.000000381	-0.0000002336
1	-0.000001409	0.000000355	-0.0000002183
1	-0.000001007	-0.000000125	-0.000000268
1	-0.000001687	-0.000000958	-0.0000002576
1	-0.000001062	-0.000000001	-0.0000003878
1	-0.000001424	0.000000101	-0.0000003499
1	-0.000001233	0.000000269	-0.000000378
6	0.00000168	0.000000291	-0.0000000924
6	0.000001994	0.000000288	0.000000159
6	0.000002058	0.000000799	-0.0000000997
1	0.000000777	0.000000422	-0.0000000632
1	0.000001395	0.000000634	0.0000000382
1	0.000001667	0.000000396	0.0000000394
1	0.000002331	0.000000645	0.000000042
1	0.000001856	0.000000063	-0.0000001739
1	0.000002608	0.000000083	-0.0000000952
1	0.000001747	0.000000674	-0.0000001013
6	0.000000754	0.000001913	-0.0000001485
6	0.000001183	0.000001003	-0.0000003252
6	0.000001847	-0.000000041	-0.0000003614
1	0.000001422	-0.000000012	-0.0000002472
1	0.000001301	0.000000114	-0.0000003442
1	0.000001203	0.000000728	-0.0000003457
1	0.000002521	0.000000865	-0.0000003384
1	0.00000008	0.000000652	-0.0000000968
1	0.000001218	0.000000773	-0.0000002234
1	0.000000875	0.000000052	-0.0000002467
6	-0.000001064	-0.000001024	0.0000003568
6	-0.000001218	-0.000001268	0.0000004349
6	-0.000000548	0.000000006	0.0000002952
6	0.000002199	0.000000885	0.0000004081
6	-0.000001187	-0.0000003079	0.000000318
1	0.000000124	-0.0000000561	0.0000004673
1	-0.000001176	-0.000000462	0.0000003085
7	0.0000006034	0.0000007102	0.0000002025
8	-0.0000003263	-0.0000005194	0.0000000703
1	0.000000834	0.000000003	0.0000003545
1	-0.000000092	-0.000000447	0.0000003966
17	0.000001015	0.000000287	0.0000002342



Zero-point correction=	1.220603 (Hartree/Particle)
Thermal correction to Energy=	1.297153
Thermal correction to Enthalpy=	1.298097
Thermal correction to Gibbs Free Energy=	1.098468
Sum of electronic and zero-point Energies=	-4408.211239
Sum of electronic and thermal Energies=	-4408.134689
Sum of electronic and thermal Enthalpies=	-4408.133745
Sum of electronic and thermal Free Energies=	-4408.333374

Re7

6	-0.000000033	-0.000001222	0.000001457
6	0.000003078	-0.00000014	-0.000003193
7	-0.000001816	0.000004741	-0.000001474
7	-0.000008332	-0.000004722	-0.000002133
16	-0.000000517	-0.000001221	-0.000002384
8	-0.000001173	0.000000454	0.000000559
8	0.000001369	-0.000000132	-0.000000255
6	0.000005283	0.000003859	-0.000003761
6	-0.000000754	0.000002342	0.000003257
6	-0.000003596	-0.000000471	-0.000002097
6	0.000006835	0.000004477	-0.000006595
6	-0.000000889	0.000002209	0.000003131
6	-0.000004076	-0.000003198	-0.000002865
1	0.000000083	0.000001448	-0.000001504
1	-0.000000021	0.000002167	-0.000001198
1	0.000000298	0.000000483	-0.000001587
1	0.000001276	0.000000389	-0.000000094
6	0.000000961	0.000001753	-0.000002909
1	-0.000000649	0.000001786	-0.000001454
1	-0.000000534	0.000002889	-0.000000819
1	-0.000000902	0.000001467	-0.000000877
6	-0.000001108	-0.000002578	0.000001515
1	0.000000432	0.000001362	0.000000431
1	-0.000000591	0.000001113	0.000000059
16	0.000007203	0.000003039	0.000001148
8	0.000000015	-0.000001408	-0.000000151
8	0.000000382	-0.000001493	0.000000095
6	0.000001732	-0.000000632	-0.000001373
6	-0.000000419	-0.00000132	0.000001487
6	-0.000001007	0.000000152	0.000000536
6	-0.000001489	0.000000089	0.000001845
1	-0.000000056	-0.000000192	0.000000231
6	0.000000035	-0.000002811	0.000000243
1	0.000000428	-0.000001967	0.000000169

6	0.000001159	-0.000000049	-0.000000572
1	-0.000000487	0.000000192	0.000001003
1	0.000000094	-0.000001476	0.000001013
6	-0.000000792	-0.000000696	0.000001841
1	-0.000000378	-0.000001207	0.000002103
1	-0.000000652	-0.000000043	0.000001783
1	-0.000000689	-0.000000486	0.000002074
6	0.000000759	0.000000361	0.000002239
1	-0.000000088	-0.000002794	-0.000000043
6	-0.000000289	0.000002537	0.000001927
6	0.000000173	0	0.000001526
6	-0.000000868	-0.000000186	-0.000000785
6	-0.00000168	0.000000084	0.000000903
1	-0.000000698	0.000000056	0.000001041
6	-0.000000599	0.000000484	0.000000563
1	-0.000000954	0.000002039	0.000000495
6	-0.000001416	0.000001777	0.00000188
1	-0.000000673	-0.000000084	0.000002041
1	-0.000000511	0.000001917	0.000001019
1	-0.000000549	0.00000102	0.000001838
6	0.000002168	-0.000002545	-0.000000919
1	-0.000000106	-0.000002903	-0.000000469
1	-0.00000047	-0.000001192	0.000000516
1	0.000001097	-0.000002236	0.000000904
6	0.00000229	-0.000001736	-0.000000171
1	0.00000146	-0.000002006	-0.000001685
1	0.000000088	-0.000001789	-0.000001372
1	0.000001354	-0.000002119	-0.000000116

**Zero-point correction=** 0.493373 (Hartree/Particle)  
**Thermal correction to Energy=** 0.527882  
**Thermal correction to Enthalpy=** 0.528826  
**Thermal correction to Gibbs Free Energy=** 0.419792  
**Sum of electronic and zero-point Energies=** -2213.755902  
**Sum of electronic and thermal Energies=** -2213.721393  
**Sum of electronic and thermal Enthalpies=** -2213.720449  
**Sum of electronic and thermal Free Energies=** -2213.829483

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6	0.000025534	-0.000024165	-0.000002218
6	-0.000017193	0.000010552	0.000013522
7	-0.000000415	0.000020603	-0.000017251
7	0.000021743	0.000007493	-0.000003164
16	0.00001097	-0.000007478	0.000000952
8	-0.000005838	-0.000003424	-0.000002612

8	-0.000002362	0.000001199	0.000002345
6	0.000005634	0.000003408	0.000001932
6	0.000000972	-0.000000246	-0.000001334
6	0.000004109	0.000002419	-0.00000232
6	0.000001642	-0.000000848	-0.000002534
6	0.000003732	-0.000000517	0.000000065
6	0.000000425	0.000001753	-0.000001742
1	0.00000267	0.000000685	-0.00000132
1	0.000002737	0.00000068	-0.000001287
1	0.00000293	-0.000000555	-0.000000283
1	0.000003605	-0.000000726	0.000001115
6	0.000004072	0.000000312	-0.000000766
1	0.000003772	-0.000000258	-0.000000869
1	0.00000381	0.000000768	-0.000001255
1	0.000003923	-0.000000083	-0.000001164
6	0.000000339	-0.000005057	-0.000001216
1	-0.000000936	0.000001632	-0.000000395
1	0.000000047	0.000001438	-0.000001179
16	-0.000014672	0.000002421	0.000000611
8	-0.000001495	-0.000000808	0.000002173
8	0.000000905	0.000000362	0.000001572
6	0.000004002	-0.000005323	0.000003756
6	0.000001659	-0.000001799	-0.000004065
6	-0.000000746	-0.000001302	0.00000128
6	0.000000019	-0.000003466	0.000000238
1	0.000002056	0.000000234	0.000002157
6	0.000001967	-0.000003794	-0.000001075
1	0.000001005	-0.000001654	0.000000542
6	0.000002693	0.000004837	0.000006793
1	0.000002041	-0.000001444	0.000000843
1	0.000002099	-0.000000415	-0.000000317
6	0.000004168	-0.000002235	0.000002553
1	0.000001782	-0.000001809	0.000000201
1	0.000002378	-0.00000027	0.000000324
1	0.000002404	-0.000001311	-0.00000041
6	-0.000009057	-0.000007128	-0.000004537
1	0.000000135	0.000001415	-0.00000081
6	0.000000225	0.000000012	-0.000001916
6	-0.000001333	-0.000001325	-0.000000256
6	0.000001817	0.000003062	0.000000033
6	0.000000903	0.000002664	-0.000000033
1	0.000003011	-0.000000929	0.000000281
6	0.000000177	-0.000000864	-0.000001843
1	0.000000878	0.000001284	-0.000001123

6	0.000004407	0.000000235	-0.000000699
1	0.000001828	-0.000000751	-0.000000442
1	0.000002153	0.000000947	-0.000001271
1	0.0000018	0.00000018	-0.000000609
6	0.000000846	0.000001194	0.000001672
1	-0.000001732	-0.000000388	0.000000344
1	-0.000001066	-0.000000694	0.000000332
1	-0.000001148	-0.000000479	0.000000843
6	0.000002944	-0.000002151	0.00000201
1	-0.000000418	0.000000553	-0.000000035
1	-0.000002556	0.000000321	0.000001155
1	-0.000001409	0.000000346	-0.000000114
79	-0.000006948	0.00000295	-0.000001741
6	-0.000002987	-0.000001683	-0.00000287
6	-0.000006403	0.000005936	-0.000000083
6	-0.000001657	-0.000003465	-0.000006171
1	-0.000002952	0.000001653	0.000001729
1	-0.00000049	-0.000001267	0.000000612
7	0.000002047	-0.000001504	0.000002007
7	0.000002766	-0.000000851	0.000005108
6	0.000000964	0.000002813	0.00000217
6	-0.000000311	-0.000000237	-0.000001771
6	-0.000001342	-0.000000733	-0.000002028
6	0.000000649	0.000000371	0.000000901
6	-0.000000449	-0.000000255	-0.000000381
6	-0.000000169	-0.000000624	-0.000000434
1	0.000000395	-0.00000113	0.000001311
1	0.000000739	-0.000000262	-0.000000494
1	0.00000096	-0.000000615	0.000000513
6	-0.000002299	0.000000176	0.000000634
6	0.000000358	0.000002053	0.000001198
6	-0.000002148	0.000001084	0.000000722
6	-0.000002453	0.000000801	-0.000000042
6	-0.000002826	0.000000378	0.000000945
6	-0.000003126	0.000000897	-0.000000596
1	-0.000002491	0.000001414	-0.000001473
1	-0.000002278	-0.000000073	0.000000674
1	-0.000002674	0.000000733	0.000000042
6	0.000000365	0.000000478	-0.000001458
6	-0.000003767	0.000000702	0.000000797
6	-0.000003314	0.000000293	-0.000001724
1	-0.0000018	0.000001793	0.000000797
1	-0.000002632	0.000001537	-0.000000769
1	-0.000002219	0.000001791	-0.000001315

1	-0.000001999	0.000002343	-0.000001787
1	-0.000001629	0.000001644	-0.00000379
1	-0.000000548	0.000001126	-0.000001098
1	-0.000000824	0.000002156	-0.000000942
6	-0.000002144	-0.000000803	-0.000000725
6	-0.000003649	-0.00000011	0.000003236
6	-0.000001689	-0.000001389	0.000001536
1	-0.000002777	-0.000000306	0.000000295
1	-0.000001446	-0.000002367	0.000002088
1	-0.000001852	-0.000000932	0.000001472
1	-0.000001661	-0.000000635	0.000000882
1	-0.000003053	-0.000000194	0.000001106
1	-0.00000355	-0.000000033	0.000000084
1	-0.000002757	-0.000000649	0.000001746
6	-0.000001976	0.000001025	-0.000002165
6	0.000001085	0.000000057	-0.000000625
6	-0.000000023	0.000001333	0.000001927
1	-0.000001715	0.000000484	-0.000001026
1	-0.000000571	0.00000238	-0.000001462
1	0.000000001	0.000001463	-0.000001361
1	-0.000001112	0.000001372	-0.000001025
1	-0.000001544	0.000000553	-0.000000837
1	-0.000000587	0.000000823	-0.000001456
1	-0.000001089	0.000001109	-0.000001049
6	0.00000107	-0.000002645	0.000002289
6	-0.000002668	-0.000001001	-0.000000648
6	-0.000001573	-0.000001456	0.000000037
1	0.000000026	-0.00000029	0.000002692
1	-0.000001223	-0.000001157	0.000001405
1	-0.000001214	-0.000001313	0.000001016
1	0.000000467	-0.00000154	0.000001961
1	0.000000146	-0.000001242	0.000000666
1	0.000000478	-0.000000379	0.000001759
1	-0.000000507	-0.000001461	0.000000092
<b>Zero-point correction=</b>			<b>1.067712 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>1.136083</b>
<b>Thermal correction to Enthalpy=</b>			<b>1.137027</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>0.952107</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-3508.607700</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-3508.539329</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-3508.538385</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-3508.723305</b>

F-2

6	-0.000003291	0.000001799	0.000002469
6	0.00000211	-0.000003282	-0.00000028
7	0.000001501	0.000000662	-0.000000401
7	-0.000000267	0.000001955	-0.000002868
16	0.000000356	0.000000523	-0.000000564
8	-0.000000451	0.000000023	-0.000000833
8	-0.000000104	-0.000000091	-0.000000514
6	-0.000000268	0.000000411	-0.000000137
6	0.000000416	-0.000001281	0.000000121
6	0.000001122	0.00000005	-0.000000806
6	0.000000145	0.000000831	0.000000504
6	0.000000034	-0.000001248	-0.000000064
6	0.00000007	0.00000053	-0.00000088
1	0.00000017	0.000000039	-0.00000031
1	0.000000241	0.000000085	-0.000000277
1	0.000000563	0.00000016	-0.00000009
1	0.000000535	0.000000096	0.000000094
6	0.000000462	0.000000439	0.000000095
1	0.000000893	-0.000000535	-0.000001047
1	-0.000000082	-0.000000172	-0.000000212
1	0.00000106	0.000000411	-0.000000102
6	-0.000000099	0.000000606	0.000000007
1	0.000000289	-0.000000333	-0.000000255
1	0.000000112	-0.000000436	0.000000224
16	0.00000011	-0.000002161	0.000001738
8	0.000000769	0.000000366	0.000000284
8	0.000000522	0.000000649	0.000000402
6	-0.00000412	0.000001865	0.00000401
6	0.000007752	0.000001588	0.000000663
6	-0.000001083	-0.000003431	-0.000006027
6	-0.000001051	-0.00000355	-0.00000689
1	-0.000000373	-0.000000129	-0.000000405
6	0.000008188	0.000001839	0.000000209
1	0.000000959	0.000000401	0.000000741
6	-0.000006127	0.000003258	0.000006762
1	0.000000854	0.000000216	0.00000039
1	0.0000001	-0.00000012	-0.00000004
6	0.000002462	-0.000001295	-0.000001855
1	0.00000125	0.000000529	-0.000000003
1	0.000000006	0.00000014	-0.000000586
1	0.000000495	0.000000148	-0.000000166
6	0.000001232	-0.00000123	0.000000168
1	-0.000000114	0.000000329	-0.000000045
6	-0.000000414	0.000001413	0.000001783

6	0.000000782	0.000000031	-0.00000023
6	-0.000000116	-0.000000681	0.000000001
6	0.000000446	-0.000000093	0.000000418
1	0.000000018	0.000000014	0.000000044
6	0.000000385	0.000000321	-0.000000293
1	-0.000000001	0.000000026	0.000000056
6	-0.000000014	0.000000335	0.000000703
1	0.000000422	0.000000215	0.000000371
1	0.000000048	0.000000048	0.000000237
1	0.000000389	0.000000043	0.000000282
6	-0.000000042	0.000000297	0.000000486
1	0.000000029	0.000000154	0.000000274
1	0.000000243	0.000000152	0.000000424
1	0.00000003	0.000000014	0.000000282
6	0.000000641	0.000000079	0.000000343
1	0.000000019	0.000000005	-0.000000012
1	0.000000155	-0.000000013	0.000000197
1	0.000000241	-0.000000008	0.000000026
79	-0.000000216	0.000001382	0.000000372
6	0.000000043	-0.000001338	-0.000001474
6	-0.000000592	0.000000324	0.000000209
6	-0.000000114	0.000000397	-0.000001183
1	-0.000000682	0.000000124	0.000000105
1	-0.000000602	-0.000000225	0.000000129
7	-0.00000011	-0.000000083	-0.000000038
7	-0.000000256	-0.000001839	0.000002791
6	-0.000001324	0.000000498	0.000000551
6	0.000000266	0.000000163	0.000000728
6	-0.000000014	-0.000000847	-0.000000223
6	-0.000000301	-0.000000322	-0.000000119
6	-0.000000177	0.000000031	-0.000000019
6	-0.000000931	0.000000046	0.000000433
1	-0.000000494	-0.000000177	0.000000452
1	-0.000000669	-0.000000181	-0.000000063
1	-0.000000447	-0.000000114	0.000000166
6	0.000000934	0.000000713	-0.000000528
6	-0.000000557	-0.000000016	-0.000000766
6	-0.000000564	0.000000275	-0.000000041
6	-0.000000266	0.000000137	-0.000000018
6	-0.000000188	0.000000025	-0.000000127
6	0.000000157	-0.000000131	0.000000068
1	0.000000019	-0.000000115	-0.000000303
1	-0.000000134	-0.000000022	0.000000079
1	0.000000142	-0.000000013	-0.000000263

6	0.000000131	0.000000749	-0.00000072
6	-0.000000407	-0.000000466	-0.000000096
6	-0.000000067	-0.000000629	0.000000052
1	-0.000000481	-0.000000011	-0.000000498
1	-0.000000315	-0.000000047	-0.000000053
1	-0.000000333	-0.000000069	-0.000000545
1	0.000000076	-0.000000079	-0.000000705
1	0.000000011	-0.000000037	-0.000000152
1	-0.000000127	0.000000338	-0.000000444
1	-0.000000193	-0.000000034	-0.000000462
6	-0.000000209	0.000000262	0.000000096
6	0.000000156	-0.000000015	0.000000211
6	-0.000000242	-0.000000019	0.000000412
1	-0.000000345	0.000000089	0.000000054
1	-0.000000055	0.000000086	0.000000378
1	-0.000000189	0.000000001	0.000000439
1	0.000000065	0.000000003	0.000000463
1	-0.000000434	-0.000000097	0.000000106
1	-0.000000423	0.000000095	0.000000084
1	-0.000000043	-0.000000119	0.000000366
6	-0.000000425	0.000000341	0.000000006
6	0.000000201	-0.000000001	-0.000000577
6	-0.000000412	-0.000000221	-0.000000192
1	-0.000000353	-0.000000404	-0.000000406
1	-0.000000803	-0.000000261	-0.000000197
1	-0.000000498	-0.000000068	-0.000000335
1	-0.000000553	0.000000197	0.000000007
1	-0.000000692	-0.000000134	-0.000000117
1	-0.000000751	-0.000000152	-0.000000219
1	-0.000000676	-0.000000008	-0.000000468
6	-0.000000544	-0.000000242	0.000000293
6	-0.000000615	-0.000000031	0.000000421
6	-0.000000056	-0.000000071	0.000000261
1	-0.000000021	0.000000234	0.000000119
1	-0.000000585	-0.000000144	0.000000475
1	-0.000000527	-0.000000067	0.000000509
1	-0.000000772	0.000000188	0.000000479
1	-0.000000336	-0.000000232	0.000000418
1	-0.000000307	-0.000000123	0.000000531
1	-0.00000003	0.000000048	0.000000059

Zero-point correction=

1.068084 (Hartree/Particle)

Thermal correction to Energy=

1.136250

Thermal correction to Enthalpy=

1.137194

Thermal correction to Gibbs Free Energy=

0.952609



Sum of electronic and zero-point Energies=	-3508.613038
Sum of electronic and thermal Energies=	-3508.544872
Sum of electronic and thermal Enthalpies=	-3508.543928
Sum of electronic and thermal Free Energies=	-3508.728513

