

Electronic supplementary information for

Sufficient driving force for quinoidal isoindigo-based diradicaloids with tunable diradical characters

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12. Coordinates and energies of the computed molecules.

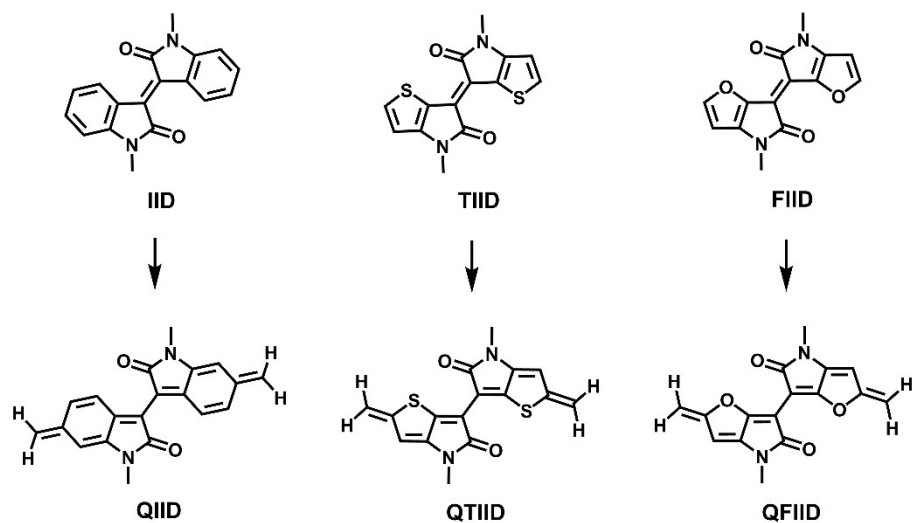
Table S1 The calculated $\Delta E(\text{OS-T}_1)$ (kcal mol⁻¹), diradical character y_0 , spin-squared values of broken-symmetry (BS) open-shell singlet ($\langle S_{\text{OS}}^2 \rangle$) and triplet state ($\langle S_{\text{T}1}^2 \rangle$) of *t*-Bu-S2IID using different functionals and 6-31G(d,p) basis set.

Functional	$\Delta E(\text{OS-T}_1)$	y_0	$\langle S_{\text{OS}}^2 \rangle$	$\langle S_{\text{T}1}^2 \rangle$
BLYP	-4.207	0	0	2.016
B3LYP	-1.150	0.574	1.055	2.060
B3LYP-GD3BJ	-1.230	0.555	1.050	2.059
PBE1PBE	-1.143	0.657	1.123	2.086
BHandHLYP	-1.427	0.819	1.415	2.217
M06-2X	-0.403	0.854	1.082	2.067
CAM-B3LYP	-0.661	0.871	1.193	2.124
ω B97XD	-0.442	0.910	1.149	2.105

Table S2. The calculated Mulliken electronegativity (χ) of different terminal end groups at the theoretical level of (U)B3LYP/6-31G(d,p).

	S1	S2	S3	S4	S5	S6
χ	6.120	5.060	5.563	4.915	5.822	5.066
	S7	S8	S9	S10		
χ	5.695	5.990	3.322	3.033		

(a)



(b)

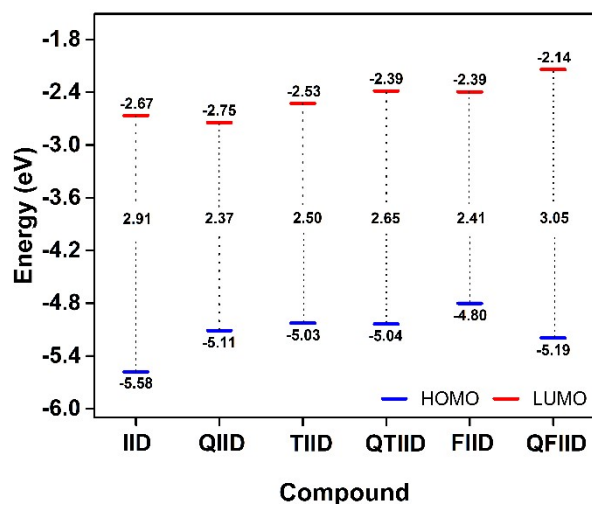


Fig. S1 Comparison between aromatic and quinoidalized IID cores: (a) molecular structures; (b) HOMO, LUMO energy levels and the corresponding HLGs (eV)

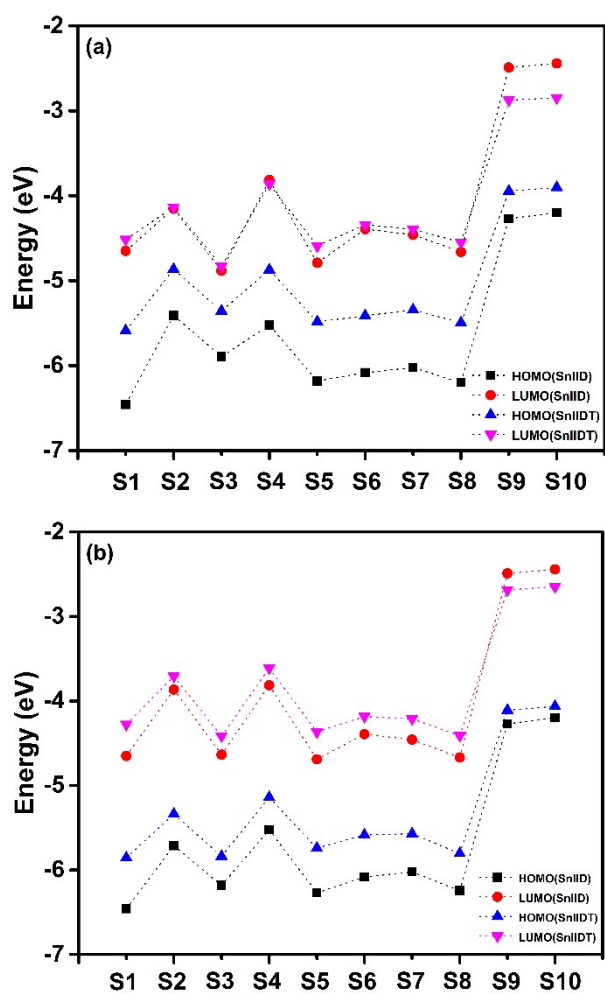


Fig. S2 HOMO, LUMO energy levels of SnIID and SnIIDT in the (a) CS and (b) OS structures.

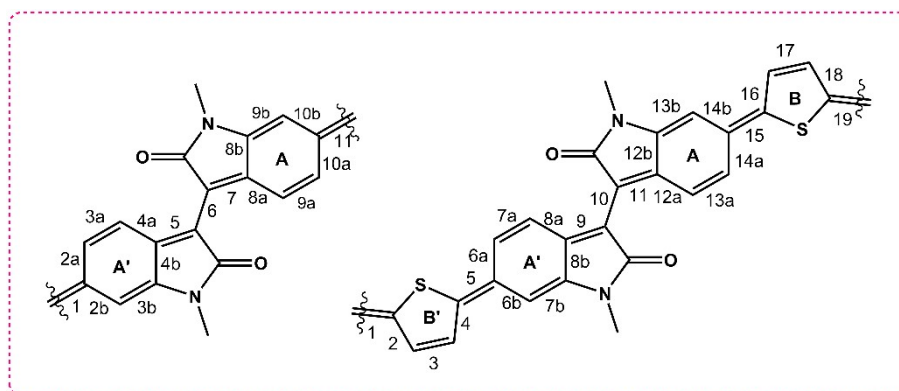


Fig. S3 Bond indexes and ring labels of quinoial IID and IIDT cores. $r_i = (r_{ia} + r_{ib})/2$

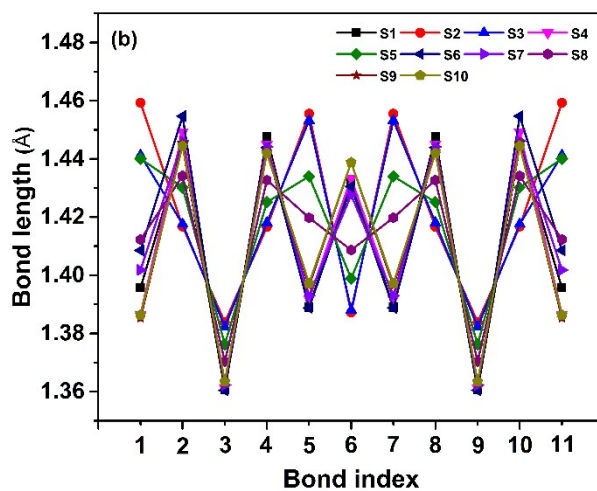
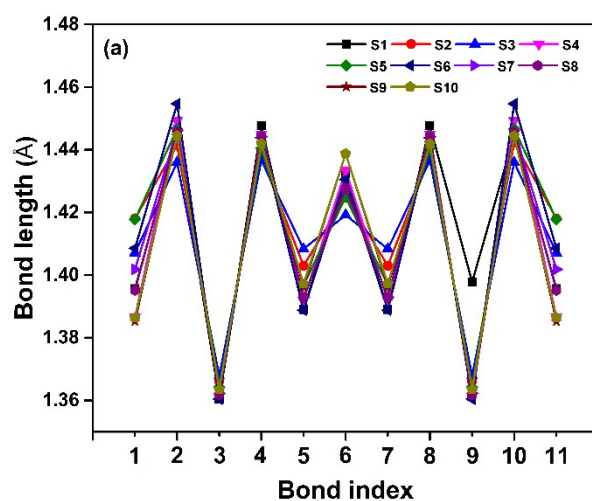


Fig. S4 Bond lengths of the highlight backbone of SnIID core in the (a) CS and (b) OS structures.

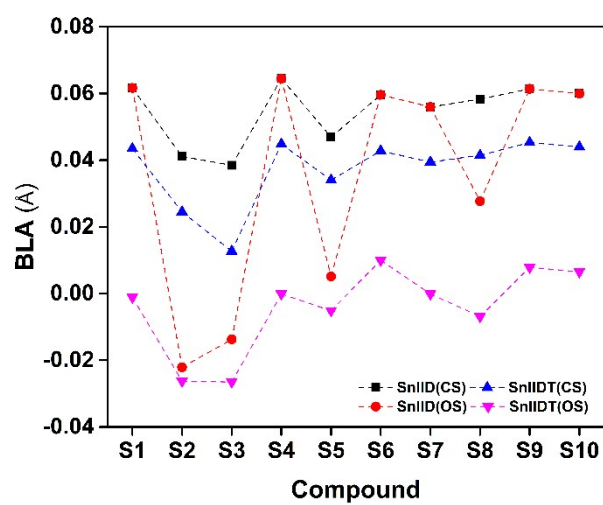


Fig. S5 BLA values of SnIID and SnIIDT compounds in the CS and OS structures.

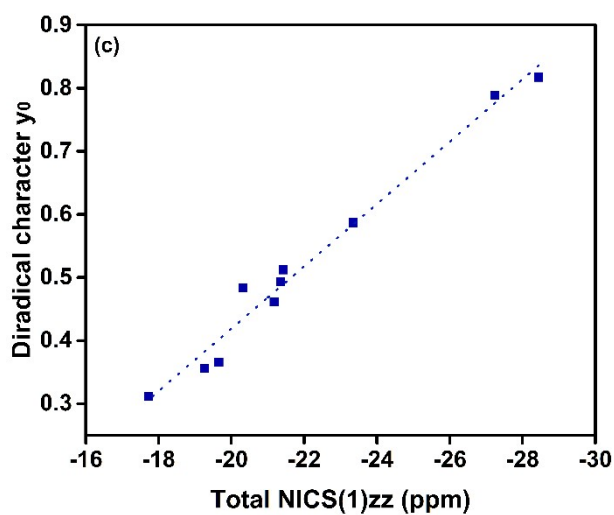
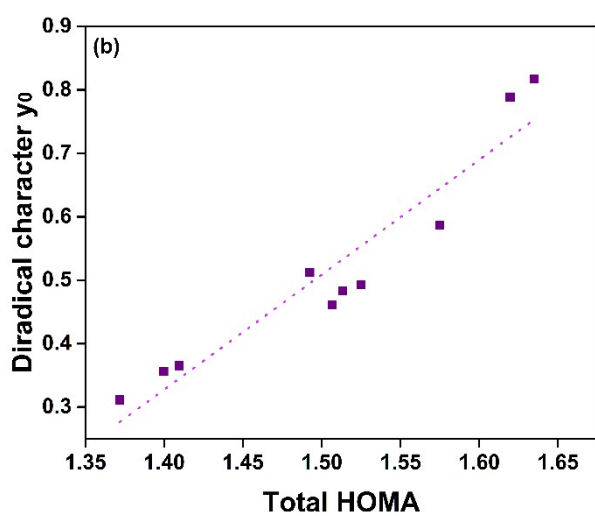
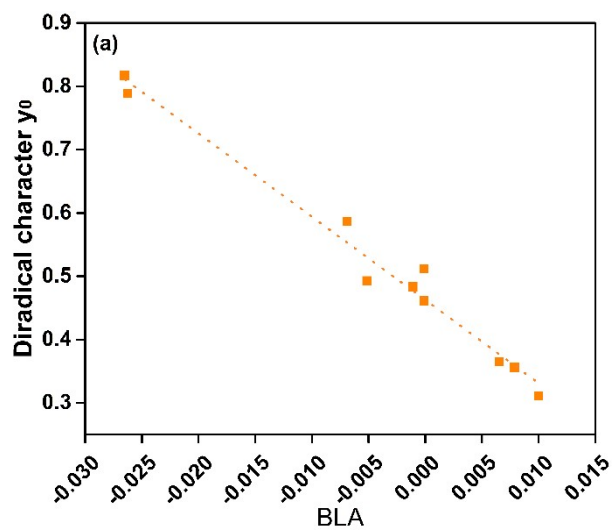


Fig. S6 Correlations between diradical character y_0 and (a) BLA, (b) total HOMA and (c) total NICS(1)zz for SnIIDT in the OS structures.

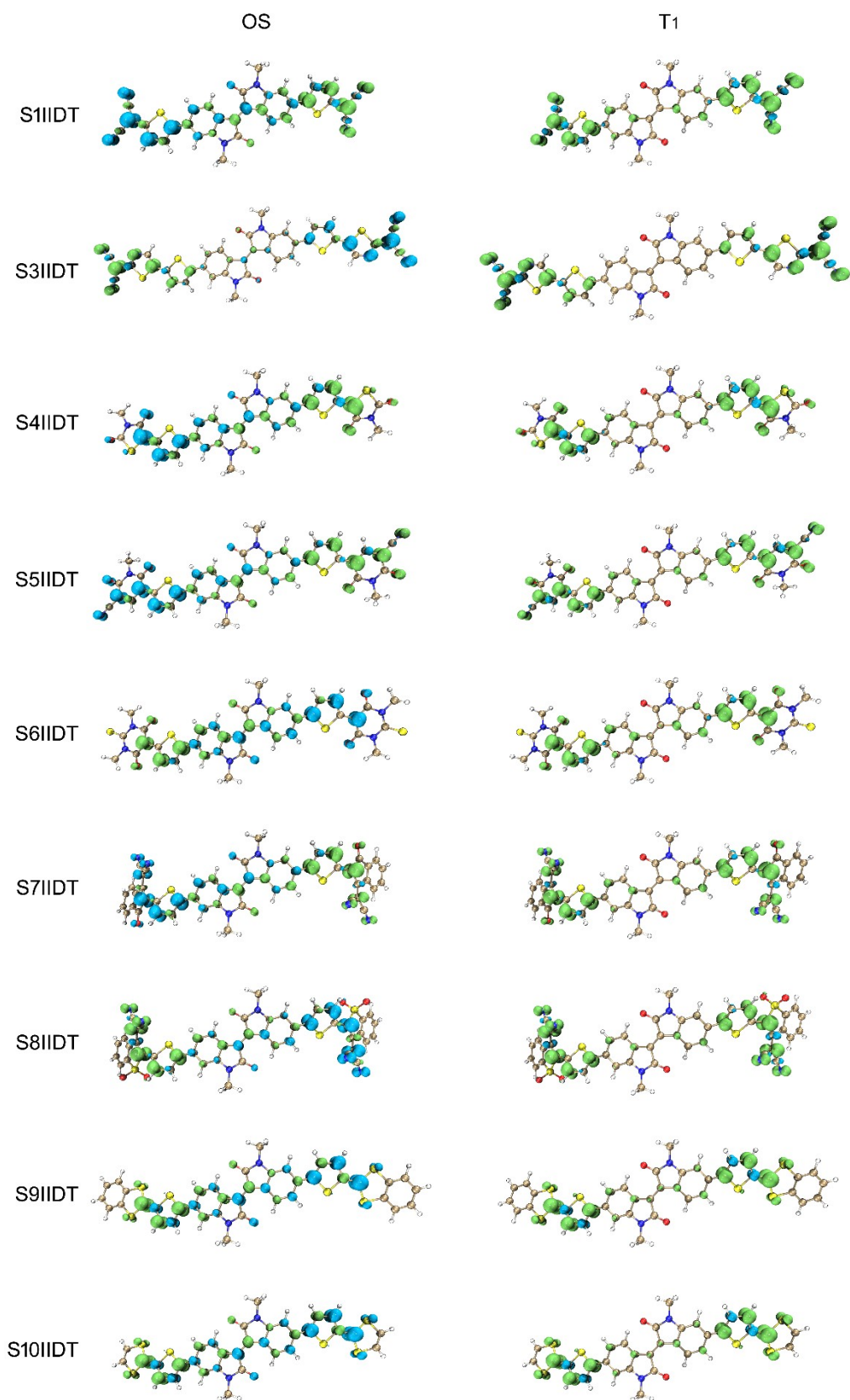


Fig. S7 Spin density distributions of SnIIDT in the OS and T₁ states (isovalue = 0.005 e-bohr⁻³)

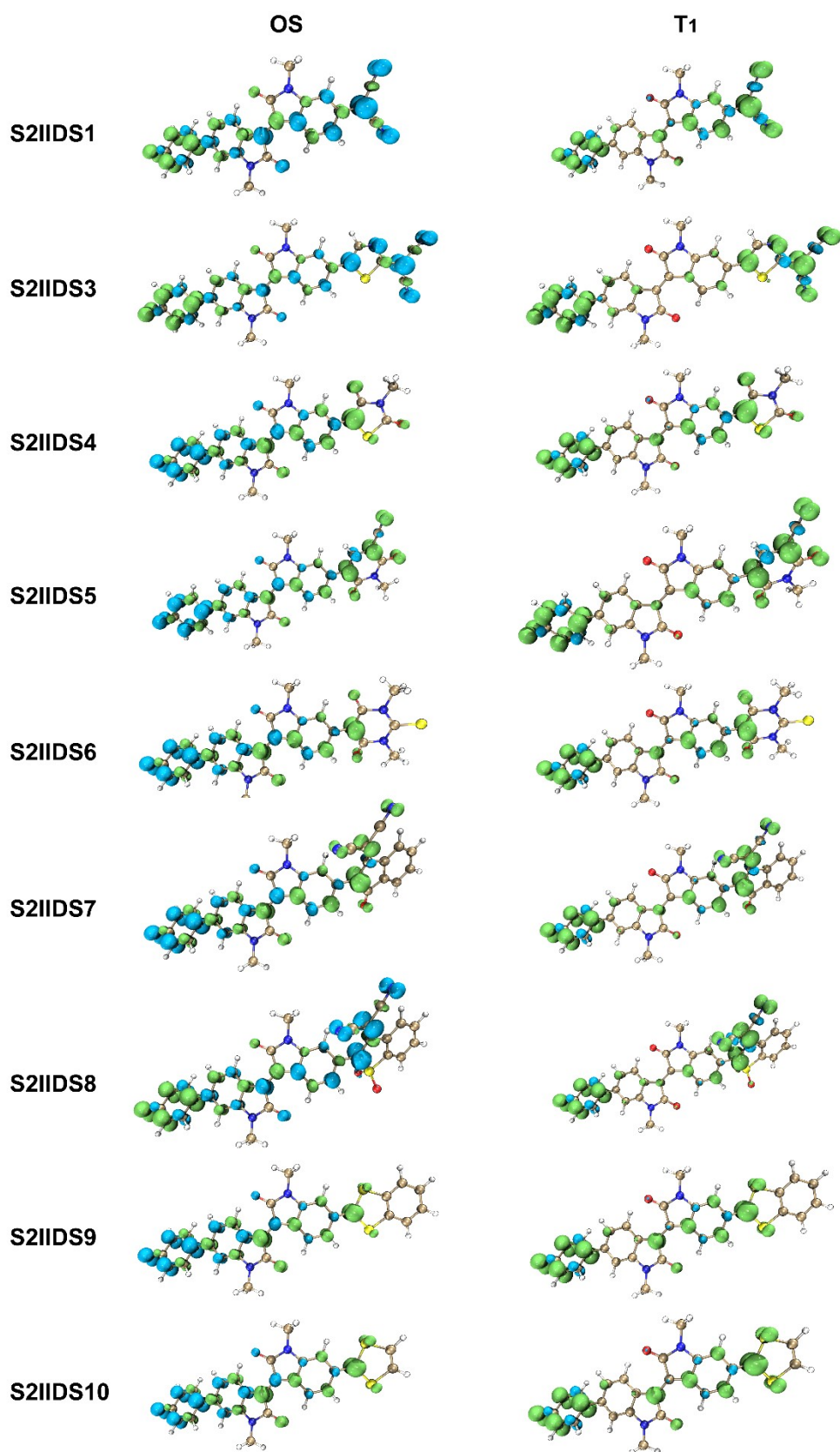


Fig. S8 Spin density distributions of S2IIDS_n in the OS and T₁ states (isovalue = 0.005 e·bohr⁻³)

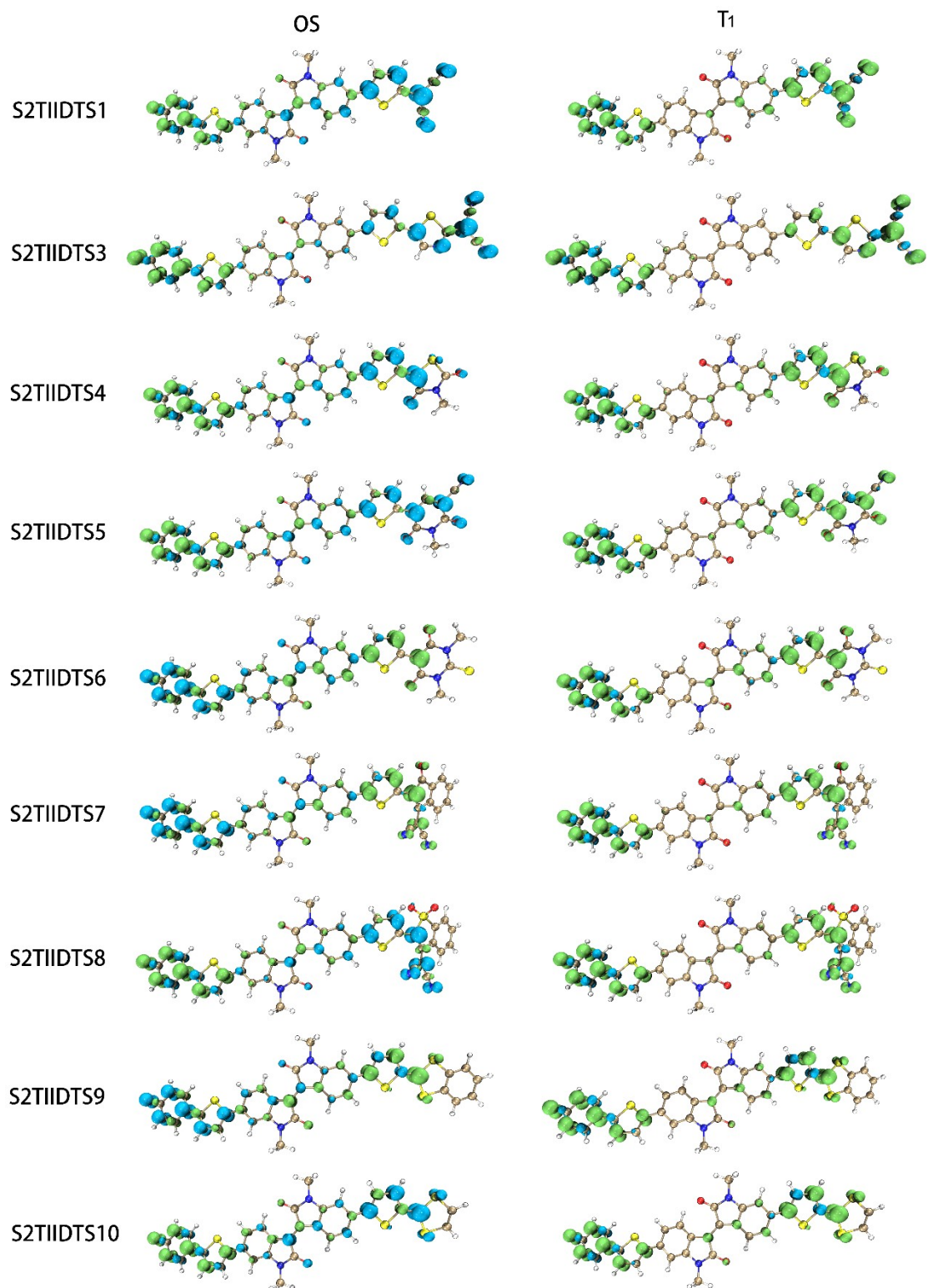


Fig. S9 Spin density distributions of S2TIIDTS_n in the OS and T₁ states (isovalue = 0.005 e-bohr⁻³)

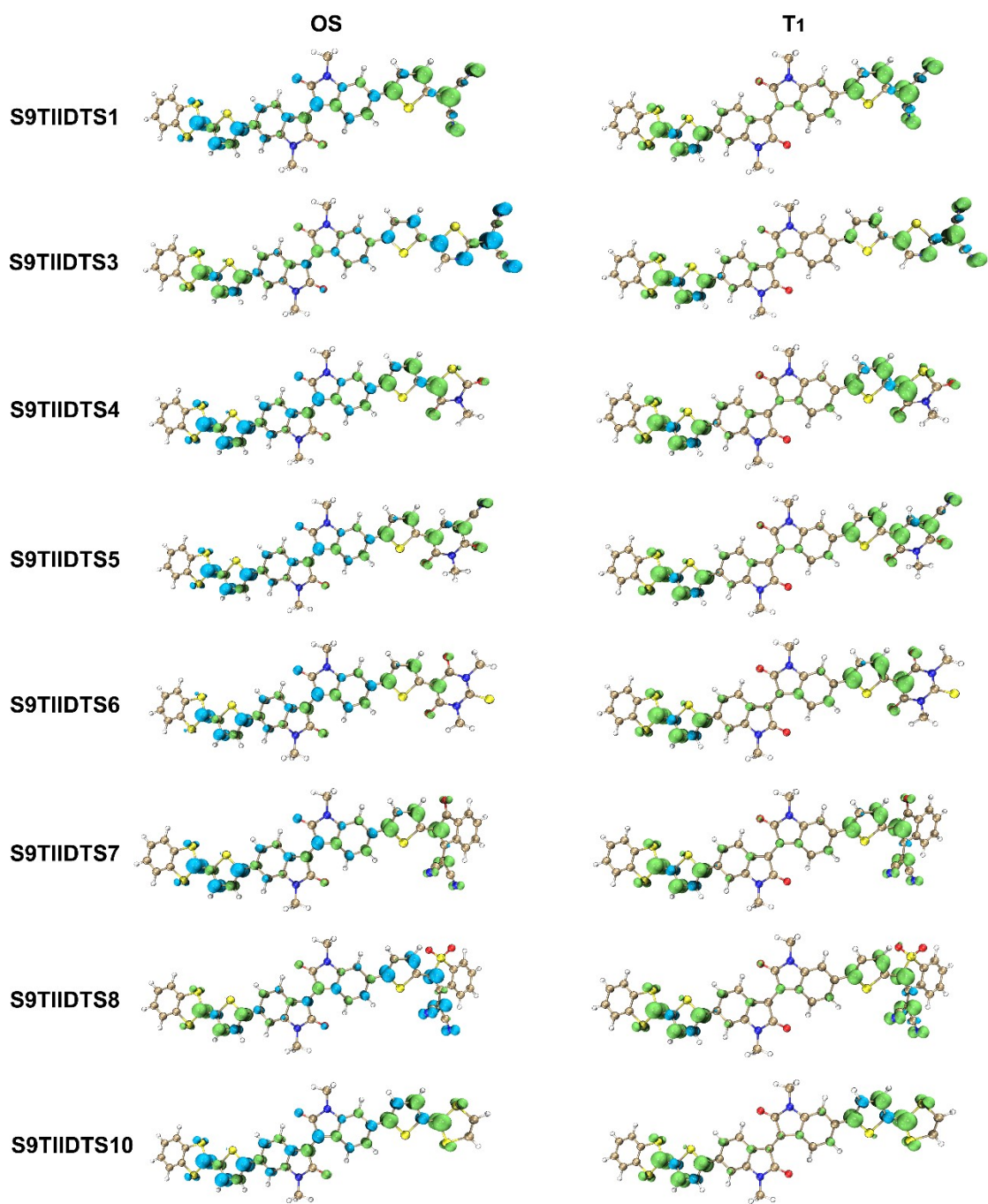


Fig. S10 Spin density distributions of S9TIIDTS_n in the OS and T₁ states (isovalue = 0.005 e-bohr⁻³)

Table S3. $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ and diradical character y_0 of S2IID, S2IIDT, S2FIID, S2FIIDT, S2TIID, S2TIIDT with the dihedral angle (φ) fixed at the specific values.

Molecule	φ	$\Delta E(\text{OS-CS})$	$\Delta E(\text{OS-T}_1)$	y_0
S2IID	0°	-6.907	-1.048	0.621
	13.7° ^a	-5.529	-1.179	0.587
	30°	-3.750	-2.016	0.428
	60°	-0.211	-8.257	0.017
S2IIDT	0°	-10.546	-0.350	0.797
	12.2° ^a	-9.786	-0.381	0.789
	30°	-7.888	-0.663	0.715
	60°	-2.880	-5.097	0.256
S2FIID	0° ^a	0	-16.033	0
	30°	0	-19.712	0
	60°	0	-23.064	0
S2FIIDT	0° ^a	-0.145	-5.873	0.018
	30°	0	-8.931	0
	60°	0	-12.036	0
S2TIID	0° ^a	0	-11.763	0
	30°	0	-16.053	0
	60°	0	-25.545	0
S2TIIDT	0° ^a	-1.023	-3.611	0.146
	30°	-0.149	-6.643	0.017
	60°	0	-14.994	0

^a In contrast to other fixed dihedral angles, the dihedral angles correspond to that of OS structure with full optimization as references, and the corresponding $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ are also obtained by the full optimized OS, CS and T₁ structures.

Table S4. HOMO, LUMO energy levels and HLGs, $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$, diradical character y_0 and N^{FOD} of SnTIID and SnTIIDT.

Compound	HOMO ^a	LUMO ^a	HLG ^a	$\Delta E(\text{OS-CS})^b$	$\Delta E(\text{OS-T}_1)^b$	y_0	N^{FOD}
S1TIID	-6.452	-4.234	2.218	0	-20.931	0	1.017
S2TIID	-5.476	-3.732	1.744	0	-11.763	0	1.631
S3TIID	-5.998	-4.512	1.486	0	-9.178	0	1.742
S4TIID	-5.497	-3.394	2.103	0	-19.983	0	1.153
S5TIID	-6.230	-4.353	1.877	0	-16.918	0	1.541
S6TIID	-6.040	-3.992	2.048	0	-21.676	0	1.667
S7TIID	-5.997	-4.041	1.956	0	-19.217	0	1.686
S8TIID	-6.152	-4.162	1.989	0	-17.533	0	1.479
S9TIID	-4.386	-2.229	2.157	0	-21.819	0	1.147
S10TIID	-4.309	-2.183	2.125	0	-21.267	0	1.121
S1TIIDT	-5.704	-4.159	1.546	0	-10.008	0	1.663
S2TIIDT	-5.017	-3.780	1.238	-1.023	-3.611	0.146	2.443
S3TIIDT	-5.507	-4.457	1.051	-1.497	-2.686	0.216	2.575
S4TIIDT	-5.008	-3.527	1.481	0	-9.044	0	1.808
S5TIIDT	-5.637	-4.309	1.328	0	-7.654	0	2.135
S6TIIDT	-5.523	-4.002	1.521	0	-11.935	0	2.125
S7TIIDT	-5.480	-4.060	1.420	0	-10.087	0	2.235
S8TIIDT	-5.627	-4.209	1.418	0	-9.114	0	2.089
S9TIIDT	-4.112	-2.591	1.522	0	-9.841	0	1.857
S10TIIDT	-4.063	-2.559	1.504	0	-9.519	0	1.828

^a HOMO, LUMO and HLG are in eV

^b $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ are in kcal mol⁻¹.

Table S5. HOMO, LUMO energy levels and HLGs, $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$, diradical character y_0 and N^{FOD} of SnFIID and SnFIIDT.

Compound	HOMO ^a	LUMO ^a	HLG ^a	$\Delta E(\text{OS-CS})^b$	$\Delta E(\text{OS-T}_1)^b$	y_0	N^{FOD}
S1FIID	-6.610	-4.069	2.541	0	-26.431	0	0.807
S2FIID	-5.519	-3.570	1.950	0	-16.033	0	1.441
S3FIID	-6.049	-4.385	1.664	0	-13.297	0	1.562
S4FIID	-5.675	-3.205	2.471	0	-25.233	0	0.942
S5FIID	-6.342	-4.123	2.219	0	-22.519	0	1.284
S6FIID	-5.945	-3.817	2.129	0	-27.890	0	1.426
S7FIID	-6.219	-3.907	2.312	0	-24.629	0	1.450
S8FIID	-6.362	-4.090	2.272	0	-23.934	0	1.290
S9FIID	-4.377	-2.014	2.363	0	-25.152	0	1.014
S10FIID	-4.281	-1.958	2.323	0	-24.402	0	0.989
S1FIIDT	-5.755	-4.039	1.716	0	-13.790	0	1.496
S2FIIDT	-5.035	-3.662	1.373	-0.145	-5.873	0.018	2.193
S3FIIDT	-5.531	-4.352	1.179	-0.336	-4.689	0.044	2.359
S4FIIDT	-5.041	-3.403	1.637	0	-12.521	0	1.653
S5FIIDT	-5.678	-4.202	1.476	0	-11.128	0	1.968
S6FIIDT	-5.578	-3.887	1.691	0	-15.826	0	1.939
S7FIIDT	-5.536	-3.958	1.578	0	-13.721	0	2.068
S8FIIDT	-5.686	-4.109	1.577	0	-12.722	0	1.925
S9FIIDT	-4.114	-2.452	1.662	0	-12.541	0	1.739
S10FIIDT	-4.056	-2.415	1.641	0	-12.154	0	1.709

^a HOMO, LUMO and HLG are in eV

^b $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ are in kcal mol⁻¹.

Table S6. HOMO, LUMO energy levels and HLGs, $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$, diradical character y_0 and N^{FOD} of SnIID and SnIIDT.

Compound	HOMO ^a	LUMO ^a	HLG ^a	$\Delta E(\text{OS-CS})^b$	$\Delta E(\text{OS-T}_1)^b$	y_0	N^{FOD}
S1IID	-6.458	-4.650	1.808	0	-7.477	0	1.414
S2IID	-5.408	-4.152	1.256	-5.529	-1.179	0.587	2.464
S3IID	-5.893	-4.884	1.010	-5.138	-1.187	0.529	2.339
S4IID	-5.524	-3.814	1.710	0	-7.043	0	1.531
S5IID	-6.181	-4.789	1.392	-1.276	-2.784	0.208	2.313
S6IID	-6.083	-4.393	1.690	0	-8.552	0	2.139
S7IID	-6.023	-4.458	1.565	0	-5.681	0	2.144
S8IID	-6.199	-4.662	1.537	-0.259	-3.120	0.081	2.200
S9IID	-4.270	-2.490	1.780	0	-11.029	0	1.370
S10IID	-4.198	-2.442	1.756	0	-10.676	0	1.344
S1IIDT	-5.589	-4.515	1.075	-4.512	-1.435	0.483	2.240
S2IIDT	-4.866	-4.136	0.730	-9.876	-0.381	0.789	2.790
S3IIDT	-5.357	-4.830	0.527	-10.041	-0.242	0.817	2.766
S4IIDT	-4.872	-3.864	1.008	-4.708	-1.216	0.512	2.339
S5IIDT	-5.484	-4.591	0.893	-4.455	-1.175	0.493	2.579
S6IIDT	-5.412	-4.341	1.070	-2.516	-2.125	0.311	2.685
S7IIDT	-5.343	-4.395	0.948	-3.736	-1.272	0.461	2.779
S8IIDT	-5.496	-4.548	0.948	-4.789	-0.840	0.587	2.709
S9IIDT	-3.945	-2.874	1.070	-3.224	-1.999	0.356	2.275
S10IIDT	-3.902	-2.847	1.055	-3.353	-1.941	0.365	2.239

^a HOMO, LUMO and HLG are in eV

^b $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ are in kcal mol⁻¹.

