

**Computational Study on Pd-Catalyzed *ipso,meta*-Dimethylation of *ortho*-
Substituted Iodoarene: Mechanisms and the Role of Base**

Supporting Information

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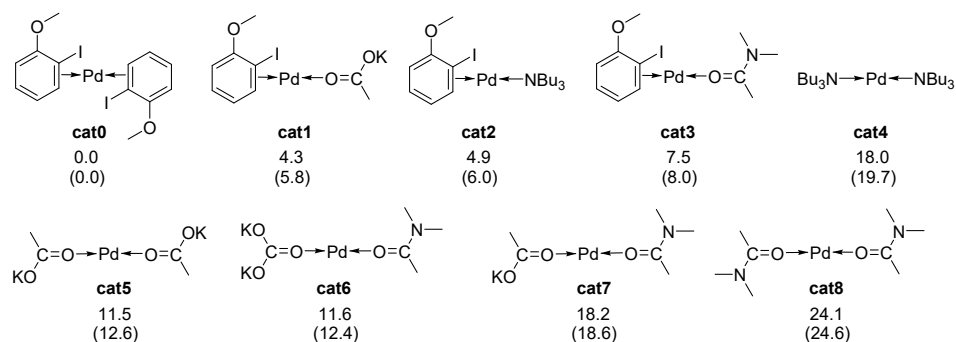
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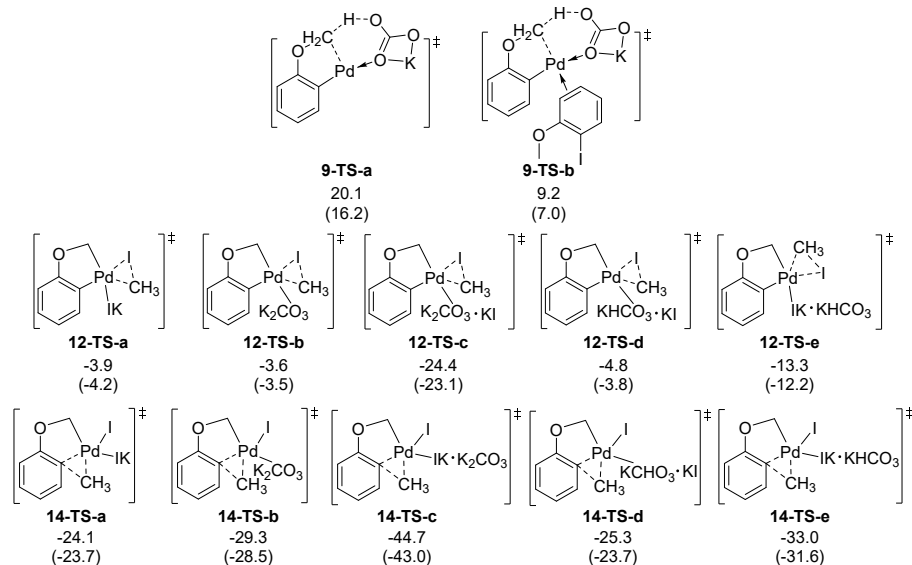
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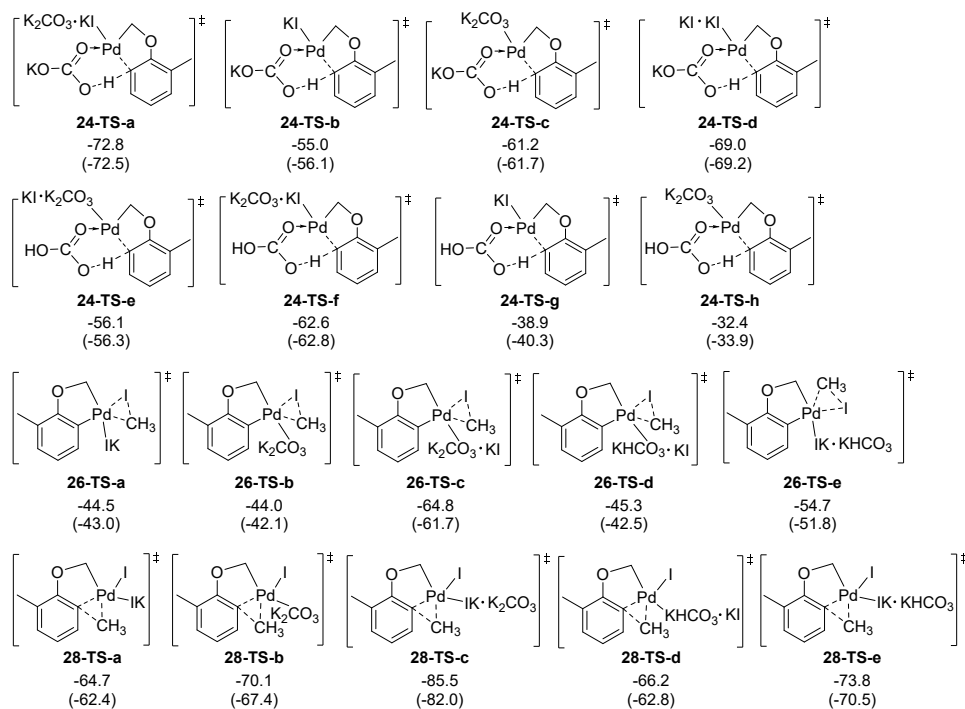
Scheme S1. Some possible Pd⁰ initial species. The free energies (enthalpies) are given in kcal/mol, where the energy of **cat0** is the zero-energy reference point.



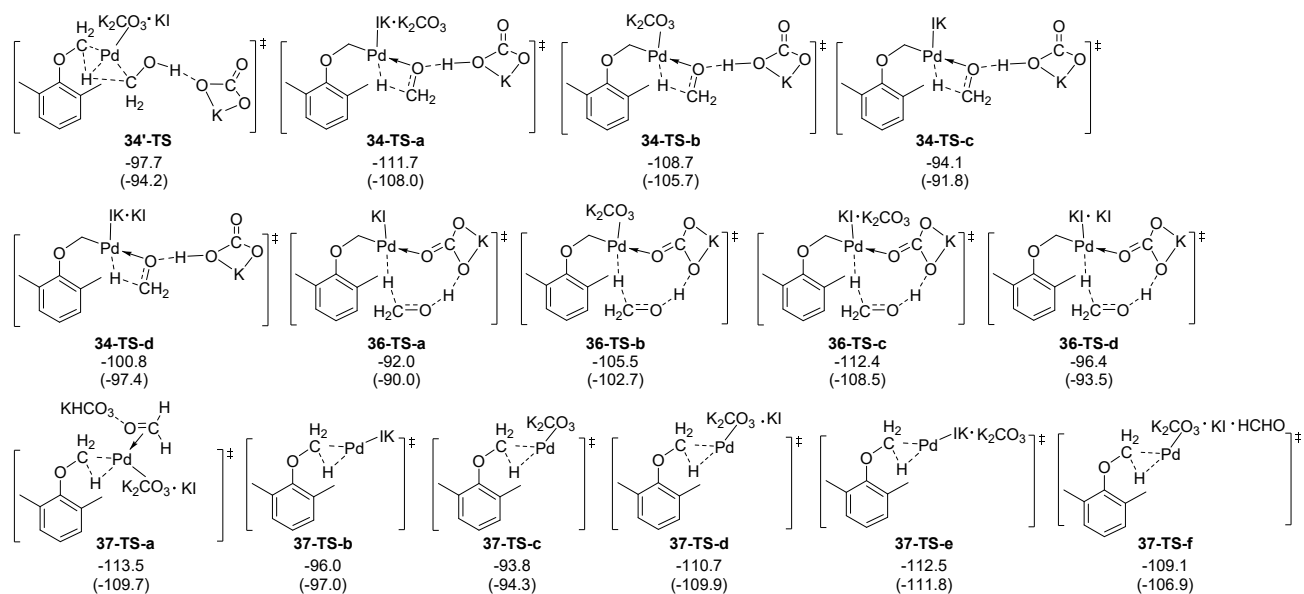
Scheme S2. Calculated relative free energies (enthalpies) of less favored transition states for the methoxyl C(sp³)-H activation, first CH₃-I oxidative addition and first Ar-C reductive elimination in the presence of K₂CO₃. The free energies (enthalpies) are given in kcal/mol.



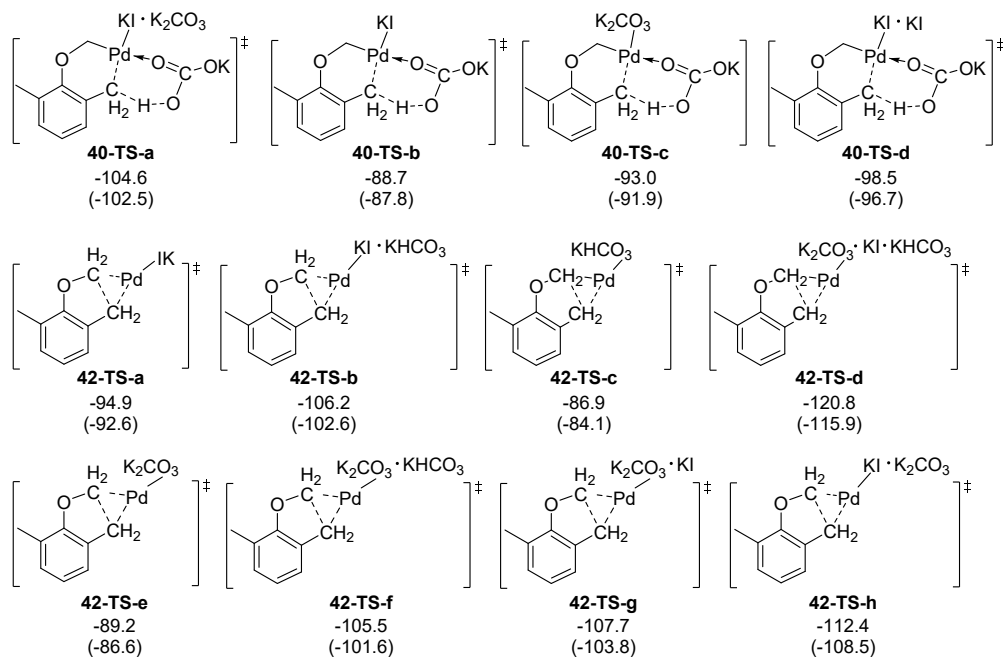
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Scheme S4. Calculated relative free energies (enthalpies) of less favored transition states for the concerted hydride transfer and C–hydride reductive elimination before the proton transfer, the hydrogen transfer and C–hydride reductive elimination in the presence of K_2CO_3 . The free energies (enthalpies) are given in kcal/mol.



Scheme S5. Calculated relative free energies (enthalpies) of less favored transition states for the third C–H activation and C–C reductive elimination in the presence of K_2CO_3 . The free energies (enthalpies) are given in kcal/mol.



Scheme S6. Calculated relative free energies (enthalpies) of transition states for the alkyPd(II) species **29** protonation by KHCO₃ in the presence of K₂CO₃. The free energies (enthalpies) are given in kcal/mol.

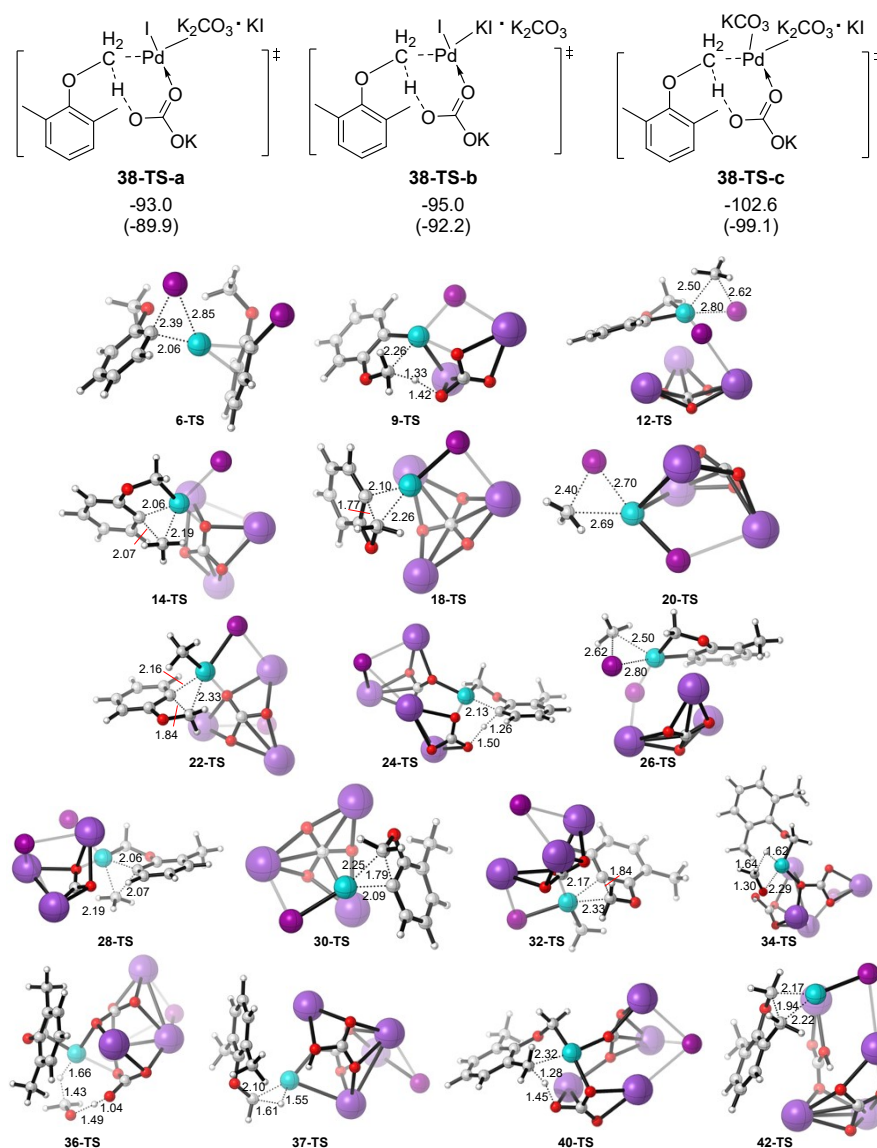


Figure S1. Optimized geometries of the key transition states in the presence of K₂CO₃. Bond

lengths are given in angstroms.

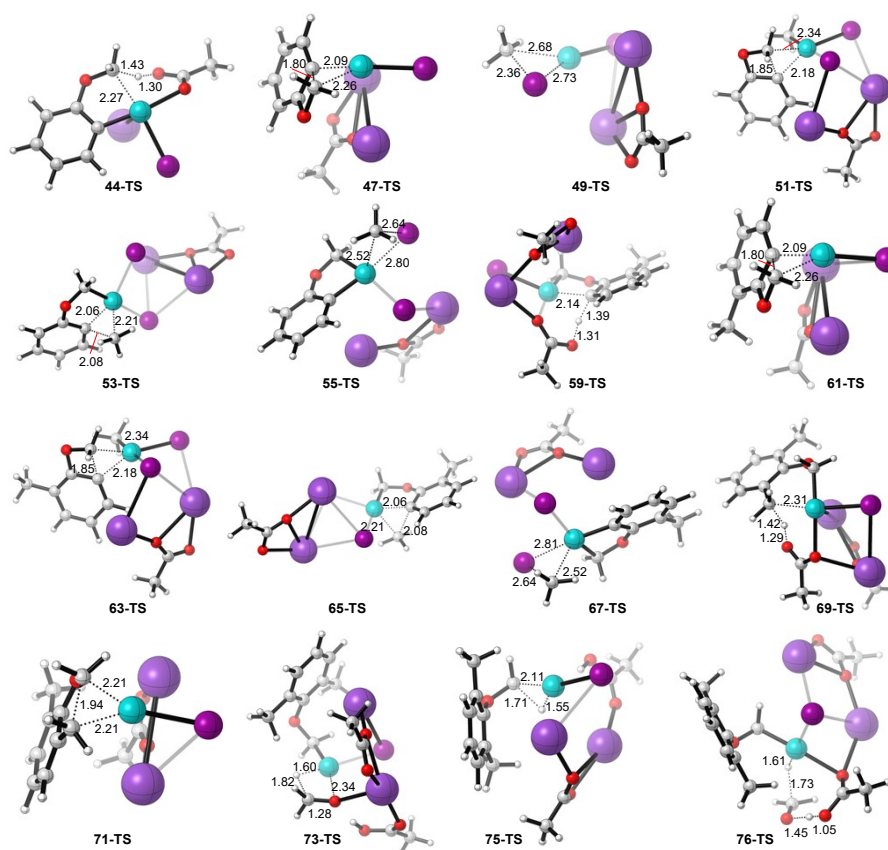


Figure S2. Optimized geometries of the key transition states in the presence of KOAc. Bond lengths are given in angstroms.

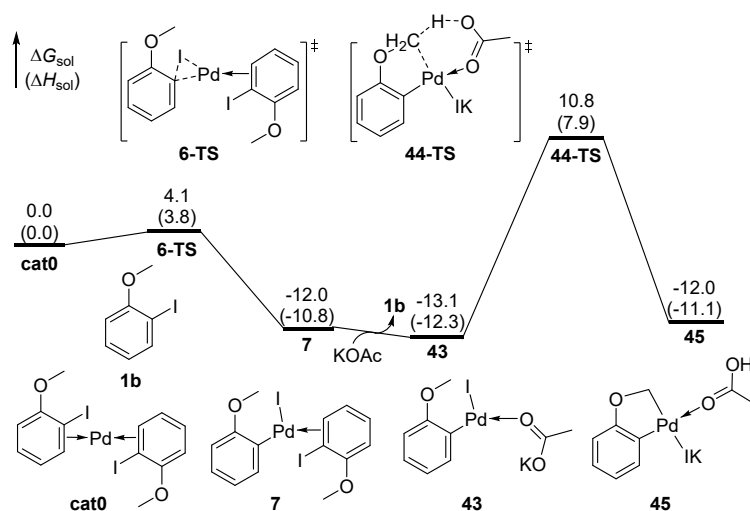


Figure S3. Calculated energy profile of the aryl-I oxidative addition and methoxyl C-H activation in Pd-catalyzed dimethylation of 1b in the presence of KOAc (in kcal/mol).

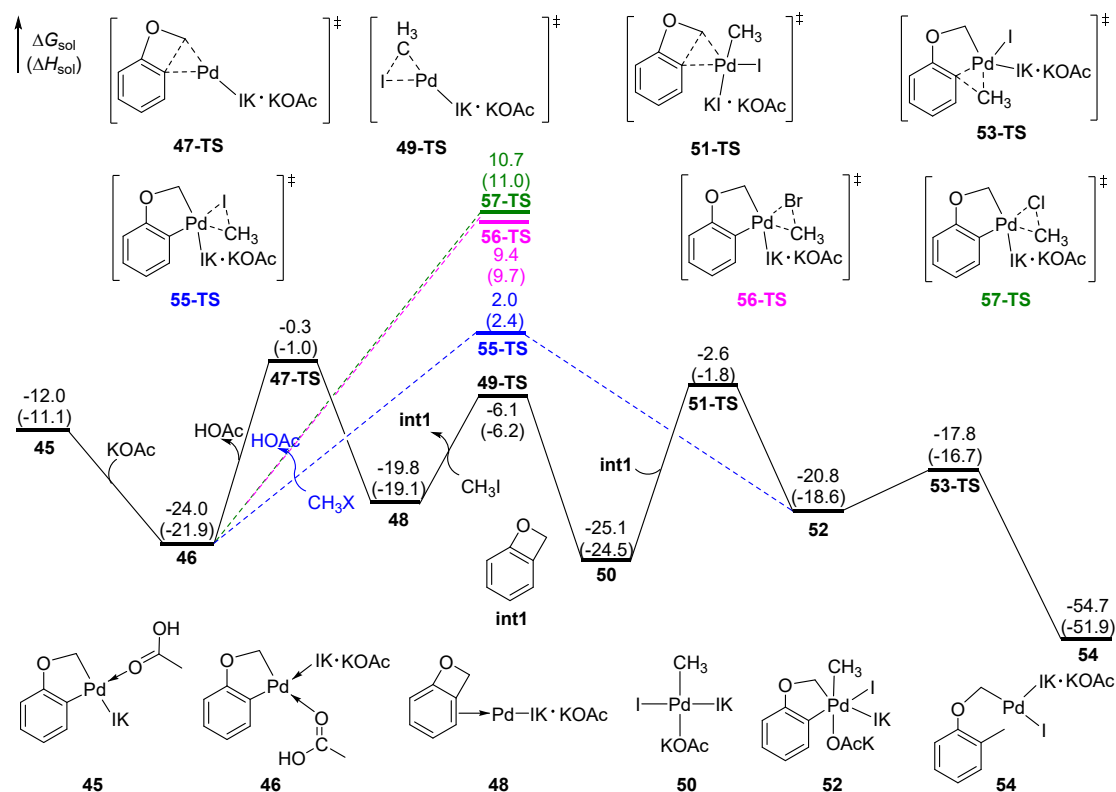


Figure S4. Calculated energy profiles of the first $\text{CH}_3\text{-X}$ oxidative addition (Ar-C reductive elimination, $\text{CH}_3\text{-I}$ oxidative addition, and Ar-C oxidative addition) and first Ar-C reductive elimination in Pd-catalyzed dimethylation of 1b in the presence of KOAc (in kcal/mol).

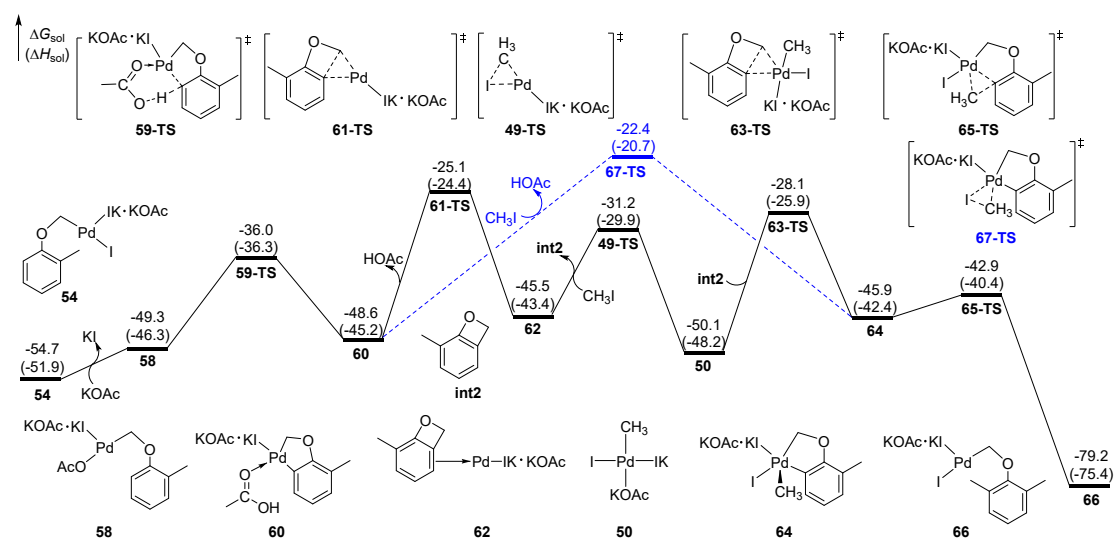
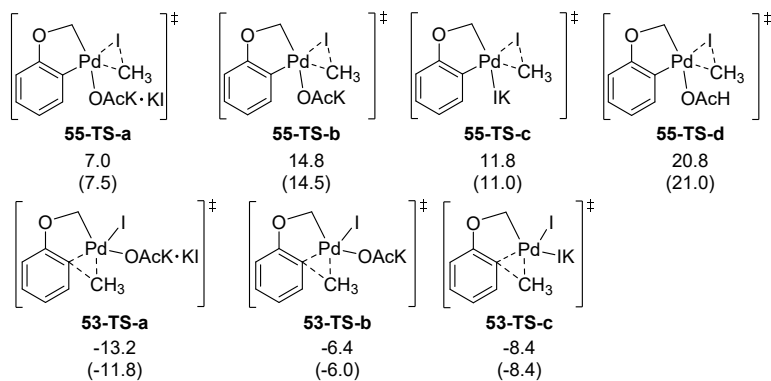
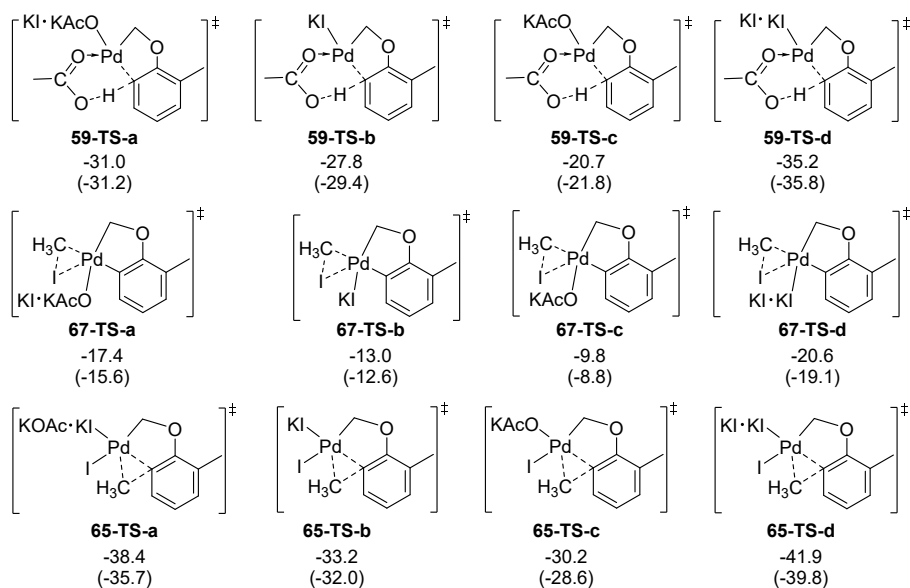


Figure S5. Calculated energy profiles of the aryl C-H activation, second $\text{CH}_3\text{-I}$ oxidative addition (Ar-C reductive elimination, $\text{CH}_3\text{-I}$ oxidative addition, and Ar-C oxidative addition) and second Ar-C reductive elimination in Pd-catalyzed dimethylation of 1b in the presence of KOAc (in kcal/mol).

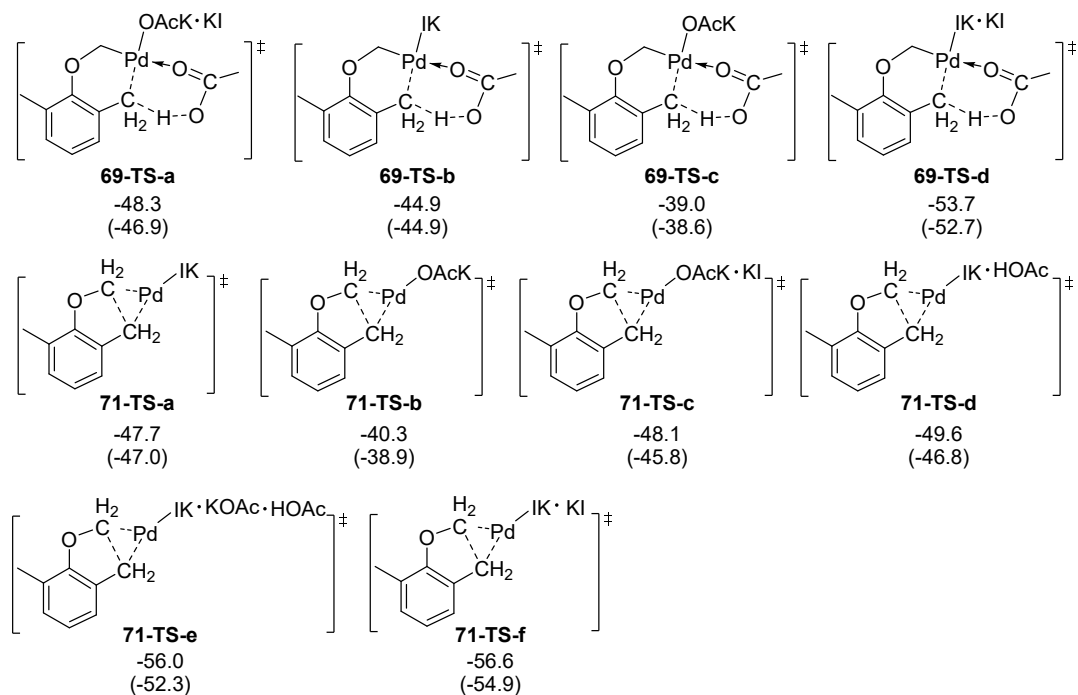
Scheme S7. Calculated relative free energies (enthalpies) of less favored transition states for the first $\text{CH}_3\text{-I}$ oxidative addition and first Ar-C reductive elimination in the presence of KOAc. The free energies (enthalpies) are given in kcal/mol.



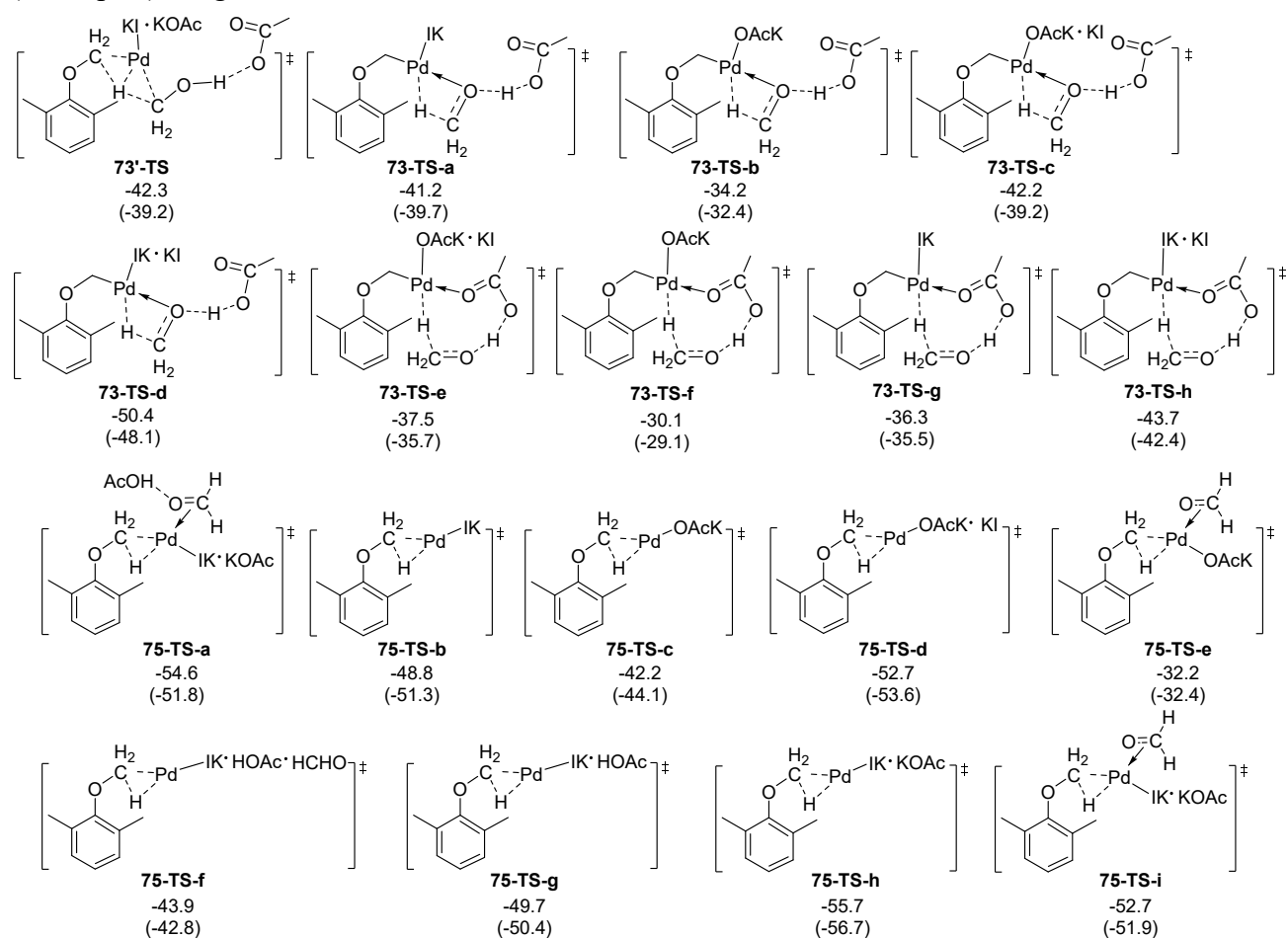
Scheme S8. Calculated relative free energies (enthalpies) of less favored transition states for the aryl C–H activation, second CH₃–I oxidative addition, and second Ar–C reductive elimination in the presence of KOAc. The free energies (enthalpies) are given in kcal/mol.



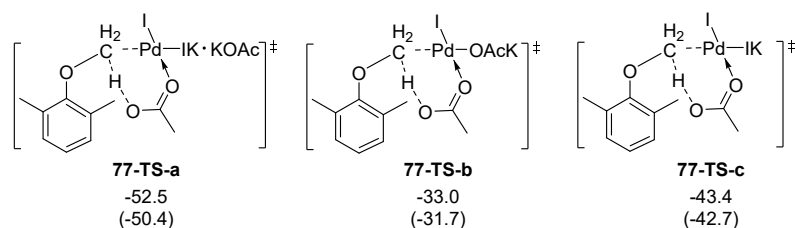
Scheme S9. Calculated relative free energies (enthalpies) of less favored transition states for the third C–H activation and C–C reductive elimination in the presence of KOAc. The free energies (enthalpies) are given in kcal/mol.



Scheme S10. Calculated relative free energies (enthalpies) of less favored transition states for the concerted hydride transfer and C–hydride reductive elimination before the proton transfer, the hydrogen transfer, and C–hydride reductive elimination in the presence of KOAc. The free energies (enthalpies) are given in kcal/mol.



Scheme S11. Calculated relative free energies (enthalpies) of transition states for the alkylPd(II) species **66** protonation by HOAc in the presence of KOAc. The free energies (enthalpies) are given in kcal/mol.



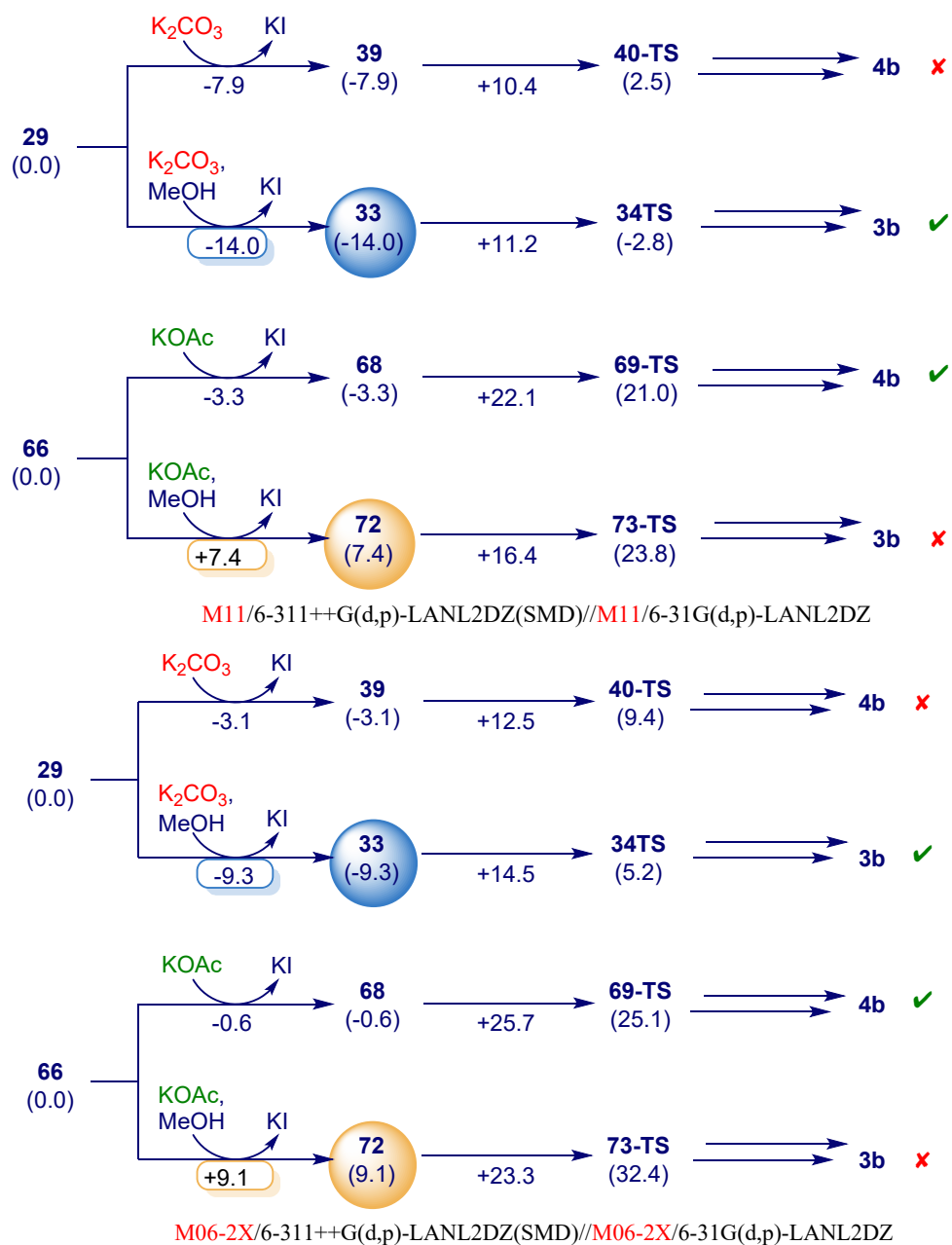


Figure S6. The calculated $\Delta\Delta G$ of key intermediates and transition states using different density functionals.

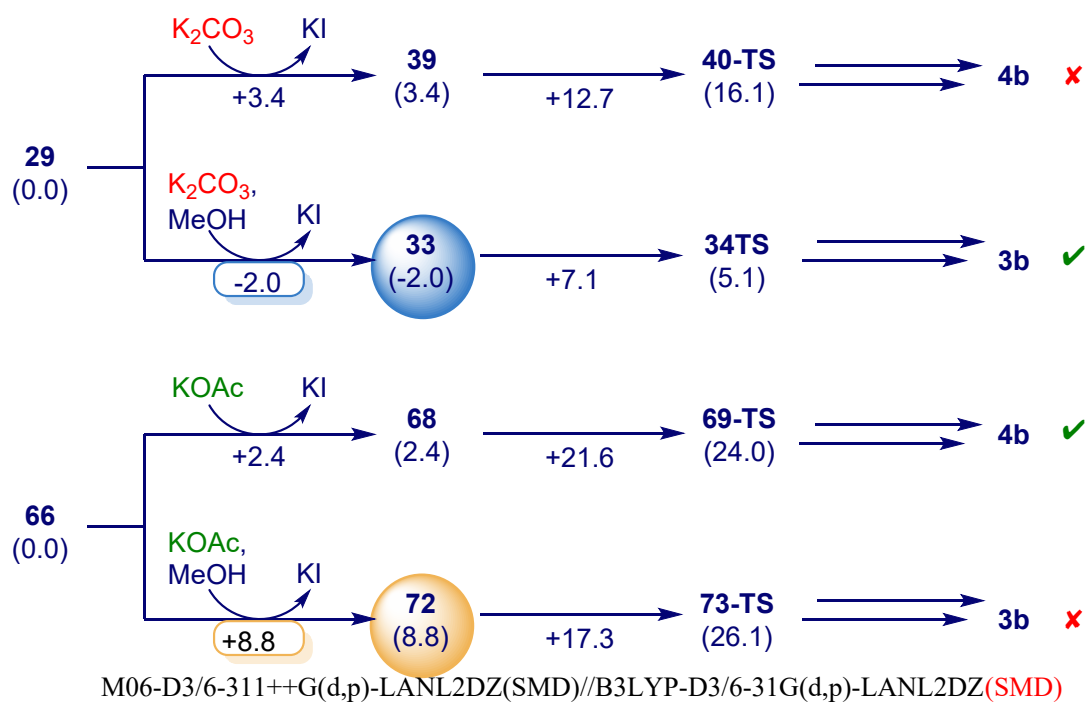


Figure S7. The calculated $\Delta\Delta G$ of key intermediates and transition states that were optimized in the solution phase (solvent = DMAc) with the SMD solvation model.

Table 1. Absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(\text{elec-B3LYP-D3/BSI})}^1$	$G_{(\text{corr-B3LYP-D3/BSI})}^2$	$H_{(\text{corr-B3LYP-D3/BSI})}^3$	$E_{(\text{sol, M06-D3/BSII})}^4$	IF ⁵
1b	-357.55998	0.087044	0.131973	-357.3649805	
3b	-425.4283563	0.152279	0.199730	-425.2027425	
4b	-424.2223834	0.134601	0.177620	-424.0073405	
int1	-345.5297888	0.081296	0.117443	-345.371363	
int2	-384.8533074	0.105993	0.146844	-384.6674039	
cat0	-841.9111026	0.189513	0.267337	-841.527353	
cat1	-1312.8126181	0.120016	0.193454	-1312.5779116	
cat2	-1012.7027159	0.435661	0.533560	-1012.1678517	
cat3	-772.1925153	0.198462	0.275296	-771.8749525	
cat4	-1183.4831916	0.685997	0.800233	-1182.8020001	
cat5	-1783.705211	0.053769	0.119894	-1783.6288366	
cat6	-1878.3387836	0.095885	0.168135	-1878.2391987	
cat7	-1243.0765286	0.133256	0.200598	-1242.9205421	
cat8	-702.4634499	0.215606	0.282703	-702.216318	
5	-3054.2663707	-0.013112	0.053221	-3054.2763957	
6-TS	-841.908773	0.191507	0.267003	-841.5228843	-90.09
6-TS'	-1948.0732285	0.085100	0.158978	-1947.8887559	-76.26
7	-841.937454	0.190296	0.269284	-841.5472439	
8	-1948.1492166	0.088181	0.160979	-1947.9459198	
9-TS	-1948.1123938	0.086224	0.154917	-1947.9043329	-1188.92
9-TS-a	-1336.6329137	0.090645	0.148979	-1336.4711972	-877.81
9-TS-b	-1694.2479549	0.202970	0.283900	-1693.8789549	-871.36
10	-1948.1664407	0.089958	0.161116	-1947.9553541	
11	-3411.981949	0.095802	0.187398	-3411.749607	
12-TS	-2598.8223098	0.105557	0.191945	-2598.5621966	-293.37
12-TS-a	-1135.0109793	0.099814	0.165638	-1134.7708308	-244.78
12-TS-b	-1987.3621213	0.113501	0.186287	-1987.1367012	-289.67
12-TS-c	-2598.8222765	0.105925	0.192413	-2598.5608374	-290.47

12-TS-d	-1999.4391537	0.119081	0.202149	-1999.1671903	-218.55
12-TS-e	-1999.4576722	0.120154	0.202260	-1999.1818126	-291.81
13	-2598.8779715	0.106539	0.194462	-2598.6049597	
14-TS	-2598.8657009	0.107014	0.193280	-2598.599306	-335.80
14-TS-a	-1135.0467091	0.101067	0.166898	-1134.8042827	-333.37
14-TS-b	-1987.4054849	0.115304	0.187337	-1987.1794945	-326.49
14-TS-c	-2598.8516013	0.107954	0.193144	-2598.595 1966	-352.99
14-TS-d	-1999.4734794	0.119164	0.203091	-1999.199903	-310.00
14-TS-e	-1999.4854709	0.119747	0.202856	-1999. 2128035	-302.23
15	-2598.9391597	0.108551	0.196314	-2598.6697845	
16-TS	-5158.8408755	0.105868	0.192196	-5161.2172 722	-329.61
17-TS	-3047.6183915	0.107196	0.192356	-3047.3860705	-373.46
18-TS	-2547.482441	0.074017	0.149302	-2547.3007899	-367.38
19	-2547.5112503	0.073074	0.151426	-2547.3307522	
20-TS	-2253.241558	0.000041	0.073912	-2253.1734204	-229.71
21	-2253.3128269	0.003030	0.075179	-2253.2296295	
22-TS	-2598.8326941	0.105820	0.192623	-2598.5742274	-343.07
23	-3451.2661846	0.119381	0.215364	-3451. 0175656	
24-TS	-3451.2612624	0.117384	0.210841	-3451.0073011	-571.94
24-TS-a	-3451.2445009	0.118804	0.210768	-3451.003 4986	-534.30
24-TS-b	-1987.452555	0.111389	0.184260	-1987.216478	-989.74
24-TS-c	-2839.8196404	0.126859	0.205098	-2839.5945341	-627.28
24-TS-d	-2598.8840907	0.102114	0.190169	-25 98.6281514	-1243.85
24-TS-e	-2851.8860101	0.131234	0.220120	-2851.6 137442	-1158.23
24-TS-f	-2851.880222	0.129684	0.220195	-2851.6226317	-853.15
24-TS-g	-1388.0733824	0.122946	0.193933	-1387.8268039	-1132.98
24-TS-h	-2240.4056815	0.134768	0.213870	-2240.18108 23	-821.54
25	-3451.3052711	0.121073	0.216768	-3451.0459 854	
26-TS	-2638.146608	0.131166	0.221332	-2637.8589411	-293.66
26-TS-a	-1174.3346313	0.125235	0.194999	-1174.067259	-244.84
26-TS-b	-2026.6856271	0.138933	0.215689	-2026.4329363	-289.82
26-TS-c	-2638.1460076	0.131426	0.221805	-2637.8569822	-290.77

26-TS-d	-2038.7634226	0.144864	0.231588	-2038.4639053	-223.93
26-TS-e	-2038.7819502	0.145374	0.231635	-2038.479401	-292.14
27	-2638.2018401	0.132482	0.223953	-2637.9015378	
28-TS	-2638.1895989	0.132242	0.222689	-2637.8956294	-334.04
28-TS-a	-1174.370625	0.126450	0.196316	-1174.1007005	-333.20
28-TS-b	-2026.7293422	0.140557	0.216745	-2026.4760444	-324.59
28-TS-c	-2638.1759639	0.133536	0.222566	-2637.8922091	-349.65
28-TS-d	-2038.7977797	0.144431	0.232504	-2038.4967814	-307.22
28-TS-e	-2038.8097673	0.145326	0.232277	-2038.5097599	-299.50
29	-2638.2444546	0.136023	0.226025	-2637.9561776	
30-TS	-2586.8088208	0.100390	0.178752	-2586.5989541	-370.92
31	-2586.8403036	0.101776	0.181015	-2586.6297513	
32-TS	-2638.1570145	0.130729	0.222068	-2637.8712702	-335.60
33	-3606.3746031	0.197108	0.302451	-3606.040 028	
34-TS	-3606.3548919	0.191011	0.298303	-3606.0228643	-591.65
34'-TS	-3606.3071069	0.194444	0.297941	-3605.9902926	-1146.25
34-TS-a	-3606.3220482	0.189858	0.298455	-3606.008153	-415.78
34-TS-b	-2994.9152877	0.201796	0.292812	-2994.6166911	-529.24
34-TS-c	-2142.5277638	0.184627	0.271774	-2142.2235033	-349.12
34-TS-d	-2753.9519228	0.175921	0.277821	-2753.6239915	-446.52
35	-3491.8292735	0.160820	0.265336	-3491.5298123	
36-TS	-3606.3498116	0.192076	0.297334	-3606.0155348	-249.68
36-TS-a	-2142.537272	0.188421	0.271331	-2142.537272	-173.99
36-TS-b	-299 4.9180625	0.202762	0.292690	-2994.6126184	-226.20
36-TS-c	-3606.3445918	0.195548	0.298568	-3606.0148355	-197.32
36-TS-d	-2753.966901	0.178809	0.277102	-2753.6278906	-143.80
37-TS	-3491.8216506	0.162040	0.264470	-3491.5311284	-709.21
37-TS-a	-3606.3415943	0.192576	0.298531	-3606.0137481	-860.85
37-TS-b	-1163.5707785	0.136795	0.201790	-1163.3314716	-649.61
37-TS-c	-20 15.9111292	0.149704	0.222567	-2015.6936226	-662.04
37-TS-d	-2627.371817	0.143522	0.228716	-2627.112794	-642.75
37-TS-e	-2627.3664528	0.143502	0.228733	-2627.1157578	-652.25

37-TS-f	-2741.9039397	0.166896	0.261476	-2741.6052645	-714.35
38-TS-a	-3502.6120759	0.150708	0.256121	-3502.2969025	-1408.19
38-TS-b	-3502.6160799	0.151461	0.255665	-3502.3008842	-1414.99
38-TS-c	-4354.9945515	0.167520	0.276832	-4354.6818385	-1295.20
39	-3490.6008201	0.146091	0.245732	-3490.3127968	
40-TS	-3490.5779422	0.145219	0.240286	-3490.2943351	-908.12
40-TS-a	-3490.5616062	0.144172	0.240160	-3490.285863	-1167.41
40-TS-b	-2026.7660414	0.139226	0.214143	-2026.5044856	-1237.01
40-TS-c	-2879.1200902	0.152828	0.234314	-2878.8775986	-901.43
40-TS-d	-2638.2002097	0.130313	0.219716	-2637.9096409	-1189.36
41	-3490.6297018	0.148664	0.246303	-3490.3421126	
42-TS	-3490.5871201	0.147714	0.243933	-3490.3200663	-480.25
42-TS-a	-1162.3388063	0.119531	0.181903	-1162.1189826	-519.16
42-TS-b	-2026.7825539	0.139824	0.218263	-2026.5329189	-479.86
42-TS-c	-1415.3302536	0.145208	0.212805	-1415.1090541	-500.58
42-TS-d	-3490.5827507	0.145794	0.244771	-3490.3134465	-470.97
42-TS-e	-2014.6691375	0.130140	0.202264	-2014.4732285	-517.66
42-TS-f	-2879.1221651	0.150653	0.238731	-2878.8952816	-481.01
42-TS-g	-2626.135724	0.124852	0.208605	-2625.89585	-492.84
42-TS-h	-2626.144793	0.128822	0.208651	-2625.9073282	-492.26
43	-1312.8538741	0.121152	0.194020	-1312.6076865	
44-TS	-1312.8157951	0.121195	0.188159	-1312.5695897	-1367.53
45	-1312.8524688	0.123011	0.194118	-1312.6076436	
46	-2141.3684432	0.159991	0.253333	-2141.0694209	
47-TS	-1912.1963161	0.106253	0.182254	-1911.9729595	-371.31
48	-1912.2296641	0.108470	0.184521	-1912.006178	
49-TS	-1617.9569882	0.031269	0.106802	-1617.8465304	-202.59
50	-1618.0083962	0.030969	0.107835	-1617.8764173	
51-TS	-1963.5267851	0.138035	0.225602	-1963.23766	-342.66
52	-1963.5804911	0.145531	0.227775	-1963.2741354	
53-TS	-1963.5602276	0.138002	0.226148	-1963.2618902	-325.45
53-TS-a	-1963.5590798	0.141051	0.226444	-1963.2575543	-341.92

53-TS-b	-1352.1304358	0.150511	0.220634	-1351.8576867	-336.51
53-TS-c	-1135.0467091	0.101067	0.166898	-1134.8042827	-333.37
54	-1963.6168847	0.137494	0.228746	-1963.3202179	
55-TS	-1963.526195	0.134430	0.225012	-1963.2268352	-298.81
55-TS-a	-1963.5252388	0.137698	0.225159	-1963.2220735	-241.14
55-TS-b	-1352.0960995	0.146692	0.219554	-1351.8201053	-244.78
55-TS-c	-1135.0109793	0.099814	0.165638	-1134.7708308	-244.78
55-TS-d	-752.7108779	0.160393	0.229545	-752.4235472	-282.78
56-TS	-4523.5454701	0.135983	0.225243	-4525.8829958	-323.52
57-TS	-2412.3249647	0.140692	0.225582	-2412.0556372	-378.87
58	-2180.6945663	0.185462	0.282158	-2180.3667268	
59-TS	-2180.6733023	0.183152	0.276875	-2180.3432415	-1199.11
59-TS-a	-2180.6659098	0.183264	0.276923	-2180.3352966	-1208.77
59-TS-b	-1352.1548517	0.144914	0.217457	-1351.8862885	-1292.34
59-TS-c	-1569.2357577	0.194397	0.271193	1568.9315248	-1209.46
59-TS-d	-1963.5921956	0.137746	0.223370	1963.2893829	-1166.99
60	-2180.6919947	0.185388	0.282726	-2180.3655027	
61-TS	-1951.5231177	0.132596	0.211867	-1951.2702346	-371.74
62	-1951.5558558	0.133205	0.214116	-1951.3034173	
63-TS	-2002.8512449	0.163153	0.255074	-2002.5348419	-336.04
64	-2002.9045897	0.170673	0.257186	-2002.5707973	
65-TS	-2002.8842137	0.163300	0.255565	-2002.5586039	-323.55
65-TS-a	-2002.8836382	0.166423	0.255855	-2002.5545166	-339.61
65-TS-b	-1174.370625	0.126450	0.196316	-1174.1007005	-333.20
65-TS-c	-1391.4535714	0.175384	0.250034	-1391.1520217	-321.54
65-TS-d	-1785.8017003	0.117090	0.201934	-1785.5037051	-318.60
66	-2002.9373683	0.164200	0.256876	-2002.6157626	
67-TS	-2002.8500515	0.160088	0.254422	-2002.5227985	-299.38
67-TS-a	-2002.848855	0.163180	0.254570	-2002.5179244	-243.08
67-TS-b	-1174.3346313	0.125235	0.194999	-1174.067259	-244.84
67-TS-c	-1391.419487	0.171917	0.248944	-1391.1160514	-244.94
67-TS-d	-1785.7671975	0.115248	0.200937	-1785.4678361	-253.76

68	-2220.0338632	0.216551	0.312242	-2219.6723957	
69-TS	-2219.9953678	0.213204	0.306689	-2219.6339333	-1291.66
69-TS-a	-2219.9774142	0.212008	0.306937	-2219.6231275	-1210.95
69-TS-b	-1391.4642581	0.172743	0.247382	-1391.1727921	-1322.59
69-TS-c	-1608.5475918	0.221607	0.301090	-1608.2194355	-1236.44
69-TS-d	-2002.9142238	0.167744	0.253099	-2002.5802176	-1300.05
70	-1990.8930143	0.161856	0.243204	-1990.5991065	
71-TS	-1990.8611747	0.161107	0.241485	-1990.5829132	-507.58
71-TS-a	-1162.3388063	0.119531	0.181903	-1162.1189826	-519.16
71-TS-b	-1379.4128965	0.166451	0.235907	-1379.1612461	-495.26
71-TS-c	-1990.8502517	0.161910	0.241774	-1990.5677121	-480.64
71-TS-d	-1391.4749549	0.177731	0.251753	-1391.1852022	-498.05
71-TS-e	-2219.9848153	0.216823	0.310547	2219.6402104	-483.94
71-TS-f	-1773.7745287	0.113134	0.187759	-1773.5252501	-505.49
72	-2335.7673202	0.262170	0.367935	-2335.3655427	
73-TS	-2335.7411399	0.256611	0.364500	-2335.3387822	-369.38
73'-TS	-2335.723019	0.262172	0.365225	-2335.3288795	-1283.61
73-TS-a	-1507.2236129	0.222655	0.305346	-1507.2236129	-403.93
73-TS-b	-1724.3010313	0.268670	0.358933	-1723.923972	-536.49
73-TS-c	-2335.7260571	0.259159	0.365052	-2335.32562	-500.88
73-TS-d	-2118.6669475	0.215507	0.310938	-2118.2879743	-486.00
73-TS-e	-2335.72196	0.260515	0.363323	-2335.3196429	-294.55
73-TS-f	-1724.2885461	0.268387	0.357559	-1723.9171314	-350.84
73-TS-g	-1507.2064875	0.219940	0.304261	-1506.8713905	-126.96
73-TS-h	-2118.6339869	0.207820	0.309335	-2118.2695948	-196.74
74	-2221.2163561	0.232138	0.332130	-2220.8508426	
75-TS	-2221.2107861	0.227000	0.330278	-2220.8512761	-621.39
75-TS-a	-2335.7398111	0.255506	0.364814	-2335.3418153	-564.50
75-TS-b	-1163.5707785	0.136795	0.201790	-1163.3314716	-694.61
75-TS-c	-1380.6472197	0.183737	0.255850	-1380.3750974	-700.47
75-TS-d	-1992.0795569	0.175252	0.261845	-1991.781866	-596.93
75-TS-e	-1495.1652009	0.212758	0.289098	-1494.859839	-796.25

75-TS-f	-1507.2135644	0.215028	0.304718	-1506.8785728	-614.84
75-TS-g	-1392.6947221	0.191131	0.271384	-1392.3922597	-688.55
75-TS-h	-1992.0837209	0.177607	0.261576	-1991.7877436	-602.03
75-TS-i	-2106.6146302	0.203505	0.295037	-2106.2817908	-586.94
76-TS	-2335.7171282	0.256207	0.362920	-2335.3237558	-294.77
77-TS-a	-2232.0271277	0.220477	0.321675	-2231.6361653	-1405.30
77-TS-b	-1620.5842307	0.229603	0.316123	-1620.2157098	-1255.71
77-TS-c	-1403.5033653	0.180540	0.262157	-1403.176055	-1426.92

¹The electronic energy calculated at B3LYP-D3/BSI level (BSI designates the basis set combination of LanL2DZ for Pd and I atoms, and 6-31G(d,p) for other atoms) in gas phase. ²The thermal correction to Gibbs free energy calculated at B3LYP-D3/BSI level in gas phase. ³The thermal correction to enthalpy calculated at B3LYP-D3/BSI level in gas phase. ⁴The electronic energy calculated at M06-D3/BSII (BSII designates the basis set combination of LANL2DZ for Pd and I atoms, and 6-311++G(d,p) for other atoms) level in DMAc solvent. ⁵The B3LYP-D3/BSI calculated imaginary frequencies for the transition states.