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6	-0.00000699	-0.00000345	0.000001344
6	0.00000513	-0.00000826	-0.000002314
7	0.00000788	-0.00000307	0.000000292
7	-0.00000765	0.00000523	0.000001753
16	0.0000069	0.00000686	0.000000597
8	0.00000414	0.00000036	-0.000000328
8	-0.00000263	0.0000004	0.000000219
6	0.00000091	-0.00000012	-0.000000837
6	0.00000445	0.00000015	-0.00000086
6	0.000001242	0.000000382	-0.000003547
6	-0.00000826	-0.00000934	0.000001781
6	-0.00000145	-0.000001433	0.000000173
6	0.00000387	0.00000053	-0.000001945
1	0.00000224	-0.00000105	-0.000000604
1	0.00000912	-0.00000554	-0.000000172
1	0.00000056	-0.00000813	-0.000000156
1	-0.00000155	-0.00000489	-0.000000308
6	0.00000577	-0.00000504	-0.000000207
1	0.00000824	0.000000412	-0.000003176
1	0.000001979	-0.000002314	-0.00000274
1	-0.00000207	0.000000127	-0.000001134
6	-0.000001055	-0.00000523	-0.000000563
1	-0.00000046	-0.00000572	-0.000000305
1	-0.00000367	-0.00000061	-0.000000216
16	-0.00000052	-0.000000126	0.000000415
8	-0.00000802	0.000001042	0.000000239
8	-0.00000862	0.00000172	0.000001117
6	-0.00000881	0.00000188	0.000001509
6	-0.00000565	0.000000496	0.000000714
6	-0.00000594	0.000000414	0.000001753
6	-0.000001197	0.00000112	0.000002106
1	-0.0000002	0.000000221	0.000000818
6	-0.000000112	0.000000372	0.000000796
1	-0.000000812	0.000000635	0.000001363
6	-0.000001511	-0.000001225	0.000001799
1	-0.000000395	0.000000596	0.000001139
1	-0.000000732	0.000000852	0.000001749
6	-0.000000115	0.000002232	0.000000771

1	-0.000001265	0.000001621	0.000000666
1	0.000000616	0.000001502	0.000003106
1	-0.000001045	0.000000328	0.000002267
6	0.000000165	0.000000399	0.000001155
1	0.000000183	0.000000596	0.000000543
6	-0.000000842	-0.000000503	-0.000000038
6	-0.000000925	-0.000000252	0.000000133
6	-0.000000864	-0.00000033	-0.000000521
6	-0.000000964	-0.000000111	-0.000000058
1	-0.000000746	-0.000000967	0.000000754
6	-0.000000742	-0.000000759	-0.000000728
1	-0.000000394	-0.000000301	-0.000001037
6	-0.000001559	-0.000000606	-0.000000329
1	-0.000001272	-0.000000222	0.00000013
1	-0.000000941	-0.000000762	-0.000000743
1	-0.000001392	-0.000000604	-0.0000003
6	-0.00000027	0.000000813	0.000001128
1	-0.00000014	0.000000951	0.0000011
1	0.000000182	0.000000667	0.000001281
1	0.000000321	0.0000006	0.000001185
6	-0.000000086	0.000000444	0.000000827
1	-0.00000024	0.00000052	0.000000484
1	-0.000000483	0.000000561	0.000000886
1	0.000000016	0.000000448	0.000000826
79	-0.000001519	0.000000658	-0.000000276
6	0.000000088	-0.000000173	-0.00000039
6	0.000000268	-0.00000037	-0.000000258
6	0.000000266	-0.000000068	-0.000000718
1	0.000000359	-0.000000259	-0.000000417
1	-0.000000356	-0.000000565	-0.000000094
7	-0.000000744	-0.00000071	-0.000000849
7	-0.000000105	0.000000982	-0.000001133
6	0.000000616	-0.000000277	-0.000000559
6	-0.000000844	-0.000000235	-0.000000512
6	-0.000000736	-0.00000088	-0.000000276
6	-0.000000996	-0.000000106	-0.000000535
6	-0.000000671	-0.000001484	-0.000000366
6	-0.000000763	-0.000000841	-0.0000002
1	-0.000001045	-0.000000709	-0.000000265
1	-0.000000399	-0.000000918	-0.000001135
1	-0.000001069	-0.000000849	-0.000000882
6	0.000000621	-0.000001602	0.000000148
6	0.000000866	0.000000269	-0.000000318
6	0.000000913	0.000001373	0.000000091

6	0.000001136	0.000000199	-0.000000063
6	0.000000738	0.000000418	0.000000332
6	0.000000094	0.000000315	0.000000418
1	0.000001272	0.000000556	-0.000000023
1	0.000000763	0.000000814	0.000000651
1	0.000001299	0.000000766	0.000000306
6	0.000000018	0.000000092	0.000000391
6	0.000001529	-0.000000792	-0.000000159
6	0.000001248	-0.000000245	-0.000000622
1	0.000000936	-0.000000484	-0.000000748
1	0.000001348	-0.000000058	-0.000000837
1	0.000001125	-0.000000355	-0.000000868
1	0.000001779	0.000000073	-0.000000551
1	0.000001464	0.000000191	0.000000511
1	0.000001509	0.000000045	-0.000000069
1	0.000001172	0.000000087	-0.000000631
6	0.000000004	-0.000000024	0.000000639
6	0.000000064	0.000000189	0.000000606
6	0.000000402	-0.000000184	0.000000418
1	-0.000000267	-0.000000315	0.000000149
1	0.000000417	0.000000266	0.000000498
1	-0.000000022	0.000000534	0.000000667
1	0.000000267	0.000000397	0.000000613
1	0.000000368	0.000000298	0.000000007
1	0.000000296	0.000000468	0.000000023
1	0.000000019	0.000000031	0.000000032
6	0.000000634	-0.000000663	-0.0000001225
6	-0.000000205	-0.000000835	-0.00000008
6	-0.000000202	-0.000001158	-0.000001262
1	-0.000000118	-0.000000499	-0.000001028
1	0.000000068	-0.000000679	-0.000001167
1	0.000000229	-0.000000053	-0.000000964
1	0.000000173	-0.000000015	-0.000001552
1	-0.000000321	-0.000000043	-0.000000756
1	-0.000000411	-0.0000000518	-0.000002443
1	0.000000493	-0.000001152	-0.000001412
6	-0.000000078	-0.000000317	-0.000000151
6	-0.000001013	-0.000000841	-0.000000466
6	-0.000000733	0.000000071	0.000000589
1	-0.000000357	0.000000354	-0.000000082
1	-0.000000705	-0.000000696	-0.000000373
1	-0.000000923	-0.000000204	0.000000175
1	-0.000001467	-0.000000456	-0.000000311
1	-0.000001129	0.000000072	0.000000168

1	-0.000001285	-0.000000356	-0.000000064
1	-0.000000898	-0.000000089	0.000000552
6	0.000000818	0.000000854	0.000000224
6	0.000000998	0.000000635	0.000000417
6	0.000001097	0.000000586	0.000000672
6	0.000001099	0.000000885	0.000000734
6	0.000000638	-0.000000048	0.000001084
1	0.000001453	0.000000858	0.000000059
1	0.000000303	0.000000193	0.000000368
7	0.000000596	0.000000831	-0.000000145
8	0.000000695	0.000001345	0.000001069
1	0.000001099	0.000000977	0.000000918
1	0.000001142	0.000000495	0.000000206
17	0.000000417	0.000000623	0.000001122
Zero-point correction=			1.152003 (Hartree/Particle)
Thermal correction to Energy=			1.227403
Thermal correction to Enthalpy=			1.228347
Thermal correction to Gibbs Free Energy=			1.027392
Sum of electronic and zero-point Energies=			-4291.535062
Sum of electronic and thermal Energies=			-4291.459662
Sum of electronic and thermal Enthalpies=			-4291.458718
Sum of electronic and thermal Free Energies=			-4291.659672

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6	0.000005983	-0.000000032	0.000001586
6	0.000000246	0.000006373	-0.000003246
7	-0.000010905	-0.000003624	0.000009106
7	-0.000001794	0.000008885	-0.000007793
16	0.000010953	-0.000003778	-0.00000915
8	-0.000000935	0.000000112	-0.000001951
8	-0.000001426	0.000003981	0.000001049
6	-0.000000899	-0.000000579	-0.00000096
6	0.000001768	0.000001419	0.000000751
6	0.000000346	0.000000046	0.000000068
6	0.000000252	0.000000903	0.000000585
6	0.000000311	0.000000223	0.000000267
6	-0.000000403	0.000000738	-0.000000263
1	0.000000162	0.000000494	0.000000441
1	0.000000057	0.000000662	0.000001016
1	0.000000297	0.000000382	0.000000336
1	0.000000055	0.000000452	0.000000356
6	0.000000714	0.000000533	0.000001018
1	0.000000281	0.000000581	0.000000969
1	0.000000858	0.000000726	0.000000867

1	0.00000388	0.00000562	0.00000193
6	0.000002684	0.000001226	0.000000165
1	-0.000000722	0.000000337	-0.000000227
1	-0.000000479	0.000000099	0.000000083
16	-0.000000054	-0.000005604	0.000008659
8	-0.000001928	0.000000071	-0.000001579
8	-0.00000015	-0.000000024	-0.000001642
6	0.000000503	-0.000000666	-0.000003224
6	-0.000001346	-0.000000065	-0.000000649
6	-0.000000298	-0.000000083	-0.000000886
6	0.000001184	0.000000024	-0.00000115
1	-0.000000075	-0.00000001	-0.000000092
6	-0.000000509	0.000000394	-0.000002011
1	-0.000000307	-0.000000398	-0.000002191
6	-0.000001012	-0.000000182	-0.000001663
1	-0.000000544	-0.000000513	-0.000001123
1	-0.000000195	-0.000000336	-0.000002271
6	-0.000000529	-0.000000371	-0.000001712
1	-0.000000049	-0.000000404	-0.000001967
1	-0.000000256	-0.000000449	-0.000001766
1	-0.000000439	-0.000000029	-0.000001795
6	-0.000001495	-0.000000393	-0.000000093
1	0.000000494	0.000001517	-0.000001488
6	-0.000000494	-0.000000851	-0.000001377
6	-0.000000169	-0.000000898	-0.000000923
6	-0.000000793	0.000000672	-0.000000149
6	0.000000112	0.000000019	-0.000001019
1	-0.000000623	-0.000000144	-0.000001179
6	-0.000000277	0.000000053	-0.000000035
1	0.000000044	-0.000000375	0.000000206
6	-0.000001086	-0.000000812	-0.000000489
1	-0.000000398	-0.000000316	-0.000001154
1	-0.000000185	-0.000000483	-0.000000116
1	-0.000000018	-0.000000476	-0.000000787
6	0.000004284	-0.000000866	-0.000000876
1	0.000000084	0.000000055	-0.000001699
1	-0.000000329	0.000000153	-0.000001838
1	-0.000000472	0.000000897	-0.000001389
6	0.000001425	-0.000000162	-0.000001396
1	-0.000000098	0.000000412	-0.000001474
1	-0.000000026	0.000000603	-0.000001203
1	0.000000253	0.000000581	-0.000001527
79	-0.000001156	0.000000795	0.000000068
6	-0.000000839	0.000002515	-0.000003127

6	0.000001111	-0.000000442	-0.000000246
6	0.000000548	0.000000838	0.000001877
1	-0.000001304	-0.000000609	0.000001989
1	-0.000000307	-0.000000323	0.000001217
7	0.000001358	-0.00000212	0.000003336
7	0.000004055	-0.000001554	0.000000615
6	-0.000001394	0.000000763	0.000001738
6	-0.000000328	0.000000062	-0.000000992
6	0.000001608	-0.00000078	0.000001332
6	0.000000818	-0.000001784	0.000000407
6	-0.000000735	-0.000001276	0.000000624
6	-0.00000098	-0.00000073	0.000000692
1	-0.000000726	-0.000000737	0.000000398
1	-0.000001066	-0.00000072	0.000000596
1	-0.000000928	-0.000001027	0.000000485
6	-0.000001591	-0.000000934	0.000000433
6	0.000000263	0.000001595	0.00000141
6	0.000001554	0.000000154	0.000000822
6	0.000000871	0.000000789	0.000000928
6	-0.000000018	-0.000000166	-0.000000381
6	0.000000587	0.000000677	0.000000783
1	0.000000613	0.000000745	0.000000891
1	0.000000141	0.000000081	0.000000323
1	0.000000577	0.000000676	0.000000398
6	-0.000000085	0.000001967	0.00000101
6	0.00000014	-0.000000192	0.000002046
6	0.000000325	-0.000000419	-0.000000322
1	0.000000654	0.000000111	0.000001261
1	0.000000574	0.000000778	0.000001312
1	0.000000729	0.000000911	0.00000146
1	0.000000656	0.000000509	0.000001626
1	0.000000339	0.00000045	0.000000482
1	0.000001266	0.000000742	0.00000156
1	0.000000969	0.000000819	0.000000805
6	-0.000000198	-0.000001592	-0.000000049
6	0.00000065	0.000000595	0.000000055
6	-0.000000181	0.00000008	0.000000793
1	-0.000000142	-0.000000418	0.000000562
1	-0.000000364	-0.000000373	0.000000607
1	-0.000000481	-0.000000573	-0.000000087
1	-0.000000488	-0.000000008	0.000000048
1	-0.000000159	-0.000000398	0.000000904
1	-0.00000007	-0.000000304	0.000000455
1	-0.000000348	-0.000000481	0.000000561

6	-0.000002266	-0.000003325	0.000000628
6	0.000000224	0.000000059	0.000002257
6	0.000000482	0.000001092	0.000000169
1	-0.000000957	-0.000000603	0.000000538
1	0.000000038	0.000000273	0.000000892
1	0.000000365	0.000000474	0.000001268
1	0.000000273	0.000000601	0.000000586
1	0.000000558	-0.000000445	0.000001483
1	-0.000000839	-0.000001535	0.000001514
1	-0.00000015	-0.00000005	0.000001785
6	-0.000000873	-0.000000946	0.000001051
6	-0.000000807	-0.00000008	0.000000765
6	-0.000001237	-0.000000894	-0.000000053
1	-0.000000221	-0.000000047	0.000000236
1	-0.00000006	-0.000001163	0.000000343
1	-0.000000978	-0.000001277	0.000000253
1	-0.000001264	-0.000001048	0.000000616
1	-0.000000033	-0.000001056	-0.000000401
1	-0.000000058	-0.000000763	-0.000000525
1	-0.000000696	-0.000001023	-0.000000402
6	0.000000291	-0.000001044	-0.000000044
6	0.000000984	0.000001791	-0.000000535
6	0.000000212	0.000000515	0.000000116
6	-0.000000041	0.000001958	-0.000002048
6	0.000002577	-0.000000831	-0.00000101
1	0.000000989	0.000001205	-0.000000037
1	0.000001233	0.000001315	-0.000000157
7	0.000000255	0.000001688	0.000000063
8	0.000003477	-0.000007017	0.000000461
1	0.000000612	0.000001155	-0.000000344
1	0.000000633	0.000000755	-0.000000123
17	-0.000002005	0.000000292	-0.000000295

Zero-point correction=	1.154281 (Hartree/Particle)
Thermal correction to Energy=	1.229160
Thermal correction to Enthalpy=	1.230104
Thermal correction to Gibbs Free Energy=	1.032819
Sum of electronic and zero-point Energies=	-4291.545092
Sum of electronic and thermal Energies=	-4291.470213
Sum of electronic and thermal Enthalpies=	-4291.469269
Sum of electronic and thermal Free Energies=	-4291.666554

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6	-0.000000018	0.000000052	-0.000000896
6	-0.000001076	0.000000563	-0.00000017

7	0.00000706	0.00000339	-0.00000636
7	-0.00000515	-0.00001144	-0.00000394
16	-0.00001032	0.00000188	-0.00002388
8	-0.00001417	0.00000206	-0.00001946
8	-0.00000826	-0.00000016	-0.00000312
6	-0.00000973	-0.00000102	-0.00001897
6	-0.00001406	0.00000096	-0.00001254
6	-0.00001835	-0.00000855	-0.00001654
6	-0.00000657	-0.00001227	0.00000072
6	-0.00000555	0.00002148	-0.00002268
6	-0.00000762	0.00000083	-0.00002089
1	-0.00001926	0.00000013	-0.00000976
1	-0.00002876	-0.00000054	-0.00000006
1	-0.00001593	-0.00000032	-0.00002445
1	-0.00000906	0.00000135	-0.00003015
6	-0.00004506	0.00000055	-0.00003077
1	-0.00002342	-0.00000429	-0.00001446
1	-0.00001671	0.00001243	-0.00001289
1	-0.00002925	-0.00000695	-0.00002027
6	0.00000717	0.00000019	-0.00001662
1	0.00000387	0.00000332	-0.000001
1	0.00000028	-0.00000193	-0.00000146
16	-0.00001461	0.00000282	-0.00000083
8	-0.00001907	0.00000079	0.00000243
8	-0.00001188	-0.00000138	0.00000584
6	-0.00001929	-0.00000275	-0.00000812
6	-0.00002982	0.00000255	-0.00001119
6	-0.00002796	0.00000025	-0.00000442
6	-0.00003169	0.00000219	-0.00002356
1	-0.00002317	0.00000191	-0.00001743
6	-0.0000041	-0.00000125	-0.00000421
1	-0.00002573	-0.00000005	0.00000057
6	-0.00003862	0.00000485	-0.00001474
1	-0.00003432	0.00000189	-0.00002561
1	-0.00003689	0.00000084	-0.00000086
6	-0.00003887	-0.00000772	-0.00002786
1	-0.00004144	0.00000283	-0.00003029
1	-0.0000482	-0.00000077	-0.00001843
1	-0.00004677	0.00000277	-0.00002296
6	0.00000182	-0.00000009	-0.00000695
1	0.00000038	-0.00000008	-0.00001426
6	0.00001497	-0.00000155	-0.00002006
6	0.00001933	-0.00000251	-0.00001267
6	0.00001764	0.00000245	-0.00002592



6	0.000002847	-0.000000036	-0.000001795
1	0.000002101	0.000000048	-0.000000739
6	0.000002132	0.000000155	-0.000003008
1	0.000000944	0.00000011	-0.000003006
6	0.000002866	0.00000011	-0.000002665
1	0.000003355	0.000000023	-0.000001469
1	0.000002293	0.000000117	-0.000003754
1	0.000003524	0.000000071	-0.000002967
6	-0.000000426	0.000000073	-0.000000977
1	-0.000000923	0.000000022	-0.000000387
1	-0.000001134	0.000000168	-0.000001424
1	-0.000000191	0.000000012	-0.000001127
6	0.000000469	-0.000000022	0.000000001
1	0.000000936	0.000000014	0.000000244
1	0.000000204	0.000000005	0.000000538
1	0.000000926	0.000000072	-0.000000252
79	0.000000306	-0.000000215	0.000000324
6	0.000000144	-0.000000238	0.000000464
6	0.000000955	-0.000000481	0.000002735
6	0.000000907	0.00000012	0.000002651
1	0.000000501	-0.000000209	0.000003827
1	0.000001958	-0.00000037	0.00000337
7	0.000002063	0.000000588	0.000002126
7	0.000000271	0.000000425	0.000002639
6	0.00000227	0.000000334	0.000001593
6	0.000003033	-0.000000126	0.000001878
6	0.000002692	-0.00000067	0.000000535
6	0.000003092	-0.000000088	0.000000453
6	0.000002933	-0.000000253	0.000001657
6	0.000003382	0.000000447	0.000000758
1	0.0000038	-0.000000282	0.00000035
1	0.000003018	-0.000000353	0.000000389
1	0.000004079	-0.000000069	-0.000000027
6	-0.00000081	-0.000000322	0.000002354
6	-0.000001258	0.000000366	0.000002473
6	-0.000000712	-0.000000496	0.000003012
6	-0.000002143	-0.00000016	0.000002662
6	-0.00000173	0.000000099	0.00000272
6	-0.000002272	-0.000000314	0.000002412
1	-0.000002734	-0.000000025	0.000002312
1	-0.000001817	0.000000022	0.000002987
1	-0.000002999	-0.000000032	0.00000269
6	-0.000001459	0.000000107	0.00000188
6	-0.000001558	-0.000000152	0.000002713