Table S7. HOMO, LUMO energy levels and HLGs, $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$, diradical character y_0 and N^{FOD} of S2IIDAr.

Compound	HOMO ^a	LUMO ^a	HLG ^a	$\Delta E(\text{OS-CS})^b$	$\Delta E(\text{OS-T}_1)^b$	y_0	N^{FOD}
S2IIDB	-4.746	-4.432	0.314	-19.095	-0.036	0.952	2.985
S2IIDF	-4.802	-4.050	0.752	-11.618	-0.241	0.732	2.705
S2IIDT	-4.866	-4.136	0.730	-9.786	-0.381	0.789	2.790
S2IIDTz	-5.079	-4.427	0.652	-9.121	-0.553	0.842	2.892

^a HOMO, LUMO and HLG are in eV, ^b $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ are in kcal mol⁻¹.

Table S8. The values of HOMA of the quinoidal IID and IIDT in CS and OS states.

Compound	HOMA(CS)			HOMA(OS)		
	Ring A	Ring B	Ring C ^a	Ring A	Ring B	Ring C ^a
S2IID	0.49		0.06	0.85		0.41
S3IID	0.55		0.56	0.83		0.70
S5IID	0.40			0.70		
S8IID	0.36			0.60		
S1IIDT	0.54	0.52		0.82	0.69	
S2IIDT	0.66	0.60	0.10	0.88	0.74	0.35
S3IIDT	0.73	0.67	0.59	0.88	0.75	0.67
S4IIDT	0.57	0.48		0.83	0.66	
S5IIDT	0.59	0.56		0.83	0.69	
S6IIDT	0.53	0.48		0.78	0.59	
S7IIDT	0.57	0.53		0.83	0.68	
S8IIDT	0.57	0.52		0.85	0.72	
S9IIDT	0.57	0.44		0.80	0.60	
S10IIDT	0.58	0.46		0.80	0.61	
S2IIDB	0.84	0.82	0.27	0.91	0.92	0.48
S2IIDF	0.67	0.20	0.13	0.87	0.28	0.35
S2IIDTz	0.69	0.62	0.10	0.89	0.73	0.37

Table S9. The values of NICS(1)zz of the quinoidal IID and IIDT in CS and OS states.

Compound	NICS(1)zz(CS)			NICS(1)zz(OS)		
	Ring A	Ring B	Ring C ^a	Ring A	Ring B	Ring C ^a
S2IID	-3.07		-2.77	-8.20	-	-4.18
S3IID	-3.16		-12.95	-7.40		-14.20
S5IID	1.90			-0.84		
S8IID	4.09			2.80		
S1IIDT	-3.74	-11.50		-7.76	-12.56	
S2IIDT	-6.75	-12.65	-3.06	-11.89	-15.35	-4.06
S3IIDT	-8.00	-13.83	-13.33	-12.43	-16.02	-14.48
S4IIDT	-4.88	-11.00		-8.95	-12.48	
S5IIDT	-4.33	-12.02		-8.25	-13.09	
S6IIDT	-3.45	-10.78		-6.60	-11.14	
S7IIDT	-4.13	-11.94		-8.28	-12.90	
S8IIDT	-3.97	-11.79		-9.11	-14.24	
S9IIDT	-6.16	-9.15		-9.02	-10.25	
S10IIDT	-6.41	-9.28		-9.28	-10.38	
S2IIDB	-12.42	-15.26	-3.66	-15.36	-18.76	-4.80
S2IIDF	-7.58	-11.55	-3.73	-11.47	-13.19	-4.46
S2IIDTz	-6.96	-14.25	-2.61	-12.25	-16.70	-3.69

^a Ring C refers to the pro-aromatic rings of S2 and S3. Ring A and B are labeled as shown in Figure S3.

Table S10. HOMO, LUMO energy levels and HLG values, $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$, diradical character y_0 of SOIIDS_n and SOIIDTS_n

Compound	HOMO ^a	LUMO ^a	HLG ^a	$\Delta E(\text{OS-CS})^b$	$\Delta E(\text{OS-T}_1)^b$	y_0	N^{FOD}
SOIIDS1	-5.818	-3.827	1.991	0	-11.381	0	1.163
SOIIDS2	-5.270	-3.601	1.670	-0.796	-4.513	0.097	1.667
SOIIDS3	-5.557	-4.088	1.470	-0.696	-4.873	0.072	1.538
SOIIDS4	-5.343	-3.389	1.954	0	-10.380	0	1.224
SOIIDS5	-5.723	-4.000	1.722	0	-7.984	0	1.479
SOIIDS6	-5.693	-3.764	1.929	0	-11.766	0	1.516
SOIIDS7	-5.645	-3.831	1.814	0	-10.118	0	1.537
SOIIDS8	-5.749	-3.991	1.759	0	-8.581	0	1.475
SOIIDS9	-4.614	-2.602	2.012	0	-12.832	0	1.124
SOIIDS10	-4.577	-2.583	1.994	0	-12.656	0	1.114
SOIIDTS1	-5.387	-3.867	1.521	-0.642	-4.906	0.070	1.608
SOIIDTS2	-4.949	-3.659	1.290	-2.738	-2.449	0.294	1.982
SOIIDTS3	-5.247	-4.117	1.130	-2.862	-2.189	0.297	2.020
SOIIDTS4	-4.963	-3.477	1.487	-0.772	-4.322	0.091	1.675
SOIIDTS5	-5.337	-3.952	1.385	-0.639	-4.642	0.069	1.783
SOIIDTS6	-5.305	-3.790	1.514	-0.177	-5.965	0.019	1.780
SOIIDTS7	-5.268	-3.844	1.424	-0.428	-4.782	0.050	1.876
SOIIDTS8	-5.370	-3.962	1.407	-0.612	-4.161	0.077	1.713
SOIIDTS9	-4.379	-2.860	1.519	-0.331	-5.717	0.033	1.582
SOIIDTS10	-4.355	-2.849	1.506	-0.365	-5.651	0.037	1.571

^a HOMO, LUMO and HLG are in eV

^b $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ are in kcal mol⁻¹.

Table S11. HOMO, LUMO energy levels and HLG values, $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ and diradical character y_0 of S2IIDS_n and S9IIDS_n.

Compound	HOMO ^a	LUMO ^a	HLG ^a	$\Delta E(\text{OS-CS})^b$	$\Delta E(\text{OS-T}_1)^b$	y_0	N^{FOD}
S2IIDS1	-5.880	-4.386	1.494	-1.770	-3.050	0.231	2.024
S2IIDS3	-5.663	-4.540	1.123	-5.156	-1.244	0.539	2.402
S2IIDS4	-5.461	-4.008	1.453	-2.018	-2.761	0.267	2.086
S2IIDS5	-5.797	-4.487	1.311	-2.992	-1.948	0.381	2.379
S2IIDS6	-5.758	-4.297	1.461	-1.367	-3.165	0.184	2.350
S2IIDS7	-5.715	-4.332	1.384	-1.873	-2.565	0.257	2.395
S2IIDS8	-5.808	-4.455	1.353	-2.477	-2.063	0.339	2.375
S2IIDS9	-4.803	-3.372	1.431	-0.962	-4.288	0.102	1.836
S2IIDS10	-4.786	-3.366	1.420	-1.007	-4.250	0.106	1.824
S9IIDS1	-5.213	-3.549	1.664	0	-10.890	0	1.395
S9IIDS3	-5.069	-3.816	1.254	-0.614	-5.205	0.051	1.811
S9IIDS4	-4.854	-3.186	1.668	0	-9.475	0	1.458
S9IIDS5	-5.181	-3.734	1.447	0	-8.274	0	1.678
S9IIDS6	-5.154	-3.547	1.607	0	-11.399	0	1.726
S9IIDS7	-5.118	-3.606	1.512	0	-10.080	0	1.761
S9IIDS8	-5.208	-3.753	1.455	0	-8.930	0	1.705
S9IIDS10	-4.235	-2.467	1.768	0	-10.853	0	1.358

^a HOMO, LUMO and HLG are in eV

^b $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ are in kcal mol⁻¹.

Table S12. Calculated Hirshfeld charges and dipole moments (D) of S2IIDS_n and S9IIDS_n in OS state.

Molecule	Fragment			μ	Molecule	Fragment			μ
	S2	IID	Sn			S9	IID	Sn	
S2IIDS1	-0.022	+0.236	-0.214	4.38	S9IIDS1	+0.252	+0.043	-0.294	20.23
S2IIDS3	-0.029	+0.142	-0.113	6.47	S9IIDS3	+0.246	-0.018	-0.228	24.97
S2IIDS4	-0.054	+0.101	-0.047	3.18	S9IIDS4	+0.209	-0.083	-0.127	12.58
S2IIDS5	-0.025	+0.187	-0.162	4.90	S9IIDS5	+0.266	+0.031	-0.297	23.90
S2IIDS6	-0.029	+0.206	-0.177	1.62	S9IIDS6	+0.252	+0.023	-0.275	19.16
S2IIDS7	-0.029	+0.217	-0.188	4.73	S9IIDS7	+0.257	+0.052	-0.309	17.91
S2IIDS8	-0.021	+0.251	-0.230	3.45	S9IIDS8	+0.275	+0.101	-0.376	19.15
S2IIDS9	-0.121	-0.079	+0.200	15.39	S9IIDS10	+0.137	-0.291	+0.154	2.51
S2IIDS10	-0.122	-0.088	+0.210	15.12					

Table S13. HOMO, LUMO energy levels and HLG values, $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T})$ and diradical character y_0 of S2TIIDTSn and S9TIIDTSn.

Compound	HOMO ^a	LUMO ^a	HLG ^a	$\Delta E(\text{OS-CS})^b$	$\Delta E(\text{OS-T}_1)^b$	y_0	N^{FOD}
S2TIIDTS1	-5.209	-4.318	0.891	-6.899	-0.788	0.644	2.528
S2TIIDTS3	-5.119	-4.500	0.619	-9.543	-0.334	0.781	2.781
S2TIIDTS4	-4.866	-4.003	0.863	-7.233	-0.680	0.677	2.553
S2TIIDTS5	-5.182	-4.376	0.806	-6.751	-0.722	0.643	2.679
S2TIIDTS6	-5.141	-4.250	0.891	-5.869	-0.943	0.588	2.735
S2TIIDTS7	-5.114	-4.284	0.830	-6.526	-0.728	0.643	2.791
S2TIIDTS8	-5.201	-4.387	0.814	-6.952	-0.632	0.666	2.745
S2TIIDTS9	-4.379	-3.515	0.864	-5.513	-1.094	0.515	2.382
S2TIIDTS10	-4.372	-3.514	0.857	-5.551	-1.092	0.513	2.366
S9TIIDTS1	-4.691	-3.678	1.013	-2.501	-2.641	0.228	2.117
S9TIIDTS3	-4.630	-3.908	0.722	-4.366	-1.446	0.351	2.346
S9TIIDTS4	-4.389	-3.377	1.011	-3.373	-1.857	0.352	2.230
S9TIIDTS5	-4.695	-3.777	0.917	-2.224	-2.706	0.193	2.221
S9TIIDTS6	-4.663	-3.651	1.012	-1.738	-3.110	0.163	2.272
S9TIIDTS7	-4.644	-3.706	0.938	-2.100	-2.625	0.194	2.363
S9TIIDTS8	-4.730	-3.834	0.895	-2.223	-2.617	0.188	2.293
S9TIIDTS10	-3.924	-2.861	1.063	-3.288	-1.968	0.361	2.258

^a HOMO, LUMO and HLG are in eV

^b $\Delta E(\text{OS-CS})$, $\Delta E(\text{OS-T}_1)$ are in kcal mol⁻¹.

Table S14. Calculated Hirshfeld charges and dipole moments (D) of S2TIIDTS_n, S9TIIDTS_n and SnIIDT in OS state.

Molecule	Fragment			μ	Molecule	Fragment			μ
	S2	T-IID-T	Sn			S9	T-IID-T	Sn	
S2TIIDTS1	-0.079	+0.326	-0.247	5.01	S9TIIDTS1	+0.163	+0.129	-0.292	22.57
S2TIIDTS3	-0.080	+0.238	-0.157	7.40	S9TIIDTS3	+0.160	+0.067	-0.227	27.09
S2TIIDTS4	-0.094	+0.196	-0.102	3.79	S9TIIDTS4	+0.131	+0.007	-0.138	12.79
S2TIIDTS5	-0.080	+0.295	-0.215	6.36	S9TIIDTS5	+0.170	+0.119	-0.289	26.03
S2TIIDTS6	-0.083	+0.311	-0.228	2.71	S9TIIDTS6	+0.165	+0.125	-0.290	21.44
S2TIIDTS7	-0.083	+0.321	-0.237	2.52	S9TIIDTS7	+0.165	+0.147	-0.312	19.22
S2TIIDTS8	-0.079	+0.364	-0.285	0.97	S9TIIDTS8	+0.177	+0.199	-0.376	21.58
S2TIIDTS9	-0.123	-0.005	0.129	15.42	S9TIIDTS10	+0.097	-0.207	+0.110	1.64
S2TIIDTS10	-0.124	-0.015	0.139	15.38					
S1IIDT	-0.237	+0.474	-0.237	1.88	S6IIDT	-0.220	+0.440	-0.220	1.14
S2IIDT	-0.091	+0.182	-0.091	2.82	S7IIDT	-0.228	+0.456	-0.228	4.21
S3IIDT	-0.144	+0.288	-0.144	0.55	S8IIDT	-0.268	+0.536	-0.268	4.82
S4IIDT	-0.105	+0.211	-0.105	0.47	S9IIDT	+0.098	-0.196	+0.098	1.62
S5IIDT	-0.203	+0.406	-0.203	1.91	S10IIDT	+0.109	-0.218	+0.109	1.60

Coordinate and energy

S1IID-CS E = -1400.685701 Hartree

6	2.813671000	1.069988000	0.254969000
6	1.920365000	-0.071623000	0.082891000
6	2.505567000	-1.318800000	-0.321206000
6	3.849658000	-1.407591000	-0.507914000
6	4.729121000	-0.270494000	-0.312006000
6	4.160924000	0.992072000	0.077447000
6	0.706446000	1.830095000	0.646842000
6	0.619327000	0.359808000	0.307544000
1	1.873756000	-2.185892000	-0.448160000
1	4.293234000	-2.349803000	-0.809762000
1	4.805977000	1.851871000	0.214878000
6	-0.619334000	-0.359503000	0.307606000
6	-1.920409000	0.071803000	0.082885000
6	-0.706330000	-1.829760000	0.647037000
6	-2.813623000	-1.069858000	0.255145000
6	-2.505725000	1.318857000	-0.321435000
6	-4.160887000	-0.992080000	0.077639000
6	-3.849828000	1.407506000	-0.508132000
1	-1.873994000	2.185977000	-0.448564000
6	-4.729198000	0.270378000	-0.311996000
1	-4.805864000	-1.851916000	0.215201000
1	-4.293485000	2.349628000	-0.810141000
8	0.188357000	-2.606189000	0.935520000
8	-0.188147000	2.606604000	0.935402000
7	-2.057510000	-2.170337000	0.601847000
7	2.057651000	2.170564000	0.601571000
6	2.559022000	3.502466000	0.886546000
1	3.244303000	3.484445000	1.739549000
1	3.078582000	3.915796000	0.016374000
1	1.699098000	4.127917000	1.126456000
6	-2.558767000	-3.502254000	0.886954000
1	-3.244031000	-3.484210000	1.739970000
1	-3.078314000	-3.915704000	0.016831000
1	-1.698788000	-4.127614000	1.126902000
6	6.104411000	-0.403010000	-0.509079000
6	-6.104501000	0.402744000	-0.509075000
6	6.989511000	0.699302000	-0.326312000
7	7.692855000	1.615480000	-0.171386000
6	6.697309000	-1.637475000	-0.903671000

7	7.177206000	-2.648716000	-1.227679000
6	-6.697559000	1.637209000	-0.903429000
7	-7.177587000	2.648447000	-1.227252000
6	-6.989454000	-0.699728000	-0.326560000
7	-7.692680000	-1.616028000	-0.171823000

S2IID-CS E=-1565.641705 Hartree

6	-2.781416000	1.152487000	-0.367158000
6	-1.936411000	-0.015428000	-0.221943000
6	-2.583025000	-1.233990000	0.141968000
6	-3.937222000	-1.264431000	0.326567000
6	-4.785246000	-0.106585000	0.157364000
6	-4.136217000	1.125203000	-0.201059000
6	-0.641932000	1.856303000	-0.710874000
6	-0.604146000	0.377824000	-0.419033000
1	-1.997737000	-2.136698000	0.238189000
1	-4.388073000	-2.215615000	0.575759000
1	-4.703790000	2.040296000	-0.301087000
6	0.604152000	-0.377775000	-0.419110000
6	1.936420000	0.015459000	-0.222013000
6	0.641944000	-1.856206000	-0.711201000
6	2.781420000	-1.152448000	-0.367313000
6	2.583034000	1.233988000	0.142005000
6	4.136218000	-1.125186000	-0.201186000
6	3.937229000	1.264408000	0.326621000
1	1.997746000	2.136688000	0.238306000
6	4.785249000	0.106571000	0.157338000
1	4.703786000	-2.040274000	-0.301279000
1	4.388081000	2.215570000	0.575900000
8	-0.273098000	-2.623160000	-0.973474000
8	0.273096000	2.623256000	-0.973204000
7	1.982049000	-2.240079000	-0.668220000
7	-1.982048000	2.240146000	-0.667970000
6	-2.429855000	3.594289000	-0.917999000
1	-3.111079000	3.628845000	-1.774751000
1	-2.937936000	4.007934000	-0.040137000
1	-1.544557000	4.191706000	-1.137346000
6	2.429846000	-3.594217000	-0.918292000
1	3.111124000	-3.628736000	-1.775003000
1	2.937863000	-4.007922000	-0.040422000
1	1.544551000	-4.191604000	-1.137730000
6	-6.189552000	-0.182186000	0.339407000
6	-7.061542000	0.920431000	-0.002813000

6	-6.830720000	-1.361626000	0.878948000
6	-8.406731000	0.862680000	0.164376000
1	-6.633792000	1.815473000	-0.439174000
6	-8.172602000	-1.436688000	1.067043000
1	-6.220654000	-2.206729000	1.174076000
6	-9.067698000	-0.325683000	0.720156000
1	-9.049756000	1.691736000	-0.113756000
1	-8.637098000	-2.322205000	1.489127000
6	6.189552000	0.182151000	0.339407000
6	7.061541000	-0.920443000	-0.002888000
6	6.830717000	1.361545000	0.879051000
6	8.406727000	-0.862711000	0.164325000
1	6.633794000	-1.815449000	-0.439325000
6	8.172596000	1.436587000	1.067170000
1	6.220651000	2.206628000	1.174237000
6	9.067692000	0.325605000	0.720208000
1	9.049752000	-1.691748000	-0.113862000
1	8.637089000	2.322067000	1.489331000
8	-10.291035000	-0.384944000	0.883167000
8	10.291026000	0.384848000	0.883241000

S3IID-CS

E=-2536.386509 Hartree

6	2.659553000	1.407590000	0.538905000
6	1.934678000	0.163179000	0.389325000
6	2.690241000	-0.993192000	0.037582000
6	4.046694000	-0.901507000	-0.120361000
6	4.763662000	0.332541000	0.055379000
6	4.014658000	1.508618000	0.389976000
6	0.461461000	1.911374000	0.854660000
6	0.563871000	0.430720000	0.570276000
1	2.189244000	-1.942918000	-0.076524000
1	4.602959000	-1.794980000	-0.383997000
1	4.508316000	2.463755000	0.515861000
6	-0.563852000	-0.430856000	0.570207000
6	-1.934639000	-0.163301000	0.389132000
6	-0.461468000	-1.911534000	0.854478000
6	-2.659570000	-1.407647000	0.538960000
6	-2.690158000	0.993052000	0.037233000
6	-4.014689000	-1.508629000	0.390124000
6	-4.046620000	0.901405000	-0.120656000
1	-2.189124000	1.942743000	-0.077006000
6	-4.763644000	-0.332576000	0.055327000
1	-4.508393000	-2.463716000	0.516211000

1	-4.602852000	1.794864000	-0.384409000
8	0.524176000	-2.589239000	1.100760000
8	-0.524269000	2.589169000	1.100353000
7	-1.759595000	-2.415471000	0.830800000
7	1.759535000	2.415429000	0.830562000
6	2.077850000	3.807726000	1.078717000
1	2.740034000	3.907371000	1.944850000
1	2.557365000	4.260736000	0.204607000
1	1.139009000	4.322912000	1.282416000
6	-2.077992000	-3.807663000	1.079438000
1	-2.740029000	-3.906995000	1.945720000
1	-2.557706000	-4.260886000	0.205548000
1	-1.139160000	-4.322874000	1.283116000
6	6.160702000	0.385276000	-0.104395000
6	7.013188000	1.524605000	0.036394000
16	7.175606000	-0.990187000	-0.525616000
1	6.642312000	2.510349000	0.296198000
6	8.597751000	0.076458000	-0.472470000
6	-6.160694000	-0.385267000	-0.104378000
6	-7.013233000	-1.524527000	0.036652000
16	-7.175545000	0.990174000	-0.525799000
1	-6.642396000	-2.510243000	0.296617000
6	-8.597743000	-0.076387000	-0.472395000
6	9.886654000	-0.367991000	-0.728676000
6	-9.886635000	0.368085000	-0.728621000
6	10.992216000	0.526980000	-0.672385000
7	11.918231000	1.232414000	-0.635042000
6	10.134290000	-1.730087000	-1.054721000
7	10.307399000	-2.851976000	-1.319762000
6	-10.134213000	1.730135000	-1.054899000
7	-10.307277000	2.851987000	-1.320127000
6	-10.992241000	-0.526819000	-0.672123000
7	-11.918291000	-1.232198000	-0.634613000
7	-8.301288000	-1.366347000	-0.156877000
7	8.301243000	1.366459000	-0.157166000

S4IID-CS E=-2468.441407 Hartree

6	2.745232000	1.237355000	0.495692000
6	1.923088000	0.044927000	0.334058000
6	2.587928000	-1.158816000	-0.067765000
6	3.935215000	-1.169807000	-0.268399000
6	4.753145000	0.018986000	-0.085885000
6	4.092257000	1.241581000	0.306002000

6	0.594018000	1.865400000	0.899794000
6	0.596441000	0.397378000	0.564432000
1	2.013044000	-2.066380000	-0.183897000
1	4.434661000	-2.080015000	-0.568729000
1	4.665359000	2.152525000	0.438001000
6	-0.596450000	-0.397296000	0.564794000
6	-1.923123000	-0.044850000	0.334604000
6	-0.594117000	-1.865078000	0.901231000
6	-2.745273000	-1.237235000	0.496502000
6	-2.587936000	1.158804000	-0.067517000
6	-4.092285000	-1.241508000	0.306723000
6	-3.935217000	1.169762000	-0.268185000
1	-2.013024000	2.066321000	-0.183903000
6	-4.753157000	-0.018990000	-0.085439000
1	-4.665396000	-2.152423000	0.438891000
1	-4.434643000	2.079894000	-0.568780000
8	0.340421000	-2.592861000	1.197611000
8	-0.340412000	2.593018000	1.196921000
7	-1.923640000	-2.290801000	0.845311000
7	1.923599000	2.290993000	0.844284000
6	2.338170000	3.650639000	1.121585000
1	3.031018000	3.683092000	1.968984000
1	2.821898000	4.098722000	0.246994000
1	1.440141000	4.217859000	1.368015000
6	-2.338142000	-3.650534000	1.122292000
1	-3.031315000	-3.683148000	1.969416000
1	-2.821472000	-4.098603000	0.247472000
1	-1.440138000	-4.217659000	1.369032000
6	-6.125198000	0.004107000	-0.283950000
6	-6.938868000	1.172433000	-0.697663000
16	-7.159874000	-1.414890000	-0.067671000
6	-8.646821000	-0.483657000	-0.515475000
6	6.125195000	-0.004147000	-0.284335000
6	6.938899000	-1.172571000	-0.697707000
16	7.159847000	1.414915000	-0.068361000
6	8.646832000	0.483572000	-0.515810000
8	-6.560819000	2.310078000	-0.937200000
8	6.560880000	-2.310288000	-0.936948000
8	9.756032000	0.960029000	-0.551144000
8	-9.756021000	-0.960117000	-0.550768000
6	-9.288080000	1.813141000	-1.191651000
1	-9.292967000	2.637809000	-0.475617000
1	-9.045760000	2.209313000	-2.180089000
1	-10.258334000	1.319357000	-1.207915000

6	9.288154000	-1.813398000	-1.191339000
1	9.292888000	-2.637944000	-0.475163000
1	9.045993000	-2.209732000	-2.179752000
1	10.258426000	-1.319648000	-1.207524000
7	-8.292045000	0.820752000	-0.798088000
7	8.292083000	-0.820912000	-0.798110000

S5IID-CS E= -2011.347011 Hartree

6	-2.781284000	1.143656000	-0.463157000
6	-1.928625000	-0.021477000	-0.303401000
6	-2.564652000	-1.237666000	0.092379000
6	-3.915507000	-1.280617000	0.287332000
6	-4.773480000	-0.127635000	0.088209000
6	-4.133180000	1.107385000	-0.293070000
6	-0.650607000	1.853795000	-0.829824000
6	-0.606000000	0.374690000	-0.514604000
1	-1.972590000	-2.133473000	0.210817000
1	-4.383611000	-2.204274000	0.589289000
1	-4.699922000	2.021692000	-0.400175000
6	0.606003000	-0.374636000	-0.514625000
6	1.928630000	0.021508000	-0.303392000
6	0.650598000	-1.853723000	-0.829926000
6	2.781280000	-1.143623000	-0.463213000
6	2.564666000	1.237667000	0.092469000
6	4.133176000	-1.107374000	-0.293120000
6	3.915521000	1.280594000	0.287428000
1	1.972613000	2.133472000	0.210962000
6	4.773485000	0.127619000	0.088236000
1	4.699910000	-2.021680000	-0.400276000
1	4.383632000	2.204228000	0.589446000
8	-0.264479000	-2.609593000	-1.108768000
8	0.264461000	2.609685000	-1.108639000
7	1.991104000	-2.231785000	-0.782925000
7	-1.991116000	2.231843000	-0.782806000
6	-2.449814000	3.580552000	-1.053656000
1	-3.132679000	3.595080000	-1.909171000
1	-2.957629000	4.002471000	-0.180194000
1	-1.570228000	4.181701000	-1.284578000
6	2.449792000	-3.580483000	-1.053844000
1	3.132659000	-3.594972000	-1.909359000
1	2.957600000	-4.002453000	-0.180403000
1	1.570201000	-4.181613000	-1.284802000
6	-6.180897000	-0.191355000	0.247072000

6	-6.869860000	-1.376741000	0.845389000
6	-7.011093000	0.891784000	-0.167945000
6	-8.371359000	0.884985000	-0.045525000
1	-6.563833000	1.757267000	-0.638504000
6	-9.087851000	-0.260551000	0.545888000
6	6.180901000	0.191323000	0.247111000
6	7.011101000	-0.891791000	-0.167965000
6	6.869858000	1.376675000	0.845501000
6	8.371367000	-0.884995000	-0.045541000
1	6.563846000	-1.757248000	-0.638576000
6	9.087855000	0.260512000	0.545935000
6	-9.151678000	1.987391000	-0.501136000
7	-9.748597000	2.910224000	-0.884322000
8	-6.299209000	-2.377409000	1.267771000
8	-10.301908000	-0.286531000	0.673652000
7	-8.267140000	-1.323763000	0.947449000
6	-8.911017000	-2.499457000	1.549644000
1	-8.677280000	-3.389145000	0.962179000
1	-8.533617000	-2.648891000	2.562939000
1	-9.982231000	-2.316769000	1.561435000
6	9.151691000	-1.987371000	-0.501216000
7	9.748614000	-2.910180000	-0.884455000
8	10.301912000	0.286492000	0.673695000
8	6.299201000	2.377326000	1.267914000
7	8.267139000	1.323700000	0.947553000
6	8.911011000	2.499367000	1.549804000
1	8.677268000	3.389084000	0.962384000
1	8.533613000	2.648748000	2.563108000
1	9.982226000	2.316683000	1.561583000

S6IID-CS

E= -2733.987173 Hartree

6	2.729301000	-1.263087000	-0.335841000
6	1.919221000	-0.065633000	-0.173741000
6	2.606016000	1.127402000	0.224270000
6	3.950068000	1.108360000	0.432150000
6	4.766364000	-0.094715000	0.263654000
6	4.077159000	-1.295769000	-0.152033000
6	0.577042000	-1.878364000	-0.742669000
6	0.591836000	-0.401621000	-0.405981000
1	2.053293000	2.050134000	0.327324000
1	4.445526000	2.015586000	0.737464000
1	4.639103000	-2.207670000	-0.274761000
6	-0.591851000	0.401700000	-0.405988000

6	-1.919231000	0.065723000	-0.173702000
6	-0.577069000	1.878422000	-0.742770000
6	-2.729318000	1.263163000	-0.335862000
6	-2.606018000	-1.127289000	0.224390000
6	-4.077173000	1.295855000	-0.152039000
6	-3.950069000	-1.108238000	0.432278000
1	-2.053295000	-2.050015000	0.327493000
6	-4.766374000	0.094824000	0.263731000
1	-4.639115000	2.207749000	-0.274817000
1	-4.445520000	-2.015452000	0.737645000
8	0.370082000	2.586706000	-1.040466000
8	-0.370116000	-2.586664000	-1.040303000
7	-1.897857000	2.312391000	-0.684495000
7	1.897830000	-2.312333000	-0.684394000
6	2.308259000	-3.675868000	-0.960122000
1	2.997248000	-3.709347000	-1.809753000
1	2.798699000	-4.116441000	-0.086523000
1	1.408921000	-4.243763000	-1.198968000
6	-2.308296000	3.675909000	-0.960293000
1	-2.997294000	3.709338000	-1.809920000
1	-2.798730000	4.116527000	-0.086714000
1	-1.408963000	4.243796000	-1.199178000
6	6.163232000	-0.060192000	0.441451000
6	6.844440000	1.141948000	0.965129000
6	7.015196000	-1.222448000	0.118126000
6	8.997170000	0.270017000	0.103842000
6	-6.163244000	0.060273000	0.441524000
6	-7.015280000	1.222478000	0.118196000
6	-6.844389000	-1.141887000	0.965243000
6	-8.997136000	-0.270148000	0.103822000
8	6.291287000	2.023000000	1.613551000
7	8.222575000	1.260366000	0.678391000
6	8.869228000	2.529382000	1.053813000
1	8.108283000	3.156047000	1.508976000
1	9.679956000	2.337764000	1.758298000
1	9.288456000	3.003813000	0.165885000
8	-6.291223000	-2.022823000	1.613811000
7	-8.222474000	-1.260473000	0.678319000
6	-8.869006000	-2.529606000	1.053550000
1	-8.108050000	-3.156185000	1.508813000
1	-9.679892000	-2.338153000	1.757896000
1	-9.288000000	-3.004049000	0.165515000
8	-6.611017000	2.375628000	0.001727000
8	6.610884000	-2.375595000	0.001798000

7	8.385318000	-0.954773000	-0.098765000
7	-8.385419000	0.954761000	-0.098511000
6	9.210651000	-2.077977000	-0.575420000
1	10.029104000	-2.256498000	0.123244000
1	8.564990000	-2.948334000	-0.639622000
1	9.636021000	-1.834417000	-1.549741000
6	-9.210864000	2.077973000	-0.574955000
1	-10.029551000	2.256004000	0.123553000
1	-8.565371000	2.948495000	-0.638629000
1	-9.635904000	1.834742000	-1.549506000
16	-10.604805000	-0.523188000	-0.279545000
16	10.604924000	0.522889000	-0.279282000

S7IID-CS

E= -2241.868986 Hartree

6	2.846841000	-0.965342000	-0.376372000
6	1.919379000	0.147492000	-0.234497000
6	2.466375000	1.409027000	0.168146000
6	3.808014000	1.540953000	0.364216000
6	4.738357000	0.443612000	0.143831000
6	4.190270000	-0.843017000	-0.186446000
6	0.773370000	-1.808365000	-0.769747000
6	0.630598000	-0.334405000	-0.451912000
1	1.810919000	2.259776000	0.285361000
1	4.221108000	2.493031000	0.665953000
1	4.831676000	-1.709715000	-0.252531000
6	-0.630590000	0.334499000	-0.451891000
6	-1.919375000	-0.147403000	-0.234489000
6	-0.773349000	1.808517000	-0.769508000
6	-2.846831000	0.965438000	-0.376287000
6	-2.466367000	-1.408972000	0.168065000
6	-4.190262000	0.843086000	-0.186391000
6	-3.808007000	-1.540912000	0.364118000
1	-1.810900000	-2.259719000	0.285215000
6	-4.738345000	-0.443567000	0.143791000
1	-4.831667000	1.709792000	-0.252391000
1	-4.221098000	-2.493012000	0.665794000
8	0.089317000	2.615816000	-1.069294000
8	-0.089308000	-2.615673000	-1.069493000
7	-2.132536000	2.102833000	-0.694307000
7	2.132548000	-2.102705000	-0.694512000
6	2.695157000	-3.396175000	-1.038373000
1	3.410960000	-3.291165000	-1.859220000
1	3.195171000	-3.846131000	-0.174361000

1	1.869737000	-4.036953000	-1.348793000
6	-2.695157000	3.396289000	-1.038218000
1	-3.410876000	3.291259000	-1.859136000
1	-3.195266000	3.846222000	-0.174252000
1	-1.869729000	4.037097000	-1.348556000
6	-6.114188000	-0.646320000	0.320076000
6	-6.688413000	-1.757333000	1.159575000
6	-7.230216000	0.222837000	-0.041214000
6	-8.068275000	-1.335091000	1.499349000
6	-8.381381000	-0.139515000	0.828294000
6	-8.962672000	-1.967306000	2.352408000
6	-9.628565000	0.456760000	1.038384000
6	-10.207686000	-1.369493000	2.556694000
1	-8.681588000	-2.896053000	2.838181000
6	-10.525923000	-0.168690000	1.910413000
1	-9.910079000	1.383516000	0.557358000
1	-10.932005000	-1.831815000	3.220037000
1	-11.493177000	0.291929000	2.086114000
6	6.114201000	0.646343000	0.320098000
6	7.230192000	-0.222860000	-0.041228000
6	6.688487000	1.757279000	1.159669000
6	8.381402000	0.139454000	0.828220000
6	8.068385000	1.335034000	1.499302000
6	9.628529000	-0.456940000	1.038324000
6	8.962833000	1.967165000	2.352368000
6	10.525945000	0.168431000	1.910347000
1	9.909959000	-1.383719000	0.557293000
6	10.207805000	1.369257000	2.556635000
1	8.681818000	2.895913000	2.838181000
1	11.493163000	-0.292265000	2.086041000
1	10.932160000	1.831514000	3.219984000
8	-6.151818000	-2.785707000	1.544467000
8	6.151947000	2.785671000	1.544596000
6	7.315114000	-1.086810000	-1.123004000
6	-7.315234000	1.086780000	-1.122998000
6	6.326732000	-1.202101000	-2.148120000
7	5.565259000	-1.329961000	-3.020666000
6	8.473978000	-1.882417000	-1.384764000
7	9.391810000	-2.560563000	-1.619382000
6	-6.326840000	1.202196000	-2.148103000
7	-5.565382000	1.330188000	-3.020644000
6	-8.474151000	1.882304000	-1.384768000
7	-9.392016000	2.560399000	-1.619410000