Table 2. B3LYP-D3 geometries for all the optimized compounds and transition states. The atomic coordinates are given at B3LYP-D3/BSI level. (BSI designates the basis set combination of LanL2DZ for Pd and I atoms, and 6-31G(d,p) for other atoms in the gas phase.

Ib				C	0.62799700	2.38765300	-0.04160200
C	-0.28023300	-0.03634600	0.03887300	C	-0.77574400	2.41467300	-0.02209500
C	1.11558500	-0.05602700	0.04054800	C	-1.45695300	1.19237000	0.00560800
C	1.82626600	1.14409000	-0.00850600	H	-1.30326800	-0.95599300	0.04034400
C	1.15223500	2.37196200	-0.05198900	H	1.17855800	-0.95638600	0.03044700
C	-0.24768000	2.37552000	-0.05191600	H	-2.54393600	1.19340300	0.02740600
C	-0.96241600	1.18072200	-0.00613600	O	1.32201900	3.58914300	-0.02129800
H	-0.82785900	-0.97299000	0.07831300	C	1.62200500	4.11311900	-1.31279300
H	1.64841200	-0.99954100	0.08059000	H	2.15956000	5.05106200	-1.15486700
H	-0.75210800	3.33658700	-0.07481700	H	2.25648500	3.42757900	-1.89007100
H	-2.04803700	1.20037400	-0.00114800	H	0.70957500	4.31408500	-1.88968500
O	1.82661500	3.56556900	-0.05361700	C	2.86176000	1.20516200	-0.01732200
C	2.06434800	4.10721100	-1.35606000	H	3.26369400	1.35060400	-1.02790500
H	2.59462300	5.04940800	-1.20632900	H	3.23895700	2.02605300	0.59806500
H	2.68492400	3.43301500	-1.95921500	H	3.26623700	0.26263400	0.36198400
H	1.12049600	4.29761100	-1.88400200	C	-1.51225200	3.73189700	-0.02204600
I	3.96781500	1.10401600	0.00430400	H	-0.98724400	4.47080500	0.58885600
				H	-1.59035900	4.14884700	-1.03403600
3b				H	-2.52955700	3.61324000	0.36121100
C	-0.76015600	-0.01563600	0.01411100				
C	0.63439500	-0.01544200	0.00731600	4b			
C	1.35282700	1.18535000	-0.02012700	C	-0.19259800	-0.77585300	0.06345100

C	1.20777900	-0.76978000	0.06373500	O	7.99320400	-0.03224000	1.26160800
C	1.86542400	0.45422000	0.03156800	C	8.23526000	1.37733200	1.36122400
C	1.12900800	1.63805800	-0.00809300	H	7.50881400	1.86882800	2.01690000
C	-0.26642100	1.67356700	-0.01565600	H	8.19345600	1.84707600	0.37066400
C	-0.90679800	0.42617700	0.02160500	H	9.23738200	1.48571400	1.77996400
H	-0.72999800	-1.71876000	0.09661400	I	5.80043500	-0.18495400	3.74437200
H	1.76654100	-1.70125900	0.09097200				
H	-1.99388700	0.40176300	0.02376000	cat1			
O	1.90929500	2.76400300	-0.04448300	Pd	4.81466300	1.19591500	0.07921200
C	-1.00416300	2.98522200	-0.06008500	C	3.29111400	3.04990200	-1.50449400
H	-0.68473100	3.64355700	0.75542600	C	4.56380400	3.03780000	-0.82932100
H	-0.80025400	3.52298500	-0.99345700	C	4.62763300	3.38847300	0.55529000
H	-2.08443400	2.83557000	0.01847800	C	3.43219400	3.74478000	1.24318600
C	3.27219200	2.34571100	0.22232000	C	2.22656600	3.75930000	0.57263200
H	3.93215600	2.92929400	-0.42343500	C	2.15753000	3.39781100	-0.79043700
H	3.50010200	2.58236200	1.26949700	H	5.57912400	3.65808500	1.00206900
C	3.33182100	0.81928900	-0.03144200	H	3.49643700	4.04597100	2.28416100
H	3.94513100	0.30572400	0.71527000	H	1.31684700	4.04797500	1.09020400
H	3.75240900	0.58853000	-1.01859200	H	1.20929300	3.37610100	-1.31779800
				O	3.16376600	2.78415400	-2.83537000
cat0				C	3.56513000	1.47739700	-3.26722500
C	3.85963300	3.16414900	-1.24517700	H	4.64289000	1.32415900	-3.15184300
C	4.19055600	3.50341300	0.10270400	H	3.03146000	0.70586200	-2.69886000
C	3.17736400	3.47313800	1.09674700	H	3.30092500	1.41520200	-4.32474200
C	1.85525100	3.13272500	0.74219000	I	6.33105200	3.69450200	-2.11391500
C	1.54094600	2.83986200	-0.57865700	O	4.99591400	-0.89262500	0.44417400
C	2.54089300	2.84289600	-1.56025000	C	6.00313000	-1.66896600	0.58512200
H	3.38987200	3.85346800	2.09011400	O	7.20658900	-1.36073700	0.41107500
H	1.08772400	3.13562300	1.50956200	C	5.65283400	-3.09304800	1.00539400
H	0.51894900	2.60092900	-0.85629200	H	5.17033000	-3.07025200	1.98773500
H	2.31820000	2.60486100	-2.59528000	H	4.92921300	-3.51676300	0.30285600
O	4.77830400	3.23256900	-2.25300900	H	6.54537800	-3.71887800	1.04799600
C	5.70455500	2.14038500	-2.32287400	K	7.93253600	0.89988500	-0.33311500
H	6.36258500	2.11503000	-1.44728400				
H	5.17272300	1.18390300	-2.38962100	cat2			
H	6.30001600	2.30277700	-3.22348900	N	4.40441800	-1.30790500	0.56282800
I	5.99562800	4.67018500	0.47728500	C	3.43593900	-1.32180500	1.69504200
Pd	4.63229800	1.54468900	0.99133400	H	3.66498200	-0.45147700	2.31846100
C	6.77158400	-0.39760700	0.77515700	H	2.44947200	-1.13097800	1.25773100
C	5.58596400	-0.32326600	1.57608800	C	5.80111700	-1.66722800	0.93715500
C	4.35832000	-0.81109400	1.04400600	H	6.46343500	-1.16341200	0.22415600
C	4.32595800	-1.36453300	-0.25592300	H	5.98710200	-1.19834900	1.90993700
C	5.48661700	-1.44193300	-1.01114300	C	3.91006200	-1.95912200	-0.68257900
C	6.69793700	-0.94787100	-0.50028900	H	3.15304400	-1.29227700	-1.11148600
H	3.49580200	-0.91714200	1.69286700	H	4.75172000	-1.96196800	-1.38508300
H	3.38809400	-1.75710900	-0.63572200	C	3.29344100	-3.36724400	-0.61306000
H	5.46619500	-1.88809100	-2.00078800	C	2.93883600	-3.87988500	-2.01553900
H	7.61586500	-0.99759300	-1.07714900	H	2.38084500	-3.33922800	-0.00478100

H	3.97189900	-4.07641400	-0.12980600	C	3.23378400	3.10804800	1.09051500
C	2.26816600	-5.25655200	-1.99090900	C	2.04582400	2.36069900	0.89841900
H	2.27722400	-3.15645400	-2.51141600	C	1.62678600	2.03886800	-0.38220800
H	3.85127200	-3.92587400	-2.62569200	C	2.39562200	2.41559300	-1.49764400
H	2.02905400	-5.60388500	-3.00108800	H	3.42530500	3.55326700	2.06124700
H	2.92083000	-6.00425500	-1.52603100	H	1.45030000	2.08721700	1.76453500
H	1.33497000	-5.23003500	-1.41681900	H	0.70414800	1.48619900	-0.53384300
C	6.21547700	-3.14823600	0.98758300	H	2.09597900	2.14681800	-2.50562300
C	7.65768100	-3.29668500	1.49086200	O	4.19996400	3.55193300	-2.49718000
H	6.14365700	-3.58469000	-0.01659800	C	5.56564700	3.15873300	-2.66210800
H	5.54680400	-3.72823000	1.63061800	H	6.22527800	3.64754900	-1.93887400
C	8.13345100	-4.75247400	1.50391600	H	5.66366300	2.06976800	-2.56028900
H	8.32709900	-2.69531100	0.86104600	H	5.84781600	3.46503300	-3.67205800
H	7.73251200	-2.87572000	2.50276300	I	5.08175000	5.47840800	0.16730500
H	9.16160300	-4.83480800	1.87054200	Pd	5.19849300	1.99907200	0.62931600
H	7.49763200	-5.36891200	2.14973500	C	8.57143000	-1.39129200	1.66173100
H	8.10161700	-5.18635300	0.49793600	H	8.63152100	-0.31444700	1.52155200
C	3.36657300	-2.54947500	2.62067800	H	9.00879500	-1.66098100	2.62993200
C	2.24426800	-2.38819300	3.65498700	H	9.13916800	-1.89575400	0.87078800
H	4.32130600	-2.66582200	3.14829000	N	7.17147900	-1.80411900	1.61675600
H	3.20617800	-3.47188500	2.05455300	C	6.94312900	-3.22533200	1.83223300
C	2.17169900	-3.55935800	4.63947600	H	5.88613500	-3.47560200	1.78100200
H	2.39095900	-1.45036700	4.20774700	H	7.47355800	-3.81275000	1.07242300
H	1.28339800	-2.28581800	3.13250900	H	7.32152700	-3.52426800	2.81753900
H	1.36270000	-3.42423800	5.36453200	C	6.19829500	-0.88809100	1.36871900
H	1.99541400	-4.50519200	4.11449200	O	6.49985700	0.30601400	1.18049100
H	3.10837000	-3.66201400	5.19918300	C	4.75266800	-1.34459800	1.33155300
Pd	4.54687100	0.91321200	-0.05694100	H	4.13229600	-0.46513400	1.14959500
C	3.38790600	3.03969200	-1.49565900	H	4.58469200	-2.06856600	0.52785500
C	4.61857000	2.84699200	-0.77591900	H	4.45351900	-1.80693200	2.27740500
C	4.64603000	3.13662400	0.62457600				
C	3.48773000	3.63215400	1.26859400	cat4			
C	2.32492300	3.84355000	0.54451200	N	-2.24044000	-0.01949500	0.01981000
C	2.27436500	3.53147500	-0.82502800	C	-2.60864200	-0.94157400	-1.09420300
H	5.59996400	3.18497000	1.13843100	H	-1.89132300	-0.75674600	-1.89915700
H	3.53825300	3.88163600	2.32430000	H	-2.40625300	-1.95555700	-0.73241300
H	1.44199000	4.24568600	1.03237500	C	-2.59720800	1.40820400	-0.22751500
H	1.36567600	3.67114800	-1.40202400	H	-1.88986600	2.00816800	0.35247800
O	3.29026900	2.85614700	-2.84681600	H	-2.36911600	1.60335900	-1.28098400
C	3.46028900	1.52200600	-3.33089600	C	-2.62335100	-0.51676000	1.37332700
H	4.46499500	1.13683200	-3.12695600	H	-1.92282300	-1.32057500	1.61820400
H	2.71882400	0.85203800	-2.87478700	H	-2.40886600	0.29863400	2.07257000
H	3.30264200	1.56731600	-4.41089900	C	-4.04913000	-1.04768100	1.61259700
I	6.52624600	3.08200400	-1.89688400	C	-4.24996000	-1.42766200	3.08577500
				H	-4.21951800	-1.93619400	0.99200400
cat3				H	-4.80783400	-0.31390100	1.32459900
C	3.56730500	3.15004400	-1.35577800	C	-5.63553000	-2.01949700	3.36191400
C	4.00598600	3.53554200	-0.03872600	H	-3.47534200	-2.14675500	3.38509600

H	-4.09741500	-0.53847500	3.71275200	H	4.78633300	-0.47307900	-1.27409500
H	-5.75897800	-2.27969900	4.41832900	C	5.57991800	-2.40822900	-3.11699400
H	-6.42689800	-1.30847300	3.09789400	H	3.41888800	-2.51554500	-3.10142200
H	-5.79942700	-2.92870700	2.77214000	H	4.05065700	-0.95919500	-3.61107900
C	-4.01664700	1.90830200	0.09997300	H	5.68848600	-2.78188000	-4.14050000
C	-4.18248800	3.37729400	-0.31197500	H	6.38119900	-1.68167700	-2.93945500
H	-4.19904300	1.82133900	1.17823700	H	5.74172100	-3.25058600	-2.43467300
H	-4.78387900	1.30739000	-0.39724700	C	4.01078100	1.88312700	-0.33314400
C	-5.55944300	3.94419900	0.04722400	C	4.19005000	3.39104200	-0.11132800
H	-3.39916000	3.98006200	0.16741800	H	4.17152400	1.66147900	-1.39573100
H	-4.01722900	3.47015400	-1.39416200	H	4.78580000	1.34464000	0.22035200
H	-5.65600600	4.99097400	-0.25926200	C	5.55897300	3.89957100	-0.57370900
H	-6.35912900	3.37718900	-0.44325100	H	3.39643900	3.93406100	-0.64246300
H	-5.73572800	3.89484300	1.12792800	H	4.05327100	3.61918800	0.95462300
C	-4.02236600	-0.87691900	-1.70247000	H	5.66705600	4.97577700	-0.40323900
C	-4.20498600	-1.96506300	-2.76922400	H	6.36932000	3.39304800	-0.03680200
H	-4.17794200	0.10421200	-2.16815100	H	5.70636900	3.71404000	-1.64385000
H	-4.79918200	-0.98843200	-0.94002700				
C	-5.57496500	-1.90377600	-3.45160500	cat5			
H	-3.41246700	-1.87128200	-3.52409700	Pd	4.60800200	1.29550700	0.68989700
H	-4.06800100	-2.95182900	-2.30608400	O	4.77415500	-0.76847400	1.12940800
H	-5.68537100	-2.69134100	-4.20429300	C	5.68586300	-1.48712100	0.58675500
H	-6.38398000	-2.02301000	-2.72173400	O	6.56860200	-1.10020900	-0.21757300
H	-5.72231500	-0.93991800	-3.95225600	C	5.68258800	-2.96169000	0.98982400
Pd	-0.00165200	-0.02499100	0.02682100	H	4.76587300	-3.23422900	1.51664200
N	2.23789100	-0.01467000	0.01659600	H	5.81584400	-3.59065300	0.10481800
C	2.59721600	1.43187700	0.07958500	H	6.53598100	-3.14846900	1.65066100
H	1.88045800	1.95749900	-0.55809300	K	6.91161300	1.29394600	-1.06500900
H	2.38734800	1.75545800	1.10471500	C	3.44613800	3.45578900	-1.00875600
C	2.60035700	-0.67755400	-1.26991600	O	4.41483000	3.19623500	-0.21094500
H	1.89833200	-1.50626300	-1.40046100	O	2.52249200	2.67647300	-1.34850600
H	2.37108300	0.04351400	-2.06196400	C	3.43130100	4.87429300	-1.57808700
C	2.62093200	-0.79093800	1.23161400	H	3.21194500	4.84459300	-2.64926100
H	1.92109000	-0.49797900	2.01972100	H	2.62409000	5.43803800	-1.09789400
H	2.40383500	-1.84067900	1.00637300	H	4.37524800	5.39206000	-1.39619200
C	4.04682100	-0.66230300	1.79985200	K	2.19384100	0.26823100	-0.53452500
C	4.24636400	-1.60688300	2.99292400				
H	4.21829900	0.36852700	2.13390300	cat6			
H	4.80661600	-0.87701600	1.04249600	Pd	4.82171100	1.35012900	0.11999000
C	5.63228600	-1.47270300	3.63109000	O	4.87284400	-0.74148500	0.30393700
H	3.47243300	-1.40938900	3.74713300	C	6.02124500	-1.43438100	0.69572800
H	4.09165700	-2.64351000	2.66349900	O	6.79160200	-1.83201700	-0.22690300
H	5.75297600	-2.15641000	4.47781600	K	5.67410200	-0.71758300	-2.13972300
H	6.42316600	-1.69608800	2.90577700	O	6.16369900	-1.65040700	1.93504400
H	5.79984400	-0.45351600	3.99795000	K	4.23610600	-0.32553600	2.75926200
C	4.02349800	-1.23317400	-1.46736900	C	2.10140100	3.18133200	-0.71015700
C	4.20322800	-1.77549500	-2.89178900	H	2.76279500	2.33348200	-0.48778400
H	4.20289500	-2.04743800	-0.75427400	H	1.25591300	3.17354000	-0.01060800

H	1.70792900	3.07588000	-1.72949700	H	-4.25530300	2.01201800	1.23725600
N	2.83165300	4.43861000	-0.58828700	C	-2.10855200	3.22140200	-0.28410800
C	2.02823300	5.61877900	-0.87514400	O	-0.95479400	2.96320000	-0.73408400
H	2.58718300	6.53976400	-0.72800700	C	-2.42643000	4.59648500	0.28367200
H	1.66911900	5.59447700	-1.91250100	H	-1.49411900	5.15854800	0.32351000
H	1.15084200	5.64309400	-0.21685300	H	-3.14001800	5.12329900	-0.36223500
C	4.15933500	4.47838600	-0.27802100	H	-2.84669800	4.54241500	1.29045100
O	4.85192500	3.47433500	-0.05009400	C	1.18289400	-0.77512700	2.08453300
C	4.84546200	5.83345500	-0.19983200	H	1.76656000	-0.06733800	2.67008600
H	5.88929200	5.64954200	0.05085400	H	1.59787300	-1.78047800	2.19541900
H	4.79686300	6.37175500	-1.15190800	H	1.23358700	-0.47289000	1.02736500
H	4.40188500	6.46984200	0.57294700	N	-0.19727300	-0.77049400	2.56166500
cat7				C	-1.04647100	-1.81453800	2.00568100
Pd	4.99161400	1.44831700	0.32611200	H	-1.96169800	-1.93097600	2.58656000
O	4.88004700	-0.59355600	0.70280100	H	-1.31523300	-1.60111100	0.95888000
C	5.75501300	-1.50573400	0.53477600	H	-0.50982600	-2.76633400	2.03545900
O	6.91814600	-1.36625200	0.07565600	C	-0.72979400	0.43914700	2.93669800
C	5.32480100	-2.91159200	0.95168900	O	0.02014800	1.43404200	3.14970900
H	5.96634000	-3.25217000	1.77135200	C	-2.19039500	0.47525400	3.36192100
H	4.28167500	-2.93594600	1.27005300	H	-2.40571400	1.48875500	3.69792200
H	5.47830800	-3.60077000	0.11557200	H	-2.86691900	0.22270800	2.54232900
K	7.75598400	0.89330500	-0.55717500	H	-2.37021000	-0.22691800	4.18569000
C	2.32386500	3.24797100	-0.37483200	Pd	-0.42989900	2.22609600	1.21505400
H	2.98311200	2.39417100	-0.17399300	int1			
H	1.64427400	3.38341400	0.47568400	C	2.92818400	2.32467600	-0.90642900
H	1.72901200	3.03852000	-1.27095300	C	2.08596500	1.46689700	-0.20999500
N	3.10953800	4.46276700	-0.58397300	C	0.80048000	1.82178200	0.14004300
C	2.29929300	5.63770200	-0.88057800	C	0.40668300	3.11726300	-0.25931200
H	2.90634700	6.49397000	-1.16536400	C	1.27166000	3.96732600	-0.96050800
H	1.62141900	5.41231800	-1.71151500	C	2.58585700	3.59855800	-1.31706800
H	1.68719000	5.91641400	-0.01231600	H	0.12278900	1.17036500	0.68367700
C	4.45553500	4.50730400	-0.38792300	H	-0.59267000	3.46636400	-0.01804600
O	5.15490800	3.52807500	-0.07485500	H	0.91607000	4.95430300	-1.24331600
C	5.16827300	5.83862300	-0.57178400	H	3.24832300	4.26305500	-1.85978100
H	6.22496700	5.66938600	-0.36783900	O	4.02939000	1.48116100	-0.97397800
H	5.06057500	6.22222300	-1.59175000	C	3.22696300	0.46962300	-0.22796500
H	4.79340100	6.60125000	0.11810700	H	3.09596300	-0.43409200	-0.83048300
cat8				H	3.70428000	0.23232200	0.72732100
C	-2.83918700	1.04463700	-1.04772800	int2			
H	-2.00899500	1.11803800	-1.74799100	C	2.90674300	2.29118200	-0.92068700
H	-2.53143200	0.37916500	-0.22494300	C	2.07515200	1.45041700	-0.19766700
H	-3.71463200	0.62315500	-1.54921100	C	0.79793300	1.82146000	0.17222300
N	-3.16487600	2.37517100	-0.54927100	C	0.41580600	3.11312000	-0.24338500
C	-4.38686500	2.45711900	0.23818200	C	1.27905000	3.94139800	-0.97478900
H	-4.71062900	3.49102800	0.35845100	C	2.58673400	3.56749100	-1.35586000
H	-5.18416400	1.91654400	-0.27892500	H	0.12270200	1.18657200	0.73755700

H	-0.57456500	3.48153100	0.00678600	C	0.70042200	2.72789200	0.18639400
H	0.92687300	4.92781200	-1.26821300	C	1.62528300	2.77452800	-0.86449200
O	4.00467900	1.43950200	-1.00129300	H	2.81607400	3.14092800	2.81270900
C	3.20988000	0.44532100	-0.22542900	H	0.39722300	2.81161000	2.32123000
H	3.06097900	-0.46624000	-0.81184600	H	-0.35433100	2.61560600	-0.04595900
H	3.70436400	0.21802100	0.72369400	H	1.27215600	2.69141000	-1.88559300
C	3.52304300	4.44796800	-2.13780700	O	3.95121100	3.00715800	-1.56309200
H	4.42231100	4.68518400	-1.55765200	C	3.56133200	2.90845400	-2.92518500
H	3.85774100	3.95341500	-3.05656400	H	3.09313400	1.93918000	-3.14075000
H	3.04076900	5.38955600	-2.41456500	H	2.87295000	3.71478400	-3.20838900
				H	4.48126500	3.00129200	-3.50396800
5				I	5.44390600	4.19111000	1.17490500
Pd	5.44334500	1.59907000	-0.43053400				
O	6.16448200	-0.45599400	-0.33275500	6-TS'			
C	5.30622100	-0.87088400	0.62940200	Pd	0.55803800	0.33599600	0.07699400
O	5.63609100	-0.69447300	1.86508500	C	-1.89332500	1.76443200	0.62092700
K	7.83676000	0.46506400	1.35234600	C	-1.31459400	0.83787000	-0.30143900
C	2.94139100	2.29637100	-1.12215400	C	-1.13498700	1.21740800	-1.66119500
O	3.82217700	3.03929100	-0.40912600	C	-1.43337600	2.51629900	-2.08159300
O	2.13836700	1.52189400	-0.50304800	C	-1.98088700	3.42027000	-1.16995800
K	3.21567600	0.76609700	1.74826500	C	-2.19904000	3.05104900	0.15737200
O	4.18230600	-1.36993800	0.28753000	H	-0.84117300	0.46431500	-2.38384200
O	2.98523300	2.36186300	-2.41059300	H	-1.27898000	2.79617500	-3.11895000
K	4.94190400	3.98658500	-2.48746600	H	-2.24453700	4.42400500	-1.49040400
K	3.44936200	-0.39300900	-2.01218900	H	-2.60972000	3.75240500	0.87736100
				O	-2.18643400	1.53847700	1.92349000
6-TS				C	-1.49134100	0.55618600	2.68673900
C	6.34204900	-0.46595100	-0.30279700	H	-1.90212600	-0.44433400	2.53509300
C	6.31260800	-0.18046500	1.09760200	H	-0.42270700	0.54128500	2.41270900
C	5.29132200	-0.75250300	1.89903300	H	-1.61259500	0.85173200	3.73200500
C	4.34569400	-1.63125900	1.31949600	I	-2.17234500	-1.52733000	-0.20106900
C	4.41329800	-1.93131600	-0.03216000	O	2.41945100	-0.55780900	0.59324000
C	5.39611500	-1.33489600	-0.83818000	C	3.40303300	-0.86070100	-0.35737300
H	5.34174100	-0.65565900	2.97848600	O	3.37009600	-2.01702200	-0.86122900
H	3.59128200	-2.08316800	1.95522800	K	1.34768100	-2.96700800	0.21676100
H	3.70065600	-2.61925700	-0.47639900	O	4.25697700	0.04301400	-0.58919200
H	5.45228700	-1.53668600	-1.90290100	K	3.47271400	1.76348400	1.00099400
O	7.30021700	0.03679400	-1.13126800				
C	7.20663600	1.44806200	-1.39919800	7			
H	7.42698100	2.04709400	-0.51113600	C	7.19638900	0.03084300	0.28843400
H	6.20217500	1.70671700	-1.75276200	C	6.12659300	0.16721200	1.18403200
H	7.94765600	1.65524500	-2.17333800	C	4.80225100	0.19630100	0.71443100
I	8.11237000	0.52918700	2.07142600	C	4.52913700	0.06136300	-0.66781800
Pd	4.69878500	1.44498500	1.20508800	C	5.60846100	-0.09758500	-1.56054000
C	2.98984400	2.92487800	-0.60429200	C	6.91538400	-0.09865900	-1.09385600
C	3.42181300	2.99739900	0.74975800	H	3.98340100	0.23880900	1.42249700
C	2.47887200	2.99123100	1.79313700	H	3.50672700	-0.01196500	-1.01909700
C	1.11743600	2.83218400	1.50937900	H	5.41625700	-0.20679600	-2.62249300

H	7.73075700	-0.20027200	-1.79925200	K	2.34258700	2.24150300	1.71250200
O	8.44414000	0.03549100	0.80101600				
C	9.56279900	-0.03982800	-0.07809100	9-TS			
H	9.57825000	0.80359900	-0.77882200	Pd	-1.13619000	-0.79871200	0.46240500
H	9.57289700	-0.98386300	-0.63666300	C	-3.90127000	-0.39873400	-0.24733700
H	10.44206100	0.00821300	0.56446200	C	-2.70841300	0.33846300	-0.03717100
I	6.47994600	0.40021300	3.26680300	C	-2.75242400	1.72556600	-0.23394600
Pd	4.66391000	2.42347700	-0.30253000	C	-3.92309800	2.35997100	-0.66405300
C	1.75049400	2.27614900	-0.56193900	C	-5.08270600	1.61201900	-0.88339900
C	2.79638200	2.60006000	0.31726700	C	-5.07750900	0.23629400	-0.66782900
C	2.53937700	2.97652100	1.62934600	H	-1.86088900	2.31692700	-0.06135200
C	1.21862400	3.00469700	2.09991700	H	-3.92439200	3.43474700	-0.82341700
C	0.17549800	2.67913100	1.23823800	H	-5.99720500	2.10027400	-1.20891600
C	0.43307400	2.31537600	-0.08701300	H	-5.97180200	-0.36480200	-0.80102600
H	3.35755500	3.25953300	2.28315400	O	-3.95578800	-1.74611200	-0.07083900
H	1.01915300	3.29662700	3.12637100	C	-2.82299900	-2.29652000	0.59751600
H	-0.85212400	2.70812700	1.58844000	H	-1.83083800	-2.51867300	-0.25369500
H	-0.39317400	2.06613500	-0.74298500	H	-2.79578000	-1.98842100	1.65468100
O	2.09933000	1.90822200	-1.83515200	H	-2.95104200	-3.38393300	0.61662200
C	1.06521300	1.75741100	-2.79736200	C	0.24230800	-2.85747800	-0.76166200
H	0.40620800	0.91146400	-2.55909900	O	-0.96635800	-3.07977300	-1.22601000
H	0.46224000	2.66980100	-2.88409400	O	1.25069200	-2.89449800	-1.53597200
H	1.56600600	1.56489900	-3.74736200	O	0.36163600	-2.48125900	0.49511600
I	4.93724500	5.00586100	-0.66822800	K	2.83889100	-1.88746700	0.29207900
				I	0.86006200	1.08385600	0.13432700
8				K	-0.67232800	-1.04056700	-2.80968300
Pd	0.44613200	-0.50654400	-0.47152000				
C	-0.96646500	1.95999000	0.28093700	9-TS-a			
C	-0.79732700	1.01691300	-0.74444700	Pd	-1.14959300	-0.64136700	0.24083700
C	-1.41213200	1.28591700	-1.97470600	C	-4.03396600	-0.27277600	0.10635100
C	-2.14171700	2.46201400	-2.18000300	C	-2.83145600	0.41360300	0.36484700
C	-2.28149000	3.39415400	-1.15008500	C	-2.87357100	1.77618400	0.65277500
C	-1.69610700	3.13502500	0.09011300	C	-4.08911100	2.47240800	0.62400400
H	-1.31729500	0.56810900	-2.78389900	C	-5.27030100	1.78475800	0.33374800
H	-2.60161100	2.64741500	-3.14736400	C	-5.25240400	0.41243100	0.08410700
H	-2.84741300	4.30839500	-1.30484700	H	-1.95136200	2.31724800	0.86711500
H	-1.79855700	3.82843500	0.92132500	H	-4.10767300	3.54170800	0.81338400
O	-0.37949100	1.77497300	1.54926800	H	-6.21681500	2.31732700	0.31497900
C	-1.13854600	0.89129900	2.38895100	H	-6.16483300	-0.14190000	-0.11150400
H	-2.13328100	1.30978400	2.58729100	O	-4.03150400	-1.61127200	-0.14621000
H	-1.24306400	-0.09464800	1.92355400	C	-2.85955200	-2.28642600	0.25923400
H	-0.59103200	0.79591700	3.33204800	H	-1.88168300	-2.18959100	-0.51251500
I	-1.48326100	-2.43284700	-0.57401800	H	-2.71475500	-2.25303200	1.34640000
O	2.14379300	0.65400200	-0.20840200	H	-2.95754300	-3.33710600	-0.02997200
C	2.84577100	-0.31763900	0.38231500	C	0.44334000	-2.70166800	-0.95346400
O	2.37970900	-1.52070900	0.14532100	O	-0.71966500	-2.85222200	-1.44579300
K	1.67710100	-3.82730200	-0.08996500	O	1.46897900	-3.37729600	-1.25448900
O	3.79352000	-0.04395800	1.14307100	O	0.61359400	-1.71439600	-0.01096700

K	3.07519000	-2.26748700	0.25072800	C	-4.68384100	-0.26439100	-0.74653400
				H	-1.95973100	2.20638900	0.56387500
9-TS-b				H	-3.50642500	2.90029800	-1.26826300
Pd	-1.20862400	-0.60173100	0.41831700	H	-5.22773100	1.31134700	-2.10704900
C	-3.99532800	-0.23145500	-0.31577900	H	-5.45131300	-0.95544500	-1.08071000
C	-2.86376800	0.51475300	0.08376100	O	-3.86101800	-1.87612900	0.83215300
C	-3.02595000	1.89733600	0.23359100	C	-3.07208600	-1.90591800	2.05805700
C	-4.24170200	2.53315000	-0.04414300	H	-2.54784200	-2.89351600	-0.41147100
C	-5.33401800	1.77522900	-0.46788300	H	-3.73318600	-1.67889600	2.90284700
C	-5.21678200	0.39251200	-0.59356200	H	-2.64460400	-2.90930200	2.13357900
H	-2.19154900	2.51689100	0.55700400	C	-0.62273000	-3.04967500	-0.46423600
H	-4.32717600	3.61089000	0.06326000	O	-1.83595300	-2.71081700	-1.05091800
H	-6.28294200	2.25611600	-0.68779100	O	0.38193700	-2.58564600	-1.08257100
H	-6.05856300	-0.22396300	-0.89321600	O	-0.63969300	-3.70513200	0.60088700
O	-3.94707600	-1.58514700	-0.45111600	K	1.80762600	-2.88548100	1.12008700
C	-2.86683600	-2.21441300	0.21985100	I	1.09968800	0.53158800	1.86151500
H	-1.75476200	-2.25888500	-0.39513600	K	-0.79066500	-0.26475300	-1.64404000
H	-2.94023700	-2.08042000	1.30973500				
H	-2.95426400	-3.28982600	0.03744800	11			
C	0.37011600	-2.97045100	-0.08040500	Pd	8.91556400	1.95526700	-1.43011300
O	-0.54231900	-2.99217700	-0.97575200	C	6.42362900	1.13940100	-2.55315600
O	1.31144900	-3.80383500	0.03927000	C	5.23431500	1.12944000	-3.28022300
O	0.31948600	-1.96902700	0.84560800	C	4.78993600	2.32593500	-3.85789000
K	2.14758100	-2.99697500	2.25887400	C	5.50909200	3.50863700	-3.67980200
C	1.42708700	0.63504300	1.46544100	C	6.69843800	3.50136000	-2.93075500
C	2.51697000	0.37447100	0.63577600	C	7.19622000	2.31169000	-2.38462300
C	2.41666800	0.49583100	-0.75366900	H	3.86715600	2.33129000	-4.43168800
C	1.23781000	0.93828900	-1.33962700	H	5.14982200	4.43567900	-4.11863400
C	0.16100800	1.31295800	-0.52602600	H	7.24673800	4.42958800	-2.77810900
C	0.23331200	1.15000800	0.88022400	O	6.90725400	-0.00811400	-1.98079100
H	3.26966600	0.24419600	-1.37403700	C	7.81682100	0.33563700	-0.90081900
H	1.16440400	1.02482400	-2.41752000	H	7.22977500	0.57202800	-0.00242800
H	-0.69963100	1.80362500	-0.96192800	H	8.44572300	-0.53945200	-0.71052400
H	-0.49823200	1.63122600	1.51891300	C	10.43021300	3.04748900	-3.76331400
O	1.55052900	0.37778700	2.78764700	O	9.35851300	2.92700700	-4.62921000
I	4.40727100	-0.18851500	1.48703900	O	10.21198000	3.56386600	-2.61858200
C	0.40344400	0.54386100	3.62496500	H	8.56107700	3.24553000	-4.16851000
H	-0.43574700	-0.06035800	3.25826800	C	11.07542100	-0.01859300	-0.75115500
H	0.71121700	0.20451000	4.61468800	O	10.73903700	1.22292200	-0.43695100
H	0.10104300	1.59513300	3.68677800	O	11.04066700	-0.92214800	0.15826300
10				K	12.69242200	2.52543000	-1.80376000
Pd	-1.51957100	-0.57943700	2.01792100	I	14.59942500	0.82004700	0.91774000
C	-3.80938500	-0.64118700	0.27480900	K	11.17497500	0.83983500	2.08452200
C	-2.79265900	0.22665800	0.73032400	O	11.49942700	2.55669600	-4.18756500
C	-2.71247000	1.51524000	0.19279200	K	9.77799400	0.15194600	-3.90115700
C	-3.58216600	1.90310900	-0.84297100	O	11.50488500	-0.27474400	-1.94580700
C	-4.55200800	1.00952100	-1.31158400	K	13.23147300	-1.92956500	-0.81317000
				H	4.66472000	0.20959500	-3.37628600

12-TS

C	3.74065900	2.45120700	-3.44920400
C	3.27775500	2.49731300	-2.11705000
C	2.01024300	1.96357100	-1.85234100
C	1.27770200	1.31771900	-2.86282900
C	1.80215700	1.22139800	-4.15715700
C	3.03380800	1.80641300	-4.46483700
H	1.60474900	2.02939400	-0.84728500
H	0.30003600	0.89821500	-2.63808500
H	1.23777500	0.71978800	-4.93837300
H	3.43300400	1.78750100	-5.47420300
O	4.93516700	3.06048700	-3.72210500
C	5.22012600	4.03535300	-2.69187000
H	4.64145100	4.94670100	-2.88648400
Pd	4.64195000	3.31700600	-0.83504500
C	4.81356700	5.45213400	0.45805100
H	3.89136300	5.29489900	-0.09706400
H	4.72300200	5.27222300	1.52171900
H	5.36874000	6.33109700	0.15546800
H	6.28784200	4.26480300	-2.74795500
I	7.05992200	4.11030400	0.33851300
K	3.47553800	-0.83147200	-1.22049400
I	3.56609700	2.12936600	1.56328800
C	6.34671900	-0.64536900	-1.03434600
O	5.73067500	-1.24310100	-0.05977000
O	7.44066900	0.02612200	-0.80204800
K	6.73154800	0.36368000	1.65103800
O	5.82392400	-0.64287400	-2.22909400
K	7.19101900	1.34671000	-2.97503900

12-TS-a

C	5.07977100	1.76794300	-3.08755800
C	4.25926800	1.75690600	-1.93472300
C	3.39166800	0.66360300	-1.77007800
C	3.41373300	-0.41349100	-2.66719500
C	4.27252300	-0.39008700	-3.77231800
C	5.10189700	0.70875300	-4.00079300
H	2.70916300	0.64899900	-0.92500800
H	2.75353200	-1.26197400	-2.50853500
H	4.27996400	-1.22045600	-4.47311700
H	5.74296300	0.76620700	-4.87486500
O	5.88926300	2.83964100	-3.26971300
C	5.42271900	3.95991600	-2.52337900
H	4.60497300	4.45769300	-3.06218300
Pd	4.54221400	3.40153200	-0.72826900
C	4.06954600	5.57597300	0.18341800
H	3.31207500	5.15371700	-0.48873300

H	3.76249500	5.57026800	1.22211600
H	4.49545700	6.50076400	-0.18750200
H	6.26606700	4.63401100	-2.37360500
I	6.47635700	4.76250800	0.76927300
K	5.89552400	0.68028600	0.36163900
I	3.17393800	2.33008100	1.62323100

12-TS-b

C	4.24384900	2.11434000	-3.40266300
C	3.93808700	2.06317000	-2.02453700
C	2.71879500	1.49296200	-1.63851200
C	1.88314400	0.88222800	-2.58988100
C	2.24638000	0.88052400	-3.93941600
C	3.42024500	1.51248600	-4.35855300
H	2.42411600	1.49767700	-0.58995000
H	0.94962000	0.42502300	-2.27203800
H	1.59830700	0.41490100	-4.67732300
H	3.68938500	1.56983600	-5.40880100
O	5.36370100	2.77489800	-3.77661900
C	5.78724200	3.68674700	-2.74426600
H	5.28979900	4.65511000	-2.89341300
Pd	5.33713900	2.98062900	-0.87056700
C	4.34896000	5.10562200	0.21378200
H	4.00587800	4.39267500	0.97257100
H	4.54635600	6.11220300	0.55838300
H	3.90674600	5.06006300	-0.77404600
H	6.86906100	3.80796900	-2.84021900
I	7.02455000	4.97709600	0.31016300
C	3.83826900	1.93032000	1.68255200
O	3.60631500	2.97392000	2.38627200
O	3.06749200	0.93490800	1.56039400
O	5.05366900	1.88049800	1.04782100
K	4.47819300	-0.37930400	-0.12195700
K	6.01220700	3.11125200	3.15078700

12-TS-c

C	3.40948700	2.88753600	-3.31520800
C	3.57325400	2.18596900	-2.10026700
C	2.90678100	0.96192000	-1.95954900
C	2.03095400	0.49285500	-2.95164800
C	1.84767800	1.24039900	-4.11960600
C	2.54748900	2.43371400	-4.31846800
H	3.05309600	0.37268800	-1.05558500
H	1.50325200	-0.44696100	-2.81262700
H	1.17566800	0.88057100	-4.89408200
H	2.44969900	2.99986800	-5.23963500
O	4.11506800	4.03212100	-3.47539900
C	5.24776400	4.06119400	-2.58143500

H	5.52352200	5.10886500	-2.44427100	C	3.53960200	2.54816400	-3.24899200
Pd	4.82985600	3.12496500	-0.80988200	C	3.21095400	2.66233800	-1.88176700
C	4.27970500	5.29442500	0.33916700	C	1.87020200	2.49298300	-1.51591900
H	3.79306200	5.36391900	-0.62851100	C	0.90378800	2.13580300	-2.47365300
H	3.77066700	4.73882100	1.12753100	C	1.27351600	1.97466200	-3.81359400
H	4.73862700	6.22585500	0.64193300	C	2.59570100	2.19496600	-4.21503600
H	6.08160300	3.50865900	-3.03440000	H	1.58241800	2.60516200	-0.47410300
I	6.78296700	4.43569400	0.62879700	H	-0.13031600	1.99176600	-2.17130900
C	3.92709700	2.30123000	2.14024800	H	0.52815900	1.70205800	-4.55566400
O	4.19630000	1.88905900	0.91075900	H	2.89478000	2.10743000	-5.25479800
O	3.03535300	3.22284900	2.31633500	O	4.84357900	2.73911600	-3.59781700
K	4.78959900	-0.47230000	1.71677400	C	5.54836900	3.48800000	-2.58452700
I	1.15725300	-0.47540100	2.46579200	H	5.44442100	4.56042100	-2.78654200
K	1.51728200	2.40460100	0.28245400	Pd	4.82307000	3.06561100	-0.70784900
O	4.47971000	1.69399400	3.12472100	C	4.66237000	5.38672700	0.23151200
K	2.42064900	2.09948600	4.61075700	H	4.46876300	5.67096400	-0.79547600
12-TS-d				H	3.87187200	4.86557700	0.76199900
C	3.68591200	2.57083200	-3.35372300	H	5.15205800	6.15010200	0.81925600
C	3.91956700	1.85539000	-2.15480900	H	6.58847200	3.16357500	-2.60398700
C	3.47513900	0.52614600	-2.11569600	I	7.03734000	4.23897100	0.55016700
C	2.73198600	-0.03341100	-3.17094500	K	3.05356300	-0.46389200	-1.29900400
C	2.45679600	0.73441000	-4.30930400	I	3.76272800	1.73528300	1.71126600
C	2.94922900	2.04108200	-4.41819200	C	6.03130600	-0.14157300	-1.76061100
H	3.69663500	-0.10408500	-1.25480000	O	5.62550600	-1.00719100	-0.93140800
H	2.38351600	-1.06066000	-3.10717100	O	7.00029600	0.64176900	-1.65452500
H	1.88818400	0.30643600	-5.13021100	K	6.97091000	0.33350400	0.96256200
H	2.79068300	2.63410500	-5.31333300	O	5.22642000	-0.03027000	-2.89219000
O	4.18038500	3.83343900	-3.42426500	H	5.47667000	0.79588600	-3.34444300
C	5.25003100	4.01335500	-2.49194000	13			
H	5.36898100	5.08317400	-2.32388300	C	3.59478700	2.52675900	-3.01072200
Pd	4.84464700	3.03662200	-0.75056200	C	4.05968800	1.84264000	-1.87315500
C	3.42728800	5.08618200	0.02329800	C	3.40007100	0.70095900	-1.42260500
H	3.09816000	4.82744600	-0.97129300	C	2.27426400	0.24684900	-2.12277400
H	3.06437800	4.54027800	0.88098600	C	1.81725800	0.93246500	-3.25333500
H	3.68253100	6.12580300	0.16994900	C	2.47497900	2.07472400	-3.71197100
H	6.17305700	3.55891300	-2.86985700	H	3.74211100	0.17668600	-0.53497500
I	6.12942500	4.81518300	0.88147300	H	1.74958900	-0.63917800	-1.77577500
C	2.69270200	2.12158900	1.59322400	H	0.94163900	0.57333100	-3.78689800
O	3.88075100	1.58934100	1.05946200	H	2.14072300	2.61307600	-4.59296000
O	2.84884300	2.97482400	2.48078100	O	4.24791600	3.65656200	-3.39235200
K	0.87808700	2.24081000	-1.41194400	C	5.56726700	3.70405400	-2.87126800
I	0.11950000	5.41949300	-0.21630500	H	5.86879000	4.74455500	-2.75922200
O	1.61535400	1.69299700	1.08107900	Pd	5.74629000	2.63961600	-1.13462900
K	0.42295400	3.74413100	2.76533400	C	4.52788700	4.01913500	-0.21202300
H	3.60505200	0.85544900	0.49136400	H	4.22984800	3.49706800	0.69779700
12-TS-e				H	5.21716700	4.84655300	-0.04241500
				H	3.69348400	4.29965200	-0.84970000

H	6.26236600	3.15441600	-3.52259300
I	8.40005100	3.64047900	-0.71153100
C	5.10789600	0.93961800	1.44325700
O	6.04103500	1.28788000	0.55826200
O	4.70505900	-0.28132900	1.43988600
K	7.23318300	2.83846400	2.48848200
I	7.78639600	-0.41783400	4.02908500
K	7.10115900	-1.07052800	0.53882000
O	4.72743900	1.79993100	2.31369800
K	4.23705000	-0.16938200	3.98826300

14-TS

C	3.68285000	2.55506200	-3.02644500
C	3.90532000	2.11175100	-1.70573900
C	3.23117800	0.98742500	-1.21865600
C	2.33602700	0.31630200	-2.05797400
C	2.10300200	0.77515900	-3.36033000
C	2.77597900	1.89413900	-3.85514500
H	3.40111000	0.66816400	-0.19168400
H	1.80282700	-0.55388700	-1.68519900
H	1.39529200	0.25487700	-3.99942500
H	2.62445400	2.25175400	-4.86823800
O	4.35666400	3.65305300	-3.44525300
C	5.66022800	3.71577700	-2.86152400
H	5.95820700	4.76273000	-2.78925900
Pd	5.72068300	2.80066900	-1.02819100
C	3.82485100	3.70230200	-0.38880400
H	3.31590500	3.14093600	0.38881800
H	4.51851600	4.42713700	0.05571200
H	3.14887700	4.21232000	-1.06828900
H	6.36172400	3.13921700	-3.47154500
I	8.51521100	2.79896600	-1.10802500
C	5.11162500	1.38501400	1.85684800
O	5.93483900	1.86162100	0.92819300
O	4.42908300	0.32347400	1.59783800
K	7.76155600	2.59184700	2.62234900
I	7.96469900	-1.04077200	3.23620700
K	6.49727800	-0.54598900	-0.03464200
O	5.13024600	1.93601600	3.01223500
K	4.61715900	-0.36784300	4.11281500

14-TS-a

C	3.63747400	2.74137700	-3.24925600
C	3.69916100	2.11502400	-1.98572300
C	2.95076500	0.94907000	-1.76915500
C	2.15587000	0.43779300	-2.79379800
C	2.09062900	1.08613900	-4.03492900
C	2.83316000	2.24091700	-4.27337400

H	2.98494500	0.46479900	-0.80032800
H	1.57608700	-0.46399800	-2.62172600
H	1.46191700	0.68319400	-4.82356900
H	2.81490200	2.74895100	-5.23173300
O	4.36314800	3.87675300	-3.42243100
C	5.57954200	3.81991100	-2.70595400
H	5.91910600	4.83204800	-2.49332300
Pd	5.40995800	2.68269400	-0.98805000
C	3.42927100	3.56052100	-0.52295000
H	2.70756900	2.94413900	0.00174100
H	4.04604800	4.10880700	0.19734000
H	2.98524300	4.24206800	-1.24243100
H	6.32294900	3.23056000	-3.25304500
I	8.10960700	3.43587300	-0.51159300
K	8.29467200	1.12788900	1.89544300
I	5.05602900	0.88549300	1.34161700

14-TS-b

C	3.66329300	2.58824500	-3.03031000
C	3.92412900	2.07545900	-1.73967900
C	3.21734500	0.95842900	-1.27690400
C	2.26872700	0.35679500	-2.11011800
C	2.00846900	0.87918600	-3.38304300
C	2.70426300	1.99427300	-3.85266400
H	3.39717000	0.57175300	-0.27546500
H	1.71676800	-0.50731800	-1.75162700
H	1.25890900	0.41383200	-4.01683800
H	2.52603100	2.40607600	-4.84059200
O	4.33969300	3.68894600	-3.43067700
C	5.65221000	3.74472000	-2.86316500
H	5.93652000	4.79209800	-2.75317900
Pd	5.76935900	2.71335800	-1.09232000
C	3.90907900	3.61164900	-0.32400700
H	3.64079200	3.04753500	0.56656700
H	4.57728100	4.44863100	-0.08833500
H	3.06102000	3.99039300	-0.88449800
H	6.35216000	3.21262900	-3.51636000
I	8.54160000	3.01327000	-1.07810000
C	5.06965400	1.08958000	1.53493800
O	4.69736800	1.92396000	2.41310000
O	4.63277500	-0.09131100	1.36842600
O	6.07793400	1.49224600	0.68733500
K	6.31687800	-0.71850000	-0.50463500
K	6.88770000	3.28341300	2.32527400

14-TS-c

C	3.92533300	2.31092800	-3.25112900
C	3.78661400	2.02904100	-1.87143100

C	2.76987300	1.14168600	-1.47189900	C	4.96047700	1.70725700	1.91544200
C	1.94191400	0.54129600	-2.42092500	O	5.88060600	1.38425000	0.86249700
C	2.10699300	0.82746500	-3.78709000	O	4.09036500	0.85224700	2.15631600
C	3.09792900	1.71194600	-4.20843800	K	7.92872500	2.89657900	2.59816300
H	2.64157200	0.93070600	-0.41580100	I	7.29149300	1.64289500	5.73472200
H	1.15711300	-0.13649800	-2.09770200	O	5.20144100	2.81107200	2.44701200
H	1.45629400	0.36205500	-4.52179500	K	4.07818400	1.76145400	4.72430700
H	3.24949300	1.94475900	-5.25721800	H	5.68174600	0.47502800	0.58875500
O	4.87944700	3.19222500	-3.63181600				
C	6.02114200	3.12544600	-2.79024300				
H	6.54001500	4.08123300	-2.82889600	14-TS-e			
Pd	5.55733900	2.46630600	-0.89035900	C	3.91049600	2.43029800	-3.24390800
C	3.76366300	3.75988300	-0.76461900	C	3.85866500	2.07945200	-1.87644300
H	2.95205800	3.41100300	-0.13506100	C	3.02159700	1.03342500	-1.46600700
H	4.47416600	4.34882000	-0.17619200	C	2.28579000	0.31871600	-2.41865600
H	3.43041800	4.32392400	-1.63119800	C	2.36269500	0.66323700	-3.77457800
H	6.63220700	2.25505700	-3.06549100	C	3.17161300	1.72132100	-4.19426100
I	8.11505400	3.34142900	-0.10724600	H	2.94913800	0.78961100	-0.41143200
K	5.21519000	-0.95903000	-2.30377200	H	1.63741500	-0.49078100	-2.09652100
I	5.00772400	0.91863300	1.45765600	H	1.78436500	0.10972800	-4.50843900
C	8.10328900	-0.58010700	-1.91036900	H	3.24522600	2.00549000	-5.23875400
O	7.42163800	-1.43342100	-1.21327900	O	4.67937000	3.48343700	-3.60193200
O	9.30307200	-0.25573000	-1.54166400	C	5.84897900	3.59598300	-2.78814100
K	8.39332400	-0.33392400	0.92649200	H	6.10701100	4.65003400	-2.67881200
K	9.48031700	1.72593900	-3.06135900	Pd	5.55405700	2.74216000	-0.91258600
O	7.54996600	0.01088700	-2.94663800	C	3.66182800	3.82751600	-0.71354700
				H	2.90839300	3.37017500	-0.08136700
				H	4.29592100	4.49955000	-0.12247300
				H	3.26045100	4.34272900	-1.58175300
				H	6.66213700	3.02909600	-3.24582700
14-TS-d				I	8.31434500	2.56573100	-0.72859600
C	3.68564400	2.56329700	-2.98829600	K	5.97192100	-0.56178800	-1.86856300
C	3.94424600	2.08760000	-1.68791500	I	5.05139600	1.49044500	1.63536900
C	3.26799000	0.95443400	-1.21636600	C	8.55080500	-1.61228300	-0.51013500
C	2.34992300	0.31274600	-2.04723400	O	7.38944200	-1.63230500	-0.01427600
C	2.09182800	0.80592800	-3.33444700	O	9.64687600	-1.45393000	0.05520200
C	2.75567700	1.93339500	-3.81575600	K	8.28796900	0.00377200	1.89484700
H	3.42150300	0.61377500	-0.19603300	O	8.55359400	-1.72398700	-1.91400600
H	1.82091400	-0.56403800	-1.68651500	H	9.47957900	-1.62328300	-2.17851800
H	1.36819200	0.30329900	-3.96908500				
H	2.58012600	2.32029400	-4.81389200				
O	4.34991600	3.67970200	-3.39281400				
C	5.65240500	3.74286200	-2.85039200	15			
H	5.96738100	4.78274500	-2.78234200	C	3.59838400	2.48023200	-1.81646100
Pd	5.76154600	2.79135000	-1.04661000	C	2.36303600	2.51224400	-1.12505600
C	3.87215600	3.70141400	-0.34404000	C	1.62569200	1.32865800	-1.02883600
H	3.17535500	3.13444500	0.26467200	C	2.08735900	0.12351300	-1.58375000
H	4.56148200	4.25259000	0.30286800	C	3.31123800	0.11007000	-2.25669500
H	3.38066100	4.35349200	-1.05976300	C	4.06781500	1.28214100	-2.37679500
H	6.34626400	3.12493300	-3.42981900	H	0.66718900	1.35206300	-0.51425400
I	8.45015400	3.42172400	-0.87456500	H	1.49091400	-0.78046600	-1.50448600

H	3.68263800	-0.81243800	-2.69411500	O	4.54127900	-0.47689400	-2.67377300
H	5.01547800	1.26757600	-2.90045200	K	6.08029900	1.10453900	-3.89310200
O	4.25202900	3.66445900	-1.86919600				
C	5.56918500	3.75039000	-2.38804000	17-TS			
H	5.79111700	4.81701400	-2.45546300	C	3.52468900	3.42736200	-3.30342400
Pd	6.90843200	2.96365100	-1.09632400	C	3.20737500	3.17998100	-1.95119900
C	1.90709300	3.80468600	-0.50071600	C	2.02872300	2.47185200	-1.68614300
H	0.95815200	3.67696200	0.02786200	C	1.24748200	1.95210600	-2.73226300
H	2.66336600	4.17562900	0.19997700	C	1.61990200	2.17098300	-4.06131000
H	1.78153700	4.58467400	-1.25892300	C	2.75466900	2.93165000	-4.35716200
H	5.65054800	3.27665200	-3.37162200	H	1.72537900	2.31162400	-0.65529100
I	8.87333900	3.05197800	-2.97392600	H	0.34335400	1.39249700	-2.50501900
C	6.51850100	2.00633100	1.30807700	H	1.01276000	1.77650500	-4.87122500
O	7.72706500	1.87886800	0.81974400	H	3.02894800	3.16042300	-5.38332600
O	5.61513600	2.52224000	0.50612600	O	4.65262100	4.15570100	-3.57305200
K	8.35244100	0.31840300	2.92732200	C	5.07441500	4.89848900	-2.40211500
I	6.61583000	-2.12886800	0.97505100	H	4.56823000	5.87197900	-2.39812200
K	7.96153800	0.01165300	-1.38463000	Pd	4.59870700	3.90135500	-0.66987400
O	6.18841300	1.59535300	2.46206600	C	4.35166500	5.91661200	0.81995900
K	4.03192300	0.50355000	1.25016600	H	3.44294000	5.66459000	0.28339300
				H	4.35620100	5.62517600	1.86162700
				H	4.78501300	6.87446400	0.56518800
16-TS				H	6.15613900	5.03858300	-2.46966600
C	3.40483400	3.19415500	-3.54804000	Cl	6.45730400	5.01796700	0.54600300
C	2.92059700	3.17397100	-2.22365900	K	3.79312000	-0.29310500	-1.15535400
C	1.56772500	2.86381500	-2.03883800	I	3.84281600	2.34704700	1.64359000
C	0.75555800	2.49606800	-3.12536400	C	6.49767400	0.42088000	-1.78347700
C	1.28510500	2.46907000	-4.41880900	O	6.31661800	-0.19960500	-0.66043700
C	2.61407000	2.84013300	-4.64223400	O	7.40453900	1.35748100	-1.87604100
H	1.14984800	2.89254900	-1.03655300	K	7.39127200	1.68113400	0.69548900
H	-0.28940200	2.24556200	-2.95895300	O	5.72009200	0.16601100	-2.79943000
H	0.65775800	2.18964800	-5.26059600	K	6.52393300	2.15081000	-4.12833500
H	3.02824700	2.87883200	-5.64580200				
O	4.71363700	3.54896500	-3.74258400	18-TS			
C	5.22202300	4.26250400	-2.58923100	Pd	2.99172300	0.60482600	1.77232700
H	4.98726100	5.32886300	-2.69632900	C	2.88036800	2.32732200	-0.80195000
Pd	4.36113800	3.58023500	-0.84731400	C	2.21743500	1.36884300	-0.01829600
C	4.57012700	5.69053400	0.49516400	C	0.81352400	1.42968100	0.05202100
H	3.64714200	5.61350000	-0.07088000	C	0.18818700	2.57676600	-0.47480200
H	4.45172900	5.53739200	1.55921400	C	0.91530200	3.57877800	-1.13487500
H	5.23306200	6.48542600	0.17980100	C	2.30158400	3.45258600	-1.35216500
H	6.30504500	4.11964000	-2.56358600	H	0.22927300	0.65664700	0.53880000
Br	6.48453900	4.19873700	0.50407100	H	0.88866400	2.68333300	-0.37399800
K	2.38335300	-0.22753200	-1.29278000	H	0.39201100	4.44052800	-1.53897000
I	2.98536500	2.47407800	1.44479100	H	2.85991900	4.17048300	-1.94315200
C	5.23172100	-0.43185100	-1.56804300	O	4.12783800	1.75763500	-0.97573400
O	4.72533200	-0.90104500	-0.47095500	C	3.71567800	0.48263500	-0.36490000
O	6.39725900	0.15859400	-1.55139200	H	3.45967000	-0.24205100	-1.13753200
K	6.16398800	0.62136900	0.98710300				