6	-0.00000222	0.000000085	0.000001429
1	-0.000000506	-0.000000187	0.000001729
1	-0.000001053	-0.000000034	0.000003364
1	-0.000001438	-0.000000004	0.000002682
1	-0.000002224	-0.000000128	0.000002955
1	-0.00000169	-0.000000153	0.000000806
1	-0.000002307	0.000000001	0.000001102
1	-0.000001288	0.000000035	0.000001048
6	-0.000000073	-0.000000092	0.000002923
6	-0.00000002	0.000000081	0.000002464
6	0.000000064	-0.000000233	0.000003809
1	0.000000389	-0.000000144	0.000002539
1	-0.000000589	-0.000000087	0.000001662
1	0.000000382	-0.000000115	0.000002549
1	-0.000000826	-0.000000064	0.000002949
1	0.000000294	-0.000000003	0.00000405
1	-0.000000411	-0.000000144	0.000004119
1	0.000000646	-0.000000013	0.000003883
6	0.00000107	-0.000000018	0.000000977
6	0.000001138	-0.000000006	0.000000505
6	0.00000196	-0.000000246	0.000001945
1	0.000000745	-0.000000565	0.00000195
1	0.000001285	0.000000318	0.000000735
1	0.000000771	-0.000000148	0.000000888
1	0.000001805	0.000000013	0.000000517
1	0.000001879	0.000000349	0.000002694
1	0.000002594	-0.000000033	0.000002164
1	0.000001482	-0.000000168	0.000002344
6	0.000002768	-0.000000228	0.000001506
6	0.000003489	-0.000000099	0.000002155
6	0.000002735	-0.000000071	0.000000713
1	0.000002105	0.000000000	0.000001565
1	0.000003234	-0.000000063	0.000002679
1	0.00000321	-0.000000134	0.000002402
1	0.000003863	-0.000000077	0.000001848
1	0.000002021	0.000000262	0.000000376
1	0.000003401	-0.000000052	0.000000237
1	0.000002633	-0.000000001	0.000000948
6	0.000000822	0.000000393	-0.000003113
6	0.000001365	-0.000000014	-0.000003164
6	0.000001424	0.000000208	-0.000003697
6	0.000000437	0.000000013	-0.000004235
6	-0.000000122	-0.000000053	-0.000003035
1	0.000001928	0.000000189	-0.000004175

1	0.000001245	0.000000205	-0.000002186
7	-0.000000265	-0.000000216	-0.000003466
8	0.000000263	0.000000203	-0.000001664
1	0.000000422	0.000000181	-0.000004313
1	0.000002155	0.000000065	-0.000003147
17	-0.000001149	0.000000003	-0.000003258
Zero-point correction=			1.153119 (Hartree/Particle)
Thermal correction to Energy=			1.228001
Thermal correction to Enthalpy=			1.228945
Thermal correction to Gibbs Free Energy=			1.032284
Sum of electronic and zero-point Energies=			-4291.548627
Sum of electronic and thermal Energies=			-4291.473745
Sum of electronic and thermal Enthalpies=			-4291.472801
Sum of electronic and thermal Free Energies=			-4291.669462

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6	-0.000003939	-0.000000028	0.000000033
6	0.000008287	0.000002213	-0.000001032
7	0.000001353	-0.000000306	-0.000003464
7	-0.000002277	-0.000001316	-0.000004532
16	-0.000001486	0.000001937	0.000001009
8	-0.000002521	-0.000000039	-0.000001286
8	0.000001226	-0.000000997	-0.000000697
6	0.000002063	-0.000000347	0.000000537
6	-0.000002156	0.000000303	0.000000432
6	-0.000002166	-0.000000204	0.000000323
6	-0.000002354	0.000000534	0.000000208
6	0.000000627	-0.000001131	0.000001474
6	-0.000002774	-0.000001599	-0.000000556
1	-0.000000679	-0.000000478	0.000000163
1	-0.000001988	-0.000001406	0.000000331
1	-0.000000759	-0.000000772	0.000000446
1	0.000000634	0.000000117	-0.000000498
6	-0.000001799	-0.000001208	0.000000827
1	-0.000001857	-0.000001647	0.000001172
1	-0.000002318	-0.000001895	0.00000146
1	-0.000002111	-0.000002331	0.000000688
6	0.000000989	0.000002864	0.000001865
1	0.000000141	-0.000000972	0.000000905
1	0.000000328	-0.000000212	0.000000595
16	0.000001069	0.000000513	-0.000005227
8	-0.000000431	-0.000000436	0.000000329
8	-0.000000957	0.000002903	0.000000298
6	-0.000000943	0.000000059	-0.000000244

6	-0.000001403	0.000000622	-0.000001904
6	-0.000000343	0.000001193	-0.000002989
6	-0.000000631	0.000000761	-0.000001892
1	-0.000000688	0.000000064	-0.000001974
6	-0.000002229	0.00000282	-0.000003519
1	-0.000000616	0.000001296	-0.000003287
6	-0.000001166	-0.000000189	-0.000005346
1	-0.000001395	0.000000921	-0.000002966
1	-0.000000747	0.000001868	-0.000004122
6	-0.000001395	0.000001358	-0.000004975
1	-0.000001809	0.000001977	-0.00000489
1	-0.000000654	0.000001246	-0.000004195
1	-0.000001899	0.00000237	-0.000003456
6	0.000004295	0.000003121	0.000004536
1	0.000001531	0.000001031	-0.000001462
6	0.000001587	-0.000000763	0.000001003
6	0.000000914	0.000000971	0.000000651
6	0.000001823	-0.000000271	0.000000576
6	0.000002301	-0.000000535	0.000001562
1	0.000001352	0.000000385	0.00000124
6	0.000001848	0.000001057	0.000000931
1	0.000001161	0.000000315	0.000000569
6	0.000002019	0.000001187	0.00000116
1	0.000002784	0.000000709	0.000001263
1	0.000002229	0.000000663	0.000001014
1	0.000003266	0.000000967	0.000001145
6	-0.000001117	0.000000277	-0.000003346
1	0.000001016	0.000001785	-0.000002004
1	0.000000881	0.00000175	-0.000002105
1	0.000001632	0.000001915	-0.00000233
6	0.000001177	0.000000158	-0.000001998
1	0.000001183	0.000000683	-0.000000874
1	0.000000487	0.000001592	-0.000001427
1	0.000001438	0.00000204	-0.000001037
79	-0.000002079	-0.000000763	0.000000091
6	-0.000000302	-0.000002337	0.000000619
6	-0.000001345	0.000001364	0.000000836
6	-0.000001228	-0.00000113	0.000002219
1	-0.000001163	-0.000001002	0.000001135
1	0.000000241	-0.000002058	0.00000261
7	0.000000421	0.000000107	0.000001422
7	0.000001982	-0.000000768	0.000002035
6	0.000001234	-0.000001999	0.000000845
6	0.000000966	-0.000001905	0.000003276

6	0.00000612	0.00000847	0.00002391
6	0.00002541	0.00000085	0.00002271
6	0.00001489	-0.00001796	0.00003454
6	0.00001406	-0.00000704	0.0000163
1	0.00002245	-0.00000195	0.00001972
1	0.00000723	-0.00001213	0.00003332
1	0.0000173	-0.00000457	0.00003195
6	-0.00001776	-0.00001746	-0.00001366
6	-0.00001468	-0.00000101	-0.00001717
6	-0.00001619	-0.00000475	0.00000189
6	-0.00002804	-0.00001552	0.00000011
6	-0.00001011	0.00000451	-0.00001443
6	-0.00001849	-0.0000067	-0.00000401
1	-0.00002434	-0.00001133	-0.00000725
1	-0.00001509	-0.00000016	-0.00001058
1	-0.00002694	-0.00000419	-0.0000181
6	-0.00002963	-0.00000332	0.00000681
6	-0.00002161	-0.00002318	0.00001305
6	-0.00001354	-0.00001335	-0.00000115
1	-0.00001736	-0.00001159	0.00000449
1	-0.00002521	-0.00001739	0.00000708
1	-0.00002608	-0.00001897	0.00000951
1	-0.00002762	-0.00001717	0.00000329
1	-0.0000144	-0.0000096	-0.00000118
1	-0.00002343	-0.00000907	-0.00000615
1	-0.00001852	-0.00001434	0.00000316
6	-0.00000324	0.00000165	0.00000637
6	-0.0000019	-0.00000273	-0.00001108
6	-0.0000064	-0.00000434	0.000007
1	-0.00000137	-0.00000415	0.00000328
1	-0.00000403	0.00000898	-0.00001072
1	0.00000056	0.0000076	-0.00000268
1	-0.00000097	0.0000051	-0.00000838
1	-0.00000449	-0.00001369	0.00000293
1	-0.00000828	-0.00000302	-0.00000112
1	-0.00000152	-0.00000088	0.00000295
6	-0.0000283	-0.0000097	0.00002156
6	0.00000282	-0.00002526	0.00001968
6	0.00000564	-0.00001653	0.00002895
1	0.00000038	-0.00001471	0.00001944
1	-0.00000506	-0.00000588	0.00001804
1	-0.00000844	-0.00001703	0.00001959
1	0.0000015	-0.00001294	0.00002111
1	-0.00000236	-0.0000165	0.00003288

1	-0.00000101	-0.000001833	0.000003261
1	-0.000000892	-0.000002247	0.000003088
6	0.000001459	0.000001146	0.000001409
6	0.00000129	0.000000302	0.00000241
6	0.000002447	0.000000417	0.000002525
1	0.000001837	-0.000000583	0.000001305
1	0.000001421	-0.000000291	0.0000022
1	0.000001672	0.000000166	0.00000158
1	0.000002542	-0.000000727	0.000001783
1	0.000001886	0.000000002	0.000000684
1	0.000002575	0.000001284	0.000001307
1	0.000001731	0.000000503	0.000000656
6	0.000001394	-0.000000961	0.000000004
6	0.000002479	0.000002366	-0.000000648
6	0.000002313	0.000002124	-0.000001841
6	0.000002634	0.000001525	-0.000001083
6	0.000000905	0.000003207	-0.000002886
1	0.000002692	0.000002208	-0.000000897
1	0.000002253	0.000001003	-0.000000059
7	0.000000339	0.000000663	-0.000000097
8	-0.000003731	0.000002715	-0.000002025
1	0.000001819	0.00000201	-0.000002347
1	0.000002516	0.00000138	-0.000000324
17	0.000000524	0.000001206	-0.000001932

Zero-point correction=	1.154412 (Hartree/Particle)
Thermal correction to Energy=	1.229338
Thermal correction to Enthalpy=	1.230282
Thermal correction to Gibbs Free Energy=	1.032776
Sum of electronic and zero-point Energies=	-4291.553518
Sum of electronic and thermal Energies=	-4291.478592
Sum of electronic and thermal Enthalpies=	-4291.477647
Sum of electronic and thermal Free Energies=	-4291.675153

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6	0.000001673	-0.000000518	-0.000000581
6	-0.000000724	0.000000756	0.000000404
7	-0.000001138	0.000000707	0.000000033
7	0.000001288	0.000000573	-0.000000575
16	-0.000000085	0.000000233	-0.000000064
8	-0.000000002	-0.000000237	0.000000636
8	-0.000000197	0.000000888	-0.000000385
6	-0.000000176	0.000000417	-0.000000625
6	-0.000000721	0.00000066	-0.000000132
6	-0.000001274	-0.000000251	-0.000000585

6	-0.00000828	0.00000709	-0.00000479
6	-0.00000081	0.00000431	-0.000001075
6	-0.00000293	0.00000806	-0.000001293
1	-0.00000393	0.00000032	-0.00000235
1	-0.00000779	-0.00000574	0.00000003
1	-0.000001189	0.00000837	-0.000001109
1	-0.00000476	0.00000934	-0.000001083
6	-0.000001627	0.00000555	-0.00000821
1	-0.000001345	0.00000053	-0.00000128
1	-0.000001518	-0.00000085	-0.000001293
1	-0.000001485	0.000000175	-0.000001442
6	0.00000028	0.000001247	-0.000000611
1	0.00000374	0.00000998	-0.00000053
1	0.00000248	0.000001199	-0.00000478
16	0.000001586	0.00000708	-0.000000107
8	0.00000775	0.000001042	-0.00000246
8	0.000001359	0.00000532	0.000000717
6	0.00000116	0.00000694	-0.000000166
6	0.00000515	0.00000465	0.00000332
6	0.00000644	0.00000345	-0.0000001
6	0.000001604	0.00000479	0.000001011
1	0.000001572	0.00000734	0.00000058
6	0.00000492	0.00000262	0.00000428
1	0.00000688	0.00000678	0.000000178
6	0.000002359	0.000001238	0.00000167
1	0.000001968	0.00000724	0.000000881
1	0.00000947	0.00000037	0.000000634
6	0.00000141	-0.000000197	0.000000392
1	0.000001361	0.00000298	0.000000774
1	0.000001836	0.00000315	0.000000337
1	0.000001333	0.000000114	0.000000723
6	0.00000028	0.00000402	0.000000929
1	0.00000773	-0.00000238	0.000000284
6	0.00000151	0.000001554	-0.000000663
6	0.00000133	0.000001358	-0.000000961
6	-0.00000097	0.000001247	-0.000000908
6	-0.00000056	0.000001666	-0.00000118
1	0.00000227	0.000001428	-0.000000728
6	-0.00000504	0.000001442	-0.000001074
1	0.00000148	0.000001117	-0.000000726
6	-0.00000493	0.000001784	-0.000001275
1	-0.00000029	0.000001755	-0.00000122
1	-0.00000589	0.000001401	-0.000001455
1	-0.00000474	0.000001795	-0.000001542

6	0.00000788	-0.00000224	0.00000292
1	0.00001184	-0.00000006	0.000000447
1	0.00000309	-0.00000378	0.000000551
1	0.00001069	-0.00000202	0.00000076
6	0.00000071	0.00000182	0.000000412
1	0.00001192	0.00000075	0.000000096
1	0.00000102	0.000000896	0.000000305
1	0.00001058	0.000000277	0.000000392
79	-0.00000213	-0.000000574	0.000000933
6	0.000000545	-0.000000375	-0.000000363
6	-0.00000058	-0.00000107	0.000000313
6	-0.000000146	-0.000000896	0.000000459
1	-0.000000101	-0.000001296	0.000000763
1	-0.000000578	-0.000001127	0.000000036
7	-0.000000425	-0.000000546	0.000000524
7	-0.000000303	-0.000000747	0.000000734
6	-0.000000775	-0.000000341	-0.000000471
6	-0.00000002	-0.000000665	0.000000179
6	-0.000000794	-0.000000272	-0.000000254
6	-0.000000303	-0.000000128	-0.000000017
6	-0.000000973	-0.000000389	-0.000000476
6	-0.000000839	-0.000000147	-0.000000604
1	-0.000000545	-0.000000057	-0.000000227
1	-0.000001236	-0.000000309	-0.000000488
1	-0.000001089	-0.000000013	-0.000000676
6	0.000000041	-0.000000643	0.000000014
6	0.000000403	-0.000001508	0.000001155
6	0.000000351	-0.000000739	0.000000916
6	0.000000494	-0.000000777	0.000000128
6	0.000001096	-0.000001384	0.000001199
6	0.000000927	-0.000000758	0.000000072
1	0.000000378	-0.000000912	0.000001047
1	0.000000859	-0.000001071	0.000001378
1	0.000000902	-0.000000094	0.000001317
6	-0.000000096	-0.000001024	0.000000624
6	-0.000000399	-0.000001377	0.000000655
6	-0.000000312	-0.000000806	0.000000211
1	-0.000000152	-0.000000973	0.000000034
1	-0.00000003	-0.000001474	0.000000744
1	-0.000000514	-0.000001347	0.000000055
1	-0.000000115	-0.000001326	0.000000905
1	0.000000207	-0.000000364	0.000000699
1	-0.000000068	-0.000000768	0.000000467
1	-0.000000298	-0.000000697	0.000000371



6	0.000000835	-0.000001166	0.000001112
6	0.000000974	-0.000000454	0.000000684
6	0.000000533	-0.000001001	0.000001309
1	0.000000716	-0.000000793	0.000000684
1	0.000001406	0.000000364	0.000000385
1	0.000000092	-0.000000336	0.000001104
1	0.000000884	-0.000000404	0.000001423
1	0.000000409	-0.000001379	0.000001286
1	0.00000007	-0.00000111	0.000001373
1	0.000000733	-0.000001198	0.00000117
6	-0.000000797	-0.00000061	-0.000000123
6	-0.000000977	-0.000000413	-0.000000281
6	-0.000001186	-0.000001016	-0.000000088
1	-0.000000744	-0.000000892	0.000000117
1	-0.000000675	-0.000000365	-0.000000028
1	-0.000001025	-0.000000593	-0.000000345
1	-0.000001174	-0.000000322	-0.000000584
1	-0.000001225	-0.000001099	-0.000000084
1	-0.000001435	-0.000000888	-0.000000363
1	-0.000001375	-0.000001062	-0.000000188
6	-0.000000114	-0.000000198	0.000000263
6	-0.000000282	-0.000000544	0.000000017
6	-0.000000007	-0.000000108	0.000000248
1	-0.000000064	-0.000000565	0.000000212
1	-0.000000529	-0.000000862	0.000000269
1	0.000000001	-0.000000561	0.000000438
1	-0.000000323	-0.000000375	0.000000059
1	0.000000366	0.000000023	-0.000000357
1	0.00000002	0.00000015	-0.00000007
1	0.000000381	-0.000000005	0.000000301
6	0.000000055	0.000000278	-0.000000376
6	-0.000001044	0.000000741	-0.000000923
6	-0.000000971	0.000000649	-0.000001118
6	-0.000000443	0.000001023	-0.000001116
6	-0.000000655	0.000000714	-0.000000864
1	-0.000001053	0.000000086	-0.000001307
1	-0.000001823	0.000000748	-0.000001403
7	-0.000001024	0.000000231	-0.000000408
8	0.000000636	0.000001186	-0.000000845
1	-0.000000508	0.000000917	-0.000000967
1	-0.00000118	0.000000561	-0.000001122
17	0.000000022	0.000000416	-0.000000357

Zero-point correction=

1.152226 (Hartree/Particle)

Thermal correction to Energy=

1.227338

Thermal correction to Enthalpy=	1.228283
Thermal correction to Gibbs Free Energy=	1.030734
Sum of electronic and zero-point Energies=	-4291.525011
Sum of electronic and thermal Energies=	-4291.449898
Sum of electronic and thermal Enthalpies=	-4291.448954
Sum of electronic and thermal Free Energies=	-4291.646503

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6	-0.000015794	0.000000147	0.000000846
6	0.000002509	0.000003671	0.000000161
7	0.000008429	0.000007624	0.000022979
7	0.000000535	-0.000004835	-0.000000961
16	0.000001103	-0.000004978	-0.000010807
8	-0.000001565	-0.000004846	-0.000001695
8	-0.000000068	0.000002382	-0.000001239
6	-0.000004317	-0.000006387	0.000003829
6	0.000001129	-0.000000033	-0.000001322
6	-0.000002453	-0.000002318	-0.000001835
6	-0.000001001	0.000000328	-0.000001063
6	0.000001295	-0.000001599	0.000004517
6	0.000000304	0.000001448	-0.000000989
1	-0.000001123	-0.000001294	-0.000000187
1	0.000000345	-0.000001672	-0.000000149
1	-0.000000002	-0.000001778	0.000000147
1	-0.000001322	-0.000001872	0.000001054
6	-0.000001666	-0.00000252	0.000001205
1	0.000001423	-0.000000222	-0.000001453
1	-0.000000788	-0.000001137	0.00000013
1	-0.000000045	-0.000002762	-0.000001492
6	-0.000000595	0.000006945	-0.000011483
1	0.000001288	-0.000002866	0.000002404
1	0.000000878	-0.000003758	0.000005454
16	0.000005812	0.000004751	-0.000001391
8	-0.00000226	0.000000705	0.000004991
8	-0.000003488	-0.000006598	0.000002357
6	0.000003895	-0.000000658	-0.000000981
6	-0.000000205	0.000000087	0.000006233
6	0.000000042	0.000000766	0.000002435
6	-0.000001519	-0.000001133	0.000000803
1	0.000000747	-0.000000427	-0.000000744
6	0.000000457	-0.00000001	-0.000001563
1	-0.000000296	0.000000518	0.000001235
6	0.000001413	0.000002569	0.000002907
1	0.00000157	0.000001124	0.000001411