S8IID-CS

E= -3112.308885 Hartree

6	2.814836000	1.055907000	0.572077000
6	1.922995000	-0.086307000	0.431368000
6	2.508141000	-1.333371000	0.037561000
6	3.850637000	-1.419337000	-0.169514000
6	4.742966000	-0.286709000	0.025438000
6	4.160880000	0.978621000	0.376180000
6	0.716276000	1.831790000	0.967866000
6	0.619908000	0.354073000	0.650781000
1	1.883558000	-2.209449000	-0.056805000
1	4.276097000	-2.380190000	-0.429663000
1	4.778156000	1.863139000	0.443000000
6	-0.619909000	-0.353973000	0.650789000
6	-1.922994000	0.086373000	0.431282000
6	-0.716266000	-1.831669000	0.967968000
6	-2.814831000	-1.055827000	0.572126000
6	-2.508143000	1.333385000	0.037314000
6	-4.160876000	-0.978570000	0.376216000
6	-3.850638000	1.419318000	-0.169783000
1	-1.883565000	2.209455000	-0.057152000
6	-4.742965000	0.286713000	0.025310000
1	-4.778149000	-1.863082000	0.443143000
1	-4.276099000	2.380138000	-0.430053000
8	0.170916000	-2.611408000	1.267554000
8	-0.170915000	2.611587000	1.267277000
7	-2.065767000	-2.168721000	0.892444000
7	2.065772000	2.168843000	0.892251000
6	2.585527000	3.483061000	1.224524000
1	3.300805000	3.410333000	2.049351000
1	3.073775000	3.939583000	0.357404000
1	1.739127000	4.100178000	1.526104000
6	-2.585522000	-3.482890000	1.224911000
1	-3.300776000	-3.410047000	2.049749000
1	-3.073798000	-3.939525000	0.357865000
1	-1.739118000	-4.099974000	1.526548000
6	-6.113673000	0.436402000	-0.187104000
6	-7.236782000	-0.401691000	0.156893000
6	-8.255698000	0.991774000	-1.531306000
6	-8.387421000	-0.173307000	-0.760998000
6	-9.208784000	1.424975000	-2.439463000
6	-9.540425000	-0.950353000	-0.949077000
6	-10.355713000	0.645549000	-2.599830000
1	-9.057473000	2.334976000	-3.010184000

6	-10.507814000	-0.533315000	-1.864397000
1	-9.688915000	-1.874663000	-0.409242000
1	-11.123493000	0.951274000	-3.303118000
1	-11.393271000	-1.144490000	-2.006345000
6	6.113675000	-0.436429000	-0.186949000
6	7.236782000	0.401708000	0.156944000
6	8.387429000	0.173195000	-0.760906000
6	8.255709000	-0.991990000	-1.531056000
6	9.540436000	0.950215000	-0.949083000
6	9.208801000	-1.425316000	-2.439147000
6	10.507830000	0.533050000	-1.864338000
1	9.688923000	1.874598000	-0.409373000
6	10.355733000	-0.645915000	-2.599611000
1	9.057493000	-2.335395000	-3.009745000
1	11.393290000	1.144203000	-2.006363000
1	11.123518000	-0.951738000	-3.302851000
6	7.305623000	1.199693000	1.296605000
6	-7.305635000	-1.199520000	1.296663000
6	6.321490000	1.193710000	2.330510000
7	5.557286000	1.224752000	3.209575000
6	8.421232000	2.032441000	1.614591000
7	9.298054000	2.740272000	1.911609000
6	-6.321522000	-1.193383000	2.330587000
7	-5.557349000	-1.224279000	3.209685000
6	-8.421247000	-2.032225000	1.614749000
7	-9.298074000	-2.740017000	1.911848000
16	-6.707952000	1.815454000	-1.218837000
16	6.707958000	-1.815622000	-1.218490000
8	6.894459000	-3.029499000	-0.408657000
8	5.935139000	-1.906780000	-2.465641000
8	-5.935123000	1.906446000	-2.465994000
8	-6.894466000	3.029441000	-0.409171000

S9IID-CS

E= -3084.207567 Hartree

6	2.763778000	1.211531000	0.555126000
6	1.928943000	0.030032000	0.407312000
6	2.586180000	-1.182900000	0.028548000
6	3.936235000	-1.201063000	-0.166681000
6	4.765278000	-0.025993000	-0.005732000
6	4.112256000	1.206782000	0.366460000
6	0.609665000	1.855935000	0.949687000
6	0.600496000	0.396246000	0.633036000
1	2.005397000	-2.089165000	-0.068279000

1	4.407205000	-2.137986000	-0.448185000
1	4.687540000	2.118617000	0.486461000
6	-0.600489000	-0.396131000	0.633067000
6	-1.928943000	-0.029950000	0.407317000
6	-0.609637000	-1.855798000	0.949815000
6	-2.763764000	-1.211447000	0.555246000
6	-2.586200000	1.182939000	0.028454000
6	-4.112246000	-1.206728000	0.366604000
6	-3.936260000	1.201073000	-0.166741000
1	-2.005426000	2.089198000	-0.068477000
6	-4.765291000	0.026012000	-0.005661000
1	-4.687518000	-2.118559000	0.486699000
1	-4.407242000	2.137960000	-0.448346000
8	0.313462000	-2.610630000	1.236759000
8	-0.313414000	2.610791000	1.236632000
7	-1.946148000	-2.273769000	0.889101000
7	1.946178000	2.273888000	0.888910000
6	2.363483000	3.632557000	1.147762000
1	3.057752000	3.678421000	1.994603000
1	2.848597000	4.072729000	0.268677000
1	1.465020000	4.202819000	1.387426000
6	-2.363430000	-3.632429000	1.148033000
1	-3.057690000	-3.678257000	1.994883000
1	-2.848546000	-4.072656000	0.268976000
1	-1.464956000	-4.202663000	1.387720000
6	6.135065000	-0.083358000	-0.203984000
6	8.603606000	-0.857669000	-0.735312000
6	8.701133000	0.506720000	-0.425769000
6	9.746689000	-1.586742000	-1.072959000
6	9.941255000	1.149381000	-0.452143000
6	10.982414000	-0.941889000	-1.098100000
1	9.670838000	-2.642635000	-1.312414000
6	11.079283000	0.418138000	-0.789559000
1	10.015472000	2.205348000	-0.212444000
1	11.872780000	-1.504474000	-1.359808000
1	12.044865000	0.913016000	-0.811370000
6	-6.135080000	0.083343000	-0.203907000
6	-8.603630000	0.857569000	-0.735318000
6	-8.701135000	-0.506800000	-0.425680000
6	-9.746722000	1.586596000	-1.073033000
6	-9.941244000	-1.149487000	-0.452027000
6	-10.982434000	0.941718000	-1.098145000
1	-9.670889000	2.642473000	-1.312560000
6	-11.079282000	-0.418290000	-0.789510000

1	-10.015444000	-2.205439000	-0.212258000
1	-11.872808000	1.504267000	-1.359903000
1	-12.044854000	-0.913188000	-0.811301000
16	-7.190673000	-1.323149000	-0.011461000
16	-6.986287000	1.563357000	-0.667862000
16	6.986245000	-1.563415000	-0.667855000
16	7.190684000	1.323122000	-0.011607000

S10IID-CS

E= -2776.890540 Hartree

6	-2.788730000	-1.153600000	0.374044000
6	-1.930040000	0.010343000	0.227258000
6	-2.562584000	1.236489000	-0.149151000
6	-3.912709000	1.282457000	-0.343519000
6	-4.764603000	0.124989000	-0.183831000
6	-4.137433000	-1.120854000	0.186070000
6	-0.647794000	-1.842500000	0.766621000
6	-0.608479000	-0.383666000	0.451947000
1	-1.963626000	2.130992000	-0.244743000
1	-4.364775000	2.229396000	-0.623068000
1	-4.731298000	-2.020953000	0.305283000
6	0.608475000	0.383833000	0.451976000
6	1.930015000	-0.010217000	0.227260000
6	0.647866000	1.842631000	0.766821000
6	2.788767000	1.153663000	0.374155000
6	2.562489000	-1.236372000	-0.149236000
6	4.137468000	1.120860000	0.186175000
6	3.912611000	-1.282398000	-0.343613000
1	1.963479000	-2.130835000	-0.244889000
6	4.764567000	-0.124986000	-0.183839000
1	4.731384000	2.020913000	0.305477000
1	4.364625000	-2.229340000	-0.623235000
8	-0.258774000	2.617989000	1.052783000
8	0.258909000	-2.617857000	1.052388000
7	1.993227000	2.232941000	0.706144000
7	-1.993133000	-2.232875000	0.705900000
6	-2.437804000	-3.582956000	0.963080000
1	-3.132842000	-3.616050000	1.809957000
1	-2.931817000	-4.012451000	0.083592000
1	-1.550916000	-4.171416000	1.201964000
6	2.437972000	3.582966000	0.963489000
1	3.133013000	3.615920000	1.810368000
1	2.932006000	4.012543000	0.084052000
1	1.551116000	4.171444000	1.202447000

6	-6.134154000	0.210473000	-0.381438000
6	-8.576629000	1.005315000	-0.895999000
6	-8.696402000	-0.295378000	-0.601901000
6	6.134112000	-0.210529000	-0.381459000
6	8.576542000	-1.005462000	-0.896091000
6	8.696387000	0.295201000	-0.601887000
16	7.230554000	1.169052000	-0.193966000
16	6.968396000	-1.703978000	-0.844858000
16	-6.968520000	1.703914000	-0.844716000
16	-7.230520000	-1.169182000	-0.194056000
1	-9.626211000	-0.850343000	-0.594177000
1	-9.395772000	1.661733000	-1.162251000
1	9.395649000	-1.661903000	-1.162398000
1	9.626226000	0.850115000	-0.594121000

S2IID-OS

E= -1565.650516 Hartree

6	-2.790964000	1.119254000	-0.242811000
6	-1.983728000	-0.052496000	-0.140024000
6	-2.648692000	-1.265990000	0.112608000
6	-4.031225000	-1.290422000	0.235517000
6	-4.826038000	-0.126004000	0.103170000
6	-4.166539000	1.104848000	-0.140701000
6	-0.642576000	1.869754000	-0.424197000
6	-0.592346000	0.360835000	-0.248670000
1	-2.083261000	-2.181785000	0.183716000
1	-4.513224000	-2.248696000	0.389376000
1	-4.726036000	2.030640000	-0.194579000
6	0.592346000	-0.360804000	-0.248699000
6	1.983730000	0.052516000	-0.140028000
6	0.642572000	-1.869705000	-0.424372000
6	2.790963000	-1.119228000	-0.242911000
6	2.648698000	1.265987000	0.112702000
6	4.166537000	-1.104835000	-0.140798000
6	4.031231000	1.290405000	0.235613000
1	2.083271000	2.181779000	0.183880000
6	4.826040000	0.125994000	0.103174000
1	4.726031000	-2.030625000	-0.194752000
1	4.513233000	2.248665000	0.389549000
8	-0.267127000	-2.670273000	-0.587289000
8	0.267121000	2.670338000	-0.587045000
7	1.979778000	-2.231973000	-0.425210000
7	-1.979783000	2.232017000	-0.425013000
6	-2.431684000	3.597238000	-0.595138000

1	-3.074719000	3.687086000	-1.477048000
1	-2.985299000	3.938900000	0.286167000
1	-1.545751000	4.218002000	-0.728966000
6	2.431676000	-3.597183000	-0.595437000
1	3.074719000	-3.686965000	-1.477347000
1	2.985280000	-3.938916000	0.285847000
1	1.545741000	-4.217933000	-0.729322000
6	-6.279902000	-0.186084000	0.213545000
6	-7.108129000	0.802245000	-0.401297000
6	-6.923314000	-1.233237000	0.942150000
6	-8.472983000	0.756295000	-0.308200000
1	-6.643033000	1.584278000	-0.992634000
6	-8.285467000	-1.293123000	1.061820000
1	-6.312947000	-1.974446000	1.446999000
6	-9.147985000	-0.298046000	0.437875000
1	-9.102154000	1.495032000	-0.794391000
1	-8.772152000	-2.076582000	1.633861000
6	6.279904000	0.186060000	0.213558000
6	7.108130000	-0.802220000	-0.401365000
6	6.923317000	1.233151000	0.942251000
6	8.472984000	-0.756282000	-0.308261000
1	6.643032000	-1.584203000	-0.992767000
6	8.285470000	1.293024000	1.061929000
1	6.312951000	1.974320000	1.447161000
6	9.147987000	0.297996000	0.437904000
1	9.102153000	-1.494980000	-0.794511000
1	8.772156000	2.076433000	1.634037000
8	-10.392515000	-0.345392000	0.536014000
8	10.392516000	0.345330000	0.536050000

S3IID-OS

E= -2536.394697 Hartree

6	2.671046000	1.380671000	0.376801000
6	1.977500000	0.136005000	0.271093000
6	2.751777000	-1.012613000	0.022414000
6	4.130367000	-0.911366000	-0.083758000
6	4.808431000	0.324412000	0.049557000
6	4.040888000	1.495885000	0.279795000
6	0.462575000	1.922879000	0.558239000
6	0.555527000	0.415987000	0.378201000
1	2.272606000	-1.975049000	-0.063723000
1	4.700758000	-1.816368000	-0.265812000
1	4.512991000	2.466406000	0.366048000
6	-0.555526000	-0.415942000	0.378267000

6	-1.977497000	-0.135975000	0.271109000
6	-0.462574000	-1.922812000	0.558493000
6	-2.671046000	-1.380624000	0.377009000
6	-2.751773000	1.012611000	0.022280000
6	-4.040888000	-1.495847000	0.280034000
6	-4.130364000	0.911351000	-0.083866000
1	-2.272598000	1.975033000	-0.063995000
6	-4.808430000	-0.324406000	0.049630000
1	-4.512994000	-2.466354000	0.366436000
1	-4.700756000	1.816329000	-0.266040000
8	0.519659000	-2.631303000	0.719027000
8	-0.519661000	2.631398000	0.718627000
7	-1.759795000	-2.409784000	0.565384000
7	1.759794000	2.409859000	0.565012000
6	2.080198000	3.812718000	0.738240000
1	2.708392000	3.961134000	1.622627000
1	2.600107000	4.205927000	-0.141843000
1	1.139307000	4.346700000	0.870326000
6	-2.080199000	-3.812622000	0.738784000
1	-2.708395000	-3.960931000	1.623188000
1	-2.600108000	-4.205936000	-0.141253000
1	-1.139309000	-4.346587000	0.870937000
6	6.244069000	0.403794000	-0.050219000
6	7.066714000	1.536471000	0.108103000
16	7.269812000	-0.969848000	-0.402345000
1	6.686617000	2.524944000	0.339141000
6	8.683669000	0.097283000	-0.304288000
6	-6.244068000	-0.403800000	-0.050126000
6	-7.066715000	-1.536454000	0.108355000
16	-7.269812000	0.969796000	-0.402433000
1	-6.686618000	-2.524896000	0.339526000
6	-8.683670000	-0.097320000	-0.304227000
6	9.996646000	-0.364691000	-0.500827000
6	-9.996647000	0.364628000	-0.500824000
6	11.097260000	0.527999000	-0.414507000
7	12.021458000	1.235628000	-0.350414000
6	10.254183000	-1.729676000	-0.789928000
7	10.439464000	-2.856949000	-1.026664000
6	-10.254183000	1.729575000	-0.790108000
7	-10.439461000	2.856810000	-1.027025000
6	-11.097262000	-0.528048000	-0.414377000
7	-12.021461000	-1.235667000	-0.350183000
7	-8.380678000	-1.374934000	-0.027683000
7	8.380677000	1.374935000	-0.027920000

S5IID-OS

E= -2011.349044 Hartree

6	-2.785165000	1.130287000	-0.339035000
6	-1.962609000	-0.041001000	-0.208983000
6	-2.615071000	-1.251894000	0.114904000
6	-3.986322000	-1.287199000	0.272165000
6	-4.804804000	-0.126816000	0.096716000
6	-4.150756000	1.106546000	-0.211079000
6	-0.642341000	1.866579000	-0.592105000
6	-0.595786000	0.366451000	-0.358120000
1	-2.040788000	-2.160234000	0.213318000
1	-4.466505000	-2.220969000	0.520500000
1	-4.709085000	2.030783000	-0.283900000
6	0.595785000	-0.366398000	-0.358134000
6	1.962610000	0.041041000	-0.208972000
6	0.642333000	-1.866515000	-0.592178000
6	2.785161000	-1.130244000	-0.339080000
6	2.615079000	1.251915000	0.114977000
6	4.150752000	-1.106516000	-0.211125000
6	3.986330000	1.287205000	0.272239000
1	2.040801000	2.160253000	0.213436000
6	4.804806000	0.126826000	0.096733000
1	4.709076000	-2.030753000	-0.283991000
1	4.466518000	2.220960000	0.520619000
8	-0.271462000	-2.646397000	-0.807202000
8	0.271451000	2.646477000	-0.807084000
7	1.980727000	-2.233834000	-0.577372000
7	-1.980736000	2.233892000	-0.577273000
6	-2.434967000	3.593153000	-0.795108000
1	-3.093526000	3.647289000	-1.668072000
1	-2.970082000	3.970932000	0.082461000
1	-1.551345000	4.206603000	-0.970976000
6	2.434952000	-3.593086000	-0.795278000
1	3.093506000	-3.647180000	-1.668248000
1	2.970070000	-3.970911000	0.082269000
1	1.551327000	-4.206524000	-0.971172000
6	-6.240762000	-0.174442000	0.194897000
6	-6.942809000	-1.287108000	0.897277000
6	-7.037344000	0.842336000	-0.376069000
6	-8.412086000	0.833921000	-0.317456000
1	-6.563713000	1.646417000	-0.925819000
6	-9.148509000	-0.246779000	0.364253000
6	6.240765000	0.174438000	0.194916000

6	7.037337000	-0.842319000	-0.376101000
6	6.942824000	1.287064000	0.897349000
6	8.412079000	-0.833927000	-0.317476000
1	6.563700000	-1.646365000	-0.925896000
6	9.148512000	0.246721000	0.364302000
6	-9.175015000	1.864227000	-0.933991000
7	-9.758600000	2.730252000	-1.449650000
8	-6.370985000	-2.211591000	1.465884000
8	-10.368383000	-0.271031000	0.433568000
7	-8.343725000	-1.248402000	0.923024000
6	-9.005944000	-2.354051000	1.628642000
1	-8.730711000	-3.303422000	1.165799000
1	-8.682431000	-2.373821000	2.671044000
1	-10.078357000	-2.190707000	1.562453000
6	9.174998000	-1.864212000	-0.934060000
7	9.758575000	-2.730219000	-1.449760000
8	10.368385000	0.270946000	0.433637000
8	6.371010000	2.211509000	1.466028000
7	8.343738000	1.248326000	0.923121000
6	9.005967000	2.353919000	1.628817000
1	8.730771000	3.303323000	1.166019000
1	8.682428000	2.373641000	2.671212000
1	10.078378000	2.190551000	1.562646000

S8IID-OS

E= -3112.309297 Hartree

6	2.814727000	1.051788000	0.494227000
6	1.947005000	-0.097485000	0.381830000
6	2.547723000	-1.340283000	0.044459000
6	3.905241000	-1.418462000	-0.137722000
6	4.767362000	-0.275395000	0.023441000
6	4.171037000	0.986915000	0.321727000
6	0.706506000	1.843512000	0.816889000
6	0.611300000	0.349921000	0.559092000
1	1.938181000	-2.227763000	-0.031116000
1	4.348280000	-2.384202000	-0.348711000
1	4.775165000	1.882389000	0.367081000
6	-0.611289000	-0.349822000	0.559147000
6	-1.946990000	0.097557000	0.381825000
6	-0.706494000	-1.843372000	0.817178000
6	-2.814716000	-1.051704000	0.494375000
6	-2.547717000	1.340312000	0.044298000
6	-4.171022000	-0.986861000	0.321874000
6	-3.905233000	1.418466000	-0.137874000

1	-1.938176000	2.227782000	-0.031402000
6	-4.767365000	0.275416000	0.023444000
1	-4.775140000	-1.882335000	0.367338000
1	-4.348268000	2.384183000	-0.348975000
8	0.180600000	-2.638853000	1.076799000
8	-0.180586000	2.639035000	1.076388000
7	-2.053927000	-2.174669000	0.759906000
7	2.053943000	2.174788000	0.759614000
6	2.566077000	3.501648000	1.049229000
1	3.265463000	3.462454000	1.889920000
1	3.071262000	3.923904000	0.174371000
1	1.713901000	4.129162000	1.309906000
6	-2.566064000	-3.501472000	1.049780000
1	-3.265419000	-3.462120000	1.890490000
1	-3.071287000	-3.923877000	0.175016000
1	-1.713883000	-4.128949000	1.310532000
6	-6.158036000	0.412360000	-0.181121000
6	-7.271065000	-0.397113000	0.213586000
6	-8.336370000	0.981060000	-1.464248000
6	-8.467162000	-0.149268000	-0.643868000
6	-9.325172000	1.426498000	-2.327037000
6	-9.663458000	-0.876772000	-0.731178000
6	-10.513160000	0.696001000	-2.387342000
1	-9.171342000	2.309596000	-2.937977000
6	-10.668464000	-0.447688000	-1.599866000
1	-9.821193000	-1.772623000	-0.148353000
1	-11.310185000	1.012458000	-3.052255000
1	-11.587265000	-1.021921000	-1.661646000
6	6.158050000	-0.412365000	-0.181137000
6	7.271085000	0.397070000	0.213552000
6	8.467248000	0.149057000	-0.643765000
6	8.336387000	-0.981243000	-1.464172000
6	9.663696000	0.876334000	-0.730884000
6	9.325229000	-1.426845000	-2.326830000
6	10.668749000	0.447085000	-1.599438000
1	9.821527000	1.772140000	-0.148016000
6	10.513352000	-0.696554000	-2.386967000
1	9.171326000	-2.309913000	-2.937796000
1	11.587667000	1.021149000	-1.661060000
1	11.310413000	-1.013139000	-3.051775000
6	7.292872000	1.203612000	1.358112000
6	-7.292928000	-1.203469000	1.358257000
6	6.265481000	1.207995000	2.347780000
7	5.470303000	1.250007000	3.198887000

6	8.393831000	2.031800000	1.726754000
7	9.255611000	2.739340000	2.067524000
6	-6.265568000	-1.207766000	2.347959000
7	-5.470401000	-1.249719000	3.199078000
6	-8.393970000	-2.031512000	1.727002000
7	-9.255818000	-2.738911000	2.067885000
16	-6.736314000	1.738781000	-1.284649000
16	6.736235000	-1.738785000	-1.284703000
8	6.821523000	-3.017574000	-0.561415000
8	6.014083000	-1.693245000	-2.564050000
8	-6.014120000	1.693386000	-2.563982000
8	-6.821749000	3.017514000	-0.561289000

S1IID-T1 E= -1400.673786 Hartree

6	2.823136000	1.041065000	0.146318000
6	1.987158000	-0.113750000	0.040667000
6	2.610373000	-1.349343000	-0.201522000
6	3.993357000	-1.421655000	-0.299795000
6	4.809030000	-0.268697000	-0.163916000
6	4.196080000	0.991904000	0.059086000
6	0.694837000	1.853486000	0.310375000
6	0.598281000	0.343029000	0.140076000
1	2.015703000	-2.244548000	-0.289705000
1	4.462778000	-2.382512000	-0.479836000
1	4.800241000	1.886941000	0.149605000
6	-0.598275000	-0.343042000	0.140103000
6	-1.987151000	0.113738000	0.040676000
6	-0.694837000	-1.853487000	0.310502000
6	-2.823136000	-1.041058000	0.146473000
6	-2.610361000	1.349310000	-0.201634000
6	-4.196082000	-0.991894000	0.059282000
6	-3.993347000	1.421623000	-0.299877000
1	-2.015689000	2.244502000	-0.289927000
6	-4.809028000	0.268688000	-0.163843000
1	-4.800249000	-1.886915000	0.149919000
1	-4.462765000	2.382464000	-0.480010000
8	0.193129000	-2.678106000	0.460202000
8	-0.193136000	2.678119000	0.459959000
7	-2.040871000	-2.173004000	0.325619000
7	2.040867000	2.173023000	0.325372000
6	2.535703000	3.526198000	0.494729000
1	3.170765000	3.596390000	1.383427000

1	3.110826000	3.840863000	-0.382112000
1	1.669939000	4.176971000	0.614544000
6	-2.535714000	-3.526151000	0.495172000
1	-3.170718000	-3.596230000	1.383920000
1	-3.110899000	-3.840913000	-0.381594000
1	-1.669951000	-4.176923000	0.615003000
6	6.239666000	-0.374725000	-0.258953000
6	-6.239665000	0.374719000	-0.258846000
6	7.069340000	0.765186000	-0.127390000
7	7.727703000	1.723425000	-0.015188000
6	6.881547000	-1.615667000	-0.489024000
7	7.400265000	-2.644442000	-0.679702000
6	-6.881542000	1.615641000	-0.489037000
7	-7.400255000	2.644399000	-0.679817000
6	-7.069347000	-0.765169000	-0.127124000
7	-7.727716000	-1.723387000	-0.014789000

S2IID-T1

E= -1565.648637 Hartree

6	-2.792873000	1.113533000	-0.210621000
6	-1.993167000	-0.058836000	-0.113721000
6	-2.661071000	-1.271454000	0.112858000
6	-4.049419000	-1.294896000	0.216306000
6	-4.833348000	-0.128870000	0.091455000
6	-4.172219000	1.102026000	-0.125285000
6	-0.642609000	1.871359000	-0.356182000
6	-0.589620000	0.357646000	-0.203659000
1	-2.098779000	-2.188930000	0.182732000
1	-4.537955000	-2.253099000	0.351814000
1	-4.731702000	2.028448000	-0.175392000
6	0.589618000	-0.357773000	-0.203694000
6	1.993149000	0.058745000	-0.113726000
6	0.642657000	-1.871469000	-0.356375000
6	2.792896000	-1.113585000	-0.210726000
6	2.661005000	1.271371000	0.112945000
6	4.172242000	-1.102034000	-0.125385000
6	4.049352000	1.294857000	0.216398000
1	2.098676000	2.188821000	0.182888000
6	4.833323000	0.128868000	0.091457000
1	4.731759000	-2.028431000	-0.175571000
1	4.537853000	2.253068000	0.351980000
8	-0.265947000	-2.678009000	-0.493642000
8	0.266029000	2.677879000	-0.493341000
7	1.979085000	-2.229780000	-0.368954000

7	-1.979025000	2.229715000	-0.368742000
6	-2.431681000	3.596675000	-0.522167000
1	-3.065699000	3.698770000	-1.409261000
1	-2.995693000	3.922981000	0.358374000
1	-1.545848000	4.221346000	-0.636617000
6	2.431788000	-3.596710000	-0.522509000
1	3.065816000	-3.698698000	-1.409608000
1	2.995804000	-3.923082000	0.358005000
1	1.545977000	-4.221399000	-0.637027000
6	-6.296983000	-0.186011000	0.182617000
6	-7.111526000	0.764263000	-0.498733000
6	-6.944827000	-1.191950000	0.957026000
6	-8.480022000	0.720939000	-0.423530000
1	-6.634466000	1.514069000	-1.121949000
6	-8.311039000	-1.249915000	1.057233000
1	-6.337575000	-1.902349000	1.508448000
6	-9.162077000	-0.292592000	0.367010000
1	-9.102982000	1.431513000	-0.957319000
1	-8.806006000	-2.003144000	1.661819000
6	6.296957000	0.186056000	0.182627000
6	7.111535000	-0.764133000	-0.498798000
6	6.944763000	1.191957000	0.957118000
6	8.480029000	-0.720766000	-0.423589000
1	6.634503000	-1.513907000	-1.122075000
6	8.310972000	1.249963000	1.057331000
1	6.337483000	1.902289000	1.508596000
6	9.162045000	0.292727000	0.367033000
1	9.103016000	-1.431274000	-0.957434000
1	8.805911000	2.003161000	1.661979000
8	-10.410852000	-0.337835000	0.448177000
8	10.410819000	0.338009000	0.448206000

S3IID-T1

E= -2536.392805 Hartree

6	2.680769000	1.360712000	0.385665000
6	1.988495000	0.119933000	0.284855000
6	2.759667000	-1.030304000	0.058769000
6	4.144320000	-0.934303000	-0.030943000
6	4.818181000	0.298173000	0.097248000
6	4.054607000	1.472368000	0.302667000
6	0.472552000	1.921925000	0.528093000
6	0.555188000	0.409594000	0.372720000
1	2.279661000	-1.992421000	-0.022693000
1	4.715976000	-1.844399000	-0.181055000

1	4.529597000	2.443733000	0.363719000
6	-0.555185000	-0.409607000	0.372825000
6	-1.988487000	-0.119942000	0.284920000
6	-0.472576000	-1.921904000	0.528564000
6	-2.680783000	-1.360685000	0.386005000
6	-2.759636000	1.030264000	0.058599000
6	-4.054624000	-1.472332000	0.303039000
6	-4.144292000	0.934272000	-0.031080000
1	-2.279610000	1.992353000	-0.023073000
6	-4.818176000	-0.298165000	0.097376000
1	-4.529634000	-2.443673000	0.364300000
1	-4.715931000	1.844348000	-0.181379000
8	0.505129000	-2.641985000	0.662864000
8	-0.505166000	2.642011000	0.662270000
7	-1.772036000	-2.398377000	0.546571000
7	1.772004000	2.398423000	0.546011000
6	2.100278000	3.801586000	0.700661000
1	2.719518000	3.959282000	1.589765000
1	2.633560000	4.176859000	-0.179271000
1	1.161922000	4.344354000	0.813096000
6	-2.100332000	-3.801504000	0.701501000
1	-2.719583000	-3.959010000	1.590630000
1	-2.633613000	-4.176947000	-0.178360000
1	-1.161986000	-4.344263000	0.814055000
6	6.263953000	0.379027000	0.019966000
6	7.092256000	1.452704000	0.380698000
16	7.271837000	-0.924142000	-0.559520000
1	6.720244000	2.383985000	0.792065000
6	8.698141000	0.087395000	-0.260547000
6	-6.263950000	-0.379007000	0.020121000
6	-7.092271000	-1.452587000	0.381097000
16	-7.271811000	0.924052000	-0.559650000
1	-6.720275000	-2.383784000	0.792670000
6	-8.698134000	-0.087390000	-0.260443000
6	10.010686000	-0.357034000	-0.525992000
6	-10.010671000	0.357004000	-0.525980000
6	11.121627000	0.490662000	-0.281720000
7	12.054506000	1.163954000	-0.091537000
6	10.251670000	-1.655313000	-1.042251000
7	10.424377000	-2.728426000	-1.467017000
6	-10.251634000	1.655173000	-1.042527000
7	-10.424322000	2.728195000	-1.467531000
6	-11.121628000	-0.490616000	-0.281513000
7	-12.054519000	-1.163848000	-0.091176000

7	-8.410895000	-1.297002000	0.230870000
7	8.410881000	1.297111000	0.230497000

S4IID-T1

E= -2468.430183 Hartree

6	2.762328000	1.193178000	0.274520000
6	1.990220000	-0.003519000	0.176369000
6	2.686928000	-1.198059000	-0.066581000
6	4.072394000	-1.197500000	-0.176064000
6	4.832011000	-0.001602000	-0.049325000
6	4.134362000	1.219060000	0.176500000
6	0.591280000	1.885866000	0.452207000
6	0.579808000	0.375047000	0.281116000
1	2.145827000	-2.127383000	-0.148601000
1	4.595917000	-2.125893000	-0.356539000
1	4.670668000	2.157623000	0.260816000
6	-0.579799000	-0.374995000	0.281193000
6	-1.990213000	0.003551000	0.176406000
6	-0.591264000	-1.885785000	0.452539000
6	-2.762319000	-1.193126000	0.274816000
6	-2.686929000	1.198044000	-0.066751000
6	-4.134357000	-1.219027000	0.176849000
6	-4.072398000	1.197465000	-0.176190000
1	-2.145832000	2.127354000	-0.148966000
6	-4.832013000	0.001592000	-0.049192000
1	-4.670661000	-2.157572000	0.261369000
1	-4.595927000	2.125824000	-0.356826000
8	0.338985000	-2.662451000	0.611284000
8	-0.338969000	2.662569000	0.610776000
7	-1.918156000	-2.281731000	0.457605000
7	1.918171000	2.281819000	0.457121000
6	2.333698000	3.659020000	0.624263000
1	2.970451000	3.767957000	1.508565000
1	2.883090000	4.010251000	-0.255930000
1	1.431602000	4.257430000	0.751292000
6	-2.333680000	-3.658896000	0.625057000
1	-2.970398000	-3.767643000	1.509408000
1	-2.883109000	-4.010313000	-0.255038000
1	-1.431581000	-4.257281000	0.752176000
6	-6.257565000	0.007768000	-0.148706000
6	-7.113646000	1.174572000	-0.397469000
16	-7.223786000	-1.446831000	0.018571000
6	-8.774730000	-0.528827000	-0.240247000
6	6.257560000	-0.007797000	-0.148886000

6	7.113634000	-1.174648000	-0.397447000
16	7.223786000	1.446836000	0.018070000
6	8.774722000	0.528782000	-0.240615000
8	-6.775628000	2.340587000	-0.563189000
8	6.775612000	-2.340697000	-0.562925000
8	9.867065000	1.044402000	-0.235185000
8	-9.867073000	-1.044445000	-0.234679000
6	-9.510490000	1.795828000	-0.667020000
1	-9.478746000	2.556346000	0.116182000
1	-9.348433000	2.280428000	-1.632211000
1	-10.470487000	1.282023000	-0.657264000
6	9.510470000	-1.795956000	-0.666953000
1	9.478665000	-2.556386000	0.116331000
1	9.348459000	-2.280661000	-1.632100000
1	10.470477000	-1.282169000	-0.657204000
7	-8.470492000	0.798427000	-0.432509000
7	8.470479000	-0.798511000	-0.432603000

S5IID-T1 E= -2011.344607 Hartree

6	-2.789304000	1.119933000	-0.243960000
6	-1.988749000	-0.054390000	-0.130923000
6	-2.651252000	-1.261649000	0.132096000
6	-4.038270000	-1.291480000	0.248020000
6	-4.826552000	-0.125493000	0.092832000
6	-4.164448000	1.106555000	-0.152649000
6	-0.637901000	1.872435000	-0.405915000
6	-0.587625000	0.360125000	-0.232023000
1	-2.087623000	-2.176463000	0.223643000
1	-4.529067000	-2.232099000	0.448337000
1	-4.720122000	2.034512000	-0.211431000
6	0.587625000	-0.360108000	-0.232050000
6	1.988750000	0.054399000	-0.130919000
6	0.637900000	-1.872406000	-0.406041000
6	2.789304000	-1.119917000	-0.244035000
6	2.651254000	1.261640000	0.132186000
6	4.164448000	-1.106547000	-0.152723000
6	4.038271000	1.291461000	0.248113000
1	2.087624000	2.176446000	0.223799000
6	4.826553000	0.125484000	0.092842000
1	4.720121000	-2.034500000	-0.211566000
1	4.529069000	2.232065000	0.448495000
8	-0.274012000	-2.669878000	-0.559982000
8	0.274009000	2.669917000	-0.559811000

7	1.974467000	-2.231586000	-0.421894000
7	-1.974469000	2.231614000	-0.421747000
6	-2.426269000	3.597454000	-0.596322000
1	-3.062436000	3.684864000	-1.483225000
1	-2.986326000	3.937963000	0.281116000
1	-1.540435000	4.219418000	-0.723757000
6	2.426267000	-3.597414000	-0.596566000
1	3.062433000	-3.684761000	-1.483476000
1	2.986324000	-3.937985000	0.280847000
1	1.540433000	-4.219369000	-0.724044000
6	-6.282980000	-0.163181000	0.139165000
6	-6.997575000	-1.204197000	0.926400000
6	-7.047458000	0.785794000	-0.551216000
6	-8.432528000	0.779033000	-0.528912000
1	-6.550276000	1.532967000	-1.159167000
6	-9.186187000	-0.233745000	0.233813000
6	6.282980000	0.163168000	0.139178000
6	7.047459000	-0.785760000	-0.551267000
6	6.997575000	1.204130000	0.926485000
6	8.432528000	-0.778998000	-0.528964000
1	6.550277000	-1.532892000	-1.159268000
6	9.186188000	0.233730000	0.233828000
6	-9.177946000	1.741705000	-1.259554000
7	-9.748105000	2.553612000	-1.870983000
8	-6.428005000	-2.063284000	1.591300000
8	-10.408410000	-0.254161000	0.268721000
7	-8.398508000	-1.173576000	0.910317000
6	-9.077671000	-2.209666000	1.700157000
1	-8.786995000	-3.197573000	1.338414000
1	-8.783842000	-2.127264000	2.748281000
1	-10.148324000	-2.059469000	1.588933000
6	9.177947000	-1.741620000	-1.259672000
7	9.748106000	-2.553485000	-1.871157000
8	10.408410000	0.254147000	0.268733000
8	6.428004000	2.063178000	1.591435000
7	8.398508000	1.173515000	0.910396000
6	9.077671000	2.209555000	1.700302000
1	8.786994000	3.197484000	1.338622000
1	8.783842000	2.127086000	2.748420000
1	10.148324000	2.059366000	1.589068000