H	4.53533900	0.09376900	0.26447300	O	6.40226000	-2.28486200	2.67779800
K	6.10584100	3.33538900	0.22728800	K	6.98015200	0.02107600	1.73006600
I	2.58498100	0.50551200	4.45965000				
C	4.82485900	4.30082200	2.65090600	21			
O	6.00432700	3.73852700	2.72840500	Pd	3.97614700	-0.12229700	1.92314500
O	4.12180400	4.48417700	3.72404500	C	2.48405300	1.06428700	1.19847400
K	5.36276500	2.64098300	4.96511400	H	1.60096000	0.43139900	1.07873800
O	4.32515700	4.60065700	1.48574600	H	2.29598000	1.88220200	1.89327300
K	1.96559800	3.99863600	2.38742200	H	2.81125900	1.43465400	0.22367000
				I	3.79972700	-1.65642000	-0.32803200
19				K	3.72147700	-2.92533300	3.47603300
Pd	1.96397800	1.11750400	1.83426300	I	4.15128800	1.40404800	4.20958500
C	2.97546900	2.35539000	-0.81192600	C	6.34085200	-1.49339200	3.68087900
C	2.39451900	1.17117700	-0.30348300	O	5.88717200	-2.10716600	4.71962100
C	0.98518200	1.09589500	-0.12258300	O	7.41121200	-0.77662800	3.72155100
C	0.28820000	2.33540100	-0.35099800	K	6.74189100	-0.13247400	6.11216200
C	0.92725200	3.48529000	-0.80009100	O	5.67123200	-1.57920700	2.54259300
C	2.32561900	3.52643900	-1.09216900	K	7.10750200	0.06321800	1.24479100
H	0.42770600	0.16356200	-0.08687900				
H	-0.78772000	2.35135200	-0.20490400	22-TS			
H	0.33370200	4.37750600	-0.98448600	Pd	0.53355100	-0.36496300	-0.70891400
H	2.80012500	4.39674800	-1.53041600	C	0.55848800	-2.13775600	0.53426200
O	4.22500600	1.80274300	-1.12499200	C	0.53594100	-1.65974000	1.85298800
C	3.67188100	0.46371700	-0.74954200	C	1.05277700	-3.42376000	0.29178900
H	3.59774700	-0.16127600	-1.64453600	C	1.13393500	-2.45332300	2.84568700
H	4.28447900	-0.01252500	0.01871800	H	0.16103200	-0.66929100	2.09154300
K	6.14487500	3.26188600	0.23594600	C	1.62619800	-4.24274800	1.25207100
I	2.06770200	0.98102100	4.55133800	C	1.67886500	-3.71120600	2.54727400
C	4.94046700	4.31608500	2.66369700	H	1.20723900	-2.06758400	3.85873800
O	6.01305500	3.56781600	2.74630100	H	1.97663900	-5.24229400	1.01945900
O	4.26694700	4.60166900	3.73254100	H	2.13142400	-4.29640700	3.34231800
K	5.18213400	2.58694500	4.97832000	C	-0.19504200	-2.54853900	-1.09149200
O	4.50862500	4.70373100	1.49800900	H	-1.22671500	-2.75463400	-0.80412800
K	2.06757000	4.39840700	2.38769400	H	-0.13768000	-2.10492500	-2.09055700
				I	1.05045900	2.28388900	-1.11290600
20-TS				C	2.42966300	-0.78419100	-1.35933700
Pd	3.69481500	0.35165900	2.13244400	H	2.48509500	-1.86351500	-1.52094700
C	1.94197300	0.94237000	0.17286300	H	2.60514600	-0.23415300	-2.28420800
H	1.02201900	0.48449300	0.51911100	H	3.12600900	-0.46220700	-0.58294000
H	2.33368800	1.70138400	0.84979600	O	0.68076700	-3.68140200	-0.99591300
H	1.90805200	1.27989500	-0.85685100	C	-2.58385700	-0.49272000	-0.71693900
I	3.36883500	-0.94585400	-0.20791400	O	-1.57588200	-0.08718900	0.05284600
K	4.04482100	-2.62207800	3.61229000	O	-3.11529700	-1.64742600	-0.46566600
I	4.27156800	1.38993900	4.55096300	K	-2.35688100	2.45621600	-0.28303200
C	6.83287400	-1.92765900	3.85025700	I	-5.19622700	1.06069100	1.79768700
O	6.25659900	-2.39304000	4.92410600	K	-2.66766200	-1.43909300	2.09968100
O	7.77174100	-1.02742500	3.95154100	O	-3.05217400	0.28814900	-1.61366600
K	6.97135500	-0.36300700	6.27001200	K	-5.42165400	-0.70423600	-1.30383500

23				H	7.26337100	0.25923500	-0.41560300
Pd	8.94305600	1.50553900	-2.09859700	H	8.36798200	-0.85241600	-1.30557100
C	6.25898700	0.99566400	-3.00289900	C	4.06881500	0.07301700	-3.07202300
C	4.88893700	1.30797700	-2.95526200	H	3.03488900	0.36906300	-3.27084100
C	4.51750800	2.60723700	-3.31003600	H	4.33865500	-0.72049000	-3.77843000
C	5.45324700	3.58393500	-3.68966900	H	4.11895600	-0.37121200	-2.07223500
C	6.79905100	3.25441000	-3.76065700	C	10.49536900	2.86617200	-3.72397300
C	7.20723400	1.94409500	-3.44869500	O	9.59026200	2.28868000	-4.47953200
H	3.46346700	2.87265900	-3.26405000	O	10.12857500	3.37587800	-2.56879500
H	5.11567800	4.58610500	-3.93564900	H	8.37799000	2.06803600	-3.62169400
H	7.55969500	3.96304300	-4.06905000	C	11.21564500	-0.07750400	-0.77795000
O	6.67708800	-0.23033200	-2.58349800	O	10.49084000	0.98114200	-0.44160200
C	7.82008100	-0.12962300	-1.70541300	O	11.33182000	-1.02333000	0.08048000
H	7.44703900	0.02048200	-0.67867900	K	12.44105800	2.92002000	-1.46833100
H	8.37677000	-1.06737400	-1.77937000	I	14.21456800	1.45421800	1.47617300
C	3.89293400	0.27275900	-2.49917700	K	10.77766000	0.59174000	2.08555000
H	2.89169500	0.70199500	-2.40429100	O	11.72827100	2.82635400	-4.05549900
H	3.83979600	-0.56492900	-3.20388000	K	11.15376300	0.21727600	-4.40569900
H	4.18568200	-0.15159300	-1.53328500	O	11.86496300	-0.08709600	-1.89532000
C	10.75856600	2.93813100	-3.69072200	K	13.80935400	-1.35854700	-0.56333900
O	10.17677800	2.27745200	-4.62498600				
O	10.06831500	3.27734800	-2.60183300	24-TS-a			
H	8.17734600	1.61622700	-3.90050300	C	-2.79926500	-0.25021800	0.27978500
C	11.28326900	-0.07906600	-0.95921900	C	-4.02982700	0.41064800	0.09022900
O	10.36848100	0.84357900	-0.67151700	C	-3.98763700	1.75523400	-0.28100200
O	11.35463900	-1.10019700	-0.18565400	C	-2.76970200	2.43443700	-0.45980400
K	12.14633800	3.12875800	-1.07214900	C	-1.57247900	1.76605600	-0.22393000
I	13.50265200	1.50947500	2.05433300	C	-1.54917000	0.41022400	0.18612200
K	10.18871600	0.16008800	1.80596500	H	-4.92494900	2.28205300	-0.44636800
O	12.02198100	3.19368000	-3.71132100	H	-2.77428900	3.48510500	-0.74067800
K	12.14320500	0.67328500	-4.49332200	H	-0.62482900	2.29433300	-0.30634700
O	12.13251900	0.12266900	-1.90643000	H	-0.65179800	0.18120800	1.01850700
K	13.93665600	-1.03815000	-0.29181200	O	-2.81665700	-1.57893300	0.55435400
				C	-1.82927200	-2.30645100	-0.18929400
24-TS				H	-2.27821700	-2.64481300	-1.13097000
Pd	8.93394900	1.68532400	-1.72912900	Pd	-0.28079100	-1.15520400	-0.73714600
C	6.36897100	1.10201800	-2.87791300	C	-5.32321100	-0.34517000	0.25420900
C	5.00502800	1.24897100	-3.18641500	H	-6.18496600	0.28400800	0.01350600
C	4.57059100	2.52507500	-3.54964800	H	-5.34410600	-1.23136700	-0.38878000
C	5.43917800	3.62837900	-3.59367900	H	-5.43680900	-0.70695400	1.28206200
C	6.78573700	3.45416200	-3.30888800	H	-1.46508900	-3.12452000	0.43160600
C	7.29259000	2.17240700	-2.99324900	K	2.43158200	1.59228900	0.86631300
H	3.51713700	2.66682900	-3.78191000	C	1.17350600	-0.73104700	1.94010500
H	5.05378500	4.60601400	-3.86854500	O	0.68491100	-1.84846900	1.52112200
H	7.49544200	4.27219400	-3.38311700	O	0.40329400	0.33400200	2.00372000
O	6.80562300	-0.09645400	-2.40729100	O	2.43684300	-0.60372500	2.18631000
C	7.78957100	0.07367300	-1.36430900	C	2.27171700	0.23827500	-2.05891000
				O	2.13206900	0.54782000	-3.30528200

O	1.27455000	0.47942700	-1.22983100	H	6.97589900	0.16989800	-0.60339500
K	3.58570500	-1.41626100	-3.97598400	H	8.30782500	-0.81347800	-1.30600700
I	0.61786500	-3.06290900	-2.71473900	C	4.29375800	-0.10733900	-3.60925600
K	-0.48570600	0.79450300	-3.17989100	H	3.24962600	0.09413200	-3.86443500
O	3.35134400	-0.31059700	-1.61131300	H	4.71370800	-0.75768000	-4.38559500
K	2.87467600	-2.34988000	0.28507300	H	4.32172300	-0.67904300	-2.67595800
				C	10.44154800	3.35452000	-3.24019500
24-TS-b				O	9.65576500	2.71088600	-4.07992300
Pd	8.92405000	1.53493200	-1.83009500	O	9.99218100	3.55711200	-2.01351100
C	6.33316500	1.12038000	-3.02024700	H	8.37515300	2.41114000	-3.37147000
C	4.97321800	1.31436700	-3.32040700	K	13.46559900	2.20665100	-2.80151600
C	4.55832400	2.62801900	-3.54527300	O	11.59996100	3.72575500	-3.57017100
C	5.44177300	3.71786400	-3.46184200	K	9.89258900	0.09065700	-3.95573700
C	6.78320800	3.49659200	-3.18637200	C	11.51499000	1.03331500	-0.96213700
C	7.27402300	2.18020100	-3.01907200	O	11.60277300	0.43176000	-2.09526400
H	3.50829100	2.80929900	-3.76490400	O	10.35612100	1.09036500	-0.30600000
H	5.06993400	4.72476100	-3.62941500	O	12.51666500	1.64769500	-0.43951400
H	7.50313100	4.30889100	-3.15945000	K	10.94909300	3.58714000	0.36108300
O	6.75877000	-0.12368200	-2.67736800				
C	7.73375800	-0.07611800	-1.62096000	24-TS-d			
H	7.22155600	0.08549300	-0.66255000	Pd	8.96135400	1.51134900	-1.67927300
H	8.26699500	-1.02770400	-1.62644800	C	6.31018800	1.16478600	-2.73608000
C	4.02092900	0.14608600	-3.33478000	C	4.95208000	1.40873600	-3.01721700
H	2.99502300	0.47399400	-3.52485000	C	4.60306000	2.69648500	-3.42738600
H	4.29618300	-0.58170400	-4.10661800	C	5.55729600	3.71771000	-3.55064100
H	4.04438300	-0.38932800	-2.37961100	C	6.89522400	3.44025500	-3.29425800
C	10.39670100	2.92832000	-3.76272800	C	7.31805300	2.14164700	-2.92272900
O	9.49757100	2.36982400	-4.54400400	H	3.55761700	2.91182500	-3.63619600
O	10.02109700	3.40271500	-2.60427800	H	5.24959700	4.70990100	-3.86941900
H	8.36075300	2.13564800	-3.73447500	H	7.65477600	4.20017600	-3.46625900
I	11.20879600	0.31447900	-0.73170400	O	6.64995600	-0.04852000	-2.22925400
K	12.37247200	3.59200500	-1.65366300	C	7.66599700	0.04812400	-1.21635900
O	11.63171200	2.90002800	-4.09782500	H	7.20235700	0.33783500	-0.26480900
K	11.07186600	0.30429400	-4.57251400	H	8.15165900	-0.92511500	-1.13987100
				C	3.93283700	0.31544500	-2.82383000
24-TS-c				H	2.92111800	0.67499900	-3.03108600
Pd	8.78006300	1.77616600	-1.52242600	H	4.13693400	-0.53681900	-3.48163300
C	6.41445300	1.14745300	-3.04506300	H	3.96448400	-0.07039800	-1.79957100
C	5.08056900	1.17255100	-3.48034200	C	10.45831500	2.85962400	-3.76525600
C	4.52080300	2.42731700	-3.74014000	O	9.48899700	2.28189700	-4.45480200
C	5.24319000	3.61593500	-3.56073400	O	10.25245900	3.15508900	-2.51997100
C	6.56874500	3.56050900	-3.14723600	H	8.46359700	2.00523600	-3.62895800
C	7.19902000	2.31947700	-2.91610300	K	12.85635300	3.42088300	-1.91569800
H	3.48472900	2.47558900	-4.06818400	I	12.05381100	6.36713500	-0.32480300
H	4.76652900	4.57119400	-3.76137200	K	9.23583200	4.48571100	-0.44753900
H	7.16593400	4.46244900	-3.05044600	O	11.57876500	3.08541500	-4.32835100
O	6.96279000	-0.05715900	-2.67860100	K	10.90084500	1.97724300	-6.52974100
C	7.69880600	0.08647200	-1.42514300	I	10.85747700	0.80770900	0.16088100

24-TS-e

Pd	8.86678500	1.83969700	-1.45506400
C	6.43127500	1.16350000	-2.84446600
C	5.10109200	1.16978900	-3.28205300
C	4.55201400	2.41880900	-3.59314100
C	5.28370500	3.60683200	-3.45896700
C	6.60779200	3.56145400	-3.03463600
C	7.23259900	2.32719600	-2.75156900
H	3.51819800	2.46269500	-3.92817300
H	4.81540500	4.55647200	-3.70092300
H	7.20050800	4.46996200	-2.97212400
O	6.99533400	-0.02722300	-2.43920500
C	7.77228700	0.18469400	-1.24303600
H	7.10325900	0.34916600	-0.39066100
H	8.40880300	-0.68868500	-1.08862600
C	4.30751700	-0.10957000	-3.36438200
H	3.26302800	0.08871300	-3.61951800
H	4.71842400	-0.78664600	-4.12269900
H	4.33728900	-0.65057600	-2.41299400
C	10.43780000	2.91525600	-3.82364300
O	9.37508000	2.38328500	-4.34030100
O	10.16065200	3.62326900	-2.67700600
H	8.38870600	2.33930800	-3.45966100
C	11.49232300	0.68873300	-0.92048400
O	10.42175700	1.12423500	-0.24914000
O	12.62072600	0.75619100	-0.32626200
I	12.89964300	4.92818600	-0.81244800
K	11.85901200	2.52764600	1.42935200
O	11.58868800	2.78867000	-4.24030400
K	9.78370100	-0.22529300	-3.99518300
O	11.37543900	0.29456500	-2.13736100
K	13.54181800	1.91359200	-2.59783900
H	10.98037600	4.02906600	-2.30428600

24-TS-f

C	-2.76713000	-0.22790300	0.34811400
C	-3.98670800	0.48755000	0.33108000
C	-3.93193800	1.82673500	-0.04430600
C	-2.72236600	2.46854500	-0.38238600
C	-1.53211300	1.75872700	-0.31474500
C	-1.52123100	0.39610400	0.07998400
H	-4.86037700	2.39307500	-0.07769600
H	-2.72845200	3.52109600	-0.65295700
H	-0.57564800	2.23744400	-0.51238800
H	-0.62130700	0.23705100	1.01377000
O	-2.79509300	-1.53346800	0.62849900
C	-1.65639600	-2.28250300	0.13175200

H	-2.00871300	-2.89226800	-0.70677200
Pd	-0.20176100	-1.09544400	-0.62885800
C	-5.27160700	-0.21420100	0.68323500
H	-6.13058900	0.45640200	0.59060600
H	-5.43345000	-1.08438200	0.03752000
H	-5.23657700	-0.59442700	1.71010500
H	-1.28400200	-2.89803700	0.95136800
K	2.71308100	0.02187600	0.72253600
C	0.30822000	-0.71242300	2.75111400
O	-0.62873200	-1.41951800	3.08583200
O	0.33400600	0.33018300	1.99115300
O	1.60754800	-1.03957200	3.17416300
C	2.14236300	0.24310000	-2.28174700
O	1.83583500	0.12290000	-3.53078300
O	1.17871000	0.51720700	-1.40927300
K	3.58320500	-1.76476100	-3.63939900
I	1.25330400	-3.30351300	-1.45230600
K	-0.69566700	0.51539700	-3.26155600
O	3.34087900	0.07193700	-1.85819000
H	1.49893300	-1.83187000	3.72060200

24-TS-g

C	-2.66403800	-0.20550900	0.24497500
C	-3.93685800	0.35781100	0.40844600
C	-4.09613800	1.66464200	-0.05394300
C	-3.04494900	2.38248700	-0.64972100
C	-1.78863300	1.80384000	-0.76634100
C	-1.55052000	0.49636100	-0.27881400
H	-5.07240600	2.13406900	0.04192400
H	-3.21913100	3.39631400	-0.99799700
H	-0.96257000	2.37222600	-1.18626800
H	-0.59682800	0.48375600	0.69261200
O	-2.44354800	-1.49300900	0.63626700
C	-1.54410800	-2.15327300	-0.22795700
H	-2.03742800	-2.45019000	-1.16153900
Pd	-0.13047200	-0.92484900	-0.98814000
C	-5.05342600	-0.43474400	1.03523700
H	-5.99342700	0.12314500	1.01970900
H	-5.20411000	-1.38599500	0.51441700
H	-4.81719000	-0.68050500	2.07690500
H	-1.10583700	-2.99966700	0.30051900
K	2.10879700	-1.46760600	1.76582600
C	-0.32882500	-0.02499500	2.79969300
O	-1.58881100	0.40142900	3.06171800
O	0.18870200	0.47330900	1.72297300
O	0.23693500	-0.83317600	3.55170700
I	1.84055600	-2.72048700	-1.57160400
H	-1.87582000	-0.08448100	3.84914900

24-TS-h

C	-2.77367600	-0.36467200	0.24160800
C	-3.95738000	0.37125100	0.44408200
C	-3.93448900	1.70617400	0.04940000
C	-2.80211400	2.30408900	-0.54086200
C	-1.63762000	1.57504200	-0.70767000
C	-1.57246400	0.23570700	-0.23730700
H	-4.83915400	2.29733600	0.17746900
H	-2.85360500	3.34183900	-0.85952000
H	-0.74855100	1.99466000	-1.17077600
H	-0.67023800	0.17986700	0.71685400
O	-2.74149400	-1.67219100	0.51985600
C	-1.76502500	-2.34910500	-0.30862900
H	-2.28372400	-2.69637900	-1.21570900
Pd	-0.27405600	-1.16247500	-0.99666800
C	-5.17964300	-0.30043800	1.01360200
H	-6.02741900	0.38939200	1.05539500
H	-5.46673900	-1.16875200	0.41050400
H	-4.98909000	-0.67346100	2.02627200
H	-1.38764000	-3.19433300	0.27490400
C	1.79941600	0.92267600	-2.11181600
O	0.89256100	1.65927500	-2.62322700
O	3.03046700	1.34360400	-1.97290500
O	1.53704100	-0.28893300	-1.67873000
C	1.27625700	-0.01920100	1.74438200
O	1.60341000	-1.17603200	1.46587900
O	0.13183900	0.54116600	1.76255000
O	2.33614700	0.85451600	2.04312800
K	3.62589300	-0.44716600	-0.15092200
K	2.46751400	3.51032400	-3.12579200
H	1.92330000	1.72001900	2.17880700

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Pd	8.91392200	1.95462400	-1.42744000
C	6.42261100	1.14513600	-2.55306400
C	5.22817900	1.11537300	-3.28316100
C	4.80049000	2.32367200	-3.85495800
C	5.51745900	3.50796500	-3.67767800
C	6.70486000	3.50634600	-2.92892500
C	7.19535200	2.31296100	-2.38243400
H	3.87835400	2.33117300	-4.43165500
H	5.15370300	4.43196900	-4.11953500
H	7.25346600	4.43389900	-2.77522900
O	6.90202900	-0.00567800	-1.97679400
C	7.81389300	0.33645200	-0.89791900
H	7.22784600	0.57346100	0.00096400
H	8.44123700	-0.54008000	-0.70835000

C	4.44871000	-0.16762100	-3.42457700
H	3.51172400	-0.00561400	-3.96544700
H	5.02445600	-0.93058000	-3.96338400
H	4.21471600	-0.59461900	-2.44313500
C	10.42407900	3.04628000	-3.76295400
O	9.35124300	2.92617600	-4.62696500
O	10.20848200	3.56257000	-2.61766900
H	8.55373000	3.24481700	-4.16556500
C	11.07621700	-0.01869400	-0.75042000
O	10.74011700	1.22247600	-0.43576600
O	11.04321800	-0.92249400	0.15906200
K	12.69005200	2.52567800	-1.80689300
I	14.60240800	0.82263600	0.91278500
K	11.17963300	0.84136500	2.08418800
O	11.49274300	2.55524400	-4.18894200
K	9.77365100	0.15149200	-3.89803100
O	11.50404900	-0.27489200	-1.94575200
K	13.23297900	-1.92826300	-0.81548400

26-TS

C	3.72774900	2.45317200	-3.42936200
C	3.25619200	2.52159300	-2.10450900
C	1.98534100	1.99622200	-1.83619900
C	1.26607100	1.33893200	-2.84631300
C	1.80942900	1.21445800	-4.13098800
C	3.04794500	1.78249600	-4.45594600
H	1.57211100	2.07629800	-0.83570500
H	0.28342700	0.92571000	-2.63128500
H	1.25178700	0.69517900	-4.90685600
O	4.92182400	3.06789200	-3.70511400
C	5.19554600	4.05583600	-2.68361900
H	4.60870300	4.95936600	-2.88918900
Pd	4.62308100	3.34102700	-0.82503200
C	4.81402700	5.45954200	0.48932500
H	3.88965700	5.31467500	-0.06596200
H	4.72581400	5.26320800	1.55036300
H	5.37066600	6.34183600	0.19938800
H	6.26136600	4.29439800	-2.73976500
I	7.05593300	4.11635800	0.33504400
K	3.46205900	-0.79836200	-1.27927100
I	3.56756600	2.12696600	1.56783900
C	6.33683100	-0.62887300	-1.11009500
O	5.72150100	-1.23477600	-0.14030400
O	7.43434300	0.03530800	-0.87339900
K	6.72876700	0.35236500	1.58589300
O	5.81020600	-0.61057900	-2.30326700
K	7.18378700	1.38608100	-3.02422900
C	3.64159700	1.70212400	-5.83889700

H 3.90758400 2.69724500 -6.21075300
H 4.56279000 1.10574000 -5.83962400
H 2.94433800 1.24135300 -6.54418300

26-TS-a

C 4.98357700 1.80154300 -3.13313700
C 4.19141900 1.78418500 -1.96444600
C 3.33237900 0.68659000 -1.77920400
C 3.34785700 -0.38395800 -2.68167800
C 4.18540600 -0.34956900 -3.80305700
C 5.00839900 0.74993600 -4.06554900
H 2.66699000 0.66582100 -0.92094600
H 2.69864300 -1.24010500 -2.51748100
H 4.18359900 -1.18092400 -4.50426600
O 5.78288600 2.88129900 -3.33212300
C 5.33266900 3.99326300 -2.56402400
H 4.49524900 4.48892700 -3.07364600
Pd 4.51061600 3.41520500 -0.74832100
C 4.11298700 5.57604900 0.23387000
H 3.85063300 5.55524400 1.28461300
H 4.53645100 6.50141900 -0.13849700
H 3.32010700 5.17757400 -0.41183800
H 6.17636500 4.67158800 -2.43580000
I 6.52648100 4.70948000 0.69909800
C 5.88139200 0.84187600 -5.29086700
H 5.62046800 1.72010400 -5.89153000
H 6.93770400 0.95582900 -5.02082200
H 5.77964800 -0.04841800 -5.91769100
K 5.83994900 0.63724200 0.26847200
I 3.20071500 2.32879300 1.63265600

26-TS-b

C 4.28857400 2.08041500 -3.40662100
C 3.97638000 2.03420600 -2.03320400
C 2.76395000 1.44772000 -1.64664300
C 1.95063000 0.82108300 -2.60400900
C 2.32738400 0.81786200 -3.95022300
C 3.49190300 1.46235600 -4.38466800
H 2.46091700 1.45544200 -0.60079000
H 1.02013800 0.35008300 -2.29701400
H 1.69039300 0.33662600 -4.68918500
O 5.40122100 2.75921800 -3.77995300
C 5.80723700 3.68050900 -2.74839300
H 5.29777100 4.64146400 -2.90466100
Pd 5.35568800 2.97581600 -0.87511000
C 4.33867800 5.09327100 0.20035100
H 4.00271900 4.37858200 0.96078600
H 4.52081200 6.10385700 0.54160500

H 3.90092300 5.03756600 -0.78896800
H 6.88789300 3.81596800 -2.83932700
I 7.01451800 4.99997400 0.30701800
C 3.86023600 1.91837700 1.68044700
O 3.61561800 2.96317400 2.37840600
O 3.10217000 0.91261200 1.56507900
O 5.07600600 1.88008200 1.04570600
K 4.52640500 -0.39285900 -0.11233000
K 6.01802000 3.12731800 3.14716000
C 3.88748300 1.53747600 -5.83722500
H 3.98742500 2.57946400 -6.16088600
H 4.86222300 1.06647200 -6.01035400
H 3.14897800 1.04457300 -6.47630700

26-TS-c

C 3.40451600 2.87589900 -3.31372900
C 3.57072500 2.17990100 -2.09988700
C 2.90556700 0.95493300 -1.95094000
C 2.03278200 0.49008200 -2.94482800
C 1.85117900 1.23800200 -4.11317500
C 2.54340300 2.43517500 -4.33299900
H 3.05261500 0.36685100 -1.04671000
H 1.50294900 -0.44945800 -2.81074300
H 1.17872200 0.87383900 -4.88660700
O 4.11133100 4.02236900 -3.47991200
C 5.24357500 4.05645100 -2.58538000
H 5.51680200 5.10522300 -2.45049400
Pd 4.82835500 3.12211500 -0.81274900
C 4.28199500 5.29314700 0.33732800
H 3.79480500 5.36305900 -0.63003200
H 3.77335600 4.73677900 1.12548200
H 4.74034000 6.22468000 0.64069100
H 6.07866300 3.50514500 -3.03748800
I 6.78501300 4.43524500 0.62170900
C 3.93031500 2.30012000 2.13906200
O 4.19871800 1.88706000 0.90989100
O 3.04076200 3.22399300 2.31495600
K 4.77623800 -0.47802500 1.71560400
I 1.14814200 -0.46600300 2.48056700
K 1.51881300 2.40239700 0.28198800
O 4.48121800 1.69154400 3.12376200
K 2.42731900 2.10948100 4.61282300
C 2.40922000 3.23096600 -5.60579100
H 2.01658600 4.23514600 -5.40761000
H 3.38595400 3.37070300 -6.08181000
H 1.74248300 2.73511900 -6.31711200

26-TS-d

C	3.68030200	2.56260800	-3.35318000	H	3.87389700	4.87408900	0.77273500
C	3.91467600	1.85308700	-2.15517200	H	5.15865900	6.15258400	0.84599200
C	3.47273100	0.52228400	-2.10765500	H	6.57894000	3.18504000	-2.59987300
C	2.73146200	-0.03174000	-3.16432300	I	7.03822500	4.23907900	0.55777600
C	2.45596800	0.73820700	-4.30206900	K	3.03756900	-0.44586500	-1.32327300
C	2.94269000	2.04782600	-4.43324800	I	3.76520600	1.72973500	1.71059600
H	3.69592400	-0.10702700	-1.24683100	C	6.01611700	-0.13397400	-1.79951700
H	2.38072700	-1.05879000	-3.10598300	O	5.60849500	-1.00397000	-0.97594700
H	1.88576400	0.30646200	-5.12122600	O	6.98718100	0.64607700	-1.68870900
O	4.17938100	3.82648500	-3.42987400	K	6.95868900	0.32564000	0.92603900
C	5.24760900	4.00729400	-2.49745200	O	5.21175200	-0.01213500	-2.93103300
H	5.36915500	5.07738500	-2.33204200	H	5.46050400	0.82227800	-3.36954100
Pd	4.84033700	3.03633900	-0.75314200	C	3.03485600	2.02837500	-5.65594400
C	3.45195500	5.09159700	0.03096800	H	3.51736400	2.94196500	-6.01872000
H	3.10237900	4.82813000	-0.95599100	H	3.77241100	1.22374100	-5.76217600
H	3.07836500	4.56282800	0.89548600	H	2.18515700	1.80136800	-6.30592600
H	3.70676900	6.13355200	0.16283300				
H	6.17006000	3.54946900	-2.87281000	27			
I	6.13169200	4.81180200	0.87784200				
C	2.69371700	2.12442800	1.59959600	C	3.68261900	2.46560700	-3.06432100
O	3.88330000	1.59726100	1.06311800	C	4.12096700	1.80137400	-1.90805800
O	2.84790700	2.98767400	2.47792100	C	3.45601600	0.66328300	-1.45399800
K	0.87228900	2.19051400	-1.39999200	C	2.35277900	0.20211500	-2.18119400
I	0.08418800	5.37044700	-0.26147000	C	1.92500600	0.87392000	-3.33160400
O	1.61734900	1.68050600	1.09884700	C	2.57786800	2.01688300	-3.80398600
K	0.41425700	3.74887600	2.74213400	H	3.77494400	0.15317200	-0.55010800
H	3.61011000	0.85744800	0.50112500	H	1.81800300	-0.68111000	-1.84199000
C	2.72370900	2.88005200	-5.67035400	H	1.06366600	0.50278100	-3.88186900
H	2.22451100	3.82536100	-5.43040200	O	4.34471800	3.59314200	-3.44814300
H	3.68101100	3.14489700	-6.13204000	C	5.65009900	3.65120200	-2.89518600
H	2.11961400	2.34444400	-6.40799700	H	5.94856000	4.69369200	-2.79353700
				Pd	5.78611500	2.61501600	-1.13878600
26-TS-e				C	4.54237900	4.00520300	-0.26773200
C	3.52956200	2.55588500	-3.23784800	H	4.23032900	3.49937800	0.64657500
C	3.20272700	2.67759300	-1.87439400	H	5.22331800	4.84010500	-0.10131500
C	1.86315800	2.50591900	-1.50231200	H	3.71793600	4.26759200	-0.92584300
C	0.90550700	2.13809800	-2.46198900	H	6.36158600	3.09075200	-3.51915400
C	1.28200400	1.96352400	-3.79897000	I	8.42654000	3.63778200	-0.66560400
C	2.60106600	2.18222600	-4.22083000	C	5.08878300	0.95825200	1.45229200
H	1.57402500	2.62352500	-0.46181900	O	6.04119700	1.28695700	0.58062900
H	-0.13055200	1.99221700	-2.16657900	O	4.68173500	-0.26126900	1.46388200
H	0.53716600	1.67736900	-4.53790900	K	7.19642700	2.86720000	2.51183500
O	4.83383300	2.75639300	-3.59125300	I	7.70144000	-0.36336400	4.12201300
C	5.53789100	3.50643800	-2.57800700	K	7.08482300	-1.07951200	0.62745400
H	5.43082000	4.57850600	-2.78029100	O	4.69284000	1.83585000	2.29846600
Pd	4.81594300	3.07928600	-0.70185300	K	4.15370800	-0.09790000	3.99704000
C	4.66873700	5.39607700	0.24959700	C	2.14224600	2.76003900	-5.04030000
H	4.47973400	5.69020300	-0.77546100	H	1.82443700	3.78041900	-4.79673200

H 2.96694600 2.85304600 -5.75517700
H 1.31000300 2.25099700 -5.53431200

28-TS

C 3.64966100 2.59281400 -3.00382000
C 3.88390700 2.13716100 -1.69229800
C 3.21182900 1.01095400 -1.20503200
C 2.30962000 0.35764500 -2.04771800
C 2.06827500 0.83427100 -3.34237100
C 2.72985500 1.95793600 -3.85025400
H 3.38815600 0.68146200 -0.18277200
H 1.77427500 -0.51619200 -1.68621700
H 1.35299900 0.32007900 -3.97954400
O 4.32800900 3.69273800 -3.41995200
C 5.63792900 3.74167300 -2.84951800
H 5.94359700 4.78604200 -2.77070100
Pd 5.71152200 2.80876200 -1.02683000
C 3.82741700 3.71628100 -0.36104500
H 3.31943300 3.15102200 0.41438100
H 4.53027200 4.43042300 0.08652400
H 3.15050100 4.23949200 -1.02945800
H 6.32919000 3.16639600 -3.47237800
I 8.50627400 2.78537500 -1.13749200
C 5.12661000 1.37628200 1.85593100
O 5.94089800 1.84862000 0.91743200
O 4.43013000 0.32255400 1.60269500
K 7.79760100 2.55252600 2.59149800
I 7.97635000 -1.08631800 3.18075300
K 6.46246600 -0.55569100 -0.06755000
O 5.16755800 1.92207100 3.01321800
K 4.64924100 -0.38229700 4.10971300
C 2.49851800 2.48569600 -5.24273100
H 2.03322400 3.47790000 -5.21732700
H 3.44481500 2.59848000 -5.78151100
H 1.84789900 1.81844700 -5.81438800

28-TS-a

C 3.59450500 2.72294400 -3.19262100
C 3.67307300 2.16768900 -1.89959600
C 2.89457600 1.04166600 -1.59279000
C 2.05675100 0.50973000 -2.56891600
C 1.97773800 1.09506200 -3.84029800
C 2.74328300 2.21154800 -4.18282200
H 2.94039400 0.60858900 -0.60080300
H 1.45106400 -0.36174400 -2.33858700
H 1.31185300 0.66927000 -4.58660700
O 4.35705400 3.82091400 -3.44990100
C 5.59141700 3.75791400 -2.76565700

H 5.97482400 4.76662300 -2.62193700
Pd 5.43132600 2.72777100 -0.98138200
C 3.49568700 3.70095900 -0.51739800
H 2.76502400 3.14323400 0.05794700
H 4.15142900 4.26253700 0.15689500
H 3.05808300 4.36022300 -1.26109200
H 6.29552900 3.10997400 -3.29800000
I 8.17483600 3.40039700 -0.63344100
C 2.69345300 2.85666100 -5.54380200
H 2.32642300 3.88731300 -5.47990400
H 3.69125500 2.90699300 -5.99218400
H 2.03701000 2.30066800 -6.21841600
K 8.35193800 1.21367500 1.88210600
I 5.08733300 1.08275200 1.45806800

28-TS-b

C 3.64774000 2.59875600 -3.02539900
C 3.91141900 2.07999000 -1.74067300
C 3.19849000 0.96775100 -1.27395500
C 2.24370800 0.38430500 -2.10988200
C 1.98450000 0.91784400 -3.37855300
C 2.67642400 2.03206300 -3.86449600
H 3.37768100 0.57583600 -0.27483100
H 1.68289700 -0.47772600 -1.75971100
H 1.22788100 0.45901400 -4.01029600
O 4.33592000 3.69550800 -3.42638100
C 5.65208100 3.73532200 -2.86620600
H 5.94841600 4.77923000 -2.75442900
Pd 5.76790800 2.69559000 -1.10146400
C 3.92133200 3.61113900 -0.31909300
H 3.65503600 3.04698200 0.57200600
H 4.59879300 4.44145000 -0.08629700
H 3.07221900 3.99875000 -0.87175500
H 6.34251400 3.19808100 -3.52535600
I 8.54402700 2.97141800 -1.09974700
C 5.06781000 1.07188300 1.52897400
O 4.71329800 1.91252000 2.40868100
O 4.61694600 -0.10464000 1.37067100
O 6.07182400 1.46146600 0.67022800
K 6.26123900 -0.74912300 -0.52886400
K 6.91904800 3.24261800 2.30260600
C 2.41823600 2.62679400 -5.22490000
H 1.99605700 3.63489300 -5.14160000
H 3.34854100 2.72503200 -5.79373200
H 1.72022500 2.01108400 -5.79857900

28-TS-c

C 3.92415400 2.30400400 -3.24506300

C	3.78565700	2.02843200	-1.86681400	H	3.39151300	4.35630400	-1.06432400
C	2.76937900	1.14331000	-1.45965700	H	6.34656000	3.10803900	-3.42915400
C	1.94832900	0.54361300	-2.41229200	I	8.45278700	3.40671300	-0.87660300
C	2.11898700	0.82650100	-3.77876100	C	4.96095800	1.70654200	1.92049300
C	3.10329600	1.71174900	-4.22325200	O	5.87429900	1.37766500	0.86395900
H	2.63876600	0.93631200	-0.40341700	O	4.09042800	0.85443700	2.16979400
H	1.16199000	-0.13559500	-2.09507700	K	7.93295700	2.89272600	2.59391600
H	1.46937900	0.35372100	-4.51112600	I	7.30299900	1.66522800	5.74332400
O	4.88209500	3.18454200	-3.62776300	O	5.20760200	2.81160800	2.44737300
C	6.02253300	3.11895700	-2.78546500	K	4.08908100	1.77534400	4.73186900
H	6.54422400	4.07320400	-2.82799300	H	5.66801100	0.46981600	0.59109800
Pd	5.55601900	2.46873400	-0.88492400	C	2.50438900	2.48423700	-5.21517900
C	3.76547700	3.76594900	-0.76704200	H	2.09375700	3.49919500	-5.17037900
H	2.94864500	3.42077200	-0.14232600	H	3.43822300	2.54843000	-5.78339700
H	4.47374300	4.35384200	-0.17472800	H	1.80334100	1.85452600	-5.76884000
H	3.43925300	4.32918800	-1.63675700				
H	6.63083300	2.24511900	-3.05583500				
I	8.12005300	3.33805200	-0.10776200	28-TS-e			
K	5.19486100	-0.95430400	-2.28556100	C	3.91173500	2.42434000	-3.24103400
I	5.01115500	0.92646200	1.46818200	C	3.86359200	2.07844300	-1.87511100
C	8.09054800	-0.58836500	-1.92216000	C	3.03314900	1.03000000	-1.45587700
O	7.41097100	-1.44045000	-1.22149400	C	2.30599000	0.31385400	-2.41148700
O	9.29198800	-0.26473000	-1.55790300	C	2.38366400	0.65825000	-3.76757300
K	8.39000100	-0.33882700	0.91467400	C	3.17784500	1.72204200	-4.21090300
K	9.46592000	1.72068000	-3.07008400	H	2.96029300	0.78928300	-0.40092200
O	7.53395500	0.00250300	-2.95685300	H	1.66135700	-0.50102400	-2.09475100
C	3.31316600	2.04067400	-5.67865200	H	1.80888900	0.09545300	-4.49857100
H	3.11252100	3.09972100	-5.87460400	O	4.68089300	3.48020800	-3.60241900
H	4.35134800	1.85890800	-5.97584600	C	5.85152100	3.59519300	-2.79088500
H	2.65614200	1.44375000	-6.31663500	H	6.10955200	4.64960600	-2.68444600
				Pd	5.55964700	2.74667700	-0.91416100
				C	3.66658300	3.82978200	-0.71671800
28-TS-d				H	2.91258700	3.37258900	-0.08508600
C	3.68266900	2.55312000	-2.98619300	H	4.29873700	4.50309800	-0.12498000
C	3.94106100	2.08099000	-1.68718500	H	3.26575600	4.34392200	-1.58577500
C	3.26500100	0.95002200	-1.20873800	H	6.66407200	3.02701100	-3.24776100
C	2.34892700	0.31494700	-2.04390100	I	8.32146700	2.55786700	-0.74036400
C	2.09453900	0.80968500	-3.33132300	K	5.94023900	-0.56941600	-1.84472200
C	2.75007500	1.93699000	-3.83321100	I	5.06320900	1.51121100	1.64425600
H	3.41595800	0.61083900	-0.18787200	C	8.53168000	-1.62213600	-0.50801900
H	1.81513500	-0.56154000	-1.68900100	O	7.37505500	-1.63702800	-0.00112100
H	1.37029000	0.30412500	-3.96450900	O	9.63358100	-1.46477700	0.04622400
O	4.35219100	3.66881800	-3.39394400	K	8.29418300	0.00999700	1.88852200
C	5.65442600	3.72963000	-2.85154800	O	8.52105100	-1.73904100	-1.91151800
H	5.97292000	4.76870600	-2.78626700	H	9.44486100	-1.64112200	-2.18456500
Pd	5.76074000	2.78164900	-1.04729800	C	3.26636000	2.12856300	-5.65936000
C	3.87441800	3.69946000	-0.34714000	H	2.76138100	1.40472700	-6.30439000
H	3.16986000	3.13640600	0.25622500	H	2.80478500	3.10952200	-5.81951800
H	4.56384400	4.24401800	0.30527400	H	4.30913400	2.21990600	-5.97970800

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C	3.69602500	2.49417000	-2.65770800
C	2.73032000	2.56226700	-1.63899800
C	1.68474900	1.63113600	-1.67245300
C	1.57611400	0.70251500	-2.70868200
C	2.50606000	0.71350900	-3.75163100
C	3.58346800	1.61395200	-3.75296700
H	0.94382000	1.64842400	-0.87820400
H	0.74984100	-0.00273200	-2.72450900
H	2.38807000	0.03669300	-4.59489200
O	4.73671500	3.41105800	-2.60864400
C	6.04006700	2.94001400	-2.53926500
H	6.67191700	3.65819700	-3.06213100
Pd	6.79347100	2.92488400	-0.65895900
C	2.77709600	3.64316600	-0.59060000
H	2.28896100	3.31357700	0.32910100
H	3.79965500	3.93058500	-0.34968700
H	2.25431500	4.53573900	-0.95743000
H	6.17076600	1.89333900	-2.83762200
I	9.27299400	3.79365300	-1.44133200
K	4.81506600	-0.88503000	-1.89102200
I	5.22191300	1.32891900	0.92150500
C	7.72053800	-0.64959900	-2.49955800
O	7.26575000	-1.36982900	-1.52722600
O	8.97717500	-0.32729600	-2.53320200
K	8.87741000	-0.04932500	0.03688600
K	8.79315800	1.41436500	-4.30689100
O	6.89973900	-0.17673800	-3.41187800
C	4.55063400	1.63961600	-4.91551600
H	4.94893500	2.64718700	-5.06759200
H	5.39059900	0.95569600	-4.74826000
H	4.04004800	1.33431900	-5.83362300

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Pd	2.94709500	0.56452300	1.77231600
C	2.85804300	2.28522100	-0.76602400
C	2.17726300	1.31062800	-0.02445300
C	0.77150400	1.36517700	0.00980500
C	0.16581500	2.51877100	-0.52139100
C	0.91689700	3.53963300	-1.12668600
C	2.31395600	3.44184000	-1.29930600
H	0.17508900	0.58760900	0.47365100
H	-0.91418800	2.62473200	-0.46054000
H	0.40534600	4.41332200	-1.52361100
O	4.11414400	1.72365600	-0.92493600
C	3.69994200	0.43617600	-0.34693600
H	3.45789100	-0.27549700	-1.13612400

H	4.51221500	0.03907200	0.28643100
K	6.13782900	3.27317300	0.13592900
I	2.60730900	0.57996700	4.47380800
C	4.80486800	4.36792500	2.48007900
O	5.99364100	3.83241900	2.59321700
O	4.09549400	4.59420900	3.54075000
K	5.34031600	2.80384000	4.86310000
O	4.30422700	4.59441600	1.29811800
K	1.94360200	3.97489900	2.28103500
C	3.15406500	4.49894200	-1.96279200
H	2.54038900	5.18695300	-2.55092800
H	3.68299000	5.07751300	-1.19510300
H	3.89704900	4.05271900	-2.63460500

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Pd	2.14008800	1.00770600	1.68215000
C	2.93889600	2.10544900	-1.00049000
C	2.25193900	0.98657900	-0.48294100
C	0.87437800	1.08341700	-0.15538100
C	0.32148500	2.39852300	-0.33292200
C	1.06814000	3.46850500	-0.82193000
C	2.44190200	3.36772400	-1.20664100
H	0.21644300	0.22731500	-0.03772700
H	-0.73281100	2.54766100	-0.11620700
H	0.57404000	4.42825800	-0.96601000
O	4.10434800	1.41929800	-1.38101600
C	3.40096500	0.14527000	-1.03684600
H	3.18634100	-0.40797400	-1.95624000
H	3.98414000	-0.46129400	-0.34083200
K	5.62624700	2.41968800	0.94088000
I	3.40442700	0.92401700	4.09233900
C	4.77401100	4.66761200	2.55576800
O	5.94855800	4.16929200	2.82427700
O	4.03720400	5.15733600	3.51224800
K	5.31949900	3.84270000	5.26639900
O	4.29453800	4.58018800	1.34981200
K	1.91584700	4.27922400	2.29867300
C	3.24894300	4.51868000	-1.73846100
H	2.60747500	5.26523400	-2.21718300
H	3.79088400	4.99554500	-0.91196000
H	3.98266600	4.17788800	-2.47695200

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Pd	0.53527400	-0.36475700	-0.71480700
C	0.56201300	-2.13117700	0.54083000
C	0.53965400	-1.64454300	1.85809900
C	1.05537300	-3.41559000	0.30784100
C	1.13340800	-2.44259900	2.84732400

H	0.17556600	-0.64970400	2.09426600	O	-1.11934400	2.51376000	-1.28168800
C	1.62824900	-4.25372300	1.25955000	C	4.14867600	0.88808100	-0.47699100
C	1.67097700	-3.70494900	2.55009700	H	3.24404400	0.98051100	-1.09184900
H	1.21140300	-2.05947500	3.86121900	H	3.98278400	1.23892800	0.58256600
H	2.11559600	-4.29191900	3.34979500	H	4.85583600	1.63022800	-0.85320500
C	-0.19137100	-2.55284100	-1.08167900	C	2.81739200	4.04342200	0.00448600
H	-1.22285000	-2.75714000	-0.79262500	H	3.44326400	4.16247200	0.90759800
H	-0.13449500	-2.11435300	-2.08303300	H	2.50473400	5.05814600	-0.30112000
I	1.04181700	2.28196200	-1.14815600	O	1.70722400	3.21628600	0.22372600
C	2.43357000	-0.78570500	-1.35591400	H	3.48095200	3.67286500	-0.79929100
H	2.49062400	-1.86608400	-1.51030400	H	1.20538400	2.53189600	-1.12831800
H	2.61256000	-0.24151300	-2.28357700	C	-0.77074600	0.50714000	1.37861100
H	3.12669500	-0.45834000	-0.57877100	O	-0.54720500	-0.51518600	0.63753800
O	0.68416700	-3.68499600	-0.98061700	O	0.22083300	1.22904400	1.87497500
C	-2.58941900	-0.50018100	-0.71908000	K	0.49984500	-1.30560400	-1.61984200
O	-1.57709800	-0.08614400	0.03969800	I	-3.00135600	-3.10796900	-1.07590600
O	-3.11412400	-1.65582400	-0.45731800	K	-0.72749000	3.54012300	1.07645100
K	-2.36329700	2.45060900	-0.30397500	O	-1.96760400	0.86363600	1.69036000
I	-5.18391600	1.05998200	1.81439200	O	-0.78562900	0.74426500	-2.63568400
K	-2.64038400	-1.43131400	2.10429400	K	-2.32129900	-1.86271200	2.01351600
O	-3.06963500	0.27435400	-1.61536000	K	-2.92468500	0.51247000	-1.09300800
K	-5.43188100	-0.72162100	-1.27234800				
C	2.10903600	-5.63711900	0.91356400				
H	2.43925400	-6.17511600	1.80585100	34-TS			
H	1.31520600	-6.21887700	0.43218400	C	7.36795700	0.40939200	-5.37833400
H	2.94674000	-5.59836800	0.20841500	C	7.03349000	-0.00120900	-6.68107700
				C	7.44369000	-1.27383500	-7.09444100
33				C	8.16788500	-2.10593600	-6.24212500
C	3.96186000	-1.62352300	-0.11789000	C	8.50894300	-1.66340900	-4.96489800
C	4.47834400	-2.92770800	-0.17099700	C	8.12318100	-0.39601600	-4.50978800
C	5.79265900	-3.10104700	-0.61804400	H	7.19776800	-1.60647300	-8.09988600
C	6.57167600	-2.00643100	-0.99135500	H	8.47617100	-3.09222200	-6.57686000
C	6.03771500	-0.72014600	-0.92889000	H	9.08568200	-2.30531400	-4.30371200
C	4.72302200	-0.50391800	-0.49862300	O	6.99427600	1.68035900	-4.96077000
H	6.20684100	-4.10476300	-0.66490100	C	5.60202800	1.85019000	-4.61584600
H	7.59222900	-2.15436800	-1.33118900	H	4.99903200	1.09507400	-5.12086900
H	6.64155900	0.13295800	-1.22672000	Pd	5.36148300	1.82664300	-2.59611600
O	2.63755900	-1.50188400	0.27082900	C	6.27833600	0.91459200	-7.61478700
C	2.36629600	-0.74064700	1.46815100	H	6.49802700	0.67009400	-8.65791700
H	3.20827100	-0.84151500	2.16712700	H	5.19355200	0.83168300	-7.47843600
Pd	2.07910200	1.18663500	0.96460500	H	6.54244400	1.96028000	-7.43436300
C	3.61468200	-4.09348200	0.24286100	H	5.32982900	2.87137300	-4.89045700
H	4.18711100	-5.02464400	0.24456100	C	7.97946200	3.43993100	-0.32145600
H	3.19584400	-3.93947000	1.24227300	O	7.81267700	2.09535600	-0.53715400
H	2.76241100	-4.22261900	-0.43489600	O	7.22122200	4.00862600	0.52343600
H	1.43337400	-1.12640500	1.87188200	C	8.54178200	0.09883000	-3.14844700
C	-0.37896700	1.71979800	-1.94234600	H	9.42219500	0.75296700	-3.21415700
O	0.97277900	1.87096300	-1.86672300	H	7.75638600	0.66929000	-2.64799600
				H	8.82282900	-0.73364700	-2.49729800

C	4.87864800	0.21841000	-1.01987700	H	6.40518800	4.33198000	-4.07627000
H	3.86662200	-0.20701400	-1.07497900	H	5.62093000	4.70492700	-2.52869600
H	5.67755100	-0.53558300	-0.98291500	O	2.75651700	0.15408900	-0.49580700
O	5.04805600	1.33769000	-0.38336600	C	5.39805700	3.98245600	0.04072500
H	4.92592200	0.26609500	-2.65684600	O	4.44893000	3.37911400	-0.67343600
H	6.96359300	1.81709900	-0.14251200	O	5.26518600	5.25200600	0.25348000
C	5.57743900	4.96533900	-2.94737800	K	2.64676700	4.91684000	0.40034300
O	5.65631700	5.02015900	-4.21570700	I	3.40698200	3.67044700	3.60207900
O	5.90043400	3.84763300	-2.31095800	O	6.34451500	3.29645700	0.55682100
K	8.36152800	3.76632800	-3.66248400	K	4.73676200	1.11822300	1.07840200
I	8.95533500	7.64738700	-3.78194100	K	6.53504700	4.98810300	2.51275200
K	4.67546800	4.00768600	-0.02455100				
O	5.27156700	5.98036100	-2.20010200				
O	8.87199200	3.98754700	-1.01885500				
K	5.57720800	7.56172400	-4.38319200				
K	7.80156300	6.37877500	-0.72788700				

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C	3.21459900	4.87387400	-3.64940800
C	3.04035500	6.00600400	-2.83070500
C	1.75352300	6.26435800	-2.32794000
C	0.67383600	5.42836100	-2.62447100
C	0.86905500	4.33187100	-3.47057700
C	2.13271600	4.04330800	-4.00715900
H	1.59280500	7.16677900	-1.73928900
H	-0.31947300	5.66415700	-2.25125800
H	0.01355200	3.73386000	-3.78413200
O	4.42230500	4.62904300	-4.25746700
C	5.51573900	4.15746300	-3.46686900
Pd	5.16490000	2.28955500	-2.42759900
C	4.18992900	6.92837300	-2.51267500
H	3.82446400	7.93530400	-2.28712800
H	4.74907700	6.56158400	-1.64164200
H	4.87990600	6.98956900	-3.35832800
C	3.50527100	0.13084500	-1.53807200
O	2.98867500	-0.08886300	-2.71324600
O	4.78788900	0.38733400	-1.43614100
C	2.33505800	2.92479600	-4.99596800
H	2.74769000	3.31620800	-5.93137000
H	3.04444700	2.16849500	-4.64800300
H	1.38431800	2.43258500	-5.23006100
C	5.68171600	0.98536200	-4.15057400
H	6.31234200	1.35584600	-4.96613600
H	5.67078400	2.64695400	-3.87257800
H	6.25216600	0.34086200	-3.47484700
O	4.52035000	0.48298800	-4.63417600
H	3.94269800	0.13923900	-3.84834400
K	0.89332300	1.10050700	-1.97052700

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C	5.42408700	-0.77952700	-4.27048500
C	4.71141900	-0.23401100	-5.35955700
C	3.43338800	0.29213200	-5.11985400
C	2.86698100	0.26250500	-3.84136100
C	3.58962100	-0.28813400	-2.77929000
C	4.87744700	-0.80940900	-2.97092000
H	2.86711400	0.69608500	-5.95599000
H	1.86042300	0.64168000	-3.68126600
H	3.15802500	-0.31688800	-1.78183000
O	6.63296400	-1.41096400	-4.45620100
C	7.79363000	-0.66001100	-4.80077200
H	7.66976600	-0.13397300	-5.74845800
Pd	8.35242100	0.80835900	-3.47859300
C	5.28240900	-0.24371100	-6.75565100
H	4.48321200	-0.18967100	-7.50083500
H	5.94857100	0.61204900	-6.91569900
H	5.86184000	-1.15418200	-6.93189700
H	8.59422100	-1.39590900	-4.87735100
C	6.34747600	2.28474500	0.02852400
O	7.65018600	2.53994400	0.44430000
O	6.22426300	1.83110800	-1.14532100
C	5.66755600	-1.34637700	-1.80633100
H	5.00406700	-1.79511600	-1.06007400
H	6.39976000	-2.08655900	-2.13213300
H	6.19907000	-0.51397700	-1.33270200
C	9.65911000	0.62879100	-1.56399200
H	9.26082600	0.03754500	-0.72661100
H	10.60112500	0.25470500	-1.98674100
O	9.39086100	1.88364800	-1.62296800
H	8.61772500	-0.42833300	-2.50732500
H	8.23818800	2.18351400	-0.25924100
K	8.15244400	4.32291300	-1.94635100
I	7.79392400	2.92295400	-5.26701400
O	5.45118200	2.57133600	0.85091500
C	5.75824200	6.14108600	-1.38733200