1	0.000000747	0.00000147	-0.000000522
6	-0.000000508	0.000000208	0.000000037
1	0.000000758	0.000001371	0.0000000374
1	0.000000483	0.000001089	0.000001446
1	0.000001588	0.000002088	0.000001242
6	0.000002549	0.000000915	0.0000008593
1	0.000001325	-0.000001675	-0.000000389
6	0.000003387	0.000000307	0.0000003543
6	0.000003172	0.000001813	0.000002497
6	-0.000001169	0.000001453	0.000000015
6	-0.000001389	-0.00000135	0.000001755
1	0.000000562	-0.000001352	0.000000887
6	0.000003898	0.000000711	0.000001696
1	-0.00000157	-0.000002422	0.000000118
6	-0.000000212	-0.000002095	0.000000174
1	0.000000394	-0.000000525	0.000001904
1	0.000000157	-0.000000059	0.000000767
1	0.000000347	-0.000000318	0.00000101
6	0.000000182	-0.000000451	-0.00000353
1	0.000001196	-0.000000134	0.000000866
1	-0.000000679	0.000000692	-0.000000039
1	-0.000000816	0.000000074	0.000001757
6	0.000001359	0.000001637	-0.000005358
1	0.000001481	-0.000001949	0.000002591
1	-0.000000766	-0.000001289	0.000001071
1	-0.000000238	-0.000002451	0.000000914
79	-0.000000263	-0.000006569	-0.000001209
6	0.000007398	-0.000000033	0.000000255
6	0.000000838	-0.00000231	0.000003547
6	-0.000004321	0.00000088	-0.000004966
1	-0.000001387	0.000000738	-0.000001501
1	-0.000000223	0.000000103	-0.000001132
7	-0.000001475	0.000006784	-0.000002634
7	0.000001311	0.000000186	0.000000741
6	-0.000001917	-0.000002448	-0.000000832
6	0.00000183	0.000003825	-0.000000031
6	0.000005238	0.000002673	-0.000001217
6	-0.000000461	0.000000468	-0.000002384
6	-0.000001147	0.000000065	-0.000001641
6	-0.000001491	0.000000066	-0.000000444
1	-0.000000018	0.000000541	-0.000000398
1	-0.000000714	0.000000238	-0.000000785
1	0.000000133	0.000001544	-0.000001156
6	-0.000005789	-0.000000039	0.00000103

6	-0.00000632	0.00000473	-0.0000049
6	0.0000048	-0.000003545	-0.000002542
6	0.000001396	-0.000002909	-0.000001062
6	-0.000000263	-0.000001108	0.000001721
6	-0.000000861	0.000001391	-0.000001298
1	-0.000001069	-0.000000568	-0.000000728
1	-0.00000113	-0.000000103	0.000001139
1	-0.000000103	-0.000001174	0.000000411
6	0.000001899	0.000002495	-0.000000867
6	-0.000001046	-0.000002753	0.000000377
6	-0.00000004	-0.000004094	-0.000002538
1	0.000000032	-0.000001079	0.00000064
1	-0.000000333	-0.000001046	-0.000001407
1	-0.000000612	-0.000001651	-0.000001117
1	-0.000001	0.000000001	-0.000001262
1	-0.000000084	0.000000983	-0.000001158
1	0.000000025	-0.000001387	-0.000000133
1	-0.000001597	0.000000286	0.000000087
6	-0.000004038	0.000004882	0.000001385
6	0.000002388	-0.000002173	0.000000666
6	0.000001474	-0.000001095	-0.000002684
1	-0.000001519	-0.00000077	-0.000000884
1	0.000001737	0.000000475	0.000001218
1	0.000000208	0.000001353	0.000000079
1	0.00000019	0.000000597	-0.000000462
1	0.000000787	0.000000098	-0.000000566
1	-0.000000801	-0.000000231	-0.000000427
1	-0.000000485	0.000001354	-0.000000034
6	-0.000000373	0.000004231	-0.000000784
6	-0.000002687	-0.000004215	-0.000002381
6	-0.000002843	-0.000001672	-0.000001427
1	0.000000171	0.000000349	-0.000001631
1	-0.000003217	0.000002358	0.000000972
1	0.000000019	-0.000000387	-0.000000701
1	-0.00000008	0.000000702	0.000000011
1	-0.000000155	-0.000000144	-0.000001205
1	0.000000256	0.000001931	-0.000002893
1	-0.000000925	-0.000000391	-0.000001664
6	0.000000813	0.000001062	-0.000002806
6	0.000000703	0.000002743	0.000001054
6	0.000000104	0.000004177	-0.000000655
1	-0.000001294	0.000001142	-0.000000746
1	-0.000000302	0.000000398	-0.00000154
1	-0.000000114	0.000001766	-0.000000971

1	-0.00000638	0.000001292	-0.000001365
1	0.000000159	-0.000000499	0.000000033
1	0.000000407	0.000001644	0.000000395
1	0.00000048	0.000001449	0.000000272
6	-0.000005324	0.000003678	0.000004088
6	-0.000003051	0.000000492	-0.000003626
6	0.000001079	0.000000036	-0.000001952
6	0.000002188	-0.000001694	-0.000001799
6	-0.000000148	0.000003868	0.000009066
1	0.000000304	0.000001083	0.000000806
1	0.000000794	0.000000568	0.000002301
7	0.000007889	-0.00000748	-0.000015785
8	-0.000003833	0.000005352	0.000005836
1	0.000000331	0.0000006	-0.000000472
1	0.000000644	-0.000001193	0.000000181
17	0.00000092	0.000002703	-0.000004588

Zero-point correction=

1.155044 (Hartree/Particle)

Thermal correction to Energy=

1.229557

Thermal correction to Enthalpy=

1.230501

Thermal correction to Gibbs Free Energy=

1.036544

Sum of electronic and zero-point Energies=

-4291.537545

Sum of electronic and thermal Energies=

-4291.463032

Sum of electronic and thermal Enthalpies=

-4291.462088

Sum of electronic and thermal Free Energies=

-4291.656045

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6	-0.00000655	0.000000412	-0.000000202
6	0.000000776	0.000000633	0.000000651
7	0.000000265	-0.000000358	0.000000715
7	0.000000353	-0.000000538	-0.000000822
16	-0.000000419	0.000000087	0.000001096
8	-0.000000499	0.000000906	-0.000000112
8	-0.00000063	0.000001081	0.00000012
6	-0.000000781	0.000000595	0.000000963
6	-0.000000983	0.000000311	0.000000501
6	-0.00000178	-0.000000159	0.000000797
6	-0.00000118	0.000000928	0.000000993
6	-0.000001333	0.000000704	0.000001024
6	-0.000001065	0.000000605	0.000001364
1	-0.000001081	0.000000658	0.000000622
1	-0.000001912	0.000000029	0.000000835
1	-0.000001464	0.000000994	0.00000014
1	-0.000000783	0.000001299	0.000001168
6	-0.000002087	0.000000525	0.000001101

1	-0.00000207	0.000000755	0.000001325
1	-0.000002237	0.000000343	0.000001316
1	-0.000002107	0.000000627	0.000001212
6	-0.000000511	0.000000638	0.000000854
1	-0.000000367	0.000000722	0.000000574
1	-0.000000875	0.000001116	0.000000091
16	0.000000765	0.000001636	-0.000000495
8	0.000001266	-0.000000056	0.000000985
8	0.000000479	0.000000268	0.000000097
6	0.00000177	0.000000466	0.00000017
6	0.0000016	0.000000371	-0.000000363
6	0.000000867	0.000000197	-0.000000503
6	0.000003039	0.000000075	-0.00000023
1	0.000001614	0.000000208	-0.000000201
6	0.000000613	0.000000111	0.000001245
1	0.000000926	0.000000237	-0.000000037
6	0.000001677	-0.000000128	-0.000000714
1	0.000002138	0.000000061	-0.000000621
1	0.000001599	-0.000000151	-0.000000695
6	0.000002423	-0.000000284	-0.000000942
1	0.000001804	-0.000000594	0.000000389
1	0.000003193	-0.000000927	-0.000001646
1	0.000001476	0.000000921	-0.000001716
6	0.000000718	-0.000000294	-0.000000127
1	0.000000155	-0.000000228	-0.000000299
6	-0.000000006	0.000000454	0.000000039
6	0.000000638	0.000001039	0.000000915
6	-0.0000002	0.000001119	0.000001086
6	0.000000205	0.00000157	0.000001426
1	0.000000547	0.000001596	0.000000546
6	0.000000208	0.000001274	0.000001157
1	-0.000000447	0.000001011	0.000001053
6	0.000000238	0.000001164	0.000001398
1	0.000000738	0.000001786	0.000001141
1	-0.000000116	0.000001594	0.000001364
1	0.000000432	0.000001828	0.000001416
6	0.000000854	-0.000000556	-0.000000434
1	0.000000846	-0.000000367	-0.000000598
1	0.000000448	0.00000017	-0.000000396
1	0.000000496	-0.000000512	-0.000000827
6	0.000000744	0.000000428	-0.000000395
1	0.000001097	0.000000624	0.000000164
1	0.000000966	0.000000047	-0.000000345
1	0.000000764	-0.000000355	-0.00000022

79	0.00000024	-0.000000623	0.000000289
6	0.000000968	-0.000000655	-0.000000366
6	-0.000000263	-0.000000775	-0.000000148
6	-0.000000413	-0.000000306	-0.000000994
1	-0.000000643	-0.000001026	-0.000000892
1	-0.000000447	-0.000001074	-0.000000401
7	-0.000000751	-0.000000334	-0.000000649
7	-0.000000763	-0.000001321	-0.000000459
6	-0.000001073	0.000000908	-0.000000882
6	0.000000382	-0.000000146	-0.000000043
6	-0.000000793	-0.000000252	-0.000000002
6	0.000000206	-0.000000325	0.000000108
6	-0.000000506	-0.000000122	0.000000602
6	-0.000000083	0.000000279	0.000000655
1	0.000000106	0.000000333	0.000000589
1	-0.000001348	0.000000182	0.000000071
1	-0.000000405	0.000000451	0.000000593
6	-0.000000306	-0.000000372	-0.000001007
6	-0.000000318	-0.000001245	-0.000000392
6	-0.000000133	-0.000002352	-0.000001358
6	-0.000000585	-0.000001234	-0.000000741
6	0.000000349	-0.000001181	-0.000000753
6	0.000000257	-0.000001013	-0.000001099
1	-0.000000448	-0.000001177	-0.000000973
1	0.000000582	-0.000001137	-0.000001175
1	0.000000109	-0.000001206	-0.000001285
6	-0.000000536	-0.000000803	-0.000000139
6	-0.000001083	-0.000001405	-0.000000671
6	-0.000000664	-0.000000488	0.000000115
1	-0.000000064	-0.000001025	-0.000000443
1	-0.000001194	-0.000001188	-0.000000685
1	-0.000001464	-0.000001085	-0.000000457
1	-0.000001192	-0.000001344	-0.000000877
1	-0.000000783	-0.000000338	-0.000000252
1	-0.000000772	-0.000000775	-0.000000423
1	-0.00000139	-0.000000597	-0.000000282
6	-0.000000359	-0.000000559	-0.000000075
6	0.000000766	-0.000000802	-0.000001241
6	0.000000422	-0.000001503	-0.000001341
1	0.000000103	-0.000001099	-0.000000088
1	0.000001141	-0.000000864	-0.000001249
1	0.00000121	-0.000000089	-0.000001031
1	0.000000913	-0.00000113	-0.000001159
1	0.000000369	-0.000001403	-0.000001319

1	0.00000058	-0.00000149	-0.000001546
1	0.000000635	-0.000001317	-0.00000137
6	-0.00000131	-0.000000676	0.000000462
6	-0.00000137	-0.000000301	-0.000000101
6	-0.000001398	-0.000000517	0.000000141
1	-0.000001099	-0.000000477	-0.000000475
1	-0.000000691	-0.000000223	0.000000168
1	-0.000001488	-0.000000386	0.000000346
1	-0.00000125	-0.000000089	0.000000336
1	-0.000001352	-0.000000439	-0.000000104
1	-0.000001378	-0.000000422	0.0000002
1	-0.000001741	-0.000000584	-0.000000097
6	0.000000786	0.000000571	-0.000000464
6	0.000000178	-0.000000315	-0.000000187
6	0.000000714	0.0000004	-0.000000416
1	0.000000153	-0.000000568	0.000000131
1	0.000000386	-0.000000584	-0.000000562
1	0.000000701	-0.00000029	-0.000000585
1	0.000000043	0.000000012	-0.000000112
1	0.000000798	0.000000434	-0.00000017
1	0.000000477	0.000000266	0.000000143
1	0.000000927	-0.000000134	-0.000000112
6	0.000000531	0.000000464	0.000000493
6	-0.000000419	0.000001092	0.000000131
6	0.000000684	0.000000585	0.000001051
6	0.000000967	0.000001109	0.000000428
6	0.000000116	0.000000962	0.000000754
1	0.000000455	0.000000766	0.0000008
1	0.0000003	0.000000151	0.00000048
7	-0.000000031	0.000001238	-0.000000031
8	0.000000666	0.000001107	0.000001219
1	0.000000875	0.000001268	0.000000906
1	-0.000000021	0.000000402	0.000000508
17	0.000000878	0.000001245	0.000001067
<b>Zero-point correction=</b>			<b>1.152791 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>1.227767</b>
<b>Thermal correction to Enthalpy=</b>			<b>1.228711</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>1.029606</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-4291.532976</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-4291.458000</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-4291.457056</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-4291.656161</b>

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6	0.000001485	-0.000003763	-0.000001434
6	-0.000001808	0.000000094	0.000002087
7	-0.000001471	0.000003328	-0.000005093
7	-0.00000174	0.000002344	-0.000002774
16	-0.000000296	-0.000000656	0.000003148
8	-0.000001003	-0.000000787	-0.000001119
8	-0.000000507	-0.000000912	0.000001879
6	0.000000912	0.000002511	0.00000184
6	0.000000321	0.00000023	-0.000000451
6	-0.00000098	0.00000092	0.000000302
6	-0.000000388	0.000001974	0.00000194
6	0.000000947	0.000001593	-0.000001048
6	-0.000001456	0.000000934	-0.000000317
1	0.000000152	0.000001256	0.000000098
1	0.000000211	0.000001164	0.00000042
1	-0.000000616	0.000001707	0.000000656
1	-0.000000135	0.000001284	0.000000248
6	-0.00000038	0.000001953	0.000000353
1	-0.000000322	0.000001772	0.000000651
1	0.000000072	0.000001784	0.000000743
1	-0.00000026	0.000001867	0.000000624
6	0.000001725	0.000001349	0.000003085
1	-0.000000452	0.000000465	-0.000000893
1	0.000000175	0.00000063	0.000000155
16	0.000003167	-0.000004477	0.00000389
8	0.000001412	0.00000125	-0.00000059
8	0.000000426	0.000001524	-0.000001741
6	0.00000023	0.000000148	0.00000062
6	0.000001735	0.000000147	0.000000814
6	0.000000131	0.000000178	-0.000001258
6	0.000001656	-0.000001192	0.000000289
1	0.000001736	0.000000002	0.000000374
6	0.000001652	-0.000000672	0.000000846
1	0.000001174	-0.000000169	-0.000000157
6	0.000001617	-0.000000395	0.000000552
1	0.000001987	-0.000000303	0.000000623
1	0.000001393	-0.000000793	0.000000127
6	0.000002053	-0.000001076	0.000000295
1	0.000001944	-0.000000754	0.000000585
1	0.000001949	-0.00000102	0.000000123
1	0.000001814	-0.000000902	0.000000014
6	0.000000664	0.000000207	0.000000915
1	0.000000264	-0.00000048	-0.000000288
6	-0.000001863	0.000000385	0.00000103

6	0.000000321	0.000002639	0.000000405
6	-0.000001622	0.000001477	-0.000000089
6	-0.000001936	0.000000983	-0.000000913
1	-0.00000131	0.000000192	0.000000269
6	0.000000509	0.000002183	0.000000698
1	-0.000000103	0.000000902	0.000000739
6	-0.00000118	0.00000073	0.000000443
1	-0.000001276	0.000001258	0.00000013
1	-0.000000567	0.000001597	0.000000434
1	-0.000001062	0.000001795	0.000000251
6	0.000001255	0.000000407	0.000000724
1	0.000001224	-0.0000001	-0.000000101
1	0.000001178	-0.000000785	0.000000405
1	0.000000555	-0.000000396	0.000000086
6	0.000000062	-0.000000362	0.000000456
1	-0.000000075	0.000000298	0.000000159
1	0.000000147	0.000000947	0.000000329
1	0.000000417	0.000000145	0.000000958
79	-0.000000355	-0.000000919	-0.000002838
6	-0.000004688	-0.000002231	0.000007025
6	-0.000000389	-0.000000453	-0.000000912
6	-0.000000568	-0.000000809	-0.000002277
1	-0.000000529	-0.000001229	-0.000000092
1	-0.0000006	-0.000001084	-0.000000322
7	0.00000237	-0.000002134	-0.000001611
7	0.00000275	0.000001319	-0.000000881
6	-0.000001582	-0.000002371	-0.00000293
6	-0.000000399	0.000000623	-0.000000697
6	-0.00000114	0.000001421	-0.000001087
6	-0.000000142	-0.000000843	0.000000106
6	-0.000001205	-0.000000559	-0.000000077
6	-0.000000173	0.000000009	0.00000015
1	-0.000000072	-0.000000923	-0.000000489
1	-0.000001245	0.000000106	-0.00000063
1	-0.000000618	-0.000000076	-0.000000361
6	-0.000000636	0.000000964	0.00000106
6	0.00000005	-0.000001018	-0.000001467
6	-0.000000427	-0.000001447	-0.000000624
6	-0.000000656	-0.000001065	-0.000000212
6	0.000000116	-0.000001129	-0.000000484
6	-0.000000101	-0.000000882	-0.000000355
1	-0.000000221	-0.000000629	-0.00000052
1	0.000000409	-0.000001089	-0.000000093
1	0.000000167	-0.000000889	-0.00000041

6	-0.00000206	-0.00000038	-0.00000069
6	-0.000001134	-0.00000081	-0.000000652
6	-0.000001478	-0.000000096	-0.000000389
1	-0.000000594	-0.000000495	-0.000000823
1	-0.000001004	-0.000000914	-0.00000072
1	-0.000001291	-0.000000511	-0.000000702
1	-0.00000096	-0.000000874	-0.0000004
1	-0.000000319	-0.000000147	-0.000000098
1	-0.000000285	-0.000000002	-0.000000005
1	-0.000000881	0.000000062	-0.000000454
6	-0.000000429	-0.000001513	-0.000000895
6	0.000000435	-0.000001194	-0.000000605
6	0.000000381	-0.000001785	-0.000000276
1	-0.000000016	-0.000001599	0.000000159
1	0.000000377	-0.000000685	-0.000000431
1	0.000000859	-0.000001237	-0.000000086
1	0.000000905	-0.000001003	-0.000000127
1	0.000000166	-0.000001623	-0.000000599
1	0.000000475	-0.000001657	-0.000000543
1	0.000000486	-0.000001651	-0.000000432
6	-0.000003491	0.000000509	0.000000301
6	-0.000000453	-0.000000786	0.000000956
6	0.000000012	-0.000001441	-0.000000636
1	-0.000000474	-0.000000023	-0.000000725
1	-0.000001024	0.000001232	-0.000001276
1	-0.000001118	0.000000162	-0.000000199
1	-0.000001325	-0.000000364	-0.00000062
1	-0.000001057	-0.00000076	-0.000000519
1	-0.000001719	-0.000000067	-0.000000543
1	-0.000001483	-0.000000616	-0.000000703
6	0.000000246	-0.000001873	0.000000496
6	0.000000111	-0.000000903	-0.000000587
6	-0.00000079	0.000000194	-0.000000206
1	0.000000619	-0.000000772	-0.000000459
1	-0.000000032	-0.00000124	-0.000000409
1	0.000000474	-0.000001098	-0.000000213
1	0.000000355	-0.000000814	-0.0000003
1	0.000000638	-0.000000156	0.000000175
1	0.00000078	-0.000000462	-0.000000368
1	0.000000801	-0.00000046	-0.000000184
6	0.000002694	0.000000126	0.000000256
6	0.00000116	0.000000928	0.000001102
6	0.000001098	0.000001168	-0.000000069
6	-0.000000051	0.000002007	0.000000844