S6IID-T1

E= -2733.973544 Hartree

6	2.753882000	-1.213134000	-0.229599000
6	1.988004000	-0.011670000	-0.130124000
6	2.691770000	1.175325000	0.120444000
6	4.074592000	1.151343000	0.246815000
6	4.837985000	-0.051602000	0.118023000
6	4.124077000	-1.259661000	-0.132533000
6	0.577956000	-1.894129000	-0.412951000
6	0.574947000	-0.380175000	-0.239731000
1	2.163680000	2.112975000	0.190081000
1	4.591467000	2.081164000	0.425754000
1	4.659177000	-2.190689000	-0.228184000
6	-0.574948000	0.380212000	-0.239713000
6	-1.988001000	0.011692000	-0.130112000
6	-0.577967000	1.894175000	-0.412850000
6	-2.753890000	1.213150000	-0.229573000
6	-2.691756000	-1.175316000	0.120427000
6	-4.124087000	1.259660000	-0.132525000
6	-4.074579000	-1.151351000	0.246786000
1	-2.163657000	-2.112963000	0.190052000
6	-4.837981000	0.051587000	0.118000000
1	-4.659197000	2.190682000	-0.228172000
1	-4.591448000	-2.081180000	0.425713000
8	0.360393000	2.658578000	-0.578787000
8	-0.360415000	-2.658527000	-0.578841000
7	-1.900263000	2.295780000	-0.412502000
7	1.900247000	-2.295753000	-0.412552000
6	2.313010000	-3.674204000	-0.589816000
1	2.967512000	-3.769981000	-1.461732000
1	2.846263000	-4.035673000	0.295554000
1	1.411695000	-4.267968000	-0.740230000
6	-2.313039000	3.674225000	-0.589780000
1	-2.967512000	3.769995000	-1.461719000
1	-2.846327000	4.035685000	0.295572000
1	-1.411727000	4.268002000	-0.740161000
6	6.278541000	-0.019412000	0.203008000
6	6.950877000	1.058201000	0.939078000
6	7.095664000	-1.063154000	-0.426199000
6	9.140984000	0.230472000	0.125903000
6	-6.278535000	0.019376000	0.202969000
6	-7.095664000	1.063125000	-0.426215000
6	-6.950852000	-1.058270000	0.939005000
6	-9.140981000	-0.230480000	0.125951000
8	6.359577000	1.869313000	1.646539000
7	8.356900000	1.132847000	0.819450000

6	9.017602000	2.251907000	1.512760000
1	8.240714000	2.825962000	2.008627000
1	9.734764000	1.865491000	2.238135000
1	9.555337000	2.866288000	0.789595000
8	-6.359523000	-1.869427000	1.646389000
7	-8.356880000	-1.132902000	0.819418000
6	-9.017570000	-2.251988000	1.512696000
1	-8.240671000	-2.826081000	2.008503000
1	-9.734697000	-1.865601000	2.238120000
1	-9.555343000	-2.866324000	0.789520000
8	-6.635655000	2.077183000	-0.946533000
8	6.635645000	-2.077139000	-0.946650000
7	8.492117000	-0.846112000	-0.451807000
7	-8.492125000	0.846119000	-0.451743000
6	9.300384000	-1.852875000	-1.161025000
1	10.020601000	-2.298594000	-0.473530000
1	8.616218000	-2.604753000	-1.542183000
1	9.849128000	-1.377357000	-1.974661000
6	-9.300417000	1.852940000	-1.160851000
1	-10.020575000	2.298641000	-0.473282000
1	-8.616260000	2.604821000	-1.542018000
1	-9.849229000	1.377477000	-1.974473000
16	-10.800192000	-0.419009000	0.009648000
16	10.800185000	0.419038000	0.009523000

S7IID-T1 E= -2241.859932 Hartree

6	2.848723000	-0.961214000	-0.116200000
6	1.981512000	0.170434000	-0.039489000
6	2.569734000	1.422045000	0.199634000
6	3.950035000	1.530585000	0.321701000
6	4.806095000	0.402076000	0.195174000
6	4.217111000	-0.873781000	0.001424000
6	0.748148000	-1.834229000	-0.315594000
6	0.607600000	-0.325801000	-0.148339000
1	1.952907000	2.304141000	0.264530000
1	4.390538000	2.500828000	0.502154000
1	4.827757000	-1.766391000	-0.022193000
6	-0.607630000	0.325939000	-0.148317000
6	-1.981544000	-0.170304000	-0.039513000
6	-0.748179000	1.834377000	-0.315491000
6	-2.848751000	0.961354000	-0.116112000
6	-2.569764000	-1.421932000	0.199526000
6	-4.217139000	0.873915000	0.001537000

6	-3.950065000	-1.530476000	0.321606000
1	-1.952939000	-2.304033000	0.264360000
6	-4.806118000	-0.401959000	0.195162000
1	-4.827783000	1.766529000	-0.021968000
1	-4.390568000	-2.500730000	0.502007000
8	0.113923000	2.680569000	-0.494562000
8	-0.113950000	-2.680400000	-0.494794000
7	-2.101217000	2.117719000	-0.292291000
7	2.101189000	-2.117564000	-0.292478000
6	2.642064000	-3.442946000	-0.525631000
1	3.312319000	-3.429991000	-1.390867000
1	3.190435000	-3.800601000	0.352445000
1	1.801308000	-4.108303000	-0.720700000
6	-2.642094000	3.443126000	-0.525302000
1	-3.312403000	3.430242000	-1.390497000
1	-3.190406000	3.800718000	0.352838000
1	-1.801343000	4.108490000	-0.720370000
6	-6.230173000	-0.564501000	0.325967000
6	-6.836987000	-1.586217000	1.246972000
6	-7.305712000	0.225922000	-0.210890000
6	-8.274068000	-1.241144000	1.353640000
6	-8.555962000	-0.145109000	0.519116000
6	-9.240605000	-1.848428000	2.141871000
6	-9.853158000	0.370809000	0.487467000
6	-10.537895000	-1.330551000	2.104957000
1	-8.976441000	-2.697713000	2.763726000
6	-10.830419000	-0.232244000	1.289955000
1	-10.121349000	1.218723000	-0.127543000
1	-11.320702000	-1.776711000	2.710284000
1	-11.839688000	0.167503000	1.274036000
6	6.230155000	0.564586000	0.325940000
6	7.305627000	-0.225943000	-0.210896000
6	6.837086000	1.586242000	1.246952000
6	8.555913000	0.144981000	0.519054000
6	8.274144000	1.241032000	1.353588000
6	9.853052000	-0.371060000	0.487314000
6	9.240774000	1.848207000	2.141788000
6	10.830408000	0.231885000	1.289766000
1	10.121112000	-1.218991000	-0.127744000
6	10.538015000	1.330203000	2.104805000
1	8.976723000	2.697513000	2.763662000
1	11.839640000	-0.167953000	1.273790000
1	11.320891000	1.776281000	2.710103000
8	-6.269577000	-2.500003000	1.825922000

8	6.269783000	2.500038000	1.825991000
6	7.264110000	-1.077945000	-1.316893000
6	-7.264211000	1.077872000	-1.316941000
6	6.146975000	-1.226209000	-2.192817000
7	5.287110000	-1.390534000	-2.962191000
6	8.395295000	-1.831975000	-1.751093000
7	9.289224000	-2.478522000	-2.128012000
6	-6.147035000	1.226194000	-2.192805000
7	-5.287138000	1.390616000	-2.962123000
6	-8.395391000	1.831816000	-1.751309000
7	-9.289095000	2.478430000	-2.128647000

S8IID-T1 E= -3112.304325 Hartree

6	2.817798000	1.045303000	0.285655000
6	1.986379000	-0.111192000	0.203220000
6	2.610212000	-1.344972000	-0.035113000
6	3.993549000	-1.412403000	-0.154698000
6	4.807809000	-0.258952000	-0.028815000
6	4.190409000	0.998793000	0.172675000
6	0.692400000	1.856432000	0.470506000
6	0.597398000	0.343702000	0.307182000
1	2.020269000	-2.245013000	-0.101270000
1	4.461254000	-2.377949000	-0.308199000
1	4.779833000	1.906003000	0.203635000
6	-0.597405000	-0.343661000	0.307238000
6	-1.986386000	0.111219000	0.203219000
6	-0.692409000	-1.856363000	0.470817000
6	-2.817803000	-1.045267000	0.285781000
6	-2.610217000	1.344967000	-0.035287000
6	-4.190412000	-0.998775000	0.172760000
6	-3.993552000	1.412380000	-0.154904000
1	-2.020273000	2.245000000	-0.101555000
6	-4.807811000	0.258944000	-0.028893000
1	-4.779834000	-1.905983000	0.203816000
1	-4.461256000	2.377906000	-0.308540000
8	0.194591000	-2.678086000	0.638494000
8	-0.194593000	2.678164000	0.638174000
7	-2.037075000	-2.179187000	0.457342000
7	2.037069000	2.179244000	0.457071000
6	2.534990000	3.525024000	0.667026000
1	3.191992000	3.554885000	1.542008000
1	3.084859000	3.878572000	-0.211587000
1	1.672014000	4.168811000	0.835492000

6	-2.534997000	-3.524949000	0.667408000
1	-3.192044000	-3.554725000	1.542357000
1	-3.084817000	-3.878592000	-0.211198000
1	-1.672025000	-4.168712000	0.835985000
6	-6.238872000	0.372623000	-0.178632000
6	-7.313009000	-0.353199000	0.375865000
6	-8.503971000	0.889705000	-1.329042000
6	-8.599464000	-0.110192000	-0.349972000
6	-9.567151000	1.311997000	-2.110470000
6	-9.849167000	-0.720438000	-0.174372000
6	-10.803377000	0.692506000	-1.916580000
1	-9.435538000	2.095065000	-2.849624000
6	-10.931893000	-0.315406000	-0.958929000
1	-9.997252000	-1.506431000	0.551471000
1	-11.659326000	0.992522000	-2.512173000
1	-11.892003000	-0.800298000	-0.814366000
6	6.238873000	-0.372652000	-0.178510000
6	7.312999000	0.353241000	0.375917000
6	8.599467000	0.110148000	-0.349868000
6	8.503994000	-0.889869000	-1.328816000
6	9.849164000	0.720420000	-0.174320000
6	9.567190000	-1.312254000	-2.110173000
6	10.931906000	0.315295000	-0.958807000
1	9.997232000	1.506503000	0.551431000
6	10.803410000	-0.692735000	-1.916337000
1	9.435593000	-2.095413000	-2.849233000
1	11.892011000	0.800209000	-0.814286000
1	11.659371000	-0.992820000	-2.511878000
6	7.212212000	1.127158000	1.557322000
6	-7.212242000	-1.126967000	1.557370000
6	6.090785000	1.092898000	2.434898000
7	5.223192000	1.105160000	3.214032000
6	8.252484000	1.957909000	2.057538000
7	9.060031000	2.671958000	2.504969000
6	-6.090828000	-1.092596000	2.434960000
7	-5.223247000	-1.104749000	3.214108000
6	-8.252522000	-1.957653000	2.057680000
7	-9.060069000	-2.671646000	2.505198000
16	-6.848251000	1.530639000	-1.437560000
16	6.848278000	-1.530822000	-1.437284000
8	6.782431000	-2.914834000	-0.940215000
8	6.252937000	-1.209955000	-2.741461000
8	-6.252887000	1.209608000	-2.741686000
8	-6.782408000	2.914712000	-0.940660000

S9IID-T1

E= -3084.189991 Hartree

6	2.780793000	1.159171000	0.299340000
6	1.989822000	-0.024803000	0.208410000
6	2.679123000	-1.229797000	-0.021706000
6	4.060956000	-1.240987000	-0.127387000
6	4.843266000	-0.056681000	-0.011846000
6	4.154374000	1.173653000	0.202582000
6	0.615357000	1.872879000	0.474755000
6	0.587865000	0.369127000	0.310836000
1	2.126974000	-2.153710000	-0.096074000
1	4.554550000	-2.192528000	-0.297867000
1	4.697225000	2.109191000	0.279824000
6	-0.587861000	-0.369099000	0.310813000
6	-1.989819000	0.024821000	0.208343000
6	-0.615342000	-1.872856000	0.474678000
6	-2.780785000	-1.159151000	0.299337000
6	-2.679128000	1.229804000	-0.021807000
6	-4.154368000	-1.173640000	0.202610000
6	-4.060962000	1.240984000	-0.127474000
1	-2.126986000	2.153718000	-0.096209000
6	-4.843266000	0.056681000	-0.011870000
1	-4.697215000	-2.109175000	0.279911000
1	-4.554562000	2.192517000	-0.297983000
8	0.302688000	-2.669619000	0.628925000
8	-0.302679000	2.669673000	0.628806000
7	-1.948969000	-2.258188000	0.474585000
7	1.948981000	2.258220000	0.474534000
6	2.375395000	3.630726000	0.631072000
1	3.015261000	3.743530000	1.513385000
1	2.926704000	3.974377000	-0.251673000
1	1.477218000	4.236092000	0.755531000
6	-2.375381000	-3.630678000	0.631272000
1	-3.015190000	-3.743405000	1.513636000
1	-2.926750000	-3.974398000	-0.251408000
1	-1.477199000	-4.236039000	0.755720000
6	6.258925000	-0.095344000	-0.110040000
6	8.759950000	-0.852882000	-0.396398000
6	8.811102000	0.535474000	-0.195449000
6	9.938287000	-1.579576000	-0.588384000
6	10.039544000	1.201542000	-0.185863000
6	11.161155000	-0.910852000	-0.577932000
1	9.898453000	-2.653048000	-0.743764000

6	11.211656000	0.472024000	-0.377823000
1	10.077779000	2.275081000	-0.030452000
1	12.078007000	-1.472170000	-0.726740000
1	12.167659000	0.985675000	-0.371076000
6	-6.258927000	0.095335000	-0.110042000
6	-8.759960000	0.852854000	-0.396394000
6	-8.811104000	-0.535493000	-0.195381000
6	-9.938302000	1.579536000	-0.588393000
6	-10.039544000	-1.201565000	-0.185746000
6	-11.161168000	0.910809000	-0.577891000
1	-9.898473000	2.653002000	-0.743822000
6	-11.211661000	-0.472058000	-0.377720000
1	-10.077773000	-2.275097000	-0.030286000
1	-12.078023000	1.472118000	-0.726709000
1	-12.167663000	-0.985711000	-0.370934000
16	-7.260972000	-1.348679000	0.038791000
16	-7.154860000	1.588797000	-0.388144000
16	7.154849000	-1.588820000	-0.388090000
16	7.260976000	1.348675000	0.038713000

S10IID-T1

E= -2776.873527 Hartree

6	-2.800840000	-1.110175000	0.208385000
6	-1.988982000	0.059558000	0.117901000
6	-2.657556000	1.276390000	-0.111483000
6	-4.039004000	1.311727000	-0.217373000
6	-4.841802000	0.141496000	-0.102647000
6	-4.174685000	-1.100456000	0.111399000
6	-0.648153000	-1.861318000	0.384150000
6	-0.594518000	-0.358806000	0.220454000
1	-2.089385000	2.190635000	-0.185222000
1	-4.516047000	2.271926000	-0.387226000
1	-4.733893000	-2.026452000	0.188423000
6	0.594516000	0.358785000	0.220450000
6	1.988978000	-0.059565000	0.117803000
6	0.648148000	1.861291000	0.384203000
6	2.800839000	1.110152000	0.208465000
6	2.657551000	-1.276367000	-0.111747000
6	4.174686000	1.100441000	0.111507000
6	4.038999000	-1.311692000	-0.217633000
1	2.089382000	-2.190603000	-0.185606000
6	4.841800000	-0.141480000	-0.102725000
1	4.733897000	2.026423000	0.188686000
1	4.516041000	-2.271868000	-0.387617000

8	-0.255440000	2.674630000	0.538530000
8	0.255449000	-2.674701000	0.538169000
7	1.988645000	2.223575000	0.383653000
7	-1.988644000	-2.223624000	0.383398000
6	-2.438633000	-3.588491000	0.539274000
1	-3.080081000	-3.691025000	1.421753000
1	-2.996145000	-3.922264000	-0.343420000
1	-1.550934000	-4.209293000	0.663048000
6	2.438639000	3.588411000	0.539784000
1	3.080028000	3.690799000	1.422323000
1	2.996216000	3.922317000	-0.342819000
1	1.550939000	4.209203000	0.663593000
6	-6.256918000	0.204794000	-0.201138000
6	-8.731043000	0.975004000	-0.477449000
6	-8.803430000	-0.349621000	-0.286085000
6	6.256917000	-0.204769000	-0.201205000
6	8.731042000	-0.974947000	-0.477600000
6	8.803432000	0.349648000	-0.286028000
16	7.296438000	1.216701000	-0.055685000
16	7.139258000	-1.709905000	-0.479977000
16	-7.139262000	1.709969000	-0.479688000
16	-7.296435000	-1.216704000	-0.055855000
1	-9.720674000	-0.924739000	-0.261531000
1	-9.582417000	1.626710000	-0.630194000
1	9.582416000	-1.626634000	-0.630434000
1	9.720679000	0.924757000	-0.261373000

S1IIDT-CS E=-2504.314091 Hartree

6	2.633679000	1.458210000	0.571177000
6	1.929760000	0.200811000	0.423871000
6	2.706399000	-0.941364000	0.069586000
6	4.059500000	-0.824543000	-0.095199000
6	4.756577000	0.422792000	0.075742000
6	3.985170000	1.584136000	0.415112000
6	0.426485000	1.917413000	0.898749000
6	0.556464000	0.442466000	0.611066000
1	2.222647000	-1.900622000	-0.039994000
1	4.628039000	-1.709930000	-0.360449000
1	4.462606000	2.547973000	0.538242000
6	-0.556459000	-0.442417000	0.611028000
6	-1.929754000	-0.200778000	0.423799000
6	-0.426455000	-1.917382000	0.898601000
6	-2.633665000	-1.458177000	0.571145000

6	-2.706406000	0.941382000	0.069492000
6	-3.985158000	-1.584114000	0.415111000
6	-4.059508000	0.824548000	-0.095276000
1	-2.222665000	1.900643000	-0.040110000
6	-4.756576000	-0.422785000	0.075713000
1	-4.462588000	-2.547950000	0.538275000
1	-4.628056000	1.709925000	-0.360541000
8	0.570210000	-2.577953000	1.151066000
8	-0.570188000	2.578021000	1.151085000
7	-1.715313000	-2.447858000	0.868249000
7	1.715335000	2.447903000	0.868268000
6	2.006108000	3.845137000	1.116117000
1	2.670826000	3.958589000	1.978906000
1	2.471826000	4.309831000	0.240383000
1	1.057560000	4.340262000	1.325222000
6	-2.006083000	-3.845077000	1.116194000
1	-2.670746000	-3.958480000	1.979032000
1	-2.471862000	-4.309811000	0.240513000
1	-1.057525000	-4.340200000	1.325261000
6	6.149704000	0.505311000	-0.090893000
6	6.982480000	1.653601000	0.045062000
16	7.144202000	-0.897459000	-0.523863000
6	8.313655000	1.427775000	-0.180777000
1	6.588368000	2.627161000	0.308111000
6	8.612639000	0.069422000	-0.512823000
1	9.090002000	2.180797000	-0.122093000
6	-6.149706000	-0.505316000	-0.090900000
6	-6.982473000	-1.653608000	0.045100000
16	-7.144218000	0.897435000	-0.523894000
6	-8.313653000	-1.427796000	-0.180727000
1	-6.588352000	-2.627157000	0.308172000
6	-8.612649000	-0.069454000	-0.512809000
1	-9.089994000	-2.180820000	-0.122011000
6	-9.866474000	0.459928000	-0.794561000
6	9.866457000	-0.459975000	-0.794576000
6	-11.016540000	-0.378811000	-0.767616000
7	-11.941637000	-1.087423000	-0.738849000
6	-10.039709000	1.834596000	-1.114575000
7	-10.152429000	2.965591000	-1.374284000
6	10.039680000	-1.834654000	-1.114553000
7	10.152393000	-2.965661000	-1.374211000
6	11.016530000	0.378756000	-0.767666000
7	11.941632000	1.087364000	-0.738930000

S2IIDT-CS

E=-2669.279874 Hartree

6	-2.565378000	1.575548000	-0.660993000
6	-1.932694000	0.286864000	-0.531796000
6	-2.772791000	-0.812349000	-0.212588000
6	-4.125790000	-0.625506000	-0.061060000
6	-4.748668000	0.653176000	-0.213403000
6	-3.913728000	1.772628000	-0.518205000
6	-0.332159000	1.938150000	-0.946181000
6	-0.532424000	0.464659000	-0.694657000
1	-2.344366000	-1.798622000	-0.116202000
1	-4.742961000	-1.485633000	0.177840000
1	-4.334730000	2.764399000	-0.627159000
6	0.532424000	-0.464686000	-0.694649000
6	1.932693000	-0.286885000	-0.531794000
6	0.332163000	-1.938182000	-0.946150000
6	2.565381000	-1.575570000	-0.660966000
6	2.772788000	0.812337000	-0.212609000
6	3.913731000	-1.772643000	-0.518173000
6	4.125787000	0.625501000	-0.061077000
1	2.344361000	1.798611000	-0.116243000
6	4.748668000	-0.653183000	-0.213394000
1	4.334735000	-2.764416000	-0.627109000
1	4.742956000	1.485634000	0.177806000
8	-0.694221000	-2.565007000	-1.172702000
8	0.694227000	2.564970000	-1.172738000
7	1.594684000	-2.526771000	-0.924208000
7	-1.594679000	2.526743000	-0.924250000
6	-1.814997000	3.939713000	-1.145350000
1	-2.462493000	4.103943000	-2.013488000
1	-2.270576000	4.409210000	-0.266370000
1	-0.840898000	4.392605000	-1.331946000
6	1.815005000	-3.939745000	-1.145278000
1	2.462503000	-4.103992000	-2.013411000
1	2.270582000	-4.409224000	-0.266287000
1	0.840907000	-4.392643000	-1.331866000
6	-6.149330000	0.814893000	-0.062650000
6	-6.910612000	2.001108000	-0.186380000
16	-7.224841000	-0.526985000	0.328438000
6	-8.262796000	1.841103000	0.019689000
1	-6.462637000	2.957389000	-0.425827000
6	-8.658116000	0.510040000	0.320939000
1	-8.970144000	2.657988000	-0.042088000
6	6.149331000	-0.814894000	-0.062638000

6	6.910615000	-2.001109000	-0.186344000
16	7.224838000	0.526993000	0.328427000
6	8.262799000	-1.841098000	0.019723000
1	6.462643000	-2.957397000	-0.425773000
6	8.658115000	-0.510028000	0.320948000
1	8.970149000	-2.657982000	-0.042039000
6	-9.948587000	0.022253000	0.580683000
6	-10.188947000	-1.368994000	0.872425000
6	-11.092806000	0.902253000	0.565761000
6	-11.435650000	-1.843877000	1.124969000
1	-9.343860000	-2.052416000	0.889026000
6	-12.347286000	0.446733000	0.815820000
1	-10.943593000	1.954991000	0.348923000
6	-12.613930000	-0.965938000	1.115635000
1	-11.611338000	-2.892213000	1.343944000
1	-13.205182000	1.111425000	0.803879000
6	9.948585000	-0.022233000	0.580685000
6	11.092806000	-0.902231000	0.565780000
6	10.188942000	1.369020000	0.872401000
6	12.347285000	-0.446703000	0.815831000
1	10.943597000	-1.954974000	0.348961000
6	11.435643000	1.843910000	1.124938000
1	9.343852000	2.052439000	0.888989000
6	12.613925000	0.965974000	1.115620000
1	13.205183000	-1.111393000	0.803904000
1	11.611328000	2.892250000	1.343895000
8	-13.753155000	-1.389409000	1.344914000
8	13.753149000	1.389452000	1.344894000

S3IIDT-CS

E=-3640.020104 Hartree

6	-2.577675000	-1.550701000	0.714778000
6	-1.944559000	-0.266385000	0.590688000
6	-2.781207000	0.836858000	0.295103000
6	-4.140842000	0.657291000	0.163077000
6	-4.762315000	-0.616574000	0.313832000
6	-3.931944000	-1.740825000	0.592085000
6	-0.345176000	-1.940964000	0.958140000
6	-0.533586000	-0.456031000	0.730917000
1	-2.351309000	1.821940000	0.198052000
1	-4.755469000	1.523892000	-0.058239000
1	-4.355027000	-2.731824000	0.698134000
6	0.533579000	0.456146000	0.730793000
6	1.944550000	0.266479000	0.590559000

6	0.345160000	1.941129000	0.957666000
6	2.577666000	1.550813000	0.714462000
6	2.781200000	-0.836807000	0.295142000
6	3.931937000	1.740918000	0.591760000
6	4.140836000	-0.657259000	0.163095000
1	2.351308000	-1.821906000	0.198247000
6	4.762310000	0.616627000	0.313674000
1	4.355020000	2.731932000	0.697670000
1	4.755464000	-1.523892000	-0.058090000
8	-0.677970000	2.579158000	1.158784000
8	0.677969000	-2.578987000	1.159198000
7	1.611558000	2.514515000	0.950576000
7	-1.611567000	-2.514366000	0.951042000
6	-1.843900000	-3.929084000	1.157502000
1	-2.477403000	-4.096222000	2.034958000
1	-2.320064000	-4.379977000	0.280111000
1	-0.872489000	-4.396042000	1.320646000
6	1.843900000	3.929246000	1.156940000
1	2.477346000	4.096446000	2.034426000
1	2.320131000	4.380057000	0.279544000
1	0.872485000	4.396233000	1.319977000
6	-6.175054000	-0.773186000	0.185621000
6	-6.936226000	-1.951189000	0.310245000
16	-7.241978000	0.583014000	-0.172546000
6	-8.297430000	-1.779016000	0.128648000
1	-6.491575000	-2.913050000	0.531840000
6	-8.673338000	-0.447447000	-0.149041000
1	-9.021122000	-2.583335000	0.191413000
6	6.175051000	0.773217000	0.185462000
6	6.936225000	1.951235000	0.309937000
16	7.241976000	-0.583035000	-0.172505000
6	8.297431000	1.779033000	0.128384000
1	6.491573000	2.913126000	0.531397000
6	8.673339000	0.447425000	-0.149119000
1	9.021124000	2.583357000	0.191051000
6	-9.960495000	0.053309000	-0.380484000
6	-10.337954000	1.394710000	-0.659305000
16	-11.416989000	-0.934646000	-0.367978000
1	-9.617506000	2.205443000	-0.722006000
6	-12.367702000	0.530213000	-0.732681000
6	9.960498000	-0.053367000	-0.380475000
6	10.337956000	-1.394808000	-0.659106000
16	11.416994000	0.934585000	-0.368082000
1	9.617507000	-2.205547000	-0.721707000

6	12.367708000	-0.530327000	-0.732570000
6	13.751023000	-0.506038000	-0.882564000
6	-13.751015000	0.505899000	-0.882691000
6	14.473630000	-1.695887000	-1.173412000
7	15.094560000	-2.652567000	-1.411799000
6	14.471881000	0.710933000	-0.748157000
7	15.033809000	1.726282000	-0.631709000
6	-14.471871000	-0.711055000	-0.748129000
7	-15.033797000	-1.726391000	-0.631551000
6	-14.473621000	1.695707000	-1.173712000
7	-15.094550000	2.652352000	-1.412238000
7	-11.616523000	1.651410000	-0.846993000
7	11.616527000	-1.651537000	-0.846740000

S4IIDT-CS E=-3572.076281 Hartree

6	-2.532756000	1.629392000	-0.832155000
6	-1.915211000	0.328867000	-0.692501000
6	-2.768614000	-0.757420000	-0.344554000
6	-4.111898000	-0.549051000	-0.175419000
6	-4.722888000	0.741902000	-0.336090000
6	-3.872530000	1.847293000	-0.671712000
6	-0.297625000	1.939934000	-1.160215000
6	-0.525526000	0.478755000	-0.879381000
1	-2.351765000	-1.748555000	-0.243247000
1	-4.739378000	-1.395234000	0.084825000
1	-4.281201000	2.843317000	-0.788207000
6	0.525526000	-0.478730000	-0.879392000
6	1.915213000	-0.328846000	-0.692520000
6	0.297624000	-1.939904000	-1.160251000
6	2.532754000	-1.629371000	-0.832184000
6	2.768619000	0.757437000	-0.344564000
6	3.872528000	-1.847277000	-0.671745000
6	4.111903000	0.549063000	-0.175434000
1	2.351773000	1.748571000	-0.243246000
6	4.722890000	-0.741891000	-0.336117000
1	4.281196000	-2.843301000	-0.788249000
1	4.739386000	1.395242000	0.084816000
8	-0.739442000	-2.538661000	-1.412503000
8	0.739436000	2.538693000	-1.412481000
7	1.548503000	-2.556451000	-1.125768000
7	-1.548508000	2.556476000	-1.125734000
6	-1.743153000	3.969819000	-1.365966000
1	-2.400004000	4.134529000	-2.227046000

1	-2.175628000	4.462617000	-0.488012000
1	-0.762623000	4.399169000	-1.573922000
6	1.743143000	-3.969793000	-1.366004000
1	2.399997000	-4.134504000	-2.227082000
1	2.175615000	-4.462596000	-0.488051000
1	0.762613000	-4.399139000	-1.573964000
6	-6.109512000	0.919245000	-0.163971000
6	-6.850520000	2.128366000	-0.296661000
16	-7.196617000	-0.412327000	0.268387000
6	-8.193309000	1.998052000	-0.068241000
1	-6.387648000	3.071478000	-0.558692000
6	-8.601402000	0.666096000	0.262556000
1	-8.902991000	2.815201000	-0.127128000
6	6.109514000	-0.919239000	-0.164002000
6	6.850519000	-2.128360000	-0.296706000
16	7.196623000	0.412327000	0.268363000
6	8.193308000	-1.998052000	-0.068285000
1	6.387645000	-3.071468000	-0.558746000
6	8.601404000	-0.666100000	0.262529000
1	8.902988000	-2.815202000	-0.127179000
6	-9.877624000	0.239176000	0.541293000
6	-10.210391000	-1.147269000	0.872350000
16	-11.316081000	1.266776000	0.549359000
6	-12.366898000	-0.149009000	0.993755000
6	9.877627000	-0.239188000	0.541274000
6	10.210397000	1.147255000	0.872338000
16	11.316081000	-1.266791000	0.549329000
6	12.366893000	0.148974000	0.993797000
7	-11.585911000	-1.282911000	1.106119000
7	11.585912000	1.282881000	1.106154000
6	-12.191523000	-2.563485000	1.456253000
1	-12.936247000	-2.844050000	0.708135000
1	-11.389404000	-3.300160000	1.485305000
1	-12.678084000	-2.494889000	2.431741000
6	12.191521000	2.563444000	1.456332000
1	12.936275000	2.844015000	0.708245000
1	11.389408000	3.300125000	1.485366000
1	12.678047000	2.494828000	2.431836000
8	-13.561138000	-0.084077000	1.160012000
8	-9.415596000	-2.077318000	0.941790000
8	9.415601000	2.077298000	0.941814000
8	13.561130000	0.084035000	1.160069000

S5IIDT-CS

E=-3115.001862 Hartree

6	-2.537219000	1.618336000	-0.869689000
6	-1.918713000	0.319299000	-0.727652000
6	-2.768654000	-0.769602000	-0.383027000
6	-4.114168000	-0.565615000	-0.222136000
6	-4.725908000	0.723426000	-0.388867000
6	-3.880123000	1.831108000	-0.718255000
6	-0.303795000	1.942660000	-1.181881000
6	-0.526378000	0.474655000	-0.905917000
1	-2.349618000	-1.758928000	-0.275907000
1	-4.740276000	-1.412899000	0.036051000
1	-4.292592000	2.825006000	-0.837454000
6	0.526375000	-0.474088000	-0.905926000
6	1.918732000	-0.318830000	-0.727695000
6	0.303668000	-1.942085000	-1.181808000
6	2.537120000	-1.617936000	-0.869653000
6	2.768780000	0.770000000	-0.383104000
6	3.880005000	-1.830826000	-0.718215000
6	4.114277000	0.565896000	-0.222220000
1	2.349841000	1.759366000	-0.276001000
6	4.725898000	-0.723206000	-0.388902000
1	4.292377000	-2.824772000	-0.837347000
1	4.740465000	1.413132000	0.035933000
8	-0.732706000	-2.541804000	-1.425746000
8	0.732479000	2.542419000	-1.426146000
7	1.556505000	-2.550584000	-1.155649000
7	-1.556692000	2.551040000	-1.155807000
6	-1.758907000	3.965001000	-1.396087000
1	-2.410249000	4.124629000	-2.261791000
1	-2.200561000	4.452119000	-0.520041000
1	-0.780375000	4.401880000	-1.596541000
6	1.758581000	-3.964600000	-1.395722000
1	2.409916000	-4.124415000	-2.261398000
1	2.200180000	-4.451637000	-0.519603000
1	0.780008000	-4.401409000	-1.596124000
6	-6.118618000	0.896148000	-0.225709000
6	-6.860662000	2.098165000	-0.364126000
16	-7.199809000	-0.439993000	0.200587000
6	-8.206481000	1.951688000	-0.141899000
1	-6.408608000	3.047239000	-0.623768000
6	-8.603755000	0.619996000	0.186352000
1	-8.910432000	2.771257000	-0.208662000
6	6.118593000	-0.896051000	-0.225744000
6	6.860524000	-2.098143000	-0.364114000

16	7.199914000	0.440013000	0.200464000
6	8.206357000	-1.951783000	-0.141891000
1	6.408380000	-3.047186000	-0.623710000
6	8.603755000	-0.620117000	0.186312000
1	8.910229000	-2.771422000	-0.208612000
6	9.906028000	-0.179666000	0.462956000
6	11.024471000	-1.053972000	0.444795000
6	10.130794000	1.240924000	0.785485000
6	12.291273000	-0.610853000	0.717142000
1	10.886233000	-2.103330000	0.210524000
6	12.564435000	0.801588000	1.044629000
6	-9.905990000	0.179430000	0.462993000
6	-11.024516000	1.053628000	0.444789000
6	-10.130626000	-1.241174000	0.785554000
6	-12.291282000	0.610394000	0.717120000
1	-10.886375000	2.102993000	0.210489000
6	-12.564312000	-0.802061000	1.044655000
6	13.400092000	-1.505921000	0.693655000
7	14.276389000	-2.271637000	0.663309000
6	-13.400189000	1.505351000	0.693568000
7	-14.276562000	2.270979000	0.663168000
8	9.210633000	2.059981000	0.821536000
8	-9.210402000	-2.060162000	0.821542000
8	-13.683744000	-1.223745000	1.291400000
8	13.683890000	1.223152000	1.291476000
7	11.435600000	1.644080000	1.054555000
7	-11.435403000	-1.644455000	1.054576000
6	-11.629219000	-3.064570000	1.372060000
1	-11.288368000	-3.679318000	0.536641000
1	-11.043547000	-3.328722000	2.254816000
1	-12.689666000	-3.218069000	1.554545000
6	11.629535000	3.064169000	1.372086000
1	11.288858000	3.678972000	0.536635000
1	11.043779000	3.328369000	2.254772000
1	12.689976000	3.217547000	1.554702000

S6IIDT-CS E=-3837.648393 Hartree

6	-2.515970000	-1.652325000	0.985113000
6	-1.908247000	-0.345521000	0.839391000
6	-2.767333000	0.734920000	0.480311000
6	-4.106736000	0.516330000	0.308427000
6	-4.709245000	-0.781079000	0.476547000
6	-3.853197000	-1.879560000	0.822225000