O	4.98168300	6.85125000	-0.61211200	34-TS-c			
O	5.41721500	4.93393900	-1.71016400	C	9.15538000	2.83893800	-3.45158900
O	6.89410900	6.63212500	-1.78897400	C	9.45039300	3.60524100	-4.58969900
K	4.93068400	2.80130400	-3.12144400	C	10.79183700	3.92035800	-4.83592500
K	6.37428300	8.91921500	-0.94505700	C	11.79605600	3.47434500	-3.97656200
K	4.15477700	4.70161700	0.62657700	C	11.47181900	2.70457800	-2.85923600
				C	10.14228600	2.36943500	-2.57007100
34-TS-b				H	11.04530400	4.51571800	-5.70949500
C	7.20633200	0.41443300	-5.68330000	H	12.83357500	3.72417400	-4.17968600
C	6.68594900	0.22905600	-6.97803300	H	12.25752800	2.35317400	-2.19553900
C	6.64840000	-1.07200000	-7.49384800	O	7.81386700	2.60058800	-3.15229200
C	7.12492700	-2.15460300	-6.75794400	C	7.22867200	1.40619400	-3.70868900
C	7.67825500	-1.94062300	-5.49664900	H	8.02005600	0.70789900	-3.98445900
C	7.73786400	-0.65701600	-4.94171400	Pd	5.94803500	0.69266600	-2.28569600
H	6.25202900	-1.22819200	-8.49418200	C	8.34502300	4.05259500	-5.51511300
H	7.08432700	-3.15736800	-7.17307900	H	8.68343000	4.85592600	-6.17527800
H	8.07728800	-2.77797500	-4.92964100	H	8.00049000	3.22534800	-6.14674200
O	7.27297200	1.68834200	-5.14577400	H	7.46849000	4.39812800	-4.95860900
C	6.00868600	2.29606200	-4.77453100	H	6.61172600	1.66447500	-4.57324100
H	5.21755300	1.97868800	-5.45526500	C	6.81204900	2.38408200	0.85252000
Pd	5.43690100	1.94024000	-2.85806300	O	7.03744400	1.06211100	1.17048200
C	6.22431900	1.39604100	-7.81972800	O	5.61191400	2.69100400	0.53625100
H	6.41570600	1.20033300	-8.87907200	C	9.77531400	1.54546000	-1.36093000
H	5.14933400	1.58190100	-7.71208900	H	9.29141600	2.14197500	-0.57857000
H	6.74340400	2.31477300	-7.53564700	H	9.06997600	0.75124900	-1.61958100
H	6.16250200	3.37563900	-4.81174300	H	10.66695200	1.08630300	-0.92479600
C	8.01559100	3.05794700	-0.03874300	C	5.99316400	-1.15401600	-0.85079300
O	7.76908000	1.78606500	-0.53415300	H	5.76896500	-2.01074100	-1.49962200
O	7.11292100	3.59911500	0.65664200	H	6.91649600	-1.22745300	-0.26141100
C	8.41784800	-0.43377800	-3.61297200	O	5.03817400	-0.40797500	-0.43248000
H	9.41371900	0.01157500	-3.75190700	H	7.08600700	-0.40338800	-2.08702800
H	7.83793700	0.21795500	-2.95644400	H	6.22829000	0.58916300	0.91116300
H	8.57162800	-1.38047400	-3.08768900	I	3.98003200	2.60971800	-3.01102000
C	5.14459700	0.10429000	-1.53781900	K	3.38868800	1.52630500	0.22251100
H	4.22450500	-0.42112700	-1.82668800	O	7.79813000	3.14440000	0.85357100
H	6.02497000	-0.54727600	-1.44757700	K	6.79730100	4.32274200	-1.29019000
O	5.05189900	1.13421100	-0.75094000				
H	5.54914300	0.35506700	-3.16494000	34-TS-d			
H	6.82908300	1.55933200	-0.35721800	C	5.99420300	-0.99644800	-4.70725900
C	5.96775900	4.89095200	-2.22831700	C	4.79212500	-0.62644400	-5.34259900
O	7.13973200	4.85375800	-2.74633900	C	3.68345600	-1.47664300	-5.20138700
O	5.06795300	3.94994100	-2.51148200	C	3.76669700	-2.66515300	-4.46990800
K	8.72613800	2.86985800	-3.01964400	C	4.98204400	-3.02982600	-3.87874800
K	4.51313700	3.73397900	0.05678800	C	6.11259400	-2.20974700	-3.99685100
O	5.60841700	5.77556800	-1.37332700	H	2.75327500	-1.21095200	-5.69770600
O	9.11432500	3.55401900	-0.39943900	H	2.90257100	-3.31939300	-4.39114900
K	8.02039800	6.02461500	-0.45211700	H	5.06346500	-3.97056800	-3.33965300
				O	7.13885900	-0.24103400	-4.82486300

C	7.17541400	1.04688600	-4.20889100	H	5.30521100	-3.64714300	-2.91382600
H	6.55064900	1.76475900	-4.74424700	H	4.53558000	-2.47950000	-1.83101100
Pd	6.47684300	1.09718700	-2.27396800	H	3.60044700	-3.87562000	-2.45663700
C	4.70026100	0.61744400	-6.18948400	I	3.95092700	2.92226600	-3.33209800
H	3.90579100	0.51744700	-6.93418000	K	1.58365000	0.32796000	-2.83264000
H	4.47626800	1.49932500	-5.57938800	C	3.39496000	-0.68998200	0.00285100
H	5.64380400	0.80017600	-6.71090000	O	2.73604900	0.28491800	-0.53561700
H	8.22202900	1.35223100	-4.23351700	O	4.65670000	-0.84156100	-0.45138700
C	7.74732400	3.42274800	0.31647700	O	2.95398300	-1.48625300	0.86752800
O	8.19201700	2.17656700	0.69736900	K	5.14281100	-2.74967200	1.11650600
O	6.49602200	3.64664900	0.47195400				
C	7.44971500	-2.63310700	-3.44211600	34-TS-partB			
H	8.09120200	-3.01326800	-4.24572800	C	-0.43716700	-0.78649700	0.68500900
H	7.98044800	-1.79160100	-2.99351600	O	-0.34530800	-0.22569100	-0.56502400
H	7.33644800	-3.42944000	-2.70053900	O	0.64122300	-1.17804700	1.23781100
C	6.96018300	-0.38020600	-0.51292200	C	1.40684200	2.17779200	0.88646100
H	6.71420400	-1.37864200	-0.90109400	H	1.29452200	1.37118500	1.62550500
H	7.97800400	-0.27516000	-0.11498200	H	0.59994600	2.91099000	1.05268700
O	6.02695700	0.38311400	-0.07052400	O	1.40705500	1.67196000	-0.44114100
H	7.70491700	0.11769700	-2.02489900	H	2.35678800	2.69588800	1.06637400
H	7.38899200	1.64915100	0.83750600	H	0.62071000	1.03417900	-0.50361200
K	3.50084000	-0.61206000	-1.83214300	K	2.18583800	-0.93868900	-0.69580900
I	1.86322500	-0.01763800	1.03633000	O	-1.59602800	-0.87057000	1.20843100
K	4.41405000	2.27577300	1.15412600	K	-2.78160700	0.33974800	-0.56912400
I	4.37452900	2.89652400	-2.76983100				
O	8.58688000	4.19802300	-0.17701800	35			
K	6.72412400	5.34168700	-1.53671200	C	3.69742100	3.78964800	-4.57610600
				C	2.61548000	4.15357900	-3.74407400
34-TS-partA				C	1.41254400	3.44459800	-3.86907600
C	4.78895500	-1.24781000	-4.31977400	C	1.26394300	2.43954200	-4.82537000
C	4.47717500	-0.49785700	-5.47017000	C	2.34291000	2.10302700	-5.65282000
C	3.24184400	-0.72907800	-6.09389400	C	3.57769600	2.75150900	-5.52723800
C	2.36020400	-1.70683200	-5.62815300	H	0.57184500	3.72098600	-3.23795500
C	2.72631100	-2.49717400	-4.53139200	H	0.30369800	1.94398900	-4.94930700
C	3.94211300	-2.28398700	-3.86966900	H	2.22319500	1.34492500	-6.42542600
H	2.98719700	-0.14733500	-6.97630700	O	4.86356000	4.52520600	-4.57545400
H	1.42073100	-1.88697300	-6.14437400	C	5.76177600	4.33094500	-3.44225900
H	2.07291000	-3.29867700	-4.19323100	Pd	5.09363400	2.71952500	-2.42744000
O	5.96130300	-1.07152500	-3.62289300	C	2.74596800	5.31231400	-2.78558100
C	6.19063800	0.19276300	-2.95989500	H	1.76270100	5.70132600	-2.50734800
H	6.44860800	0.97385000	-3.67688100	H	3.26488800	5.01575800	-1.86704500
Pd	4.58444700	0.72065700	-1.85226900	H	3.33162200	6.11616400	-3.24054500
C	5.45303500	0.49301200	-6.04927000	C	5.69726100	-1.08803800	-2.96145800
H	5.27702200	0.62142500	-7.12129300	O	4.87328000	-2.00663400	-3.22384300
H	5.35181800	1.47325100	-5.57250400	O	5.77178500	-0.09830400	-3.92240600
H	6.48137800	0.15072000	-5.90335300	C	4.76393200	2.37024800	-6.37378800
H	7.02301200	0.00153900	-2.27661700	H	4.46200500	1.73948200	-7.21482200
C	4.36440700	-3.12871500	-2.69567800	H	5.27492200	3.25753400	-6.75528200

H	5.48815400	1.80741900	-5.77491600	H	5.84046900	4.93137900	-2.03113900
H	6.52563900	2.77379700	-1.85131200	O	5.50607100	0.33753300	-1.00184200
H	6.21358600	0.66984700	-3.51643600	C	5.49474900	3.08544900	0.79738100
K	2.76820900	-0.38142700	-3.51125700	O	4.75640700	3.23932900	-0.27329400
H	6.76479400	4.24177400	-3.86548900	O	4.89767100	2.95358000	1.93903000
H	5.71175000	5.21843200	-2.79863600	K	7.99835600	1.17955500	-0.61204700
O	6.41004300	-0.97088400	-1.92835700	I	8.87850000	0.56121000	2.97714600
C	3.58598200	0.58132100	-0.59380100	K	5.47476600	0.28125600	2.19674600
O	3.95187100	1.03069800	-1.76943300	O	6.77817700	3.04593400	0.70785000
O	2.85326400	-0.49613300	-0.56436300	K	7.26152000	3.69563100	3.13093300
K	6.57351100	0.76738200	0.06677800				
I	5.64165600	-2.02690300	2.60260800	36-TS-a			
K	4.72367900	-2.74165400	-0.68730900	C	3.04470100	4.51665000	-3.04963200
O	3.98612100	1.16413800	0.47295100	C	2.67620800	5.42548200	-2.03591400
K	2.68935200	-0.26442600	2.12758900	C	1.39022000	5.31574800	-1.48377400
				C	0.47687800	4.36605100	-1.94892200
36-TS				C	0.84482900	3.51262700	-2.99629400
C	3.15637100	4.61532000	-2.84596400	C	2.12711100	3.57173100	-3.56189800
C	2.84455300	5.41539400	-1.72922000	H	1.09527700	6.01502800	-0.70525000
C	1.55671500	5.31658300	-1.18153800	H	-0.52728500	4.32396400	-1.53439500
C	0.60248700	4.45028600	-1.72468500	H	0.12469000	2.80485300	-3.40100800
C	0.93493100	3.66719000	-2.83504900	O	4.26765000	4.57360300	-3.66944400
C	2.20996300	3.73714300	-3.41515900	C	5.46459400	4.31274900	-2.92947200
H	1.29840100	5.94690900	-0.33338500	Pd	5.53874100	2.51037200	-1.98611300
H	-0.40073800	4.41058200	-1.30726800	C	3.59765200	6.53466100	-1.59517100
H	0.19420100	3.00400900	-3.27475800	H	3.02066300	7.37054200	-1.18902800
O	4.36037900	4.72806500	-3.50484100	H	4.28980600	6.19769200	-0.81677400
C	5.57770700	4.30749900	-2.88971600	H	4.19036900	6.90041300	-2.43817900
Pd	5.50933100	2.44984200	-2.10033600	C	4.37576400	0.00465000	-0.80083200
C	3.85896100	6.35077600	-1.12500900	O	3.94639300	-0.08916300	0.38107600
H	3.36825500	7.13067900	-0.53511100	O	3.46084400	-0.14219100	-1.78390500
H	4.52957400	5.78652900	-0.46772000	C	2.52088200	2.66491400	-4.69811200
H	4.46540600	6.82943200	-1.89924800	H	3.07449300	3.21901000	-5.46041900
C	4.26527800	0.05559900	-0.78842200	H	3.17005700	1.84844900	-4.36626900
O	3.76344600	-0.12557600	0.35461500	H	1.63532900	2.21796200	-5.15992200
O	3.41540900	0.03119300	-1.82118600	C	5.57622800	0.53961800	-4.18346800
C	2.56535600	2.90678300	-4.62039500	H	5.91670300	1.01813900	-5.11808100
H	3.13436600	3.49696000	-5.34339000	H	5.59916200	1.93309700	-3.49723200
H	3.18494300	2.04235100	-4.35297100	H	6.37681700	0.14777800	-3.54078900
H	1.66211700	2.52695300	-5.10692800	O	4.41752900	0.04068000	-4.13582000
C	5.65183900	0.59419700	-4.19504800	H	3.90216100	-0.13351200	-2.70907700
H	6.02254700	0.97545700	-5.16436500	K	2.23973200	1.95852000	-0.47161800
H	5.92932000	1.85514500	-3.58715500	I	5.29588000	3.65956600	0.65248200
H	6.42516200	0.03446600	-3.63738600	H	6.26404300	4.36265600	-3.67055600
O	4.43374500	0.21739900	-4.12154200	H	5.62534600	5.05680000	-2.14706100
H	3.89355500	0.06687100	-2.74011400	O	5.58250100	0.30167200	-1.12314700
K	2.39853700	2.23958700	0.02079700	K	6.32915500	0.45741700	1.38145200
H	6.32838500	4.38775100	-3.67764700				

36-TS-b

C	4.21178800	4.86194000	-4.47649000
C	3.16378400	5.42569100	-3.71524000
C	1.85917400	5.33539300	-4.22842600
C	1.58977500	4.71871300	-5.45294900
C	2.64446400	4.17753000	-6.19624800
C	3.96005900	4.24050200	-5.72147800
H	1.04646500	5.77252300	-3.65345400
H	0.57252400	4.67660300	-5.83228900
H	2.44976700	3.70173900	-7.15440600
O	5.52835100	4.93369200	-4.12494800
C	6.01056400	4.44899800	-2.86023300
Pd	5.48907800	2.60974700	-2.19638700
C	3.41236200	6.11454700	-2.39810900
H	2.53389700	6.69273600	-2.09809200
H	3.63008300	5.38599600	-1.61035400
H	4.26484000	6.79720700	-2.47101200
C	4.21702400	-0.00524700	-0.80661900
O	3.84897800	-0.20917000	0.37594300
O	3.34812200	-0.38769500	-1.79112200
C	5.11462200	3.66565000	-6.50110600
H	5.73309400	3.03396300	-5.85850700
H	4.76184500	3.07874500	-7.35394800
H	5.76827500	4.46199300	-6.87414900
C	5.58485300	0.49483900	-4.21381500
H	6.05264000	0.84033700	-5.14813300
H	6.04496200	1.99156800	-3.59167300
H	6.25287000	0.00032700	-3.49795700
O	4.34419700	0.26925100	-4.18709700
H	3.80095200	-0.25772800	-2.67221500
K	2.60045900	2.19415400	-3.40359700
H	7.09705400	4.45489500	-2.97921700
H	5.71311400	5.10619300	-2.04071400
O	5.31162700	0.54200800	-1.16181300
C	3.44107100	3.08937100	-0.05404100
O	4.64812400	3.48907400	-0.43092700
O	2.53779900	2.81720200	-0.93296800
K	5.63953500	1.75921600	1.30703700
K	1.55427400	0.99635100	0.67615200
O	3.23567600	2.92196200	1.20264700

36-TS-c

C	5.34416800	4.25500100	-5.40866400
C	4.09147300	4.69643300	-5.87867600
C	3.60890700	4.13329000	-7.07253100
C	4.34567200	3.17734600	-7.77501800
C	5.60993200	2.80104700	-7.31366800
C	6.13526800	3.34721700	-6.13799900

H	2.65070400	4.47255100	-7.46062700
H	3.95267000	2.75505300	-8.69568700
H	6.20356700	2.08595900	-7.87741800
O	5.89789400	4.76465800	-4.25838600
C	5.27875800	4.44724200	-3.02188800
Pd	5.52164800	2.62040600	-2.14943200
C	3.28921600	5.75465600	-5.15703000
H	2.71874600	6.35030000	-5.87677200
H	2.58036900	5.30318400	-4.45225200
H	3.94918700	6.42693300	-4.60152400
C	4.30500000	-0.07962100	-0.90472500
O	3.81191800	-0.21666200	0.24943000
O	3.51333600	-0.47973800	-1.92645300
C	7.52900000	3.02730900	-5.65906100
H	7.53072800	2.76902200	-4.59661700
H	7.96455400	2.20459800	-6.23358300
H	8.18009600	3.90176300	-5.77062100
C	5.59966700	0.46365900	-4.25900300
H	6.06666900	0.87292300	-5.16381300
H	5.54822000	1.97382100	-3.65216200
H	6.28387500	0.11581400	-3.47536300
O	4.42680800	-0.00390600	-4.32638800
H	3.94174000	-0.33863400	-2.82465400
K	2.35629900	5.05995000	-0.81072700
H	5.68012700	5.16956600	-2.30983500
H	4.18566300	4.48382900	-3.09678100
O	5.46302200	0.39949500	-1.16217800
C	1.20215200	2.78903600	-2.26492500
O	1.81141400	3.72411600	-2.95012200
O	1.01255500	2.94392200	-0.98441200
K	5.93277600	0.69707400	1.43140100
I	5.49646600	3.93089300	0.49055500
K	1.23015800	0.38130100	-0.63136800
O	0.84575600	1.68678500	-2.84227400
K	2.50086600	1.90408000	-4.77246500

36-TS-d

C	2.99397000	4.45860700	-3.29668400
C	2.62969500	5.42959400	-2.34180000
C	1.32965900	5.37953700	-1.81436900
C	0.40143600	4.43191400	-2.25230900
C	0.76891600	3.51532700	-3.24479700
C	2.06517100	3.51093200	-3.78121000
H	1.03608700	6.12573100	-1.08049100
H	-0.61286200	4.43920900	-1.86146800
H	0.03783300	2.80918000	-3.63225300
O	4.23260100	4.44846400	-3.89682200
C	5.40903600	4.24048600	-3.12434600

Pd	5.41696400	2.48163500	-2.09287000	H	5.08443400	1.44969500	-6.69240300
C	3.56477600	6.54169300	-1.93768200	H	5.45806000	3.17937500	-6.87166100
H	2.99591600	7.40726500	-1.58688600	H	5.92726600	2.33515500	-5.40429500
H	4.23266600	6.23255500	-1.12705800	H	6.38648100	3.01529600	-2.96185600
H	4.18178800	6.85614100	-2.78403900	H	5.49884100	0.62729000	-3.69654400
C	4.23784500	0.06737900	-0.80090700	K	2.23566300	0.11858900	-2.94941600
O	3.72573700	0.03943100	0.34457200	H	6.57506500	4.84199800	-3.31080500
O	3.37894600	-0.11202100	-1.83340800	H	5.11042600	5.00214300	-2.34088900
C	2.45920000	2.53252100	-4.85656700	O	5.96734700	-1.11197800	-2.25910100
H	3.03850200	3.02845100	-5.63962600	C	3.87988900	0.62485300	-0.10372200
H	3.08207500	1.72133900	-4.46606000	O	3.85798100	1.15108700	-1.30742700
H	1.57240500	2.07990300	-5.30951100	O	3.08127600	-0.37000300	0.13134300
C	5.50141700	0.48618700	-4.35387500	K	6.97779400	0.47244100	-0.41335800
H	5.71146600	1.04662500	-5.28166400	I	6.53384500	-2.37511300	2.21232700
H	5.61590800	1.81325900	-3.56486000	K	4.46327700	-2.72291100	-0.60916800
H	6.40195200	0.06321300	-3.87157600	O	4.69936300	1.07046900	0.77549300
O	4.38053400	-0.05856000	-4.19302200	K	3.82568500	-0.27645200	2.74260900
H	3.85924900	-0.16523200	-2.72390900				
K	2.02455500	1.99586000	-0.64599400	37-TS-a			
H	6.22620600	4.24327800	-3.84697900	C	3.27820600	3.99789600	-3.64317000
H	5.55612800	5.01680500	-2.37287500	C	2.77934200	4.46496900	-2.40528300
O	5.46433800	0.33234100	-1.06917500	C	1.48283000	4.08642500	-2.02968000
K	8.02237700	0.82807700	-1.17326900	C	0.68351800	3.28627900	-2.85008300
I	8.93980800	-0.28879900	1.84930400	C	1.18763600	2.85259600	-4.07760800
K	5.63426700	0.46981900	2.09236700	C	2.48254600	3.19740400	-4.49168300
I	5.15280400	3.68518600	0.43454600	H	1.09124900	4.44914200	-1.08244900
				H	-0.32923400	3.03119700	-2.54917900
				H	0.56992200	2.24905500	-4.73888100
37-TS				O	4.49219600	4.39967900	-4.15494100
C	3.75407000	3.80271300	-4.59478400	C	5.72784800	4.23670500	-3.46377400
C	2.54119200	4.17343000	-3.98493100	Pd	6.02431500	2.25605000	-2.63088900
C	1.38287700	3.46598700	-4.33516900	C	3.58130200	5.34935100	-1.48527100
C	1.42470000	2.43062100	-5.27405900	H	2.91928400	5.86751000	-0.78493600
C	2.64328400	2.07924800	-5.86525100	H	4.27986200	4.73419900	-0.90641900
C	3.82221800	2.75629200	-5.53342800	H	4.14098900	6.10678500	-2.04167100
H	0.43473900	3.75578600	-3.88787100	C	6.40181500	-0.54906200	-1.04516700
H	0.50820500	1.92306000	-5.56734000	O	6.76718600	-1.04889200	0.05009600
H	2.68489600	1.27401800	-6.59433400	O	5.26751600	-1.08844700	-1.59063800
O	4.91421500	4.52338200	-4.38491100	C	2.99219200	2.69972700	-5.82223900
C	5.59165600	4.40485000	-3.12951200	H	2.21219700	2.77343400	-6.58685400
Pd	5.12213600	2.60552700	-2.15578200	H	3.86237100	3.26588500	-6.15406100
C	2.48647100	5.30789000	-2.99395700	H	3.27766900	1.64508400	-5.74067900
H	1.47222400	5.70863600	-2.91146000	C	5.53523300	0.84750100	-4.24601400
H	2.79655700	4.97321600	-1.99659900	H	5.34163500	1.51570400	-5.09362400
H	3.15888600	6.11756600	-3.29150400	H	6.68206500	3.07289700	-3.79850300
C	4.99064300	-1.11165100	-3.05547100	H	6.51613700	0.35186300	-4.25784800
O	4.02620600	-1.92241500	-3.09158600	O	4.53680100	0.24231500	-3.70381000
O	4.90605500	-0.09230200	-3.98631800	H	5.07198700	-0.64656900	-2.47517900
C	5.14375500	2.40392300	-6.16388600				

K	2.80260600	0.88645600	-1.72506600	H	-0.50627500	5.00532000	-1.52311100
H	6.42765900	4.81666800	-4.06760100	H	-0.02453500	3.22745900	-3.20445600
H	5.72867700	4.67073900	-2.46283500	O	4.12033000	4.81959500	-3.99288900
O	6.97857400	0.41338700	-1.63733100	C	5.36052000	4.42070100	-3.40479100
C	4.66332700	1.98640400	0.46041000	Pd	5.22665300	3.21205600	-1.70261300
O	4.62962200	2.37839500	-0.77053700	C	3.80331300	6.80887500	-1.84101700
O	3.75430100	1.12801300	0.88044400	H	3.36017100	7.74326600	-1.48453600
K	7.80256100	1.19367100	1.02146700	H	4.37504600	6.37718200	-1.00882700
I	6.16092100	-0.36788800	4.38780800	H	4.48304900	7.03986200	-2.66469300
K	4.62977300	-1.43053900	1.40362500	C	2.30751700	2.84208700	-4.60850800
O	5.55030900	2.43588700	1.27894900	H	2.53713200	3.30361600	-5.57428400
K	4.10956900	2.16261300	3.36128400	H	3.19382600	2.27045600	-4.31312000
				H	1.47019400	2.15115400	-4.74226900
				H	5.35824300	2.80810000	-3.19381800
37-TS-b				H	6.02022900	4.24382300	-4.25607200
C	2.96156200	4.80356300	-3.17903200	H	5.80271500	5.22901300	-2.80327200
C	2.76160900	5.82450900	-2.22811800	K	2.46411500	3.26067300	0.11439400
C	1.56440000	5.81967800	-1.49448600	C	5.18347900	4.03724000	1.09297900
C	0.58726900	4.84129300	-1.70403900	O	5.04022100	2.83623000	0.38898700
C	0.80017300	3.84464800	-2.66559500	O	4.20517100	4.84218800	1.04809300
C	1.98588900	3.81112000	-3.41272500	O	6.26769700	4.19782500	1.72250200
H	1.39175900	6.61007300	-0.76826200	K	7.49824400	2.27383600	0.71291700
H	-0.34643000	4.87500100	-1.14915300				
H	0.03249700	3.09779800	-2.85489100				
O	4.06573200	4.76703700	-3.98515700	37-TS-d			
C	5.35971100	4.47159800	-3.42984400	C	3.80982500	6.18376400	-2.69473300
Pd	5.57931200	3.53942100	-1.54314000	C	4.35845100	7.48546100	-2.72428500
C	3.79637100	6.89952300	-2.01881900	C	3.87458300	8.43729800	-1.81559200
H	3.35407100	7.78358200	-1.55192600	C	2.85541100	8.11471800	-0.91304300
H	4.60484100	6.54289400	-1.37037900	C	2.31312700	6.82753000	-0.91612800
H	4.24471900	7.19329900	-2.97205600	C	2.77904900	5.83850600	-1.79728500
C	2.24494100	2.75407300	-4.45587200	H	4.27729800	9.44727400	-1.84274800
H	2.38724100	3.20821000	-5.44124900	H	2.47193500	8.86900700	-0.23095100
H	3.16526900	2.20396600	-4.23298900	H	1.51534800	6.57168300	-0.22317700
H	1.41511700	2.04431600	-4.51534700	O	4.22769700	5.26084200	-3.62623300
H	5.14666500	2.91872800	-2.89777500	C	5.48804600	4.61043200	-3.40015600
I	5.90092200	3.24156800	1.17468100	Pd	5.58489300	3.57384800	-1.55955100
H	5.94958200	4.11387200	-4.27454400	C	5.41162600	7.85614300	-3.74193500
H	5.83233400	5.38710500	-3.04447400	H	5.37563900	8.92643500	-3.96496200
K	2.79470500	2.86172000	-0.16571800	H	6.42440400	7.62874300	-3.38746000
				H	5.26228300	7.29661600	-4.66850000
				C	2.20702300	4.44559800	-1.73845000
37-TS-c				H	2.50565900	3.85833000	-2.60667600
C	2.96878900	4.84657900	-3.23709600	H	2.57701300	3.94590700	-0.83526400
C	2.73253600	5.83847000	-2.26625800	H	1.11281100	4.48190900	-1.68662600
C	1.46672700	5.87012300	-1.65737800	H	5.35846100	3.05272300	-2.99367700
C	0.47449200	4.94355900	-1.98791400	H	5.76394200	4.21456500	-4.37856800
C	0.74304500	3.95012000	-2.93769400	H	6.26657000	5.33266900	-3.11724800
C	1.98856200	3.89037900	-3.57382200	K	5.23025900	6.19545800	0.66131700
H	1.26513600	6.64159700	-0.91838100				

C	4.74524000	3.29578200	1.39334600	H	1.90286200	1.05958200	-5.20242500
O	5.77368800	3.48612500	0.56309100	H	2.83415500	0.21792500	-7.34759500
O	3.75316400	4.11087600	1.36658200	H	4.79708200	1.35798600	-8.37442200
I	6.55697400	5.60246900	4.04588400	O	4.94875500	4.47013400	-5.11260900
K	7.45388600	2.54624600	2.26277600	C	5.70428200	4.46099800	-3.89219500
O	4.85295000	2.36574400	2.27302200	Pd	6.48647200	2.66156200	-3.15116200
K	3.45230900	3.77868200	3.92833900	C	2.75980300	3.14074700	-3.68485100

37-TS-e

C	3.24352200	4.24123600	-4.25008900	H	1.70805900	2.85715200	-3.58123900
C	2.78727000	5.26576800	-3.39656800	H	3.31744100	2.67446200	-2.86304500
C	1.48287700	5.16170800	-2.88529500	H	2.83778200	4.22664500	-3.58892800
C	0.66352600	4.07654800	-3.20719800	C	6.14389300	3.55844200	-7.42152100
C	1.13960500	3.07581900	-4.06145500	H	6.47518100	3.07328500	-8.34392300
C	2.43058700	3.14494000	-4.60130100	H	5.89445500	4.60070200	-7.64397600
H	1.10923300	5.95164500	-2.23801500	H	6.98098400	3.58090100	-6.71569800
H	-0.34683100	4.02070700	-2.81114200	C	8.11658200	1.80892100	-0.03413600
H	0.50078700	2.23683300	-4.32531300	H	8.23060300	2.73435600	-0.62740700
O	4.48401500	4.32832000	-4.84171900	H	7.02768600	3.61508000	-4.24639500
C	5.61991100	4.06373800	-4.01932000	K	8.17389800	-1.24254200	-1.04534300
Pd	5.86897400	2.12708300	-3.16401400	H	6.29356600	5.37913700	-3.92685200
C	3.66971800	6.43113400	-3.02084000	H	5.03553100	4.52693100	-3.01915000
H	3.06504600	7.31611500	-2.80112400	C	5.62396200	0.29861500	-1.48144100
H	4.26077100	6.19304000	-2.12702800	O	6.73111800	0.85778300	-1.97334800
H	4.35993100	6.67219000	-3.83345500	O	5.73410100	-0.37608600	-0.39528900
C	2.95618700	2.09786500	-5.54887600	I	6.10878900	-3.30886000	-3.23637500
H	3.24958000	2.55158300	-6.50096900	K	3.70644500	-1.84495200	-1.03851800
H	3.85165700	1.61826800	-5.13981300	O	4.52322200	0.38710300	-2.13896200
H	2.20317200	1.32922300	-5.74319400	K	5.56487500	-0.02416400	-4.59137800
H	6.17118000	2.57586400	-4.61168800				

38-TS-a

I	5.88734800	0.24429800	-1.11731600	Pd	3.01290800	-0.69484600	-2.00563000
H	6.46063400	4.53458700	-4.53104400	C	3.20995900	2.52709400	-3.44126300
H	5.49762400	4.51257800	-3.02648800	C	1.90425600	2.18897400	-3.85023800
K	3.13547400	2.98825300	-1.02372900	C	0.85310000	3.03118400	-3.45605400
C	5.43839300	3.93832300	0.54033100	C	1.08618500	4.20219200	-2.73090000
O	6.62618800	3.81446000	1.06641300	C	2.40066600	4.54947900	-2.39045100
O	4.40542200	3.44737400	1.15961100	C	3.47498800	3.72113400	-2.73335900
K	5.88125900	1.72768100	2.31652200	H	-0.15811300	2.78280600	-3.76958100
O	5.30269800	4.46908800	-0.64101700	H	0.26094600	4.86680800	-2.48542700
K	7.78402000	3.91116800	-1.19134000	H	2.60142500	5.48292600	-1.86850600
				O	4.31695500	1.80415000	-3.79053500
				C	4.45450400	0.40878200	-3.48554800
				H	3.92717400	-0.21218700	-4.21006700
				H	5.51921700	0.19297000	-3.62797700
				C	1.62693500	1.00244200	-4.74257400
				H	2.41823200	0.86081800	-5.48456000
				H	1.54957700	0.07668600	-4.15854100

37-TS-f

C	4.41351700	3.30735600	-5.60971200
C	3.31346800	2.66952200	-5.00416100
C	2.76282900	1.55127500	-5.65102000
C	3.28741800	1.07404900	-6.85521500
C	4.38803300	1.71789500	-7.43335200
C	4.96274300	2.83936600	-6.82181700

H	0.68120000	1.14112200	-5.27515600	O	4.88172500	2.26554200	0.74087800
C	4.89628100	4.07677700	-2.38019200	K	2.22112300	3.19957300	0.26810800
H	5.34820400	3.30509100	-1.75249400	C	5.79343100	-1.68128200	1.51367600
H	5.50777100	4.15585000	-3.28504800	O	6.96554200	-1.63607800	0.95448000
H	4.93791600	5.02967300	-1.84523800	O	5.45904500	-0.80159700	2.41534300
H	4.70982400	0.41634300	-2.14123400	K	5.91027000	-2.59358100	-1.20556800
C	4.16311900	1.37444200	-0.38792700	I	2.72505900	-2.46705700	-3.43434800
O	2.97577000	0.89044200	-0.75361400	K	7.16167800	0.88346700	1.50418700
O	5.21164000	0.83892400	-0.97646700	O	4.91310900	-2.55483100	1.10878500
O	4.20482900	2.28968800	0.45543700	K	2.95890400	-1.18375000	1.94031900
K	1.51740900	2.65181700	0.19778400	I	0.50971300	-0.53497800	-0.67230900
K	5.40128500	-1.81502400	-0.38190100				
C	4.26339200	-2.90108300	-3.45606900	38-TS-c			
O	3.08637300	-2.31710500	-3.22490400	Pd	2.98085400	-0.72743800	-1.94479500
O	4.27234500	-3.81921700	-4.33793200	C	2.67294500	1.90805900	-3.90408700
I	4.01366500	-1.21475800	-7.50636200	C	1.63280600	1.25156300	-4.59858200
K	1.96057800	-3.06653300	-5.43731300	C	0.33305500	1.77040900	-4.50130800
O	5.32161600	-2.48003000	-2.86088100	C	0.06728500	2.92409400	-3.75608300
K	6.34300200	-2.58111100	-5.38057600	C	1.11588100	3.56945900	-3.09389000
I	1.26802600	-1.94586700	-0.35012300	C	2.42636100	3.07568400	-3.15125400
				H	-0.46861500	1.28427500	-5.05305900
38-TS-b				H	-0.93856200	3.33594900	-3.72493200
Pd	2.98064000	-0.31373800	-1.81772400	H	0.92369900	4.47842400	-2.52750500
C	4.01714700	2.86616000	-3.10889600	O	3.97741000	1.49988400	-4.01846100
C	2.67469600	2.89253600	-3.54655900	C	4.38914300	0.22345300	-3.49920700
C	1.87843800	3.98148900	-3.15571100	H	4.05583700	-0.60009000	-4.13041900
C	2.39623600	5.03544000	-2.39785500	H	5.48223900	0.22561600	-3.58336700
C	3.74477300	5.01203600	-2.01973100	C	1.90939400	0.04542000	-5.46031300
C	4.57011600	3.93540300	-2.36533300	H	2.84059600	0.14607400	-6.02358500
H	0.84621600	4.01643700	-3.49475200	H	2.01399100	-0.85230200	-4.84025600
H	1.77090700	5.89023900	-2.15141000	H	1.09662900	-0.11984500	-6.17384500
H	4.17127900	5.84577500	-1.46651000	C	3.53513200	3.78042800	-2.41099200
O	4.91377400	1.89840500	-3.46978900	H	3.36428600	3.73645200	-1.33064000
C	4.67265200	0.49413900	-3.28094900	H	4.49900000	3.31437200	-2.60986400
H	3.95820000	0.11633900	-4.00635000	H	3.58626700	4.83522800	-2.70335700
H	5.62959300	0.01637800	-3.52153600	H	4.59967600	0.36692000	-2.18375700
C	2.10414400	1.85100200	-4.47863500	C	4.05267600	1.35262300	-0.36109200
H	2.83291600	1.57370000	-5.24584900	O	2.85332000	1.01943300	-0.84671900
H	1.81196500	0.93587900	-3.95207000	O	5.09019300	0.85763100	-0.98397000
H	1.21374800	2.23838100	-4.98072600	O	4.12387200	2.07482400	0.65785500
C	6.03124700	3.91135800	-1.99658400	K	0.22251000	0.80227100	-1.10890000
H	6.29090800	2.96627600	-1.51669200	K	5.17548100	-1.78627000	0.00795100
H	6.65255700	3.99965300	-2.89512600	C	4.26818300	-3.11986400	-3.00208400
H	6.27618400	4.73754500	-1.32359200	O	3.08246800	-2.50813700	-2.94298400
H	4.90814400	0.39189700	-1.93769100	O	4.32599000	-4.19177800	-3.69045900
C	4.63206500	1.38314700	-0.12064400	I	4.52315500	-2.43112200	-7.40057400
O	3.36273700	1.05964200	-0.33354900	K	2.22999000	-3.71059600	-5.15284200
O	5.54276600	0.78277200	-0.83117200	O	5.29566000	-2.58763200	-2.44695300

K	6.54364300	-3.18240900	-4.72984800	C	-3.46513100	1.53914900	-1.14330200
C	1.75567900	-1.09872000	0.60196600	C	-4.65211200	1.46855900	-0.42273700
O	2.87852500	-1.34126700	1.16487500	C	-4.77132700	0.55405400	0.62608600
O	1.54555700	-1.47048900	-0.67409200	C	-3.71262000	-0.29378600	0.95156800
O	0.80745200	-0.45835400	1.17743600	H	-3.36499300	2.26543400	-1.94529800
K	2.62041500	0.96336400	2.44082900	H	-5.48097900	2.12375300	-0.67402500
39				H	-5.69577100	0.48943800	1.19444800
Pd	1.45798400	-0.16215700	-0.48060900	O	-1.52000000	-1.04677900	0.65404700
C	-2.58750400	0.26009600	0.05055300	C	-0.54365500	-1.55474900	-0.25281800
C	-2.96816900	1.16624200	-0.95248100	H	-0.03273400	-2.36010300	0.27864300
C	-4.34047400	1.33409600	-1.18523400	H	-1.03243600	-1.92460800	-1.16342700
C	-5.29079600	0.62895200	-0.44847500	C	-1.07143900	0.92334700	-1.58940600
C	-4.88266800	-0.26124000	0.54656600	H	-1.12984900	1.79973800	-2.24316800
C	-3.52399500	-0.45928400	0.81075100	H	-0.79492300	0.10355000	-2.26572300
H	-4.66012800	2.03324800	-1.95425600	C	-3.81162900	-1.28729600	2.08366200
H	-6.34907000	0.77459100	-0.64605600	H	-3.58771600	-2.30264900	1.74080800
H	-5.62240300	-0.81130900	1.12323100	H	-3.08800700	-1.06994200	2.88009800
O	-1.24714200	0.10262800	0.36929700	H	-4.81184200	-1.27856700	2.52543800
C	-0.46327700	-0.74911000	-0.51827600	H	-0.34395400	1.57346700	-0.75729200
H	-0.52448000	-1.78336800	-0.16042500	C	1.39458500	2.45180900	0.29940000
H	-0.85398800	-0.65977400	-1.53876500	O	2.02290500	1.77249300	-0.64075700
C	-1.93859000	1.92611700	-1.75417000	O	0.08805600	2.55460100	0.21815200
H	-2.33226900	2.89823600	-2.06685400	O	2.01401400	2.88847200	1.32086200
H	-1.67006700	1.37844500	-2.66613900	K	-0.05988700	1.13366600	2.40636000
C	-3.04694100	-1.39969900	1.89089500	C	2.17152300	-1.55252600	1.55834600
H	-2.30140300	-2.10337000	1.50878600	O	2.30281500	-1.24543200	0.26909700
H	-2.56494500	-0.85312400	2.71159000	O	2.37958800	-2.77010200	1.89912800
H	-3.87981600	-1.97013900	2.31162700	K	3.99297300	1.18050800	0.94614800
H	-1.00901300	2.07895000	-1.20202000	I	6.21310200	-1.58464700	2.00247400
C	2.51162000	2.01231800	-0.01086200	K	3.91127800	-3.22208900	-0.18661000
O	3.32930200	1.05084000	-0.37304500	O	1.93728600	-0.62604600	2.42249100
O	1.31061200	1.96725400	-0.57352500	K	3.44919100	-2.01145400	4.12929400
O	2.77811300	2.81904700	0.92886500	40-TS-a			
K	0.35505000	1.55422000	1.93541000	Pd	0.99545300	-0.11240100	-0.56889500
C	1.92140300	-1.85483000	1.84533000	C	-2.38141600	-0.26901000	0.03202600
O	1.92257000	-1.93395500	0.52498800	C	-2.19730700	0.55906800	-1.09576400
O	2.06512600	-2.96524900	2.47604300	C	-3.30638200	1.32014300	-1.50625300
K	4.55711500	0.92505300	1.83992600	C	-4.52700700	1.26420000	-0.84296900
I	5.94929000	-2.04377700	3.18119900	C	-4.67182500	0.44011300	0.27522000
K	3.84529300	-3.66955500	0.66448400	C	-3.60313700	-0.33288000	0.73011700
O	1.86206800	-0.71802100	2.46689900	H	-3.18985000	1.97630900	-2.36465000
K	2.77207600	-1.97549600	4.68428000	H	-5.36408100	1.86060000	-1.19361000
40-TS				H	-5.62370400	0.38754600	0.79713100
Pd	0.78803000	-0.09089700	-0.64358000	O	-1.36843500	-1.01667500	0.60971400
C	-2.52436300	-0.21475100	0.19691900	C	-0.34680300	-1.58321600	-0.19157100
C	-2.36749500	0.70626100	-0.86220000	H	0.10175100	-2.37979200	0.39848200
				H	-0.75477000	-1.96090000	-1.13642400

C	-0.86312800	0.77214700	-1.74679100	K	3.88540600	1.37932000	1.34750900
H	-0.91332100	1.58829700	-2.47650400	I	2.66301100	-1.79379700	0.55150900
H	-0.50273300	-0.08973000	-2.32290700	O	1.64598200	2.79331900	1.51786100
C	-3.73098400	-1.22978700	1.93757600	K	-0.97815900	2.35166500	2.21808700
H	-3.45940200	-2.26232100	1.69569400				
H	-3.05902200	-0.92148400	2.74889900				
H	-4.75273800	-1.21856300	2.32599300	40-TS-c			
H	-0.26199700	1.53529900	-0.85985400	Pd	0.80069200	-0.08967300	-0.67163300
C	1.32563900	2.53286200	0.20719800	C	-2.54294500	-0.17515300	0.15996500
O	2.03685800	1.92432900	-0.71589900	C	-2.38788600	0.67534500	-0.95436300
O	0.01264700	2.51635500	0.06666300	C	-3.50831100	1.43431200	-1.33375100
O	1.84963000	3.02755000	1.24604400	C	-4.71759700	1.35552600	-0.65126100
K	-0.06020800	1.31112600	2.37703200	C	-4.83533000	0.51043600	0.45426900
C	5.25321600	1.53198700	-2.04075600	C	-3.75244100	-0.26138000	0.87671900
O	5.89416800	0.93627400	-1.07691200	H	-3.40964300	2.10804300	-2.18066000
O	4.73593700	0.81665300	-3.01454500	H	-5.56516600	1.95237200	-0.97540700
K	4.48417800	2.45043000	0.57247300	H	-5.77682300	0.44196500	0.99340700
I	2.80913700	-1.21080200	1.16560600	O	-1.51412200	-0.92410000	0.70101600
K	5.07218500	-1.34626100	-1.73018300	C	-0.53906800	-1.51989100	-0.15277700
O	5.03790400	2.80689500	-1.99044700	H	-0.04674300	-2.26720500	0.47638200
K	2.80390400	2.51304700	-3.16709800	H	-1.03670700	-1.97735100	-1.02013600
				C	-1.07200600	0.88791600	-1.64415000
				H	-1.11238100	1.74582400	-2.32289300
40-TS-b				H	-0.77406700	0.04734200	-2.28754200
Pd	0.80291200	-0.20813500	-0.72203600	C	-3.84784100	-1.17615800	2.07340000
C	-2.38743700	-0.33985500	0.18476600	H	-3.56327500	-2.20113400	1.81417700
C	-2.25622600	0.74371300	-0.71961700	H	-3.16662600	-0.86706700	2.87614600
C	-3.16429000	1.81344400	-0.56318100	H	-4.86339900	-1.18610700	2.47850500
C	-4.13420000	1.83340800	0.43512100	H	-0.37974800	1.54150900	-0.78800000
C	-4.22840700	0.75431700	1.32489300	C	1.34726600	2.47495100	0.23479800
C	-3.36692400	-0.33840600	1.20890400	O	1.97828600	1.80993400	-0.71696400
H	-3.07521300	2.65743500	-1.24179700	O	0.03553600	2.51615200	0.19612400
H	-4.82192300	2.67096600	0.51243800	O	1.97976500	2.95473700	1.22708100
H	-4.98961300	0.74792000	2.10124300	K	0.01427700	1.16606600	2.47668800
O	-1.56457600	-1.42556900	0.24501600	C	2.13868200	-1.46114700	1.52690700
C	-0.55840600	-1.71232000	-0.70767900	O	2.40348900	-1.15980200	0.20607200
H	-0.10929700	-2.64649500	-0.37860900	O	2.02636100	-2.68923100	1.81369600
H	-0.98361600	-1.81392400	-1.71298900	K	3.82686500	1.10729200	0.97238300
C	-1.10061700	0.91758500	-1.65317100	K	2.36577300	-3.59277500	-0.51484900
H	-1.23936000	1.80820400	-2.27669500	O	2.04886800	-0.48761900	2.34012900
H	-0.92329900	0.11117800	-2.36291800				
C	-3.44637400	-1.51378700	2.15175900	40-TS-d			
H	-3.65886700	-2.43918600	1.60621900	Pd	0.95865300	-0.01454800	-0.65019600
H	-2.49239400	-1.68033500	2.66445500	C	-2.38459500	-0.44313600	-0.12724700
H	-4.22916000	-1.36461100	2.90082200	C	-2.23568600	0.46254000	-1.19973000
H	-0.26951500	1.64827700	-0.91497400	C	-3.37755200	1.19912600	-1.56438800
C	1.28675600	2.39422000	0.35372900	C	-4.59447900	1.04793900	-0.90997300
O	2.06132400	1.67646300	-0.40057600	C	-4.70449000	0.14722200	0.15195000
O	0.06361800	2.64349600	-0.06100500	C	-3.60395400	-0.60657700	0.56043900

H	-3.28953900	1.91265000	-2.37897300	C	1.16179000	2.64904600	0.15476600
H	-5.45634900	1.62863900	-1.22463800	O	1.73008700	1.97778000	-0.76326600
H	-5.65408200	0.01851400	0.66456200	O	-0.12984100	3.08576200	-0.09046500
O	-1.33935400	-1.17309700	0.41744300	O	1.59401900	2.91464100	1.29781000
C	-0.26173200	-1.61139000	-0.38595200	K	-0.47007600	0.99758600	2.03377800
H	0.24651500	-2.39305900	0.17476400	C	1.97567400	-1.36652100	1.62316000
H	-0.61328200	-1.97131900	-1.35907500	O	2.30601700	-0.94039400	0.41754300
C	-0.91659800	0.77276400	-1.84299400	O	2.06596700	-2.62033300	1.88820800
H	-1.01353200	1.61492500	-2.53717400	K	3.68386000	1.26006200	1.13128900
H	-0.51468100	-0.04157400	-2.45696500	I	5.89829300	-1.44741400	2.40469000
C	-3.69579800	-1.58813800	1.70396000	K	3.76637700	-3.02960000	-0.04573900
H	-3.38906500	-2.59120400	1.39078200	O	1.64645300	-0.50417700	2.53339500
H	-3.03282000	-1.31518000	2.53501800	K	2.93556300	-2.02595600	4.26004800
H	-4.71631000	-1.64026600	2.09191800				
H	-0.34270300	1.56811100	-0.95541500	42-TS			
C	1.15009500	2.61553900	0.22189500	C	-0.65631600	0.76472400	0.59184500
O	1.96823600	2.06613700	-0.65025900	C	-0.33908200	1.30597600	-0.65700900
O	-0.13965500	2.54708900	-0.01963600	C	-0.52623000	2.67686900	-0.85609800
O	1.56531900	3.09306900	1.31960800	C	-1.03308400	3.46357300	0.18649100
K	-0.39171700	1.23205900	2.22565100	C	-1.28267400	2.89436700	1.44539100
K	4.13821500	2.60294400	1.16403300	C	-1.07568500	1.52924800	1.68740500
I	2.93070800	-1.03713200	0.89710600	H	-0.29908000	3.11925900	-1.82209000
K	3.51552000	1.28600300	-2.52507000	H	-1.25199900	4.51522800	0.01567600
I	6.33352900	2.76364100	-1.46692600	H	-1.66401800	3.51468100	2.25353000
				O	-0.52234000	-0.59691600	0.69310500
41				C	-0.43852200	-1.17194600	-0.61587500
Pd	0.62884800	-0.14338000	-0.82063100	H	-0.18917100	-2.24011100	-0.47916400
C	-2.45207400	-0.49792600	0.10311100	H	-1.41553500	-1.12944300	-1.10478700
C	-2.21774800	0.49143500	-0.88683700	C	0.20605500	0.32903700	-1.66076300
C	-3.06097100	1.62054800	-0.86187400	H	1.22102000	0.65980000	-1.96970900
C	-4.08882600	1.76454300	0.06411200	H	-0.40718200	0.23028100	-2.55724500
C	-4.31326000	0.75619800	1.00766300	C	-1.27127500	0.89266700	3.03821900
C	-3.50575700	-0.38255000	1.03951500	H	-1.83033700	-0.04495000	2.95256300
H	-2.89265400	2.40049000	-1.60088800	H	-0.29897700	0.66075600	3.49254600
H	-4.71958100	2.64855500	0.04681000	H	-1.81226200	1.55988400	3.71488900
H	-5.12396900	0.84990500	1.72633100	Pd	1.59883800	-1.36796000	-1.34996100
O	-1.62810200	-1.56206800	0.32693000	C	2.54415300	1.16052700	2.94173300
C	-0.48358400	-1.81128200	-0.50879700	O	2.83441700	2.35718100	3.24266500
H	0.11388800	-2.52713900	0.06157400	O	2.65499500	0.80598700	1.60061000
H	-0.81752600	-2.25621900	-1.45335400	O	2.15696800	0.24070500	3.69595900
C	-1.07504300	0.40454500	-1.84556900	K	1.86677000	-1.68937000	1.95195400
H	-0.92728300	1.36065100	-2.36638800	C	4.62401800	3.14968900	0.77707700
H	-1.23294800	-0.35521000	-2.61791100	O	5.64456600	2.39243200	1.01131600
C	-3.70441500	-1.47133300	2.06604500	O	3.61865000	2.65257500	0.05871600
H	-3.88212500	-2.43909800	1.58522200	K	5.34662500	3.13768400	3.48214000
H	-2.81185700	-1.60985600	2.68947200	I	3.89325300	-2.84021300	-1.04429500
H	-4.55203500	-1.24498500	2.71934000	K	4.94429800	0.52304900	-0.66600600
H	-0.36567500	2.76806800	-0.97476500	O	4.51041600	4.31797900	1.29507600

K	1.89442400	4.07412600	1.35261200	H	-2.55354400	-0.82181300	3.22632100
H	3.01558900	1.56507400	1.02325300	H	-4.23896600	-0.31739800	3.07021900
				H	-0.84929900	2.34402200	1.34880400
42-TS-a				C	1.05678000	2.24911800	1.15322900
C	2.85802600	0.51563000	0.00631200	O	0.96467400	2.92707700	0.10637800
C	3.07183400	-0.77613400	-0.49331800	O	-0.11263700	1.96997400	1.85916700
C	4.15886500	-1.50840500	-0.00382000	K	3.34336800	1.94960500	-0.63924400
C	5.01532300	-0.93536000	0.94118200	I	3.79617200	-1.55020600	-0.49764100
C	4.78776700	0.36863400	1.40127500	O	2.08253900	1.70868700	1.65590800
C	3.70219800	1.12898400	0.94520500	K	0.98376800	-0.62720600	2.14219900
H	4.32842500	-2.52040800	-0.36086200				
H	5.86668500	-1.49707400	1.31327700	42-TS-c			
H	5.46594000	0.80909200	2.12801100	Pd	1.10031200	1.22806500	-0.33053400
O	1.69160700	1.11869900	-0.35817800	C	-2.32747700	0.32256700	-0.94358400
C	0.96523800	0.36546400	-1.33793300	C	-2.12779000	1.47975200	-0.18320400
H	-0.10123900	0.60852800	-1.18054600	C	-3.03025600	1.76353200	0.84604400
H	1.24265900	0.69293000	-2.33996900	C	-4.11511900	0.91169700	1.07115600
C	2.00995400	-1.26084200	-1.42717700	C	-4.29607900	-0.22830400	0.27800500
H	1.78698200	-2.33380100	-1.24761300	C	-3.40448300	-0.55474600	-0.75206900
H	2.26289600	-1.16973400	-2.48365700	H	-2.88249700	2.64494200	1.46382000
C	3.41237600	2.52690700	1.42990800	H	-4.82570700	1.13603000	1.86072200
H	3.48910100	3.24927800	0.61000400	H	-5.14774200	-0.87968700	0.45780100
H	2.39036900	2.61693900	1.81714100	O	-1.33097000	0.01181000	-1.82566000
H	4.11005800	2.82583500	2.21656800	C	-0.39204600	1.08718200	-1.96052300
Pd	-0.02055700	-1.45390200	-0.51839000	H	0.55087600	0.62259300	-2.30735300
I	-1.65942400	-2.56089900	1.36976900	H	-0.72714700	1.77749600	-2.73574900
K	1.22792300	-0.91210800	2.29804100	C	-0.87495800	2.22900900	-0.52015800
				H	-0.35552000	2.54089100	0.41541100
42-TS-b				H	-1.03884500	3.13817000	-1.09946200
Pd	1.17048900	-1.10044900	-1.05439800	C	-3.55740500	-1.77755100	-1.62063400
C	-2.11295000	-0.18452800	0.39109700	H	-3.69698300	-1.49783700	-2.67052500
C	-1.69457900	0.63202300	-0.66029900	H	-2.66278100	-2.41177800	-1.59335900
C	-2.18117900	1.94074100	-0.72072100	H	-4.41460500	-2.37963800	-1.30823900
C	-3.08904400	2.38505400	0.24522700	H	4.69543000	-0.03766200	1.67751400
C	-3.49165400	1.53431700	1.28305900	C	2.88897200	-0.48191100	1.44350200
C	-3.00417900	0.22712400	1.38737900	O	2.85558100	0.54142600	0.68281300
H	-1.83742000	2.60826400	-1.50397700	O	4.11130500	-0.73596700	2.00703300
H	-3.48226900	3.39565100	0.19398800	O	1.96831800	-1.27019300	1.73614700
H	-4.19385700	1.89303000	2.03108100	K	-0.38241500	-1.25003900	0.96178000
O	-1.51867100	-1.42298200	0.44957000				
C	-0.91169800	-1.73704700	-0.80388400	42-TS-d			
H	-0.28674500	-2.63166100	-0.63197200	C	-2.06587400	-0.16334300	0.43198000
H	-1.67637500	-1.99667800	-1.53937300	C	-1.57236900	0.70041300	-0.54415500
C	-0.66862300	0.03223400	-1.57335200	C	-1.99686100	2.03157900	-0.53633100
H	0.19020200	0.73246000	-1.63752900	C	-2.92065600	2.45209800	0.42563500
H	-1.02823200	-0.15853000	-2.58497700	C	-3.39529900	1.55592000	1.39147300
C	-3.38028100	-0.70094000	2.51308300	C	-2.97114200	0.22282300	1.42452900
H	-3.62202000	-1.70023000	2.13818500	H	-1.59531300	2.73133200	-1.26225200