6	0.000001693	0.000000841	0.000001521
1	0.00000083	0.000001749	0.000001045
1	-0.000000469	0.000000994	-0.000000151
7	-0.000003744	0.00000192	0.000000441
8	0.000003614	0.000002454	0.000001379
1	0.000000587	0.000001451	0.000000825
1	0.000000301	0.000000761	0.000000418
17	-0.000000251	0.000001387	0.000000035

Zero-point correction=

1.154833 (Hartree/Particle)

Thermal correction to Energy=

1.229538

Thermal correction to Enthalpy=

1.230483

Thermal correction to Gibbs Free Energy=

1.033800

Sum of electronic and zero-point Energies=

-4291.550093

Sum of electronic and thermal Energies=

-4291.475387

Sum of electronic and thermal Enthalpies=

-4291.474443

Sum of electronic and thermal Free Energies=

-4291.671126

Re8

6	-0.000000673	0.000001255	0.000001806
6	-0.000003083	-0.000000729	0.000001396
7	0.000001891	0.000000695	-0.000000716
7	0.000003874	0.000001103	0.000001114
16	-0.000001663	0.000004778	0.000002857
8	0.000001188	0.000002804	0.000000792
8	0.00000112	0.000002171	0.000000485
6	0.000001543	0.00000049	0.000001203
6	0.00000421	0.00000051	0.000001624
6	0.000000864	0.00000011	0.00000206
6	0.000003437	0.00000528	-0.000002717
6	0.000003572	-0.000001499	0.0000008
6	0.000003348	-0.000001471	0.000000082
1	0.000000978	0.000002219	0.00000195
1	0.000002631	0.000000567	0.000000743
1	0.00000256	0.000000072	0.000000975
1	0.000000864	0.000001361	0.000000413
6	0.000004273	0.000000066	-0.000000489
1	0.000003356	-0.000002346	0.0000019
1	0.000004245	-0.000001746	0.000001751
1	0.00000308	-0.000002402	0.000000413
16	0.000000884	-0.000001364	-0.000001432
8	0.000003298	0.000001158	-0.000000272
8	-0.000000911	-0.000000942	0.000001362
6	0.00000038	-0.000001764	-0.000002674
6	0.000000342	-0.000001986	0.000000282

6	-0.00000822	-0.000001897	-0.000000595
6	0.000000955	-0.000001276	-0.000000546
1	0.000001269	-0.000001088	-0.000000147
6	-0.000002094	-0.000003574	-0.000002102
1	-0.000001011	-0.000001894	-0.000001383
6	0.000000181	-0.000003154	-0.000003134
1	0.000000035	-0.000001575	-0.000000761
1	-0.000001612	-0.000002863	-0.000001944
6	-0.000000773	-0.000003071	-0.000003772
1	-0.000001534	-0.000002446	-0.000000245
1	-0.00000128	-0.00000289	-0.000001149
1	-0.000001907	-0.000004166	-0.000001832
6	-0.000000691	-0.000002626	-0.000001673
1	-0.000001049	0.000000727	-0.000000265
6	-0.000001732	0.000001365	-0.000000112
1	-0.000000666	-0.000000698	-0.000000293
1	-0.00000173	0.000000014	-0.000000887
1	-0.000002183	0.000000359	-0.000000141
6	-0.000000683	0.000000509	0.000000143
1	0.000000871	0.000001114	0.000000095
1	0.000001242	0.000000696	0.000000304
1	0.000000395	0.000001382	0.000000561
6	-0.000001006	0.000001018	-0.000000037
6	-0.000001972	-0.000000979	0.000001203
1	-0.000000866	0.000002492	0.000000928
1	-0.000001094	0.000000326	0.000000477
6	-0.000002543	0.000003145	0.000000013
1	-0.000001721	0.000001709	0.000000802
1	-0.000002137	0.000001769	0.000000053
6	-0.000003827	0.000001364	-0.000000026
1	-0.000002321	0.000000932	-0.000000452
1	-0.000001908	0.000001596	0.000000708
1	-0.000004181	0.000001567	-0.000000267
1	-0.000003576	0.00000242	0.000000279
1	-0.00000364	0.000001301	-0.000000013

Zero-point correction=

0.497543 (Hartree/Particle)

Thermal correction to Energy=

0.531772

Thermal correction to Enthalpy=

0.532716

Thermal correction to Gibbs Free Energy=

0.423728

Sum of electronic and zero-point Energies=

-2100.647004

Sum of electronic and thermal Energies=

-2100.612775

Sum of electronic and thermal Enthalpies=

-2100.611831

Sum of electronic and thermal Free Energies=

-2100.720819

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6	-0.000011935	-0.000000013	0.000001885
6	0.000009607	0.000004801	0.000000422
7	0.00000183	0.000000858	-0.000002498
7	-0.000000494	-0.000016543	0.000006113
16	0.000000085	-0.000001007	-0.000000627
8	0.000000683	-0.000002039	-0.000000259
8	-0.000000349	-0.000000825	-0.000001367
6	0.000002241	-0.000000466	-0.000000958
6	0.00000197	-0.000001604	-0.000000946
6	0.000002834	-0.000001947	-0.000001241
6	0.000002542	-0.000000189	-0.000001751
6	0.000002598	-0.000001439	-0.000000808
6	0.000001667	-0.000001684	-0.000000808
1	0.000002105	-0.000001843	-0.000001573
1	0.000003398	-0.000002065	-0.000001487
1	0.000002438	-0.000001318	-0.000000731
1	0.000001804	-0.000000962	-0.000000151
6	0.000003685	-0.000002035	-0.000001315
1	0.000003614	-0.000002395	-0.000001701
1	0.000004125	-0.000002073	-0.00000139
1	0.000003841	-0.000001709	-0.000001089
16	0.000004281	0.000008634	-0.000003837
8	-0.000000175	0.000000162	0.000001552
8	0.000000097	0.000003131	0.000000329
6	0.000002493	0.000002115	0.000002328
6	0.00000271	-0.000000157	-0.000000055
6	0.000002223	0.000002257	0.000001709
6	0.000003206	0.000001073	0.000001092
1	0.000002209	0.000000517	0.000000286
6	0.000003486	0.000001626	0.00000171
1	0.000002495	0.000001982	0.000001602
6	0.000003805	0.000000766	0.000000891
1	0.000003607	0.000000154	0.000000407
1	0.000003716	0.000002292	0.000001869
6	0.000004641	0.00000149	0.000001139
1	0.000004846	0.000001456	0.000001632
1	0.00000498	0.000001069	0.000001339
1	0.000004827	0.000000683	0.000000934
6	0.000005347	0.000005832	0.000002044
1	-0.00000021	0.000001144	0.000001452
6	0.000000022	0.000002281	0.000002027
1	0.000001236	0.00000195	0.000002264
1	0.000001573	0.00000179	0.000001487
1	0.0000006	0.000002564	0.000001875

6	-0.000001185	0.00000228	0.000001178
1	-0.000000422	0.000001838	0.000001264
1	0.000000045	0.000001885	0.000001845
1	-0.000000494	0.000002278	0.00000191
6	0.000002148	-0.000001854	0.000001321
6	0.00000191	0.00000117	-0.000000673
1	0.000002031	0.000000141	-0.000000554
1	0.000001942	-0.000000325	-0.000000087
6	0.000001813	-0.000000059	0.000001026
1	0.000000703	-0.000000025	-0.000000117
1	0.000000689	0.000000532	0.000000391
6	0.000001733	0.000000919	0.000000274
1	0.000002061	0.000000799	0.00000077
1	0.000002489	-0.000000022	0.000000105
1	0.000002133	0.000000822	0.000000884
1	0.000001228	0.000000323	0.000000412
1	0.000001168	0.000000977	0.000001042
79	-0.000000599	0.000001784	0.000000616
6	-0.000002834	-0.000000736	0.000000632
6	-0.000000835	-0.000000452	0.000000649
6	-0.000003458	0.000000118	-0.000001486
1	-0.000003013	-0.00000137	-0.000000829
1	-0.000003287	0.000000169	-0.000000127
7	-0.000002089	0.000000269	-0.000002775
7	-0.000001117	-0.000002021	0.000000265
6	-0.000003181	-0.000000546	0.000001645
6	-0.000002115	0.00000244	0.000000272
6	-0.000000539	0.000001374	0.000001392
6	0.00000038	0.000001465	0.000000805
6	-0.000003317	0.000003005	0.000000579
6	-0.000002376	0.000000362	0.000001971
1	-0.000001374	0.000001527	0.000001174
1	-0.000002154	0.00000187	0.0000014
1	-0.000001544	0.000002684	0.000001782
6	-0.000002089	-0.000002446	-0.000001937
6	-0.000002163	-0.000000423	-0.000001033
6	-0.000000273	-0.000002414	-0.000002246
6	-0.000001167	-0.000001624	-0.000001495
6	-0.000001425	-0.000001419	-0.000002294
6	-0.000001363	-0.000002872	-0.00000173
1	-0.000002082	-0.000001893	-0.000001813
1	-0.000000794	-0.000002893	-0.00000212
1	-0.000001168	-0.000002533	-0.000002282
6	-0.000002797	-0.000000876	-0.000000208

6	-0.000002864	-0.000001279	-0.000001002
6	-0.000001982	-0.000000806	-0.000001898
1	-0.000002613	-0.000000279	-0.000000061
1	-0.000003546	-0.000001057	-0.000001144
1	-0.000003501	-0.000000598	-0.000000781
1	-0.000002983	-0.000001313	-0.000001339
1	-0.000001258	-0.000000591	-0.000000384
1	-0.000001823	-0.000001011	-0.000000831
1	-0.000002099	-0.000000191	-0.000000126
6	-0.000000976	-0.000001212	-0.000001663
6	-0.000000679	-0.000001559	-0.000001118
6	-0.00000184	-0.000002011	-0.000001179
1	-0.000001238	-0.000001214	-0.000001192
1	0.00000072	-0.000001803	-0.000002129
1	-0.000000168	-0.00000018	-0.000001364
1	0.000000033	-0.000002496	-0.000001876
1	-0.000002344	-0.000002114	-0.000001884
1	-0.000001511	-0.000002558	-0.000002408
1	-0.000001546	-0.000001994	-0.000001715
6	-0.000002665	0.000001097	0.000001095
6	-0.00000208	0.000001362	0.000000687
6	-0.00000035	0.000001585	0.000001071
1	-0.000002818	0.000000443	0.000000263
1	-0.000001688	0.000001102	0.000000605
1	-0.000002652	0.000001165	0.000000743
1	-0.000002245	0.000001739	0.000001278
1	-0.000003783	0.000001187	0.000000634
1	-0.000003693	0.000001713	0.000001065
1	-0.000003855	0.000001197	0.000000675
6	-0.00000141	0.000000313	0.000000923
6	-0.000001624	0.000000032	-0.000000705
6	0.000000783	0.000000356	0.000000474
1	-0.000001251	-0.000000251	-0.000000436
1	-0.000002317	0.000000187	0.000000141
1	-0.00000153	-0.000000099	-0.000000151
1	-0.000001681	0.000000681	0.000000678
1	-0.000000538	0.000000372	-0.000000558
1	-0.000000434	0.000000673	0.000000746
1	-0.000000323	-0.000000097	-0.000000177

Zero-point correction=

1.071576 (Hartree/Particle)

Thermal correction to Energy=

1.139791

Thermal correction to Enthalpy=

1.140736

Thermal correction to Gibbs Free Energy=

0.955651

Sum of electronic and zero-point Energies=

-3395.499026



Sum of electronic and thermal Energies=	-3395.430811
Sum of electronic and thermal Enthalpies=	-3395.429867
Sum of electronic and thermal Free Energies=	-3395.614952

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6	0.000004564	-0.000007401	0.000006636
6	-0.000007169	0.000008822	-0.000005451
7	0.000003807	0.000016714	-0.000006645
7	0.000001285	-0.000005399	-0.00000128
16	-0.00000564	-0.000008273	0.000002029
8	-0.000001405	0.000002403	0.000002121
8	-0.0000027	0.000001246	0.000000296
6	-0.000001169	0.000000674	0.000001511
6	-0.000001414	0.000002003	-0.000000093
6	-0.000003016	0.00000243	0.000000957
6	-0.000002947	0.000001083	0.000000887
6	-0.000003825	0.000000552	0.00000036
6	-0.000001773	0.000000562	-0.00000006
1	-0.000002303	0.000000811	0.00000197
1	-0.000002866	0.000001652	0.000001528
1	-0.000003401	0.000000238	0.000000212
1	-0.000002996	0.000000017	0.000000822
6	-0.000004061	0.000001373	0.000000762
1	-0.000003785	0.00000122	0.000000947
1	-0.000003967	0.000001396	0.00000127
1	-0.000004015	0.000001143	0.000000394
16	-0.000003673	0.000002538	0.000003171
8	-0.000001532	-0.000003384	-0.000004939
8	0.000000237	-0.000001453	-0.000001417
6	0.000000015	-0.000001179	-0.000000146
6	-0.000000206	-0.000000021	-0.00000209
6	-0.000002772	-0.000002758	-0.000002699
6	-0.000002403	-0.000001568	-0.00000108
1	-0.000000878	-0.000001287	0.000000678
6	-0.000002815	-0.000001255	-0.000001175
1	-0.0000015	-0.000001639	-0.00000115
6	-0.000001314	-0.000001988	0.000000494
1	-0.000001823	-0.000000055	-0.000000115
1	-0.000001998	-0.000001706	-0.000001568
6	-0.00000243	-0.000000629	-0.000001893
1	-0.000002939	-0.000001417	-0.000001177
1	-0.000002437	-0.00000104	-0.000001063
1	-0.000002939	-0.000000858	-0.000000544
6	0.000000297	0.000000073	-0.000002869

1	-0.000002101	0.000000284	-0.000000584
6	-0.000003818	-0.000000755	0.000000286
1	-0.000001825	-0.000001901	-0.000001809
1	-0.000002302	-0.000000198	0.000000412
1	-0.000001207	-0.000000131	-0.000001072
6	-0.000001285	-0.000001364	-0.000001719
1	-0.000001036	-0.000001042	-0.000000537
1	-0.000001591	-0.000000877	-0.000001361
1	-0.000001681	-0.000000982	-0.000000475
6	0.000000799	-0.000006795	0.000006025
6	-0.000000189	0.000001988	-0.000000515
1	-0.000000933	0.000002507	-0.000000702
1	-0.000000968	0.000001478	0.000001079
6	0.000000806	0.000000105	0.000001138
1	0.000000863	0.000000512	0.000000564
1	-0.000000054	0.000000072	0.000000158
6	-0.000000259	0.000000911	0.000000267
1	-0.000000701	0.000001183	0.000000808
1	0.000000298	0.000001278	0.000001132
1	0.000000189	0.000000057	0.000000621
1	0.000000412	0.000000163	0.000000035
1	0.000000143	0.000000662	0.000000293
79	0.000002983	-0.000001322	0.000002165
6	0.000001108	0.000003943	-0.000001956
6	0.000003883	-0.000001771	-0.000000228
6	0.000000652	0.000000219	0.000000797
1	0.000002672	0.000000058	0.000000668
1	0.000003258	0.000001507	-0.000000783
7	0.000001813	-0.000002281	0.000000037
7	0.000002673	0.000000215	-0.000000265
6	0.000001048	0.000000686	0.000001
6	0.000003087	-0.000004486	0.000001061
6	-0.00000153	-0.000002931	-0.00000363
6	-0.000000696	-0.000001229	-0.000001685
6	0.000002994	-0.000002977	-0.000000033
6	0.00000184	-0.000000594	-0.000001772
1	0.000000772	-0.000000675	-0.000001044
1	0.000001071	-0.000002242	-0.000001356
1	0.000000831	-0.000002053	-0.000001256
6	0.000000466	-0.000002317	0.000000907
6	0.000001112	0.000004227	0.000000405
6	0.000001606	0.000002813	0.00000373
6	0.000003434	0.000001103	0.000000916
6	-0.000000385	0.000001915	0.000000094

6	0.000001044	0.000000145	0.000001441
1	0.00000143	0.000001499	0.000000772
1	0.000001214	0.000001425	0.000000782
1	0.000000815	0.000002234	0.000001642
6	0.000002408	-0.000000747	0.00000102
6	0.000003089	0.000000933	0.000000236
6	0.000000492	-0.000000364	0.000001033
1	0.000001728	0.000000575	-0.000000947
1	0.000003065	0.000000584	0.000000695
1	0.000002872	0.000000066	0.0000002
1	0.000002611	0.000000078	0.000000654
1	0.000001365	-0.000000079	-0.000000225
1	0.000001266	0.000000458	-0.000000014
1	0.000002032	-0.000000121	-0.000000215
6	0.000002682	-0.000000067	-0.000002058
6	-0.000000541	0.000002208	0.000001799
6	-0.000000343	0.000002278	0.000000306
1	0.000001561	-0.000000166	0.000000059
1	0.000000766	0.000001104	0.000001243
1	-0.000000033	0.000001401	0.000001135
1	-0.000000225	0.000000804	0.000001377
1	0.000001779	0.00000174	0.00000136
1	0.00000178	0.000002581	0.000001103
1	0.000001001	0.000001967	0.000001786
6	0.000002586	0.000000458	0.00000194
6	0.000001342	-0.000001407	-0.000002947
6	0.000002435	-0.000001582	-0.000000634
1	0.000001805	-0.000001186	-0.000000082
1	0.000001163	-0.000001425	-0.000000046
1	0.000002387	-0.000001405	-0.000000931
1	0.000001378	-0.000001581	-0.000001479
1	0.000002768	-0.000001253	-0.000001042
1	0.000002506	-0.000001742	-0.00000156
1	0.000002882	-0.000001416	-0.000001386
6	0.000000563	0.00000209	0.000001673
6	0.000000096	-0.000000677	-0.000001348
6	0.000000631	-0.000001077	-0.000000504
1	0.000001259	-0.000000068	-0.000001147
1	0.000001613	-0.000000082	0.000000341
1	0.000001198	0.000000346	0.000000356
1	0.000001611	-0.000000829	-0.000000684
1	-0.000000416	0.000000782	0.000000541
1	-0.000000362	-0.000000709	0.000000171
1	-0.000000027	0.000000036	0.000000557

Zero-point correction=	1.072324 (Hartree/Particle)
Thermal correction to Energy=	1.140131
Thermal correction to Enthalpy=	1.141075
Thermal correction to Gibbs Free Energy=	0.959431
Sum of electronic and zero-point Energies=	-3395.499247
Sum of electronic and thermal Energies=	-3395.431441
Sum of electronic and thermal Enthalpies=	-3395.430497
Sum of electronic and thermal Free Energies=	-3395.612140

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6	-0.00000338	0.000001185	0.000000709
6	0.00000002	0.000000897	0.000001632
7	-0.000001356	0.000000242	0.000000498
7	0.000000026	0.000000945	0.000001465
16	-0.000000974	-0.000000041	0.000000458
8	-0.000001421	0.00000014	-0.000000516
8	-0.000000638	0.000000137	0.000000029
6	-0.00000183	0.000000749	0.000000462
6	-0.00000278	0.000000056	-0.000000153
6	-0.00000297	0.000000935	0.000000447
6	-0.000002751	0.00000102	0.000001292
6	-0.000002049	0.000000744	0.00000102
6	-0.000001353	0.000001312	0.000001012
1	-0.00000268	0.000000315	-0.000000194
1	-0.000003417	0.000000752	0.000000329
1	-0.000001773	0.000001283	0.000001735
1	-0.00000106	0.000000986	0.000001291
6	-0.000003191	0.000001363	0.000001597
1	-0.000002725	0.000001228	0.00000082
1	-0.000003711	0.00000126	0.000000834
1	-0.000003036	0.000001763	0.000001719
16	0.000000059	0.000001462	0.000001963
8	0.000000189	0.000001726	0.000002789
8	-0.000000445	0.000001046	0.00000188
6	0.000001256	0.00000063	0.000001507
6	0.000001407	0.000001262	0.000002236
6	0.000001098	0.000000481	0.000001497
6	0.000002535	0.000000563	0.000002118
1	0.000001448	0.000001357	0.000002457
6	0.000001244	0.000000428	0.000001048
1	0.000000196	0.000000522	0.000000801
6	0.000002251	0.0000001	0.000001005
1	0.000002606	0.000000874	0.000002094
1	0.000001113	0.000000177	0.000000403