6	-0.281615000	-1.943688000	1.322579000
6	-0.521686000	-0.483045000	1.031613000
1	-2.356321000	1.727781000	0.372669000
1	-4.740667000	1.354306000	0.039570000
1	-4.258160000	-2.876192000	0.943490000
6	0.521689000	0.483066000	1.031620000
6	1.908252000	0.345536000	0.839420000
6	0.281622000	1.943708000	1.322599000
6	2.515972000	1.652346000	0.985098000
6	2.767338000	-0.734915000	0.480372000
6	3.853197000	1.879579000	0.822195000
6	4.106740000	-0.516329000	0.308480000
1	2.356326000	-1.727779000	0.372758000
6	4.709247000	0.781087000	0.476554000
1	4.258159000	2.876216000	0.943425000
1	4.740671000	-1.354312000	0.039648000
8	-0.761259000	2.526293000	1.580760000
8	0.761256000	-2.526254000	1.580821000
7	1.526441000	2.569877000	1.287689000
7	-1.526441000	-2.569847000	1.287735000
6	-1.712490000	-3.984297000	1.536994000
1	-2.370460000	-4.146142000	2.397285000
1	-2.139065000	-4.484009000	0.660551000
1	-0.730217000	-4.406502000	1.750483000
6	1.712484000	3.984340000	1.536873000
1	2.370472000	4.146232000	2.397141000
1	2.139036000	4.484014000	0.660396000
1	0.730212000	4.406548000	1.750364000
6	-6.092606000	-0.968426000	0.299698000
6	-6.825451000	-2.180381000	0.435945000
16	-7.184740000	0.354924000	-0.146062000
6	-8.167577000	-2.058080000	0.199574000
1	-6.363715000	-3.122210000	0.705753000
6	-8.580644000	-0.725792000	-0.142346000
1	-8.890247000	-2.857837000	0.252461000
6	6.092607000	0.968432000	0.299694000
6	6.825449000	2.180393000	0.435897000
16	7.184742000	-0.354930000	-0.146028000
6	8.167574000	2.058087000	0.199523000
1	6.363712000	3.122230000	0.705676000
6	8.580643000	0.725789000	-0.142354000
1	8.890243000	2.857848000	0.252381000
6	9.875494000	0.288802000	-0.437648000
6	11.009566000	1.212922000	-0.425838000

6	10.083928000	-1.114505000	-0.761305000
6	12.495740000	-0.681510000	-1.051776000
6	-9.875495000	-0.288812000	-0.437650000
6	-11.009570000	-1.212928000	-0.425804000
6	-10.083927000	1.114486000	-0.761352000
6	-12.495741000	0.681487000	-1.051799000
8	9.159070000	-1.929048000	-0.785173000
8	-9.159066000	1.929025000	-0.785254000
7	11.396552000	-1.523599000	-1.051626000
7	-11.396551000	1.523573000	-1.051682000
6	-11.591630000	2.946018000	-1.375099000
1	-12.286423000	3.394334000	-0.663701000
1	-10.617747000	3.423822000	-1.318116000
1	-12.013494000	3.042677000	-2.376386000
6	11.591634000	-2.946054000	-1.374996000
1	12.286430000	-3.394344000	-0.663586000
1	10.617752000	-3.423858000	-1.317994000
1	12.013494000	-3.042746000	-2.376282000
7	12.269439000	0.648431000	-0.741918000
7	-12.269442000	-0.648444000	-0.741897000
6	13.418798000	1.568421000	-0.734277000
1	14.157681000	1.229925000	-0.006663000
1	13.887267000	1.581824000	-1.719309000
1	13.040313000	2.551909000	-0.472377000
6	-13.418803000	-1.568431000	-0.734221000
1	-14.157683000	-1.229908000	-0.006616000
1	-13.887276000	-1.581866000	-1.719251000
1	-13.040320000	-2.551911000	-0.472289000
8	-10.931407000	-2.410642000	-0.165990000
8	10.931402000	2.410645000	-0.166064000
16	14.028212000	-1.251273000	-1.411565000
16	-14.028213000	1.251243000	-1.411601000

S7IIDT-CS

E=-3345.507171 Hartree

6	-2.488087000	1.694236000	-1.236766000
6	-1.907373000	0.376886000	-1.094856000
6	-2.789537000	-0.687550000	-0.751614000
6	-4.126904000	-0.443152000	-0.584340000
6	-4.699262000	0.864976000	-0.744765000
6	-3.822894000	1.947364000	-1.080648000
6	-0.246778000	1.950674000	-1.553919000
6	-0.512695000	0.490695000	-1.276481000
1	-2.401334000	-1.690548000	-0.655837000

1	-4.780243000	-1.274094000	-0.339996000
1	-4.205949000	2.953922000	-1.190790000
6	0.512678000	-0.489841000	-1.276513000
6	1.907372000	-0.376176000	-1.094853000
6	0.246609000	-1.949783000	-1.553962000
6	2.487952000	-1.693578000	-1.236882000
6	2.789656000	0.688119000	-0.751470000
6	3.822733000	-1.946864000	-1.080799000
6	4.126997000	0.443560000	-0.584230000
1	2.401568000	1.691146000	-0.655564000
6	4.699219000	-0.864608000	-0.744812000
1	4.205676000	-2.953455000	-1.191030000
1	4.780425000	1.274403000	-0.339787000
8	-0.806739000	-2.518286000	-1.799795000
8	0.806476000	2.519290000	-1.799888000
7	1.480664000	-2.596078000	-1.524949000
7	-1.480895000	2.596849000	-1.524813000
6	-1.641226000	4.015687000	-1.767704000
1	-2.290774000	4.192790000	-2.631331000
1	-2.064789000	4.518039000	-0.891286000
1	-0.650639000	4.422252000	-1.972793000
6	1.640846000	-4.014923000	-1.767897000
1	2.290345000	-4.192059000	-2.631554000
1	2.064389000	-4.517348000	-0.891511000
1	0.650211000	-4.421381000	-1.972967000
6	-6.080277000	1.086805000	-0.564767000
6	-6.804516000	2.295207000	-0.755521000
16	-7.185090000	-0.187377000	-0.052866000
6	-8.146811000	2.202390000	-0.500139000
1	-6.332135000	3.210214000	-1.090119000
6	-8.576273000	0.895450000	-0.092115000
1	-8.857830000	3.012010000	-0.580681000
6	6.080212000	-1.086604000	-0.564844000
6	6.804319000	-2.295064000	-0.755731000
16	7.185163000	0.187404000	-0.052808000
6	8.146626000	-2.202418000	-0.500345000
1	6.331838000	-3.209984000	-1.090426000
6	8.576230000	-0.895568000	-0.092182000
1	8.857558000	-3.012106000	-0.580978000
6	9.863525000	-0.578911000	0.341749000
6	10.827479000	-1.662855000	0.732806000
6	10.453835000	0.686809000	0.741312000
6	11.856435000	-1.004466000	1.572046000
6	11.611218000	0.379484000	1.626853000

6	12.912802000	-1.602007000	2.245115000
6	12.445205000	1.190475000	2.401382000
6	13.743306000	-0.787260000	3.018042000
1	13.069469000	-2.672710000	2.163116000
6	13.501778000	0.589034000	3.095078000
1	12.291259000	2.257660000	2.484753000
1	14.576291000	-1.219474000	3.563762000
1	14.148476000	1.211320000	3.706063000
6	-9.863531000	0.578606000	0.341787000
6	-10.827603000	1.662402000	0.732963000
6	-10.453699000	-0.687222000	0.741216000
6	-11.856496000	1.003807000	1.572120000
6	-11.611123000	-0.380121000	1.626781000
6	-12.912937000	1.601157000	2.245241000
6	-12.445026000	-1.191289000	2.401216000
6	-13.743357000	0.786234000	3.018073000
1	-13.069724000	2.671851000	2.163355000
6	-13.501674000	-0.590041000	3.094966000
1	-12.290961000	-2.258465000	2.484475000
1	-14.576396000	1.218296000	3.563830000
1	-14.148308000	-1.212465000	3.705878000
8	-10.780420000	2.855639000	0.468463000
8	10.780154000	-2.856061000	0.468192000
6	-10.141123000	-1.955887000	0.273002000
6	10.141406000	1.955559000	0.273229000
6	-9.327272000	-2.202977000	-0.872500000
7	-8.718124000	-2.454278000	-1.833684000
6	-10.732449000	-3.143261000	0.804076000
7	-11.179479000	-4.132836000	1.226991000
6	10.732866000	3.142809000	0.804432000
7	11.180009000	4.132286000	1.227457000
6	9.327598000	2.202864000	-0.872256000
7	8.718506000	2.454335000	-1.833431000

S8IIDT-CS

E=-4215.945304 Hartree

6	2.523131000	-1.640296000	-1.304964000
6	1.914614000	-0.335561000	-1.160526000
6	2.773633000	0.747432000	-0.816289000
6	4.115968000	0.531682000	-0.651293000
6	4.716043000	-0.763641000	-0.815353000
6	3.863404000	-1.864600000	-1.151576000
6	0.287942000	-1.944710000	-1.619344000
6	0.522878000	-0.478896000	-1.341112000

1	2.363778000	1.741473000	-0.717713000
1	4.750942000	1.376264000	-0.405197000
1	4.267957000	-2.862384000	-1.264078000
6	-0.522987000	0.479427000	-1.340903000
6	-1.914707000	0.336023000	-1.160249000
6	-0.288083000	1.945336000	-1.618658000
6	-2.523240000	1.640809000	-1.304165000
6	-2.773691000	-0.747095000	-0.816321000
6	-3.863499000	1.865054000	-1.150571000
6	-4.116012000	-0.531408000	-0.651124000
1	-2.363824000	-1.741170000	-0.718137000
6	-4.716105000	0.763973000	-0.814665000
1	-4.268066000	2.862878000	-1.262677000
1	-4.750961000	-1.376080000	-0.405272000
8	0.753428000	2.535350000	-1.862705000
8	-0.753590000	-2.534630000	-1.863528000
7	-1.535673000	2.564618000	-1.591744000
7	1.535535000	-2.564002000	-1.592782000
6	1.726390000	-3.979239000	-1.837211000
1	2.376741000	-4.141126000	-2.703102000
1	2.163605000	-4.472180000	-0.962292000
1	0.744461000	-4.407528000	-2.039450000
6	-1.726552000	3.979944000	-1.835638000
1	-2.376992000	4.142146000	-2.701405000
1	-2.163678000	4.472568000	-0.960496000
1	-0.744643000	4.408307000	-2.037821000
6	6.101535000	-0.955110000	-0.638526000
6	6.851379000	-2.147121000	-0.831357000
16	7.178513000	0.345402000	-0.131209000
6	8.191142000	-2.024564000	-0.580993000
1	6.399417000	-3.073485000	-1.161847000
6	8.592732000	-0.707942000	-0.172631000
1	8.897742000	-2.837519000	-0.676613000
6	-6.101580000	0.955375000	-0.637643000
6	-6.851446000	2.147451000	-0.829985000
16	-7.178509000	-0.345319000	-0.130691000
6	-8.191186000	2.024803000	-0.579544000
1	-6.399517000	3.073933000	-1.160191000
6	-8.592733000	0.708036000	-0.171602000
1	-8.897796000	2.837789000	-0.674817000
6	-9.864161000	0.351990000	0.254537000
6	-10.441438000	-0.899148000	0.667543000
6	-11.976412000	0.646974000	1.712538000
6	-11.542322000	-0.686069000	1.648908000

6	-13.006266000	1.084097000	2.529940000
6	-12.179168000	-1.615230000	2.484959000
6	-13.630863000	0.141552000	3.349104000
1	-13.303867000	2.127245000	2.536542000
6	-13.210914000	-1.190937000	3.324312000
1	-11.877721000	-2.652831000	2.502392000
1	-14.436397000	0.447009000	4.008952000
1	-13.691104000	-1.917432000	3.972015000
6	9.864201000	-0.352065000	0.253529000
6	10.441546000	0.898912000	0.666922000
6	11.976527000	-0.647643000	1.711280000
6	11.542474000	0.685440000	1.648170000
6	13.006404000	-1.085115000	2.528466000
6	12.179377000	1.614248000	2.484574000
6	13.631065000	-0.142909000	3.347969000
1	13.303970000	-2.128275000	2.534654000
6	13.211147000	1.189597000	3.323718000
1	11.877959000	2.651846000	2.502448000
1	14.436616000	-0.448648000	4.007667000
1	13.691378000	1.915824000	3.971691000
6	10.100543000	2.140643000	0.132367000
6	-10.100444000	-2.140705000	0.132598000
6	9.348486000	2.284712000	-1.069889000
7	8.775566000	2.446814000	-2.071893000
6	10.578328000	3.385040000	0.641218000
7	10.929103000	4.425097000	1.033652000
6	-10.578251000	-3.385232000	0.641110000
7	-10.929158000	-4.425317000	1.033354000
6	-9.348466000	-2.284421000	-1.069750000
7	-8.775573000	-2.446218000	-2.071819000
16	11.047794000	-1.690282000	0.606388000
16	-11.047761000	1.690051000	0.607987000
8	11.827184000	-2.021502000	-0.596368000
8	10.407917000	-2.784402000	1.353385000
8	-10.407871000	2.783899000	1.355371000
8	-11.827236000	2.021717000	-0.594590000

S9IIDT-CS

E=-4187.828756 Hartree

6	2.521663000	1.653674000	0.942572000
6	1.912426000	0.348850000	0.809184000
6	2.776501000	-0.729556000	0.464823000
6	4.118048000	-0.508970000	0.289352000

6	4.719315000	0.786174000	0.438902000
6	3.858246000	1.884485000	0.774227000
6	0.281595000	1.938145000	1.282342000
6	0.521885000	0.486351000	1.002698000
1	2.368356000	-1.725633000	0.373560000
1	4.752187000	-1.352316000	0.032609000
1	4.257609000	2.885504000	0.884764000
6	-0.521879000	-0.486427000	1.002650000
6	-1.912413000	-0.348917000	0.809095000
6	-0.281591000	-1.938242000	1.282188000
6	-2.521669000	-1.653729000	0.942515000
6	-2.776475000	0.729497000	0.464723000
6	-3.858258000	-1.884522000	0.774193000
6	-4.118026000	0.508926000	0.289261000
1	-2.368320000	1.725568000	0.373454000
6	-4.719312000	-0.786206000	0.438844000
1	-4.257636000	-2.885532000	0.884760000
1	-4.752156000	1.352277000	0.032513000
8	0.758389000	-2.535954000	1.539625000
8	-0.758418000	2.535877000	1.539600000
7	-1.528159000	-2.570389000	1.238350000
7	1.528140000	2.570328000	1.238382000
6	1.706134000	3.984246000	1.473842000
1	2.366641000	4.162076000	2.330303000
1	2.127340000	4.483257000	0.593106000
1	0.720505000	4.400032000	1.686887000
6	-1.706184000	-3.984285000	1.473920000
1	-2.366650000	-4.162038000	2.330429000
1	-2.127453000	-4.483341000	0.593240000
1	-0.720556000	-4.400086000	1.686938000
6	6.100823000	0.981090000	0.260960000
6	6.845368000	2.189017000	0.378733000
16	7.205206000	-0.342154000	-0.168288000
6	8.189529000	2.070104000	0.144764000
1	6.375660000	3.129793000	0.636864000
6	8.614308000	0.743548000	-0.178989000
1	8.884577000	2.900641000	0.197570000
6	-6.100825000	-0.981104000	0.260919000
6	-6.845388000	-2.189016000	0.378727000
16	-7.205190000	0.342147000	-0.168348000
6	-8.189549000	-2.070087000	0.144770000
1	-6.375692000	-3.129794000	0.636874000
6	-8.614310000	-0.743532000	-0.179008000
1	-8.884610000	-2.900613000	0.197603000

6	-9.885246000	-0.312563000	-0.461239000
16	-10.265587000	1.369094000	-0.846432000
16	-11.279571000	-1.406403000	-0.467651000
6	-12.003756000	1.128048000	-1.066745000
6	-12.481120000	-0.179208000	-0.888269000
6	-12.883733000	2.160049000	-1.400691000
6	-13.840778000	-0.459448000	-1.043175000
6	-14.240089000	1.875856000	-1.554378000
1	-12.513424000	3.170944000	-1.538260000
6	-14.715632000	0.573799000	-1.376644000
1	-14.209969000	-1.470678000	-0.904950000
1	-14.926838000	2.675070000	-1.813710000
1	-15.772602000	0.359654000	-1.497695000
6	9.885248000	0.312593000	-0.461226000
16	10.265610000	-1.369066000	-0.846387000
16	11.279555000	1.406455000	-0.467679000
6	12.003773000	-1.127997000	-1.066727000
6	12.481118000	0.179270000	-0.888285000
6	12.883763000	-2.159991000	-1.400662000
6	13.840770000	0.459529000	-1.043214000
6	14.240112000	-1.875779000	-1.554372000
1	12.513468000	-3.170895000	-1.538205000
6	14.715636000	-0.573711000	-1.376672000
1	14.209946000	1.470768000	-0.905015000
1	14.926870000	-2.674989000	-1.813695000
1	15.772602000	-0.359551000	-1.497741000

S10IIDT-CS E=-3880.511261 Hartree

6	-2.590865000	-1.543077000	0.728798000
6	-1.926265000	-0.265756000	0.596202000
6	-2.743511000	0.848646000	0.253210000
6	-4.093627000	0.685800000	0.078176000
6	-4.749624000	-0.582153000	0.226888000
6	-3.936362000	-1.716351000	0.560838000
6	-0.364857000	-1.924077000	1.067269000
6	-0.542334000	-0.463204000	0.789076000
1	-2.293244000	1.826469000	0.162626000
1	-4.691057000	1.555889000	-0.177534000
1	-4.378179000	-2.699474000	0.670825000
6	0.542340000	0.463388000	0.789018000
6	1.926270000	0.265894000	0.596196000
6	0.364879000	1.924301000	1.067015000
6	2.590878000	1.543236000	0.728551000

6	2.743505000	-0.848577000	0.253404000
6	3.936374000	1.716471000	0.560544000
6	4.093621000	-0.685772000	0.078331000
1	2.293228000	-1.826412000	0.162998000
6	4.749627000	0.582204000	0.226801000
1	4.378198000	2.699612000	0.670345000
1	4.691042000	-1.555912000	-0.177225000
8	-0.648293000	2.566947000	1.323656000
8	0.648316000	-2.566659000	1.324068000
7	1.637577000	2.502157000	1.022946000
7	-1.637558000	-2.501939000	1.023363000
6	-1.876130000	-3.906971000	1.257916000
1	-2.543380000	-4.056927000	2.114518000
1	-2.318792000	-4.386875000	0.377052000
1	-0.909168000	-4.364845000	1.470259000
6	1.876158000	3.907232000	1.257232000
1	2.543433000	4.057344000	2.113787000
1	2.318794000	4.386975000	0.376268000
1	0.909203000	4.365146000	1.469520000
6	-6.138911000	-0.717794000	0.049663000
6	-6.934806000	-1.891727000	0.166076000
16	-7.185719000	0.652609000	-0.376983000
6	-8.273492000	-1.713826000	-0.067005000
1	-6.506273000	-2.852455000	0.422368000
6	-8.639919000	-0.370763000	-0.388165000
1	-9.004000000	-2.513551000	-0.015094000
6	6.138913000	0.717804000	0.049540000
6	6.934816000	1.891753000	0.165732000
16	7.185708000	-0.652685000	-0.376862000
6	8.273499000	1.713800000	-0.067329000
1	6.506292000	2.852531000	0.421850000
6	8.639915000	0.370676000	-0.388244000
1	9.004013000	2.513530000	-0.015570000
6	9.891486000	-0.117863000	-0.669155000
16	10.208744000	-1.817134000	-1.052774000
16	11.344642000	0.901896000	-0.680108000
6	11.941559000	-1.620483000	-1.266200000
6	12.453068000	-0.394824000	-1.098115000
6	-9.891496000	0.117716000	-0.669153000
16	-10.208769000	1.816914000	-1.053083000
16	-11.344645000	-0.902055000	-0.679906000
6	-11.941584000	1.620213000	-1.266458000
6	-12.453084000	0.394581000	-1.098142000
1	-13.500349000	0.138437000	-1.199920000

1	-12.513814000	2.502549000	-1.524548000
1	12.513781000	-2.502870000	-1.524134000
1	13.500334000	-0.138705000	-1.199949000

S1IIDT-OS

E=-2504.321281 Hartree

6	2.645987000	1.429652000	0.403890000
6	1.972893000	0.172895000	0.299739000
6	2.767963000	-0.961519000	0.046793000
6	4.143105000	-0.835288000	-0.065826000
6	4.802023000	0.412679000	0.064877000
6	4.012424000	1.569199000	0.300524000
6	0.427975000	1.929358000	0.596945000
6	0.548753000	0.426711000	0.412417000
1	2.305875000	-1.932558000	-0.037144000
1	4.726518000	-1.731256000	-0.251592000
1	4.468017000	2.547648000	0.386681000
6	-0.548753000	-0.426705000	0.412431000
6	-1.972893000	-0.172890000	0.299757000
6	-0.427977000	-1.929345000	0.597018000
6	-2.645988000	-1.429645000	0.403937000
6	-2.767962000	0.961519000	0.046788000
6	-4.012425000	-1.569193000	0.300571000
6	-4.143105000	0.835287000	-0.065829000
1	-2.305873000	1.932555000	-0.037172000
6	-4.802023000	-0.412677000	0.064899000
1	-4.468019000	-2.547640000	0.386750000
1	-4.726517000	1.731250000	-0.251616000
8	0.566302000	-2.619963000	0.764934000
8	-0.566302000	2.619975000	0.764877000
7	-1.716396000	-2.441378000	0.598208000
7	1.716394000	2.441390000	0.598135000
6	2.010232000	3.849032000	0.773031000
1	2.639455000	4.008395000	1.654991000
1	2.518770000	4.254758000	-0.108217000
1	1.059539000	4.364191000	0.910360000
6	-2.010233000	-3.849021000	0.773101000
1	-2.639467000	-4.008385000	1.655052000
1	-2.518758000	-4.254749000	-0.108154000
1	-1.059541000	-4.364178000	0.910444000
6	6.234226000	0.518738000	-0.042300000
6	7.033851000	1.665147000	0.100487000
16	7.244784000	-0.882264000	-0.392927000
6	8.392439000	1.441279000	-0.061095000

1	6.623335000	2.641829000	0.323774000
6	8.706754000	0.090946000	-0.340581000
1	9.157713000	2.204155000	0.015340000
6	-6.234226000	-0.518739000	-0.042280000
6	-7.033852000	-1.665145000	0.100527000
16	-7.244783000	0.882257000	-0.392933000
6	-8.392439000	-1.441279000	-0.061061000
1	-6.623336000	-2.641823000	0.323830000
6	-8.706754000	-0.090951000	-0.340569000
1	-9.157714000	-2.204154000	0.015386000
6	-9.983339000	0.453015000	-0.555404000
6	9.983340000	-0.453023000	-0.555406000
6	-11.129480000	-0.385280000	-0.502340000
7	-12.053355000	-1.095509000	-0.453199000
6	-10.170151000	1.833093000	-0.828374000
7	-10.297617000	2.971196000	-1.051374000
6	10.170153000	-1.833106000	-0.828349000
7	10.297622000	-2.971219000	-1.051296000
6	11.129481000	0.385273000	-0.502351000
7	12.053355000	1.095503000	-0.453220000

S2IIDT-OS

E=-2669.295469 Hartree

6	-2.593592000	1.522331000	-0.624118000
6	-1.975817000	0.242736000	-0.527839000
6	-2.818497000	-0.856741000	-0.298109000
6	-4.193559000	-0.674523000	-0.199258000
6	-4.792598000	0.596491000	-0.319652000
6	-3.957129000	1.718666000	-0.529731000
6	-0.354629000	1.944681000	-0.781340000
6	-0.530832000	0.443342000	-0.622368000
1	-2.398959000	-1.847423000	-0.223344000
1	-4.820376000	-1.548099000	-0.051972000
1	-4.373284000	2.717504000	-0.582517000
6	0.530835000	-0.443302000	-0.622394000
6	1.975820000	-0.242708000	-0.527841000
6	0.354624000	-1.944636000	-0.781413000
6	2.593585000	-1.522310000	-0.624112000
6	2.818512000	0.856767000	-0.298142000
6	3.957118000	-1.718657000	-0.529712000
6	4.193572000	0.674536000	-0.199289000
1	2.398977000	1.847452000	-0.223395000
6	4.792598000	-0.596487000	-0.319650000
1	4.373264000	-2.717500000	-0.582480000

1	4.820399000	1.548109000	-0.052026000
8	-0.664477000	-2.605365000	-0.925311000
8	0.664470000	2.605434000	-0.925152000
7	1.622461000	-2.502385000	-0.790132000
7	-1.622474000	2.502415000	-0.790119000
6	-1.862582000	3.921624000	-0.943710000
1	-2.477796000	4.118928000	-1.828141000
1	-2.365484000	4.331752000	-0.061000000
1	-0.892270000	4.403630000	-1.063545000
6	1.862562000	-3.921588000	-0.943789000
1	2.477819000	-4.118849000	-1.828200000
1	2.365415000	-4.331771000	-0.061077000
1	0.892251000	-4.403577000	-1.063699000
6	-6.233311000	0.771449000	-0.230148000
6	-6.995068000	1.865777000	-0.623026000
16	-7.274391000	-0.470210000	0.438323000
6	-8.371360000	1.713978000	-0.404564000
1	-6.564172000	2.744580000	-1.087244000
6	-8.726505000	0.491048000	0.169704000
1	-9.096596000	2.471479000	-0.673851000
6	6.233308000	-0.771459000	-0.230133000
6	6.995056000	-1.865801000	-0.622988000
16	7.274396000	0.470195000	0.438337000
6	8.371349000	-1.714009000	-0.404526000
1	6.564155000	-2.744606000	-1.087198000
6	8.726503000	-0.491073000	0.169723000
1	9.096581000	-2.471517000	-0.673806000
6	-10.031304000	0.012900000	0.522300000
6	-10.231020000	-1.301553000	1.050871000
6	-11.184348000	0.847032000	0.355011000
6	-11.473775000	-1.757780000	1.388021000
1	-9.371540000	-1.953532000	1.181338000
6	-12.435249000	0.410761000	0.685479000
1	-11.058358000	1.850557000	-0.037841000
6	-12.662205000	-0.926082000	1.225882000
1	-11.623369000	-2.756102000	1.786413000
1	-13.307956000	1.043782000	0.560548000
6	10.031307000	-0.012928000	0.522307000
6	11.184339000	-0.847084000	0.355067000
6	10.231038000	1.301550000	1.050812000
6	12.435244000	-0.410816000	0.685524000
1	11.058337000	-1.850626000	-0.037737000
6	11.473798000	1.757775000	1.387949000
1	9.371567000	1.953551000	1.181231000

6	12.662213000	0.926044000	1.225879000
1	13.307943000	-1.043855000	0.560628000
1	11.623404000	2.756118000	1.786285000
8	-13.800770000	-1.332676000	1.530115000
8	13.800786000	1.332647000	1.530070000

S3IIDT-OS

E=-3640.036105 Hartree

6	-2.589690000	-1.528671000	0.230878000
6	-1.977059000	-0.246146000	0.142595000
6	-2.823890000	0.854203000	-0.062812000
6	-4.199829000	0.669552000	-0.150700000
6	-4.792474000	-0.604052000	-0.037653000
6	-3.954827000	-1.726433000	0.155630000
6	-0.350703000	-1.947396000	0.381745000
6	-0.529415000	-0.443967000	0.230453000
1	-2.406861000	1.845413000	-0.141771000
1	-4.826131000	1.537349000	-0.331016000
1	-4.373355000	-2.719469000	0.266301000
6	0.529421000	0.443998000	0.230469000
6	1.977062000	0.246176000	0.142582000
6	0.350709000	1.947441000	0.381658000
6	2.589703000	1.528692000	0.230928000
6	2.823882000	-0.854163000	-0.062919000
6	3.954840000	1.726447000	0.155703000
6	4.199823000	-0.669515000	-0.150818000
1	2.406864000	-1.845367000	-0.141976000
6	4.792478000	0.604075000	-0.037667000
1	4.373380000	2.719471000	0.266443000
1	4.826116000	-1.537301000	-0.331216000
8	-0.669803000	2.606729000	0.516076000
8	0.669800000	-2.606644000	0.516385000
7	1.617177000	2.506889000	0.393212000
7	-1.617163000	-2.506875000	0.393104000
6	-1.854837000	-3.927780000	0.542877000
1	-2.459081000	-4.129468000	1.433646000
1	-2.367514000	-4.332723000	-0.336351000
1	-0.883224000	-4.410117000	0.648973000
6	1.854848000	3.927834000	0.542638000
1	2.458970000	4.129757000	1.433435000
1	2.367654000	4.332526000	-0.336631000
1	0.883227000	4.410211000	0.648472000
6	-6.234620000	-0.782334000	-0.122201000
6	-6.946436000	-1.948785000	-0.373060000

16	-7.337793000	0.561342000	0.102651000
6	-8.338669000	-1.775587000	-0.397617000
1	-6.465577000	-2.899831000	-0.565468000
6	-8.742861000	-0.463321000	-0.162016000
1	-9.040110000	-2.578373000	-0.594357000
6	6.234625000	0.782351000	-0.122201000
6	6.946451000	1.948807000	-0.373014000
16	7.337785000	-0.561340000	0.102616000
6	8.338682000	1.775596000	-0.397571000
1	6.465600000	2.899861000	-0.565392000
6	8.742862000	0.463318000	-0.162024000
1	9.040132000	2.578382000	-0.594284000
6	-10.065016000	0.059673000	-0.116796000
6	-10.469610000	1.393941000	0.083075000
16	-11.495326000	-0.932470000	-0.314160000
1	-9.769561000	2.210327000	0.230061000
6	-12.490223000	0.530383000	-0.112991000
6	10.065012000	-0.059694000	-0.116830000
6	10.469590000	-1.393982000	0.082945000
16	11.495334000	0.932447000	-0.314112000
1	9.769531000	-2.210371000	0.229864000
6	12.490213000	-0.530429000	-0.113028000
6	13.893319000	-0.496273000	-0.160594000
6	-13.893327000	0.496219000	-0.160592000
6	14.652599000	-1.684571000	0.005727000
7	15.303924000	-2.642220000	0.138442000
6	14.583606000	0.724630000	-0.375462000
7	15.124327000	1.743059000	-0.553709000
6	-14.583598000	-0.724671000	-0.375581000
7	-15.124306000	-1.743088000	-0.553932000
6	-14.652619000	1.684504000	0.005764000
7	-15.303955000	2.642138000	0.138530000
7	-11.775533000	1.647988000	0.085136000
7	11.775510000	-1.648040000	0.085009000

S4IIDT-OS

E=-3572.083784 Hartree

6	-2.549293000	1.596867000	-0.630174000
6	-1.959281000	0.300245000	-0.530215000
6	-2.828384000	-0.778378000	-0.278892000
6	-4.192805000	-0.561673000	-0.162318000
6	-4.769089000	0.726232000	-0.287448000
6	-3.903488000	1.826587000	-0.522360000
6	-0.302136000	1.951372000	-0.825438000

6	-0.520293000	0.461010000	-0.643600000
1	-2.431653000	-1.778370000	-0.199741000
1	-4.834837000	-1.417571000	0.018377000
1	-4.292396000	2.834372000	-0.599576000
6	0.520297000	-0.461020000	-0.643606000
6	1.959282000	-0.300256000	-0.530178000
6	0.302148000	-1.951376000	-0.825510000
6	2.549300000	-1.596872000	-0.630185000
6	2.828375000	0.778358000	-0.278785000
6	3.903494000	-1.826592000	-0.522352000
6	4.192794000	0.561652000	-0.162189000
1	2.431639000	1.778345000	-0.199596000
6	4.769086000	-0.726245000	-0.287368000
1	4.292407000	-2.834372000	-0.599607000
1	4.834819000	1.417543000	0.018561000
8	-0.734162000	-2.578902000	-0.994929000
8	0.734183000	2.578905000	-0.994783000
7	1.554547000	-2.546778000	-0.822936000
7	-1.554532000	2.546780000	-0.822855000
6	-1.755455000	3.969702000	-0.994272000
1	-2.374934000	4.172975000	-1.874473000
1	-2.235474000	4.407194000	-0.111859000
1	-0.772865000	4.421222000	-1.132221000
6	1.755479000	-3.969690000	-0.994426000
1	2.374974000	-4.172913000	-1.874627000
1	2.235484000	-4.407227000	-0.112028000
1	0.772893000	-4.421208000	-1.132416000
6	-6.193834000	0.927266000	-0.175495000
6	-6.910187000	2.119445000	-0.358963000
16	-7.287304000	-0.392532000	0.233147000
6	-8.280071000	1.990630000	-0.183751000
1	-6.438673000	3.057231000	-0.625246000
6	-8.691257000	0.678030000	0.148416000
1	-8.984377000	2.807530000	-0.291355000
6	6.193829000	-0.927280000	-0.175392000
6	6.910189000	-2.119448000	-0.358898000
16	7.287283000	0.392498000	0.233359000
6	8.280071000	-1.990633000	-0.183669000
1	6.438683000	-3.057224000	-0.625230000
6	8.691248000	-0.678042000	0.148548000
1	8.984383000	-2.807523000	-0.291308000
6	-9.988574000	0.237816000	0.385557000
6	-10.332646000	-1.141207000	0.722041000
16	-11.420228000	1.263474000	0.318555000

6	-12.493846000	-0.146390000	0.739280000
6	9.988562000	-0.237827000	0.385698000
6	10.332623000	1.141181000	0.722253000
16	11.420224000	-1.263470000	0.318647000
6	12.493851000	0.146423000	0.739253000
7	-11.718924000	-1.276031000	0.900310000
7	11.718920000	1.276049000	0.900339000
6	-12.336547000	-2.552690000	1.243685000
1	-13.049023000	-2.846041000	0.469493000
1	-11.535000000	-3.286967000	1.316661000
1	-12.863085000	-2.471342000	2.197203000
6	12.336554000	2.552740000	1.243577000
1	13.048925000	2.846076000	0.469282000
1	11.534997000	3.286999000	1.316625000
1	12.863215000	2.471446000	2.197032000
8	-13.693828000	-0.075413000	0.853458000
8	-9.542197000	-2.070948000	0.839303000
8	9.542182000	2.070941000	0.839416000
8	13.693852000	0.075487000	0.853257000

S5IIDT-OS

E=-3115.008962 Hartree

6	-2.557915000	1.580694000	-0.709614000
6	-1.960324000	0.287548000	-0.602664000
6	-2.819945000	-0.797076000	-0.344595000
6	-4.185778000	-0.590103000	-0.230048000
6	-4.769946000	0.693765000	-0.364500000
6	-3.914177000	1.800136000	-0.604870000
6	-0.313964000	1.950923000	-0.901060000
6	-0.522455000	0.457526000	-0.715360000
1	-2.415637000	-1.793462000	-0.259609000
1	-4.822326000	-1.449201000	-0.046776000
1	-4.311602000	2.804302000	-0.684274000
6	0.522456000	-0.457475000	-0.715376000
6	1.960325000	-0.287507000	-0.602670000
6	0.313955000	-1.950870000	-0.901091000
6	2.557905000	-1.580659000	-0.709612000
6	2.819957000	0.797114000	-0.344624000
6	3.914165000	-1.800113000	-0.604861000
6	4.185789000	0.590129000	-0.230074000
1	2.415655000	1.793503000	-0.259655000
6	4.769944000	-0.693746000	-0.364502000
1	4.311583000	-2.804283000	-0.684250000
1	4.822345000	1.449225000	-0.046818000

8	-0.719103000	-2.582014000	-1.069324000
8	0.719094000	2.582084000	-1.069246000
7	1.570197000	-2.536651000	-0.904323000
7	-1.570212000	2.536693000	-0.904313000
6	-1.781726000	3.958532000	-1.081058000
1	-2.400510000	4.153065000	-1.963407000
1	-2.266473000	4.394342000	-0.200703000
1	-0.802656000	4.417489000	-1.218561000
6	1.781704000	-3.958489000	-1.081085000
1	2.400515000	-4.153012000	-1.963417000
1	2.266417000	-4.394320000	-0.200722000
1	0.802634000	-4.417434000	-1.218627000
6	-6.196976000	0.883942000	-0.255465000
6	-6.922971000	2.061990000	-0.485053000
16	-7.275372000	-0.426348000	0.209313000
6	-8.289660000	1.919549000	-0.299711000
1	-6.466407000	2.993950000	-0.794136000
6	-8.686686000	0.618141000	0.086921000
1	-8.991792000	2.731077000	-0.443591000
6	6.196972000	-0.883936000	-0.255463000
6	6.922957000	-2.061991000	-0.485046000
16	7.275378000	0.426346000	0.209316000
6	8.289648000	-1.919560000	-0.299705000
1	6.466386000	-2.993947000	-0.794129000
6	8.686684000	-0.618155000	0.086925000
1	8.991773000	-2.731095000	-0.443582000
6	10.005308000	-0.178991000	0.349050000
6	11.120669000	-1.042653000	0.249539000
6	10.236511000	1.225955000	0.739961000
6	12.398469000	-0.606431000	0.503529000
1	10.978660000	-2.079263000	-0.033607000
6	12.678062000	0.788107000	0.894523000
6	-10.005307000	0.178967000	0.349046000
6	-11.120674000	1.042623000	0.249545000
6	-10.236499000	-1.225982000	0.739952000
6	-12.398470000	0.606391000	0.503536000
1	-10.978671000	2.079237000	-0.033589000
6	-12.678054000	-0.788153000	0.894517000
6	13.507756000	-1.493039000	0.397187000
7	14.385152000	-2.252065000	0.298264000
6	-13.507762000	1.492994000	0.397211000
7	-14.385163000	2.252017000	0.298302000
8	9.316777000	2.036783000	0.850977000
8	-9.316757000	-2.036798000	0.850987000