H	-3.26624600	3.48123700	0.43013700	H	-2.98062000	-1.77619500	-2.40904200
H	-4.10533300	1.89830800	2.13978200	H	-2.38768500	-2.52471200	-0.93645100
O	-1.53817300	-1.43282500	0.40394600	H	-4.13002800	-2.43588000	-1.22458400
C	-0.92233800	-1.66825200	-0.86476900	C	3.48810200	-0.11466300	0.00496900
H	-0.36413200	-2.61994900	-0.75785500	O	2.66489500	0.64490000	0.82845300
H	-1.68656300	-1.81814200	-1.63202600	O	4.68102700	0.29546800	-0.12928000
C	-0.53181500	0.10878100	-1.44888100	O	2.99817100	-1.16205500	-0.51152300
H	0.37577100	0.74210600	-1.36674400	K	0.75496800	-1.37057000	0.52784200
H	-0.83274000	0.06181400	-2.49623800	K	4.39844600	2.45771700	1.04253900
C	-3.42559400	-0.75785000	2.47366900				
H	-3.70051000	-1.71789500	2.02564300	42-TS-f			
H	-2.62669600	-0.96260900	3.19910300	C	-2.00413000	-0.13688000	0.34025900
H	-4.28348200	-0.37127900	3.03020700	C	-1.72256500	0.57986900	-0.82240200
Pd	1.20363900	-1.22009200	-1.02910100	C	-2.28905500	1.84717200	-0.97916300
H	-0.61705000	2.15030500	1.49266800	C	-3.14385900	2.34641000	0.00835800
C	1.28678700	1.93250500	1.53909900	C	-3.41054300	1.59484100	1.15798600
O	1.35031300	2.51004700	0.43098700	C	-2.83581000	0.33472300	1.35881600
O	0.02087100	1.75415500	2.10733500	H	-2.05892200	2.43712800	-1.86138600
O	2.21115000	1.39958400	2.21216500	H	-3.59795200	3.32493700	-0.11321500
K	1.02641300	-0.98272900	2.23328800	H	-4.06663000	1.99859200	1.92462300
C	3.76007200	-2.21111200	0.30031000	O	-1.33659700	-1.33393900	0.46305200
O	3.27143200	-1.70844800	-0.82504600	C	-0.81480200	-1.73154800	-0.80516600
O	4.65546000	-3.12787200	0.21395700	H	-0.11271700	-2.56012800	-0.59754800
K	3.67970000	1.09057600	0.01733000	H	-1.61684400	-2.12604600	-1.43432200
I	7.17028600	-0.03092400	-0.41391900	C	-0.74620200	-0.07596100	-1.75341400
K	5.31655100	-2.48555600	-2.21061600	H	0.08011000	0.64065200	-1.96184900
O	3.41232600	-1.70641000	1.43542100	H	-1.18050800	-0.37628400	-2.70801900
K	5.91007300	-2.04937100	2.22068900	C	-3.04171100	-0.46231900	2.62002500
				H	-3.10601400	-1.53372200	2.40878800
42-TS-e				H	-2.20449600	-0.31327400	3.31564300
Pd	1.00269900	1.63266900	-0.06993800	H	-3.95185100	-0.15155200	3.14039000
C	-2.21889900	0.38105600	-0.82494500	Pd	1.20431700	-0.99342600	-1.25964600
C	-2.20413700	1.63874400	-0.21433400	C	1.26056800	2.13589200	1.27105800
C	-3.26761800	1.98029900	0.62436100	O	1.44350900	2.58607500	0.11807700
C	-4.31919100	1.08054700	0.81455500	O	-0.06028900	1.96833500	1.70021900
C	-4.30328800	-0.16772800	0.18342200	O	2.11055400	1.72682700	2.10842500
C	-3.24657800	-0.55222500	-0.65060700	K	1.14705100	-0.73238900	2.28153000
H	-3.27285900	2.94740400	1.11982800	C	3.52378500	-1.97942600	0.15770900
H	-5.15503400	1.35055100	1.45300500	O	3.31516000	-1.26345600	-1.00052700
H	-5.12844000	-0.85920700	0.33525000	O	3.81735200	-3.20530600	0.04532600
O	-1.11300700	0.06598500	-1.57359000	K	3.79414500	1.12721700	0.13460600
C	-0.31591200	1.22919200	-1.81488800	K	3.32913200	-3.37340300	-2.40803000
H	0.67758800	0.87046700	-2.12456800	O	3.41870000	-1.33877000	1.25668700
H	-0.73928600	1.80525500	-2.64114000	H	-0.62638500	2.26375200	0.97056400
C	-0.98143700	2.46013600	-0.49711600				
H	-0.56152500	2.85986600	0.46238100	42-TS-g			
H	-1.15288700	3.31879100	-1.14773300	C	-1.76066300	-0.05495400	0.45849900
C	-3.18905400	-1.89145100	-1.34052600	C	-1.69957100	0.53273900	-0.80861000

C	-2.26830500	1.79707000	-0.98028000	H	-3.50443100	-0.19632200	3.46669500
C	-2.89674200	2.42849800	0.09572600	Pd	0.98901800	-0.83896400	-1.28939800
C	-2.94471300	1.80817300	1.34868300	C	1.67295300	0.36692300	3.35326200
C	-2.37108500	0.54917800	1.56429900	O	0.41998000	0.26182500	3.01442900
H	-2.22215800	2.28020500	-1.95248300	O	2.33263400	-0.69245300	3.72567300
H	-3.35360100	3.40420500	-0.03961400	K	0.66986400	2.13447900	1.28834400
H	-3.44058400	2.30624800	2.17823600	I	3.55683000	-0.47958300	-0.42972300
O	-1.10227600	-1.25050600	0.59517900	K	0.81366800	-2.13991000	2.20606800
C	-0.73034300	-1.78259000	-0.68090500	O	2.28488500	1.50845400	3.21869200
H	0.07337500	-2.51118200	-0.48944700	K	4.53654500	0.34700500	2.97039200
H	-1.57577000	-2.31553500	-1.12085300				
C	-0.95158700	-0.26448900	-1.83459600	43			
H	-0.24064500	0.40327000	-2.38471300	Pd	0.82960100	0.07092200	0.68211000
H	-1.58516800	-0.73346500	-2.58862200	C	2.63199200	2.24909600	-0.01018800
C	-2.39602300	-0.14640500	2.90214600	C	1.27384700	1.90965400	0.09928400
H	-2.74498000	-1.17921500	2.80252600	C	0.32517600	2.85072800	-0.32439100
H	-1.39779500	-0.20011000	3.35732500	C	0.72468300	4.06137000	-0.89841000
H	-3.04877400	0.37751100	3.60548600	C	2.08208300	4.36917100	-1.01898900
Pd	1.14199900	-0.85282700	-1.47686500	C	3.04079800	3.45950700	-0.57037100
K	1.53072400	0.10267700	1.43712900	H	-0.73161700	2.63790000	-0.19449800
C	3.83593200	-1.46360900	-0.07970500	H	-0.02607400	4.77176600	-1.23321800
O	3.25426200	-0.77657800	-1.04734500	H	2.39424000	5.31645000	-1.44859500
O	5.12316100	-1.57522700	-0.12966200	H	4.10366200	3.67537800	-0.64047400
I	4.67689600	1.69128100	2.30106600	O	3.61722900	1.36455200	0.46308800
K	5.28157600	0.78483600	-1.19741800	C	4.16034200	0.51279600	-0.55698000
O	3.15487400	-1.90653100	0.91983100	H	3.38579200	-0.14251500	-0.97446900
K	5.29847400	-1.86448100	2.39894200	H	4.60620000	1.10720000	-1.36281600
				H	4.93041800	-0.10473300	-0.08813100
42-TS-h				C	1.63629900	-2.56723700	1.55946100
C	-2.00841000	-0.19129100	0.39806100	O	0.60087500	-2.02994600	1.03922600
C	-1.80915300	0.58884900	-0.74770100	O	2.69545600	-1.95203100	1.85856600
C	-2.25228100	1.91730100	-0.74157600	C	1.53801900	-4.05477900	1.86198900
C	-2.89497500	2.42749800	0.39151300	H	1.13405500	-4.17813200	2.87349500
C	-3.07272800	1.61858300	1.52189100	H	0.85616600	-4.54796100	1.16676800
C	-2.62500500	0.29175500	1.56003600	H	2.52590300	-4.51914400	1.82883100
H	-2.10123500	2.53841000	-1.62082200	K	3.38112800	0.19797300	2.97631100
H	-3.26418100	3.44913200	0.39405800	I	-0.08302400	1.09090000	2.98901100
H	-3.55950200	2.02673700	2.40383100				
O	-1.47042200	-1.45441200	0.36521200	44-TS			
C	-0.97604200	-1.78377100	-0.93530500	Pd	1.09287900	-0.06274100	0.03401700
H	-0.23263100	-2.59283900	-0.80384500	C	2.85253000	2.21651700	-0.24704000
H	-1.78124500	-2.18305800	-1.55402300	C	1.47463500	1.89588000	-0.21496800
C	-1.02324900	-0.06600800	-1.84059600	C	0.56100500	2.95108900	-0.34366800
H	-0.25730200	0.63436500	-2.23829100	C	0.99898600	4.27632600	-0.44966000
H	-1.61275900	-0.39896500	-2.69491800	C	2.36502100	4.56890600	-0.44314000
C	-2.70700400	-0.54810800	2.80590500	C	3.30004500	3.53782000	-0.35148500
H	-2.89499700	-1.59939100	2.56558300	H	-0.50118900	2.73642700	-0.33224800
H	-1.75256800	-0.47132600	3.34258600	H	0.26942400	5.07701200	-0.53184400

H	2.70618200	5.59675500	-0.52875300	C	4.75362600	2.75538100	-3.74820400
H	4.36810000	3.73020000	-0.38812300	C	5.85234400	3.49502400	-4.19383000
O	3.79721500	1.22803400	-0.13335500	C	7.13673300	3.19684800	-3.71427900
C	3.29105500	-0.05844500	-0.53502100	C	7.34064200	2.18521000	-2.76700800
H	2.86605000	-0.79352000	0.61837000	H	3.75985600	2.97523000	-4.12809600
H	2.97235300	-0.04256200	-1.58514800	H	5.71225600	4.29935800	-4.91054900
H	4.14018000	-0.74913000	-0.49221200	H	7.98267400	3.78523700	-4.06173000
C	1.96943800	-2.46411800	1.37230000	O	6.38029500	0.55579700	-1.33027100
O	1.05879800	-2.24489800	0.54685700	C	7.77026200	0.19580100	-1.15387500
O	2.90588900	-1.59666400	1.63999900	H	7.92868200	-0.00054900	-0.09168700
C	2.03072100	-3.77628800	2.11578800	H	7.99244900	-0.70274600	-1.74203800
H	1.93136600	-3.58719700	3.18973200	C	10.75488600	2.94270900	-4.01661400
H	1.23092700	-4.43803500	1.78462600	O	10.23166000	1.92205400	-4.67118600
H	3.00646500	-4.24410900	1.95574800	O	10.43096300	3.23679000	-2.86144600
K	2.21137300	1.08439200	2.70150600	C	11.79480000	3.69178300	-4.79736800
I	-1.26620000	0.28723400	1.36633100	H	12.72097700	3.10707800	-4.78444300
				H	11.48513600	3.80442200	-5.83827900
				H	11.97724900	4.66429100	-4.34065800
45				H	9.57893700	1.47262600	-4.07469200
Pd	1.88010400	0.23050700	0.74374500	K	10.80358900	4.18255700	-0.30183800
C	2.97552200	2.42397000	-0.75792500	I	11.25984900	0.72521200	-0.37682300
C	1.82067700	2.08631500	-0.00874000	C	7.81741900	6.07679000	0.78705500
C	0.82869600	3.06961200	0.13361500	O	8.63477400	5.16375500	0.40480500
C	1.01508700	4.36591000	-0.37548500	O	6.57239500	5.95124000	0.82900800
C	2.18946500	4.68142800	-1.06671400	C	8.44331100	7.40608100	1.21578100
C	3.17236600	3.70964000	-1.27522500	H	9.02378000	7.82405800	0.38551900
H	-0.08697500	2.82569400	0.66635700	H	7.67876300	8.12156000	1.52138400
H	0.24135500	5.11713000	-0.24108700	H	9.13734000	7.23464100	2.04599000
H	2.33426100	5.68162000	-1.46637800	K	6.47913400	3.52608100	-0.11466100
H	4.07285600	3.92633700	-1.84181100	H	4.08042500	1.13178500	-2.46822700
O	3.92109200	1.47192000	-0.92523700				
C	3.41337100	0.16311500	-0.59048900				
H	0.34781300	-1.80632900	2.53153800	47-TS			
H	3.03055100	-0.31937900	-1.49973700	Pd	2.68593600	0.64063500	2.11091500
H	4.23899900	-0.41902200	-0.17186300	C	1.88885000	2.89121900	0.24594600
C	1.71200600	-2.87495600	1.73430800	C	1.70065600	1.52134800	0.49619000
O	2.32584500	-1.93612900	1.22727600	C	0.44001600	0.96074100	0.23151500
O	0.59467400	-2.75950800	2.42876500	C	-0.61545700	1.85265800	-0.04659800
C	2.17961500	-4.30106500	1.61367700	C	-0.40548600	3.23557800	-0.14816800
H	1.40950400	-4.89188000	1.10867300	C	0.88374000	3.79008700	-0.04458700
H	3.11115000	-4.34018100	1.05089900	H	0.26287300	-0.10807700	0.28938500
H	2.31712700	-4.72881000	2.61080200	H	-1.61833000	1.45790600	-0.18691500
K	2.63153500	2.80620100	2.66937900	H	-1.24680700	3.89047200	-0.34970000
I	-0.04344600	0.61174300	2.98626800	H	1.07138300	4.84467600	-0.21170300
				O	3.26733600	3.01270300	0.22286300
46				C	3.47533400	1.56131000	0.20277900
Pd	9.04159200	1.60600500	-1.83908500	H	3.55397200	1.19741600	-0.82205900
C	6.20639800	1.46082200	-2.33317400	H	4.38734100	1.29574500	0.76034000
C	4.92091700	1.72403200	-2.81729200	K	3.65199400	3.60017000	3.20992400

I	2.63677600	0.27595800	4.80540900	O	8.48398200	-1.79977400	1.75511600
C	0.35922500	5.27100900	3.03365200	C	8.26149200	-4.19129700	1.80649700
O	1.39393100	4.57431200	3.33065300	H	9.25125800	-4.18023400	1.34798400
O	-0.81812100	4.84383700	3.04122300	H	8.28697300	-4.77673300	2.73147000
C	0.62016300	6.71967100	2.61803200	H	7.55322700	-4.68332900	1.13015300
H	-0.31379100	7.25412700	2.43856300	K	6.91841700	0.09299100	2.61720400
H	1.19815800	7.23201100	3.39404400				
H	1.22572900	6.72823300	1.70405900	50			
K	-0.21770500	2.33707700	3.44538000	Pd	3.72898600	0.14894200	1.46875600
				C	1.95820500	1.09367200	1.23117700
48				H	1.33876400	0.43847800	0.61878100
Pd	1.56092000	0.57848500	2.10747400	H	1.55530800	1.26585600	2.22766900
C	1.91425900	2.91226900	0.23733100	H	2.22094400	2.01748300	0.71235400
C	1.96575100	1.50006300	0.18119400	I	4.07034200	-0.64570400	-1.06449200
C	0.77288600	0.74726600	0.03405500	K	4.20634900	-3.05444300	2.12458200
C	-0.43227600	1.53446900	0.05339300	I	4.04663200	0.38727000	4.11458600
C	-0.42181200	2.92293500	0.14246900	C	7.88393400	-2.80957300	2.04378600
C	0.78388600	3.68260500	0.21098000	O	6.62161400	-2.57925200	2.01444600
H	0.74620500	-0.28225400	-0.31160300	O	8.77127700	-1.94335400	1.86646500
H	-1.38297900	1.01870700	-0.04713300	C	8.30129900	-4.25555900	2.31405500
H	-1.36427400	3.46296500	0.13855800	H	9.38729500	-4.35390700	2.33657100
H	0.77698200	4.76535800	0.22173200	H	7.88312400	-4.58661400	3.27099900
O	3.29511700	3.12855800	0.12331700	H	7.89189000	-4.90654700	1.53358800
C	3.44868300	1.66454900	-0.14899000	K	7.19347000	0.05778900	1.48468300
H	3.72098500	1.52196600	-1.19897800				
H	4.18747500	1.20636700	0.51193400	51-TS			
K	3.40198600	3.40736500	3.12898500	Pd	0.46590700	-0.35244100	-0.74873300
I	2.15466300	0.34422400	4.75028700	C	0.47504000	-2.04757200	0.62189600
C	0.38709900	5.48509400	3.04360700	C	0.43489200	-1.50809500	1.91531600
O	1.29853400	4.68272900	3.45358500	C	1.01701700	-3.32494900	0.43871100
O	-0.82552300	5.19180500	2.92291400	C	1.06322900	-2.23549800	2.94146100
C	0.85191500	6.88908600	2.65108500	H	0.01302300	-0.53501400	2.14560200
H	0.00554800	7.53224300	2.40591900	C	1.62199200	-4.07607000	1.43324800
H	1.43364500	7.33085300	3.46628000	C	1.65657100	-3.48331400	2.70269000
H	1.51592600	6.81916100	1.78076000	H	1.11482500	-1.79398400	3.93283100
K	-0.57088500	2.67195700	3.59608600	H	2.01237300	-5.06991900	1.24419000
				H	2.13365500	-4.01263600	3.52225200
49-TS				C	-0.24449000	-2.56647000	-1.00394300
Pd	3.60353300	0.12736200	2.24268300	H	-1.26214700	-2.81700900	-0.70927600
C	2.23824000	0.82376500	0.04269200	H	-0.21389000	-2.17493800	-2.02516600
H	1.36949400	0.21510700	-0.18197300	I	1.10305300	2.23933600	-1.26745000
H	2.19206500	1.27449100	1.03952100	C	2.41797400	-0.82826300	-1.21465600
H	2.47890700	1.55254700	-0.72324800	H	2.43213800	-1.90688700	-1.37896900
I	3.99141700	-0.70803400	-0.33023900	H	2.69111100	-0.27677100	-2.11233500
K	4.26456800	-2.87943200	3.31183300	H	3.03723500	-0.53542900	-0.36665000
I	3.95346300	0.35463800	4.90440400	O	0.67220600	-3.65480600	-0.84202800
C	7.77561900	-2.77234400	2.10721800	K	-2.59410900	-1.29499400	2.76063100
O	6.64678000	-2.67518800	2.70669000	I	-2.48722100	0.09450000	-0.38009200

C	-0.75609800	1.43701200	4.44668000	H	2.94412400	0.66471800	-0.60264600
O	-1.36427600	0.67217200	3.61020800	H	1.44138400	-0.35181000	-2.29958700
O	-0.37168200	2.59965200	4.20023400	H	1.39289200	0.53783000	-4.61942100
C	-0.49141300	0.84200800	5.83151200	H	2.90164500	2.42500800	-5.27092100
H	0.02836200	1.55396700	6.47368400	O	4.56040200	3.62575500	-3.61023000
H	-1.43969100	0.55258600	6.29807800	C	5.77744400	3.55753800	-2.89376300
H	0.11232400	-0.06714000	5.73048600	H	6.19463900	4.55846900	-2.79646400
K	-0.91131400	2.71741000	1.64028600	Pd	5.53359400	2.64071800	-1.05408700
				C	3.64457800	3.72598100	-0.68719800
52				H	2.89509300	3.23179400	-0.07870200
C	3.60443800	1.83424400	-3.32990000	H	4.31346600	4.31898200	-0.05347400
C	3.18801000	2.21810000	-2.04252500	H	3.23091700	4.34055200	-1.48111600
C	1.82756800	2.20354500	-1.73861800	H	6.46920700	2.85960600	-3.37649500
C	0.90689300	1.69540200	-2.67345600	I	8.29305900	3.08572900	-0.68182000
C	1.35129200	1.24415400	-3.92113600	K	8.30832800	-0.26684200	0.71714300
C	2.70504800	1.32668800	-4.26818600	I	5.12765100	1.15544500	1.44635800
H	1.49103300	2.54658500	-0.76453500	C	9.88417700	0.92431900	3.87657400
H	-0.15028200	1.66007600	-2.42485000	O	9.27556500	0.61839700	2.79057600
H	0.63902100	0.85594600	-4.64366800	O	9.68391200	1.97087200	4.53689400
H	3.06010900	1.02930000	-5.24986100	C	10.92238600	-0.08099000	4.37625300
O	4.93414300	1.94124800	-3.61889900	H	11.39088300	0.26303300	5.29935500
C	5.56639800	2.88114300	-2.77218600	H	10.44108800	-1.05004700	4.54723700
H	5.33992000	3.90783300	-3.06835100	H	11.68857200	-0.22979300	3.60771300
Pd	4.80799200	2.61488200	-0.86709200	K	7.85978600	3.00063100	3.00653200
C	4.21663300	4.58368100	-0.79674700				
H	3.47006200	4.78832700	-1.56264600	53-TS-a			
H	3.80827200	4.67386900	0.20962200	C	3.79278800	2.51668500	-3.28440900
H	5.11756700	5.18092900	-0.92668900	C	3.75681700	2.11481100	-1.93266300
H	6.63162100	2.67034300	-2.73650100	C	2.84938100	1.11616700	-1.54438100
I	7.31382500	3.24818300	0.36255300	C	2.03277100	0.50724600	-2.49755300
K	2.92289100	-0.57039000	-0.71284400	C	2.09876500	0.90557900	-3.84249700
I	3.23327000	1.86054500	1.79348800	C	2.97151300	1.91365000	-4.24250800
C	6.41035600	-0.30552400	-0.91336200	H	2.75203600	0.86292000	-0.49215500
O	5.29211200	0.34587800	-0.83800500	H	1.31816500	-0.25193600	-2.19113100
O	6.76802100	-1.11658400	-0.03379000	H	1.45453700	0.43381600	-4.57828500
C	7.30494200	-0.03155000	-2.10823100	H	3.03281000	2.24168500	-5.27466000
H	7.92531000	0.83894200	-1.86511000	O	4.60566200	3.54475900	-3.62136000
H	7.96369700	-0.88118700	-2.29559800	C	5.77249100	3.60676100	-2.81497400
H	6.70978100	0.20887800	-2.99149200	H	6.09027000	4.64436900	-2.72818200
K	6.39163100	0.40847200	2.08135900	Pd	5.51273000	2.67471700	-1.01315200
				C	3.61001400	3.76683100	-0.68516700
53-TS				H	2.89192200	3.28868500	-0.02564400
C	3.74940900	2.57950400	-3.30503900	H	4.28311200	4.41948900	-0.12046800
C	3.77623100	2.09797300	-1.97855900	H	3.13768500	4.32717100	-1.48628300
C	2.93852500	1.03232300	-1.62230000	H	6.55500600	2.96588900	-3.23763700
C	2.09132500	0.47224900	-2.57790200	I	8.06140300	3.54979000	-0.30738900
C	2.06311000	0.97587400	-3.88566300	C	4.41527800	1.26322700	1.55456500
C	2.89345400	2.03080900	-4.26027500	O	5.41026600	1.20338000	0.71727500

O	3.53345500	0.38777200	1.62788300	H	1.46191700	0.68319400	-4.82356900
C	4.37834500	2.45423400	2.50323400	H	2.81490200	2.74895100	-5.23173300
H	3.35396400	2.81747500	2.61417100	O	4.36314800	3.87675300	-3.42243100
H	4.70683900	2.11833400	3.49356100	C	5.57954200	3.81991100	-2.70595400
H	5.03824700	3.25577600	2.16591200	H	5.91910600	4.83204800	-2.49332300
K	8.00358200	0.55536400	1.39189000	Pd	5.40995800	2.68269400	-0.98805000
I	7.51859800	-2.69267500	0.61721000	C	3.42927100	3.56052100	-0.52295000
K	4.50907100	-1.40128200	-0.16472600	H	2.70756900	2.94413900	0.00174100
				H	4.04604800	4.10880700	0.19734000
				H	2.98524300	4.24206800	-1.24243100
				H	6.32294900	3.23056000	-3.25304500
				I	8.10960700	3.43587300	-0.51159300
				K	8.29467200	1.12788900	1.89544300
				I	5.05602900	0.88549300	1.34161700
53-TS-b				54			
C	3.63485700	2.75175100	-3.22866600	C	3.79282500	3.11854900	-2.13873800
C	3.66820000	2.09390000	-1.98312100	C	2.70485100	3.34364500	-1.28259900
C	2.99470600	0.88222900	-1.80577600	C	1.87189800	2.25187700	-1.01929000
C	2.26519700	0.34830800	-2.86908400	C	2.10246800	0.98299300	-1.57111100
C	2.20731500	1.02586600	-4.09511200	C	3.16882800	0.78437700	-2.43963900
C	2.89365100	2.22596200	-4.28788000	C	4.00421100	1.86934500	-2.74792700
H	3.04858800	0.38740500	-0.84127800	H	1.03188000	2.39274600	-0.34355300
H	1.73379800	-0.59026200	-2.74225900	H	1.43886900	0.16046400	-1.32349100
H	1.62968000	0.60762700	-4.91431700	H	3.36770500	-0.18107800	-2.89156200
H	2.87929700	2.74686900	-5.23945400	H	4.64611500	1.82523900	-3.64807800
O	4.31846400	3.91672700	-3.34100200	O	4.68716600	4.13090800	-2.37829300
C	5.50155800	3.91499200	-2.53504000	C	6.01192000	3.77096900	-2.03488700
H	5.71919000	4.94027700	-2.23435500	H	6.12136600	3.68259100	-0.94609800
Pd	5.31524100	2.66117800	-0.92537500	Pd	6.42998900	1.85826400	-2.62511300
C	3.31562200	3.45692900	-0.48006000	C	2.49236000	4.70126200	-0.66393900
H	2.66577600	2.78247500	0.06825100	H	1.65906700	4.68537200	0.04311900
H	3.89921200	4.07437400	0.21321300	H	3.39040600	5.03798100	-0.13645100
H	2.78273900	4.09535000	-1.17827000	H	2.27774400	5.45417000	-1.43016800
H	6.32722100	3.47403300	-3.10136200	H	6.68348900	4.50918200	-2.46838000
I	8.03635800	2.85706800	-0.37642100	I	6.52651800	-0.93614100	-3.48417200
C	5.27421200	1.11988400	1.85930500	K	9.47697900	-1.13630300	-1.54350600
O	5.82432400	0.19805700	2.49247000	I	9.08373000	2.42070000	-2.31313500
O	5.07286700	1.05379200	0.57719600	C	11.75271600	-1.59143500	-4.45957200
C	4.85002200	2.38963600	2.57768700	O	10.88854100	-1.36576900	-3.54006800
H	4.92555400	2.26001900	3.65753900	O	11.69126900	-1.13417900	-5.62516400
H	5.51378600	3.20313300	2.26351000	C	12.93043500	-2.48814000	-4.07557500
H	3.82927300	2.66640900	2.30111300	H	13.61786300	-2.61490700	-4.91300400
K	7.19830000	-0.52073300	0.39606300	H	13.46311000	-2.05017000	-3.22457000
				H	12.55609400	-3.46684900	-3.75617000
				K	9.47288400	0.18328300	-5.35567100
53-TS-c				55-TS			
C	3.63747400	2.74137700	-3.24925600				
C	3.69916100	2.11502400	-1.98572300				
C	2.95076500	0.94907000	-1.76915500				
C	2.15587000	0.43779300	-2.79379800				
C	2.09062900	1.08613900	-4.03492900				
C	2.83316000	2.24091700	-4.27337400				
H	2.98494500	0.46479900	-0.80032800				
H	1.57608700	-0.46399800	-2.62172600				

C	3.41945700	2.68283200	-3.47392700	H	4.74117600	6.56154200	0.25533900
C	3.02202900	2.68230700	-2.11616500	H	3.48592300	5.43733100	-0.40707000
C	1.74602400	2.19069400	-1.80669700	H	6.20011900	4.65223300	-2.48534600
C	0.93333900	1.62152600	-2.80089400	I	6.59601400	4.54494100	0.78684000
C	1.38418100	1.57001600	-4.12578700	C	2.41612900	2.46229200	1.43336700
C	2.62327100	2.11336800	-4.47561700	O	3.63933300	2.76566300	1.11759700
H	1.39920300	2.21955700	-0.77795100	O	2.14994600	1.66953400	2.35327400
H	-0.04503400	1.22685100	-2.54042400	C	1.30245300	3.12845900	0.63717900
H	0.75744900	1.13036700	-4.89697300	H	1.40110600	2.87336100	-0.42251800
H	2.96851700	2.12360600	-5.50463700	H	0.32665900	2.81238600	1.00644400
O	4.62111300	3.21486700	-3.78404800	H	1.39181700	4.21694900	0.71842400
C	5.13331500	4.02872800	-2.71825300	K	6.90584200	1.08910100	-1.42285100
H	4.79779800	5.06511000	-2.85282000	I	7.41441700	-0.53998800	1.43426100
Pd	4.46534500	3.39911900	-0.86611900	K	4.77575200	1.10788200	2.83285900
C	4.31348100	5.59043900	0.36434800				
H	3.53390500	5.44611900	-0.37736900	55-TS-b			
H	4.05912700	5.27857100	1.36991200	C	4.48768200	1.80782300	-3.07036100
H	4.84627100	6.52680300	0.26376300	C	3.78385500	2.01127000	-1.86310800
H	6.22208800	3.97092800	-2.75442000	C	2.72160700	1.15417400	-1.55543300
I	6.71429100	4.49670000	0.40056700	C	2.40127900	0.09009200	-2.40812100
K	3.75473700	-0.21248300	-1.54265000	C	3.12776400	-0.10458800	-3.58940700
I	3.46335800	2.07356900	1.55106700	C	4.17289500	0.75554900	-3.93771600
C	7.20110000	-1.32400600	-0.78901900	H	2.17110600	1.30920000	-0.63250300
O	6.00000300	-0.87457200	-0.72986300	H	1.58992700	-0.58601800	-2.15301000
O	8.12395200	-0.99812600	-0.00711200	H	2.87162400	-0.92606300	-4.25313800
C	7.49518300	-2.32075700	-1.91108500	H	4.72683300	0.63285600	-4.86339800
H	8.52318600	-2.68158300	-1.85802000	O	5.54271200	2.62363700	-3.32482500
H	6.80272500	-3.16684100	-1.84565500	C	5.45757100	3.83573400	-2.53322400
H	7.32940900	-1.83700900	-2.88040300	H	4.83977000	4.56486000	-3.07443600
K	6.75169700	0.71595800	1.38287500	Pd	4.53407400	3.50114100	-0.71604000
				C	4.15751800	5.65637900	0.25514100
55-TS-a				H	3.68846400	5.32785300	1.17545900
C	4.58785100	1.99068300	-3.19866900	H	4.66186500	6.61333000	0.28187700
C	3.99209200	1.95586100	-1.91801000	H	3.55567200	5.52275400	-0.64661000
C	3.17608400	0.86124800	-1.60479000	H	6.47565700	4.21559400	-2.43099600
C	2.98235000	-0.17193200	-2.52979200	I	6.56403700	4.68461700	0.76966900
C	3.58176800	-0.10662600	-3.79258300	C	3.73495800	1.91834200	1.74486400
C	4.38757200	0.97980800	-4.14408800	O	4.64957200	1.11238800	1.45375900
H	2.71392200	0.79341400	-0.62510900	O	3.39551400	2.95175900	1.06859500
H	2.37042800	-1.02880300	-2.26366500	K	6.13901800	0.72592500	-0.52305600
H	3.41800500	-0.90379100	-4.51209500	C	2.92724000	1.65758700	3.01241600
H	4.84829700	1.05459700	-5.12422400	H	2.43902200	0.68102900	2.93037600
O	5.46907000	3.00078200	-3.45213700	H	3.60864500	1.60728000	3.86712100
C	5.25589900	4.10798600	-2.55410900	H	2.17648400	2.43056300	3.18139700
H	4.47254300	4.75705000	-2.96826600				
Pd	4.51554300	3.52080600	-0.72889500	55-TS-c			
C	4.22838300	5.61564300	0.37837300	C	5.07977100	1.76794300	-3.08755800
H	3.87204900	5.39290700	1.37704300	C	4.25926800	1.75690600	-1.93472300

C	3.39166800	0.66360300	-1.77007800	H	4.78793800	0.82806600	3.70604400
C	3.41373300	-0.41349100	-2.66719500	H	3.26572800	1.76855700	3.70070700
C	4.27252300	-0.39008700	-3.77231800				
C	5.10189700	0.70875300	-4.00079300				
H	2.70916300	0.64899900	-0.92500800				
H	2.75353200	-1.26197400	-2.50853500				
H	4.27996400	-1.22045600	-4.47311700				
H	5.74296300	0.76620700	-4.87486500				
O	5.88926300	2.83964100	-3.26971300				
C	5.42271900	3.95991600	-2.52337900				
H	4.60497300	4.45769300	-3.06218300				
Pd	4.54221400	3.40153200	-0.72826900				
C	4.06954600	5.57597300	0.18341800				
H	3.31207500	5.15371700	-0.48873300				
H	3.76249500	5.57026800	1.22211600				
H	4.49545700	6.50076400	-0.18750200				
H	6.26606700	4.63401100	-2.37360500				
I	6.47635700	4.76250800	0.76927300				
K	5.89552400	0.68028600	0.36163900				
I	3.17393800	2.33008100	1.62323100				
55-TS-d							
C	4.03536700	2.22427300	-3.21550000				
C	3.73315400	2.06450300	-1.84505100				
C	2.80198500	1.08463600	-1.48196500				
C	2.19043400	0.28503400	-2.45426900				
C	2.51818100	0.45622200	-3.80303900				
C	3.44480100	1.42260700	-4.19602400				
H	2.52960100	0.95542700	-0.43819500				
H	1.45624400	-0.46020600	-2.16185300				
H	2.04820800	-0.16848400	-4.55761500				
H	3.71137200	1.56456800	-5.23823600				
O	4.89146700	3.21024200	-3.56748800				
C	5.60572200	3.73875300	-2.45028700				
H	5.72754000	4.81433200	-2.60052100				
Pd	4.73405300	3.34481900	-0.64903100				
C	3.88821100	5.55484500	0.04669900				
H	3.27917400	5.06048500	0.79612700				
H	4.18704900	6.56210500	0.30226500				
H	3.56230700	5.45595800	-0.98352100				
H	6.58723400	3.25359400	-2.37287000				
I	6.37144300	5.02348100	0.82354200				
H	4.98968900	0.99620900	0.16374000				
C	4.17017600	1.51009000	1.78703200				
O	4.85681100	0.62906500	1.06582800				
O	3.82892400	2.61278900	1.36369400				
C	3.85349900	1.02089300	3.17065100				
H	3.30783800	0.07504000	3.11148000				
56-TS							
C	3.39404000	2.63481900	-3.49376400				
C	2.97991500	2.63664800	-2.14042400				
C	1.69027900	2.16830100	-1.85014500				
C	0.87791600	1.62345300	-2.85747000				
C	1.34212800	1.57408300	-4.17770700				
C	2.59641900	2.09250100	-4.50901100				
H	1.33190400	2.19801300	-0.82533700				
H	-0.11109900	1.24652500	-2.61132800				
H	0.71501700	1.15404000	-4.95945100				
H	2.95453100	2.10138400	-5.53364200				
O	4.61459800	3.13443600	-3.78791900				
C	5.14828800	3.91233800	-2.70754700				
H	4.85780800	4.96384800	-2.83028900				
Pd	4.43318700	3.29182300	-0.87479100				
C	4.47307600	5.45636100	0.36221700				
H	3.56390600	5.29764500	-0.21096800				
H	4.37042300	5.28633600	1.42574200				
H	5.05565400	6.31384500	0.05256800				
H	6.23408700	3.80825300	-2.72540100				
K	3.68986600	-0.24963000	-1.49364900				
I	3.34530100	2.06646600	1.55503300				
C	7.18172200	-1.20702100	-0.76441800				
O	5.96076400	-0.82034900	-0.67924800				
O	8.09976800	-0.84922000	0.00912000				
C	7.50898000	-2.16418800	-1.91191400				
H	8.54973900	-2.48814100	-1.87007200				
H	6.84775200	-3.03623000	-1.86876000				
H	7.32463500	-1.66079900	-2.86794200				
K	6.68597000	0.81300200	1.42152000				
Br	6.54881900	4.18855900	0.31879900				
57-TS							
C	3.70826500	2.03377500	-3.25064300				
C	3.15724200	2.33553600	-1.98323200				
C	1.77903100	2.15525800	-1.80684300				
C	0.98920400	1.59618900	-2.82595700				
C	1.57689300	1.23841800	-4.04525400				
C	2.93760200	1.46641300	-4.27235000				
H	1.32694500	2.41822200	-0.85468500				
H	-0.07534300	1.44673200	-2.66672900				
H	0.97000800	0.80401600	-4.83506000				
H	3.39993100	1.23446600	-5.22664700				
O	5.02540600	2.27030000	-3.44614500				
C	5.58539200	3.10480400	-2.41574900				

H	5.56542200	4.15159400	-2.74227500	O	9.64947200	5.50585600	0.30263700
Pd	4.55244700	2.93666400	-0.64759600	O	7.75461600	6.56384800	-0.27985200
C	4.64235300	5.30940300	0.16883300	C	9.55217500	7.87229400	0.63008200
H	3.94275800	5.20695700	-0.65365200	H	10.45385700	8.06672900	0.03864200
H	4.22001700	5.21146200	1.16102800	H	8.85439200	8.70273200	0.51406100
H	5.39477200	6.07232100	0.02511800	H	9.86301400	7.79264300	1.67698100
H	6.60989800	2.77191500	-2.23723400	K	7.56917000	4.02812500	-0.80889000
K	3.15314200	-0.49780500	-0.90326900	H	8.17072500	1.16422100	-3.96671200
I	3.08885800	2.17365800	1.77744400				
C	6.74415700	-0.39677500	-0.91705200	59-TS			
O	5.59048400	-0.56704300	-0.37373800	Pd	8.95698700	1.48430000	-1.65018500
O	7.77294800	-0.04012800	-0.29889000	C	6.33696900	1.16682500	-2.80549300
C	6.81701400	-0.59974500	-2.43043100	C	4.98595200	1.45065300	-3.07923700
H	7.85154800	-0.59763700	-2.77709500	C	4.66237500	2.77110200	-3.40286200
H	6.33562300	-1.54300300	-2.71151400	C	5.63492800	3.78101600	-3.45175800
H	6.27222200	0.21479800	-2.92231200	C	6.96906300	3.46468400	-3.21068700
K	6.46695600	0.81141100	1.78657600	C	7.36255600	2.13745500	-2.91696900
Cl	6.44254900	3.93100900	0.62408400	H	3.62264100	3.01934600	-3.60223400
				H	5.34754900	4.79877000	-3.69903600
58				H	7.73433200	4.23249300	-3.29281800
Pd	8.74133000	1.14805800	-1.86628900	O	6.66269500	-0.07182500	-2.35525700
C	6.20035300	0.76516800	-3.11992600	C	7.64592200	-0.01461100	-1.31088800
C	4.87284600	1.21280500	-2.99391400	H	7.14088600	0.16241200	-0.35170400
C	4.59933600	2.52615000	-3.38894100	H	8.17300200	-0.96957800	-1.28923700
C	5.59407900	3.37447500	-3.90503100	C	3.94705300	0.36407900	-2.97082100
C	6.89697800	2.90651600	-4.04952700	H	2.93957000	0.76213100	-3.11902400
C	7.20514600	1.59131200	-3.65562900	H	4.11962100	-0.41976200	-3.71662300
H	3.58350800	2.89982300	-3.28455800	H	3.99206000	-0.12530300	-1.99231300
H	5.33590900	4.38416500	-4.21056100	C	10.40275800	2.96533000	-3.76882000
H	7.68715000	3.51423800	-4.47612000	O	9.52089400	2.34396800	-4.44253600
O	6.53439600	-0.49227000	-2.69196900	O	10.41083100	3.04405400	-2.50101900
C	7.48452800	-0.43360900	-1.62044700	C	11.51917100	3.64985700	-4.53045900
H	6.95574700	-0.24600400	-0.67934400	H	12.46713800	3.16078000	-4.28410400
H	8.02859400	-1.37872000	-1.59740700	H	11.35081500	3.59743800	-5.60583000
C	3.81971800	0.29569600	-2.42777800	H	11.59036100	4.69519300	-4.21419300
H	2.87389600	0.82308300	-2.27946500	H	8.54542400	1.99729700	-3.63749600
H	3.63896500	-0.55148100	-3.09811000	K	11.29160300	4.19698000	-0.32158200
H	4.14052400	-0.12729800	-1.47080200	I	10.42432800	0.87184600	0.59293100
C	10.26929400	3.30670600	-3.33142100	C	8.30408900	6.25011700	0.52732100
O	9.99777400	2.63015100	-4.32502800	O	9.16936300	5.33434500	0.28781800
O	9.94237300	3.00624100	-2.10156500	O	7.06831000	6.06059300	0.61636200
C	11.05080100	4.61567400	-3.47124600	C	8.85130600	7.66723700	0.70922200
H	12.10750000	4.43614600	-3.23295000	H	9.36332300	7.98212700	-0.20703800
H	11.00125600	4.97813400	-4.49911400	H	8.05112600	8.37221300	0.93844800
H	10.66695400	5.37575900	-2.78307700	H	9.59226900	7.67534200	1.51582300
K	11.38517000	3.76322300	0.06432100	K	7.12725800	3.49871000	0.18686300
I	9.75693800	0.66099800	0.60346900				
C	8.92157800	6.55384300	0.18015300	59-TS-a			

Pd	8.88389800	1.61605100	-1.60669400	O	6.64267500	-0.12264100	-2.34736300
C	6.27575500	1.14481300	-2.72329000	C	7.58426600	-0.00546800	-1.27734500
C	4.94456600	1.33216300	-3.13312700	H	7.06647700	0.28694700	-0.35550800
C	4.59939000	2.59897900	-3.60607300	H	8.09205900	-0.96369900	-1.16859700
C	5.52557200	3.65140700	-3.65508200	C	3.97744000	0.16707400	-3.20667900
C	6.84027200	3.43045300	-3.26684400	H	2.98028800	0.50134700	-3.50654300
C	7.26952300	2.14958400	-2.84607700	H	4.27841000	-0.65379500	-3.86708300
H	3.57340300	2.77496400	-3.92070900	H	3.91647300	-0.25325800	-2.19715200
H	5.21505700	4.62776800	-4.01506300	C	10.31507400	3.02816500	-3.77018800
H	7.57598100	4.22514300	-3.35581800	O	9.46310200	2.35476900	-4.42938500
O	6.61381300	-0.03069000	-2.13348000	O	10.28835600	3.17265500	-2.50755800
C	7.58454500	0.17018600	-1.10014500	C	11.44626800	3.67484300	-4.54158800
H	7.07730800	0.51118600	-0.18564400	H	12.35835700	3.09374000	-4.36816100
H	8.09439000	-0.78293400	-0.93488900	H	11.23174200	3.69077100	-5.61014100
C	3.94549300	0.21154300	-3.00272500	H	11.62146700	4.68903500	-4.17257300
H	2.94810900	0.53267100	-3.31492200	H	8.49654000	1.99721000	-3.62918200
H	4.23587600	-0.65057100	-3.61335900	I	10.68765800	0.59204100	0.28850400
H	3.88970300	-0.14369600	-1.96821700	K	10.66741900	3.92533200	-0.13459900
C	10.32203100	2.98608100	-3.79094300				
O	9.41961200	2.35330500	-4.41975700				
O	10.37024300	3.09359600	-2.52277500	59-TS-c			
C	11.40672200	3.66756200	-4.59912700	Pd	8.87667400	1.64242700	-1.55154500
H	12.38780500	3.36379800	-4.22275400	C	6.28900700	1.13268400	-2.70664200
H	11.31818500	3.42297800	-5.65731200	C	4.96370500	1.30124500	-3.14498100
H	11.32289900	4.75130600	-4.46676000	C	4.61462200	2.55667600	-3.64388400
H	8.43367300	2.01250000	-3.57398900	C	5.53221400	3.61668300	-3.69122700
C	11.08453800	-0.04898700	-0.27175400	C	6.84106100	3.41385400	-3.27291300
O	10.31336800	0.99823200	-0.11303600	C	7.27445300	2.14534400	-2.82190900
O	11.44639800	-0.74690100	0.68697100	H	3.59329800	2.71709400	-3.98189600
C	11.52466100	-0.38642400	-1.68735700	H	5.22026000	4.58433300	-4.07359300
H	11.75765700	0.52582500	-2.24343100	H	7.57180800	4.21357700	-3.35872200
H	12.38279400	-1.05940200	-1.66564000	O	6.62831500	-0.03208800	-2.10120700
H	10.69877600	-0.87908900	-2.21211100	C	7.59059100	0.18339700	-1.05990700
K	11.07303900	3.69825500	-0.08459600	H	7.07618600	0.52923400	-0.15294700
I	10.67919700	3.69137100	3.27331600	H	8.10556200	-0.76266700	-0.88554300
K	10.00743200	0.44216500	2.58687300	C	3.97491600	0.17117600	-3.01738500
				H	2.98092900	0.47432700	-3.35796000
				H	4.28950900	-0.69845600	-3.60504800
				H	3.89998500	-0.16675300	-1.97820800
59-TS-b				C	10.33969700	2.98131700	-3.77288500
Pd	8.89412000	1.48033500	-1.64594000	O	9.43490400	2.33324900	-4.38403600
C	6.30120000	1.09000200	-2.85185000	O	10.38204200	3.14777400	-2.51340900
C	4.97138900	1.29854500	-3.25877100	C	11.46122700	3.57114700	-4.60739000
C	4.62340300	2.59027800	-3.65679600	H	12.35605900	2.95180100	-4.47788400
C	5.54849700	3.64414700	-3.63875600	H	11.19524800	3.58763800	-5.66444500
C	6.86194700	3.40030300	-3.25490400	H	11.69619900	4.58064700	-4.25912100
C	7.29121300	2.10058400	-2.90383800	H	8.45868200	2.00484700	-3.52790300
H	3.59864700	2.78189100	-3.96679300	C	11.39857100	0.37663000	-0.34510200
H	5.23944300	4.63930200	-3.94618700	O	10.40012200	1.17753600	-0.11552700
H	7.59789800	4.20000900	-3.29371800				

O	12.58536900	0.74196500	-0.23431000	H	5.70929000	4.28488200	-4.91991300
C	11.07097100	-1.05051500	-0.75651200	H	7.98621100	3.78631500	-4.06888600
H	10.59635400	-1.04303300	-1.74303600	O	6.37959400	0.55483400	-1.33579900
H	11.97654400	-1.65703600	-0.78976200	C	7.76941100	0.19969600	-1.15227400
H	10.35276100	-1.48250800	-0.05371700	H	7.92395900	0.00508300	-0.08909900
K	11.94238300	3.28812400	-0.41676000	H	7.99690000	-0.69911700	-1.73810300
				C	3.74603200	0.88815100	-2.31727700
59-TS-d				H	2.81783200	1.16729500	-2.82371300
Pd	8.90113200	1.54668800	-1.61796200	H	3.92318000	-0.18050300	-2.47833900
C	6.29492000	1.12361600	-2.77387900	H	3.59686300	1.01375500	-1.23760700
C	4.93416100	1.36868100	-3.03772700	C	10.74889400	2.94341500	-4.01961300
C	4.57542400	2.67324000	-3.39070400	O	10.20883400	1.93366600	-4.67728300
C	5.52333900	3.70421200	-3.47783000	O	10.43411900	3.23613100	-2.86159100
C	6.86833100	3.42632600	-3.24428900	C	11.79652800	3.68165500	-4.80049300
C	7.29505800	2.11645400	-2.91963000	H	12.71629300	3.08686100	-4.78795600
H	3.52799200	2.89123100	-3.58536600	H	11.48786600	3.79864400	-5.84117400
H	5.21063200	4.70793400	-3.75046100	H	11.99011100	4.65162900	-4.34291300
H	7.61241000	4.21152100	-3.34944100	H	9.54987300	1.49213000	-4.08165200
O	6.65506600	-0.09323400	-2.29005000	K	10.81401100	4.19641500	-0.31153100
C	7.62640200	0.02374500	-1.23899000	I	11.25209400	0.73837800	-0.35652100
H	7.10548000	0.20119100	-0.28800200	C	7.82478300	6.08110300	0.79502000
H	8.18670100	-0.91132300	-1.18865200	O	8.64747100	5.17958200	0.39757400
C	3.92269700	0.26055300	-2.89231800	O	6.58125100	5.94362000	0.84519500
H	2.90275000	0.63544000	-3.01278700	C	8.44178700	7.41163900	1.23263100
H	4.08993900	-0.52266700	-3.63998500	H	9.01683400	7.84065800	0.40429900
H	4.00832800	-0.22347300	-1.91403200	H	7.67279100	8.11869600	1.54659500
C	10.32793200	2.98535400	-3.77770900	H	9.13945000	7.23851000	2.05946200
O	9.45154800	2.34283600	-4.43680100	K	6.50146400	3.52939100	-0.12924800
O	10.35412700	3.06437700	-2.50860800				
C	11.39445000	3.72556800	-4.55780700	61-TS			
H	12.38056300	3.49738800	-4.14324000	Pd	2.68994900	0.56641500	2.06112500
H	11.36201800	3.45862400	-5.61391000	C	1.91721500	2.91976500	0.35694700
H	11.22410500	4.80274800	-4.45330400	C	1.70549800	1.54154900	0.50315200
H	8.47834600	1.98695100	-3.62083800	C	0.43141900	1.02559600	0.20861200
K	11.39180500	4.31893500	-0.45640200	C	-0.59790900	1.96253900	-0.00239700
I	8.70704700	6.31355200	0.09505500	C	-0.35513200	3.34579900	0.00577900
K	6.89875400	3.49568100	0.06719100	C	0.94090500	3.88127600	0.15780700
I	10.28907200	1.12769500	0.71393500	H	0.22752100	-0.03960400	0.19798000
				H	-1.61071800	1.60713400	-0.17398600
60				H	-1.18313100	4.03172500	-0.15211300
Pd	9.03992300	1.61052600	-1.83569500	O	3.30010300	3.02378400	0.32972400
C	6.20732100	1.46315500	-2.34032500	C	3.48484100	1.57448000	0.20392600
C	4.90887400	1.70804900	-2.81693700	H	3.54594000	1.28363800	-0.84517400
C	4.76069100	2.74190500	-3.75171500	H	4.39854100	1.25529200	0.72922700
C	5.85671600	3.48448700	-4.19996200	K	3.76249600	3.49145700	3.26285100
C	7.14169400	3.19631000	-3.72162900	I	2.66446600	0.14874800	4.74977500
C	7.34035800	2.18556100	-2.77114400	C	0.54854300	5.33213700	3.75004400
H	3.76702600	2.96110800	-4.13521600	O	1.58599900	4.62396000	3.48726800

O	-0.61280800	4.87950300	3.87280100	C	1.60505200	-4.11419300	1.37342600
C	0.76684800	6.84046400	3.87844200	C	1.63417100	-3.52473900	2.64689100
H	-0.08253400	7.31538900	4.37206800	H	1.11224300	-1.85218000	3.90522300
H	1.69010800	7.05163000	4.42596100	H	2.10584300	-4.06939800	3.46094900
H	0.87218000	7.27190700	2.87596600	C	-0.26727100	-2.55627400	-1.03121800
K	-0.11066500	2.36192200	3.46344000	H	-1.28431800	-2.80508500	-0.73321100
C	1.25934600	5.34995600	0.11995200	H	-0.24046800	-2.15572600	-2.04899300
H	2.06792900	5.56407800	-0.58760700	I	1.10368100	2.24428600	-1.27048900
H	0.38406100	5.93892500	-0.16582100	C	2.40447300	-0.83177100	-1.23218400
H	1.58437700	5.67480800	1.11441000	H	2.41124900	-1.90863200	-1.40844200
62				H	2.68243300	-0.27243100	-2.12350600
Pd	1.56419700	0.58983000	2.08115500	H	3.02542600	-0.55296500	-0.38062100
C	2.03073000	2.90990500	0.23046200	O	0.64606600	-3.64882100	-0.88319200
C	2.01110700	1.49996000	0.16204100	K	-2.58487900	-1.29553300	2.74879500
C	0.78088200	0.81136300	0.00412300	I	-2.49440400	0.11301200	-0.38326100
C	-0.37429700	1.66693500	0.01511300	C	-0.73468300	1.41858300	4.44917900
C	-0.28487800	3.05390500	0.10865800	O	-1.35940100	0.66934500	3.61100500
C	0.95486600	3.76178400	0.19425600	O	-0.33656200	2.57816600	4.20989100
H	0.69841000	-0.21402600	-0.34415300	C	-0.46645600	0.80749600	5.82638100
H	-1.35312500	1.21037000	-0.10194900	H	0.06289600	1.50872200	6.47259200
H	-1.19982600	3.64203100	0.07304800	H	-1.41404300	0.52032900	6.29567200
O	3.42334800	3.06000500	0.12298400	H	0.12991800	-0.10498600	5.71196100
C	3.50321700	1.59174000	-0.15648900	K	-0.89071900	2.71115900	1.65235100
H	3.77520800	1.44014200	-1.20524300	C	2.14557800	-5.48408700	1.06353700
H	4.21123100	1.09299200	0.50840500	H	2.46790000	-5.99660500	1.97349900
K	3.49067700	3.38075700	3.12030700	H	1.38969500	-6.10151800	0.56638200
I	2.18660200	0.32829100	4.71209300	H	3.00354400	-5.42369600	0.38457300
C	0.55515600	5.59548900	3.86068900	64			
O	1.47966200	4.76121300	3.54909700	C	3.59418500	2.07182400	-3.27694500
O	-0.65697100	5.30435600	3.98286700	C	3.19149100	2.39145200	-1.97150500
C	0.99184400	7.04770100	4.05504400	C	1.83373100	2.36347800	-1.65256100
H	0.18752700	7.64453400	4.48749400	C	0.91319300	1.89868300	-2.60701300
H	1.87986400	7.09411600	4.69285000	C	1.35225400	1.50642600	-3.87691500
H	1.26625200	7.47243600	3.08215300	C	2.70086300	1.60321600	-4.25054700
K	-0.46774600	2.74500800	3.53882900	H	1.50440700	2.66031900	-0.66122700
C	1.06727200	5.26088300	0.22391300	H	-0.14364700	1.84760800	-2.35882000
H	1.83885900	5.61386400	-0.46920900	H	0.63259500	1.14953800	-4.60968100
H	0.11964400	5.73256900	-0.04976100	O	4.92393400	2.19572400	-3.57459000
H	1.33567600	5.59611900	1.23138400	C	5.56432700	3.08978200	-2.68618900
63-TS				H	5.33582400	4.13021900	-2.92725400
Pd	0.45619100	-0.34751600	-0.76060500	Pd	4.82276000	2.72876900	-0.79213400
C	0.45999200	-2.05343300	0.59708800	C	4.23164500	4.69191100	-0.62362600
C	0.42556100	-1.52541600	1.89687200	H	3.48080900	4.93374200	-1.37437800
C	0.99589800	-3.32791800	0.40147200	H	3.82801500	4.73126400	0.38785600
C	1.05105100	-2.27526100	2.90615100	H	5.13130400	5.29607800	-0.72803100
H	0.01774000	-0.54975800	2.13981500	H	6.62981300	2.87771800	-2.66915700
				I	7.34674700	3.30304000	0.43425400