6	0.000002682	0.000000101	0.000000775
1	0.000002591	-0.000000187	0.000000494
1	0.000002631	0.000000228	0.000000992
1	0.000003222	0.000000187	0.00000124
6	-0.000000203	0.000001446	0.000002169
1	-0.000000531	0.000001656	0.000002517
6	0.000000574	0.000001468	0.000002486
1	0.000000646	0.000001232	0.000002239
1	0.000000875	0.000001502	0.000002754
1	0.000000265	0.000001778	0.000002903
6	-0.000000629	0.0000013	0.000001905
1	-0.000001229	0.000001256	0.000001677
1	-0.000000508	0.000000931	0.000001499
1	-0.000000835	0.000001522	0.000002247
6	-0.000001734	0.000001024	0.00000062
6	-0.000002024	0.000000784	0.000000629
1	-0.000001963	0.000000848	0.000001149
1	-0.000001516	0.000001276	0.000001492
6	-0.000002707	0.000001141	0.000001016
1	-0.000002196	0.000000472	0.000000158
1	-0.000001632	0.0000007	0.000000655
6	-0.000003066	0.000000989	0.00000072
1	-0.000002472	0.000001352	0.000001538
1	-0.000003047	0.000001188	0.000001059
1	-0.000003527	0.000001225	0.000000972
1	-0.00000329	0.000000725	0.000000244
1	-0.000002729	0.000000893	0.000000645
79	0.000000137	-0.000000141	-0.000000265
6	0.000000356	-0.000000415	-0.000001051
6	0.000000659	-0.000001228	-0.000001902
6	0.000000561	-0.000001422	-0.000002176
1	0.000000288	-0.000001736	-0.000002668
1	0.000001188	-0.000001604	-0.000002208
7	0.000000709	-0.000001213	-0.000001507
7	-0.000000218	-0.00000093	-0.000001677
6	0.000001295	-0.000000696	-0.000000508
6	0.000001928	-0.000000779	-0.000000893
6	0.000001091	-0.00000093	-0.000000767
6	0.000002645	-0.00000095	-0.000000478
6	0.000001431	-0.000000432	-0.000000473
6	0.000002147	-0.000000608	-0.000000049
1	0.000002866	-0.000000593	-0.000000378
1	0.000001237	-0.000000443	-0.000000496
1	0.000002567	-0.000000425	-0.000000005

6	-0.00000558	-0.00000122	-0.0000017
6	-0.000001181	-0.000000854	-0.00000195
6	-0.000000395	-0.000001023	-0.000001534
6	-0.000001817	-0.000001087	-0.000001977
6	-0.000000773	-0.000001048	-0.000001959
6	-0.000001638	-0.000000851	-0.000001933
1	-0.000002298	-0.000000898	-0.000002117
1	-0.000000698	-0.000000925	-0.000001784
1	-0.000001984	-0.00000088	-0.000002048
6	-0.00000138	-0.000000957	-0.000002067
6	-0.000001691	-0.000001373	-0.000002685
6	-0.00000199	-0.000000548	-0.000001583
1	-0.000000846	-0.000000891	-0.000001803
1	-0.000001223	-0.000001596	-0.000002953
1	-0.000001814	-0.000001353	-0.000002706
1	-0.00000218	-0.000001367	-0.000002826
1	-0.000001952	-0.000000309	-0.000001079
1	-0.000002521	-0.000000615	-0.000001722
1	-0.000002141	-0.000000605	-0.000001573
6	0.000000257	-0.000000975	-0.00000157
6	0.000000461	-0.000000617	-0.000001055
6	0.0000007	-0.00000147	-0.000002069
1	0.000000852	-0.000001019	-0.0000013
1	0.000000397	-0.000000473	-0.000000533
1	0.000001084	-0.000000812	-0.000000964
1	0.000000281	-0.000000821	-0.000001223
1	0.000000791	-0.000001655	-0.000002511
1	0.000000522	-0.000001526	-0.000002268
1	0.000001394	-0.000001489	-0.000002075
6	0.000000257	-0.000000829	-0.000001126
6	-0.000000233	-0.000000298	-0.000000588
6	0.000000375	-0.000001072	-0.000001584
1	0.000000111	-0.000000792	-0.000001275
1	-0.000000146	-0.000000079	-0.000000335
1	-0.000000724	-0.000000363	-0.000000788
1	0.000000143	-0.000000154	-0.000000257
1	0.000000668	-0.000001319	-0.000001966
1	0.00000062	-0.000000905	-0.000001406
1	-0.000000141	-0.000001059	-0.000001766
6	0.000002255	-0.000000924	-0.000001128
6	0.000002903	-0.000001266	-0.000001314
6	0.000002421	-0.000000696	-0.000000389
1	0.00000174	-0.000000974	-0.000001076
1	0.000002723	-0.000001547	-0.000001676

1	0.00000308	-0.000001408	-0.000001436
1	0.000003399	-0.000001312	-0.00000097
1	0.000002117	-0.000000309	0.000000048
1	0.00000288	-0.00000058	0.000000025
1	0.000002635	-0.0000007	-0.000000474
6	0.000001648	0.000000383	0.000000882
6	0.000002333	0.00000031	0.000001381
6	0.000002563	0.00000068	0.000001557
6	0.00000222	0.000000464	0.000001218
6	0.000001326	0.000000254	0.000001438
1	0.000003093	0.000000575	0.000001846
1	0.000001219	0.000000318	0.000000968
7	0.000001237	0.000000444	0.00000081
8	0.000000439	0.00000041	0.000000981
1	0.000002266	0.000000603	0.000001636
1	0.000002639	0.000000384	0.000001542
17	0.000000793	0.000000627	0.000001206

Zero-point correction=

1.156519 (Hartree/Particle)

Thermal correction to Energy=

1.231225

Thermal correction to Enthalpy=

1.232169

Thermal correction to Gibbs Free Energy=

1.036316

Sum of electronic and zero-point Energies=

-4178.423273

Sum of electronic and thermal Energies=

-4178.348567

Sum of electronic and thermal Enthalpies=

-4178.347622

Sum of electronic and thermal Free Energies=

-4178.543476

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6	-0.000011395	0.000004494	0.000002948
6	0.000004918	-0.000008041	0.000002314
7	0.000003309	-0.000003623	-0.000003287
7	0.000001542	0.000002325	0.000004702
16	-0.000001621	0.000002748	-0.000001388
8	-0.000000244	0.000000105	-0.00000211
8	0.00000083	0.000001	-0.000000775
6	-0.000000919	0.000002411	0.000000027
6	0.000002349	0.000000609	-0.000002668
6	-0.000000975	0.000000213	-0.000002725
6	-0.000000626	0.000003268	-0.000001143
6	0.000001253	0.00000043	-0.00000242
6	0.000000022	0.00000041	-0.000002038
1	-0.000000097	0.000001137	-0.000001647
1	0.000000105	0.000001626	-0.000002361
1	-0.000000063	0.000001253	-0.000001827
1	0.000000038	0.000000024	-0.000001067

6	0.00000136	0.000001473	-0.000003029
1	0.000000453	0.000001716	-0.000002812
1	-0.000000262	0.000001892	-0.000002962
1	-0.000000266	0.00000177	-0.000002643
16	0.000004079	-0.000001166	-0.00000037
8	-0.00000151	-0.00000164	-0.000000395
8	-0.000004565	0.000002537	0.000000863
6	-0.000001237	0.000002482	-0.000000799
6	-0.000000889	-0.000001633	0.000001669
6	0.000000439	-0.000000719	-0.000000301
6	0.000000107	0.000001376	-0.000001201
1	-0.000000808	0.000000341	0.000000947
6	-0.000000792	0.000001037	0.000000306
1	0.000000801	0.000000861	-0.000001123
6	0.000002131	-0.000003559	0.000000845
1	0.000000366	-0.000000385	0.000000652
1	0.000001393	0.000000013	0.000000185
6	0.000002249	0.000000474	0.000000549
1	0.000001047	-0.000000816	0.000000404
1	0.000000616	-0.000000164	0.000000232
1	0.000000588	-0.000001098	0.000000634
6	-0.000007056	0.000003699	-0.000006127
1	-0.000002764	-0.000000625	0.000000711
6	-0.000000309	-0.00000386	0.000002196
1	-0.000001586	0.000000551	0.00000104
1	-0.000001023	0.000000505	0.000000833
1	-0.000001979	0.000000368	0.000000764
6	-0.000001296	0.000000526	0.000004147
1	-0.000001093	0.000000959	0.000000308
1	-0.000002475	-0.000000683	-0.000000199
1	-0.000002595	0.000000048	-0.000000281
6	-0.000001863	-0.000000668	0.000000129
6	-0.000001789	0.000001191	-0.000001179
1	-0.000000237	0.000000541	-0.000000865
1	-0.000001129	0.000000076	-0.000000683
6	-0.000001961	0.000001192	0.000000033
1	-0.000000654	0.000000494	-0.000000833
1	-0.000000957	0.000000726	-0.000000454
6	-0.000001878	0.000000753	-0.000001275
1	-0.000001572	0.000000914	-0.000001195
1	-0.000001463	0.000001346	-0.000001364
1	-0.000002267	0.000001237	-0.000001108
1	-0.000001559	0.000001096	-0.000001113
1	-0.000001988	0.000000804	-0.000000557



79	0.000003908	0.000003135	0.000003566
6	-0.000003067	-0.000002507	-0.000008898
6	-0.000000597	-0.000002475	0.000004897
6	0.000003643	0.000000026	-0.000002726
1	0.000000532	-0.000000677	0.000000435
1	0.00000114	-0.00000039	0.000001107
7	0.00000245	-0.000001108	0.000004008
7	0.000000458	0.000002801	0.000006539
6	-0.0000015	-0.000001387	0.000001108
6	-0.000000047	-0.000004104	0.000001382
6	-0.000001704	0.000001756	-0.000001991
6	-0.000001318	0.000000115	-0.000000093
6	0.000002722	-0.000002797	0.000001118
6	-0.000001136	-0.000002021	0.000004887
1	0.000000734	-0.000000968	0.000002455
1	-0.000001254	-0.000000784	0.000001893
1	-0.000000555	-0.000001435	0.000002043
6	0.000000866	-0.000002847	-0.000003787
6	0.000002055	0.000000898	0.000000001
6	-0.000000307	0.000000319	-0.000000795
6	0.00000093	0.000001142	-0.000000834
6	0.000002612	-0.000000849	-0.000001214
6	0.000001603	0.000000683	-0.000000603
1	0.000000698	0.000001201	-0.000001666
1	0.000001086	-0.000000053	-0.000001122
1	0.000001362	0.000000704	-0.000001961
6	0.000001351	0.000004485	-0.000002999
6	0.000000688	-0.000002339	-0.000000604
6	-0.00000201	-0.00000178	0.000001452
1	0.000000309	-0.000000093	0.000000066
1	0.000000499	0.000000654	-0.000000262
1	-0.000000109	0.000000471	-0.000000378
1	0.000000558	0.000000974	-0.000000713
1	-0.0000002	0.000001292	-0.000000084
1	0.000000099	0.000000819	-0.000001833
1	-0.000000185	0.000000722	-0.000000991
6	0.000002234	-0.00000235	-0.000000398
6	0.000001782	0.000001034	-0.000000432
6	0.000002513	0.000000935	0.000000104
1	0.000000145	-0.00000048	-0.000000132
1	0.000001623	-0.000000422	0.000000053
1	0.000001709	0.000000002	0.000000045
1	0.000002105	0.000000032	-0.000001044
1	0.000002089	-0.000000793	-0.000000081

1	0.000001922	-0.000000617	-0.000000104
1	0.000002375	-0.000000513	-0.000000067
6	0.000000929	0.000000365	0.000002421
6	-0.000002913	-0.000000795	-0.000000278
6	-0.000001171	-0.000001481	0.000001758
1	0.000000549	0.000001857	-0.000000088
1	-0.000000702	-0.000000593	0.00000134
1	-0.000001668	-0.000000503	0.000000811
1	0.00000022	-0.000000446	0.000000324
1	-0.000000598	-0.000000876	0.000000862
1	-0.000001319	0.000000289	0.000002346
1	-0.000001177	-0.000000898	0.00000085
6	0.000003638	0.000001151	0.000001104
6	0.000001293	-0.000001244	0.000001961
6	0.000000771	-0.000001948	-0.000000411
1	0.000000237	-0.000000481	0.000001202
1	0.000000848	-0.000001659	0.000001841
1	0.0000017	-0.000001522	0.000001582
1	0.000001219	-0.000001268	0.000001853
1	0.000002309	-0.000001124	0.000000917
1	0.000000222	-0.000001518	0.000001917
1	0.000001508	-0.000001133	0.000001288
6	0.00000057	0.000001123	-0.000003595
6	-0.000001107	-0.000001755	0.000001887
6	-0.000000003	-0.000001049	0.000002552
6	0.000000006	0.00000023	0.000000381
6	-0.000000956	-0.000000878	0.000003447
1	0.000000228	-0.000001102	0.000001836
1	-0.000001144	-0.000001525	0.000001501
7	0.000001657	-0.000000699	0.000006416
8	-0.000000254	0.000000385	-0.000011694
1	-0.000000741	-0.000001358	0.000001732
1	0.000001654	0.00000001	0.000000951
17	-0.000001623	-0.000000481	0.000000998

Zero-point correction=

1.158573 (Hartree/Particle)

Thermal correction to Energy=

1.232829

Thermal correction to Enthalpy=

1.233774

Thermal correction to Gibbs Free Energy=

1.041479

Sum of electronic and zero-point Energies=

-4178.435221

Sum of electronic and thermal Energies=

-4178.360964

Sum of electronic and thermal Enthalpies=

-4178.360020

Sum of electronic and thermal Free Energies=

-4178.552314

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6	0.00000104	-0.00000877	-0.000001505
6	-0.000001345	-0.000001021	0.00000159
7	0.000000218	0.00000029	0.000000285
7	0.000000521	0.000000803	0.000000881
16	0.000001372	-0.000001028	-0.000001944
8	0.000001406	-0.000000036	-0.000001616
8	0.000000653	-0.000001385	-0.000001198
6	0.00000111	-0.000001227	-0.000002173
6	0.000001885	-0.000000683	-0.000002163
6	0.000001621	-0.000001515	-0.00000261
6	0.000000988	-0.000001004	-0.0000032
6	0.000001932	-0.000002412	-0.000001919
6	0.000001018	-0.000002203	-0.00000186
1	0.00000157	-0.000000434	-0.000002602
1	0.000002116	-0.000001277	-0.000003314
1	0.00000165	-0.000003188	-0.000002024
1	0.000001071	-0.000002314	-0.000001307
6	0.00000383	-0.000004625	-0.000002552
1	0.000001372	-0.000003547	-0.000002859
1	0.000002151	-0.000002308	-0.000003415
1	0.00000305	-0.000002491	-0.000003241
16	-0.000000845	0.000000617	0.000001158
8	-0.000000668	0.000001258	0.000001675
8	-0.000000788	0.000000955	0.000000349
6	-0.000000891	0.000000904	0.000001463
6	-0.00000146	0.000001252	0.000002467
6	-0.000001278	0.000000932	0.000001163
6	-0.000001897	0.000000996	0.000002557
1	-0.000001521	0.000001096	0.000002635
6	-0.000001118	0.000001075	0.000001973
1	-0.000000516	0.000000881	0.000000814
6	-0.000002026	0.00000092	0.000002803
1	-0.000002168	0.000001396	0.000003242
1	-0.000001054	0.000001146	0.000001544
6	-0.000001792	0.000001825	0.000002456
1	-0.000001164	0.000001043	0.000002784
1	-0.000002159	0.000002457	0.000002403
1	-0.000002449	0.000001432	0.00000298
6	-0.000000801	-0.000000952	0.000001802
1	-0.000001261	0.000000173	0.000001558
6	-0.000001358	-0.000000905	0.000002185
1	-0.000001267	-0.000001087	0.000002092
1	-0.000001715	0.000000042	0.000002075
1	-0.000001374	-0.000001051	0.000002611

6	-0.000000712	-0.000001454	0.000001413
1	0.000000551	-0.000001918	0.00000037
1	-0.000000483	-0.000001601	0.000001293
1	-0.000000596	-0.000001832	0.000001566
6	0.000000437	-0.000000202	-0.000000844
6	0.000000738	0.000000849	-0.000001174
1	0.000001131	-0.000000202	-0.000001163
1	0.000000405	-0.000000128	-0.00000118
6	0.000000488	0.000001554	-0.000001246
1	0.000000451	0.000001037	-0.000001466
1	0.000000389	0.000000973	-0.000000498
6	0.000000642	0.000002117	-0.000001405
1	0.000000419	0.000001129	-0.000000911
1	0.000000888	0.000001068	-0.000001724
1	0.000000592	0.000002462	-0.000001524
1	0.000000725	0.00000232	-0.000001803
1	0.000000226	0.000002386	-0.000000932
79	-0.000000494	-0.000000385	0.000000182
6	0.000000581	0.000000483	-0.00000099
6	-0.000000065	0.000000259	0.000000046
6	0.000000159	0.000001033	-0.000000523
1	0.000000216	0.000001268	-0.000000653
1	-0.000000223	0.000000349	0.000000244
7	-0.000000175	0.000000035	0.000000068
7	-0.000000299	0.000001259	-0.000000552
6	-0.000000715	-0.00000095	0.000000938
6	-0.000000358	-0.000001532	0.000000402
6	-0.000000605	-0.000000328	0.000001157
6	-0.000000151	-0.000002004	0.00000102
6	-0.000001068	-0.00000107	0.000001817
6	-0.000000733	-0.000001841	0.000001916
1	-0.000000198	-0.000002588	0.000000983
1	-0.000001318	-0.000000794	0.000002434
1	-0.000000921	-0.000002263	0.000002077
6	0.000000353	0.000001394	-0.000000855
6	0.000000312	0.000001991	-0.000001063
6	0.000000812	0.000001575	-0.000001509
6	0.000000659	0.000002506	-0.000001284
6	0.000001142	0.000001671	-0.000002304
6	0.00000095	0.000002511	-0.000002014
1	0.000000244	0.00000314	-0.000001028
1	0.000001397	0.000001782	-0.000002711
1	0.000001007	0.000002901	-0.00000232
6	-0.000000254	0.000002256	0.000000013

6	-0.000000426	0.000002913	-0.000000041
6	-0.000000061	0.000002862	0.000000022
1	-0.00000002	0.000001865	0.000000254
1	-0.000000377	0.000002657	-0.000000145
1	-0.000000077	0.000003025	0.000000515
1	-0.000000259	0.000003576	-0.000000251
1	-0.000000488	0.000002345	0.000000019
1	-0.000000418	0.000002973	-0.000000058
1	-0.000000652	0.00000264	0.000000595
6	0.00000121	0.000000647	-0.000001997
6	0.000001571	0.000000466	-0.000002473
6	0.000001243	0.000000805	-0.000002159
1	0.000001009	-0.000000111	-0.000001603
1	0.000001214	0.000000003	-0.00000243
1	0.000001609	-0.000000386	-0.000002599
1	0.000001632	0.000000054	-0.000003048
1	0.000000992	0.000001045	-0.000001916
1	0.000001449	0.000001216	-0.000002586
1	0.000001441	0.000000412	-0.000002374
6	-0.000001134	0.000000429	0.000001632
6	-0.000001308	0.000000069	0.000002045
6	-0.000001149	0.000000527	0.000001767
1	-0.000000943	0.000000832	0.000001123
1	-0.000001016	0.000000514	0.000001925
1	-0.000001497	0.000001285	0.000002256
1	-0.000001653	0.000000248	0.000002616
1	-0.000000886	0.000000371	0.000001531
1	-0.000001489	0.000000093	0.000002332
1	-0.000001343	0.000001098	0.000001972
6	0.000000422	-0.000001335	-0.000000084
6	0.000000371	-0.000001753	-0.000000267
6	0.000000354	-0.000002019	-0.000000044
1	0.000000607	-0.000000069	-0.000000414
1	0.000000391	-0.000001318	-0.000000223
1	0.000000776	-0.000001866	-0.000000871
1	0.000000376	-0.000002313	-0.000000074
1	0.000000666	-0.000002238	-0.000000097
1	0.000000407	-0.000002609	-0.000000214
1	0.000000845	-0.000002146	-0.000000927
6	-0.000000746	-0.000001068	0.000001404
6	-0.000001051	-0.000001576	0.000001717
6	-0.000000785	-0.000002337	0.000001684
6	-0.000000268	-0.000002565	0.000001056
6	0.000000198	-0.000001912	0.000000491