8	-13.805199000	-1.199663000	1.124911000
8	13.805213000	1.199613000	1.124902000
7	11.548786000	1.622139000	0.985989000
7	-11.548773000	-1.622182000	0.985961000
6	-11.747110000	-3.025010000	1.371525000
1	-11.375813000	-3.680642000	0.581471000
1	-11.190239000	-3.238471000	2.285987000
1	-12.812359000	-3.175336000	1.526505000
6	11.747133000	3.024964000	1.371562000
1	11.376081000	3.680612000	0.581404000
1	11.190051000	3.238479000	2.285881000
1	12.812356000	3.175218000	1.526787000

S6IIDT-OS E=-3837.652402 Hartree

6	-2.530468000	-1.625639000	0.740258000
6	-1.946866000	-0.322066000	0.630529000
6	-2.819764000	0.751949000	0.353807000
6	-4.177540000	0.526385000	0.224524000
6	-4.750481000	-0.768326000	0.360712000
6	-3.879783000	-1.863389000	0.620856000
6	-0.283982000	-1.953812000	0.966417000
6	-0.516801000	-0.468805000	0.760648000
1	-2.426329000	1.752758000	0.266578000
1	-4.823394000	1.373106000	0.018538000
1	-4.266548000	-2.870300000	0.714228000
6	0.516805000	0.468797000	0.760681000
6	1.946872000	0.322058000	0.630597000
6	0.283991000	1.953794000	0.966538000
6	2.530471000	1.625636000	0.740288000
6	2.819772000	-0.751959000	0.353888000
6	3.879782000	1.863390000	0.620857000
6	4.177546000	-0.526394000	0.224592000
1	2.426335000	-1.752769000	0.266671000
6	4.750483000	0.768322000	0.360742000
1	4.266543000	2.870306000	0.714190000
1	4.823401000	-1.373117000	0.018616000
8	-0.758509000	2.563116000	1.156803000
8	0.758497000	-2.563110000	1.156872000
7	1.530574000	2.562525000	0.958297000
7	-1.530576000	-2.562523000	0.958302000
6	-1.720179000	-3.985605000	1.148925000
1	-2.346128000	-4.180975000	2.026015000
1	-2.186821000	-4.439623000	0.268004000

1	-0.735049000	-4.425966000	1.303330000
6	1.720166000	3.985624000	1.148801000
1	2.346160000	4.181067000	2.025842000
1	2.186753000	4.439586000	0.267822000
1	0.735038000	4.425982000	1.303231000
6	-6.164164000	-0.974187000	0.234110000
6	-6.869885000	-2.187910000	0.360037000
16	-7.272948000	0.351545000	-0.119184000
6	-8.232156000	-2.069305000	0.183219000
1	-6.390636000	-3.134015000	0.579522000
6	-8.665460000	-0.737377000	-0.094215000
1	-8.943055000	-2.879216000	0.240758000
6	6.164163000	0.974186000	0.234120000
6	6.869881000	2.187917000	0.360003000
16	7.272949000	-0.351551000	-0.119151000
6	8.232150000	2.069312000	0.183177000
1	6.390629000	3.134026000	0.579464000
6	8.665458000	0.737377000	-0.094220000
1	8.943046000	2.879227000	0.240686000
6	9.977687000	0.294570000	-0.321196000
6	11.105938000	1.226435000	-0.294643000
6	10.209067000	-1.118630000	-0.586821000
6	12.629073000	-0.676639000	-0.789335000
6	-9.977688000	-0.294570000	-0.321195000
6	-11.105945000	-1.226427000	-0.294607000
6	-10.209062000	1.118623000	-0.586862000
6	-12.629071000	0.676641000	-0.789349000
8	9.292078000	-1.940670000	-0.621676000
8	-9.292066000	1.940655000	-0.621760000
7	11.535876000	-1.526434000	-0.806372000
7	-11.535869000	1.526428000	-0.806421000
6	-11.753726000	2.957854000	-1.071300000
1	-12.420089000	3.375621000	-0.315533000
1	-10.781483000	3.441216000	-1.039414000
1	-12.218836000	3.085645000	-2.049649000
6	11.753741000	-2.957868000	-1.071202000
1	12.420110000	-3.375605000	-0.315424000
1	10.781501000	-3.441235000	-1.039294000
1	12.218847000	-3.085689000	-2.049549000
7	12.381445000	0.661504000	-0.536660000
7	-12.381451000	-0.661495000	-0.536633000
6	13.523523000	1.590444000	-0.512745000
1	14.232695000	1.283556000	0.257185000
1	14.033431000	1.572993000	-1.476888000

1	13.128006000	2.579525000	-0.302145000
6	-13.523534000	-1.590428000	-0.512681000
1	-14.232699000	-1.283511000	0.257243000
1	-14.033449000	-1.573003000	-1.476822000
1	-13.128022000	-2.579505000	-0.302054000
8	-11.007845000	-2.431559000	-0.080892000
8	11.007830000	2.431573000	-0.080968000
16	14.178890000	-1.246716000	-1.062991000
16	-14.178886000	1.246719000	-1.063018000

S7IIDT-OS

E=-3345.513124 Hartree

6	-2.515814000	1.648193000	-1.067348000
6	-1.952378000	0.338842000	-0.962805000
6	-2.840538000	-0.724136000	-0.709365000
6	-4.200170000	-0.481709000	-0.591801000
6	-4.747974000	0.818630000	-0.719516000
6	-3.865347000	1.903716000	-0.959584000
6	-0.263251000	1.958894000	-1.258475000
6	-0.510746000	0.471189000	-1.075740000
1	-2.463315000	-1.731853000	-0.634623000
1	-4.862909000	-1.325146000	-0.428625000
1	-4.238126000	2.918345000	-1.025624000
6	0.510743000	-0.470987000	-1.075814000
6	1.952375000	-0.338663000	-0.962838000
6	0.263246000	-1.958661000	-1.258801000
6	2.515809000	-1.647996000	-1.067615000
6	2.840535000	0.724267000	-0.709198000
6	3.865341000	-1.903541000	-0.959889000
6	4.200166000	0.481815000	-0.591669000
1	2.463314000	1.731971000	-0.634278000
6	4.747969000	-0.818501000	-0.719618000
1	4.238117000	-2.918159000	-1.026114000
1	4.862905000	1.325221000	-0.428335000
8	-0.785634000	-2.563224000	-1.425722000
8	0.785631000	2.563494000	-1.425249000
7	1.503619000	-2.577700000	-1.259668000
7	-1.503624000	2.577934000	-1.259222000
6	-1.677628000	4.005086000	-1.434675000
1	-2.292254000	4.216343000	-2.316036000
1	-2.149661000	4.452904000	-0.553443000
1	-0.686901000	4.437995000	-1.573158000
6	1.677623000	-4.004819000	-1.435393000
1	2.292248000	-4.215909000	-2.316794000

1	2.149656000	-4.452804000	-0.554246000
1	0.686895000	-4.437701000	-1.573956000
6	-6.165515000	1.052306000	-0.601833000
6	-6.881575000	2.214743000	-0.932027000
16	-7.256713000	-0.177239000	0.003538000
6	-8.244746000	2.126654000	-0.706948000
1	-6.408912000	3.092925000	-1.354017000
6	-8.663449000	0.868929000	-0.194332000
1	-8.959195000	2.916064000	-0.891188000
6	6.165509000	-1.052201000	-0.601968000
6	6.881567000	-2.214583000	-0.932360000
16	7.256706000	0.177236000	0.003621000
6	8.244738000	-2.126535000	-0.707260000
1	6.408904000	-3.092691000	-1.354501000
6	8.663442000	-0.868899000	-0.194429000
1	8.959185000	-2.915916000	-0.891632000
6	9.964501000	-0.560080000	0.234624000
6	10.943391000	-1.655046000	0.553885000
6	10.559631000	0.689300000	0.663242000
6	12.000384000	-1.024351000	1.379168000
6	11.752351000	0.355565000	1.492865000
6	13.082472000	-1.640739000	1.991331000
6	12.610701000	1.141766000	2.265531000
6	13.938102000	-0.850385000	2.762519000
1	13.239655000	-2.707118000	1.865497000
6	13.694627000	0.520757000	2.897844000
1	12.456426000	2.204453000	2.393576000
1	14.791851000	-1.298046000	3.261647000
1	14.361062000	1.123991000	3.506715000
6	-9.964509000	0.560033000	0.234664000
6	-10.943408000	1.654938000	0.554107000
6	-10.559634000	-0.689423000	0.663065000
6	-12.000384000	1.024100000	1.379303000
6	-11.752349000	-0.355836000	1.492756000
6	-13.082462000	1.640382000	1.991591000
6	-12.610688000	-1.142171000	2.265295000
6	-13.938081000	0.849893000	2.762653000
1	-13.239648000	2.706783000	1.865945000
6	-13.694605000	-0.521273000	2.897733000
1	-12.456410000	-2.204881000	2.393154000
1	-14.791823000	1.297466000	3.261871000
1	-14.361031000	-1.124614000	3.506508000
8	-10.884206000	2.835987000	0.244322000
8	10.884203000	-2.836034000	0.243864000

6	-10.220575000	-1.974776000	0.257628000
6	10.220577000	1.974725000	0.258026000
6	-9.353573000	-2.264643000	-0.838324000
7	-8.700860000	-2.559560000	-1.757478000
6	-10.830008000	-3.143542000	0.807929000
7	-11.291697000	-4.118781000	1.248347000
6	10.830020000	3.143392000	0.808525000
7	11.291715000	4.118555000	1.249107000
6	9.353580000	2.264785000	-0.837878000
7	8.700873000	2.559869000	-1.756983000

S8IIDT-OS

E=-4215.952936 Hartree

6	2.562460000	-1.573121000	-1.110109000
6	1.965590000	-0.280680000	-1.004255000
6	2.824075000	0.806184000	-0.760372000
6	4.192870000	0.601866000	-0.653939000
6	4.771692000	-0.681652000	-0.783677000
6	3.920791000	-1.791156000	-1.012926000
6	0.318607000	-1.951734000	-1.279946000
6	0.522834000	-0.454544000	-1.107032000
1	2.419842000	1.803078000	-0.684135000
1	4.834361000	1.463874000	-0.503126000
1	4.322556000	-2.795128000	-1.073617000
6	-0.522933000	0.455022000	-1.106815000
6	-1.965679000	0.281109000	-1.003997000
6	-0.318729000	1.952281000	-1.279163000
6	-2.562565000	1.573588000	-1.109283000
6	-2.824137000	-0.805859000	-0.760478000
6	-3.920891000	1.791575000	-1.011900000
6	-4.192925000	-0.601593000	-0.653849000
1	-2.419890000	-1.802781000	-0.684673000
6	-4.771765000	0.681973000	-0.783025000
1	-4.322667000	2.795569000	-1.072153000
1	-4.834398000	-1.463665000	-0.503330000
8	0.712816000	2.588888000	-1.432042000
8	-0.712953000	-2.588270000	-1.433019000
7	-1.576308000	2.533416000	-1.288419000
7	1.576182000	-2.532872000	-1.289550000
6	1.791478000	-3.955694000	-1.458128000
1	2.404744000	-4.153260000	-2.343486000
1	2.284149000	-4.383199000	-0.578249000
1	0.813248000	-4.419129000	-1.585616000
6	-1.791625000	3.956306000	-1.456398000

1	-2.404970000	4.154230000	-2.341621000
1	-2.284220000	4.383451000	-0.576301000
1	-0.813409000	4.419798000	-1.583783000
6	6.200752000	-0.878701000	-0.679725000
6	6.949386000	-1.989754000	-1.088924000
16	7.245513000	0.338403000	0.017220000
6	8.311975000	-1.869529000	-0.854769000
1	6.505920000	-2.846676000	-1.579973000
6	8.682399000	-0.642393000	-0.256338000
1	9.044630000	-2.615488000	-1.136659000
6	-6.200817000	0.878972000	-0.678875000
6	-6.949495000	1.990175000	-1.087586000
16	-7.245509000	-0.338406000	0.017696000
6	-8.312063000	1.869852000	-0.853357000
1	-6.506078000	2.847286000	-1.578350000
6	-8.682424000	0.642487000	-0.255357000
1	-9.044748000	2.615912000	-1.134899000
6	-9.972660000	0.321082000	0.199498000
6	-10.603792000	-0.892758000	0.590295000
6	-12.182620000	0.706506000	1.493765000
6	-11.804263000	-0.643881000	1.442715000
6	-13.289835000	1.173647000	2.183919000
6	-12.591526000	-1.560022000	2.155587000
6	-14.062195000	0.243228000	2.881423000
1	-13.538017000	2.229706000	2.184184000
6	-13.704786000	-1.107014000	2.866383000
1	-12.349783000	-2.612755000	2.175571000
1	-14.933778000	0.571283000	3.438378000
1	-14.300969000	-1.826754000	3.418164000
6	9.972679000	-0.321172000	0.198522000
6	10.603856000	0.892511000	0.589730000
6	12.182734000	-0.707115000	1.492471000
6	11.804385000	0.643295000	1.441970000
6	13.289992000	-1.174533000	2.182368000
6	12.591706000	1.559154000	2.155143000
6	14.062408000	-0.244391000	2.880179000
1	13.538164000	-2.230594000	2.182208000
6	13.705010000	1.105860000	2.865687000
1	12.349973000	2.611881000	2.175552000
1	14.934027000	-0.572670000	3.436947000
1	14.301237000	1.825381000	3.417706000
6	10.228021000	2.162267000	0.119066000
6	-10.227971000	-2.162332000	0.119129000
6	9.376863000	2.353466000	-1.007252000

7	8.724918000	2.567143000	-1.949966000
6	10.752581000	3.387378000	0.621069000
7	11.135777000	4.418043000	1.010392000
6	-10.752471000	-3.387637000	0.620718000
7	-11.135631000	-4.418447000	1.009691000
6	-9.376890000	-2.353097000	-1.007321000
7	-8.724997000	-2.566406000	-1.950154000
16	11.052646000	-1.735406000	0.581891000
16	-11.052606000	1.735159000	0.583503000
8	11.662674000	-2.265860000	-0.648214000
8	10.370491000	-2.669602000	1.489056000
8	-10.370387000	2.669004000	1.490980000
8	-11.662731000	2.266091000	-0.646349000

S9IIDT-OS

E=-4187.833894 Hartree

6	2.531162000	1.631879000	0.689724000
6	1.949673000	0.328488000	0.589608000
6	2.832342000	-0.740154000	0.328682000
6	4.190983000	-0.508185000	0.201365000
6	4.759374000	0.786746000	0.323728000
6	3.879861000	1.877255000	0.570576000
6	0.279681000	1.949976000	0.910636000
6	0.517000000	0.471151000	0.716073000
1	2.444889000	-1.744397000	0.251507000
1	4.840644000	-1.356316000	0.008156000
1	4.258841000	2.888595000	0.655159000
6	-0.517001000	-0.471127000	0.716087000
6	-1.949675000	-0.328468000	0.589626000
6	-0.279681000	-1.949947000	0.910689000
6	-2.531161000	-1.631859000	0.689755000
6	-2.832346000	0.740168000	0.328685000
6	-3.879859000	-1.877240000	0.570604000
6	-4.190987000	0.508195000	0.201368000
1	-2.444895000	1.744411000	0.251495000
6	-4.759375000	-0.786736000	0.323745000
1	-4.258836000	-2.888581000	0.655195000
1	-4.840649000	1.356322000	0.008147000
8	0.762810000	-2.567215000	1.095497000
8	-0.762805000	2.567245000	1.095472000
7	-1.525631000	-2.566178000	0.897776000
7	1.525634000	2.566201000	0.897737000
6	1.705776000	3.989191000	1.075768000
1	2.330363000	4.199226000	1.951333000

1	2.171169000	4.441501000	0.192408000
1	0.716749000	4.423258000	1.225372000
6	-1.705769000	-3.989168000	1.075806000
1	-2.330364000	-4.199204000	1.951365000
1	-2.171150000	-4.441481000	0.192442000
1	-0.716741000	-4.423230000	1.225421000
6	6.172288000	1.004201000	0.200763000
6	6.888728000	2.206531000	0.312080000
16	7.295316000	-0.322355000	-0.134928000
6	8.259325000	2.090864000	0.141067000
1	6.404387000	3.152942000	0.519477000
6	8.695418000	0.766511000	-0.117378000
1	8.945213000	2.928223000	0.199154000
6	-6.172288000	-1.004195000	0.200779000
6	-6.888725000	-2.206526000	0.312109000
16	-7.295318000	0.322353000	-0.134931000
6	-8.259321000	-2.090865000	0.141091000
1	-6.404382000	-3.152934000	0.519518000
6	-8.695417000	-0.766516000	-0.117369000
1	-8.945208000	-2.928224000	0.199187000
6	-9.988340000	-0.319981000	-0.330906000
16	-10.384388000	1.372735000	-0.640989000
16	-11.376197000	-1.419121000	-0.312224000
6	-12.130507000	1.133203000	-0.789524000
6	-12.597248000	-0.181202000	-0.634591000
6	-13.026841000	2.173133000	-1.047165000
6	-13.962369000	-0.459568000	-0.736948000
6	-14.388354000	1.890454000	-1.148527000
1	-12.664723000	3.189321000	-1.166555000
6	-14.853333000	0.581562000	-0.994285000
1	-14.323256000	-1.476143000	-0.616970000
1	-15.087424000	2.696056000	-1.348535000
1	-15.914426000	0.368387000	-1.074272000
6	9.988340000	0.319971000	-0.330907000
16	10.384384000	-1.372750000	-0.640970000
16	11.376199000	1.419108000	-0.312236000
6	12.130505000	-1.133223000	-0.789505000
6	12.597248000	0.181182000	-0.634586000
6	13.026836000	-2.173158000	-1.047132000
6	13.962370000	0.459544000	-0.736944000
6	14.388350000	-1.890484000	-1.148496000
1	12.664717000	-3.189347000	-1.166511000
6	14.853332000	-0.581591000	-0.994268000
1	14.323260000	1.476120000	-0.616978000

1	15.087418000	-2.696089000	-1.348493000
1	15.914425000	-0.368420000	-1.074256000

S10IIDT-OS E=-3880.516605 Hartree

6	-2.599668000	-1.520568000	0.533407000
6	-1.962613000	-0.243587000	0.434038000
6	-2.798715000	0.862034000	0.174741000
6	-4.166367000	0.688780000	0.048071000
6	-4.789795000	-0.580360000	0.169541000
6	-3.957855000	-1.707676000	0.414836000
6	-0.363846000	-1.935986000	0.752824000
6	-0.536892000	-0.448143000	0.559594000
1	-2.368592000	1.848791000	0.098135000
1	-4.778965000	1.564356000	-0.143928000
1	-4.379911000	-2.701889000	0.498793000
6	0.536900000	0.448221000	0.559535000
6	1.962617000	0.243656000	0.433988000
6	0.363844000	1.936103000	0.752501000
6	2.599662000	1.520666000	0.533068000
6	2.798728000	-0.862021000	0.174953000
6	3.957846000	1.707756000	0.414447000
6	4.166377000	-0.688784000	0.048238000
1	2.368599000	-1.848793000	0.098566000
6	4.789794000	0.580389000	0.169409000
1	4.379896000	2.701992000	0.498166000
1	4.778983000	-1.564401000	-0.143553000
8	-0.650914000	2.598437000	0.936195000
8	0.650912000	-2.598303000	0.936604000
7	1.635266000	2.497838000	0.739503000
7	-1.635279000	-2.497704000	0.740044000
6	-1.876689000	-3.911662000	0.916929000
1	-2.509473000	-4.095327000	1.792560000
1	-2.361593000	-4.342704000	0.033407000
1	-0.907266000	-4.388170000	1.065743000
6	1.876676000	3.911820000	0.916199000
1	2.509500000	4.095596000	1.791779000
1	2.361536000	4.342757000	0.032602000
1	0.907257000	4.388342000	1.065000000
6	-6.211316000	-0.737103000	0.047288000
6	-6.979015000	-1.906391000	0.157600000
16	-7.276638000	0.637149000	-0.286541000
6	-8.344379000	-1.730748000	-0.012766000
1	-6.536411000	-2.873332000	0.363678000

6	-8.721943000	-0.389673000	-0.269413000
1	-9.065962000	-2.537714000	0.044628000
6	6.211313000	0.737116000	0.047114000
6	6.979003000	1.906435000	0.157162000
16	7.276644000	-0.637203000	-0.286409000
6	8.344368000	1.730763000	-0.013167000
1	6.536393000	2.873419000	0.363025000
6	8.721942000	0.389634000	-0.269514000
1	9.065945000	2.537747000	0.044046000
6	9.994993000	-0.115253000	-0.482376000
16	10.327921000	-1.825442000	-0.791598000
16	11.441248000	0.911057000	-0.466552000
6	12.067723000	-1.629068000	-0.937115000
6	12.568928000	-0.396033000	-0.790550000
6	-9.994991000	0.115176000	-0.482383000
16	-10.327907000	1.825297000	-0.791995000
16	-11.441255000	-0.911119000	-0.466317000
6	-12.067711000	1.628905000	-0.937457000
6	-12.568926000	0.395907000	-0.790608000
1	-13.619390000	0.141082000	-0.856681000
1	-12.653214000	2.517127000	-1.139616000
1	12.653232000	-2.517332000	-1.139073000
1	13.619389000	-0.141214000	-0.856686000

S1IIDT-T1

E= -2504.318994 Hartree

6	2.658193000	1.405474000	0.425597000
6	1.986307000	0.153446000	0.328286000
6	2.777580000	-0.983183000	0.102608000
6	4.160071000	-0.863108000	0.009059000
6	4.814448000	0.380793000	0.132308000
6	4.029478000	1.540683000	0.338715000
6	0.440286000	1.928668000	0.573806000
6	0.548556000	0.418803000	0.418470000
1	2.314542000	-1.953923000	0.025007000
1	4.745268000	-1.765025000	-0.138530000
1	4.487943000	2.520171000	0.397105000
6	-0.548555000	-0.418800000	0.418480000
6	-1.986305000	-0.153444000	0.328282000
6	-0.440288000	-1.928661000	0.573858000
6	-2.658194000	-1.405466000	0.425643000
6	-2.777575000	0.983179000	0.102562000
6	-4.029480000	-1.540674000	0.338771000
6	-4.160066000	0.863104000	0.009021000

1	-2.314535000	1.953915000	0.024925000
6	-4.814446000	-0.380790000	0.132319000
1	-4.487947000	-2.520159000	0.397202000
1	-4.745262000	1.765017000	-0.138603000
8	0.548918000	-2.632847000	0.711724000
8	-0.548924000	2.632860000	0.711613000
7	-1.731562000	-2.427751000	0.587254000
7	1.731559000	2.427763000	0.587167000
6	2.035298000	3.835973000	0.739602000
1	2.654165000	4.005943000	1.626891000
1	2.559846000	4.220158000	-0.141900000
1	1.087661000	4.362111000	0.853943000
6	-2.035306000	-3.835952000	0.739768000
1	-2.654161000	-4.005872000	1.627075000
1	-2.559868000	-4.220181000	-0.141707000
1	-1.087670000	-4.362087000	0.854123000
6	6.258892000	0.487113000	0.047851000
6	7.066446000	1.575219000	0.394677000
16	7.245790000	-0.841174000	-0.546134000
6	8.428708000	1.361257000	0.202589000
1	6.665875000	2.494880000	0.802709000
6	8.722753000	0.081420000	-0.309501000
1	9.204403000	2.084075000	0.424871000
6	-6.258891000	-0.487109000	0.047870000
6	-7.066447000	-1.575201000	0.394737000
16	-7.245788000	0.841159000	-0.546159000
6	-8.428709000	-1.361243000	0.202645000
1	-6.665878000	-2.494849000	0.802800000
6	-8.722753000	-0.081424000	-0.309490000
1	-9.204405000	-2.084051000	0.424954000
6	-9.995330000	0.441401000	-0.613953000
6	9.995332000	-0.441412000	-0.613949000
6	-11.154145000	-0.354619000	-0.414396000
7	-12.089564000	-1.029772000	-0.240663000
6	-10.160815000	1.755403000	-1.120971000
7	-10.271780000	2.839998000	-1.537314000
6	10.160818000	-1.755432000	-1.120919000
7	10.271785000	-2.840044000	-1.537219000
6	11.154145000	0.354617000	-0.414421000
7	12.089563000	1.029778000	-0.240713000

S2IIDT-T1

E=-2669.294862 Hartree

6	-2.598492000	1.513527000	-0.631880000
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6	-1.979625000	0.235711000	-0.537785000
6	-2.820119000	-0.865593000	-0.316034000
6	-4.197331000	-0.686568000	-0.223047000
6	-4.796466000	0.582956000	-0.340685000
6	-3.963571000	1.707205000	-0.541889000
6	-0.359978000	1.944280000	-0.778209000
6	-0.531370000	0.440682000	-0.626616000
1	-2.399065000	-1.855619000	-0.242454000
1	-4.823815000	-1.561752000	-0.084190000
1	-4.382559000	2.705182000	-0.590188000
6	0.531373000	-0.440674000	-0.626642000
6	1.979629000	-0.235704000	-0.537828000
6	0.359982000	-1.944264000	-0.778306000
6	2.598495000	-1.513521000	-0.631923000
6	2.820124000	0.865598000	-0.316067000
6	3.963573000	-1.707201000	-0.541920000
6	4.197335000	0.686571000	-0.223076000
1	2.399069000	1.855623000	-0.242479000
6	4.796468000	-0.582953000	-0.340713000
1	4.382559000	-2.705179000	-0.590216000
1	4.823819000	1.561754000	-0.084211000
8	-0.657228000	-2.609369000	-0.914425000
8	0.657225000	2.609376000	-0.914412000
7	1.629218000	-2.497310000	-0.789897000
7	-1.629216000	2.497317000	-0.789854000
6	-1.873589000	3.916444000	-0.937911000
1	-2.486621000	4.115399000	-1.823471000
1	-2.380976000	4.320747000	-0.055101000
1	-0.904604000	4.402378000	-1.052294000
6	1.873587000	-3.916441000	-0.937917000
1	2.486644000	-4.115416000	-1.823455000
1	2.380946000	-4.320730000	-0.055084000
1	0.904603000	-4.402372000	-1.052319000
6	-6.240611000	0.756417000	-0.258090000
6	-7.004825000	1.830482000	-0.693030000
16	-7.274765000	-0.461702000	0.459673000
6	-8.382338000	1.681343000	-0.467423000
1	-6.576699000	2.690684000	-1.193439000
6	-8.730829000	0.481705000	0.153928000
1	-9.111106000	2.423916000	-0.767178000
6	6.240613000	-0.756417000	-0.258110000
6	7.004827000	-1.830483000	-0.693046000
16	7.274764000	0.461700000	0.459659000
6	8.382339000	-1.681347000	-0.467431000

1	6.576703000	-2.690684000	-1.193458000
6	8.730828000	-0.481709000	0.153921000
1	9.111108000	-2.423921000	-0.767183000
6	-10.034962000	0.010192000	0.526681000
6	-10.228522000	-1.287440000	1.095413000
6	-11.189980000	0.835732000	0.338488000
6	-11.469312000	-1.736798000	1.451011000
1	-9.366903000	-1.933163000	1.241743000
6	-12.439006000	0.406247000	0.686763000
1	-11.067846000	1.827599000	-0.084058000
6	-12.659909000	-0.913758000	1.267970000
1	-11.614593000	-2.723054000	1.879877000
1	-13.313799000	1.033110000	0.546337000
6	10.034960000	-0.010198000	0.526681000
6	11.189979000	-0.835739000	0.338493000
6	10.228520000	1.287435000	1.095414000
6	12.439003000	-0.406256000	0.686775000
1	11.067845000	-1.827605000	-0.084055000
6	11.469308000	1.736791000	1.451017000
1	9.366901000	1.933159000	1.241738000
6	12.659905000	0.913747000	1.267988000
1	13.313796000	-1.033119000	0.546351000
1	11.614589000	2.723047000	1.879882000
8	-13.796932000	-1.314142000	1.588664000
8	13.796927000	1.314133000	1.588679000

S3IIDT-T1

E=-3640.035719 Hartree

6	-2.591948000	-1.524791000	0.193864000
6	-1.979420000	-0.242959000	0.107784000
6	-2.825658000	0.858056000	-0.091240000
6	-4.202786000	0.674435000	-0.176267000
6	-4.794638000	-0.598641000	-0.065694000
6	-3.957946000	-1.721729000	0.122169000
6	-0.352958000	-1.947365000	0.338047000
6	-0.529523000	-0.442661000	0.192087000
1	-2.408414000	1.849238000	-0.168588000
1	-4.829392000	1.542716000	-0.353152000
1	-4.377609000	-2.714426000	0.232222000
6	0.529523000	0.442621000	0.192091000
6	1.979422000	0.242925000	0.107801000
6	0.352952000	1.947324000	0.338058000
6	2.591942000	1.524762000	0.193849000
6	2.825666000	-0.858090000	-0.091203000

6	3.957938000	1.721708000	0.122141000
6	4.202794000	-0.674462000	-0.176236000
1	2.408428000	-1.849275000	-0.168531000
6	4.794638000	0.598621000	-0.065696000
1	4.377596000	2.714410000	0.232166000
1	4.829404000	-1.542742000	-0.353104000
8	-0.666696000	2.608897000	0.467468000
8	0.666682000	-2.608937000	0.467522000
7	1.619956000	2.504719000	0.350719000
7	-1.619967000	-2.504749000	0.350760000
6	-1.859389000	-3.925838000	0.496042000
1	-2.461726000	-4.129755000	1.387593000
1	-2.375035000	-4.326728000	-0.383306000
1	-0.888280000	-4.410076000	0.597878000
6	1.859369000	3.925815000	0.495953000
1	2.461720000	4.129764000	1.387486000
1	2.374998000	4.326681000	-0.383416000
1	0.888259000	4.410049000	0.597789000
6	-6.238688000	-0.777180000	-0.148086000
6	-6.949114000	-1.935827000	-0.430619000
16	-7.341275000	0.557023000	0.124795000
6	-8.342882000	-1.763656000	-0.441742000
1	-6.467298000	-2.879184000	-0.655937000
6	-8.746507000	-0.460684000	-0.163591000
1	-9.044425000	-2.560956000	-0.659418000
6	6.238686000	0.777167000	-0.148099000
6	6.949103000	1.935811000	-0.430666000
16	7.341284000	-0.557021000	0.124814000
6	8.342872000	1.763650000	-0.441791000
1	6.467279000	2.879158000	-0.656009000
6	8.746507000	0.460688000	-0.163607000
1	9.044408000	2.560949000	-0.659493000
6	-10.069758000	0.060618000	-0.094713000
6	-10.473862000	1.387096000	0.148426000
16	-11.499613000	-0.926329000	-0.314821000
1	-9.773938000	2.199372000	0.316810000
6	-12.494854000	0.528331000	-0.063148000
6	10.069762000	-0.060604000	-0.094721000
6	10.473876000	-1.387072000	0.148449000
16	11.499609000	0.926348000	-0.314860000
1	9.773958000	-2.199349000	0.316855000
6	12.494861000	-0.528299000	-0.063154000
6	13.898905000	-0.493398000	-0.104275000
6	-13.898898000	0.493439000	-0.104262000

6	14.658636000	-1.674780000	0.102856000
7	15.310362000	-2.627025000	0.268729000
6	14.588816000	0.721071000	-0.353172000
7	15.129492000	1.734147000	-0.560015000
6	-14.588819000	-0.721032000	-0.353126000
7	-15.129503000	-1.734109000	-0.559940000
6	-14.658621000	1.674832000	0.102843000
7	-15.310339000	2.627085000	0.268695000
7	-11.780794000	1.639533000	0.165461000
7	11.780810000	-1.639500000	0.165484000

S4IIDT-T1

E=-3572.081846 Hartree

6	-2.568420000	1.564162000	-0.713018000
6	-1.973239000	0.274623000	-0.616798000
6	-2.833675000	-0.810085000	-0.386549000
6	-4.205956000	-0.604937000	-0.287279000
6	-4.784143000	0.676274000	-0.408817000
6	-3.928387000	1.783843000	-0.619781000
6	-0.321963000	1.950077000	-0.869133000
6	-0.522696000	0.451380000	-0.710823000
1	-2.431102000	-1.807655000	-0.310519000
1	-4.846519000	-1.467866000	-0.137429000
1	-4.326180000	2.789978000	-0.674434000
6	0.522692000	-0.451411000	-0.710782000
6	1.973240000	-0.274637000	-0.616814000
6	0.321962000	-1.950119000	-0.868955000
6	2.568425000	-1.564177000	-0.712979000
6	2.833673000	0.810081000	-0.386595000
6	3.928395000	-1.783850000	-0.619743000
6	4.205953000	0.604942000	-0.287314000
1	2.431105000	1.807655000	-0.310602000
6	4.784146000	-0.676270000	-0.408818000
1	4.326194000	-2.789984000	-0.674361000
1	4.846514000	1.467877000	-0.137487000
8	-0.707963000	-2.593803000	-1.012475000
8	0.707958000	2.593731000	-1.012816000
7	1.580321000	-2.528065000	-0.878625000
7	-1.580314000	2.528037000	-0.878730000
6	-1.796976000	3.950864000	-1.032380000
1	-2.407327000	4.158442000	-1.917890000
1	-2.295008000	4.368768000	-0.150524000
1	-0.818727000	4.417107000	-1.150134000
6	1.796979000	-3.950916000	-1.032053000
1	2.407308000	-4.158634000	-1.917544000

1	2.295033000	-4.368681000	-0.150143000
1	0.818728000	-4.417179000	-1.149709000
6	-6.220925000	0.872278000	-0.317564000
6	-6.955142000	1.996564000	-0.701101000
16	-7.279043000	-0.371965000	0.331543000
6	-8.327196000	1.873555000	-0.493412000
1	-6.501666000	2.872937000	-1.147839000
6	-8.706037000	0.636664000	0.067875000
1	-9.049218000	2.642122000	-0.744402000
6	6.220930000	-0.872265000	-0.317571000
6	6.955152000	-1.996540000	-0.701130000
16	7.279041000	0.371975000	0.331550000
6	8.327206000	-1.873527000	-0.493438000
1	6.501679000	-2.872905000	-1.147885000
6	8.706040000	-0.636644000	0.067873000
1	9.049233000	-2.642086000	-0.744441000
6	-9.995764000	0.215226000	0.394604000
6	-10.308221000	-1.089495000	0.968913000
16	-11.446353000	1.185631000	0.165169000
6	-12.490028000	-0.150419000	0.834096000
6	9.995764000	-0.215208000	0.394615000
6	10.308213000	1.089499000	0.968961000
16	11.446356000	-1.185608000	0.165179000
6	12.490031000	0.150461000	0.834068000
7	-11.691148000	-1.218906000	1.181091000
7	11.691141000	1.218923000	1.181117000
6	-12.279261000	-2.428448000	1.747089000
1	-12.989459000	-2.866708000	1.042371000
1	-11.461633000	-3.122344000	1.939384000
1	-12.802141000	-2.192974000	2.676724000
6	12.279247000	2.428455000	1.747146000
1	12.989421000	2.866752000	1.042427000
1	11.461612000	3.122329000	1.939486000
1	12.802153000	2.192956000	2.676760000
8	-13.690513000	-0.082322000	0.944889000
8	-9.498099000	-1.969486000	1.239273000
8	9.498086000	1.969484000	1.239330000
8	13.690512000	0.082352000	0.944898000

S5IIDT-T1

E=-3115.007089 Hartree

6	-2.575563000	1.550969000	-0.772187000
6	-1.973853000	0.264111000	-0.671852000
6	-2.826132000	-0.826234000	-0.437788000
6	-4.199428000	-0.629628000	-0.339324000