K	2.92058200	-0.43677600	-0.76352800				
I	3.26996500	1.86109100	1.85358700	65-TS-a			
C	6.42020800	-0.19209800	-0.98761100	C	3.79205000	2.50345800	-3.27875500
O	5.30333900	0.45305600	-0.85493900	C	3.75671200	2.10881900	-1.92771800
O	6.80570300	-1.03445400	-0.15067700	C	2.84966500	1.11247800	-1.53024300
C	7.27975900	0.12816000	-2.19703300	C	2.03721200	0.50647900	-2.48612200
H	7.92402400	0.97438200	-1.93137300	C	2.10630300	0.90284500	-3.83159700
H	7.91750500	-0.72148900	-2.44723800	C	2.97240600	1.91106900	-4.25612800
H	6.66172000	0.42239400	-3.04753500	H	2.74936700	0.86471500	-0.47733000
K	6.42940500	0.39426000	2.03045000	H	1.32015100	-0.25270000	-2.18470900
C	3.19568400	1.25468400	-5.63079100	H	1.46077900	0.42575500	-4.56413000
H	3.62623100	2.13347500	-6.12327000	O	4.60979000	3.52995100	-3.62036500
H	3.99059300	0.50171400	-5.58956000	C	5.77567400	3.59456800	-2.81308900
H	2.38576600	0.87153000	-6.25741100	H	6.09483000	4.63222200	-2.73091000
65-TS				Pd	5.51365700	2.66952600	-1.00984000
C	3.74599900	2.56940000	-3.30501300	C	3.61308000	3.76848900	-0.68944900
C	3.77655400	2.08816200	-1.98097800	H	2.88873000	3.29552100	-0.03316600
C	2.93791000	1.02489300	-1.61802900	H	4.28609000	4.41860400	-0.12167200
C	2.08974900	0.47510100	-2.57595900	H	3.14828800	4.32951300	-1.49446700
C	2.06059300	0.98454700	-3.88158500	H	6.55799400	2.95100300	-3.23210700
C	2.88539400	2.04002000	-4.27746500	I	8.06275000	3.54612400	-0.30059600
H	2.94510100	0.65534800	-0.59942800	C	4.41802900	1.26330200	1.56426000
H	1.43641500	-0.34874100	-2.30438100	O	5.40776600	1.20067400	0.72100000
H	1.38536200	0.54725800	-4.61259000	O	3.54335200	0.38244900	1.65378600
O	4.56382400	3.61332400	-3.61236800	C	4.37597300	2.46620300	2.49782000
C	5.78228500	3.53867700	-2.89949600	H	3.35389800	2.84407600	2.57890400
H	6.20570600	4.53725200	-2.80411400	H	4.67438400	2.13842400	3.50008200
Pd	5.53931900	2.62405000	-1.06043200	H	5.05292000	3.25552900	2.16596300
C	3.65460000	3.71700300	-0.69055000	K	8.00092400	0.53765400	1.37413800
H	2.90149300	3.22606600	-0.08391200	I	7.51090000	-2.70204900	0.56636900
H	4.32623700	4.30435900	-0.05439700	K	4.49102700	-1.39746200	-0.16178200
H	3.24541300	4.33603100	-1.48329600	C	3.05178500	2.37819500	-5.68580300
H	6.46861600	2.83638200	-3.38364200	H	2.73957600	3.42482100	-5.77350000
I	8.30351000	3.05992700	-0.69499500	H	4.07978300	2.32635300	-6.05856100
K	8.31070600	-0.28047100	0.72811300	H	2.41346900	1.77337400	-6.33454700
I	5.13395600	1.14704600	1.44627900				
C	9.88713000	0.92975300	3.88081600	65-TS-b			
O	9.28047100	0.61629800	2.79594700	C	3.59450500	2.72294400	-3.19262100
O	9.68718600	1.98175500	4.53260100	C	3.67307300	2.16768900	-1.89959600
C	10.92240600	-0.07344200	4.39082500	C	2.89457600	1.04166600	-1.59279000
H	11.39079200	0.27790000	5.31122500	C	2.05675100	0.50973000	-2.56891600
H	10.43843200	-1.03962100	4.57032900	C	1.97773800	1.09506200	-3.84029800
H	11.68893200	-0.23137800	3.62447800	C	2.74328300	2.21154800	-4.18282200
K	7.86650700	3.00175500	2.99115900	H	2.94039400	0.60858900	-0.60080300
C	2.88496400	2.60463500	-5.67457900	H	1.45106400	-0.36174400	-2.33858700
H	2.55786600	3.65053000	-5.67768700	H	1.31185300	0.66927000	-4.58660700
H	3.89152400	2.59035700	-6.10533100	O	4.35705400	3.82091400	-3.44990100
H	2.21865500	2.03586300	-6.32831600	C	5.59141700	3.75791400	-2.76565700

H	5.97482400	4.76662300	-2.62193700
Pd	5.43132600	2.72777100	-0.98138200
C	3.49568700	3.70095900	-0.51739800
H	2.76502400	3.14323400	0.05794700
H	4.15142900	4.26253700	0.15689500
H	3.05808300	4.36022300	-1.26109200
H	6.29552900	3.10997400	-3.29800000
I	8.17483600	3.40039700	-0.63344100
C	2.69345300	2.85666100	-5.54380200
H	2.32642300	3.88731300	-5.47990400
H	3.69125500	2.90699300	-5.99218400
H	2.03701000	2.30066800	-6.21841600
K	8.35193800	1.21367500	1.88210600
I	5.08733300	1.08275200	1.45806800

65-TS-c

C	3.67950300	2.72710100	-3.14892000
C	3.69760500	2.19498600	-1.84422400
C	2.99894700	1.01841700	-1.55245600
C	2.30538300	0.37307100	-2.58045800
C	2.29030400	0.91464400	-3.87286400
C	2.97016900	2.09828200	-4.18541600
H	3.02318100	0.61125200	-0.54927900
H	1.76128500	-0.54301800	-2.36944800
H	1.73773900	0.40795700	-4.66011500
O	4.36514700	3.86906600	-3.38250000
C	5.53226800	3.98918800	-2.54134100
H	5.64847400	5.03975300	-2.26482900
Pd	5.36631500	2.82611200	-0.84772600
C	3.40589900	3.69300100	-0.43393000
H	2.78347400	3.07034200	0.20039600
H	4.01883200	4.36502500	0.18144400
H	2.85335400	4.26589700	-1.17293300
H	6.40052800	3.64181400	-3.10512000
I	8.11933200	2.47785300	-0.80928200
C	5.21736600	0.48484400	1.12443500
O	5.34995800	-0.33686400	0.18705600
O	5.07422600	1.75007900	0.99392400
C	2.96998200	2.70145200	-5.56657700
H	2.42198000	3.65044900	-5.58083200
H	3.98906100	2.92789100	-5.89667100
H	2.50494300	2.02878000	-6.29227800
C	5.24145600	-0.01993100	2.56086100
H	4.89832800	-1.05551300	2.60743700
H	6.27711300	0.01716100	2.91692900
H	4.63989500	0.61771500	3.21152400
K	6.12304400	-0.18742500	-2.18027400

65-TS-d

C	3.75372900	2.57335600	-3.29585500
C	3.78962400	2.09681100	-1.97038900
C	2.96294200	1.02648400	-1.60179600
C	2.12177600	0.46242500	-2.55788100
C	2.08791000	0.96556400	-3.86579300
C	2.90004400	2.02934600	-4.26626800
H	2.97180400	0.66283700	-0.58101000
H	1.47696300	-0.36686800	-2.28267300
H	1.41818800	0.51713700	-4.59502000
O	4.55834200	3.62681200	-3.60596300
C	5.77669800	3.57128400	-2.89184000
H	6.18567700	4.57600400	-2.79653200
Pd	5.54267000	2.65933800	-1.04962200
C	3.64940600	3.73353400	-0.68248500
H	2.90523500	3.23475700	-0.07123300
H	4.31440600	4.33533100	-0.05266600
H	3.22910700	4.34032500	-1.47878700
H	6.47407700	2.87915400	-3.37456200
I	8.30845200	3.05748400	-0.69057400
K	8.14147200	-0.51336700	0.30904400
I	5.17444700	1.18390600	1.45817400
K	7.95218600	2.88943400	2.92415700
C	2.89256700	2.58799800	-5.66571200
H	2.55058500	3.62907100	-5.67312200
H	3.89947800	2.58618300	-6.09582600
H	2.23473900	2.00718400	-6.31734800
I	9.86720500	0.11440400	3.13803700

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C	3.54262300	2.87481000	-2.79949500
C	2.72072400	3.00253600	-1.65068800
C	1.98760900	1.88341400	-1.24744900
C	2.05299400	0.68946200	-1.96379700
C	2.84258100	0.58889300	-3.10890000
C	3.59722100	1.67565200	-3.55664900
H	1.36366200	1.95142800	-0.36129500
H	1.48607600	-0.17166000	-1.62483100
H	2.87666400	-0.34334100	-3.66471500
O	4.14386900	4.03451600	-3.32420400
C	5.47729400	4.10048700	-2.82517900
H	5.63773000	5.02473000	-2.26370600
Pd	5.58212200	2.50350000	-1.58605600
C	2.58686200	4.33795800	-0.96174100
H	1.99143800	4.24496400	-0.05013100
H	3.55952900	4.75983800	-0.69661400
H	2.09660400	5.06020800	-1.62409200
H	6.20967900	3.96552000	-3.62727500

I	8.11026900	3.25636500	-0.91591400	H	4.10871500	1.60562700	-5.99175700
K	8.76062100	-0.28839900	-0.28971600	H	2.42956000	1.61035300	-6.57405600
I	5.26111600	0.09395000	0.00533300				
C	9.59602400	0.52933200	3.24709300	67-TS-a			
O	9.16681000	0.27317000	2.06664300	C	4.62942500	1.81813600	-3.16642700
O	9.02646500	1.29011700	4.06474400	C	4.03178300	1.80804200	-1.88898500
C	10.90196600	-0.15351000	3.65497300	C	3.23524100	0.70813300	-1.54366700
H	11.17824400	0.10466200	4.67819800	C	3.06913200	-0.34754400	-2.44544600
H	10.79338600	-1.23955900	3.56430800	C	3.67394500	-0.30089200	-3.70669600
H	11.70207500	0.15152800	2.97156400	C	4.46452400	0.78426800	-4.10315600
K	7.05758000	2.01302900	2.53868700	H	2.77154300	0.65612500	-0.56412800
C	4.38714900	1.63111900	-4.84093900	H	2.47388100	-1.21181200	-2.16516500
H	4.08524600	2.45003700	-5.50188800	H	3.52756800	-1.12233600	-4.40381300
H	5.46007600	1.74608400	-4.66023400	O	5.48939300	2.84280400	-3.44842300
H	4.23080000	0.68240200	-5.36000700	C	5.25246000	3.96882900	-2.58043300
				H	4.45985000	4.59240200	-3.01562200
67-TS				Pd	4.51270600	3.41855900	-0.74427500
C	3.42145400	2.67839300	-3.46136000	C	4.15274600	5.53883100	0.29824900
C	3.02421400	2.68506700	-2.10708700	H	3.79157600	5.33295600	1.29874800
C	1.75001800	2.18986700	-1.79174800	H	4.63738600	6.49630400	0.15378700
C	0.94968100	1.61119200	-2.78774100	H	3.42618000	5.31494400	-0.49006200
C	1.40882600	1.55251100	-4.11013900	H	6.18626500	4.53221600	-2.52243600
C	2.64330600	2.09914800	-4.48103800	I	6.54551100	4.55347700	0.75870200
H	1.39954000	2.22465200	-0.76468100	C	5.12070500	0.86606900	-5.45826900
H	-0.02867000	1.21132300	-2.53424900	H	4.81451400	1.77444400	-5.98805100
H	0.78544400	1.10126100	-4.87872200	H	6.21360700	0.91160500	-5.37607600
O	4.62036300	3.22153800	-3.77575800	H	4.86210300	0.00121700	-6.07521000
C	5.12485400	4.04447200	-2.71331900	C	2.41896800	2.37540200	1.42968900
H	4.77891100	5.07683700	-2.85253000	O	3.63809500	2.69921000	1.11859000
Pd	4.46325900	3.41498700	-0.85971800	O	2.16132500	1.59732000	2.36459800
C	4.29930300	5.60586200	0.37184800	C	1.29847700	2.99630800	0.60693600
H	3.52306800	5.45887200	-0.37282900	H	1.40566500	2.70367700	-0.44226800
H	4.04468500	5.28769500	1.37540100	H	0.32621700	2.67801100	0.98354900
H	4.82457300	6.54703500	0.27707500	H	1.37073300	4.08822200	0.64845900
H	6.21425200	3.99773000	-2.74943900	K	6.95254700	1.03562700	-1.34774300
I	6.70763400	4.53280700	0.40361300	I	7.48886500	-0.52143300	1.54475300
K	3.72206700	-0.21483500	-1.51341000	K	4.79181400	1.09509700	2.87211100
I	3.47819600	2.08403000	1.56332900				
C	7.18560600	-1.32341600	-0.81949700	67-TS-b			
O	5.98722800	-0.86859300	-0.75022600	C	4.98357700	1.80154300	-3.13313700
O	8.11974000	-0.99259300	-0.05316700	C	4.19141900	1.78418500	-1.96444600
C	7.46148500	-2.33407800	-1.93383400	C	3.33237900	0.68659000	-1.77920400
H	8.48834000	-2.69927900	-1.88902600	C	3.34785700	-0.38395800	-2.68167800
H	6.76582100	-3.17596600	-1.85069800	C	4.18540600	-0.34956900	-3.80305700
H	7.28636300	-1.86034800	-2.90646200	C	5.00839900	0.74993600	-4.06554900
K	6.77062700	0.73925900	1.33928300	H	2.66699000	0.66582100	-0.92094600
C	3.13786000	2.10677100	-5.90469800	H	2.69864300	-1.24010500	-2.51748100
H	3.28841000	3.13253700	-6.25875500	H	4.18359900	-1.18092400	-4.50426600

O	5.78288600	2.88129900	-3.33212300	K	6.07320600	0.71839900	-0.60480300
C	5.33266900	3.99326300	-2.56402400				
H	4.49524900	4.48892700	-3.07364600				
Pd	4.51061600	3.41520500	-0.74832100				
C	4.11298700	5.57604900	0.23387000				
H	3.85063300	5.55524400	1.28461300				
H	4.53645100	6.50141900	-0.13849700				
H	3.32010700	5.17757400	-0.41183800				
H	6.17636500	4.67158800	-2.43580000				
I	6.52648100	4.70948000	0.69909800				
C	5.88139200	0.84187600	-5.29086700				
H	5.62046800	1.72010400	-5.89153000				
H	6.93770400	0.95582900	-5.02082200				
H	5.77964800	-0.04841800	-5.91769100				
K	5.83994900	0.63724200	0.26847200				
I	3.20071500	2.32879300	1.63265600				
67-TS-c							
C	4.40656100	1.89020200	-3.11524700				
C	3.73412100	2.06357200	-1.88880200				
C	2.67355100	1.20418300	-1.57739200				
C	2.33490000	0.17025300	-2.45668000				
C	3.03454500	0.01139000	-3.65996000				
C	4.07855700	0.86959500	-4.02457800				
H	2.14449500	1.33396600	-0.63849500				
H	1.52710500	-0.51326400	-2.20927400				
H	2.75711100	-0.78993400	-4.34125100				
O	5.46069700	2.70942900	-3.37471200				
C	5.40669400	3.89651200	-2.54476100				
H	4.78652700	4.64889800	-3.05056100				
Pd	4.51423000	3.52153400	-0.72110700				
C	4.18001800	5.66061900	0.30581200				
H	3.71957300	5.31501900	1.22425600				
H	4.69501800	6.61137400	0.34840500				
H	3.56470500	5.55465100	-0.59048200				
H	6.43098800	4.26233400	-2.45193100				
I	6.58188200	4.64946300	0.75800000				
C	3.74449100	1.90705000	1.73394500				
O	4.64180300	1.09183400	1.41627000				
O	3.40139500	2.94854800	1.07208700				
C	2.97846000	1.66193800	3.03023400				
H	2.62045200	0.62846600	3.05186000				
H	3.66585400	1.78494900	3.87384400				
H	2.14130700	2.35230800	3.14232400				
C	4.82716800	0.74085800	-5.32696800				
H	4.75720500	1.66508800	-5.91087700				
H	5.89679800	0.56322600	-5.16161700				
H	4.43310100	-0.08079200	-5.93178900				
67-TS-d							
C	3.78703300	2.73948300	-3.59494600				
C	3.29510500	2.54144400	-2.28563100				
C	2.18793400	1.69391500	-2.12998100				
C	1.64989300	1.03221700	-3.23857700				
C	2.18321700	1.23427700	-4.51626400				
C	3.25890200	2.10332200	-4.72942600				
H	1.76952300	1.53124600	-1.14316500				
H	0.81134000	0.35404000	-3.10662600				
H	1.74795500	0.72117300	-5.37046800				
O	4.88800900	3.53960800	-3.73513000				
C	4.98314400	4.44463600	-2.63063300				
H	4.29220800	5.28415800	-2.78019600				
Pd	4.34530100	3.57629800	-0.85522200				
C	4.55718000	5.56866800	0.53175400				
H	4.48119200	5.41350300	1.60070900				
H	5.11041500	6.44315700	0.21015200				
H	3.60360400	5.43582300	0.01367700				
H	6.01498700	4.79451000	-2.58007700				
I	6.76992400	4.17496600	0.41352100				
C	3.83230100	2.37640800	-6.09730000				
H	3.79245000	3.44544600	-6.33209000				
H	4.88818700	2.08652300	-6.15949500				
H	3.28364800	1.83185700	-6.87061400				
K	5.84480600	0.92598500	-2.20523800				
I	7.76987400	-0.65872700	0.05783000				
K	6.10347800	0.94197700	2.47344100				
I	3.15301300	2.30204400	1.44692700				
68							
Pd	1.84858000	-0.03509300	-0.66506300				
C	-1.80138900	0.29216700	0.75238700				
C	-2.15062800	1.36318300	-0.08373800				
C	-3.50465400	1.72192200	-0.13290500				
C	-4.46198100	1.04460000	0.62094500				
C	-4.08080000	-0.01450400	1.44450900				
C	-2.74132900	-0.41056100	1.52097400				
H	-3.80372600	2.54833100	-0.77216200				
H	-5.50515600	1.34172000	0.56636400				
H	-4.82595100	-0.54738100	2.02934600				
O	-0.46522300	-0.08932600	0.89619500				
C	0.10540600	-0.87768700	-0.14795700				
H	0.32448800	-1.87790000	0.23467600				
H	-0.55200000	-0.91688800	-1.02096500				
C	-1.11323200	2.09915000	-0.89332000				
H	-1.53871900	3.00559400	-1.33225600				

H	-0.73244300	1.47974200	-1.71399900	O	2.82213000	1.70020800	-0.90428700
C	-2.29970400	-1.55489900	2.40110200	O	1.19443400	2.47055000	0.42440600
H	-1.69100600	-2.27524700	1.84607900	C	3.28365100	3.61416300	0.48099200
H	-1.68862400	-1.20546100	3.24333200	H	2.70309700	4.49168500	0.76850700
H	-3.16107900	-2.08323400	2.81781400	H	3.76617600	3.19981800	1.37398500
H	-0.24577600	2.36984300	-0.28696000	H	4.04607900	3.88551500	-0.25323100
C	3.08559800	2.14491400	0.20099400	K	5.14585200	0.50066300	-0.07380100
O	3.78357900	1.38263300	-0.52766700	I	3.15209100	-2.03261300	-1.20246400
O	1.86783000	1.84656100	0.47934800	C	4.00392400	0.94221200	3.43553900
C	3.66065700	3.40099500	0.80540100	O	2.99591700	0.60576200	4.09535900
H	2.97121500	4.23521900	0.64986500	O	4.08540600	0.91568100	2.15360400
H	3.76058700	3.24917300	1.88657600	C	5.25115300	1.42398700	4.18050100
H	4.63321400	3.63134400	0.36844300	H	5.55847500	2.40309900	3.79760400
K	4.87933100	-0.84354900	0.45335100	H	5.06849700	1.48830000	5.25396800
I	2.53588500	-2.24726700	-2.03657900	H	6.07800800	0.72834600	3.99655800
C	4.28893400	0.98576900	3.40974300	K	1.35810100	0.00226700	2.15620600
O	3.48394000	1.81468100	3.90210100				
O	3.96293700	-0.02613000	2.69781400				
C	5.78857500	1.22834200	3.61799900	69-TS-a			
H	6.19355900	1.71953600	2.72319600	Pd	0.82022100	-0.16554600	-0.73136100
H	5.96349100	1.88652100	4.47060300	C	-2.44496000	-0.71236900	-0.04729600
H	6.32181900	0.28306400	3.75713300	C	-2.28600300	0.52519400	-0.70380200
K	1.28472000	0.80815700	2.86742400	C	-3.35180400	1.43920000	-0.59806600
				C	-4.51299200	1.14071600	0.10251200
69-TS				C	-4.63713300	-0.09689700	0.73945200
Pd	1.24024800	-0.05767600	-1.12785800	C	-3.60882700	-1.03446900	0.67963000
C	-1.69387700	-0.21983200	0.62521300	H	-3.25109800	2.40543900	-1.08555200
C	-1.62837400	1.01602800	-0.05350400	H	-5.31864400	1.86685200	0.15585600
C	-2.48461200	2.03481300	0.40654700	H	-5.54131500	-0.33952500	1.29148400
C	-3.36199200	1.83843700	1.46571000	O	-1.47366700	-1.68652800	0.00518700
C	-3.40111500	0.60097100	2.11437100	C	-0.45719600	-1.72277300	-0.95579600
C	-2.56768900	-0.44098500	1.71011600	H	0.11304000	-2.63431000	-0.76122900
H	-2.44575500	3.00082100	-0.08957200	H	-0.86589200	-1.72442100	-1.97379400
H	-4.01569700	2.64380200	1.78691100	C	-1.03341000	0.94682900	-1.41543300
H	-4.08796600	0.43808100	2.94067300	H	-1.12962400	1.99320600	-1.72988800
O	-0.85052300	-1.28081600	0.36572700	H	-0.84204000	0.41938600	-2.35354700
C	-0.24463100	-1.43778700	-0.89899100	C	-3.70596800	-2.36979200	1.37318400
H	0.18209700	-2.43780800	-0.90695100	H	-3.58236300	-3.19547200	0.66398000
H	-0.97244700	-1.30602800	-1.70621800	H	-2.91498300	-2.48453200	2.12292800
C	-0.61447000	1.31938500	-1.11217500	H	-4.67212500	-2.48214200	1.87212400
H	-0.64942400	2.38270900	-1.37477500	H	-0.18314200	1.54921000	-0.46595200
H	-0.77193200	0.79954900	-2.05970700	C	1.53286400	2.55268500	0.24508600
C	-2.58205400	-1.78395600	2.39858700	O	2.21967000	1.60635000	-0.25075000
H	-2.75661900	-2.59357200	1.68282300	O	0.26464700	2.55944500	0.26680700
H	-1.62235300	-2.00626200	2.88156100	C	2.26371700	3.74107300	0.83324100
H	-3.36011400	-1.82014400	3.16537400	H	3.01236800	3.39221000	1.55041200
H	0.51093100	1.68739600	-0.33661600	H	2.79169100	4.26833900	0.03179300
C	2.38380200	2.52876600	-0.06055000	H	1.56972400	4.42526300	1.32084100
				C	2.39811800	-2.28606100	0.78337600

O	2.42151400	-1.54240000	-0.29680800	C	-4.50744300	1.16698300	0.19280400
O	2.98618900	-3.37767000	0.83298700	C	-4.65003600	-0.09105300	0.78424700
C	1.60718100	-1.77708400	1.97600800	C	-3.63515100	-1.04025700	0.68961800
H	0.53568100	-1.85617600	1.75954000	H	-3.22607900	2.45430600	-0.94915800
H	1.84227500	-2.36785800	2.86211800	H	-5.30215200	1.90296000	0.27264300
H	1.82023600	-0.71851500	2.15184500	H	-5.55770800	-0.34071600	1.32769000
K	4.31759400	0.32444700	-1.04362600	O	-1.51221700	-1.70055500	-0.00680900
I	5.73170500	-1.81380900	-3.24839900	C	-0.47655000	-1.70651200	-0.94823200
K	3.45593300	-3.78685300	-1.72744300	H	0.10402400	-2.61276300	-0.77760800
				H	-0.86475400	-1.66498400	-1.97301100
				C	-1.03094100	0.97689600	-1.33652300
69-TS-b				H	-1.12520500	2.03012100	-1.62859400
Pd	0.80057000	-0.20438200	-0.66704100	H	-0.84401400	0.46862800	-2.28587300
C	-2.51647300	-0.45240900	0.18092700	C	-3.75064300	-2.39810900	1.33500800
C	-2.32144900	0.69013000	-0.62130100	H	-3.63891000	-3.19935200	0.59642300
C	-3.36133800	1.63927500	-0.63680100	H	-2.95936700	-2.55086900	2.07758800
C	-4.53460500	1.45818900	0.08396800	H	-4.71769800	-2.51462000	1.83175100
C	-4.69702900	0.31017100	0.86473800	H	-0.15640200	1.58177200	-0.38847800
C	-3.69263600	-0.65283100	0.93181100	C	1.56575000	2.54669400	0.36692700
H	-3.23076900	2.53521900	-1.23856300	O	2.25736800	1.59255000	-0.09821900
H	-5.32170000	2.20550400	0.04050900	O	0.29687000	2.58491400	0.32719200
H	-5.61188100	0.15959800	1.43206700	C	2.28049900	3.70077900	1.04209500
O	-1.56356500	-1.42386200	0.37148700	H	2.62215400	3.37067200	2.02952200
C	-0.58828500	-1.69138000	-0.58480800	H	3.15981400	3.99025400	0.46023000
H	-0.07725400	-2.59792500	-0.26725800	H	1.61371200	4.55383000	1.16874900
H	-1.01176700	-1.78702900	-1.59184600	C	2.62292600	-1.92613800	1.05184500
C	-1.04974300	0.97000700	-1.35502600	O	3.71481900	-1.76293700	1.63037700
H	-1.07181400	1.98581500	-1.76761900	O	2.41009700	-1.48900000	-0.15738800
H	-0.89231000	0.33218300	-2.23003500	C	1.50219100	-2.69345800	1.73754300
C	-3.82782200	-1.88844200	1.78529500	H	0.55893300	-2.14378400	1.67943200
H	-3.71414800	-2.79866000	1.18672700	H	1.35261600	-3.64454900	1.21491700
H	-3.04669500	-1.92449300	2.55269900	H	1.76335500	-2.89419300	2.77700100
H	-4.80194000	-1.91692300	2.28110300	K	4.43878100	0.16319200	-0.00630000
H	-0.17481500	1.59112400	-0.37350400				
C	1.54169200	2.65566700	0.09901600				
O	2.21962700	1.79596400	-0.53644300	69-TS-d			
O	0.28855300	2.56709900	0.29807500	Pd	1.27677800	-0.08753900	-1.26825300
C	2.25295400	3.85326800	0.69709800	C	-1.71338500	-0.44672700	0.36330600
H	2.79683400	3.52344800	1.58910200	C	-1.60139300	0.87689300	-0.11395000
H	2.98175100	4.25457400	-0.01272200	C	-2.44948500	1.83362300	0.47591800
H	1.54162000	4.62746000	0.98507700	C	-3.36395500	1.49730200	1.46636000
K	4.33017200	0.80063000	-1.48469800	C	-3.45211500	0.17507000	1.91057200
I	2.94217900	-1.97165600	-0.30100300	C	-2.62886800	-0.81309800	1.37196900
				H	-2.37521900	2.86355100	0.13777100
				H	-4.01031100	2.25948100	1.89090500
69-TS-c				H	-4.17182600	-0.09674800	2.67808600
Pd	0.79960000	-0.17043000	-0.64865500	O	-0.88055300	-1.47522700	-0.03202500
C	-2.46517600	-0.71073700	-0.02506100	C	-0.24136100	-1.45220200	-1.29272200
C	-2.28797600	0.54835800	-0.63640700	H	0.16375000	-2.45001200	-1.44158300
C	-3.34134500	1.47246300	-0.49689300				

H	-0.94506200	-1.18270900	-2.08656100	C	0.59318300	2.93142100	3.61434100
C	-0.55262000	1.31249600	-1.08939800	H	0.38213900	2.38464700	4.53838700
H	-0.55619800	2.40393700	-1.18531400	H	1.64341200	2.75154800	3.35607900
H	-0.69764500	0.94744900	-2.10828800	H	0.44009300	4.00073000	3.76635200
C	-2.70288400	-2.24862400	1.83298300	K	-1.62143800	1.44996100	-0.03306200
H	-2.86730600	-2.92598300	0.98905900				
H	-1.77068000	-2.57887300	2.30885800	71-TS			
H	-3.51243200	-2.38454300	2.55454300	C	2.19450800	0.89665800	-0.54757300
H	0.56332000	1.52687900	-0.24072600	C	2.68511800	-0.40377500	-0.38323700
C	2.43106100	2.31746600	0.15625600	C	3.60467400	-0.64754800	0.64569500
O	2.88271300	1.58694000	-0.76918000	C	4.02930600	0.40940200	1.45701800
O	1.24481200	2.17534800	0.63544500	C	3.54917600	1.70527200	1.23210900
C	3.29626700	3.37955000	0.78794000	C	2.62027000	1.98599500	0.22265800
H	2.69131100	4.24180400	1.07326000	H	4.00088600	-1.65049200	0.78815900
H	3.73720700	2.95233100	1.69738000	H	4.75680800	0.23211000	2.24376600
H	4.09444700	3.68382000	0.10730600	H	3.90529400	2.52438400	1.85134600
K	5.27855500	0.28052100	-0.29928700	O	1.19280000	1.04805100	-1.47520300
I	3.14181900	-2.06471600	-1.59508400	C	1.01948000	-0.12843600	-2.26501000
I	4.38428700	0.16260300	2.98127700	H	-0.01095000	-0.10132400	-2.66497900
K	1.22024500	-0.59876200	1.95139000	H	1.70048200	-0.11707800	-3.11654100
				C	2.09423500	-1.42636300	-1.30152300
70				H	1.88162900	-2.37636400	-0.76321800
C	2.16045700	0.77976700	-0.53656100	H	2.72440900	-1.69600100	-2.14898300
C	2.68469500	-0.52175100	-0.33411800	C	2.08943500	3.37311300	-0.03047900
C	3.60960400	-0.67761700	0.72327500	H	2.00922100	3.56801200	-1.10442000
C	4.02370700	0.40129500	1.50068800	H	1.09391100	3.50649200	0.40799200
C	3.53466800	1.68245800	1.22170200	H	2.74974300	4.12539800	0.40976400
C	2.60267700	1.89480200	0.20457600	Pd	-0.10075600	-1.68898200	-1.16989200
H	4.03226300	-1.66538700	0.89547600	I	-2.34165400	-2.41288500	0.18823400
H	4.75221400	0.25532300	2.29323600	K	0.51686000	-1.27369600	2.20616500
H	3.88055600	2.53434900	1.80091600	C	-0.24202100	2.33765200	2.43728200
O	1.11383700	1.02741000	-1.38995300	O	-0.83587800	3.12725000	1.66035700
C	0.66456600	-0.00434100	-2.25791400	O	-0.23670100	1.06497000	2.31276800
H	-0.26856400	0.35835700	-2.70200900	C	0.58196000	2.91303000	3.58737000
H	1.39723600	-0.18953200	-3.04692200	H	0.36815600	2.37375300	4.51517100
C	2.25030900	-1.69826800	-1.13998700	H	1.64388900	2.76592600	3.35830500
H	2.53858400	-2.64018900	-0.65613500	H	0.38729900	3.97846500	3.71789400
H	2.65373700	-1.70100100	-2.15527900	K	-1.57405700	1.30179700	-0.07244900
C	2.06015800	3.27172300	-0.08841000				
H	1.97609200	3.43848200	-1.16623000	71-TS-a			
H	1.06658500	3.41753800	0.35011700	C	2.85802600	0.51563000	0.00631200
H	2.71685400	4.03865300	0.33153700	C	3.07183400	-0.77613400	-0.49331800
Pd	0.18178100	-1.72225800	-1.25108800	C	4.15886500	-1.50840500	-0.00382000
I	-2.32774200	-2.23950800	-0.12796300	C	5.01532300	-0.93536000	0.94118200
K	0.61436900	-1.13182200	2.15730400	C	4.78776700	0.36863400	1.40127500
C	-0.27748900	2.40608800	2.47541900	C	3.70219800	1.12898400	0.94520500
O	-0.85506900	3.22783100	1.72129900	H	4.32842500	-2.52040800	-0.36086200
O	-0.32594200	1.13407700	2.33347600	H	5.86668500	-1.49707400	1.31327700

H	5.46594000	0.80909200	2.12801100	C	2.56973400	0.62624800	-0.03626200
O	1.69160700	1.11869900	-0.35817800	C	2.67402700	-0.65739000	-0.58536900
C	0.96523800	0.36546400	-1.33793300	C	3.69714500	-1.49989200	-0.13415300
H	-0.10123900	0.60852800	-1.18054600	C	4.60049300	-1.03345800	0.82972300
H	1.24265900	0.69293000	-2.33996900	C	4.47722500	0.26612300	1.34134500
C	2.00995400	-1.26084200	-1.42717700	C	3.46041000	1.13385200	0.91911600
H	1.78698200	-2.33380100	-1.24761300	H	3.79677000	-2.49919900	-0.55058900
H	2.26289600	-1.16973400	-2.48365700	H	5.41567300	-1.66937500	1.16366400
C	3.41237600	2.52690700	1.42990800	H	5.18778700	0.62272600	2.08179800
H	3.48910100	3.24927800	0.61000400	O	1.48521100	1.36114000	-0.44420300
H	2.39036900	2.61693900	1.81714100	C	0.84130500	0.75177500	-1.56693900
H	4.11005800	2.82583500	2.21656800	H	-0.18876700	1.16183100	-1.60622600
Pd	-0.02055700	-1.45390200	-0.51839000	H	1.33995000	1.04421600	-2.49209700
I	-1.65942400	-2.56089900	1.36976900	C	1.60730200	-1.00806800	-1.57622000
K	1.22792300	-0.91210800	2.29804100	H	1.21403900	-2.02819400	-1.37120400
				H	1.93957800	-1.00611600	-2.61466800
				C	3.30091500	2.52697300	1.46427300
71-TS-b				H	2.99935600	3.22360400	0.67654200
C	2.87823600	0.49604600	-0.00873000	H	2.53597700	2.54442200	2.24967600
C	3.09168700	-0.79314900	-0.50742300	H	4.23382000	2.88001600	1.91116300
C	4.21848600	-1.49632500	-0.07261100	Pd	-0.50549900	-0.85552800	-0.92106000
C	5.11125500	-0.89366400	0.81736400	C	-1.73171300	-2.25385400	1.40829400
C	4.87528400	0.40474600	1.28488100	O	-0.66523900	-1.98386800	2.03542700
C	3.74881700	1.13500000	0.88526700	O	-2.09921100	-1.70583000	0.32010300
H	4.39398300	-2.50662100	-0.43169700	C	-2.65803600	-3.31103700	1.99438500
H	5.99557900	-1.43124700	1.14550800	H	-3.64997900	-3.26211500	1.54346500
H	5.58055600	0.86589800	1.97185800	H	-2.23100000	-4.29951200	1.78965600
O	1.69052400	1.07966000	-0.35725600	H	-2.72039900	-3.19826700	3.07970000
C	1.02486200	0.33434600	-1.38643800	K	-0.86444200	0.83010900	1.75752900
H	-0.04467500	0.60869400	-1.31598000	I	1.17389500	0.94724200	4.49968500
H	1.38577200	0.65240800	-2.36565700	K	1.76410000	-1.90368200	2.74177500
C	2.00020100	-1.30013800	-1.39984000				
H	1.74261400	-2.34834400	-1.12311800				
H	2.25868500	-1.31305000	-2.45923200	71-TS-d			
C	3.45725000	2.53283100	1.36976900	Pd	1.20514200	0.34680700	-1.62121900
H	3.41361700	3.23742000	0.53225600	C	-1.90073000	0.44342400	-0.01209700
H	2.48329300	2.59862500	1.87094000	C	-1.88886900	0.02160100	-1.34846100
H	4.22376800	2.87566900	2.06956700	C	-2.90009500	0.47177800	-2.20503600
Pd	-0.09388800	-1.43705300	-0.66779700	C	-3.90714400	1.30761700	-1.71177500
C	-2.02057000	-2.33354600	1.52428800	C	-3.89983200	1.69750000	-0.36536600
O	-1.77339000	-2.34591000	0.27444700	C	-2.89575900	1.27870300	0.51847000
O	-1.32411400	-1.78984100	2.42109800	H	-2.89471300	0.16668100	-3.24792400
C	-3.29455600	-3.05431500	1.96010700	H	-4.70348500	1.64583000	-2.36800900
H	-3.03809300	-3.83006100	2.68863400	H	-4.68903600	2.34327400	0.01164800
H	-3.95412300	-2.34275200	2.46725100	O	-0.82080500	0.09691800	0.74132500
H	-3.81542900	-3.50026700	1.11189400	C	0.12727500	-0.71041600	0.03499300
K	0.82200300	-0.55695200	2.18949700	H	1.11718600	-0.43216400	0.43243600
				H	-0.04414100	-1.76526500	0.24756100
				C	-0.69602500	-0.79045900	-1.73046200
71-TS-c							

H	-0.35970900	-0.54391300	-2.76139800	I	-2.33916500	-2.37688300	-0.27859900
H	-0.85379500	-1.86877200	-1.71004200	C	-1.64274200	3.17975700	-0.90086400
C	-2.82145000	1.74225200	1.94924600	O	-0.54075900	3.25103500	-1.50325900
H	-2.65485500	0.90057600	2.62897300	O	-2.26032400	2.09152600	-0.63428600
H	-1.98059500	2.43223700	2.07818500	C	-2.28897000	4.47130800	-0.39733800
H	-3.74112500	2.25287500	2.24724300	H	-2.19674300	4.50930800	0.69499800
H	2.27539500	2.07728500	0.34470000	H	-1.80051600	5.34930000	-0.82256700
C	0.99094000	2.39900500	1.73462400	H	-3.35636300	4.47996400	-0.63728300
O	0.26322800	3.11822600	1.05645000	K	-0.32950700	0.66261300	-1.99120500
O	2.12852700	1.87077100	1.29927700				
C	0.66691000	1.98071800	3.14349500	71-TS-f			
H	1.57306700	1.78854500	3.71964800	C	2.05008000	0.84470500	-0.50862800
H	0.05278900	2.74261700	3.62434800	C	2.58176000	-0.43611800	-0.31021800
H	0.08816200	1.05351600	3.07619400	C	3.43986100	-0.64441700	0.77753300
I	2.85367900	2.43611200	-2.26459100	C	3.76100700	0.42635100	1.61871200
K	-0.54303500	3.12725700	-1.43917500	C	3.23018900	1.69785800	1.37291500
				C	2.36227000	1.94240800	0.30136900
71-TS-e				H	3.86515900	-1.63085200	0.94678900
Pd	0.37317800	-2.27084900	-0.12173800	H	4.43915400	0.27717200	2.45375400
C	3.03195700	0.13348000	-0.51483800	H	3.48753300	2.52352300	2.03012400
C	3.15458500	-0.65747200	0.62926100	O	1.11125200	0.95871300	-1.51025200
C	3.77517100	-0.10560500	1.75228500	C	1.04982400	-0.22547000	-2.30552400
C	4.27089500	1.19891300	1.69953400	H	0.06325700	-0.23804100	-2.80414800
C	4.11448000	1.96622000	0.54007800	H	1.80671800	-0.19529300	-3.08992200
C	3.47331700	1.45681100	-0.59502700	C	2.08584600	-1.48866500	-1.25029800
H	3.86641900	-0.69401000	2.66114800	H	1.86278700	-2.43405000	-0.71005500
H	4.77597200	1.62253300	2.56255600	H	2.77550200	-1.75294000	-2.05169600
H	4.48817500	2.98689600	0.51421000	C	1.74826000	3.29377800	0.05363300
O	2.33045100	-0.43143600	-1.55880200	H	1.60702400	3.47506300	-1.01590500
C	2.15297200	-1.82690400	-1.34849600	H	0.77268100	3.35740100	0.55180100
H	1.39825700	-2.17274000	-2.07423800	H	2.37621900	4.08919300	0.46377400
H	3.07995700	-2.36491400	-1.55712200	Pd	-0.10731300	-1.77655400	-1.24094200
C	2.47030300	-1.99178900	0.57581700	I	-2.39968000	-2.48538200	0.01539800
H	1.82548400	-2.11603400	1.47219500	K	0.28412700	-1.11467100	2.24819700
H	3.13687200	-2.85343300	0.53740900	K	-1.85876600	1.11435200	-0.61349700
C	3.19955500	2.29727600	-1.81652700	I	-1.09426400	1.95624900	2.56859900
H	3.27929200	1.70566100	-2.73374700				
H	2.18830900	2.72545700	-1.77820800	72			
H	3.90153500	3.13325900	-1.88465700	C	4.90506600	-1.20496700	-4.42952800
H	0.10764000	-0.20086600	0.90354900	C	3.97846200	-1.06156500	-5.48178100
C	-0.10243700	1.56166700	1.72907700	C	2.68799400	-1.58049000	-5.29141300
O	-1.06188800	1.25048200	2.42144500	C	2.34050200	-2.23284500	-4.10471000
O	0.46962100	0.72368400	0.85630200	C	3.29016000	-2.39039800	-3.09270000
C	0.57726400	2.90109700	1.72075100	C	4.59022100	-1.88372600	-3.23555000
H	1.64237100	2.76416000	1.92868100	H	1.96462500	-1.49872300	-6.09925500
H	0.49236300	3.32767500	0.71557400	H	1.34032000	-2.63751400	-3.97839800
H	0.11802300	3.55794500	2.45874700	H	3.02954500	-2.89122800	-2.16619800
K	-3.31499900	0.63752500	1.14745100	O	6.19449900	-0.71172200	-4.58357200

C	6.34775600	0.70379900	-4.54215600	H	6.53203200	1.19020900	-4.45515200
H	5.48525700	1.23263800	-4.95197800	Pd	6.55769200	0.61479700	-1.97539300
Pd	6.73279900	0.97556400	-2.60196100	C	4.86975700	0.74992700	-6.31868300
C	4.36910200	-0.42264600	-6.79484400	H	4.24824800	0.91109700	-7.20392300
H	3.77200400	-0.83534700	-7.61252500	H	4.84728000	1.66971500	-5.72250700
H	4.21682800	0.66324200	-6.79321000	H	5.90087900	0.58864000	-6.64450200
H	5.42544400	-0.59802900	-7.01276100	H	8.06292700	0.33571600	-4.08417500
H	7.27106800	0.95494700	-5.07687600	C	6.88553900	3.88980000	0.77966800
C	6.99332100	3.44394000	1.33521000	O	7.75439200	2.98031100	0.34282000
O	7.83009000	2.99964800	0.43282400	O	5.87594300	3.60887200	1.41398200
O	6.00570600	2.82660500	1.74796700	C	5.70143200	-3.10463400	-3.12793800
C	5.60589000	-2.06226300	-2.13938400	H	6.50284300	-3.53563600	-3.73720300
H	6.42742200	-2.71057000	-2.46129300	H	6.18416000	-2.45795200	-2.39109800
H	6.05818400	-1.10075200	-1.84966100	H	5.18410800	-3.91570900	-2.60819400
H	5.13601600	-2.46849000	-1.24187300	C	7.27443600	-0.43946300	-0.02335500
C	8.37920400	-0.03225600	-0.28312300	H	6.83023500	-1.44172800	0.01693600
H	8.17068000	-1.09061500	-0.50972400	H	8.36790800	-0.40167500	0.05979400
H	8.69388500	0.02088900	0.77147500	O	6.57527000	0.56803300	0.36000600
O	7.24423900	0.78146200	-0.50471300	H	7.51880700	-0.64953500	-1.81354400
H	9.24756400	0.27306600	-0.89243100	H	7.36866400	2.07240200	0.47420700
H	7.53783700	2.05169500	0.03272700	I	4.83946000	2.78024400	-2.40375900
I	5.38555500	3.30631400	-2.53530300	K	4.19149200	1.52609700	1.37114600
K	4.86490400	0.66177900	0.74839300	C	7.26013000	5.29083900	0.37779900
C	7.33086500	4.83413200	1.83189300	H	6.72174000	6.01185000	0.99255800
H	6.73752800	5.07466500	2.71441400	H	8.33928200	5.44306100	0.44952400
H	8.39871100	4.91089400	2.05239200	H	6.96910000	5.42140300	-0.67041800
H	7.10838900	5.55307700	1.03628000	K	2.66101700	0.03521000	-2.35582600
K	2.58766100	1.13820700	-2.90534100	C	2.17549600	-0.78092500	1.20822300
C	2.43066700	-1.01750000	-0.15279800	O	2.42999300	-0.23756000	0.07283600
O	2.46442500	0.16683500	-0.64378000	O	2.66975800	-0.42768400	2.30087700
O	3.40097600	-1.60682500	0.37605100	C	1.18744000	-1.95117600	1.18367300
C	1.08470800	-1.74382700	-0.24966000	H	1.57992500	-2.74973800	0.54371200
H	0.83131300	-1.89971100	-1.30521900	H	1.01391000	-2.34195300	2.18736200
H	1.11852800	-2.70904900	0.25825100	H	0.23757200	-1.62266300	0.74776600
H	0.29538100	-1.12167600	0.18357400				

73'-TS

73-TS				C	3.03710100	4.66163100	-3.58734500
C	5.21138800	-1.17281600	-4.67560100	C	2.76039900	5.45971600	-2.46014000
C	4.36562500	-0.43080300	-5.52607800	C	1.43322200	5.52024900	-2.01354900
C	3.02970900	-0.84797800	-5.65282100	C	0.40846300	4.85721400	-2.68968400
C	2.54737600	-1.96953300	-4.97312300	C	0.70098400	4.12565000	-3.84305200
C	3.40958900	-2.69930600	-4.14624600	C	2.01875500	4.01298400	-4.31320900
C	4.74721500	-2.31438600	-3.98648700	H	1.20426600	6.11379400	-1.13302500
H	2.37264000	-0.29713800	-6.32156600	H	-0.61205400	4.92213500	-2.32568300
H	1.51801300	-2.29007200	-5.10909400	H	-0.09922300	3.64325500	-4.39984400
H	3.04871600	-3.58529800	-3.62982900	O	4.32097000	4.56678900	-4.10622000
O	6.55151000	-0.89951500	-4.55709000	C	5.33966100	3.95639400	-3.34751500
C	6.97945400	0.32451800	-3.96835300	Pd	4.93525400	2.07747200	-2.17991300

C	3.83192300	6.26984500	-1.77599600	C	5.68160500	-1.89843300	-5.10406100
H	3.39190300	7.14202000	-1.28522700	H	5.60713800	-2.96870700	-5.31686200
H	4.34563300	5.68434200	-1.00589800	H	4.66543400	-1.52711500	-4.92183200
H	4.57712100	6.62136700	-2.49533600	H	6.05940900	-1.39195000	-5.99673600
C	3.96023700	-0.26076200	-0.27439400	H	5.93093600	2.24026100	-5.13294400
O	2.86112100	-0.06342500	0.27897500	C	7.45333600	2.42449500	1.01441000
O	4.20846600	0.07581700	-1.50399000	O	7.23276500	1.34592000	0.28147700
C	2.31925900	3.21912700	-5.56271500	O	6.56278300	3.17864400	1.40290800
H	3.22864900	3.57620400	-6.04899200	C	8.82191000	1.14861600	-2.56709100
H	2.45173900	2.15690000	-5.32974700	H	9.40085200	1.36385600	-3.47075200
H	1.49144100	3.29829500	-6.27355900	H	8.10559100	1.96758400	-2.45132500
C	5.10950200	-0.88856500	0.48811500	H	9.49527200	1.15481500	-1.70613600
H	4.75750200	-1.37537000	1.39962300	C	4.67863100	0.05509000	-1.20240800
H	5.64244500	-1.60262300	-0.14417800	H	3.71614000	-0.46160000	-1.28430800
H	5.80949800	-0.08712100	0.74996400	H	5.55950900	-0.59601200	-1.23688300
C	4.69784100	1.04958900	-4.14138000	O	4.71723500	1.14240100	-0.47457400
H	4.73633900	1.53076600	-5.12212900	H	4.47254600	0.18333800	-3.00182000
H	4.96796300	2.52875100	-3.71973100	H	6.25756500	1.28774800	0.02966200
H	5.57331900	0.40951900	-3.99113600	I	5.78042900	4.30563400	-2.71685500
O	3.47912000	0.40997300	-3.99959700	K	4.24356200	3.61590900	0.30056900
H	3.53253300	-0.04585400	-3.12601600	C	8.91494600	2.64520600	1.30388700
K	1.67793800	1.81593400	-1.56564500	H	9.03566300	3.42754600	2.05236100
I	5.20710400	3.14338800	0.36221500	H	9.38097800	1.71444900	1.63689200
H	6.22822500	3.92997700	-3.98123700	H	9.40927300	2.94643200	0.37434200
H	5.56410400	4.47018600	-2.41619700				
C	-0.04055500	3.36452800	1.36365700	73-TS-b			
O	0.48866100	2.64600300	0.44483000	C	7.46962900	1.91416700	-5.62987600
O	0.29923600	3.34943900	2.57035000	C	7.57049600	1.20969800	-6.84317800
C	-1.15212100	4.31807000	0.91925500	C	8.77932300	0.56942900	-7.13428100
H	-1.62999300	4.79469900	1.77648300	C	9.85591600	0.63823500	-6.25045900
H	-0.72147000	5.09024200	0.27157100	C	9.73731100	1.36653300	-5.06879800
H	-1.89588300	3.77532800	0.32717600	C	8.54515000	2.02260100	-4.73456800
K	2.30676600	1.69798400	2.24266800	H	8.87656000	0.02475800	-8.07010000
				H	10.79069500	0.14027500	-6.49185000
73-TS-a				H	10.58294800	1.43891200	-4.38897600
C	7.23296100	-0.41715100	-3.74898100	O	6.28683300	2.58888400	-5.35414000
C	6.58339400	-1.64899300	-3.92059600	C	5.21422400	1.81170800	-4.86228000
C	6.80082300	-2.64459700	-2.95839600	H	5.28527700	0.77758100	-5.20322200
C	7.64343600	-2.42187700	-1.87011900	Pd	5.16182500	1.93976500	-2.82304400
C	8.30539800	-1.19879300	-1.74333500	C	6.41376700	1.17547800	-7.81310700
C	8.12014400	-0.18029700	-2.68330200	H	6.75910000	0.93131200	-8.82146300
H	6.30560700	-3.60565000	-3.07522600	H	5.66516200	0.42540400	-7.53122800
H	7.79701300	-3.20372600	-1.13170900	H	5.90175100	2.14155900	-7.84121400
H	8.96540100	-1.02088000	-0.89917400	H	4.28282800	2.27777100	-5.19440700
O	7.04683300	0.63112000	-4.63377100	C	8.13043300	2.49434900	0.30802400
C	5.77687200	1.26139400	-4.68086400	O	7.59667800	1.38612600	-0.18628200
H	5.04346500	0.67827900	-5.23967200	O	7.47137400	3.45356800	0.69859300
Pd	5.09935500	1.61348200	-2.75335000	C	8.43105800	2.81193200	-3.45442400

H	7.68817100	3.60721500	-3.53081000	C	4.62556900	0.55727900	-1.07352000
H	8.11730600	2.16406300	-2.62632000	H	3.55866500	0.36397000	-1.23601900
H	9.40000600	3.24746000	-3.18657700	H	5.23056400	-0.34071100	-0.89052500
C	4.61715900	0.48103700	-1.16991300	O	4.97672400	1.66752800	-0.50049500
H	3.53974800	0.30365800	-1.26703900	H	5.06342400	0.36219100	-2.69228700
H	5.21726000	-0.43258900	-1.06867200	H	6.55423800	1.58868300	-0.10321700
O	5.01251700	1.54880300	-0.53218500	C	9.58512000	2.51139100	0.60940600
H	4.93847000	0.35389400	-2.82488500	H	9.84884600	1.62368400	1.18997500
H	6.58971000	1.47308200	-0.24506200	H	10.03593900	2.40161000	-0.38225900
C	9.63769200	2.46354500	0.31252400	H	9.96696400	3.41204700	1.08881200
H	9.99852300	1.51642800	0.72129000	C	5.00026200	5.12378500	-3.33578800
H	9.98848800	2.52998600	-0.72260100	O	4.79909900	6.22288800	-2.76452700
H	10.02695800	3.30495800	0.88480200	O	5.41429800	4.09452500	-2.69322500
C	4.68271000	5.02401600	-2.98228100	C	4.74222300	4.99112700	-4.82610900
O	4.28629800	5.86171300	-2.15304400	H	5.58179400	4.48582400	-5.30725100
O	5.47005700	4.04109500	-2.65141800	H	3.85479600	4.36686300	-4.97847500
C	4.25813200	5.11568300	-4.43890900	H	4.56929700	5.96965700	-5.27699500
H	5.05104200	4.74456400	-5.09083600	K	3.77733600	8.28943200	-1.82268400
H	3.37482300	4.48354500	-4.58798200	I	3.06238400	7.14646900	1.20285900
H	3.98686500	6.14280400	-4.68804600	K	4.99982200	4.48059700	0.00388300
K	5.09951900	4.36737200	-0.04000900				

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73-TS-c				C	5.41370000	-0.73115300	-4.11103200
C	7.81641600	1.72492300	-5.33967800	C	4.73093300	-0.21370800	-5.22937700
C	8.04456200	0.91057700	-6.46347500	C	3.45595400	0.33803500	-5.02331100
C	9.28061000	0.26437000	-6.56749500	C	2.86785100	0.35588100	-3.75580100
C	10.26109800	0.43345600	-5.59022000	C	3.56226700	-0.17697500	-2.66417600
C	10.01848900	1.26898200	-4.50236800	C	4.84256800	-0.72261700	-2.82200900
C	8.79444800	1.93461600	-4.35541500	H	2.90882700	0.72389200	-5.87988100
H	9.47607700	-0.36549800	-7.43168100	H	1.86441900	0.75282100	-3.62533700
H	11.21808900	-0.07124300	-5.68658900	H	3.10598600	-0.18122500	-1.67753800
H	10.78929500	1.41800200	-3.75003100	O	6.62175700	-1.38596900	-4.23390900
O	6.60853400	2.40655600	-5.24961400	C	7.78520600	-0.69248200	-4.64101500
C	5.48730200	1.66294400	-4.80404400	H	7.65998500	-0.18688300	-5.59822700
H	5.59374300	0.60648100	-5.05434100	Pd	8.38727900	0.83004700	-3.38639800
Pd	5.24523400	1.95056200	-2.79939500	C	5.31340500	-0.28037100	-6.61923500
C	6.99345700	0.76534200	-7.53773300	H	4.51997500	-0.24260600	-7.37068300
H	7.44375600	0.44244000	-8.48032400	H	5.98992900	0.56136400	-6.80722200
H	6.23127700	0.02492100	-7.26704800	H	5.87958900	-1.20496500	-6.76190300
H	6.47309900	1.71299100	-7.70330900	H	8.57254500	-1.44262500	-4.69567700
H	4.59736200	2.09063600	-5.27357700	C	6.67137100	2.34780900	0.01496100
C	8.08893700	2.60724100	0.45122100	O	7.95604600	2.50169100	0.31902800
O	7.54392300	1.46608200	0.04196800	O	6.29662200	1.92604200	-1.07773400
O	7.44742500	3.63067600	0.65609400	C	5.60499800	-1.28832800	-1.65215800
C	8.54527700	2.83321400	-3.17013400	H	4.95596900	-1.39179500	-0.77813400
H	7.81167800	3.60968300	-3.39100400	H	6.03258800	-2.26409600	-1.89680400
H	8.15211600	2.25439700	-2.32618800	H	6.43206200	-0.62270100	-1.38874900
H	9.47730200	3.30588900	-2.84245400	C	9.89430200	0.73897300	-1.70990400

H	9.70470800	0.11683900	-0.82650400	K	7.16408800	1.30951300	0.59471800
H	10.78250600	0.45679600	-2.28602600	I	10.29519600	2.57854600	0.36851500
O	9.54828300	1.99193200	-1.66396100	O	6.39137700	5.40018200	-0.39979900
H	8.68784500	-0.38827300	-2.41151500	K	8.82858700	5.17773300	-1.14876500
H	8.53190000	2.22169800	-0.46567800	C	3.28006400	0.79985500	0.39866600
C	5.73271800	2.78905600	1.10084600	H	3.66226800	0.21079000	1.23848400
H	6.18994000	2.70154900	2.08741500	H	2.19569400	0.70639500	0.34657400
H	5.49787600	3.84324800	0.90617800	H	3.56978600	1.84454000	0.55621000
H	4.80839600	2.21163000	1.04555300	C	4.18235000	5.06816500	0.48267500
K	8.88033500	4.55754200	-2.15687300	H	4.25825800	6.10916300	0.79906300
I	5.80860200	5.86600300	-1.49605300	H	3.40625300	4.98729800	-0.28524500
K	4.85665700	2.92170500	-3.08912500	H	3.88706500	4.43546200	1.32492100
I	7.76474500	2.89211300	-5.17867000				