1	-0.00000087	-0.000002841	0.000002067
1	-0.000000822	-0.00000043	0.000001506
7	0.000000101	-0.00000094	0.000000773
8	-0.000000274	-0.00000188	0.000000389
1	-0.000000097	-0.00000318	0.00000094
1	-0.000001219	-0.000001435	0.000002322
17	0.000000597	-0.000002286	-0.00000034
Zero-point correction=			1.157252 (Hartree/Particle)
Thermal correction to Energy=			1.231685
Thermal correction to Enthalpy=			1.232629
Thermal correction to Gibbs Free Energy=			1.036797
Sum of electronic and zero-point Energies=			-4178.434457
Sum of electronic and thermal Energies=			-4178.360024
Sum of electronic and thermal Enthalpies=			-4178.359080
Sum of electronic and thermal Free Energies=			-4178.554912

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6	-0.000000952	0.000012905	-0.000002118
6	0.000001189	-0.000016857	0.000004591
7	-0.000002934	-0.000004763	-0.000001855
7	0.000000745	0.000012451	0.000010835
16	0.000004251	0.000000837	0.000000614
8	-0.000002948	-0.000000189	0.000000166
8	-0.00000044	0.000000749	-0.00000173
6	0.000000663	-0.000000327	-0.000000916
6	-0.00000124	-0.000001095	-0.000001258
6	-0.000000449	-0.000000296	-0.000001731
6	-0.000000719	-0.000000266	-0.00000045
6	-0.000000994	0.000001271	-0.000002265
6	0.000000523	0.000000514	-0.000000106
1	-0.000000243	0.00000065	-0.000001559
1	-0.000000786	-0.000000432	-0.000001723
1	0.000000145	0.00000049	-0.000001279
1	0.000000083	0.000000396	-0.000001257
6	-0.000000753	-0.000000425	-0.00000182
1	-0.00000055	0.000000346	-0.000002069
1	-0.000000478	-0.000000214	-0.000001773
1	-0.000000216	0.000000305	-0.000001639
16	0.000001656	-0.000006277	-0.000006751
8	-0.000000394	-0.000000985	0.000001421
8	-0.000000593	-0.000000373	0.0000006
6	-0.00000071	0.000000812	-0.000000495
6	0.000000594	-0.000001106	0.000002206
6	0.000000691	-0.000000994	0.000000951

6	0.000001373	-0.000000975	0.000001726
1	0.000000142	-0.000000028	0.000001364
6	-0.000000335	-0.000001282	0.00000167
1	-0.000000404	-0.000000902	0.000001004
6	-0.000000471	0.000000285	0.000000899
1	0.000000242	-0.000000072	0.000001913
1	0.000000003	-0.000001198	0.000001262
6	-0.000000252	-0.000000938	0.000001809
1	0.000000267	-0.000001113	0.000001579
1	0.000000261	-0.000001696	0.000002145
1	0.000000129	-0.000000855	0.000002398
6	-0.000001446	0.000000009	-0.00000299
1	0.000000434	0.000000738	0.00000079
6	0.000000885	0.000000168	0.000000896
1	0.000000432	0.000000165	0.000001398
1	0.000000057	0.000000109	0.000000834
1	0.000000431	0.000000032	0.000000889
6	0.000000855	0.000000619	0.00000077
1	0.000000127	0.000001225	-0.000000551
1	0.000000067	0.000001195	0.000000064
1	0.000000233	0.000000537	0.00000008
6	0.000001222	-0.000002036	0.000000942
6	-0.000000198	-0.000000526	-0.000001328
1	-0.000000352	-0.000000313	-0.000000769
1	-0.000000999	-0.000000881	0.000000127
6	-0.000000244	-0.000001083	0.000000402
1	-0.000000052	-0.000000155	-0.000000167
1	-0.000000506	-0.000000351	-0.000000283
6	-0.000000634	-0.000001195	-0.000000486
1	-0.000000599	-0.000001048	-0.000000217
1	-0.000000073	-0.00000111	-0.000000781
1	-0.000000728	-0.000001621	-0.000000239
1	-0.000000394	-0.000001539	-0.000000297
1	-0.000000508	-0.000001419	-0.000000022
79	-0.000000891	-0.000003086	-0.000002414
6	0.000001693	0.000003052	0.000001269
6	0.000000008	-0.000001022	-0.000000416
6	-0.000000658	0.000000006	0.000001152
1	0.000000038	0.000000156	-0.000000341
1	0.000000434	0.000000744	-0.000000241
7	-0.000002556	0.000001615	-0.000001712
7	0.000003429	-0.000002427	-0.000001893
6	0.00000106	-0.000002911	0.000000055
6	-0.000000727	0.000003512	0.000003897

6	0.000003004	0.0000045	-0.00000204
6	0.000001107	0.000003069	-0.000001715
6	0.000000258	0.000001442	0.000002645
6	-0.00000009	-0.000001576	-0.000000468
1	0.000000306	0.0000016	-0.000000052
1	0.000000828	0.000000954	0.000000744
1	0.000000903	0.000001623	0.000000697
6	-0.000003593	-0.000001486	0.000000121
6	0.000000458	-0.000000122	-0.00000023
6	0.000000012	0.000002173	-0.00000109
6	-0.000000662	-0.000000431	-0.000000229
6	-0.000000128	-0.000000738	0.00000042
6	-0.000001316	-0.000002268	-0.000000959
1	-0.000000618	-0.000000962	-0.000000607
1	-0.000000797	-0.000000453	-0.00000123
1	-0.000000556	-0.000000901	-0.000000766
6	-0.000000875	-0.000000296	0.000000731
6	-0.000000144	-0.000000631	0.000000289
6	-0.000000103	0.00000018	0.000000128
1	0.00000047	0.000000367	-0.000000035
1	0.000000182	-0.0000005	0.000000348
1	-0.000000042	-0.00000045	0.000000671
1	-0.000000368	-0.000000555	0.000000385
1	0.000000463	-0.000000929	0.000000993
1	0.000000106	-0.000001027	0.000000426
1	-0.000000194	-0.000000769	0.000000724
6	-0.000000216	-0.000000347	-0.000000569
6	-0.000000065	0.000000024	-0.000001211
6	0.000000797	-0.000000526	-0.000000932
1	-0.000000278	0.000000132	-0.000001067
1	-0.000000148	0.000000476	-0.000001469
1	-0.000000132	0.000000306	-0.000001372
1	-0.000000442	0.000000004	-0.000001314
1	-0.000000466	0.000000051	-0.000000847
1	-0.000001035	0.000000198	-0.000001339
1	-0.000000286	0.000000325	-0.000001412
6	0.000000477	-0.000000264	0.000001708
6	0.000001011	0.000001347	0.000001233
6	0.000000365	0.000000325	0.00000053
1	0.000001344	0.000000101	0.000000371
1	-0.000000144	-0.000000042	0.000000584
1	0.000000212	0.000000126	0.000000901
1	0.000000404	0.000000807	0.000001357
1	0.00000018	0.000001117	0.000000473



1	0.000001007	0.000000864	0.000000795
1	0.000000196	0.000000613	0.000000958
6	-0.000000899	-0.00000052	-0.000002002
6	0.000000708	0.000001195	-0.000000816
6	0.000002312	0.000001147	-0.000000453
1	-0.000000027	0.000000756	0.000000354
1	0.000000545	0.000001658	-0.000000297
1	0.000000236	0.000001318	-0.000000955
1	0.000000026	0.000001607	-0.000000293
1	-0.000000398	0.000001253	0.000000034
1	0.000000206	0.000000922	-0.000000191
1	-0.000000255	0.000000651	-0.000001216
6	0.000000562	-0.000000482	0.000000047
6	-0.000000251	-0.000000051	0.000001489
6	0.000000232	0.000000066	0.000000658
6	0.000000059	0.000000368	-0.000000298
6	-0.000000091	-0.000000004	0.000000329
1	0.000000388	0.000000044	0.000000954
1	-0.000000075	0.000000426	0.000001274
7	-0.000000772	-0.000000393	0.000001202
8	-0.000000687	0.0000003073	-0.000002914
1	0.000000001	0.000000465	0.000000196
1	0.000000196	-0.000000059	0.000001014
17	-0.000000042	-0.000000246	-0.000000599

Zero-point correction=

1.158934 (Hartree/Particle)

Thermal correction to Energy=

1.233149

Thermal correction to Enthalpy=

1.234094

Thermal correction to Gibbs Free Energy=

1.039370

Sum of electronic and zero-point Energies=

-4178.437421

Sum of electronic and thermal Energies=

-4178.363206

Sum of electronic and thermal Enthalpies=

-4178.362262

Sum of electronic and thermal Free Energies=

-4178.556985

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6	0.000000339	-0.000000305	-0.000000277
6	0.000000335	-0.000000253	0.000000073
7	0.000000583	-0.000000024	0.000000122
7	-0.000000128	0.000000334	0.000000297
16	0.000000328	0.000000396	0.000000901
8	0.000000015	0.000000515	0.000001001
8	0.000000506	0.000000515	0.000001572
6	0.000000253	0.000000042	0.000001559
6	-0.000000171	0.000000563	0.000001133
6	-0.000000007	0.000000658	0.000001317

6	0.000000144	0.000000493	0.000002186
6	0.000000435	0.000000453	0.000001891
6	0.000000054	0.000000515	0.000001657
1	-0.000000258	0.000000697	0.000001117
1	-0.000000164	0.000000757	0.000001403
1	0.000000889	0.000000386	0.00000216
1	0.000000814	0.000000305	0.000001791
6	0.000000575	0.000000471	0.000001953
1	0.000000202	0.000001047	0.00000201
1	-0.000000064	0.000000757	0.000001711
1	0.000000647	0.00000071	0.000001843
16	0.000000331	0.000000041	0.000000335
8	-0.000000177	0.000000191	0.000000119
8	0.000000435	-0.000000088	0.000000305
6	0.000000182	0.000000609	0.000000091
6	-0.000000924	0.000000744	0.000000788
6	0.000000268	0.000000298	0.000001228
6	-0.000000077	0.000000417	0.000001609
1	-0.000000119	0.000000516	0.000000989
6	-0.000000636	0.000000722	0.000001069
1	0.000000242	0.000000214	0.000000837
6	-0.000000021	0.000001256	0.000001543
1	-0.000000342	0.000000931	0.000001532
1	0.000000027	0.000000058	0.000001384
6	-0.000000008	0.000000846	0.000001818
1	0.000000196	0.000000916	0.000002437
1	-0.000000423	0.000001365	0.000001723
1	-0.000000509	0.000001252	0.000001985
6	0.000000957	-0.000000071	0.00000008
1	0.000000071	-0.000000025	0.000000864
6	0.000000801	-0.000000092	0.000001062
1	0.000000826	-0.000000078	0.000000892
1	0.000000621	0.000000138	0.000001217
1	0.000001103	-0.000000209	0.000001173
6	0.000000944	-0.000000509	0.000000293
1	0.000000876	-0.000000541	0.000000205
1	0.000000882	-0.000000445	0.000000255
1	0.000001232	-0.000000579	0.000000523
6	0.000000925	-0.000000122	0.000000884
6	0.00000103	-0.000000455	0.000000562
1	0.000000073	-0.000000111	0.000000846
1	0.000000946	-0.000000078	0.000001135
6	0.000001309	-0.000000653	0.000000552
1	0.000000837	-0.000000435	0.000000239

1	0.000000977	-0.000000437	0.000000442
6	0.00000152	-0.000000977	0.000000201
1	0.000001511	-0.000000621	0.000000841
1	0.00000121	-0.000000566	0.000000524
1	0.000001733	-0.000001051	0.000000249
1	0.000001335	-0.000000932	-0.000000072
1	0.000001592	-0.000001018	0.000000187
79	-0.000000379	-0.000000002	-0.000000522
6	-0.000000002	-0.000000401	-0.000000656
6	-0.000000474	-0.000000385	-0.000001455
6	-0.000000615	-0.000000227	-0.000001434
1	-0.000000919	-0.000000163	-0.000001707
1	-0.000000395	-0.000000647	-0.000001823
7	-0.000000265	-0.000000403	-0.000001252
7	-0.000000668	0.000000021	-0.000001244
6	0.000000047	-0.000000581	-0.000001098
6	0.000000181	-0.000000907	-0.000001039
6	0.000000477	-0.000000892	-0.000001187
6	0.000000642	-0.000000934	-0.000001062
6	0.000000765	-0.000001065	-0.000000919
6	0.000000928	-0.00000097	-0.000000826
1	0.000000607	-0.000000798	-0.000000865
1	0.000001068	-0.00000116	-0.000000901
1	0.000001136	-0.00000115	-0.000000819
6	-0.000000848	0.000000083	-0.000000911
6	-0.000000832	0.000000278	-0.000001099
6	-0.000001168	0.000000343	-0.000000731
6	-0.000001091	0.000000379	-0.000000804
6	-0.000001373	0.00000008	-0.000000563
6	-0.000001421	0.000000643	-0.000000717
1	-0.000001201	0.000000362	-0.000000844
1	-0.000001592	0.000000084	-0.000000543
1	-0.000001647	0.000000802	-0.000000605
6	-0.000000674	-0.000000006	-0.000001118
6	-0.000000828	-0.000000152	-0.00000151
6	-0.000000424	-0.000000029	-0.000000834
1	-0.00000047	-0.000000349	-0.000001257
1	-0.000001009	-0.000000139	-0.000001745
1	-0.000000637	-0.000000034	-0.000001674
1	-0.00000101	-0.000000001	-0.000001447
1	-0.000000199	-0.000000173	-0.000000537
1	-0.000000551	0.000000027	-0.000000785
1	-0.000000218	-0.000000335	-0.000001011
6	-0.000001102	0.000000388	-0.000000711

6	-0.000001105	0.000000608	-0.000000373
6	-0.000001506	0.000000493	-0.000001059
1	-0.000000927	0.000000232	-0.000000985
1	-0.000000886	0.000000489	-0.000000114
1	-0.000001152	0.000000625	-0.000000033
1	-0.000001349	0.000000804	-0.000000296
1	-0.00000152	0.000000437	-0.000001364
1	-0.000001744	0.000000703	-0.000001002
1	-0.000001535	0.000000505	-0.000001098
6	0.000000481	-0.000000834	-0.000001225
6	0.000000611	-0.000000782	-0.000000875
6	0.000000585	-0.000001125	-0.000001528
1	0.000000252	-0.000000702	-0.000001057
1	0.000000083	-0.000000638	-0.000000246
1	0.000000692	-0.000000779	-0.000000738
1	0.000000918	-0.000000902	-0.000000702
1	0.000000421	-0.000001098	-0.000001701
1	0.000000889	-0.000001329	-0.00000145
1	0.000000549	-0.000001086	-0.000001553
6	-0.000000151	-0.000000487	-0.000001076
6	-0.000000188	-0.000000059	-0.00000149
6	-0.000000072	-0.000000313	-0.000000666
1	-0.000000331	-0.000000207	-0.000001002
1	-0.000000229	-0.000000572	-0.00000169
1	-0.000000418	-0.000000438	-0.000001454
1	0.000000036	-0.000000719	-0.000001485
1	0.000000092	-0.000000307	-0.000000503
1	0.000000146	-0.000000459	-0.000000688
1	-0.000000025	-0.000000012	-0.000000717
6	-0.000000479	0.000000451	0.000000321
6	-0.000000744	0.000000069	0.000000227
6	-0.000000847	0.000000743	0.000000024
6	-0.000000524	0.000000473	0.000000496
6	-0.000000298	0.000000187	0.000000252
1	-0.000001103	0.000000845	0.000000331
1	-0.00000006	0.000000523	-0.000000007
7	-0.000000102	0.000000328	0.000000294
8	0.000000251	0.000000015	0.000000283
1	-0.000000546	0.000000048	0.000000287
1	-0.000001015	0.000000864	0.000000302
17	0.000000224	0.000000047	0.000000101

Zero-point correction=

1.156091 (Hartree/Particle)

Thermal correction to Energy=

1.231161

Thermal correction to Enthalpy=

1.232106

Thermal correction to Gibbs Free Energy=	1.033238
Sum of electronic and zero-point Energies=	-4178.426811
Sum of electronic and thermal Energies=	-4178.351741
Sum of electronic and thermal Enthalpies=	-4178.350797
Sum of electronic and thermal Free Energies=	-4178.549664

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6	0.000005067	-0.000000748	-0.000001351
6	-0.000002146	0.000002453	-0.000000188
7	-0.000003423	0.000000297	0.000000899
7	-0.000001031	-0.000001981	0.000000963
16	0.000002358	-0.000001767	-0.000000089
8	-0.000000772	-0.00000155	0.000000073
8	-0.00000089	-0.000000329	-0.000001365
6	0.000000003	-0.000000598	0.000001304
6	0.000000124	-0.000001758	-0.000000171
6	0.000000391	-0.000001725	0.000000596
6	-0.00000001	-0.000000799	0.000001101
6	-0.000000142	-0.000001525	-0.000000436
6	0.00000004	-0.000001004	-0.000001092
1	0.000000498	-0.0000016	0.000000754
1	0.000000748	-0.000001658	0.000001388
1	0.000000073	-0.000001075	-0.000000252
1	-0.000000235	-0.000000764	-0.000000514
6	0.000000083	-0.000001816	0.000001279
1	0.000000339	-0.000001886	0.000000397
1	0.000000589	-0.000001294	0.000000924
1	0.000000164	-0.000001337	0.000000328
16	0.000002155	0.000001232	-0.000002119
8	-0.000001489	-0.000002292	-0.000000047
8	-0.000000396	-0.000000466	-0.000000985
6	-0.00000157	-0.000000548	-0.000001718
6	-0.000001239	-0.000001325	-0.000001997
6	-0.000000535	-0.000000899	-0.000002637
6	-0.000000871	-0.000001449	-0.000002262
1	-0.000000749	-0.000001671	-0.000001277
6	-0.000002017	-0.000000991	-0.000003048
1	-0.000001079	-0.000000387	-0.000002164
6	0.000000026	-0.000000538	-0.000002982
1	-0.000000892	-0.000001745	-0.000002611
1	-0.000001221	-0.000000849	-0.000003585
6	-0.000000871	-0.000001539	-0.000004825
1	-0.000001864	-0.000001228	-0.000003326
1	-0.000001964	-0.000001718	-0.00000347

1	-0.000001658	-0.000002445	-0.000003097
6	-0.000000911	-0.000000041	-0.000002061
1	-0.000000972	0.000001055	-0.000000724
6	-0.000000127	0.000000061	-0.000001506
1	-0.000001173	0.00000002	-0.000002001
1	-0.000000587	-0.000000127	-0.000001721
1	-0.000000711	0.000000745	-0.000001988
6	-0.00000007	0.000001811	-0.000000816
1	-0.000000282	0.000000852	-0.000000771
1	-0.000000799	0.000000058	-0.000001532
1	-0.000000316	0.000001432	-0.000001401
6	0.000000177	-0.000001062	-0.000001779
6	-0.000000312	0.000000812	-0.000000103
1	-0.000000216	0.000000715	-0.000000441
1	-0.000000201	0.000000889	-0.000000054
6	0.000000016	0.000001633	0.000000328
1	0.000000641	0.000000708	0.000000895
1	0.000000175	0.000000981	0.000000302
6	0.000000021	0.000001928	0.000000717
1	-0.00000002	0.000001629	-0.000000387
1	0.000000004	0.000001214	0.000000233
1	0.00000001	0.000002358	0.000000581
1	0.000000403	0.00000018	0.000001143
1	0.000000152	0.000002128	0.000000633
79	-0.000000582	-0.000000278	-0.000000063
6	0.000001481	-0.000000247	-0.000002524
6	0.000000435	-0.000000155	0.000001815
6	0.000001203	0.000002026	-0.000000283
1	0.000000054	0.000000351	0.000001141
1	0.000000198	0.000001366	0.000000929
7	-0.000001806	0.000002951	0.000000285
7	-0.000000418	-0.000000645	0.000003114
6	0.000000912	0.000001751	-0.000000671
6	-0.000000541	0.000001209	-0.000000819
6	0.000000328	0.000001976	0.000001044
6	-0.000000503	0.000001965	-0.000000061
6	-0.000000024	0.000002313	-0.000000122
6	-0.000000563	0.00000288	-0.000000859
1	-0.000000528	0.000002243	-0.000001437
1	-0.000000362	0.000002826	0.000000045
1	-0.000000498	0.00000291	-0.000001
6	-0.000000012	0.000000608	0.000000914
6	0.000000747	-0.000001411	0.000000904
6	0.000001474	-0.000001169	0.000001245