6	-4.784427000	0.648462000	-0.466204000
6	-3.937054000	1.761657000	-0.681323000
6	-0.332022000	1.949651000	-0.926893000
6	-0.524439000	0.448802000	-0.765946000
1	-2.416967000	-1.820779000	-0.358368000
1	-4.834796000	-1.495552000	-0.186209000
1	-4.342069000	2.764560000	-0.740135000
6	0.524441000	-0.448824000	-0.765932000
6	1.973856000	-0.264131000	-0.671844000
6	0.332025000	-1.949678000	-0.926834000
6	2.575565000	-1.550992000	-0.772131000
6	2.826135000	0.826222000	-0.437814000
6	3.937056000	-1.761678000	-0.681255000
6	4.199430000	0.629618000	-0.339339000
1	2.416970000	1.820770000	-0.358429000
6	4.784428000	-0.648476000	-0.466173000
1	4.342070000	-2.764583000	-0.740029000
1	4.834799000	1.495547000	-0.186252000
8	-0.694815000	-2.596825000	-1.070194000
8	0.694816000	2.596791000	-1.070295000
7	1.593543000	-2.519793000	-0.939847000
7	-1.593541000	2.519764000	-0.939936000
6	-1.818869000	3.941757000	-1.097271000
1	-2.429371000	4.142668000	-1.983964000
1	-2.319712000	4.358004000	-0.216462000
1	-0.843655000	4.413979000	-1.215430000
6	1.818870000	-3.941793000	-1.097117000
1	2.429376000	-4.142746000	-1.983798000
1	2.319708000	-4.358001000	-0.216287000
1	0.843655000	-4.414020000	-1.215259000
6	-6.222357000	0.834118000	-0.375958000
6	-6.961973000	1.952423000	-0.770638000
16	-7.271628000	-0.407962000	0.283880000
6	-8.330351000	1.816318000	-0.559093000
1	-6.518601000	2.828899000	-1.226919000
6	-8.702573000	0.582840000	0.014994000
1	-9.046443000	2.584520000	-0.822846000
6	6.222358000	-0.834130000	-0.375914000
6	6.961975000	-1.952448000	-0.770556000
16	7.271626000	0.407968000	0.283893000
6	8.330353000	-1.816338000	-0.559009000
1	6.518605000	-2.828938000	-1.226812000
6	8.702573000	-0.582841000	0.015040000
1	9.046446000	-2.584547000	-0.822736000

6	10.015658000	-0.163625000	0.348739000
6	11.143602000	-0.986798000	0.137753000
6	10.222328000	1.175967000	0.936290000
6	12.414475000	-0.570320000	0.459253000
1	11.019741000	-1.975980000	-0.287714000
6	12.669799000	0.759821000	1.043032000
6	-10.015659000	0.163634000	0.348703000
6	-11.143603000	0.986802000	0.137689000
6	-10.222331000	-1.175939000	0.936295000
6	-12.414476000	0.570334000	0.459201000
1	-11.019740000	1.975971000	-0.287806000
6	-12.669803000	-0.759789000	1.043019000
6	13.537940000	-1.416108000	0.237894000
7	14.427981000	-2.140439000	0.039991000
6	-13.537940000	1.416117000	0.237816000
7	-14.427980000	2.140444000	0.039893000
8	9.289198000	1.947922000	1.156023000
8	-9.289200000	-1.947884000	1.156063000
8	-13.789586000	-1.151920000	1.335620000
8	13.789584000	1.151965000	1.335614000
7	11.527040000	1.554669000	1.243359000
7	-11.527043000	-1.554630000	1.243374000
6	-11.700306000	-2.892105000	1.824166000
1	-11.320089000	-3.646395000	1.132556000
1	-11.137290000	-2.965041000	2.756681000
1	-12.762373000	-3.036623000	2.004403000
6	11.700302000	2.892164000	1.824102000
1	11.320096000	3.646431000	1.132460000
1	11.137274000	2.965137000	2.756608000
1	12.762367000	3.036684000	2.004346000

S6IIDT-T1

E=-3837.649015 Hartree

6	-2.551985000	-1.590043000	0.768022000
6	-1.968994000	-0.294105000	0.666460000
6	-2.837205000	0.783441000	0.429445000
6	-4.206598000	0.566248000	0.329465000
6	-4.775115000	-0.721042000	0.458716000
6	-3.909233000	-1.821300000	0.677311000
6	-0.302453000	-1.954297000	0.926087000
6	-0.517494000	-0.456988000	0.762269000
1	-2.442483000	1.783664000	0.347915000
1	-4.853596000	1.421983000	0.168897000
1	-4.298324000	-2.829748000	0.743681000
6	0.517497000	0.457088000	0.762268000

6	1.968994000	0.294188000	0.666460000
6	0.302474000	1.954400000	0.926089000
6	2.552000000	1.590121000	0.768003000
6	2.837190000	-0.783372000	0.429461000
6	3.909250000	1.821360000	0.677284000
6	4.206586000	-0.566197000	0.329474000
1	2.442455000	-1.783591000	0.347945000
6	4.775118000	0.721088000	0.458703000
1	4.298353000	2.829804000	0.743640000
1	4.853574000	-1.421943000	0.168918000
8	-0.734236000	2.585268000	1.071756000
8	0.734265000	-2.585152000	1.071752000
7	1.555119000	2.543392000	0.939065000
7	-1.555093000	-2.543302000	0.939088000
6	-1.759322000	-3.968045000	1.100204000
1	-2.366890000	-4.175580000	1.987379000
1	-2.254183000	-4.393805000	0.220567000
1	-0.777200000	-4.425445000	1.219467000
6	1.759364000	3.968135000	1.100158000
1	2.366943000	4.175678000	1.987324000
1	2.254221000	4.393878000	0.220510000
1	0.777249000	4.425547000	1.219425000
6	-6.206382000	-0.926033000	0.366791000
6	-6.923988000	-2.086214000	0.692106000
16	-7.285998000	0.339607000	-0.201197000
6	-8.291413000	-1.973331000	0.503284000
1	-6.458273000	-2.983527000	1.080954000
6	-8.701053000	-0.702672000	0.010772000
1	-9.015164000	-2.748149000	0.704463000
6	6.206388000	0.926061000	0.366770000
6	6.924008000	2.086242000	0.692055000
16	7.285988000	-0.339606000	-0.201189000
6	8.291431000	1.973338000	0.503234000
1	6.458304000	2.983571000	1.080880000
6	8.701056000	0.702661000	0.010755000
1	9.015191000	2.748153000	0.704392000
6	10.008175000	0.276390000	-0.286737000
6	11.152954000	1.170859000	-0.108228000
6	10.216234000	-1.079081000	-0.778913000
6	12.645607000	-0.655474000	-0.895981000
6	-10.008177000	-0.276426000	-0.286732000
6	-11.152944000	-1.170906000	-0.108199000
6	-10.216256000	1.079029000	-0.778944000
6	-12.645624000	0.655387000	-0.895992000

8	9.285328000	-1.867043000	-0.951544000
8	-9.285362000	1.867000000	-0.951597000
7	11.537298000	-1.469904000	-1.056842000
7	-11.537327000	1.469826000	-1.056881000
6	-11.731410000	2.842621000	-1.551559000
1	-12.381381000	3.392195000	-0.869449000
1	-10.750102000	3.305025000	-1.607188000
1	-12.204915000	2.817161000	-2.533835000
6	11.731361000	-2.842715000	-1.551483000
1	12.381332000	-3.392277000	-0.869363000
1	10.750048000	-3.305109000	-1.607091000
1	12.204859000	-2.817289000	-2.533764000
7	12.420038000	0.628578000	-0.431576000
7	-12.420037000	-0.628650000	-0.431553000
6	13.578155000	1.519977000	-0.251980000
1	14.275318000	1.079610000	0.462104000
1	14.095569000	1.648762000	-1.203578000
1	13.198494000	2.469408000	0.113406000
6	-13.578141000	-1.520059000	-0.251925000
1	-14.275306000	-1.079681000	0.462149000
1	-14.095559000	-1.648877000	-1.203517000
1	-13.198466000	-2.469475000	0.113484000
8	-11.073501000	-2.328062000	0.294615000
8	11.073528000	2.328027000	0.294551000
16	14.187215000	-1.203473000	-1.249577000
16	-14.187241000	1.203357000	-1.249594000

S7IIDT-T1

E=-3345.511097 Hartree

6	-2.534746000	1.618305000	-1.054749000
6	-1.967694000	0.315190000	-0.957325000
6	-2.849642000	-0.753615000	-0.733891000
6	-4.217877000	-0.521478000	-0.638728000
6	-4.765940000	0.773096000	-0.758930000
6	-3.890299000	1.865290000	-0.966717000
6	-0.281409000	1.958444000	-1.201991000
6	-0.512852000	0.462173000	-1.047527000
1	-2.467863000	-1.759463000	-0.662128000
1	-4.879155000	-1.371312000	-0.505119000
1	-4.270335000	2.878282000	-1.019871000
6	0.512853000	-0.462002000	-1.047596000
6	1.967694000	-0.315034000	-0.957352000
6	0.281411000	-1.958249000	-1.202297000
6	2.534747000	-1.618131000	-1.055000000
6	2.849640000	0.753734000	-0.733731000

6	3.890301000	-1.865129000	-0.967008000
6	4.217875000	0.521582000	-0.638602000
1	2.467860000	1.759569000	-0.661797000
6	4.765939000	-0.772971000	-0.759027000
1	4.270338000	-2.878112000	-1.020339000
1	4.879152000	1.371394000	-0.504846000
8	-0.761778000	-2.579828000	-1.338992000
8	0.761784000	2.580050000	-1.338538000
7	1.527506000	-2.561185000	-1.215929000
7	-1.527502000	2.561386000	-1.215507000
6	-1.715243000	3.989286000	-1.369573000
1	-2.318297000	4.208098000	-2.257074000
1	-2.207265000	4.416066000	-0.488842000
1	-0.727757000	4.436161000	-1.484264000
6	1.715250000	-3.989056000	-1.370259000
1	2.318301000	-4.207703000	-2.257802000
1	2.207276000	-4.415995000	-0.489608000
1	0.727765000	-4.435913000	-1.485027000
6	-6.196349000	1.001026000	-0.669400000
6	-6.920332000	2.114709000	-1.109266000
16	-7.268037000	-0.180605000	0.043823000
6	-8.288536000	2.027800000	-0.882284000
1	-6.454562000	2.952452000	-1.613535000
6	-8.689840000	0.819611000	-0.261065000
1	-9.011992000	2.786738000	-1.143528000
6	6.196348000	-1.000914000	-0.669534000
6	6.920334000	-2.114521000	-1.109590000
16	7.268035000	0.180597000	0.043890000
6	8.288538000	-2.027648000	-0.882594000
1	6.454566000	-2.952179000	-1.614003000
6	8.689840000	-0.819564000	-0.261169000
1	9.011995000	-2.786541000	-1.143967000
6	9.990743000	-0.525981000	0.190025000
6	10.982733000	-1.629911000	0.429150000
6	10.574654000	0.696962000	0.696472000
6	12.042013000	-1.043854000	1.283666000
6	11.780822000	0.322922000	1.489835000
6	13.136850000	-1.686937000	1.843224000
6	12.639126000	1.066260000	2.303452000
6	13.992759000	-0.939186000	2.655705000
1	13.303658000	-2.741070000	1.646504000
6	13.736565000	0.417295000	2.882650000
1	12.475480000	2.116558000	2.502379000
1	14.856420000	-1.409059000	3.115808000

1	14.403353000	0.987012000	3.522621000
6	-9.990744000	0.525952000	0.190079000
6	-10.982732000	1.629843000	0.429395000
6	-10.574655000	-0.697076000	0.696319000
6	-12.042015000	1.043639000	1.283805000
6	-11.780825000	-0.323172000	1.489742000
6	-13.136855000	1.686627000	1.843469000
6	-12.639131000	-1.066649000	2.303229000
6	-13.992766000	0.938737000	2.655820000
1	-13.303662000	2.740793000	1.646928000
6	-13.736572000	-0.417782000	2.882534000
1	-12.475485000	-2.116981000	2.501979000
1	-14.856429000	1.408531000	3.116000000
1	-14.403362000	-0.987609000	3.522407000
8	-10.929345000	2.787838000	0.042128000
8	10.929343000	-2.787841000	0.041693000
6	-10.214421000	-2.003480000	0.383341000
6	10.214422000	2.003419000	0.383715000
6	-9.329210000	-2.357574000	-0.678774000
7	-8.660547000	-2.709998000	-1.565657000
6	-10.816674000	-3.139433000	1.004892000
7	-11.272344000	-4.088387000	1.505153000
6	10.816674000	3.139266000	1.005461000
7	11.272342000	4.088135000	1.505884000
6	9.329216000	2.357694000	-0.678342000
7	8.660556000	2.710270000	-1.565169000

S8IIDT-T1

E=-4215.951598 Hartree

6	2.574251000	-1.552964000	-1.094750000
6	1.975237000	-0.264567000	-0.994393000
6	2.829493000	0.826130000	-0.771107000
6	4.203745000	0.628690000	-0.679404000
6	4.782321000	-0.651250000	-0.802752000
6	3.936284000	-1.765405000	-1.010060000
6	0.330484000	-1.950545000	-1.236180000
6	0.524022000	-0.448219000	-1.082362000
1	2.422241000	1.821743000	-0.697266000
1	4.844229000	1.494662000	-0.548076000
1	4.343148000	-2.767991000	-1.062670000
6	-0.524175000	0.449569000	-1.082175000
6	-1.975350000	0.265720000	-0.994119000
6	-0.330841000	1.951965000	-1.235630000
6	-2.574545000	1.554058000	-1.094062000
6	-2.829419000	-0.825172000	-0.771087000

6	-3.936601000	1.766281000	-1.009179000
6	-4.203689000	-0.627954000	-0.679188000
1	-2.422006000	-1.820750000	-0.697597000
6	-4.782456000	0.651943000	-0.802100000
1	-4.343616000	2.768822000	-1.061478000
1	-4.844039000	-1.494056000	-0.548059000
8	0.696476000	2.599802000	-1.368465000
8	-0.696959000	-2.598210000	-1.368886000
7	-1.591887000	2.522498000	-1.252924000
7	1.591451000	-2.521240000	-1.253736000
6	1.815664000	-3.944376000	-1.407088000
1	2.421726000	-4.148006000	-2.296043000
1	2.320721000	-4.357136000	-0.527181000
1	0.839850000	-4.416773000	-1.518891000
6	-1.816304000	3.945637000	-1.405947000
1	-2.422480000	4.149381000	-2.294799000
1	-2.321328000	4.358140000	-0.525901000
1	-0.840563000	4.418188000	-1.517743000
6	6.219807000	-0.844424000	-0.717075000
6	6.971776000	-1.919869000	-1.196354000
16	7.252833000	0.333858000	0.052340000
6	8.337862000	-1.802798000	-0.957464000
1	6.531359000	-2.746230000	-1.739972000
6	8.697433000	-0.614056000	-0.288779000
1	9.076892000	-2.523458000	-1.285484000
6	-6.219963000	0.844887000	-0.716228000
6	-6.972131000	1.920361000	-1.195129000
16	-7.252746000	-0.333762000	0.052949000
6	-8.338179000	1.803026000	-0.956144000
1	-6.531884000	2.746938000	-1.738558000
6	-8.697511000	0.614048000	-0.287754000
1	-9.077344000	2.523667000	-1.283900000
6	-9.988602000	0.304921000	0.184291000
6	-10.617092000	-0.894737000	0.610252000
6	-12.208986000	0.727188000	1.449860000
6	-11.829662000	-0.623913000	1.439406000
6	-13.326512000	1.211622000	2.110728000
6	-12.628224000	-1.521533000	2.162859000
6	-14.109448000	0.299313000	2.820378000
1	-13.574931000	2.267170000	2.079494000
6	-13.752160000	-1.050692000	2.844968000
1	-12.388044000	-2.573619000	2.212723000
1	-14.989275000	0.641367000	3.355501000
1	-14.357030000	-1.756429000	3.405320000

6	9.988610000	-0.305281000	0.183264000
6	10.617368000	0.894143000	0.609504000
6	12.208909000	-0.728330000	1.448723000
6	11.829863000	0.622850000	1.438612000
6	13.326327000	-1.213166000	2.109480000
6	12.628606000	1.520121000	2.162298000
6	14.109443000	-0.301200000	2.819373000
1	13.574528000	-2.268757000	2.077977000
6	13.752435000	1.048873000	2.844301000
1	12.388646000	2.572245000	2.212421000
1	14.989192000	-0.643573000	3.354418000
1	14.357447000	1.754342000	3.404838000
6	10.227681000	2.179389000	0.187442000
6	-10.227068000	-2.179783000	0.187897000
6	9.367917000	2.405725000	-0.925667000
7	8.709321000	2.652313000	-1.855721000
6	10.744661000	3.388886000	0.731690000
7	11.121066000	4.407838000	1.157313000
6	-10.743720000	-3.389552000	0.731852000
7	-11.119847000	-4.408719000	1.157208000
6	-9.367078000	-2.405612000	-0.925140000
7	-8.708237000	-2.651757000	-1.855137000
16	11.064763000	-1.732002000	0.528410000
16	-11.065034000	1.731337000	0.529826000
8	11.659928000	-2.239820000	-0.718490000
8	10.383946000	-2.679632000	1.422194000
8	-10.384405000	2.678856000	1.423870000
8	-11.660294000	2.239378000	-0.716937000

S9IIDT-T1

E=-4187.830708 Hartree

6	2.542429000	1.611163000	0.684764000
6	1.966905000	0.311298000	0.596302000
6	2.850841000	-0.757062000	0.372220000
6	4.217638000	-0.526237000	0.269310000
6	4.777570000	0.766019000	0.380281000
6	3.896512000	1.857106000	0.587002000
6	0.288236000	1.952644000	0.850206000
6	0.516349000	0.461732000	0.693398000
1	2.467199000	-1.762731000	0.302164000
1	4.871598000	-1.379222000	0.116991000
1	4.272448000	2.871493000	0.645192000
6	-0.516351000	-0.461799000	0.693387000
6	-1.966906000	-0.311355000	0.596303000
6	-0.288246000	-1.952717000	0.850157000

6	-2.542436000	-1.611222000	0.684700000
6	-2.850837000	0.757019000	0.372266000
6	-3.896519000	-1.857154000	0.586918000
6	-4.217633000	0.526205000	0.269340000
1	-2.467188000	1.762689000	0.302255000
6	-4.777572000	-0.766054000	0.380246000
1	-4.272458000	-2.871543000	0.645062000
1	-4.871588000	1.379200000	0.117052000
8	0.752175000	-2.581616000	0.997702000
8	-0.752185000	2.581527000	0.997821000
7	-1.536257000	-2.556492000	0.851361000
7	1.536246000	2.556421000	0.851468000
6	1.724626000	3.982068000	1.001728000
1	2.334935000	4.205034000	1.883963000
1	2.210815000	4.409950000	0.117579000
1	0.737144000	4.427961000	1.122926000
6	-1.724642000	-3.982147000	1.001533000
1	-2.334964000	-4.205163000	1.883747000
1	-2.210819000	-4.409977000	0.117353000
1	-0.737163000	-4.428049000	1.122720000
6	6.204436000	0.988380000	0.283697000
6	6.925122000	2.158762000	0.523002000
16	7.311541000	-0.305360000	-0.189669000
6	8.303393000	2.047321000	0.345973000
1	6.450050000	3.079244000	0.840710000
6	8.722295000	0.756758000	-0.047296000
1	8.997774000	2.864746000	0.501858000
6	-6.204438000	-0.988403000	0.283643000
6	-6.925128000	-2.158807000	0.522840000
16	-7.311543000	0.305386000	-0.189590000
6	-8.303396000	-2.047349000	0.345813000
1	-6.450057000	-3.079321000	0.840457000
6	-8.722296000	-0.756750000	-0.047342000
1	-8.997778000	-2.864789000	0.501612000
6	-10.015494000	-0.313254000	-0.302903000
16	-10.391272000	1.344537000	-0.779299000
16	-11.413714000	-1.389940000	-0.173978000
6	-12.141745000	1.115299000	-0.885445000
6	-12.623004000	-0.171931000	-0.599693000
6	-13.028190000	2.137367000	-1.233400000
6	-13.992673000	-0.440200000	-0.661231000
6	-14.394116000	1.864596000	-1.293634000
1	-12.654873000	3.132423000	-1.453731000
6	-14.873551000	0.582999000	-1.009123000

1	-14.364780000	-1.435499000	-0.439859000
1	-15.085336000	2.656505000	-1.563498000
1	-15.938053000	0.377371000	-1.057541000
6	10.015496000	0.313283000	-0.302882000
16	10.391276000	-1.344464000	-0.779427000
16	11.413715000	1.389955000	-0.173841000
6	12.141753000	-1.115223000	-0.885516000
6	12.623011000	0.171981000	-0.599639000
6	13.028202000	-2.137262000	-1.233545000
6	13.992681000	0.440251000	-0.661125000
6	14.394130000	-1.864490000	-1.293727000
1	12.654885000	-3.132297000	-1.453973000
6	14.873563000	-0.582920000	-1.009092000
1	14.364787000	1.435528000	-0.439656000
1	15.085353000	-2.656377000	-1.563648000
1	15.938066000	-0.377292000	-1.057470000

S10IIDT-T1

E=-3880.513512 Hartree

6	-2.608702000	-1.501773000	0.516845000
6	-1.978341000	-0.227523000	0.428902000
6	-2.816459000	0.877386000	0.205638000
6	-4.191808000	0.704721000	0.102884000
6	-4.806217000	-0.562624000	0.213201000
6	-3.971970000	-1.690062000	0.419155000
6	-0.370994000	-1.938474000	0.682620000
6	-0.535613000	-0.439398000	0.525983000
1	-2.390572000	1.865943000	0.135971000
1	-4.808948000	1.584789000	-0.049179000
1	-4.390531000	-2.687628000	0.477410000
6	0.535613000	0.439555000	0.525862000
6	1.978340000	0.227650000	0.428833000
6	0.370999000	1.938675000	0.682089000
6	2.608707000	1.501919000	0.516447000
6	2.816453000	-0.877321000	0.205856000
6	3.971976000	1.690177000	0.418713000
6	4.191803000	-0.704690000	0.103059000
1	2.390562000	-1.865894000	0.136448000
6	4.806218000	0.562681000	0.213051000
1	4.390542000	2.687755000	0.476708000
1	4.808940000	-1.584800000	-0.048772000
8	-0.641699000	2.611470000	0.829695000
8	0.641710000	-2.611229000	0.830375000
7	1.643517000	2.489099000	0.682616000
7	-1.643508000	-2.488906000	0.683269000

6	-1.892127000	-3.905225000	0.833421000
1	-2.511332000	-4.102291000	1.715652000
1	-2.396077000	-4.312113000	-0.050714000
1	-0.924392000	-4.392533000	0.954546000
6	1.892143000	3.905455000	0.832414000
1	2.511342000	4.102738000	1.714601000
1	2.396102000	4.312118000	-0.051818000
1	0.924409000	4.392799000	0.953410000
6	-6.241239000	-0.724377000	0.116956000
6	-7.010915000	-1.863510000	0.350976000
16	-7.293734000	0.617358000	-0.349282000
6	-8.384069000	-1.692456000	0.175469000
1	-6.575501000	-2.805240000	0.663262000
6	-8.747480000	-0.384448000	-0.211054000
1	-9.112402000	-2.480637000	0.327537000
6	6.241240000	0.724403000	0.116767000
6	7.010924000	1.863584000	0.350526000
16	7.293727000	-0.617446000	-0.349163000
6	8.384077000	1.692481000	0.175059000
1	6.575516000	2.805387000	0.662598000
6	8.747480000	0.384382000	-0.211163000
1	9.112415000	2.480692000	0.326948000
6	10.021430000	-0.116849000	-0.464106000
16	10.337995000	-1.792870000	-0.932889000
16	11.475662000	0.888954000	-0.340316000
6	12.081108000	-1.603200000	-1.040323000
6	12.593329000	-0.394966000	-0.772854000
6	-10.021433000	0.116716000	-0.464113000
16	-10.338009000	1.792626000	-0.933286000
16	-11.475659000	-0.889067000	-0.340089000
6	-12.081120000	1.602920000	-1.040677000
6	-12.593334000	0.394746000	-0.772927000
1	-13.647214000	0.147423000	-0.804081000
1	-12.660173000	2.474404000	-1.319713000
1	12.660156000	-2.474752000	-1.319157000
1	13.647211000	-0.147657000	-0.804065000

S2FIIDT-CS E=-2664.824588 Hartree

6	0.076910000	-1.987950000	0.000183000
6	-0.431471000	-0.568943000	0.000032000
6	-1.796992000	-0.706594000	0.000035000
6	-2.181469000	-2.088584000	0.000020000

6	-3.994901000	-0.792416000	-0.000009000
6	-3.550647000	-2.153141000	-0.000030000
1	-4.199472000	-3.016328000	-0.000063000
6	0.431471000	0.568933000	-0.000045000
6	-0.076913000	1.987939000	-0.000151000
6	1.796992000	0.706586000	-0.000064000
6	2.181466000	2.088577000	-0.000079000
6	3.550644000	2.153137000	-0.000073000
6	3.994901000	0.792413000	-0.000055000
1	4.199468000	3.016325000	-0.000074000
7	-1.052052000	-2.857333000	0.000013000
7	1.052047000	2.857324000	-0.000083000
8	1.226257000	-2.383839000	-0.000014000
8	-1.226261000	2.383825000	0.000014000
6	-0.951460000	-4.303056000	-0.000030000
1	-1.420933000	-4.729364000	-0.892494000
1	0.110930000	-4.549940000	-0.000134000
1	-1.420759000	-4.729414000	0.892504000
6	0.951453000	4.303047000	0.000029000
1	1.421017000	4.729450000	-0.892340000
1	-0.110937000	4.549928000	-0.000161000
1	1.420659000	4.729310000	0.892657000
8	-2.902130000	0.074040000	-0.000005000
8	2.902132000	-0.074045000	-0.000046000
6	5.245252000	0.218205000	-0.000040000
6	5.534343000	-1.177974000	-0.000029000
16	6.743307000	1.154335000	-0.000052000
6	6.871292000	-1.465006000	-0.000003000
1	4.739958000	-1.914561000	-0.000028000
6	7.734403000	-0.322321000	0.000004000
1	7.258115000	-2.475718000	0.000019000
6	-5.245251000	-0.218205000	-0.000026000
6	-5.534339000	1.177974000	-0.000038000
16	-6.743308000	-1.154333000	-0.000078000
6	-6.871288000	1.465009000	-0.000030000
1	-4.739953000	1.914559000	-0.000030000
6	-7.734401000	0.322325000	-0.000022000
1	-7.258109000	2.475722000	-0.000014000
6	9.128363000	-0.290942000	0.000037000
6	9.862416000	0.953218000	0.000020000
6	9.903948000	-1.512174000	0.000063000
6	11.217902000	0.987504000	0.000054000
1	9.305109000	1.886946000	-0.000024000
6	11.260125000	-1.497263000	0.000097000

1	9.383597000	-2.464521000	0.000051000
6	12.024264000	-0.242377000	0.000153000
1	11.763155000	1.925984000	0.000029000
1	11.836975000	-2.416681000	0.000102000
6	-9.128361000	0.290949000	0.000005000
6	-9.862416000	-0.953210000	0.000005000
6	-9.903943000	1.512182000	0.000053000
6	-11.217902000	-0.987493000	0.000029000
1	-9.305111000	-1.886939000	-0.000013000
6	-11.260121000	1.497274000	0.000075000
1	-9.383591000	2.464529000	0.000073000
6	-12.024262000	0.242390000	0.000013000
1	-11.763157000	-1.925973000	0.000041000
1	-11.836969000	2.416692000	0.000122000
8	13.259957000	-0.219544000	0.000074000
8	-13.259955000	0.219558000	0.000133000

S3FIIDT-CS E=-3635.563838 Hartree

6	0.196108000	-1.981282000	0.000145000
6	-0.396425000	-0.592170000	0.000088000
6	-1.750805000	-0.811727000	0.000096000
6	-2.050565000	-2.214176000	0.000137000
6	-3.936663000	-1.029096000	0.000099000
6	-3.415285000	-2.359849000	0.000139000
1	-4.011447000	-3.260210000	0.000167000
6	0.396425000	0.592170000	0.000043000
6	-0.196108000	1.981281000	-0.000014000
6	1.750804000	0.811726000	0.000033000
6	2.050565000	2.214175000	-0.000012000
6	3.415285000	2.359849000	-0.000014000
6	3.936663000	1.029096000	0.000027000
1	4.011447000	3.260210000	-0.000039000
7	-0.879459000	-2.915436000	0.000150000
7	0.879459000	2.915435000	-0.000039000
8	1.366585000	-2.304087000	0.000136000
8	-1.366585000	2.304086000	-0.000001000
6	-0.694532000	-4.354517000	0.000214000
1	-1.138573000	-4.805735000	-0.892549000
1	0.380115000	-4.539843000	0.000095000
1	-1.138353000	-4.805639000	0.893138000
6	0.694532000	4.354517000	-0.000044000
1	1.138583000	4.805692000	-0.892824000
1	-0.380115000	4.539843000	-0.000185000

1	1.138342000	4.805681000	0.892863000
8	-2.901070000	-0.099123000	0.000071000
8	2.901070000	0.099123000	0.000057000
6	5.221063000	0.526273000	0.000045000
6	5.588111000	-0.848115000	0.000092000
16	6.659605000	1.552695000	0.000017000
6	6.942560000	-1.058335000	0.000098000
1	4.837510000	-1.629200000	0.000119000
6	7.724373000	0.134523000	0.000048000
1	7.402833000	-2.039384000	0.000132000
6	-5.221063000	-0.526273000	0.000083000
6	-5.588111000	0.848115000	0.000046000
16	-6.659605000	-1.552695000	0.000116000
6	-6.942560000	1.058335000	0.000034000
1	-4.837509000	1.629200000	0.000027000
6	-7.724373000	-0.134523000	0.000056000
1	-7.402832000	2.039384000	0.000005000
6	-9.107482000	-0.239750000	0.000046000
6	-9.894786000	-1.429407000	0.000101000
16	-10.211677000	1.141926000	0.000012000
1	-9.451681000	-2.422057000	0.000142000
6	-11.580184000	-0.001752000	-0.000080000
6	9.107482000	0.239750000	0.000036000
6	9.894786000	1.429407000	0.000024000
16	10.211677000	-1.141926000	0.000096000
1	9.451681000	2.422057000	0.000002000
6	11.580184000	0.001752000	-0.000082000
6	-12.903909000	0.411777000	-0.000196000
6	12.903909000	-0.411776000	-0.000185000
6	-13.966156000	-0.536155000	-0.000252000
7	-14.857875000	-1.285549000	-0.000290000
6	-13.227838000	1.796511000	-0.000250000
7	-13.458521000	2.939426000	-0.000325000
6	13.227838000	-1.796510000	-0.000153000
7	13.458521000	-2.939426000	-0.000170000
6	13.966156000	0.536155000	-0.000311000
7	14.857875000	1.285549000	-0.000403000
7	-11.200598000	-1.309587000	0.000014000
7	11.200598000	1.309587000	-0.000063000

S2FIIDT-OS E=-2664.824819 Hartree

6	-0.075789000	1.986755000	0.000208000
6	0.430771000	0.565994000	0.000193000

6	1.801048000	0.703945000	0.000174000
6	2.182732000	2.080400000	0.000183000
6	3.996922000	0.788571000	0.000115000
6	3.556737000	2.144693000	0.000167000
1	4.205580000	3.007850000	0.000181000
6	-0.430772000	-0.566005000	0.000196000
6	0.075786000	-1.986767000	0.000227000
6	-1.801049000	-0.703953000	0.000174000
6	-2.182735000	-2.080407000	0.000181000
6	-3.556740000	-2.144697000	0.000152000
6	-3.996922000	-0.788574000	0.000097000
1	-4.205585000	-3.007852000	0.000158000
7	1.053653000	2.852857000	0.000185000
7	-1.053659000	-2.852867000	0.000190000
8	-1.225552000	2.382945000	0.000243000
8	1.225547000	-2.382961000	0.000257000
6	0.956638000	4.298631000	0.000297000
1	1.427192000	4.724202000	-0.892017000
1	-0.105149000	4.548104000	0.000068000
1	1.426765000	4.724062000	0.892905000
6	-0.956646000	-4.298640000	0.000297000
1	-1.427194000	-4.724208000	-0.892023000
1	0.105140000	-4.548116000	0.000077000
1	-1.426783000	-4.724074000	0.892899000
8	2.907344000	-0.076744000	0.000138000
8	-2.907343000	0.076739000	0.000129000
6	-5.253052000	-0.207755000	0.000040000
6	-5.539775000	1.182525000	0.000010000
16	-6.747641000	-1.143871000	0.000015000
6	-6.882754000	1.469211000	-0.000066000
1	-4.746512000	1.920239000	0.000033000
6	-7.739210000	0.329601000	-0.000086000
1	-7.270034000	2.479797000	-0.000111000
6	5.253053000	0.207755000	0.000075000
6	5.539779000	-1.182525000	0.000077000
16	6.747641000	1.143874000	0.000062000
6	6.882759000	-1.469209000	-0.000005000
1	4.746517000	-1.920240000	0.000114000
6	7.739213000	-0.329597000	-0.000056000
1	7.270040000	-2.479793000	-0.000040000
6	-9.140287000	0.292645000	-0.000165000
6	-9.867355000	-0.952375000	-0.000161000
6	-9.917210000	1.509764000	-0.000258000
6	-11.224696000	-0.991558000	-0.000239000

1	-9.307319000	-1.884367000	-0.000090000
6	-11.275145000	1.490554000	-0.000337000
1	-9.400016000	2.463778000	-0.000265000
6	-12.033214000	0.234271000	-0.000336000
1	-11.766324000	-1.932110000	-0.000232000
1	-11.854753000	2.408219000	-0.000404000
6	9.140290000	-0.292638000	-0.000164000
6	9.867356000	0.952383000	-0.000175000
6	9.917215000	-1.509756000	-0.000273000
6	11.224697000	0.991569000	-0.000281000
1	9.307318000	1.884374000	-0.000092000
6	11.275150000	-1.490544000	-0.000378000
1	9.400022000	-2.463770000	-0.000270000
6	12.033217000	-0.234259000	-0.000387000
1	11.766323000	1.932121000	-0.000287000
1	11.854759000	-2.408208000	-0.000460000
8	-13.270904000	0.207446000	-0.000399000
8	13.270907000	-0.207432000	-0.000490000

S3FIIDT-OS E=-3635.564374 Hartree

6	0.193433000	-1.980119000	-0.000001000
6	-0.395937000	-0.587463000	-0.000033000
6	-1.757432000	-0.807229000	-0.000040000
6	-2.054175000	-2.201155000	-0.000005000
6	-3.940435000	-1.021692000	-0.000052000
6	-3.425505000	-2.346785000	-0.000010000
1	-4.020922000	-3.247628000	0.000011000
6	0.395937000	0.587464000	-0.000060000
6	-0.193433000	1.980119000	-0.000079000
6	1.757432000	0.807230000	-0.000068000
6	2.054175000	2.201155000	-0.000106000
6	3.425505000	2.346786000	-0.000114000
6	3.940435000	1.021693000	-0.000082000
1	4.020922000	3.247629000	-0.000135000
7	-0.883201000	-2.908523000	0.000011000
7	0.883200000	2.908524000	-0.000136000
8	1.364532000	-2.303542000	0.000048000
8	-1.364532000	2.303543000	-0.000093000
6	-0.704640000	-4.348096000	0.000130000
1	-1.150616000	-4.797933000	-0.892478000
1	0.369189000	-4.538236000	-0.000127000
1	-1.150148000	-4.797756000	0.893064000
6	0.704639000	4.348097000	-0.000110000