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73-TS-e				C	4.97017800	5.59717100	-3.18662900
C	4.04163800	4.96826100	-3.57016500	C	5.58928300	6.83170300	-2.92320100
C	4.08348500	6.27801500	-3.05882500	C	4.86109400	7.79585200	-2.21591500
C	2.92581300	6.78712100	-2.45998800	C	3.55763700	7.53877200	-1.79156200
C	1.76539400	6.01930000	-2.37150400	C	2.96432200	6.31078500	-2.07956900
C	1.74657500	4.73002200	-2.90066400	C	3.65535600	5.31710400	-2.78275900
C	2.87899100	4.18158600	-3.51699800	H	5.32117100	8.75933600	-2.01104000
H	2.94025500	7.79946300	-2.06392600	H	3.00253600	8.29827500	-1.24828700
H	0.87489300	6.43041900	-1.90458500	H	1.94479700	6.11219700	-1.75835800
H	0.83795000	4.13475800	-2.85207300	O	5.64636100	4.66141000	-3.95759200
O	5.15916800	4.45049900	-4.21749300	C	6.65512900	3.89654400	-3.33613900
C	6.20259300	3.99128100	-3.38704000	Pd	5.89062100	2.27758700	-2.38915100
Pd	5.75863400	2.34665300	-2.28227700	C	6.98767400	7.11905000	-3.41423500
C	5.33218400	7.12293600	-3.13875600	H	7.15888400	8.19649200	-3.49061400
H	5.07613500	8.18015700	-3.25808500	H	7.74785500	6.71250300	-2.73632000
H	5.91071900	7.01974000	-2.21329800	H	7.15666100	6.66658200	-4.39544700
H	5.96068700	6.82188900	-3.98107000	C	3.93615000	0.50988300	-0.89443400
C	3.94649900	0.35709800	-0.87919600	O	3.09181400	0.34983500	-1.86265800
O	3.15545500	-0.02287400	-1.82873500	C	3.01168000	3.98662700	-3.07486300
C	2.83117700	2.79262400	-4.10350800	H	3.40903700	3.53609000	-3.98674900
H	3.69711100	2.58980700	-4.73176900	H	3.20819000	3.28856300	-2.25399600
H	2.81613600	2.03114000	-3.31808500	H	1.92667700	4.08958300	-3.17381600
H	1.92245400	2.65759700	-4.69992800	C	5.40817900	0.06043200	-4.12183200
C	5.47645600	0.03950400	-4.06232600	H	5.92534500	0.12900900	-5.08852600
H	5.96686100	0.21531500	-5.02963100	H	6.26038400	1.43387800	-3.71723500
H	5.86040400	1.58723200	-3.69380800	H	5.93403400	-0.50350100	-3.33901100
H	6.11945900	-0.35160800	-3.26347500	O	4.15438100	0.17810300	-4.09268600
O	4.23146700	-0.15156800	-4.03754400	H	3.57186400	0.20116800	-2.80965100
H	3.66784800	-0.16957100	-2.76688900	H	7.35306300	3.59570300	-4.11655500
H	7.05466600	3.79638700	-4.04255100	H	7.15365500	4.44277900	-2.52753000
H	6.43176200	4.72537900	-2.60542900	O	5.17507100	0.37027400	-1.01949500
O	5.19493700	0.40084800	-0.98501000	C	6.05284100	4.14083700	0.07480300
C	5.49308800	4.58131800	-0.10889400	O	5.26442800	3.45865100	-0.68248600
O	5.58735600	3.30415000	-0.29129900	O	7.25369300	3.86034900	0.29522500

K	7.43713300	1.30629900	0.08670900
C	3.34772100	0.96165900	0.41516700
H	3.82086600	0.43115600	1.24561700
H	2.26610100	0.83065600	0.44427300
H	3.59791200	2.02628200	0.49887100
C	5.42617200	5.36984800	0.71219300
H	6.05513000	5.75531700	1.51622600
H	5.30920500	6.13534300	-0.06114700
H	4.42408600	5.13783800	1.08214200

73-TS-g

C	4.48274200	4.88101100	-4.38196800
C	4.59582500	6.16922200	-3.84032500
C	3.43359000	6.76624700	-3.33629400
C	2.20641400	6.11053100	-3.38455400
C	2.11892500	4.84333600	-3.96127700
C	3.25351500	4.20714500	-4.47389600
H	3.50176500	7.76223200	-2.90624800
H	1.31654600	6.59163900	-2.98862600
H	1.15920100	4.33625500	-4.02080900
O	5.58895000	4.22742100	-4.92528200
C	6.59354000	3.78893300	-4.05339200
Pd	5.87256400	2.50534300	-2.63831200
C	5.91213600	6.90442900	-3.79532900
H	5.74892900	7.98599200	-3.81907200
H	6.45729200	6.67456300	-2.87185300
H	6.54866800	6.63403000	-4.64270400
C	3.77397200	0.79089100	-0.88394900
O	2.95724700	0.45851700	-1.84098700
C	3.17052100	2.84298300	-5.11095700
H	3.68757400	2.82564700	-6.07518800
H	3.64440200	2.07478500	-4.49314300
H	2.12847500	2.55016000	-5.26664300
C	5.36504400	-0.26166200	-3.95579400
H	5.93782100	-0.30283300	-4.89322300
H	6.07143100	1.39681600	-3.78343100
H	5.90611200	-0.52512700	-3.03684400
O	4.12145100	-0.23484900	-3.98519300
H	3.45636100	0.11921100	-2.68150800
H	7.35179700	3.30466700	-4.66723800
H	7.01183400	4.58938300	-3.43964800
O	5.01255900	0.65357800	-0.95730400
C	3.12314600	1.39997600	0.32660300
H	3.53727700	0.95286300	1.23413500
H	2.03985000	1.28401200	0.30405200
H	3.38561000	2.46482600	0.33198400
I	5.78235100	4.37140200	-0.49138800
K	7.32373700	1.38091600	-0.03776200

73-TS-h

C	4.47099500	4.65769500	-5.28506000
C	4.78694600	5.90540200	-5.84745600
C	3.79346900	6.88998700	-5.85981400
C	2.52703700	6.63247100	-5.33615200
C	2.23660700	5.37813000	-4.80306700
C	3.20149700	4.36355100	-4.76815900
H	4.01661700	7.86114400	-6.29419600
H	1.76378400	7.40501500	-5.35548800
H	1.24557900	5.17261800	-4.40657600
O	5.43929000	3.65668200	-5.31432100
C	6.42634200	3.71278700	-4.31442000
Pd	5.96009200	2.50448500	-2.73513900
C	6.15278600	6.15851400	-6.43873400
H	6.13737600	7.03107900	-7.09717000
H	6.90358800	6.34662000	-5.66119900
H	6.49570500	5.29212800	-7.01245500
C	3.69707100	0.95816300	-1.09323600
O	2.96986100	0.50794400	-2.06678900
C	2.89397100	3.01446200	-4.17515100
H	3.39936400	2.20531700	-4.70669700
H	3.23199800	2.97164200	-3.13306200
H	1.81800200	2.81845800	-4.17530200
C	5.48912700	-0.21892500	-3.97752600
H	6.11953700	-0.32907200	-4.87040500
H	6.23533800	1.35489200	-3.81895000
H	5.94676000	-0.48881800	-3.01661600
O	4.24833200	-0.14344200	-4.10522700
H	3.53829000	0.17649700	-2.89197000
H	7.36598700	3.38815300	-4.77429500
H	6.50400000	4.72135800	-3.89366400
O	4.94640300	0.91037700	-1.06941100
C	2.92807800	1.59951700	0.03483900
H	3.19027600	1.12414100	0.98565000
H	1.85175700	1.53200700	-0.12061000
H	3.23636500	2.65005800	0.08707800
I	5.93619400	4.49445100	-0.72176600
K	6.71164000	1.30349400	0.90611500
K	9.12310100	3.34661100	-2.21457400
I	9.94085600	0.97851400	-0.00289600

73-TS-partA

C	4.51631700	-1.17667400	-4.46603700
C	5.04520300	-0.79568800	-5.70944100
C	4.48399900	-1.35902400	-6.86066100
C	3.43052000	-2.26801500	-6.76957500
C	2.92666400	-2.62876000	-5.52091600

C	3.45906600	-2.09117000	-4.34179000	C	5.67484800	-3.26960500	-2.99615600
H	4.87810000	-1.07733700	-7.83351900	C	6.46549400	-2.12276600	-3.15598500
H	3.00041600	-2.69305500	-7.67161500	H	2.78614400	-2.20501500	-4.44842400
H	2.09936200	-3.32997900	-5.45200800	H	3.75598100	-4.20039100	-3.31996500
O	5.10972600	-0.65800400	-3.31369700	H	6.10749600	-4.13483600	-2.50377500
C	4.66186300	0.66983200	-2.91162200	O	6.70138100	0.09748000	-3.96033800
H	4.10880000	1.12390300	-3.73329500	C	6.44132900	1.28409600	-3.21260400
Pd	3.61478700	0.52317000	-1.20895300	H	5.57177100	1.82497400	-3.62011600
C	6.18151000	0.19381400	-5.78687400	Pd	5.95460200	1.26071000	-1.21295200
H	6.60501000	0.22702000	-6.79384400	C	3.98125600	0.18570000	-4.97035000
H	5.84836400	1.20490100	-5.52809300	H	3.15872900	-0.11849500	-5.62387500
H	6.98022600	-0.06142400	-5.08186300	H	3.58886600	0.93543200	-4.27261900
H	5.55797600	1.25642800	-2.67377600	H	4.74476100	0.67829300	-5.57854500
C	2.90354100	-2.47074700	-2.99179900	H	7.33863900	1.89770400	-3.34058600
H	3.61532100	-3.06110400	-2.39885500	C	9.95104500	0.49131600	-0.57937400
H	2.66004800	-1.58424000	-2.39562300	O	9.22563000	1.19191800	-1.45214400
H	1.99883100	-3.07391400	-3.10068300	O	9.46573000	-0.17497400	0.32275100
I	2.11656800	2.57500800	-1.99078500	C	7.89975300	-2.11647000	-2.68667300
C	3.77635200	-1.02642100	0.93647000	H	8.24363900	-1.10198100	-2.48326200
O	2.88682100	-0.15531200	0.88622000	H	8.00547500	-2.73501500	-1.79029600
O	4.61554400	-1.19470700	-0.03720200	H	8.55612100	-2.52881200	-3.46348700
K	6.38908200	-2.04416800	-1.50780900	H	6.40204700	-0.19372800	-1.30317300
C	3.91709900	-1.93455400	2.14113800	H	8.25953300	1.07629800	-1.26373800
H	3.82580700	-2.98001600	1.82798500	I	4.98078100	1.59576000	1.36374600
H	3.15168000	-1.70612700	2.88295900	K	7.38854400	-1.42027700	1.34897700
H	4.90944100	-1.80648500	2.58626400	C	11.42906900	0.60826900	-0.84642300
73-TS-partB				H	11.98669100	0.06807500	-0.08246800
C	-1.55070500	0.09889000	-0.03480500	H	11.65043200	0.19431000	-1.83496200
O	-0.69650400	0.37106200	-0.95105000	H	11.72220200	1.66166500	-0.86045000
O	-1.43211700	-0.82282500	0.81419300	K	3.73869700	-1.27004000	-0.67852200
C	2.18063700	1.94251700	0.45174300	C	5.92999700	-3.88813600	0.32814400
H	3.17788600	1.79200100	0.87864400	O	5.17266600	-2.88376500	0.56886800
H	1.49500300	2.20663800	1.27171600	O	7.18447000	-3.85207300	0.30303800
O	1.79533800	0.75030300	-0.20649700	C	5.22169300	-5.21866100	0.06064100
H	2.23478700	2.79808700	-0.23715700	H	4.53552800	-5.10683100	-0.78619600
H	0.85951300	0.84314800	-0.53436700	H	5.93939300	-6.01284400	-0.15112900
K	0.82289200	-1.68081400	-0.05542000	H	4.61662000	-5.49120600	0.93157300
C	-2.80050100	0.97738900	0.00335100	75-TS			
H	-3.50684100	0.62789200	0.75812200	C	5.54903600	-1.50597000	-3.99361300
H	-2.50813700	2.00990500	0.22319200	C	4.34204400	-0.80952400	-4.20138000
H	-3.27399400	0.98398800	-0.98320900	C	3.13715400	-1.48077200	-3.94267100
74				C	3.13098900	-2.81101100	-3.51162400
C	5.89250400	-0.99598100	-3.78060500	C	4.34291700	-3.48427900	-3.32233100
C	4.56209100	-1.00649700	-4.24857400	C	5.56983200	-2.84408000	-3.54860700
C	3.80426100	-2.17322200	-4.06608600	H	2.19796300	-0.96128300	-4.11668800
C	4.35187400	-3.29972200	-3.44124500	H	2.18845400	-3.32935700	-3.35541600
				H	4.34214100	-4.52370200	-3.00496700

O	6.76283400	-0.94721400	-4.31705900	H	4.10145900	1.20790200	-6.79009400
C	7.28871400	0.12990900	-3.54875000	H	4.73704300	1.80894200	-5.25244400
H	6.90051500	1.09937100	-3.89779600	H	5.81052800	0.96204600	-6.37765700
Pd	6.56219400	0.50386200	-1.60249300	H	8.17647200	0.57387700	-4.04052400
C	4.34287500	0.60633700	-4.72068200	C	6.76739600	3.64798000	1.39389300
H	3.37791800	0.85934800	-5.16793700	O	7.57857500	2.79217800	0.77658100
H	4.53664300	1.32616100	-3.91654000	O	5.74488700	3.30906100	1.97691600
H	5.12309400	0.74048500	-5.47544000	C	6.17765700	-3.12131600	-3.34619800
H	8.36655200	0.11143400	-3.71319300	H	6.99486400	-3.34949400	-4.03775300
C	10.05492000	1.50408900	-0.04161000	H	6.61437800	-2.54884800	-2.52293200
O	9.29042400	2.05627600	-0.98233600	H	5.78282000	-4.06061600	-2.94983900
O	9.75771700	0.48576600	0.56687200	C	7.14779000	-0.53323600	0.03225600
C	6.88103000	-3.55226000	-3.31949900	H	6.74924400	-1.55132900	-0.06137300
H	7.59419000	-3.31995700	-4.11376500	H	8.23680600	-0.44359800	0.13054200
H	7.33551900	-3.24861000	-2.36954300	O	6.38581900	0.39931900	0.49420000
H	6.73676400	-4.63494500	-3.27567500	H	7.60488200	-0.42129100	-2.39292000
H	7.50307400	-0.64417000	-2.03678100	H	7.15476000	1.89162600	0.76383500
H	8.44720200	1.53629300	-1.07876100	I	4.64721700	2.67208900	-2.00733500
I	5.31198700	1.55321500	0.57840000	K	4.02765200	1.27009700	1.64704000
K	7.94685100	-1.39620200	1.00816500	C	7.22845200	5.07635100	1.27103300
C	11.32252900	2.28622400	0.19162300	H	6.70043800	5.70099400	1.99104900
H	11.96697100	1.74741900	0.88523600	H	8.30948300	5.14798800	1.41163400
H	11.83806800	2.45589800	-0.75742100	H	6.99985100	5.41953600	0.25617400
H	11.06778500	3.26698500	0.60522700	K	2.81174300	-0.29512100	-2.07396300
K	4.02778500	-1.60377200	-0.54101600	C	2.15943700	-1.16692600	1.46027400
C	6.55607900	-3.99879800	0.23098300	O	2.44022700	-0.65298800	0.31769400
O	5.73753300	-3.06145400	0.53728300	O	2.56863800	-0.73814300	2.56101800
O	7.79881900	-3.86328100	0.12723100	C	1.25024400	-2.39920100	1.43447800
C	5.94071800	-5.37384100	-0.04159900	H	1.71388200	-3.18629300	0.82914500
H	5.31476000	-5.31790700	-0.93951100	H	1.06595400	-2.77426700	2.44224700
H	6.71447000	-6.12795900	-0.19240100	H	0.29731100	-2.14279100	0.95857800
H	5.28991900	-5.66286700	0.78952500				

75-TS-b

75-TS-a				C	2.96156200	4.80356300	-3.17903200
C	5.40903900	-1.08663600	-4.62892700	C	2.76160900	5.82450900	-2.22811800
C	4.44526900	-0.32824100	-5.32131500	C	1.56440000	5.81967800	-1.49448600
C	3.14260600	-0.84713100	-5.40866800	C	0.58726900	4.84129300	-1.70403900
C	2.81011900	-2.07707400	-4.83397100	C	0.80017300	3.84464800	-2.66559500
C	3.78706700	-2.81115900	-4.15128800	C	1.98588900	3.81112000	-3.41272500
C	5.09831500	-2.32938300	-4.04030200	H	1.39175900	6.61007300	-0.76826200
H	2.39232300	-0.28669900	-5.96097800	H	-0.34643000	4.87500100	-1.14915300
H	1.80405900	-2.47421400	-4.93968700	H	0.03249700	3.09779800	-2.85489100
H	3.53857200	-3.77637800	-3.71751000	O	4.06573200	4.76703700	-3.98515700
O	6.73355500	-0.70804900	-4.60185600	C	5.35971100	4.47159800	-3.42984400
C	7.12040300	0.41421600	-3.83132500	Pd	5.57931200	3.53942100	-1.54314000
H	6.55687800	1.31193500	-4.08702700	C	3.79637100	6.89952300	-2.01881900
Pd	6.57119000	0.53935500	-1.74382000	H	3.35407100	7.78358200	-1.55192600
C	4.79455300	0.98509900	-5.97434400	H	4.60484100	6.54289400	-1.37037900

H	4.24471900	7.19329900	-2.97205600	C	2.70399800	8.32738700	-1.57131500
C	2.24494100	2.75407300	-4.45587200	C	2.10901700	7.06627600	-1.44665100
H	2.38724100	3.20821000	-5.44124900	C	2.59512100	5.96741900	-2.16838800
H	3.16526900	2.20396600	-4.23298900	H	4.23770300	9.48471200	-2.55244700
H	1.41511700	2.04431600	-4.51534700	H	2.30581500	9.17473700	-1.01960300
H	5.14666500	2.91872800	-2.89777500	H	1.25222800	6.93067100	-0.79163200
I	5.90092200	3.24156800	1.17468100	O	4.13456200	5.09144100	-3.76667600
H	5.94958200	4.11387200	-4.27454400	C	5.35380400	4.46329500	-3.37741200
H	5.83233400	5.38710500	-3.04447400	Pd	5.42222800	3.53264200	-1.47352000
K	2.79470500	2.86172000	-0.16571800	C	5.46845100	7.62763800	-4.11913700
75-TS-c				H	5.46864700	8.64665400	-4.51667600
C	2.92267800	4.75848100	-3.34655200	H	6.42608000	7.47254000	-3.60713900
C	2.67200800	5.74237900	-2.36965800	H	5.41440800	6.92437400	-4.95358400
C	1.43397600	5.71773800	-1.70872900	C	1.95793400	4.60549600	-2.06988800
C	0.46525400	4.75794000	-2.01655600	H	1.61631400	4.26594800	-3.05297500
C	0.72719400	3.80149500	-3.00540100	H	2.68284800	3.86482800	-1.71420600
C	1.95571200	3.78694400	-3.68023000	H	1.10531700	4.61909500	-1.38584800
H	1.22490600	6.47608200	-0.95838500	H	4.86281400	2.97568400	-2.79493900
H	-0.49655200	4.77237500	-1.51134700	H	5.70497800	3.92918100	-4.25992200
H	-0.03156900	3.06790100	-3.26829700	H	6.11702300	5.19810700	-3.08952200
O	4.07659600	4.74218100	-4.08208400	K	5.19363200	6.73135700	0.15347600
C	5.33235400	4.40910200	-3.45624700	C	5.43983500	3.67409900	1.60868400
Pd	5.49128200	3.49287500	-1.56044400	O	6.13220900	3.30865100	0.57364200
C	3.69875800	6.80061100	-2.05893500	O	4.71627300	4.68225100	1.66014600
H	3.23496800	7.66990300	-1.58494000	C	5.58903500	2.77336100	2.82781600
H	4.46759800	6.41332600	-1.38013000	H	4.96407800	3.12458300	3.64938900
H	4.20405300	7.12644100	-2.97256900	H	5.31404900	1.74869200	2.56031800
C	2.26949800	2.77047500	-4.74886400	H	6.63666700	2.75540500	3.14790400
H	2.47657500	3.26222500	-5.70435300	I	8.38893300	6.73035400	-1.14050000
H	3.16913900	2.19940300	-4.49495100	K	8.47280300	3.42701900	-0.52695700
H	1.43854700	2.07325600	-4.88849900	75-TS-e			
H	4.99891600	2.93890400	-2.92170800	C	6.19698500	2.18798100	-5.30619100
H	5.95363300	4.02823100	-4.26880800	C	4.86164600	2.37213400	-5.71478500
H	5.80833100	5.32003200	-3.06233800	C	4.15895900	1.25540900	-6.19300500
K	2.65549800	2.64951100	-0.45882400	C	4.76455400	-0.00104000	-6.27939100
C	5.31134900	3.04507500	1.53507900	C	6.09841000	-0.15767500	-5.88064900
O	5.99844600	3.20770500	0.46608400	C	6.83059800	0.93065000	-5.38546500
O	4.07720700	2.83754500	1.59654600	H	3.12932900	1.38369800	-6.51645900
C	6.12444100	3.09834800	2.82469600	H	4.21192600	-0.84584500	-6.68207700
H	5.47499100	3.02811400	3.69846300	H	6.58448100	-1.12653700	-5.97189200
H	6.84268700	2.27218100	2.83208000	O	6.97457000	3.24107400	-4.89744300
H	6.70276700	4.02631100	2.85809000	C	6.70748500	3.85411800	-3.62844900
75-TS-d				H	5.84106100	4.52201500	-3.68781800
C	3.70470600	6.16344800	-3.01563300	Pd	5.76333800	2.72686100	-2.03675400
C	4.30866400	7.42664500	-3.17579700	C	4.22157100	3.73488700	-5.66626300
C	3.79062500	8.50098300	-2.43290600	H	3.33965500	3.77417800	-6.31170500
				H	3.91343500	3.98539800	-4.64615400

H	4.92993100	4.50157900	-5.99469800	H	2.03225000	0.52011800	-0.69893800
H	7.59119400	4.45370500	-3.41144100	I	5.50217900	1.95623400	0.55597100
C	8.26878500	0.79562300	-4.95287900	H	6.02892600	4.08563800	-4.46636100
H	8.91299600	1.46394900	-5.53239800	H	5.72025100	5.08818200	-3.02468200
H	8.38740100	1.08060300	-3.90241300	O	3.21213300	-1.46039500	-0.25352600
H	8.62496800	-0.23055600	-5.08111400	K	4.80488000	-0.41232600	-2.01169400
C	4.88394700	1.83671500	-0.14396100	C	2.18679200	-1.36531300	1.92708800
O	5.64993700	0.94385600	-0.60431900	H	2.76146100	-0.72272300	2.60312200
K	4.51517400	-0.09942400	-2.94664600	H	1.13109900	-1.26383700	2.18772000
C	2.68479500	2.86650000	-2.51544300	H	2.52014300	-2.39638600	2.04263100
O	3.67009000	3.64175500	-2.29229100				
O	2.71790600	1.60633000	-2.48262100	75-TS-g			
C	1.36932600	3.54083400	-2.89824500	C	2.83675800	4.42284700	-2.94899200
H	1.32293600	4.56177800	-2.51492800	C	2.80742700	5.70215100	-2.35780300
H	1.30934900	3.58349900	-3.99232100	C	1.63304000	6.09940100	-1.70018200
H	0.52062700	2.95417800	-2.53939600	C	0.51544300	5.26065800	-1.63657500
H	5.25333600	2.54098500	0.61861800	C	0.56339300	3.99681900	-2.23680000
H	3.80460700	1.80655600	-0.33422300	C	1.72123400	3.56198600	-2.89498300
H	7.23591700	2.71175200	-2.59782500	H	1.59189500	7.09022500	-1.25443800
				H	-0.39438800	5.60007200	-1.14881500
75-TS-f				H	-0.30578300	3.34429400	-2.20317100
C	3.77685800	5.87597300	-4.32718100	O	3.90619800	3.98283100	-3.68075300
C	4.12124000	6.44334800	-5.56274500	C	5.15884600	3.69246700	-3.03403100
C	3.82791800	7.79727700	-5.76590500	Pd	5.26278700	3.34602400	-0.94775800
C	3.22111600	8.55596400	-4.76622400	C	3.99510200	6.62496500	-2.44960800
C	2.88769500	7.96546200	-3.54698500	H	3.69849200	7.66329100	-2.27878700
C	3.15661700	6.61363400	-3.30625300	H	4.75279000	6.36244300	-1.70241500
H	4.07985500	8.25484700	-6.71927600	H	4.46532600	6.55214000	-3.43438100
H	3.00304400	9.60601500	-4.93802700	C	3.21410400	0.22329100	-0.32466700
H	2.41044600	8.55612100	-2.76936800	O	3.26505600	-0.35029400	-1.53642500
O	4.02397400	4.52334200	-4.10865900	C	1.80259100	2.20996700	-3.55584800
C	5.34395000	4.24918900	-3.63049000	H	1.79579200	2.30333900	-4.64719500
Pd	5.35052400	2.94194600	-1.98184400	H	2.74411000	1.71569000	-3.29827900
C	4.78587200	5.61062400	-6.63094000	H	0.95754600	1.57842600	-3.26300000
H	4.61015700	6.03265200	-7.62438900	H	4.75643400	2.40336400	-2.06923500
H	5.87162700	5.56466500	-6.48137500	H	2.51143100	-0.00715100	-2.04661700
H	4.41237800	4.58311700	-6.61267800	I	5.57614400	3.70161900	1.76280700
C	2.43742400	-0.89779800	0.51826300	H	5.67666700	3.02326900	-3.72220300
O	1.76171100	0.19759000	0.20847100	H	5.76197600	4.60643500	-2.93043400
C	2.77824300	5.95030500	-2.00557800	O	2.30259600	0.97952700	-0.01268800
H	1.95800200	5.23843800	-2.15453200	K	2.32666000	3.53385600	0.59717400
H	3.61265300	5.38611500	-1.57617000	C	4.37604400	-0.13022800	0.55157500
H	2.45069200	6.68843700	-1.26911500	H	4.85435300	-1.05656700	0.23261400
C	2.71163200	2.39022700	-2.15176700	H	5.09726400	0.69406700	0.48454900
H	2.82130500	2.97090000	-3.07483700	H	4.04515700	-0.19417300	1.58921500
H	5.28236100	2.52587600	-3.47194900				
H	2.58925200	2.95617300	-1.21583900	75-TS-h			
O	2.53284500	1.15731000	-2.17306800	C	3.30536200	4.38301200	-3.65740900

C	3.13268500	5.57708200	-2.92697400	H	3.81062700	1.01428100	-6.58356300
C	2.05098200	5.65230600	-2.03521800	H	4.51365900	1.65557600	-5.09393200
C	1.15792600	4.58593600	-1.89042600	H	5.57451100	1.07595600	-6.38912700
C	1.33025200	3.42582100	-2.65582000	H	8.27602200	0.94435600	-4.16792000
C	2.40174700	3.30595200	-3.55425200	C	7.09601100	-3.04728500	-3.86330700
H	1.89275200	6.57132100	-1.47637600	H	7.71431100	-3.26403200	-4.74169000
H	0.30956200	4.67359800	-1.21664500	H	7.67937300	-2.37849700	-3.22729200
H	0.61535100	2.61022300	-2.57627700	H	6.92272700	-3.98726500	-3.33135800
O	4.32477800	4.28979000	-4.57538200	C	6.69748700	-1.23040500	-0.56424700
C	5.64557600	4.09338500	-4.06578200	H	6.55992800	-2.16916700	-1.11939700
Pd	5.95392400	2.14687700	-3.26748800	H	7.67293200	-1.10728000	-0.07411300
C	4.05033500	6.75447200	-3.15045800	O	5.67519100	-0.58478800	-0.12986900
H	3.57543000	7.68131300	-2.81721200	H	7.85717200	-0.13601900	-2.55498100
H	4.99869800	6.65131700	-2.61281200	I	4.41448700	2.39087500	-2.03730000
H	4.29083000	6.84461300	-4.21370300	K	4.13940600	1.05849100	1.39285600
C	2.58696100	2.08162000	-4.41252300	K	3.19477700	-0.99841200	-1.74604400
H	2.61330800	2.35454800	-5.47195200	C	1.76659500	-0.80958300	1.70023000
H	3.54335900	1.59137400	-4.19165500	O	2.20299400	-0.73397700	0.49820600
H	1.77960000	1.36197200	-4.25255400	O	2.26213100	-0.20499600	2.68116000
H	6.29332400	2.63039100	-4.69302000	C	0.55021900	-1.70999500	1.92241900
I	5.83776100	0.38146000	-1.12356000	H	0.78672800	-2.73145700	1.60475100
H	6.31336300	4.54305200	-4.79910800	H	0.24790700	-1.71290400	2.97066700
H	5.79464200	4.61585400	-3.11256100	H	-0.28059100	-1.36189700	1.29949600
K	3.64886000	3.00614800	-0.26489700				
C	5.88424000	5.69301000	-0.22841400	76-TS			
O	6.77873600	5.90580300	-1.08797900	C	3.62449200	4.93514300	-3.36936600
O	5.58390600	4.53974200	0.23663100	C	3.69214400	6.29425800	-3.01678200
C	5.06385300	6.87423200	0.29071100	C	2.57386300	6.87273500	-2.40823400
H	4.05099600	6.81027700	-0.12347000	C	1.42327300	6.12254100	-2.16844700
H	4.97793700	6.82278800	1.37988000	C	1.37534800	4.78521300	-2.55385900
H	5.50692800	7.82446000	-0.01066400	C	2.47162500	4.16343800	-3.16352300
K	7.85275200	3.50452900	-0.95300000	H	2.60433100	7.92549500	-2.13698500
				H	0.56082800	6.58499900	-1.69708700
				H	0.47489500	4.20177000	-2.37899800
75-TS-i				O	4.71792400	4.35544900	-4.00556200
C	5.78371400	-1.09362600	-4.77978400	C	5.80583600	3.99883900	-3.18384900
C	4.61108200	-0.49262400	-5.27264300	Pd	5.50786700	2.20950800	-2.26339800
C	3.42223500	-1.23803600	-5.22282500	C	4.92326200	7.11870600	-3.31348100
C	3.40151300	-2.53812700	-4.70972600	H	4.65925000	8.16970500	-3.46288600
C	4.58636600	-3.11939900	-4.24281800	H	5.65224200	7.08661900	-2.49154000
C	5.79419400	-2.41092100	-4.28084600	H	5.43377700	6.75515600	-4.20881900
H	2.51071200	-0.79690500	-5.61850500	C	4.10025800	-0.44311100	-1.26964300
H	2.47592100	-3.10836300	-4.70688500	O	3.32725600	-0.60480100	-2.29936700
H	4.58233400	-4.14113100	-3.87108800	C	2.40579900	2.70918200	-3.55466100
O	7.00492300	-0.45311200	-4.86137600	H	3.16548700	2.44203800	-4.28964700
C	7.24400400	0.64434100	-3.99686300	H	2.56009000	2.06854700	-2.67814100
H	6.58227500	1.49030700	-4.19377600	H	1.42098300	2.46237400	-3.96496200
Pd	6.49568900	0.37154400	-1.99772000	C	5.58191600	0.24046600	-4.46836400
C	4.63018300	0.89059300	-5.87031200				

H	6.08518900	0.67408000	-5.34322600	O	0.00213600	1.78474400	0.35149300
H	6.15972600	1.62454800	-3.61391900	O	0.01071300	1.74103300	2.57406800
H	6.20968300	-0.35839100	-3.79337200	C	1.24263100	3.48332300	1.48872800
O	4.33680600	0.10494400	-4.47667200	H	2.27463200	3.13242900	1.37542700
H	3.78082500	-0.32929500	-3.21039900	H	1.00237400	4.14765600	0.65648200
H	6.68989400	3.95539000	-3.81945500	H	1.15341700	4.01175900	2.43800500
H	5.93731500	4.72914300	-2.37626000	K	0.84526400	1.49356500	-2.18107000
O	5.27847300	-0.03070400	-1.33776600	I	-3.22337700	-1.85089600	0.52978900
K	7.36878100	0.92422800	0.06198800	I	-2.73830300	1.44226000	-1.54026200
K	7.36665200	5.18169100	0.08994400	C	0.79303100	-1.47574300	-4.39221200
I	4.43118600	3.23076700	0.16002100	O	0.45903300	-0.45701100	-3.69171600
C	3.46314400	-0.74358900	0.05988200	O	0.16790800	-2.56326500	-4.41341700
H	4.17974800	-1.24655100	0.71359400	C	2.06000000	-1.33520500	-5.23858400
H	3.21171100	0.22121200	0.51682900	H	2.21453200	-2.21451200	-5.86520700
H	2.55873600	-1.34166600	-0.05167500	H	1.99272900	-0.43864500	-5.86330000
C	9.92782500	3.60515000	0.21738500	H	2.92802100	-1.20751600	-4.58063300
O	8.87304400	2.89278700	0.37635900	K	-1.90441900	-1.81885100	-3.01349400
O	9.93034000	4.84530600	0.03074200				
C	11.26248600	2.85917800	0.25080800	77-TS-b			
H	11.30908100	2.16111400	-0.59305100	Pd	-1.39597500	0.58646400	0.42213700
H	12.10248100	3.55240700	0.18990900	C	1.03531500	-1.66404400	0.18300000
H	11.33463100	2.26675800	1.16880600	C	0.52825000	-2.05640900	-1.07162200
				C	1.37094000	-1.94996100	-2.18658900
77-TS-a				C	2.67622500	-1.46136100	-2.05822900
Pd	-1.45399400	0.19433400	0.55134700	C	3.16801300	-1.13287200	-0.79491800
C	1.72643100	-0.99118300	1.10343800	C	2.36999200	-1.25676000	0.35151600
C	1.82931700	-1.37568000	-0.24716900	H	1.00878800	-2.28836300	-3.15647700
C	2.82897100	-0.78302600	-1.03012200	H	3.32189200	-1.39207400	-2.92959700
C	3.70516800	0.16015300	-0.48079500	H	4.20241300	-0.81668200	-0.68273000
C	3.61994300	0.47557400	0.87722000	O	0.18800200	-1.81106600	1.25752000
C	2.65101400	-0.11532800	1.70070200	C	-0.28613100	-0.67280000	1.98231300
H	2.92147200	-1.07846400	-2.07222600	H	-1.20819600	-0.97970200	2.46577700
H	4.48500600	0.60331400	-1.09510900	H	0.40933100	-0.43673600	2.80473800
H	4.34596200	1.15225100	1.32229500	C	-0.87797500	-2.59034800	-1.18526900
O	0.75063600	-1.61484900	1.84443500	H	-1.10286200	-2.89201500	-2.21232800
C	-0.36527400	-0.88013700	2.35068200	H	-1.01974900	-3.45312500	-0.52764600
H	-1.19159000	-1.58052700	2.41944900	H	-1.61775100	-1.84602300	-0.87046200
H	-0.16252800	-0.57409700	3.39219800	C	2.94091400	-1.02077400	1.72877900
C	0.91882600	-2.44402200	-0.79590300	H	2.72296400	-0.01282500	2.09268700
H	-0.12045100	-2.25562200	-0.51024700	H	2.51128200	-1.72956200	2.44284300
H	0.99932100	-2.52287000	-1.88207600	H	4.02643300	-1.15240300	1.72264400
H	1.17340800	-3.41681100	-0.35952500	H	0.15731700	0.61068300	1.65595400
C	2.64983700	0.10743700	3.19402600	C	1.23684500	1.84400400	0.37823900
H	1.95034700	0.89142300	3.49544600	O	0.40915100	1.44699400	-0.49854500
H	2.35334000	-0.81090200	3.70932200	O	1.10042800	1.58454700	1.61064700
H	3.64770200	0.39111500	3.54015800	C	2.45987900	2.60321700	-0.07682200
H	-0.36164900	0.53999300	2.28264200	H	3.20357300	1.86706800	-0.40143400
C	0.34790400	2.27039300	1.47011900	H	2.21775800	3.24893100	-0.92341500

H	2.87686900	3.18803200	0.74319900
C	-3.13291500	0.97639500	-2.18094300
O	-2.79705100	0.65713600	-3.33629500
O	-2.23692400	1.36990200	-1.31200600
C	-4.59305100	0.97615800	-1.78663100
H	-4.86318700	-0.01721200	-1.41610700
H	-4.78250100	1.68673100	-0.98211700
H	-5.20279200	1.19619700	-2.66539800
K	-0.18267400	0.85534900	-2.97934400
I	-3.69222900	-0.19183200	1.55279800

77-TS-c

Pd	-1.47440100	0.53405900	0.42182600
C	0.65514900	-2.04100300	0.18353500
C	-0.03298900	-2.61891300	-0.90719200
C	0.65695500	-2.78350800	-2.11701300
C	1.99012900	-2.37133100	-2.25055100
C	2.65676100	-1.83212700	-1.14744200
C	2.01622100	-1.68835200	0.09255800
H	0.15139300	-3.26908400	-2.94992600
H	2.52039900	-2.52635700	-3.18676500
H	3.70898800	-1.56982300	-1.22814200
O	-0.03282600	-1.97588400	1.36184400
C	-0.31925900	-0.72955300	2.02048500
H	-1.22000300	-0.90211900	2.60092800
H	0.47388400	-0.52885800	2.76008600
C	-1.46075400	-3.07045800	-0.73646500
H	-1.84442500	-3.51736200	-1.65811200
H	-1.53589600	-3.80864800	0.06777200
H	-2.11319100	-2.24084500	-0.44685800
C	2.78913600	-1.27230100	1.32073800
H	2.61734300	-0.22896700	1.59616100
H	2.48448900	-1.88317600	2.17618800
H	3.86260700	-1.40933900	1.16452000
H	0.20932600	0.55670400	1.61647300
C	1.17996700	1.75243100	0.28788800
O	0.35146200	1.32256800	-0.56860900
O	1.07111900	1.49712000	1.52868100
C	2.37374700	2.54718300	-0.17809700
H	3.17593100	1.84310200	-0.42783000
H	2.12315700	3.12557200	-1.06894200
H	2.72873000	3.20283500	0.61758600
K	-0.07099900	0.18294100	-2.83760300
I	-3.74425300	-0.29316100	1.57371300
I	-2.89363200	1.67029400	-1.62879100

Table 3. Cartesian Coordinates and Energies for key intermediates and transition states using different DFT functionals.

29 (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.393440	1.220146	-1.309941
2	6	0	3.321338	0.176051	-1.428691
3	6	0	4.500457	0.269595	-0.684687
4	6	0	4.770517	1.389372	0.099410
5	6	0	3.860347	2.443386	0.136481
6	6	0	2.652734	2.383857	-0.567574
7	1	0	5.219493	-0.542203	-0.744526
8	1	0	5.701603	1.454632	0.653856
9	1	0	4.084914	3.339442	0.708995
10	8	0	1.229987	1.110734	-2.050761
11	6	0	0.026254	1.188634	-1.387395
12	1	0	-0.714076	1.626706	-2.057428
13	46	0	-0.595297	-0.649112	-0.995531
14	6	0	3.094858	-0.959390	-2.388121
15	1	0	3.657709	-1.841797	-2.078172
16	1	0	2.041842	-1.232815	-2.455815
17	1	0	3.431429	-0.663138	-3.387819
18	1	0	0.086073	1.600486	-0.370656
19	53	0	-3.240577	0.103840	-1.165039
20	19	0	2.201834	0.395389	1.811246
21	53	0	1.074172	-2.503114	0.307411
22	6	0	-0.603166	1.037795	2.452116
23	8	0	0.065141	0.118558	3.048573
24	8	0	-1.891242	1.042603	2.523184
25	19	0	-1.767913	-1.497205	2.314481
26	19	0	-2.292961	2.784406	0.836620
27	8	0	0.012405	1.924520	1.708391
28	6	0	1.698584	3.550245	-0.523919
29	1	0	1.126279	3.624497	-1.452533
30	1	0	1.008166	3.437394	0.320401
31	1	0	2.258950	4.478835	-0.393347
Zero-point correction=			0.200936 (Hartree/Particle)		
Thermal correction to Energy=			0.226058		
Thermal correction to Enthalpy=			0.227002		
Thermal correction to Gibbs Free Energy=			0.140249		
Sum of electronic and zero-point Energies=			-2637.435097		
Sum of electronic and thermal Energies=			-2637.409976		

Sum of electronic and thermal Enthalpies= -2637.409031

Sum of electronic and thermal Free Energies= -2637.495784

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2638.00845

33 (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.007625	2.081413	0.129135
2	6	0	-3.210922	3.436796	0.406673
3	6	0	-4.436957	4.001341	0.057467
4	6	0	-5.430816	3.233986	-0.541726
5	6	0	-5.205587	1.886739	-0.800424
6	6	0	-3.989520	1.285541	-0.471954
7	1	0	-4.610714	5.053496	0.264637
8	1	0	-6.380545	3.686060	-0.807373
9	1	0	-5.978182	1.285878	-1.271583
10	8	0	-1.764182	1.559824	0.437542
11	6	0	-1.725527	0.604613	1.495699
12	1	0	-2.571200	0.763000	2.179140
13	46	0	-1.827358	-1.187714	0.690058
14	6	0	-2.118076	4.237503	1.062682
15	1	0	-2.466321	5.244841	1.298269
16	1	0	-1.781733	3.759756	1.987246
17	1	0	-1.241599	4.324104	0.412671
18	1	0	-0.757243	0.691603	1.983396
19	6	0	0.511536	-1.722028	-2.047981
20	8	0	-0.833488	-1.600688	-2.035060
21	8	0	1.025674	-2.735190	-1.488062
22	6	0	-3.748111	-0.170160	-0.765019
23	1	0	-2.805948	-0.342635	-1.305825
24	1	0	-3.809438	-0.777412	0.168885
25	1	0	-4.541603	-0.589606	-1.386639
26	6	0	-3.131949	-3.573708	-0.775302
27	1	0	-3.877678	-3.569311	0.039142
28	1	0	-3.100672	-4.602007	-1.170493
29	8	0	-1.874843	-3.146753	-0.348258
30	1	0	-3.539040	-2.943276	-1.587911
31	1	0	-1.225418	-2.357947	-1.445673
32	6	0	1.036910	-1.292788	1.318292
33	8	0	1.085381	-0.158247	0.721250
34	8	0	-0.100846	-1.796622	1.719345
35	19	0	0.390037	1.280993	-1.266783
36	53	0	3.822971	2.135017	-0.430859
37	19	0	0.342857	-4.042145	0.571402
38	8	0	2.113507	-1.945782	1.560398

39	8	0	1.157566	-0.779616	-2.573954
40	19	0	3.021552	0.470195	2.328335
41	19	0	3.108612	-1.255281	-0.928528

Zero-point correction=	0.272417 (Hartree/Particle)
Thermal correction to Energy=	0.305342
Thermal correction to Enthalpy=	0.306287
Thermal correction to Gibbs Free Energy=	0.203372
Sum of electronic and zero-point Energies=	-3605.364649
Sum of electronic and thermal Energies=	-3605.331724
Sum of electronic and thermal Enthalpies=	-3605.330780
Sum of electronic and thermal Free Energies=	-3605.433695

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -3606.1808127

34-TS (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.477533	-1.731195	-0.082368
2	6	0	4.325035	-2.502087	0.722451
3	6	0	5.626607	-2.729169	0.271136
4	6	0	6.064575	-2.212841	-0.942470
5	6	0	5.190826	-1.476432	-1.736329
6	6	0	3.881011	-1.227911	-1.324768
7	1	0	6.295424	-3.330138	0.881799
8	1	0	7.080378	-2.396457	-1.277373
9	1	0	5.522591	-1.087162	-2.695057
10	8	0	2.177329	-1.501640	0.326056
11	6	0	2.036745	-0.585385	1.416674
12	1	0	2.912446	-0.640996	2.063988
13	46	0	1.666758	1.283621	0.778191
14	6	0	3.843453	-3.104348	2.017895
15	1	0	4.318518	-4.074576	2.182301
16	1	0	4.086676	-2.469535	2.876557
17	1	0	2.759956	-3.242070	2.004498
18	1	0	1.116319	-0.855248	1.942686
19	6	0	-0.486388	1.934587	-2.057310
20	8	0	0.871086	2.085332	-2.083517
21	8	0	-1.165787	2.920052	-1.647075
22	6	0	2.910524	-0.480920	-2.198072
23	1	0	2.198513	-1.168196	-2.672873
24	1	0	2.331795	0.264096	-1.645344
25	1	0	3.431995	0.038717	-3.005016
26	6	0	2.943351	3.178001	0.375806
27	1	0	3.481124	3.527712	1.264788
28	1	0	3.567651	3.008680	-0.510533

29	8	0	1.713373	3.499244	0.220277
30	1	0	3.250210	1.578389	0.881051
31	1	0	1.081521	2.897788	-1.593195
32	6	0	-1.344208	0.500211	1.379646
33	8	0	-1.145526	-0.655008	1.858180
34	8	0	-0.461999	1.030625	0.560681
35	19	0	-0.287294	-1.244215	-0.826574
36	53	0	-3.792564	-2.075142	-0.695264
37	19	0	-0.897395	3.514031	0.830227
38	8	0	-2.424501	1.182149	1.582224
39	8	0	-0.916883	0.821038	-2.424023
40	19	0	-3.545703	-1.046581	2.470678
41	19	0	-3.116514	1.221793	-1.097608

Zero-point correction=	0.268404 (Hartree/Particle)
Thermal correction to Energy=	0.301418
Thermal correction to Enthalpy=	0.302362
Thermal correction to Gibbs Free Energy=	0.198607
Sum of electronic and zero-point Energies=	-3605.341372
Sum of electronic and thermal Energies=	-3605.308358
Sum of electronic and thermal Enthalpies=	-3605.307414
Sum of electronic and thermal Free Energies=	-3605.411169

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -3606.1528391

39 (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	0.884578	1.137460	1.051140
2	6	0	4.204548	-0.842015	-0.051923
3	6	0	5.195671	0.089187	0.274836
4	6	0	6.521775	-0.350910	0.256801
5	6	0	6.841932	-1.663391	-0.071699
6	6	0	5.832270	-2.566243	-0.393362
7	6	0	4.496514	-2.168302	-0.387008
8	1	0	7.310084	0.356111	0.501270
9	1	0	7.878944	-1.983366	-0.079954
10	1	0	6.078430	-3.593323	-0.649304
11	8	0	2.879847	-0.446198	-0.099404
12	6	0	2.232738	-0.298524	1.173446
13	1	0	1.725677	-1.235084	1.436997
14	1	0	2.974667	-0.025296	1.933745
15	6	0	4.841566	1.508984	0.633732
16	1	0	5.654908	2.184607	0.357344
17	1	0	4.688977	1.611889	1.714425
18	6	0	3.378812	-3.113503	-0.741890

19	1	0	2.590371	-3.102597	0.015541
20	1	0	2.909057	-2.833127	-1.691526
21	1	0	3.753648	-4.134599	-0.841283
22	1	0	3.920429	1.843175	0.148259
23	6	0	0.557693	2.910641	-0.589747
24	8	0	-0.249021	2.981331	0.429925
25	8	0	1.797802	2.544633	-0.311665
26	8	0	0.150476	2.985721	-1.785186
27	19	0	1.461932	0.652223	-2.063851
28	6	0	-0.897873	-1.019456	0.273718
29	8	0	-0.653898	-0.321875	1.359235
30	8	0	-1.407508	-2.180854	0.419933
31	19	0	-2.128774	1.860314	-0.792033
32	53	0	-4.749728	-0.322134	-0.093864
33	19	0	-2.699149	-1.341352	2.483010
34	8	0	-0.704754	-0.509425	-0.900787
35	19	0	-2.538094	-2.207181	-1.805073

Zero-point correction=	0.218406 (Hartree/Particle)
Thermal correction to Energy=	0.247838
Thermal correction to Enthalpy=	0.248783
Thermal correction to Gibbs Free Energy=	0.152517
Sum of electronic and zero-point Energies=	-3489.708114
Sum of electronic and thermal Energies=	-3489.678682
Sum of electronic and thermal Enthalpies=	-3489.677738
Sum of electronic and thermal Free Energies=	-3489.774003

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -3490.439456

40-TS (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	-1.127103	-0.862707	1.051096
2	6	0	-3.926262	0.908296	0.304259
3	6	0	-4.350347	-0.386865	0.650120
4	6	0	-5.698770	-0.687534	0.408323
5	6	0	-6.575796	0.234766	-0.142111
6	6	0	-6.119012	1.506559	-0.478796
7	6	0	-4.791088	1.858371	-0.261190
8	1	0	-6.050127	-1.684985	0.655946
9	1	0	-7.613152	-0.035288	-0.310263
10	1	0	-6.797941	2.239370	-0.906150
11	8	0	-2.618548	1.338115	0.420766
12	6	0	-1.856402	0.909573	1.529414
13	1	0	-1.026471	1.611855	1.635282
14	1	0	-2.479081	0.873917	2.431080

15	6	0	-3.421445	-1.463484	1.125518
16	1	0	-3.936591	-2.427821	1.148944
17	1	0	-3.074802	-1.317282	2.157832
18	6	0	-4.267973	3.227949	-0.606966
19	1	0	-3.801239	3.701158	0.261155
20	1	0	-3.498497	3.184263	-1.386395
21	1	0	-5.076171	3.868613	-0.965828
22	1	0	-2.736768	-1.780082	0.083089
23	6	0	-1.053366	-2.360320	-1.233666
24	8	0	-0.507266	-2.714079	-0.102235
25	8	0	-2.322151	-2.035553	-1.236117
26	8	0	-0.360564	-2.188706	-2.282297
27	19	0	-1.537149	0.258167	-2.096695
28	6	0	1.057599	0.979662	0.285942
29	8	0	0.855334	-0.037912	1.104033
30	8	0	1.628830	2.020012	0.751616
31	19	0	1.763594	-1.785271	-0.860616
32	53	0	4.763688	-0.064304	-0.167080
33	19	0	2.844467	0.637531	2.554347
34	8	0	0.755165	0.864072	-0.957388
35	19	0	2.825557	2.391126	-1.458717

Zero-point correction= 0.214213 (Hartree/Particle)
Thermal correction to Energy= 0.242525
Thermal correction to Enthalpy= 0.243469
Thermal correction to Gibbs Free Energy= 0.151172
Sum of electronic and zero-point Energies= -3489.690721
Sum of electronic and thermal Energies= -3489.662409
Sum of electronic and thermal Enthalpies= -3489.661464
Sum of electronic and thermal Free Energies= -3489.753762

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -3490.4181203

66 (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.621351	0.298023	0.189077
2	6	0	-3.565727	-0.581700	1.286725
3	6	0	-3.645765	-1.950160	1.026395
4	6	0	-3.775762	-2.421505	-0.274757
5	6	0	-3.835336	-1.534368	-1.345187
6	6	0	-3.760146	-0.157845	-1.137791
7	1	0	-3.587904	-2.648960	1.855012
8	1	0	-3.820382	-3.489589	-0.457970
9	1	0	-3.943468	-1.909450	-2.358520
10	8	0	-3.645345	1.673927	0.445863

11	6	0	-2.352347	2.204139	0.241502
12	1	0	-2.043083	2.800808	1.102079
13	46	0	-1.221850	0.579874	0.080818
14	6	0	-3.490467	-0.035840	2.688617
15	1	0	-3.247406	-0.831875	3.394643
16	1	0	-2.736173	0.750068	2.776422
17	1	0	-4.449550	0.404778	2.978217
18	1	0	-2.281905	2.757176	-0.701185
19	53	0	0.983476	2.195648	-0.041178
20	19	0	2.308580	-0.326281	-2.092540
21	53	0	0.084713	-2.016779	-0.123735
22	6	0	5.158534	-0.507382	0.253607
23	8	0	4.109403	-0.480594	-0.473623
24	8	0	5.155485	-0.518668	1.499570
25	6	0	6.492473	-0.532675	-0.482900
26	1	0	7.323154	-0.517394	0.221320
27	1	0	6.547124	-1.433915	-1.099817
28	1	0	6.555779	0.328415	-1.153390
29	19	0	2.616857	-0.447630	1.740078
30	6	0	-3.868162	0.832234	-2.268256
31	1	0	-4.475803	1.689556	-1.967799
32	1	0	-2.883848	1.212115	-2.562181
33	1	0	-4.320762	0.363445	-3.143963

Zero-point correction= 0.233073 (Hartree/Particle)

Thermal correction to Energy= 0.259408

Thermal correction to Enthalpy= 0.260353

Thermal correction to Gibbs Free Energy= 0.168362

Sum of electronic and zero-point Energies= -2002.121904

Sum of electronic and thermal Energies= -2002.095568

Sum of electronic and thermal Enthalpies= -2002.094624

Sum of electronic and thermal Free Energies= -2002.186614

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2002.6593252

68 (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	0.319854	0.571181	0.469264
2	6	0	-3.337955	-0.305434	-0.164839
3	6	0	-3.640703	-0.174009	1.192907
4	6	0	-4.991886	-0.161713	1.547233
5	6	0	-5.991458	-0.278206	0.587831
6	6	0	-5.654338	-0.407756	-0.755439
7	6	0	-4.318374	-0.419146	-1.153945
8	1	0	-5.254081	-0.063303	2.596822

9	1	0	-7.034328	-0.266885	0.887214
10	1	0	-6.431986	-0.492507	-1.509189
11	8	0	-2.012933	-0.355982	-0.588689
12	6	0	-1.308548	0.869919	-0.594451
13	1	0	-0.991881	1.109848	-1.614164
14	1	0	-1.901102	1.677625	-0.155743
15	6	0	-2.555587	-0.060468	2.229719
16	1	0	-2.979615	-0.154841	3.231734
17	1	0	-2.047911	0.910505	2.176337
18	6	0	-3.921072	-0.544867	-2.600831
19	1	0	-3.263389	0.274495	-2.905401
20	1	0	-3.382311	-1.480240	-2.788603
21	1	0	-4.802720	-0.533872	-3.244450
22	1	0	-1.791231	-0.830275	2.092022
23	6	0	1.353537	-1.553268	1.690456
24	8	0	2.100330	-0.540536	1.598990
25	8	0	0.180759	-1.557305	1.192121
26	6	0	1.833357	-2.805156	2.380455
27	1	0	1.066461	-3.151613	3.075902
28	1	0	1.971756	-3.577896	1.617032
29	1	0	2.768579	-2.621966	2.908905
30	19	0	3.463459	0.394174	-0.393136
31	53	0	1.217050	3.028820	-0.265936
32	6	0	2.638631	-2.757584	-0.946367
33	8	0	1.883546	-3.744462	-0.832424
34	8	0	2.307323	-1.624238	-1.422528
35	6	0	4.067147	-2.882712	-0.407278
36	1	0	4.112832	-2.379115	0.567525
37	1	0	4.339197	-3.927759	-0.261719
38	1	0	4.782882	-2.407024	-1.084815
39	19	0	-0.257501	-2.363880	-1.222306

Zero-point correction= 0.286110 (Hartree/Particle)

Thermal correction to Energy= 0.314269

Thermal correction to Enthalpy= 0.315213

Thermal correction to Gibbs Free Energy= 0.222916

Sum of electronic and zero-point Energies= -2219.113969

Sum of electronic and thermal Energies= -2219.085811

Sum of electronic and thermal Enthalpies= -2219.084867

Sum of electronic and thermal Free Energies= -2219.177163

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2219.7686156

69-TS (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

1	46	0	-0.226972	-1.171174	0.740446
2	6	0	2.966585	-0.824723	-0.344990
3	6	0	2.952921	-0.570707	1.038600
4	6	0	4.062027	0.121161	1.556857
5	6	0	5.119319	0.527352	0.758369
6	6	0	5.099421	0.252589	-0.608660
7	6	0	4.025137	-0.421176	-1.178699
8	1	0	4.073616	0.339454	2.621038
9	1	0	5.960449	1.053702	1.197028
10	1	0	5.926504	0.558376	-1.242964
11	8	0	1.903454	-1.368589	-1.025003
12	6	0	1.019437	-2.248877	-0.388211
13	1	0	0.453105	-2.744774	-1.172463
14	1	0	1.553600	-2.962155	0.246183
15	6	0	1.783358	-0.867377	1.919345
16	1	0	1.977308	-0.469353	2.921405
17	1	0	1.596506	-1.930728	2.081462
18	6	0	3.966966	-0.723091	-2.653031
19	1	0	3.826586	-1.793032	-2.827270
20	1	0	3.125172	-0.217720	-3.138895
21	1	0	4.886689	-0.402734	-3.145975
22	1	0	0.950599	0.276201	1.788776
23	6	0	-0.685715	1.495653	2.091913
24	8	0	-1.430089	0.511832	1.887688
25	8	0	0.583662	1.463500	1.897579
26	6	0	-1.265532	2.809358	2.545807
27	1	0	-0.559983	3.341653	3.183058
28	1	0	-1.437332	3.398827	1.639380
29	1	0	-2.209396	2.647743	3.068102
30	19	0	-3.238887	1.025599	0.061959
31	53	0	-2.410800	-2.094161	-0.690307
32	6	0	-0.976780	3.544759	-1.305572
33	8	0	0.171398	3.677188	-1.763396
34	8	0	-1.386209	2.529836	-0.640528
35	6	0	-1.993733	4.659981	-1.531852
36	1	0	-2.375191	5.012225	-0.568702
37	1	0	-1.543764	5.490105	-2.074398
38	1	0	-2.843741	4.271289	-2.100674
39	19	0	1.116476	1.498398	-0.809291

Zero-point correction=	0.281686 (Hartree/Particle)
Thermal correction to Energy=	0.309074
Thermal correction to Enthalpy=	0.310018
Thermal correction to Gibbs Free Energy=	0.218643
Sum of electronic and zero-point Energies=	-2219.076068
Sum of electronic and thermal Energies=	-2219.048681
Sum of electronic and thermal Enthalpies=	-2219.047737
Sum of electronic and thermal Free Energies=	-2219.139112