6	0.000001026	-0.000001401	0.00000204
6	-0.000000078	-0.000001648	0.000001178
6	0.000000653	-0.000001551	0.000001581
1	0.000001175	-0.000001035	0.000002341
1	0.000000329	-0.000001928	0.000000739
1	0.000000788	-0.000002017	0.000001757
6	0.000002733	-0.000000715	0.000001207
6	0.000000123	0.000000726	0.000002958
6	-0.000000331	0.000000529	0.000003037
1	0.00000126	-0.000000204	0.000001645
1	0.000001081	0.000000187	0.000002575
1	0.000000898	0.000000568	0.000002912
1	0.000001461	-0.000000778	0.000003329
1	0.000000861	0.000000366	0.000001893
1	0.00000149	-0.000000313	0.000001517
1	0.000000885	0.00000058	0.000002385
6	-0.000000245	-0.000001121	0.000000026
6	-0.00000015	-0.000001292	0.000000231
6	0.000000059	-0.000001365	0.000000166
1	0.000000438	-0.00000049	0.000000223
1	-0.000000282	-0.000001468	-0.000000697
1	-0.000000128	-0.000001344	-0.000000868
1	-0.000000117	-0.000002221	-0.000000341
1	0.000000256	-0.000000929	0.000000065
1	0.000000447	-0.000001558	0.000000031
1	-0.000000114	-0.000001076	-0.000000167
6	0.000000394	0.000001539	0.000000949
6	0.000000075	0.000002038	0.000001036
6	0.000000194	0.000002774	0.000001198
1	0.000000341	0.00000159	0.00000125
1	0.000000422	0.000001532	0.000000721
1	0.000000534	0.000001916	0.000001414
1	0.000000233	0.000002459	0.000000081
1	0.000000426	0.000002637	0.000001239
1	0.000000321	0.000002965	0.000001061
1	0.000000592	0.000002604	0.000001731
6	0.000000732	0.000000982	-0.000000664
6	-0.000001055	0.000001553	-0.000000831
6	-0.000001386	0.000000864	-0.000000924
1	-0.000000151	0.000000656	-0.000000056
1	-0.000000305	0.000001441	-0.000000423
1	-0.000000528	0.000001135	-0.000000984
1	-0.000000397	0.000001855	-0.000001226
1	-0.000000645	0.000000491	-0.00000183

1	-0.000000649	0.00000118	-0.000001579
1	-0.000000805	0.000000526	-0.000001617
6	-0.000000064	-0.000001	0.000001034
6	0.000000221	-0.000001905	0.000000965
6	0.000000717	-0.000002347	0.000001163
6	0.000000719	-0.000001891	0.00000167
6	0.000001194	-0.000000586	0.000001543
1	0.000000911	-0.000002479	0.000001436
1	0.000000555	-0.000001415	-0.000000402
7	0.000001324	0.000000542	0.000001098
8	-0.000002444	-0.000000661	0.000000096
1	0.000000089	-0.000001669	0.000002252
1	0.000000444	-0.000002085	0.000000529
17	0.000000694	-0.000000738	0.000001783
Zero-point correction=			1.158520 (Hartree/Particle)
Thermal correction to Energy=			1.233151
Thermal correction to Enthalpy=			1.234095
Thermal correction to Gibbs Free Energy=			1.035614
Sum of electronic and zero-point Energies=			-4178.446560
Sum of electronic and thermal Energies=			-4178.371929
Sum of electronic and thermal Enthalpies=			-4178.370985
Sum of electronic and thermal Free Energies=			-4178.569466

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6	0.000001716	-0.000002818	-0.000000682
6	0.000001943	0.000001997	0.000003324
7	-0.000001078	0.000001545	0.000000272
7	-0.000002425	0.00000003	-0.000001197
16	-0.000000056	0.000000782	-0.000000795
8	-0.000000285	0.000000327	0.000000276
8	0.000000084	0.000001361	0.000000478
6	0.000000802	0.000000385	-0.000000583
6	0.000000416	0.000000626	0.000000068
6	0.000000504	0.000000826	0.000000324
6	0.000000769	0.000000246	-0.000000536
6	0.000000598	0.000000635	0.000000149
6	0.000000249	0.000000848	0.000000916
1	0.000000096	0.000000507	-0.00000014
1	0.000000409	0.000000078	-0.000000247
1	0.000000736	0.000000406	-0.00000004
1	0.00000006	0.000000208	-0.000000319
6	0.000000076	0.000001142	0.000000396
1	0.000000761	0.000000908	0.000000125
1	0.000000504	0.000000905	0.000000198



1	0.000000852	0.000000952	0.000000246
16	-0.000000523	-0.000000486	0.000000135
8	-0.000000863	0.000000003	0.000000109
8	0.000000067	-0.000000108	-0.000000157
6	-0.000000538	0.000000115	-0.000000285
6	-0.000000036	0.000000246	-0.000000063
6	-0.000000675	-0.000000161	-0.000000544
6	-0.000000833	0.000000026	-0.000000126
1	-0.000000343	-0.000000041	-0.000000022
6	-0.000000805	0.000000092	-0.000000271
1	-0.000000699	-0.000000034	-0.000000122
6	-0.000001209	0.000000033	-0.000000029
1	-0.000000897	0.000000538	-0.000000094
1	-0.000001066	-0.000000012	-0.000000057
6	-0.000001114	0.000000234	-0.000000272
1	-0.000001174	0.000000023	-0.00000003
1	-0.000001017	0.000000214	-0.000000257
1	-0.00000105	0.000000377	-0.000000385
6	0.000001817	0.000001267	-0.000002319
1	-0.000002211	-0.000000744	0.000002177
6	0.000000146	0.000000013	0.000000061
1	-0.000000443	0.000000007	-0.000000246
1	-0.000000539	0.000000198	-0.000000013
1	-0.000000509	0.000000129	-0.000000133
6	-0.000000135	0.000000474	-0.000000316
1	0.000000208	-0.000000059	0.000000842
1	-0.000000447	-0.000000031	-0.000000158
1	-0.000000177	-0.000000039	-0.000000022
6	-0.000000029	0.000000581	-0.000000474
6	-0.000000522	0.000000592	-0.000000194
1	0.000000033	0.000000635	0.000000066
1	-0.000000412	-0.000000147	-0.000000708
6	0.000000465	-0.000000053	0.000000016
1	0.000000183	0.000000905	-0.000000546
1	-0.000000539	0.000000106	0.000000627
6	-0.000000136	0.000000588	-0.000000075
1	-0.000000362	0.000000295	0.000000123
1	0.000000127	0.000000587	-0.000000025
1	-0.000000144	0.000000558	-0.000000005
1	-0.000000177	0.000000677	-0.000000044
1	-0.000000248	0.000000464	-0.000000083
79	0.000000363	0.000000026	-0.000000597
6	0.000000119	-0.000000081	0.000000357
6	0.000000049	-0.000000558	0.000000502

6	0.000000149	-0.000000454	-0.000000509
1	0.000000152	-0.000000823	0.000000256
1	0.000000532	-0.000000596	0.000000066
7	0.000000028	-0.000000294	-0.000000847
7	0.000000019	-0.000000566	0.000001582
6	0.000000173	-0.000000526	0.000000331
6	0.000000597	-0.000000104	0.000000358
6	0.000000163	-0.000000527	-0.000000413
6	0.000000486	-0.000000144	0.000000497
6	0.000000282	-0.000000268	-0.000000016
6	0.000000712	-0.000000445	-0.000000141
1	0.000000639	-0.000000355	0.000000083
1	0.000000034	-0.000000331	0.000000543
1	0.000000952	0.000000126	0.000000167
6	-0.000002005	-0.000000777	-0.000000272
6	0.000000233	-0.000000965	-0.000000127
6	-0.000000067	-0.000000116	0.000000235
6	-0.000000213	-0.000000669	-0.000000209
6	0.000000368	-0.000000026	-0.000000491
6	-0.000000387	-0.000000763	-0.000000211
1	-0.000000384	-0.000000104	0.000000038
1	-0.000000486	-0.000000058	-0.000000046
1	-0.000000647	-0.000000526	-0.000000052
6	-0.000000246	-0.000000467	0.000000414
6	0.000000019	-0.000000589	-0.000000013
6	-0.000000229	-0.000000161	-0.000000025
1	0.000000461	0.000000023	-0.000000288
1	-0.000000068	-0.000000044	-0.000000059
1	-0.000000206	-0.000000546	-0.000000001
1	-0.000000038	-0.000000473	-0.000000053
1	-0.000000435	-0.000000203	-0.000000167
1	-0.000000287	0.000000037	-0.000000121
1	-0.000000047	-0.000000051	0.000000015
6	-0.000000477	-0.000000574	0.000000195
6	-0.000000066	-0.000000369	0.000000148
6	-0.000000003	-0.000001445	0.000000384
1	0.000000842	-0.000000279	-0.000000298
1	-0.000000565	-0.000000072	-0.000000106
1	-0.000000274	-0.000000615	0.000000006
1	-0.000000291	-0.000000712	-0.000000038
1	0.000000033	-0.000000781	-0.000000001
1	-0.000000228	-0.000001009	-0.000000039
1	0.000000012	-0.000000915	0.000000096
6	0.000000786	0.000000131	-0.000000102

6	0.000000603	0.000000049	0.000000005
6	0.000001111	-0.000000479	0.000000397
1	-0.000000158	-0.000000522	0.000000027
1	0.000000986	-0.000000114	0.000000613
1	0.000000629	0.000000367	-0.000000121
1	0.000000254	0.000000026	0.000000193
1	0.000000063	-0.000000405	0.000000123
1	0.000000682	-0.000000224	0.000000136
1	0.000000463	-0.000000296	0.000000161
6	0.000002046	0.000000434	-0.000000047
6	0.000000721	-0.000000945	-0.000000566
6	0.000000353	0.000000545	0.000000691
1	0.000000007	-0.000001701	-0.000000457
1	0.000000097	-0.000000518	0.000000034
1	0.000000097	-0.000000691	0.000000308
1	0.000000344	-0.000000634	0.000000959
1	0.000000151	-0.000001085	-0.000000094
1	0.000000241	-0.000000698	-0.000000256
1	0.000000007	-0.000000063	0.000000075
6	0.000000512	0.000000345	-0.000002806
6	-0.000000272	0.000001299	-0.000000537
6	-0.000000213	0.000000463	-0.000000451
6	-0.000000319	0.000001065	0.000000409
6	-0.000000823	0.000001011	0.000000236
1	-0.000000003	0.000000955	-0.000000073
1	0.000000003	-0.000002166	0.000003307
7	-0.000001303	-0.000001124	0.000000769
8	0.000000215	0.000001074	-0.000001332
1	-0.000000158	0.000000954	-0.000000072
1	-0.000000043	0.000000916	-0.000000202
17	-0.000000362	0.000000608	-0.000000423

Zero-point correction=

1.156665 (Hartree/Particle)

Thermal correction to Energy=

1.231430

Thermal correction to Enthalpy=

1.232375

Thermal correction to Gibbs Free Energy=

1.034452

Sum of electronic and zero-point Energies=

-4178.428418

Sum of electronic and thermal Energies=

-4178.353652

Sum of electronic and thermal Enthalpies=

-4178.352708

Sum of electronic and thermal Free Energies=

-4178.550631

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6	0.00000462	-0.000002668	0.000000893
6	-0.000001016	0.000007686	-0.000004621
7	-0.000002975	0.000000394	0.000001538

7	-0.000012019	0.000001896	0.000003695
16	0.000002485	0.000004033	-0.000000956
8	0.000000234	-0.000000044	-0.000000697
8	-0.000002308	-0.000000339	0.000001272
6	-0.000000243	-0.000001293	0.000003434
6	-0.000001325	-0.000001467	-0.000000878
6	-0.000000827	-0.000001335	0.000000039
6	-0.000000008	-0.000000547	-0.000000008
6	-0.000001238	0.000000441	0.000000667
6	0.000000723	-0.000000451	-0.000001338
1	-0.000000537	-0.000000811	0.000000418
1	-0.000001101	-0.000000938	-0.000000186
1	0.000000001	0.000000357	0.000000837
1	0.000000975	-0.000000355	0.000001909
6	-0.000000787	-0.000000634	0.000000172
1	-0.000000739	-0.000000558	0.000000488
1	-0.000000642	-0.000000063	-0.000000002
1	-0.000000277	-0.000000223	0.000000129
16	0.000007025	-0.000010869	-0.000001348
8	0.000000401	-0.000000284	-0.000000832
8	0.000000062	0.000000208	-0.000000355
6	-0.000000692	0.000001558	-0.000004568
6	0.000000896	0.000000196	-0.000001914
6	-0.000000036	-0.000002152	-0.000000598
6	0.000000162	-0.000000842	-0.000000196
1	0.000000479	0.000000125	-0.000001735
6	-0.000000064	-0.000001295	-0.000003098
1	-0.000000364	-0.000001158	-0.000002645
6	0.000001027	-0.000000125	-0.000003837
1	0.000001023	0.000000038	-0.000002691
1	-0.000000204	-0.000001125	-0.000003268
6	0.000000643	0.000000136	-0.000004031
1	0.000000448	-0.000000849	-0.000004255
1	0.000000963	-0.000000261	-0.000003543
1	0.000001269	-0.000000279	-0.000003845
6	0.000002778	-0.000000054	-0.000004784
1	-0.000001651	-0.000000422	-0.000001673
6	-0.000001174	-0.000002446	0.000000014
1	-0.000000938	-0.000001633	-0.000001531
1	-0.000000863	-0.000001343	-0.000002219
1	-0.000001589	-0.000001871	-0.000002109
6	-0.000000687	-0.000001157	-0.000000202
1	-0.000001183	-0.000000132	-0.000000456
1	-0.000001441	-0.000001479	0.000000486

1	-0.000001301	-0.000002103	-0.000000046
6	0.00000056	-0.000004638	-0.000002333
6	0.000001542	0.000000528	-0.000001178
1	-0.000000848	0.000000847	0.000001157
1	0.000002634	0.000000395	-0.000000724
6	0.000000772	0.000001843	-0.000000692
1	0.000000027	0.00000067	-0.000001771
1	0.000001276	0.000000836	-0.00000137
6	0.000002039	0.000001539	-0.000000779
1	0.000001555	0.000000475	0.000000056
1	0.000001298	0.00000118	-0.000000182
1	0.000002013	0.00000225	-0.000000975
1	0.000001335	0.000001138	-0.00000197
1	0.000001356	0.000001686	-0.000001564
79	-0.000002508	0.000001322	-0.000000061
6	0.000005053	-0.00000426	0.000007458
6	0.00000139	0.000001823	0.000000809
6	-0.00000053	-0.000001311	0.000001481
1	0.000000866	0.000001532	0.000002311
1	-0.000001068	0.000001093	0.000002781
7	-0.000003545	0.000003511	-0.000001384
7	-0.000003308	0.000004725	-0.000000892
6	-0.000000353	-0.000001456	0.000002495
6	-0.000000844	-0.000001891	0.000000828
6	0.000000964	-0.000000201	0.000001434
6	-0.000001176	-0.000001023	0.0000016
6	-0.000001914	-0.000000996	0.000000854
6	-0.000002054	-0.000001651	0.000001125
1	-0.0000015	-0.00000143	0.000000557
1	-0.000002218	-0.000000661	0.000002219
1	-0.000001914	-0.000001376	0.000001378
6	0.000002432	0.000002568	0.000001844
6	0.000001597	0.00000007	0.000004871
6	0.00000027	-0.000002451	-0.000003231
6	0.0000004	0.000000826	-0.000001149
6	0.000001776	0.00000245	0.000002924
6	0.000001279	0.000002983	0.000000482
1	0.000001544	0.000002163	0.000000913
1	0.00000173	0.000001804	0.000000417
1	0.000002124	0.000002309	0.000000489
6	0.000002309	0.00000082	0.000000621
6	-0.000000327	0.000002048	0.000003213
6	-0.000000512	0.000001511	0.000002047
1	-0.000000084	0.000000474	0.000002205

1	0.00000072	0.000001409	0.000002825
1	0.000000779	0.000001484	0.000002702
1	0.000000947	0.000001784	0.000002428
1	0.000000382	0.000000315	0.000001017
1	0.000000489	0.000001313	0.000001566
1	0.000000579	0.000000688	0.000002173
6	-0.000000751	0.000003379	0.000002008
6	0.000001615	0.000001074	-0.000001517
6	0.000002358	0.000001352	0.000000587
1	-0.000000152	-0.000000012	0.000000269
1	0.000000903	0.000001508	-0.000000244
1	0.000001344	0.000001119	-0.000000422
1	0.000001491	0.000000985	-0.000000145
1	0.000001322	0.000001244	0.000001094
1	0.00000101	0.000002021	0.000000492
1	0.000001238	0.000001397	0.000000586
6	-0.000002318	-0.000000008	0.000000939
6	-0.000000701	-0.000003082	0.000001368
6	-0.00000122	0.000000186	0.000003366
1	-0.000000066	-0.000000473	0.000001246
1	-0.000001875	-0.000001072	0.000001301
1	-0.000001378	-0.000000177	0.000002022
1	-0.000001516	-0.000001351	0.000002415
1	-0.000001175	-0.000000765	0.000002615
1	-0.000001167	-0.000000478	0.000002632
1	-0.000001167	-0.00000005	0.000002957
6	-0.000000347	0.000000485	0.000000798
6	-0.000001238	-0.000000815	0.000001749
6	-0.000000382	-0.000000113	0.000000186
1	-0.000000177	-0.000000537	0.000001192
1	-0.000000445	0.000000117	0.000001706
1	-0.000000138	0.000000353	0.000001248
1	-0.000000798	-0.000000474	0.000001567
1	-0.000000736	-0.000000797	-0.000000092
1	-0.000000433	-0.000000848	0.000000845
1	-0.000000348	-0.000000089	0.000000214
6	-0.000001572	-0.000001633	-0.000001757
6	0.000001984	0.000000226	-0.000000875
6	-0.000000544	-0.000002068	-0.000003611
6	0.000000142	0.000000079	-0.000002388
6	-0.000000431	0.000001273	-0.000000779
1	0.000000619	-0.000000003	-0.000002394
1	-0.00000199	0.000000104	-0.000002301
7	0.00000308	-0.000000189	0.000000528

<b>8</b>	<b>-0.000003092</b>	<b>-0.000002795</b>	<b>-0.000003419</b>
<b>1</b>	<b>0.000001279</b>	<b>-0.000000241</b>	<b>-0.000002749</b>
<b>1</b>	<b>-0.000000056</b>	<b>-0.000000477</b>	<b>-0.000001329</b>
<b>17</b>	<b>0.000000826</b>	<b>-0.000000357</b>	<b>-0.000002799</b>
<b>Zero-point correction=</b>			<b>1.158658 (Hartree/Particle)</b>
<b>Thermal correction to Energy=</b>			<b>1.233139</b>
<b>Thermal correction to Enthalpy=</b>			<b>1.234083</b>
<b>Thermal correction to Gibbs Free Energy=</b>			<b>1.038545</b>
<b>Sum of electronic and zero-point Energies=</b>			<b>-4178.434486</b>
<b>Sum of electronic and thermal Energies=</b>			<b>-4178.360005</b>
<b>Sum of electronic and thermal Enthalpies=</b>			<b>-4178.359061</b>
<b>Sum of electronic and thermal Free Energies=</b>			<b>-4178.554599</b>