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2219.725315

72 (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.746272	-1.088547	0.915002
2	6	0	-3.690974	-1.573617	-0.003180
3	6	0	-4.543846	-0.645151	-0.610703
4	6	0	-4.465169	0.712963	-0.300980
5	6	0	-3.537908	1.159509	0.638351
6	6	0	-2.663562	0.267267	1.267413
7	1	0	-5.296893	-1.002326	-1.308473
8	1	0	-5.143785	1.418438	-0.770455
9	1	0	-3.472305	2.212047	0.898170
10	8	0	-1.890085	-1.980046	1.537964
11	6	0	-0.852924	-2.479176	0.725073
12	1	0	-1.168839	-2.639771	-0.308039
13	46	0	0.489633	-1.078149	1.017273
14	6	0	-3.817846	-3.049069	-0.289563
15	1	0	-4.855112	-3.297996	-0.523424
16	1	0	-3.203993	-3.360252	-1.141784
17	1	0	-3.503687	-3.637951	0.574592
18	1	0	-0.464056	-3.394592	1.182687
19	6	0	4.422344	0.600216	0.026739
20	8	0	3.985074	-0.104684	1.029356
21	8	0	3.862293	1.599735	-0.420352
22	6	0	-1.662777	0.753169	2.278831
23	1	0	-1.513053	0.018808	3.074065
24	1	0	-0.695830	0.976059	1.804628
25	1	0	-1.989485	1.699880	2.711802
26	6	0	1.719348	0.660654	3.128632
27	1	0	1.131030	1.529088	3.460660
28	1	0	2.735736	0.765105	3.534790
29	8	0	1.744739	0.561341	1.728258
30	1	0	1.274437	-0.231497	3.608082
31	1	0	2.997874	0.223060	1.339526
32	53	0	1.360540	-1.292658	-1.545762
33	19	0	1.399947	2.329426	-0.140665
34	6	0	5.692685	0.061643	-0.585397
35	1	0	6.133109	0.802152	-1.250953
36	1	0	6.396481	-0.228979	0.196132
37	1	0	5.436805	-0.836146	-1.155645
38	19	0	-1.714737	0.219950	-1.879188
39	6	0	-1.420347	3.307333	-0.472698
40	8	0	-1.011518	2.513960	-1.385021

41	8	0	-0.951093	3.374533	0.678936
42	6	0	-2.569161	4.238303	-0.859493
43	1	0	-3.418599	3.648503	-1.219431
44	1	0	-2.875305	4.853605	-0.013467
45	1	0	-2.252095	4.878663	-1.686746

Zero-point correction= 0.338060 (Hartree/Particle)
 Thermal correction to Energy= 0.370675
 Thermal correction to Enthalpy= 0.371619
 Thermal correction to Gibbs Free Energy= 0.266639
 Sum of electronic and zero-point Energies= -2334.729138
 Sum of electronic and thermal Energies= -2334.696523
 Sum of electronic and thermal Enthalpies= -2334.695579
 Sum of electronic and thermal Free Energies= -2334.800559

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2335.4794931

73-TS (M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.023163	-0.910325	0.887920
2	6	0	-3.545988	-1.816006	-0.055709
3	6	0	-4.344915	-1.311971	-1.087801
4	6	0	-4.627888	0.050960	-1.179202
5	6	0	-4.114760	0.926819	-0.223990
6	6	0	-3.307840	0.465843	0.822814
7	1	0	-4.776041	-2.007016	-1.804247
8	1	0	-5.269096	0.422990	-1.972304
9	1	0	-4.352262	1.986152	-0.275084
10	8	0	-2.302382	-1.374919	1.948336
11	6	0	-0.972956	-1.803174	1.673725
12	1	0	-0.955083	-2.460442	0.798270
13	46	0	0.432736	-0.391069	1.308623
14	6	0	-3.306624	-3.298582	0.075978
15	1	0	-4.162678	-3.854479	-0.313321
16	1	0	-2.419165	-3.620592	-0.479618
17	1	0	-3.156455	-3.567587	1.123452
18	1	0	-0.652454	-2.358542	2.556335
19	6	0	4.531667	-0.002454	0.054640
20	8	0	4.095381	-0.273989	1.274227
21	8	0	4.192215	0.987108	-0.572063
22	6	0	-2.789317	1.413488	1.872320
23	1	0	-2.534629	0.869269	2.782689
24	1	0	-1.888298	1.932028	1.523660
25	1	0	-3.545775	2.169385	2.101881
26	6	0	1.135332	1.544156	2.487385

27	1	0	0.338553	2.276761	2.325439
28	1	0	1.422916	1.300961	3.516885
29	8	0	1.954743	1.326730	1.543312
30	1	0	-0.119461	0.221969	2.663464
31	1	0	3.385277	0.373182	1.507663
32	53	0	1.334521	-1.513603	-1.156966
33	19	0	1.850063	2.062606	-0.991511
34	6	0	5.456496	-1.055913	-0.481577
35	1	0	6.013048	-0.662103	-1.329920
36	1	0	6.128352	-1.412076	0.300042
37	1	0	4.835914	-1.895718	-0.809752
38	19	0	-1.594033	-0.017229	-1.861065
39	6	0	-0.952910	3.085643	-0.687823
40	8	0	-0.767949	2.322548	-1.688085
41	8	0	-0.191202	3.163082	0.302698
42	6	0	-2.177932	3.997391	-0.704967
43	1	0	-2.837148	3.772129	-1.544186
44	1	0	-2.716983	3.907355	0.241908
45	1	0	-1.840232	5.034651	-0.781433

Zero-point correction= 0.335595 (Hartree/Particle)

Thermal correction to Energy= 0.367242

Thermal correction to Enthalpy= 0.368186

Thermal correction to Gibbs Free Energy= 0.269290

Sum of electronic and zero-point Energies= -2334.703575

Sum of electronic and thermal Energies= -2334.671928

Sum of electronic and thermal Enthalpies= -2334.670984

Sum of electronic and thermal Free Energies= -2334.769881

M06-2X/6-311++G(d,p)-LANL2DZ(SMD)//M06-2X/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2335.4450284

29 (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.404273	0.958704	-1.421180
2	6	0	3.363847	-0.063881	-1.422885
3	6	0	4.552596	0.160517	-0.722890
4	6	0	4.804075	1.382132	-0.099826
5	6	0	3.868689	2.410731	-0.195033
6	6	0	2.652792	2.223513	-0.861385
7	1	0	5.298899	-0.635840	-0.692859
8	1	0	5.746694	1.545452	0.424869
9	1	0	4.081257	3.389921	0.239740
10	8	0	1.216790	0.718684	-2.087289
11	6	0	0.034130	0.912548	-1.391129
12	1	0	-0.697516	1.375017	-2.065824

13	46	0	-0.715958	-0.856784	-0.916478
14	6	0	3.157543	-1.321453	-2.226063
15	1	0	3.679675	-2.167986	-1.764296
16	1	0	2.096866	-1.575436	-2.313090
17	1	0	3.559712	-1.173459	-3.239465
18	1	0	0.163058	1.400414	-0.407864
19	53	0	-3.265989	0.023090	-1.107216
20	19	0	2.272902	0.585256	1.795804
21	53	0	1.047289	-2.406707	0.524342
22	6	0	-0.521165	1.361132	2.350057
23	8	0	0.093283	0.466839	3.039103
24	8	0	-1.811428	1.430130	2.380907
25	19	0	-1.823812	-1.125379	2.412909
26	19	0	-2.076425	2.963602	0.460367
27	8	0	0.153102	2.156441	1.551532
28	6	0	1.679057	3.371365	-0.987792
29	1	0	1.083351	3.279151	-1.905917
30	1	0	1.013622	3.392409	-0.111329
31	1	0	2.229916	4.319420	-1.031495

Zero-point correction= 0.199601 (Hartree/Particle)

Thermal correction to Energy= 0.224591

Thermal correction to Enthalpy= 0.225536

Thermal correction to Gibbs Free Energy= 0.139806

Sum of electronic and zero-point Energies= -2637.289704

Sum of electronic and thermal Energies= -2637.264713

Sum of electronic and thermal Enthalpies= -2637.263769

Sum of electronic and thermal Free Energies= -2637.349498

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent =-2637.8876218

33 (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.083816	-2.025198	0.116997
2	6	0	3.342604	-3.378608	0.356503
3	6	0	4.604334	-3.874361	0.029093
4	6	0	5.580956	-3.042480	-0.510714
5	6	0	5.300787	-1.698540	-0.733537
6	6	0	4.047438	-1.168041	-0.425340
7	1	0	4.820653	-4.929443	0.208866
8	1	0	6.563771	-3.443093	-0.760578
9	1	0	6.062079	-1.043147	-1.161589
10	8	0	1.813823	-1.561772	0.408894
11	6	0	1.724974	-0.608444	1.480616
12	1	0	2.557150	-0.770857	2.187318

13	46	0	1.798413	1.194038	0.681737
14	6	0	2.264946	-4.246710	0.954073
15	1	0	2.647697	-5.251181	1.170409
16	1	0	1.881730	-3.807955	1.885435
17	1	0	1.408229	-4.344942	0.272513
18	1	0	0.745786	-0.733021	1.950290
19	6	0	-0.644881	1.702256	-2.035185
20	8	0	0.700841	1.531921	-1.993017
21	8	0	-1.129933	2.717361	-1.451846
22	6	0	3.739447	0.284100	-0.678868
23	1	0	2.792548	0.419240	-1.234709
24	1	0	3.773384	0.863727	0.280858
25	1	0	4.516207	0.766886	-1.283363
26	6	0	3.021014	3.558252	-0.892996
27	1	0	3.860909	3.469014	-0.172191
28	1	0	2.983860	4.620424	-1.203460
29	8	0	1.803249	3.131830	-0.355771
30	1	0	3.309054	2.980143	-1.797790
31	1	0	1.101544	2.292146	-1.420911
32	6	0	-1.043426	1.286083	1.294111
33	8	0	-1.088938	0.172523	0.660408
34	8	0	0.099385	1.782974	1.700828
35	19	0	-0.323303	-1.232948	-1.333769
36	53	0	-3.780044	-2.228713	-0.401089
37	19	0	-0.423594	4.061326	0.592575
38	8	0	-2.121472	1.927169	1.572229
39	8	0	-1.309811	0.797066	-2.601253
40	19	0	-2.965923	-0.506267	2.357299
41	19	0	-3.217627	1.224503	-0.893765

Zero-point correction= 0.270089 (Hartree/Particle)
Thermal correction to Energy= 0.303033
Thermal correction to Enthalpy= 0.303977
Thermal correction to Gibbs Free Energy= 0.201155
Sum of electronic and zero-point Energies= -3605.211227
Sum of electronic and thermal Energies= -3605.178283
Sum of electronic and thermal Enthalpies= -3605.177339
Sum of electronic and thermal Free Energies= -3605.280161

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -
3606.0660532

34-TS (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.452326	-1.785710	-0.037236
2	6	0	4.443982	-2.343500	0.777052

3	6	0	5.750536	-2.381158	0.282596
4	6	0	6.054462	-1.891129	-0.982137
5	6	0	5.040202	-1.377235	-1.786124
6	6	0	3.723625	-1.322636	-1.330441
7	1	0	6.534977	-2.819318	0.904085
8	1	0	7.080040	-1.928078	-1.351745
9	1	0	5.265171	-1.014601	-2.791503
10	8	0	2.144437	-1.725850	0.409569
11	6	0	1.904237	-0.752718	1.440511
12	1	0	2.712289	-0.792536	2.181256
13	46	0	1.644368	1.116902	0.750790
14	6	0	4.114641	-2.935142	2.126974
15	1	0	4.724669	-3.830039	2.306471
16	1	0	4.320147	-2.228083	2.944293
17	1	0	3.055438	-3.215695	2.181583
18	1	0	0.937717	-1.004935	1.900038
19	6	0	-0.211514	1.876214	-2.050134
20	8	0	1.142360	2.055214	-2.114969
21	8	0	-0.892401	2.873083	-1.660589
22	6	0	2.600887	-0.827969	-2.203447
23	1	0	1.952239	-1.665321	-2.509694
24	1	0	1.984318	-0.069854	-1.702215
25	1	0	2.984801	-0.367299	-3.121625
26	6	0	3.086249	2.833554	0.317585
27	1	0	3.717946	3.140323	1.167374
28	1	0	3.634999	2.619415	-0.616592
29	8	0	1.883909	3.298248	0.234544
30	1	0	3.243698	1.271727	0.790105
31	1	0	1.337116	2.867532	-1.616492
32	6	0	-1.406689	0.551926	1.411857
33	8	0	-1.291893	-0.591335	1.948230
34	8	0	-0.471256	0.991981	0.594106
35	19	0	-0.349479	-1.363581	-0.689835
36	53	0	-3.926927	-1.932377	-0.721435
37	19	0	-0.727179	3.535407	0.826721
38	8	0	-2.447116	1.309643	1.550801
39	8	0	-0.637770	0.741926	-2.360057
40	19	0	-3.761227	-0.810940	2.461076
41	19	0	-2.938916	1.301485	-1.207488

Zero-point correction=	0.266771 (Hartree/Particle)
Thermal correction to Energy=	0.299505
Thermal correction to Enthalpy=	0.300449
Thermal correction to Gibbs Free Energy=	0.198048
Sum of electronic and zero-point Energies=	-3605.192799
Sum of electronic and thermal Energies=	-3605.160065
Sum of electronic and thermal Enthalpies=	-3605.159121
Sum of electronic and thermal Free Energies=	-3605.261522

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -
3606.0451266

39 (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	0.875832	1.156696	0.963202
2	6	0	4.227548	-0.829742	-0.041503
3	6	0	5.189693	0.077247	0.414762
4	6	0	6.513835	-0.365154	0.473403
5	6	0	6.860348	-1.658061	0.093810
6	6	0	5.879370	-2.536882	-0.358194
7	6	0	4.546561	-2.134756	-0.430330
8	1	0	7.283687	0.328352	0.819183
9	1	0	7.900773	-1.981615	0.146037
10	1	0	6.145994	-3.552931	-0.657705
11	8	0	2.908446	-0.428075	-0.159858
12	6	0	2.172134	-0.332190	1.076065
13	1	0	1.630525	-1.276796	1.251242
14	1	0	2.875740	-0.139204	1.902266
15	6	0	4.801257	1.478559	0.818299
16	1	0	5.638847	2.169166	0.656296
17	1	0	4.545982	1.522156	1.888563
18	6	0	3.455799	-3.051338	-0.926219
19	1	0	2.600669	-3.062455	-0.237162
20	1	0	3.075380	-2.719982	-1.904814
21	1	0	3.829371	-4.076544	-1.041164
22	1	0	3.925425	1.838880	0.262050
23	6	0	0.598600	2.901798	-0.679738
24	8	0	-0.198824	3.024343	0.345153
25	8	0	1.831910	2.504721	-0.391406
26	8	0	0.184307	2.944805	-1.875734
27	19	0	1.440702	0.582932	-2.113160
28	6	0	-0.919649	-1.001580	0.325998
29	8	0	-0.693800	-0.208494	1.355560
30	8	0	-1.415571	-2.154708	0.562455
31	19	0	-2.092651	1.836679	-0.812322
32	53	0	-4.767298	-0.326086	-0.090687
33	19	0	-2.724986	-1.192626	2.580037
34	8	0	-0.717801	-0.581645	-0.882951
35	19	0	-2.529181	-2.335903	-1.697162

Zero-point correction= 0.216699 (Hartree/Particle)
 Thermal correction to Energy= 0.245148
 Thermal correction to Enthalpy= 0.246092
 Thermal correction to Gibbs Free Energy= 0.153590

Sum of electronic and zero-point Energies= -3489.559220
 Sum of electronic and thermal Energies= -3489.530771
 Sum of electronic and thermal Enthalpies= -3489.529827
 Sum of electronic and thermal Free Energies= -3489.622329

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -
 3490.3279961

40-TS (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	-1.118150	-0.861840	1.023710
2	6	0	-3.904500	0.922708	0.314455
3	6	0	-4.316199	-0.364112	0.700140
4	6	0	-5.666938	-0.679964	0.496232
5	6	0	-6.561391	0.223058	-0.059384
6	6	0	-6.116427	1.486836	-0.442331
7	6	0	-4.786626	1.850845	-0.262067
8	1	0	-6.006768	-1.678890	0.776765
9	1	0	-7.605662	-0.058087	-0.199737
10	1	0	-6.809722	2.208418	-0.879884
11	8	0	-2.600154	1.361896	0.410540
12	6	0	-1.815041	0.924573	1.510624
13	1	0	-0.976462	1.626789	1.600973
14	1	0	-2.428260	0.914206	2.426115
15	6	0	-3.366719	-1.426045	1.180749
16	1	0	-3.872793	-2.399738	1.219803
17	1	0	-3.011588	-1.266512	2.212147
18	6	0	-4.272113	3.212743	-0.656785
19	1	0	-3.794720	3.713877	0.195745
20	1	0	-3.506558	3.143988	-1.445055
21	1	0	-5.088525	3.843544	-1.029373
22	1	0	-2.717882	-1.751140	0.128305
23	6	0	-1.080733	-2.353765	-1.240803
24	8	0	-0.523178	-2.704392	-0.108366
25	8	0	-2.350514	-2.037113	-1.230720
26	8	0	-0.392565	-2.180582	-2.295175
27	19	0	-1.567828	0.258912	-2.107563
28	6	0	1.050727	0.952782	0.241407
29	8	0	0.848744	-0.071346	1.058074
30	8	0	1.594906	2.005016	0.717306
31	19	0	1.770164	-1.832478	-0.894534
32	53	0	4.774097	-0.053408	-0.124755
33	19	0	2.787263	0.668096	2.584067
34	8	0	0.768408	0.830269	-1.006800
35	19	0	2.824994	2.381829	-1.504957

Zero-point correction= 0.213129 (Hartree/Particle)
 Thermal correction to Energy= 0.241174
 Thermal correction to Enthalpy= 0.242118
 Thermal correction to Gibbs Free Energy= 0.150281
 Sum of electronic and zero-point Energies= -3489.541885
 Sum of electronic and thermal Energies= -3489.513840
 Sum of electronic and thermal Enthalpies= -3489.512896
 Sum of electronic and thermal Free Energies= -3489.604733

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -
 3490.3080797

66 (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.567405	0.198718	0.333752
2	6	0	-3.430546	-0.637497	1.458099
3	6	0	-3.461253	-2.014969	1.251961
4	6	0	-3.614320	-2.538952	-0.029298
5	6	0	-3.741927	-1.696329	-1.127559
6	6	0	-3.720041	-0.309109	-0.971205
7	1	0	-3.350741	-2.682527	2.108126
8	1	0	-3.616205	-3.619472	-0.173751
9	1	0	-3.855255	-2.113767	-2.129418
10	8	0	-3.643676	1.580118	0.545369
11	6	0	-2.372700	2.162925	0.304528
12	1	0	-2.038857	2.735174	1.179826
13	46	0	-1.218941	0.569305	0.011126
14	6	0	-3.314051	-0.018235	2.828371
15	1	0	-3.150398	-0.789819	3.589899
16	1	0	-2.482650	0.699059	2.872183
17	1	0	-4.229424	0.536407	3.076635
18	1	0	-2.376373	2.773434	-0.610977
19	53	0	0.874319	2.235041	-0.128306
20	19	0	2.521650	-0.178387	-2.108851
21	53	0	0.115928	-1.938838	-0.386902
22	6	0	5.090597	-0.571207	0.542900
23	8	0	4.118350	-0.406181	-0.271838
24	8	0	4.965730	-0.660435	1.782233
25	6	0	6.485699	-0.673683	-0.068991
26	1	0	7.246617	-0.727892	0.715022
27	1	0	6.539262	-1.573227	-0.697108
28	1	0	6.670331	0.193510	-0.716068
29	19	0	2.416642	-0.417381	1.797271
30	6	0	-3.901307	0.638676	-2.132102
31	1	0	-4.496458	1.507980	-1.824119
32	1	0	-2.933200	1.009792	-2.499905

33 1 0 -4.405689 0.134123 -2.964915

 Zero-point correction= 0.230962 (Hartree/Particle)
 Thermal correction to Energy= 0.257276
 Thermal correction to Enthalpy= 0.258220
 Thermal correction to Gibbs Free Energy= 0.166407
 Sum of electronic and zero-point Energies= -2001.978985
 Sum of electronic and thermal Energies= -2001.952671
 Sum of electronic and thermal Enthalpies= -2001.951727
 Sum of electronic and thermal Free Energies= -2002.043540

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2002.5307387

68 (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	0.351755	0.577577	0.447296
2	6	0	-3.329388	-0.329401	-0.147047
3	6	0	-3.646224	-0.071139	1.188829
4	6	0	-5.000176	-0.038857	1.531297
5	6	0	-5.990467	-0.260291	0.579775
6	6	0	-5.639881	-0.519855	-0.741834
7	6	0	-4.300227	-0.554183	-1.126527
8	1	0	-5.273352	0.157637	2.570127
9	1	0	-7.041346	-0.233391	0.870183
10	1	0	-6.413092	-0.692456	-1.493356
11	8	0	-2.000153	-0.399567	-0.550042
12	6	0	-1.290475	0.833112	-0.614520
13	1	0	-1.001883	1.037033	-1.656290
14	1	0	-1.893317	1.657353	-0.208387
15	6	0	-2.561525	0.142094	2.214048
16	1	0	-2.974949	0.069357	3.227649
17	1	0	-2.100635	1.137421	2.114313
18	6	0	-3.882063	-0.824718	-2.550099
19	1	0	-3.195287	-0.049188	-2.916344
20	1	0	-3.361682	-1.791046	-2.636579
21	1	0	-4.754080	-0.856297	-3.214230
22	1	0	-1.760814	-0.601435	2.099038
23	6	0	1.372337	-1.486540	1.725578
24	8	0	2.121459	-0.475213	1.598384
25	8	0	0.195338	-1.492656	1.231137
26	6	0	1.854588	-2.724227	2.442660
27	1	0	1.088816	-3.054484	3.154209
28	1	0	1.988202	-3.517575	1.692568
29	1	0	2.797592	-2.526490	2.962002
30	19	0	3.487427	0.417554	-0.422121

31	53	0	1.151326	2.998919	-0.319617
32	6	0	2.646379	-2.752233	-0.875964
33	8	0	1.893806	-3.739773	-0.729086
34	8	0	2.305539	-1.634183	-1.385673
35	6	0	4.081762	-2.855162	-0.340737
36	1	0	4.144777	-2.286069	0.601850
37	1	0	4.342709	-3.896537	-0.128322
38	1	0	4.797485	-2.433466	-1.060475
39	19	0	-0.256158	-2.367661	-1.190742

Zero-point correction= 0.283754 (Hartree/Particle)
Thermal correction to Energy= 0.311764
Thermal correction to Enthalpy= 0.312708
Thermal correction to Gibbs Free Energy= 0.221224
Sum of electronic and zero-point Energies= -2218.962891
Sum of electronic and thermal Energies= -2218.934881
Sum of electronic and thermal Enthalpies= -2218.933937
Sum of electronic and thermal Free Energies= -2219.025420

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -
2219.6384682

69-TS (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	0.031375	-1.218899	0.799769
2	6	0	3.086397	-0.371371	-0.355958
3	6	0	3.050516	-0.155048	1.032048
4	6	0	4.053368	0.670893	1.565687
5	6	0	5.036569	1.242821	0.773471
6	6	0	5.039160	1.008098	-0.601617
7	6	0	4.065964	0.205037	-1.183877
8	1	0	4.040610	0.863082	2.640512
9	1	0	5.803279	1.873807	1.223893
10	1	0	5.809784	1.450216	-1.236365
11	8	0	2.127784	-1.089090	-1.030981
12	6	0	1.409570	-2.097497	-0.356146
13	1	0	0.929442	-2.708354	-1.123359
14	1	0	2.085434	-2.701546	0.265948
15	6	0	1.937195	-0.641160	1.913341
16	1	0	2.037376	-0.183044	2.908101
17	1	0	1.950518	-1.719756	2.110097
18	6	0	4.036685	-0.072374	-2.666186
19	1	0	4.053019	-1.152788	-2.861593
20	1	0	3.119267	0.314238	-3.134859
21	1	0	4.895723	0.392768	-3.164306
22	1	0	0.971934	0.364459	1.694708

23	6	0	-0.790987	1.343935	2.095055
24	8	0	-1.367005	0.231930	1.989608
25	8	0	0.435022	1.517292	1.761755
26	6	0	-1.547213	2.553256	2.586695
27	1	0	-0.880120	3.223299	3.137692
28	1	0	-1.909561	3.074490	1.688989
29	1	0	-2.392313	2.248676	3.214429
30	19	0	-3.493140	0.517366	0.448444
31	53	0	-1.943859	-2.175056	-0.794924
32	6	0	-1.752544	3.230924	-1.321715
33	8	0	-0.699556	3.405136	-1.962280
34	8	0	-1.982887	2.229674	-0.552574
35	6	0	-2.869519	4.268885	-1.437695
36	1	0	-3.139167	4.637986	-0.438616
37	1	0	-2.554765	5.103981	-2.070077
38	1	0	-3.763386	3.799098	-1.870760
39	19	0	0.539791	1.324148	-1.056113

Zero-point correction= 0.279376 (Hartree/Particle)
Thermal correction to Energy= 0.306689
Thermal correction to Enthalpy= 0.307633
Thermal correction to Gibbs Free Energy= 0.216838
Sum of electronic and zero-point Energies= -2218.923536
Sum of electronic and thermal Energies= -2218.896223
Sum of electronic and thermal Enthalpies= -2218.895279
Sum of electronic and thermal Free Energies= -2218.986075

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2219.5952156

72 (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.810451	-1.056919	0.921925
2	6	0	-3.810063	-1.506713	0.043200
3	6	0	-4.646597	-0.549304	-0.538588
4	6	0	-4.499797	0.807676	-0.241692
5	6	0	-3.526236	1.219027	0.665019
6	6	0	-2.665258	0.293984	1.266943
7	1	0	-5.441252	-0.881046	-1.210916
8	1	0	-5.166210	1.542066	-0.696947
9	1	0	-3.406019	2.274599	0.918898
10	8	0	-1.940715	-1.985738	1.468209
11	6	0	-0.932212	-2.424702	0.567182
12	1	0	-1.316821	-2.520247	-0.459198
13	46	0	0.402671	-1.026162	0.930027
14	6	0	-3.991636	-2.981637	-0.228828

15	1	0	-5.043416	-3.200482	-0.449916
16	1	0	-3.394835	-3.323842	-1.087626
17	1	0	-3.681913	-3.572497	0.641623
18	1	0	-0.536246	-3.384559	0.926678
19	6	0	4.475062	0.539607	0.118886
20	8	0	3.980218	-0.173427	1.091078
21	8	0	3.939076	1.548756	-0.341738
22	6	0	-1.609043	0.755152	2.236556
23	1	0	-1.263659	-0.065973	2.880337
24	1	0	-0.754671	1.205570	1.704233
25	1	0	-2.006075	1.549739	2.880951
26	6	0	1.660748	0.617721	3.114760
27	1	0	1.035140	1.466132	3.449490
28	1	0	2.674094	0.761669	3.531208
29	8	0	1.702726	0.525101	1.711714
30	1	0	1.247954	-0.297960	3.590106
31	1	0	2.986209	0.157918	1.354213
32	53	0	1.446039	-1.305846	-1.481955
33	19	0	1.459571	2.324993	-0.174213
34	6	0	5.769563	-0.004997	-0.441100
35	1	0	6.278088	0.762287	-1.031735
36	1	0	6.410831	-0.371624	0.367926
37	1	0	5.521665	-0.857956	-1.088098
38	19	0	-1.730016	0.114708	-1.820243
39	6	0	-1.354019	3.295655	-0.541729
40	8	0	-0.972765	2.405922	-1.377288
41	8	0	-0.858646	3.467133	0.590370
42	6	0	-2.499285	4.204296	-0.996805
43	1	0	-3.358711	3.592472	-1.307266
44	1	0	-2.794453	4.888607	-0.194896
45	1	0	-2.177940	4.779047	-1.875190

Zero-point correction= 0.334964 (Hartree/Particle)

Thermal correction to Energy= 0.367465

Thermal correction to Enthalpy= 0.368409

Thermal correction to Gibbs Free Energy= 0.265810

Sum of electronic and zero-point Energies= -2334.574411

Sum of electronic and thermal Energies= -2334.541910

Sum of electronic and thermal Enthalpies= -2334.540966

Sum of electronic and thermal Free Energies= -2334.643565

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2335.3466842

73-TS (M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ)

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-3.231565	-1.007135	0.416474
2	6	0	-3.481274	-1.124787	-0.962190
3	6	0	-4.130350	-0.062042	-1.605455
4	6	0	-4.535080	1.074616	-0.907666
5	6	0	-4.295736	1.160163	0.465368
6	6	0	-3.644546	0.126208	1.142102
7	1	0	-4.348999	-0.154067	-2.671847
8	1	0	-5.060238	1.878467	-1.425635
9	1	0	-4.631572	2.033734	1.028591
10	8	0	-2.676874	-2.020865	1.141690
11	6	0	-1.339204	-2.420880	0.851771
12	1	0	-1.247697	-2.787968	-0.176844
13	46	0	0.115546	-1.024324	1.039860
14	6	0	-3.145218	-2.384858	-1.720492
15	1	0	-3.807162	-2.490096	-2.589047
16	1	0	-2.107080	-2.373361	-2.085027
17	1	0	-3.272393	-3.263286	-1.074474
18	1	0	-1.121543	-3.234324	1.551864
19	6	0	4.106821	-1.329927	0.328157
20	8	0	3.333510	-1.679884	1.351969
21	8	0	4.259226	-0.166024	-0.003054
22	6	0	-3.429642	0.161133	2.632977
23	1	0	-4.049120	-0.603238	3.122007
24	1	0	-2.387379	-0.074590	2.880770
25	1	0	-3.692427	1.142923	3.046006
26	6	0	0.884775	0.226090	2.826142
27	1	0	0.121760	0.992595	3.039493
28	1	0	1.184765	-0.413895	3.671767
29	8	0	1.689555	0.403495	1.852742
30	1	0	-0.429271	-1.021194	2.525262
31	1	0	2.852400	-0.870559	1.657921
32	53	0	0.853577	-1.052133	-1.632438
33	19	0	2.592059	1.859814	-0.269793
34	6	0	4.720944	-2.503633	-0.380421
35	1	0	5.556103	-2.166834	-0.999990
36	1	0	5.040426	-3.264388	0.339862
37	1	0	3.942913	-2.941221	-1.021981
38	19	0	-1.450308	1.408751	-0.827974
39	6	0	0.808792	4.270061	-0.149569
40	8	0	0.202721	3.160953	-0.357118
41	8	0	2.039116	4.389813	0.004187
42	6	0	-0.068982	5.521379	-0.094669
43	1	0	-0.819337	5.409306	0.699467
44	1	0	0.539759	6.411030	0.091624
45	1	0	-0.608329	5.631993	-1.045017

Zero-point correction=

0.332068 (Hartree/Particle)

Thermal correction to Energy=

0.364537

Thermal correction to Enthalpy= 0.365481
 Thermal correction to Gibbs Free Energy= 0.261128
 Sum of electronic and zero-point Energies= -2334.548959
 Sum of electronic and thermal Energies= -2334.516490
 Sum of electronic and thermal Enthalpies= -2334.515546
 Sum of electronic and thermal Free Energies= -2334.619899

M11/6-311++G(d,p)-LANL2DZ(SMD)//M11/6-31G(d,p)-LANL2DZ energy in DMAc solvent = -2335.3158192

29 (M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.474226	0.354813	-1.734774
2	6	0	3.364168	-0.707007	-1.500892
3	6	0	4.600095	-0.401759	-0.917944
4	6	0	4.952256	0.918249	-0.626687
5	6	0	4.081432	1.960261	-0.954804
6	6	0	2.823751	1.703062	-1.527426
7	1	0	5.293092	-1.210060	-0.700956
8	1	0	5.915114	1.138496	-0.174520
9	1	0	4.378291	2.992677	-0.785830
10	8	0	1.237622	0.034182	-2.288022
11	6	0	0.094597	0.377358	-1.588430
12	1	0	-0.685514	0.591696	-2.319536
13	46	0	-0.667435	-1.165979	-0.525572
14	6	0	3.019648	-2.111071	-1.923313
15	1	0	3.666683	-2.838174	-1.426012
16	1	0	1.980210	-2.360320	-1.703176
17	1	0	3.159421	-2.221988	-3.006474
18	1	0	0.235941	1.135985	-0.810383
19	53	0	-3.291439	-0.638543	-1.212448
20	19	0	2.172074	1.530741	1.775707
21	53	0	1.200161	-1.959976	1.374080
22	6	0	-0.739348	2.276651	1.803765
23	8	0	-0.177890	1.722895	2.831676
24	8	0	-2.034987	2.307779	1.711577
25	19	0	-2.110632	-0.070398	2.789877
26	19	0	-2.123781	3.106153	-0.710346
27	8	0	-0.004185	2.760426	0.833432
28	6	0	1.919424	2.848619	-1.921538
29	1	0	1.283022	2.580874	-2.770365
30	1	0	1.270387	3.150474	-1.092255
31	1	0	2.521624	3.716138	-2.207206

Zero-point correction= 0.197811 (Hartree/Particle)
 Thermal correction to Energy= 0.224555

Thermal correction to Enthalpy= 0.225499
 Thermal correction to Gibbs Free Energy= 0.133792
 Sum of electronic and zero-point Energies= -2638.077331
 Sum of electronic and thermal Energies= -2638.050586
 Sum of electronic and thermal Enthalpies= -2638.049642
 Sum of electronic and thermal Free Energies= -2638.141349

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -2637.9559024

33 (M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.061098	2.167868	0.127823
2	6	0	-3.223091	3.555806	0.264816
3	6	0	-4.424823	4.125973	-0.172046
4	6	0	-5.434656	3.333661	-0.720271
5	6	0	-5.248566	1.956873	-0.848128
6	6	0	-4.056483	1.347986	-0.433614
7	1	0	-4.567605	5.198834	-0.071988
8	1	0	-6.365092	3.787715	-1.048932
9	1	0	-6.029984	1.339763	-1.283721
10	8	0	-1.833292	1.656162	0.523219
11	6	0	-1.833212	0.662771	1.561926
12	1	0	-2.685227	0.818945	2.237409
13	46	0	-1.940799	-1.147279	0.695674
14	6	0	-2.114886	4.384363	0.862318
15	1	0	-2.430500	5.423246	0.991318
16	1	0	-1.806405	3.990754	1.836941
17	1	0	-1.222059	4.377263	0.224803
18	1	0	-0.876674	0.744690	2.075251
19	6	0	0.721183	-1.906788	-2.100841
20	8	0	-0.620391	-1.692198	-2.167032
21	8	0	1.144046	-2.961096	-1.531920
22	6	0	-3.854812	-0.131873	-0.628749
23	1	0	-2.978452	-0.346024	-1.256120
24	1	0	-3.830071	-0.676306	0.354216
25	1	0	-4.705652	-0.598021	-1.129990
26	6	0	-3.159418	-3.494442	-0.954956
27	1	0	-3.911018	-3.653153	-0.161009
28	1	0	-3.039222	-4.463600	-1.473376
29	8	0	-1.934635	-3.030132	-0.449995
30	1	0	-3.617057	-2.805882	-1.689356
31	1	0	-1.124273	-2.337459	-1.531974
32	6	0	0.935055	-1.282365	1.414441
33	8	0	1.046675	-0.173766	0.776510
34	8	0	-0.250741	-1.798728	1.696328

35	19	0	0.242686	1.090693	-1.353686
36	53	0	4.064575	2.190570	-0.495750
37	19	0	0.188554	-4.182247	0.599912
38	8	0	1.966060	-1.932951	1.817824
39	8	0	1.450641	-0.998026	-2.597625
40	19	0	2.781922	0.698324	2.566477
41	19	0	3.303971	-1.554098	-0.685044

Zero-point correction=	0.266339 (Hartree/Particle)
Thermal correction to Energy=	0.300409
Thermal correction to Enthalpy=	0.301354
Thermal correction to Gibbs Free Energy=	0.194815
Sum of electronic and zero-point Energies=	-3606.146569
Sum of electronic and thermal Energies=	-3606.112499
Sum of electronic and thermal Enthalpies=	-3606.111555
Sum of electronic and thermal Free Energies=	-3606.218093

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -3606.0407755

34-TS (M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.583533	-1.766675	-0.097642
2	6	0	4.369141	-2.642925	0.675207
3	6	0	5.647842	-2.967951	0.203890
4	6	0	6.126752	-2.443422	-0.996860
5	6	0	5.319348	-1.595592	-1.755536
6	6	0	4.031658	-1.246709	-1.325237
7	1	0	6.266361	-3.646935	0.785739
8	1	0	7.122387	-2.703148	-1.345849
9	1	0	5.684868	-1.195411	-2.698103
10	8	0	2.301884	-1.454219	0.332327
11	6	0	2.215060	-0.524856	1.437312
12	1	0	3.123883	-0.571425	2.039062
13	46	0	1.802022	1.348559	0.756254
14	6	0	3.848957	-3.234066	1.963144
15	1	0	4.310596	-4.207563	2.153643
16	1	0	4.072428	-2.591923	2.823634
17	1	0	2.763094	-3.361871	1.931106
18	1	0	1.326484	-0.803460	2.007615
19	6	0	-0.797377	1.990090	-2.044824
20	8	0	0.569976	1.956696	-2.177980
21	8	0	-1.327448	3.034440	-1.565387
22	6	0	3.144711	-0.376647	-2.179641
23	1	0	2.453429	-0.986188	-2.779085
24	1	0	2.548341	0.319575	-1.584472

25	1	0	3.738858	0.209273	-2.887330
26	6	0	3.057592	3.157988	0.041532
27	1	0	3.600675	3.667859	0.848163
28	1	0	3.672940	2.910753	-0.834080
29	8	0	1.800640	3.442075	-0.134650
30	1	0	3.385416	1.712891	0.722614
31	1	0	0.961083	2.664788	-1.619916
32	6	0	-1.188020	0.468034	1.440348
33	8	0	-0.960764	-0.735465	1.794048
34	8	0	-0.295111	1.127678	0.716283
35	19	0	-0.191818	-1.087641	-1.007177
36	53	0	-4.021576	-2.206934	-0.750928
37	19	0	-0.765122	3.697226	0.952839
38	8	0	-2.296291	1.087706	1.683556
39	8	0	-1.393453	0.944999	-2.423089
40	19	0	-3.344248	-1.172514	2.727672
41	19	0	-3.495178	1.477754	-0.806086

Zero-point correction=	0.262516 (Hartree/Particle)
Thermal correction to Energy=	0.296943
Thermal correction to Enthalpy=	0.297887
Thermal correction to Gibbs Free Energy=	0.189005
Sum of electronic and zero-point Energies=	-3606.128267
Sum of electronic and thermal Energies=	-3606.093840
Sum of electronic and thermal Enthalpies=	-3606.092896
Sum of electronic and thermal Free Energies=	-3606.201777

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -3606.0237406

39 (M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	0.863859	1.152994	1.101340
2	6	0	4.282973	-0.821424	-0.067950
3	6	0	5.355876	0.069849	0.094380
4	6	0	6.654650	-0.452225	0.002573
5	6	0	6.868012	-1.808551	-0.244676
6	6	0	5.780603	-2.670240	-0.413814
7	6	0	4.468820	-2.189629	-0.329289
8	1	0	7.502366	0.218620	0.121512
9	1	0	7.881457	-2.194852	-0.311806
10	1	0	5.947572	-3.726001	-0.613385
11	8	0	2.982175	-0.338425	-0.045265
12	6	0	2.400596	-0.134822	1.271004
13	1	0	2.027730	-1.092893	1.652720
14	1	0	3.161545	0.280200	1.945144

15	6	0	5.117543	1.536952	0.357198
16	1	0	5.881675	2.147864	-0.134720
17	1	0	5.171387	1.758615	1.430923
18	6	0	3.272774	-3.084659	-0.539490
19	1	0	2.549485	-2.990066	0.276828
20	1	0	2.741015	-2.826017	-1.464013
21	1	0	3.576248	-4.133079	-0.611002
22	1	0	4.130805	1.857069	0.012423
23	6	0	0.490970	3.077352	-0.412530
24	8	0	-0.439428	2.873626	0.492429
25	8	0	1.720346	2.730946	-0.033674
26	8	0	0.236658	3.446952	-1.589786
27	19	0	1.517540	0.677249	-2.028074
28	6	0	-0.806292	-1.055484	0.342902
29	8	0	-0.430399	-0.437989	1.457626
30	8	0	-1.353575	-2.202910	0.482673
31	19	0	-2.274894	1.913867	-1.050544
32	53	0	-4.962181	-0.366392	-0.156069
33	19	0	-2.611495	-1.353638	2.656015
34	8	0	-0.676192	-0.489032	-0.814958
35	19	0	-2.260046	-2.415712	-1.927333

Zero-point correction=	0.213290 (Hartree/Particle)
Thermal correction to Energy=	0.244156
Thermal correction to Enthalpy=	0.245100
Thermal correction to Gibbs Free Energy=	0.142677
Sum of electronic and zero-point Energies=	-3490.433149
Sum of electronic and thermal Energies=	-3490.402283
Sum of electronic and thermal Enthalpies=	-3490.401339
Sum of electronic and thermal Free Energies=	-3490.503762

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -3490.3148002

40-TS (M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	-1.142123	-0.727636	1.114980
2	6	0	-3.984306	0.986239	0.266079
3	6	0	-4.347234	-0.304184	0.713562
4	6	0	-5.679243	-0.702634	0.492903
5	6	0	-6.603758	0.127977	-0.133422
6	6	0	-6.209748	1.394264	-0.575272
7	6	0	-4.898854	1.837981	-0.388681
8	1	0	-5.981131	-1.694145	0.821530
9	1	0	-7.626959	-0.207605	-0.278249
10	1	0	-6.924785	2.049835	-1.065895

11	8	0	-2.701872	1.492244	0.345267
12	6	0	-1.856298	1.129408	1.433377
13	1	0	-1.021351	1.832806	1.410314
14	1	0	-2.404129	1.192903	2.381780
15	6	0	-3.366564	-1.285492	1.286100
16	1	0	-3.826091	-2.275074	1.390992
17	1	0	-3.045653	-1.038863	2.308097
18	6	0	-4.447031	3.192172	-0.875746
19	1	0	-3.995913	3.778153	-0.067574
20	1	0	-3.683471	3.105499	-1.659348
21	1	0	-5.287643	3.758014	-1.286893
22	1	0	-2.681466	-1.703362	0.243213
23	6	0	-1.095035	-2.635630	-0.952027
24	8	0	-0.543719	-2.731107	0.235810
25	8	0	-2.350548	-2.228929	-1.020181
26	8	0	-0.434433	-2.847690	-2.013516
27	19	0	-1.547434	0.049330	-2.222773
28	6	0	1.029383	0.925316	0.050903
29	8	0	0.827940	0.042566	1.032934
30	8	0	1.493663	2.073168	0.361328
31	19	0	1.848346	-2.058069	-0.707795
32	53	0	4.997027	-0.049889	-0.043534
33	19	0	2.567675	1.209452	2.622398
34	8	0	0.816280	0.570420	-1.170108
35	19	0	2.713911	2.291884	-1.968604

Zero-point correction= 0.209340 (Hartree/Particle)

Thermal correction to Energy= 0.238789

Thermal correction to Enthalpy= 0.239734

Thermal correction to Gibbs Free Energy= 0.142604

Sum of electronic and zero-point Energies= -3490.412846

Sum of electronic and thermal Energies= -3490.383397

Sum of electronic and thermal Enthalpies= -3490.382452

Sum of electronic and thermal Free Energies= -3490.479582

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -3490.2944896

66 (M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.551875	0.383647	0.309741
2	6	0	-3.453508	-0.419680	1.476150
3	6	0	-3.596402	-1.804056	1.325103
4	6	0	-3.846185	-2.365152	0.073154
5	6	0	-3.960081	-1.558739	-1.061382
6	6	0	-3.827670	-0.170326	-0.969894

7	1	0	-3.520264	-2.440450	2.202056
8	1	0	-3.956733	-3.441513	-0.020586
9	1	0	-4.168283	-2.007241	-2.028436
10	8	0	-3.615260	1.785040	0.461889
11	6	0	-2.293080	2.289357	0.298808
12	1	0	-1.947814	2.785121	1.211594
13	46	0	-1.203620	0.625323	0.003468
14	6	0	-3.307011	0.213223	2.836458
15	1	0	-3.005302	-0.532393	3.577002
16	1	0	-2.573096	1.022194	2.840752
17	1	0	-4.263621	0.641307	3.160973
18	1	0	-2.220352	2.930404	-0.585348
19	53	0	1.047771	2.183793	-0.243204
20	19	0	2.684115	-0.494829	-2.189232
21	53	0	-0.015051	-2.071941	-0.358247
22	6	0	5.083124	-0.476888	0.586122
23	8	0	4.075254	-0.835008	-0.114404
24	8	0	5.049842	-0.235264	1.819533
25	6	0	6.405294	-0.318211	-0.166217
26	1	0	7.245060	-0.174357	0.517639
27	1	0	6.589167	-1.194452	-0.796553
28	1	0	6.339107	0.552315	-0.830384
29	19	0	2.410314	-0.584288	2.041565
30	6	0	-4.053216	0.733103	-2.154886
31	1	0	-4.932725	1.366816	-1.991525
32	1	0	-3.204377	1.400699	-2.327180
33	1	0	-4.217590	0.145997	-3.061992

Zero-point correction= 0.229445 (Hartree/Particle)

Thermal correction to Energy= 0.256295

Thermal correction to Enthalpy= 0.257239

Thermal correction to Gibbs Free Energy= 0.161795

Sum of electronic and zero-point Energies= -2002.734648

Sum of electronic and thermal Energies= -2002.707798

Sum of electronic and thermal Enthalpies= -2002.706854

Sum of electronic and thermal Free Energies= -2002.802298

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -2002.6153078

68 (M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	0.318444	0.835825	0.478694
2	6	0	-3.262537	-0.562723	-0.169918
3	6	0	-3.652892	-0.376896	1.164498
4	6	0	-5.021497	-0.477988	1.453427

5	6	0	-5.952122	-0.755971	0.451743
6	6	0	-5.528777	-0.940718	-0.865381
7	6	0	-4.172271	-0.845293	-1.200194
8	1	0	-5.352009	-0.339390	2.479531
9	1	0	-7.007717	-0.830304	0.697880
10	1	0	-6.252657	-1.155864	-1.647128
11	8	0	-1.910302	-0.522579	-0.524557
12	6	0	-1.317583	0.753151	-0.678718
13	1	0	-0.940889	0.858830	-1.701410
14	1	0	-2.010713	1.554822	-0.409589
15	6	0	-2.643763	-0.083324	2.243560
16	1	0	-3.104436	-0.153415	3.233057
17	1	0	-2.230532	0.927428	2.138760
18	6	0	-3.686214	-1.051447	-2.612929
19	1	0	-3.002737	-0.255353	-2.924805
20	1	0	-3.143578	-2.000208	-2.715208
21	1	0	-4.526238	-1.077282	-3.312482
22	1	0	-1.795926	-0.771938	2.195817
23	6	0	1.563636	-1.084969	1.830418
24	8	0	2.221543	-0.009518	1.719323
25	8	0	0.388980	-1.187027	1.320178
26	6	0	2.124004	-2.283916	2.550202
27	1	0	1.444325	-2.572757	3.358506
28	1	0	2.184692	-3.126064	1.852757
29	1	0	3.111627	-2.069559	2.961276
30	19	0	3.415312	0.291876	-0.759473
31	53	0	0.880058	3.350400	-0.382266
32	6	0	2.848746	-3.186771	-0.781111
33	8	0	2.069230	-4.127445	-0.478093
34	8	0	2.487977	-2.063424	-1.272365
35	6	0	4.343586	-3.364233	-0.497139
36	1	0	4.598039	-2.825860	0.425383
37	1	0	4.599438	-4.416622	-0.352863
38	1	0	4.949427	-2.946145	-1.307571
39	19	0	-0.190308	-2.711505	-0.828864

Zero-point correction=	0.281654 (Hartree/Particle)
Thermal correction to Energy=	0.310676
Thermal correction to Enthalpy=	0.311620
Thermal correction to Gibbs Free Energy=	0.216420
Sum of electronic and zero-point Energies=	-2219.776607
Sum of electronic and thermal Energies=	-2219.747586
Sum of electronic and thermal Enthalpies=	-2219.746642
Sum of electronic and thermal Free Energies=	-2219.841841

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -2219.6724306

69-TS (M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	0.076123	-1.217788	0.753419
2	6	0	3.216002	-0.386246	-0.341132
3	6	0	3.119878	-0.129452	1.044403
4	6	0	4.084214	0.736530	1.597605
5	6	0	5.093497	1.301610	0.826322
6	6	0	5.159793	1.024694	-0.543182
7	6	0	4.224108	0.184639	-1.147971
8	1	0	4.025363	0.960466	2.659651
9	1	0	5.828790	1.955418	1.286781
10	1	0	5.947184	1.461748	-1.151704
11	8	0	2.286155	-1.121804	-1.045236
12	6	0	1.497417	-2.104851	-0.409483
13	1	0	1.017093	-2.663783	-1.210920
14	1	0	2.106965	-2.762402	0.219040
15	6	0	1.983004	-0.608438	1.889702
16	1	0	2.036990	-0.160020	2.888502
17	1	0	1.974443	-1.684729	2.078202
18	6	0	4.264199	-0.108429	-2.627049
19	1	0	4.284379	-1.186114	-2.821787
20	1	0	3.379851	0.283830	-3.145244
21	1	0	5.147625	0.343873	-3.085755
22	1	0	0.995081	0.363552	1.661252
23	6	0	-0.799868	1.331555	2.081693
24	8	0	-1.359546	0.209992	1.930759
25	8	0	0.436989	1.536892	1.790653
26	6	0	-1.588156	2.515942	2.581197
27	1	0	-0.962347	3.160981	3.201364
28	1	0	-1.907854	3.091869	1.705092
29	1	0	-2.467443	2.194258	3.144068
30	19	0	-3.697090	0.602751	0.326513
31	53	0	-2.000315	-2.323480	-0.710379
32	6	0	-1.833709	3.361340	-1.256098
33	8	0	-0.725126	3.767706	-1.683127
34	8	0	-2.041803	2.201570	-0.753989
35	6	0	-3.045237	4.292179	-1.320002
36	1	0	-3.434271	4.460187	-0.309018
37	1	0	-2.793115	5.253981	-1.772495
38	1	0	-3.844434	3.818688	-1.901773
39	19	0	0.547435	1.452489	-1.201300

Zero-point correction= 0.276950 (Hartree/Particle)
 Thermal correction to Energy= 0.304994
 Thermal correction to Enthalpy= 0.305938
 Thermal correction to Gibbs Free Energy= 0.213210

Sum of electronic and zero-point Energies= -2219.741706
 Sum of electronic and thermal Energies= -2219.713662
 Sum of electronic and thermal Enthalpies= -2219.712718
 Sum of electronic and thermal Free Energies= -2219.805446

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -2219.6348756

72(M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.925757	-0.938034	0.996870
2	6	0	-3.982665	-1.358344	0.166796
3	6	0	-4.855385	-0.372391	-0.321148
4	6	0	-4.689894	0.972203	0.021884
5	6	0	-3.645495	1.352742	0.868250
6	6	0	-2.741072	0.406463	1.372844
7	1	0	-5.680822	-0.673268	-0.961017
8	1	0	-5.378043	1.719521	-0.362330
9	1	0	-3.514708	2.396442	1.135959
10	8	0	-2.051126	-1.892233	1.520344
11	6	0	-1.143479	-2.486471	0.626856
12	1	0	-1.497129	-2.518249	-0.404198
13	46	0	0.467266	-1.367248	0.939519
14	6	0	-4.193002	-2.811400	-0.184610
15	1	0	-5.255332	-3.010811	-0.350724
16	1	0	-3.660093	-3.085499	-1.102850
17	1	0	-3.835991	-3.473081	0.609251
18	1	0	-0.858945	-3.472161	1.014696
19	6	0	4.749023	0.767499	0.033770
20	8	0	4.338453	-0.220196	0.738359
21	8	0	4.096795	1.807301	-0.222855
22	6	0	-1.608178	0.833038	2.267262
23	1	0	-1.761383	0.503069	3.300912
24	1	0	-0.652309	0.395359	1.941330
25	1	0	-1.489503	1.918718	2.247671
26	6	0	2.259491	0.027700	3.112831
27	1	0	1.316497	0.299374	3.599081
28	1	0	3.024365	0.759283	3.405765
29	8	0	2.077181	0.029728	1.696793
30	1	0	2.567860	-0.960779	3.481942
31	1	0	3.040675	-0.081849	1.242072
32	53	0	1.216951	-1.439729	-1.682834
33	19	0	1.518717	2.262548	0.176427
34	6	0	6.151226	0.609904	-0.549054
35	1	0	6.523522	1.556167	-0.947928
36	1	0	6.841379	0.227436	0.209343

37	1	0	6.119939	-0.126792	-1.360939
38	19	0	-1.890767	0.564763	-2.167434
39	6	0	-1.234916	3.563595	-0.363384
40	8	0	-0.873374	2.635209	-1.166518
41	8	0	-0.636512	3.875809	0.696576
42	6	0	-2.478870	4.359231	-0.770547
43	1	0	-3.297299	3.683200	-1.038518
44	1	0	-2.807209	5.027730	0.028798
45	1	0	-2.246621	4.956961	-1.660170

Zero-point correction=	0.333502 (Hartree/Particle)
Thermal correction to Energy=	0.366768
Thermal correction to Enthalpy=	0.367712
Thermal correction to Gibbs Free Energy=	0.261260
Sum of electronic and zero-point Energies=	-2335.465646
Sum of electronic and thermal Energies=	-2335.432380
Sum of electronic and thermal Enthalpies=	-2335.431436
Sum of electronic and thermal Free Energies=	-2335.537888

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -2335.3722995

73-TS(M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.173585	-0.980061	0.867250
2	6	0	-3.946876	-1.644472	-0.110332
3	6	0	-4.811288	-0.877821	-0.905748
4	6	0	-4.927814	0.503571	-0.720085
5	6	0	-4.167671	1.136586	0.267082
6	6	0	-3.272075	0.411358	1.070629
7	1	0	-5.415477	-1.377581	-1.658756
8	1	0	-5.616459	1.079762	-1.331816
9	1	0	-4.259491	2.208608	0.419781
10	8	0	-2.366958	-1.715475	1.711023
11	6	0	-1.155890	-2.235184	1.172522
12	1	0	-1.282189	-2.526030	0.126683
13	46	0	0.432653	-0.935311	1.151211
14	6	0	-3.871396	-3.141495	-0.286069
15	1	0	-4.818290	-3.531246	-0.670890
16	1	0	-3.086994	-3.425215	-0.997658
17	1	0	-3.646204	-3.639932	0.660703
18	1	0	-0.889721	-3.102981	1.779142
19	6	0	4.789921	-0.215325	0.143510
20	8	0	4.158951	-0.744057	1.187316
21	8	0	4.463243	0.846875	-0.377977
22	6	0	-2.412688	1.124781	2.083754

23	1	0	-2.077801	0.448824	2.871903
24	1	0	-1.521961	1.535979	1.593358
25	1	0	-2.956528	1.960748	2.534875
26	6	0	1.304688	0.489363	2.771615
27	1	0	0.506932	1.196919	3.021485
28	1	0	1.749075	-0.049070	3.617045
29	8	0	2.014426	0.690962	1.713519
30	1	0	0.120110	-0.885999	2.709569
31	1	0	3.365574	-0.176509	1.427190
32	53	0	1.112230	-1.371485	-1.573010
33	19	0	2.160038	2.312258	-0.476696
34	6	0	5.939101	-1.061705	-0.333099
35	1	0	6.492698	-0.541466	-1.114954
36	1	0	6.603433	-1.302878	0.502024
37	1	0	5.549338	-2.006801	-0.726603
38	19	0	-1.800765	0.756662	-2.014117
39	6	0	-0.556065	3.740955	-0.254802
40	8	0	-0.561350	2.583934	-0.802053
41	8	0	0.472986	4.356232	0.117932
42	6	0	-1.925566	4.384030	-0.023307
43	1	0	-2.439439	3.850821	0.784414
44	1	0	-1.832445	5.436135	0.256543
45	1	0	-2.547765	4.296164	-0.920328

Zero-point correction= 0.329318 (Hartree/Particle)

Thermal correction to Energy= 0.362539

Thermal correction to Enthalpy= 0.363483

Thermal correction to Gibbs Free Energy= 0.257631

Sum of electronic and zero-point Energies= -2335.438216

Sum of electronic and thermal Energies= -2335.404995

Sum of electronic and thermal Enthalpies= -2335.404051

Sum of electronic and thermal Free Energies= -2335.509903

M06-D3/6-311++G(d,p)-LANL2DZ(SMD)//B3LYP-D3/6-31G(d,p)-LANL2DZ(SMD) energy in DMAc solvent = -2335.3412389