1	1.150614000	4.797876000	-0.892748000
1	-0.369189000	4.538237000	-0.000377000
1	1.150150000	4.797814000	0.892794000
8	-2.909079000	-0.093878000	-0.000070000
8	2.909080000	0.093879000	-0.000057000
6	5.233324000	0.510276000	-0.000063000
6	5.596834000	-0.856341000	-0.000007000
16	6.666867000	1.536325000	-0.000098000
6	6.959545000	-1.065498000	-0.000001000
1	4.848511000	-1.639459000	0.000019000
6	7.732554000	0.122522000	-0.000046000
1	7.419212000	-2.046904000	0.000036000
6	-5.233323000	-0.510275000	-0.000086000
6	-5.596834000	0.856342000	-0.000163000
16	-6.666867000	-1.536324000	-0.000063000
6	-6.959545000	1.065499000	-0.000165000
1	-4.848511000	1.639460000	-0.000202000
6	-7.732554000	-0.122522000	-0.000086000
1	-7.419213000	2.046904000	-0.000212000
6	-9.124270000	-0.239270000	-0.000049000
6	-9.902400000	-1.428073000	-0.000017000
16	-10.228621000	1.136855000	-0.000078000
1	-9.458049000	-2.419732000	-0.000012000
6	-11.594075000	-0.009091000	0.000081000
6	9.124270000	0.239270000	-0.000058000
6	9.902401000	1.428072000	-0.000154000
16	10.228620000	-1.136855000	-0.000009000
1	9.458050000	2.419732000	-0.000216000
6	11.594075000	0.009090000	0.000036000
6	-12.922392000	0.406389000	0.000181000
6	12.922392000	-0.406391000	0.000156000
6	-13.982904000	-0.541855000	0.000298000
7	-14.873720000	-1.292762000	0.000390000
6	-13.247285000	1.789887000	0.000167000
7	-13.480095000	2.932640000	0.000178000
6	13.247284000	-1.789889000	0.000253000
7	13.480093000	-2.932642000	0.000354000
6	13.982904000	0.541853000	0.000187000
7	14.873721000	1.292759000	0.000206000
7	-11.213914000	-1.310613000	0.000068000
7	11.213915000	1.310613000	-0.000085000

S2FIIDT-T1

E=-2664.815459 Hartree

6	0.070158000	-1.984134000	0.000395000
6	-0.426263000	-0.545050000	-0.000032000
6	-1.827012000	-0.685468000	0.000012000
6	-2.191102000	-2.030899000	-0.000037000
6	-4.011223000	-0.763238000	-0.000094000
6	-3.589197000	-2.099071000	-0.000166000
1	-4.233521000	-2.965416000	-0.000277000
6	0.426262000	0.545041000	-0.000246000
6	-0.070161000	1.984124000	-0.000615000
6	1.827012000	0.685462000	-0.000276000
6	2.191100000	2.030892000	-0.000341000
6	3.589195000	2.099067000	-0.000274000
6	4.011222000	0.763236000	-0.000204000
1	4.233518000	2.965413000	-0.000270000
7	-1.060305000	-2.826073000	-0.000084000
7	1.060301000	2.826065000	-0.000384000
8	1.221735000	-2.377927000	-0.000275000
8	-1.221739000	2.377915000	-0.000194000
6	-0.988883000	-4.272576000	-0.000376000
1	-1.466551000	-4.690980000	-0.892695000
1	0.068075000	-4.541931000	-0.000358000
1	-1.466657000	-4.691333000	0.891721000
6	0.988877000	4.272568000	-0.000210000
1	1.466827000	4.691251000	-0.892246000
1	-0.068081000	4.541921000	-0.000452000
1	1.466368000	4.691047000	0.892170000
8	-2.938903000	0.096588000	-0.000080000
8	2.938904000	-0.096593000	-0.000167000
6	5.294672000	0.154551000	-0.000124000
6	5.574197000	-1.211167000	-0.000052000
16	6.771761000	1.094473000	-0.000139000
6	6.942957000	-1.494297000	0.000056000
1	4.788400000	-1.956503000	-0.000061000
6	7.770183000	-0.364238000	0.000077000
1	7.333014000	-2.504134000	0.000141000
6	-5.294671000	-0.154553000	-0.000122000
6	-5.574194000	1.211166000	-0.000125000
16	-6.771762000	-1.094472000	-0.000250000
6	-6.942952000	1.494299000	-0.000061000
1	-4.788396000	1.956501000	-0.000125000
6	-7.770182000	0.364241000	-0.000090000
1	-7.333008000	2.504136000	-0.000030000
6	9.198854000	-0.299332000	0.000212000
6	9.894777000	0.951467000	0.000172000

6	9.984989000	-1.498250000	0.000337000
6	11.258920000	1.014261000	0.000302000
1	9.320904000	1.874560000	0.000026000
6	11.349390000	-1.457670000	0.000468000
1	9.482544000	-2.459933000	0.000317000
6	12.079719000	-0.193362000	0.000571000
1	11.783438000	1.964356000	0.000247000
1	11.942881000	-2.366357000	0.000536000
6	-9.198851000	0.299338000	0.000144000
6	-9.894777000	-0.951459000	0.000165000
6	-9.984984000	1.498258000	0.000314000
6	-11.258921000	-1.014251000	0.000306000
1	-9.320906000	-1.874554000	0.000070000
6	-11.349385000	1.457681000	0.000456000
1	-9.482537000	2.459940000	0.000336000
6	-12.079717000	0.193374000	0.000371000
1	-11.783441000	-1.964344000	0.000342000
1	-11.942874000	2.366369000	0.000605000
8	13.324999000	-0.146940000	0.000483000
8	-13.324997000	0.146955000	0.000670000

S3FIIDT-T1 E=-3635.556902 Hartree

6	0.188715000	-1.978045000	0.000813000
6	-0.392822000	-0.570007000	0.000246000
6	-1.780301000	-0.792843000	0.000343000
6	-2.064137000	-2.160017000	0.000375000
6	-3.954385000	-0.999949000	0.000278000
6	-3.454822000	-2.309562000	0.000280000
1	-4.046477000	-3.212769000	0.000228000
6	0.392822000	0.570007000	-0.000094000
6	-0.188715000	1.978045000	-0.000644000
6	1.780301000	0.792843000	-0.000185000
6	2.064137000	2.160017000	-0.000263000
6	3.454822000	2.309562000	-0.000184000
6	3.954385000	0.999949000	-0.000135000
1	4.046477000	3.212769000	-0.000166000
7	-0.890019000	-2.886192000	0.000334000
7	0.890018000	2.886192000	-0.000269000
8	1.361336000	-2.300058000	-0.000003000
8	-1.361336000	2.300058000	0.000081000
6	-0.732885000	-4.327248000	0.000049000
1	-1.184982000	-4.771753000	-0.892565000
1	0.337935000	-4.534011000	0.000062000

1	-1.185057000	-4.772099000	0.892453000
6	0.732885000	4.327248000	0.000016000
1	1.185293000	4.772110000	-0.892261000
1	-0.337935000	4.534011000	-0.000272000
1	1.184746000	4.771742000	0.892756000
8	-2.935223000	-0.078003000	0.000229000
8	2.935223000	0.078003000	-0.000060000
6	5.269841000	0.466001000	-0.000069000
6	5.624714000	-0.882505000	0.000025000
16	6.690078000	1.491801000	-0.000082000
6	7.007674000	-1.089072000	0.000066000
1	4.881579000	-1.670158000	0.000058000
6	7.759556000	0.088677000	0.000003000
1	7.466723000	-2.070958000	0.000135000
6	-5.269841000	-0.466001000	0.000227000
6	-5.624714000	0.882505000	0.000187000
16	-6.690079000	-1.491801000	0.000211000
6	-7.007674000	1.089072000	0.000138000
1	-4.881579000	1.670158000	0.000195000
6	-7.759556000	-0.088677000	0.000130000
1	-7.466723000	2.070958000	0.000103000
6	-9.170853000	-0.235209000	0.000078000
6	-9.925824000	-1.424474000	0.000093000
16	-10.277729000	1.125458000	0.000030000
1	-9.476154000	-2.412665000	0.000146000
6	-11.634235000	-0.028442000	-0.000113000
6	9.170853000	0.235209000	0.000010000
6	9.925824000	1.424474000	-0.000029000
16	10.277729000	-1.125458000	0.000129000
1	9.476154000	2.412665000	-0.000075000
6	11.634235000	0.028442000	-0.000054000
6	-12.974262000	0.389763000	-0.000269000
6	12.974263000	-0.389763000	-0.000124000
6	-14.029105000	-0.560784000	-0.000361000
7	-14.916572000	-1.316733000	-0.000435000
6	-13.304060000	1.769645000	-0.000332000
7	-13.544872000	2.911386000	-0.000389000
6	13.304060000	-1.769645000	-0.000063000
7	13.544872000	-2.911386000	-0.000015000
6	14.029105000	0.560784000	-0.000248000
7	14.916573000	1.316733000	-0.000345000
7	-11.250963000	-1.314797000	-0.000021000
7	11.250963000	1.314797000	-0.000076000

S2TIIDT-CS E=-3310.800160 Hartree

6	0.362824000	-1.936318000	-0.000022000
6	0.550628000	-0.450120000	-0.000054000
6	1.917674000	-0.244978000	-0.000019000
6	2.587087000	-1.523086000	-0.000015000
6	4.429088000	-0.125045000	0.000009000
6	3.954971000	-1.472160000	-0.000001000
1	4.618110000	-2.328249000	0.000005000
6	-0.550611000	0.449518000	-0.000095000
6	-0.362660000	1.935692000	-0.000099000
6	-1.917687000	0.244500000	-0.000150000
6	-2.586966000	1.522685000	-0.000125000
6	-3.954855000	1.471917000	-0.000126000
6	-4.429125000	0.124858000	-0.000115000
1	-4.617896000	2.328082000	-0.000102000
7	1.639951000	-2.521358000	-0.000027000
7	-1.639728000	2.520860000	-0.000109000
8	-0.682142000	-2.570512000	-0.000023000
8	0.682384000	2.569757000	-0.000087000
6	1.874010000	-3.951705000	-0.000031000
1	2.429857000	-4.257264000	0.892377000
1	0.897819000	-4.438011000	-0.000034000
1	2.429859000	-4.257261000	-0.892440000
6	-1.873641000	3.951230000	-0.000100000
1	-2.429468000	4.256836000	0.892305000
1	-0.897400000	4.437434000	-0.000084000
1	-2.429447000	4.256852000	-0.892512000
16	-3.077868000	-1.056159000	-0.000234000
16	3.077697000	1.055818000	-0.000002000
6	-5.745762000	-0.301619000	-0.000079000
6	-6.234096000	-1.641220000	-0.000110000
16	-7.115933000	0.823907000	-0.000003000
6	-7.597902000	-1.748127000	-0.000058000
1	-5.565021000	-2.494411000	-0.000166000
6	-8.297436000	-0.500304000	0.000010000
1	-8.115633000	-2.698418000	-0.000067000
6	5.745676000	0.301584000	0.000025000
6	6.233857000	1.641241000	0.000033000
16	7.115976000	-0.823785000	0.000037000
6	7.597651000	1.748303000	0.000048000
1	5.564685000	2.494355000	0.000027000
6	8.297327000	0.500561000	0.000054000
1	8.115273000	2.698654000	0.000057000

6	-9.675762000	-0.283571000	0.000073000
6	-10.236268000	1.047727000	0.000133000
6	-10.607240000	-1.390302000	0.000078000
6	-11.575018000	1.263047000	0.000195000
1	-9.558429000	1.897826000	0.000128000
6	-11.949263000	-1.194303000	0.000139000
1	-10.218988000	-2.403678000	0.000031000
6	-12.538356000	0.151784000	0.000208000
1	-11.990055000	2.265916000	0.000239000
1	-12.644074000	-2.028134000	0.000140000
6	9.675677000	0.283985000	0.000069000
6	10.236334000	-1.047250000	0.000073000
6	10.607030000	1.390821000	0.000081000
6	11.575109000	-1.262418000	0.000089000
1	9.558592000	-1.897426000	0.000064000
6	11.949075000	1.194974000	0.000096000
1	10.218663000	2.404153000	0.000077000
6	12.538321000	-0.151045000	0.000102000
1	11.990260000	-2.265240000	0.000092000
1	12.643791000	2.028885000	0.000104000
8	-13.759803000	0.339515000	0.000254000
8	13.759789000	-0.338638000	0.000114000

S3TIIDT-CS E=-4281.538963 Hartree

6	0.286237000	1.949697000	-0.000007000
6	0.531683000	0.469368000	-0.000025000
6	1.906222000	0.318051000	-0.000029000
6	2.522716000	1.621496000	-0.000028000
6	4.415411000	0.295870000	-0.000039000
6	3.893383000	1.622773000	-0.000035000
1	4.522512000	2.504106000	-0.000035000
6	-0.531681000	-0.469309000	-0.000032000
6	-0.286225000	-1.949635000	-0.000048000
6	-1.906222000	-0.318001000	-0.000028000
6	-2.522707000	-1.621451000	-0.000033000
6	-3.893373000	-1.622739000	-0.000024000
6	-4.415412000	-0.295841000	-0.000013000
1	-4.522494000	-2.504077000	-0.000025000
7	1.539556000	2.583065000	-0.000022000
7	-1.539539000	-2.583012000	-0.000044000
8	-0.783403000	2.538690000	-0.000010000
8	0.783420000	-2.538619000	-0.000058000
6	1.719578000	4.022769000	-0.000023000

1	2.263042000	4.347668000	-0.892815000
1	0.726125000	4.472391000	-0.000015000
1	2.263058000	4.347667000	0.892760000
6	-1.719550000	-4.022717000	-0.000054000
1	-2.263023000	-4.347613000	-0.892842000
1	-0.726093000	-4.472331000	-0.000061000
1	-2.263016000	-4.347627000	0.892733000
16	-3.114735000	0.936284000	-0.000017000
16	3.114724000	-0.936243000	-0.000040000
6	-5.750836000	0.082141000	-0.000001000
6	-6.289018000	1.398607000	0.000012000
16	-7.072112000	-1.101401000	0.000004000
6	-7.659500000	1.452147000	0.000021000
1	-5.654834000	2.277890000	0.000012000
6	-8.295485000	0.177535000	0.000017000
1	-8.228723000	2.374248000	0.000031000
6	5.750832000	-0.082124000	-0.000044000
6	6.289001000	-1.398596000	-0.000050000
16	7.072119000	1.101405000	-0.000046000
6	7.659482000	-1.452149000	-0.000051000
1	5.654808000	-2.277872000	-0.000052000
6	8.295480000	-0.177544000	-0.000041000
1	8.228696000	-2.374256000	-0.000055000
6	-9.658105000	-0.087709000	0.000024000
6	-10.300474000	-1.361495000	0.000022000
16	-10.915357000	1.154793000	0.000038000
1	-9.744089000	-2.295214000	0.000015000
6	-12.141066000	-0.140790000	0.000039000
6	9.658103000	0.087686000	-0.000035000
6	10.300486000	1.361465000	-0.000045000
16	10.915341000	-1.154830000	-0.000048000
1	9.744111000	2.295190000	-0.000047000
6	12.141064000	0.140740000	0.000039000
6	-13.504180000	0.115661000	0.000048000
6	13.504174000	-0.115727000	0.000103000
6	-14.448440000	-0.949726000	0.000049000
7	-15.246489000	-1.798184000	0.000051000
6	-13.987644000	1.453024000	0.000058000
7	-14.350425000	2.561101000	0.000066000
6	13.987624000	-1.453095000	0.000094000
7	14.350391000	-2.561176000	0.000116000
6	14.448447000	0.949650000	0.000152000
7	15.246505000	1.798098000	0.000186000
7	-11.611653000	-1.394897000	0.000030000

7	11.611664000	1.394852000	0.000008000
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S2TIIDT-OS E=-3310.801790 Hartree

6	-0.365206000	-1.932923000	0.000014000
6	-0.546083000	-0.442353000	0.000004000
6	-1.926796000	-0.234207000	0.000023000
6	-2.586105000	-1.498734000	-0.000002000
6	-4.428888000	-0.108122000	0.000023000
6	-3.965568000	-1.445469000	-0.000006000
1	-4.628113000	-2.302060000	-0.000026000
6	0.546088000	0.442571000	-0.000008000
6	0.365264000	1.933149000	-0.000006000
6	1.926791000	0.234380000	-0.000024000
6	2.586148000	1.498879000	-0.000046000
6	3.965608000	1.445556000	-0.000061000
6	4.428874000	0.108190000	-0.000033000
1	4.628190000	2.302120000	-0.000076000
7	-1.642598000	-2.507713000	-0.000024000
7	1.642678000	2.507894000	-0.000055000
8	0.680035000	-2.568497000	-0.000034000
8	-0.679948000	2.568771000	-0.000047000
6	-1.887619000	-3.935957000	-0.000071000
1	-2.445735000	-4.237905000	-0.892409000
1	-0.915295000	-4.430021000	-0.000075000
1	-2.445755000	-4.237957000	0.892237000
6	1.887751000	3.936128000	-0.000100000
1	2.445869000	4.238058000	-0.892443000
1	0.915446000	4.430229000	-0.000092000
1	2.445908000	4.238105000	0.892203000
16	3.086078000	-1.064628000	-0.000046000
16	-3.086140000	1.064752000	0.000047000
6	5.762763000	-0.331574000	-0.000015000
6	6.245305000	-1.657429000	-0.000002000
16	7.122438000	0.794986000	-0.000012000
6	7.623273000	-1.760013000	0.000015000
1	5.581314000	-2.514453000	-0.000003000
6	8.306740000	-0.520256000	0.000012000
1	8.142483000	-2.709670000	0.000028000
6	-5.762795000	0.331586000	0.000030000
6	-6.245391000	1.657421000	0.000058000
16	-7.122423000	-0.795030000	0.000003000
6	-7.623364000	1.759948000	0.000058000
1	-5.581436000	2.514472000	0.000078000

6	-8.306779000	0.520163000	0.000029000
1	-8.142612000	2.709584000	0.000077000
6	9.698854000	-0.285506000	0.000025000
6	10.240917000	1.046517000	0.000020000
6	10.634168000	-1.380802000	0.000045000
6	11.582021000	1.275887000	0.000032000
1	9.556080000	1.890744000	0.000005000
6	11.978500000	-1.172069000	0.000058000
1	10.255241000	-2.397615000	0.000050000
6	12.550926000	0.176269000	0.000053000
1	11.986395000	2.283051000	0.000027000
1	12.680507000	-1.999813000	0.000073000
6	-9.698884000	0.285356000	0.000020000
6	-10.240892000	-1.046689000	-0.000012000
6	-10.634242000	1.380613000	0.000043000
6	-11.581987000	-1.276114000	-0.000020000
1	-9.556021000	-1.890888000	-0.000030000
6	-11.978566000	1.171826000	0.000035000
1	-10.255357000	2.397442000	0.000068000
6	-12.550937000	-0.176535000	0.000003000
1	-11.986319000	-2.283295000	-0.000044000
1	-12.680607000	1.999541000	0.000053000
8	13.775430000	0.375962000	0.000063000
8	-13.775433000	-0.376279000	-0.000005000

S3TIIDT-OS E=-4281.541349 Hartree

6	-0.289530000	-1.946510000	-0.000082000
6	-0.526732000	-0.460760000	-0.000211000
6	-1.917548000	-0.306003000	-0.000211000
6	-2.523494000	-1.593216000	-0.000125000
6	-4.416594000	-0.275245000	-0.000208000
6	-3.906992000	-1.592038000	-0.000123000
1	-4.535707000	-2.473779000	-0.000068000
6	0.526727000	0.460620000	-0.000295000
6	0.289499000	1.946364000	-0.000422000
6	1.917548000	0.305885000	-0.000350000
6	2.523469000	1.593112000	-0.000249000
6	3.906968000	1.591963000	-0.000180000
6	4.416596000	0.275181000	-0.000242000
1	4.535663000	2.473718000	-0.000082000
7	-1.543402000	-2.567515000	-0.000066000
7	1.543359000	2.567392000	-0.000193000
8	0.780470000	-2.537468000	-0.000050000

8	-0.780514000	2.537298000	-0.000145000
6	-1.736649000	-4.005015000	0.000014000
1	-2.283040000	-4.325931000	-0.892622000
1	-0.747447000	-4.464027000	0.000051000
1	-2.283057000	-4.325826000	0.892678000
6	1.736579000	4.004896000	0.000029000
1	2.283066000	4.325888000	-0.892521000
1	0.747368000	4.463889000	-0.000014000
1	2.282881000	4.325651000	0.892778000
16	3.124177000	-0.946730000	-0.000398000
16	-3.124149000	0.946638000	-0.000303000
6	5.771511000	-0.117258000	-0.000190000
6	6.302023000	-1.419790000	-0.000260000
16	7.081458000	1.065826000	-0.000036000
6	7.687794000	-1.468491000	-0.000163000
1	5.672901000	-2.302480000	-0.000369000
6	8.307425000	-0.203915000	-0.000014000
1	8.257072000	-2.390712000	-0.000188000
6	-5.771501000	0.117223000	-0.000233000
6	-6.301982000	1.419768000	-0.000352000
16	-7.081474000	-1.065831000	-0.000141000
6	-7.687752000	1.468500000	-0.000338000
1	-5.672841000	2.302443000	-0.000442000
6	-8.307412000	0.203938000	-0.000190000
1	-8.257009000	2.390733000	-0.000416000
6	9.682721000	0.086569000	0.000122000
6	10.306857000	1.357876000	0.000269000
16	10.940911000	-1.144103000	0.000143000
1	9.746846000	2.288586000	0.000288000
6	12.158651000	0.156770000	0.000323000
6	-9.682714000	-0.086514000	-0.000118000
6	-10.306881000	-1.357805000	-0.000055000
16	-10.940874000	1.144188000	-0.000257000
1	-9.746891000	-2.288529000	-0.000025000
6	-12.158645000	-0.156656000	0.000247000
6	13.531060000	-0.100068000	0.000403000
6	-13.531047000	0.100215000	0.000557000
6	14.470391000	0.967045000	0.000537000
7	15.265144000	1.819292000	0.000653000
6	14.018354000	-1.434155000	0.000339000
7	14.387152000	-2.540738000	0.000283000
6	-14.018308000	1.434314000	0.000505000
7	-14.387079000	2.540905000	0.000520000
6	-14.470405000	-0.966874000	0.000908000

7	-15.265178000	-1.819101000	0.001178000
7	11.627828000	1.398618000	0.000373000
7	-11.627852000	-1.398517000	0.000188000

S2TIIDT-T1 E=-3310.796035 Hartree

6	0.366436000	-1.930765000	0.000046000
6	0.538044000	-0.430769000	0.000060000
6	1.941437000	-0.219133000	0.000051000
6	2.584319000	-1.465229000	0.000042000
6	4.430562000	-0.086032000	0.000026000
6	3.979347000	-1.411324000	0.000030000
1	4.640570000	-2.268971000	0.000019000
6	-0.538042000	0.430711000	0.000074000
6	-0.366421000	1.930705000	0.000067000
6	-1.941438000	0.219087000	0.000104000
6	-2.584308000	1.465190000	0.000093000
6	-3.979337000	1.411302000	0.000095000
6	-4.430565000	0.086014000	0.000090000
1	-4.640550000	2.268955000	0.000079000
7	1.642713000	-2.489647000	0.000046000
7	-1.642692000	2.489600000	0.000078000
8	-0.679579000	-2.565876000	0.000047000
8	0.679602000	2.565804000	0.000048000
6	1.904264000	-3.914576000	0.000043000
1	2.466054000	-4.210710000	0.892220000
1	0.938086000	-4.420613000	0.000045000
1	2.466049000	-4.210707000	-0.892139000
6	-1.904229000	3.914531000	0.000069000
1	-2.466005000	4.210677000	0.892251000
1	-0.938046000	4.420558000	0.000056000
1	-2.466021000	4.210662000	-0.892108000
16	-3.099308000	-1.076006000	0.000159000
16	3.099292000	1.075974000	0.000057000
6	-5.786145000	-0.370121000	0.000057000
6	-6.262657000	-1.680450000	0.000067000
16	-7.132072000	0.758895000	0.000000000
6	-7.657333000	-1.777025000	0.000025000
1	-5.604746000	-2.542022000	0.000104000
6	-8.321527000	-0.545227000	-0.000018000
1	-8.179479000	-2.725299000	0.000025000
6	5.786136000	0.370118000	0.000006000
6	6.262634000	1.680452000	0.000005000
16	7.132076000	-0.758884000	-0.000021000

6	7.657309000	1.777042000	-0.000019000
1	5.604713000	2.542016000	0.000020000
6	8.321517000	0.545251000	-0.000036000
1	8.179445000	2.725321000	-0.000023000
6	-9.728470000	-0.287072000	-0.000068000
6	-10.247637000	1.046854000	-0.000107000
6	-10.670274000	-1.368037000	-0.000080000
6	-11.590546000	1.294581000	-0.000156000
1	-9.553100000	1.882832000	-0.000098000
6	-12.016437000	-1.142388000	-0.000128000
1	-10.303317000	-2.389138000	-0.000050000
6	-12.567773000	0.209649000	-0.000171000
1	-11.981133000	2.307121000	-0.000186000
1	-12.728143000	-1.961787000	-0.000137000
6	9.728462000	0.287111000	-0.000062000
6	10.247644000	-1.046808000	-0.000077000
6	10.670254000	1.368087000	-0.000075000
6	11.590555000	-1.294521000	-0.000104000
1	9.553116000	-1.882794000	-0.000068000
6	12.016419000	1.142452000	-0.000101000
1	10.303286000	2.389183000	-0.000064000
6	12.567771000	-0.209579000	-0.000118000
1	11.981153000	-2.307057000	-0.000115000
1	12.728116000	1.961860000	-0.000110000
8	-13.795142000	0.424913000	-0.000214000
8	13.795142000	-0.424829000	-0.000141000

S3TIIDT-T1 E=-4281.537069 Hartree

6	0.290568000	1.944489000	-0.000448000
6	0.520650000	0.451561000	-0.000206000
6	1.929645000	0.294409000	-0.000336000
6	2.523623000	1.566602000	-0.000210000
6	4.418918000	0.256829000	-0.000189000
6	3.918901000	1.565028000	-0.000114000
1	4.546620000	2.447544000	0.000031000
6	-0.520651000	-0.451628000	-0.000036000
6	-0.290583000	-1.944559000	0.000218000
6	-1.929645000	-0.294464000	-0.000001000
6	-2.523635000	-1.566651000	0.000086000
6	-3.918913000	-1.565062000	0.000077000
6	-4.418916000	-0.256858000	0.000005000
1	-4.546641000	-2.447571000	0.000131000
7	1.544016000	2.552970000	-0.000114000

7	-1.544037000	-2.553028000	0.000131000
8	-0.780044000	2.535569000	0.000029000
8	0.780022000	-2.535651000	0.000112000
6	1.750123000	3.988144000	0.000220000
1	2.299680000	4.305065000	-0.892119000
1	0.765266000	4.456522000	0.000166000
1	2.299419000	4.304708000	0.892848000
6	-1.750157000	-3.988200000	0.000136000
1	-2.299535000	-4.304954000	-0.892374000
1	-0.765305000	-4.456588000	0.000202000
1	-2.299638000	-4.304922000	0.892593000
16	-3.133931000	0.955552000	-0.000129000
16	3.133945000	-0.955594000	-0.000428000
6	-5.790209000	0.148324000	-0.000010000
6	-6.314694000	1.440414000	-0.000099000
16	-7.090503000	-1.034592000	0.000094000
6	-7.712705000	1.485170000	-0.000093000
1	-5.689477000	2.325676000	-0.000171000
6	-8.319368000	0.227805000	0.000000000
1	-8.282370000	2.407280000	-0.000158000
6	5.790215000	-0.148338000	-0.000085000
6	6.314714000	-1.440423000	-0.000151000
16	7.090497000	1.034592000	0.000185000
6	7.712725000	-1.485164000	-0.000025000
1	5.689506000	-2.325692000	-0.000295000
6	8.319375000	-0.227793000	0.000124000
1	8.282400000	-2.407268000	-0.000059000
6	-9.703792000	-0.084052000	0.000026000
6	-10.312536000	-1.354750000	0.000121000
16	-10.963795000	1.135708000	-0.000064000
1	-9.748432000	-2.282297000	0.000188000
6	-12.174081000	-0.170699000	0.000048000
6	9.703796000	0.084079000	0.000248000
6	10.312527000	1.354783000	0.000488000
16	10.963811000	-1.135668000	0.000277000
1	9.748413000	2.282325000	0.000597000
6	12.174084000	0.170751000	0.000146000
6	-13.554118000	0.085391000	0.000042000
6	13.554123000	-0.085324000	-0.000079000
6	-14.488668000	-0.983746000	0.000131000
7	-15.280085000	-1.839681000	0.000202000
6	-14.045741000	1.416352000	-0.000054000
7	-14.420668000	2.521281000	-0.000135000
6	14.045760000	-1.416279000	-0.000242000

7	14.420699000	-2.521204000	-0.000405000
6	14.488662000	0.983824000	-0.000111000
7	15.280070000	1.839766000	-0.000130000
7	-11.641146000	-1.402661000	0.000133000
7	11.641135000	1.402709000	0.000398000

S2IIDS0-CS E=-1298.683180 Hartree

6	-1.161315000	1.195028000	-0.273365000
6	-0.283480000	0.047492000	-0.130535000
6	-0.908405000	-1.212005000	0.130536000
6	-2.266673000	-1.294905000	0.230514000
6	-3.146453000	-0.155119000	0.071626000
6	-2.519878000	1.115225000	-0.188187000
6	0.972045000	1.971225000	-0.462826000
6	1.035706000	0.486273000	-0.229187000
1	-0.296316000	-2.098784000	0.213218000
1	-2.698666000	-2.271181000	0.404554000
1	-3.113301000	2.014579000	-0.280688000
6	2.270776000	-0.243453000	-0.188933000
6	3.553626000	0.164669000	0.164229000
6	2.375343000	-1.681312000	-0.609139000
6	4.458358000	-0.968885000	-0.008390000
6	4.106184000	1.382421000	0.689587000
6	5.783141000	-0.911499000	0.278921000
6	5.430071000	1.451178000	0.986370000
1	3.463451000	2.242050000	0.813932000
6	6.338923000	0.327156000	0.795007000
1	6.435686000	-1.767173000	0.139661000
1	5.849478000	2.372701000	1.379226000
8	1.507130000	-2.442164000	-1.013932000
8	1.879215000	2.772519000	-0.637519000
7	3.719188000	-2.037802000	-0.482583000
7	-0.380954000	2.317875000	-0.478002000
6	-0.853895000	3.668797000	-0.692853000
1	-1.486682000	3.725348000	-1.585034000
1	-1.422915000	4.028525000	0.171443000
1	0.024632000	4.299177000	-0.833989000
6	4.227505000	-3.351909000	-0.811493000
1	4.978609000	-3.294293000	-1.606725000
1	4.674672000	-3.831360000	0.066343000
1	3.381635000	-3.947269000	-1.156818000
6	-4.552261000	-0.284482000	0.169526000
6	-5.443484000	0.813702000	-0.139030000

6	-5.184450000	-1.518494000	0.585508000
6	-6.792741000	0.704304000	-0.050594000
1	-5.024701000	1.752728000	-0.481778000
6	-6.531121000	-1.646369000	0.691876000
1	-4.564764000	-2.367010000	0.849357000
6	-7.443758000	-0.540162000	0.378705000
1	-7.446632000	1.533827000	-0.301051000
1	-6.987255000	-2.575061000	1.020143000
6	7.658534000	0.443055000	1.099114000
8	-8.671886000	-0.647111000	0.468785000
1	8.347804000	-0.384135000	0.963674000
1	8.068165000	1.369273000	1.488040000

S3IIDS0-CS E=-1784.057381 Hartree

6	5.305557000	-1.166314000	-0.008754000
6	4.507492000	0.038712000	0.196064000
6	5.158464000	1.179009000	0.775825000
6	6.479656000	1.115593000	1.089240000
6	7.283878000	-0.077933000	0.862207000
6	6.626693000	-1.240685000	0.294095000
6	3.175696000	-1.666817000	-0.655710000
6	3.195322000	-0.239039000	-0.187404000
1	4.595080000	2.087907000	0.929097000
1	6.974778000	1.979053000	1.523349000
1	7.200766000	-2.146335000	0.128783000
6	2.035793000	0.599650000	-0.219195000
6	0.677084000	0.281974000	-0.171882000
6	2.113845000	2.096169000	-0.392071000
6	-0.084280000	1.512867000	-0.286299000
6	-0.060689000	-0.927863000	0.018926000
6	-1.447482000	1.556647000	-0.238920000
6	-1.424634000	-0.892855000	0.072642000
1	0.469597000	-1.866520000	0.090634000
6	-2.175761000	0.331338000	-0.057789000
1	-1.968630000	2.501366000	-0.328538000
1	-1.967801000	-1.821401000	0.214039000
8	3.095244000	2.813950000	-0.511610000
8	2.247535000	-2.330670000	-1.095308000
7	0.800277000	2.565340000	-0.428010000
7	4.479725000	-2.145697000	-0.530239000
6	4.872995000	-3.488755000	-0.901475000

1	5.636459000	-3.469908000	-1.686428000
1	5.263346000	-4.035915000	-0.036497000
1	3.982340000	-3.993691000	-1.276542000
6	0.457354000	3.962429000	-0.597527000
1	-0.141268000	4.110946000	-1.502329000
1	-0.100733000	4.337128000	0.267232000
1	1.392471000	4.515370000	-0.690254000
6	8.604947000	-0.093268000	1.183587000
6	-3.577665000	0.325286000	-0.002459000
6	-4.462240000	1.440976000	-0.116412000
16	-4.571437000	-1.115954000	0.230074000
1	-4.111911000	2.456654000	-0.267975000
6	-6.024894000	-0.094218000	0.153663000
6	-7.311770000	-0.598402000	0.275338000
6	-7.531663000	-1.989495000	0.472872000
7	-7.683167000	-3.134145000	0.634742000
6	-8.443293000	0.263029000	0.206803000
7	-9.390392000	0.939271000	0.155861000
7	-5.754424000	1.227092000	-0.034906000
1	9.218756000	-0.973672000	1.023129000
1	9.090946000	0.776824000	1.612123000

S2IIDS0-OS E=-1298.684448 Hartree

6	-1.160413000	1.175277000	-0.231549000
6	-0.300716000	0.026437000	-0.122281000
6	-0.927865000	-1.225807000	0.100408000
6	-2.298967000	-1.304169000	0.194971000
6	-3.152599000	-0.162974000	0.061609000
6	-2.529234000	1.102052000	-0.157236000
6	0.971841000	1.970914000	-0.367189000
6	1.045225000	0.476307000	-0.192115000
1	-0.325123000	-2.120001000	0.160319000
1	-2.742689000	-2.283034000	0.326602000
1	-3.120546000	2.007019000	-0.211771000
6	2.269681000	-0.239845000	-0.164227000
6	3.582225000	0.178942000	0.138292000
6	2.370205000	-1.697317000	-0.539140000
6	4.468365000	-0.959807000	-0.024946000
6	4.157250000	1.397815000	0.614041000
6	5.806026000	-0.908068000	0.222843000
6	5.495888000	1.464373000	0.873560000
1	3.527262000	2.266357000	0.736414000
6	6.385085000	0.333967000	0.686050000

1	6.443876000	-1.775498000	0.088813000
1	5.929473000	2.393752000	1.230735000
8	1.497705000	-2.474315000	-0.901150000
8	1.872427000	2.787798000	-0.510744000
7	3.715082000	-2.044455000	-0.443746000
7	-0.379697000	2.308583000	-0.387107000
6	-0.857792000	3.663487000	-0.561027000
1	-1.483011000	3.746033000	-1.456569000
1	-1.437270000	3.990847000	0.309236000
1	0.018193000	4.303025000	-0.672800000
6	4.217734000	-3.366816000	-0.747926000
1	4.947851000	-3.329711000	-1.563599000
1	4.689375000	-3.819309000	0.131391000
1	3.365174000	-3.973855000	-1.053749000
6	-4.584690000	-0.283878000	0.145836000
6	-5.454679000	0.758638000	-0.323727000
6	-5.210832000	-1.449488000	0.705983000
6	-6.812492000	0.656507000	-0.252404000
1	-5.020756000	1.636379000	-0.790187000
6	-6.565930000	-1.566877000	0.803196000
1	-4.587848000	-2.242867000	1.103290000
6	-7.464239000	-0.517870000	0.324980000
1	-7.461550000	1.439503000	-0.631754000
1	-7.028593000	-2.441471000	1.249515000
6	7.723720000	0.444532000	0.948041000
8	-8.701478000	-0.616865000	0.403289000
1	8.399443000	-0.393693000	0.813293000
1	8.153040000	1.376672000	1.299387000

S3IIDS0-OS E=-1784.058489 Hartree

6	5.320089000	-1.158976000	-0.012562000
6	4.539254000	0.052292000	0.169858000
6	5.212710000	1.201296000	0.688243000
6	6.547450000	1.139357000	0.967023000
6	7.332967000	-0.062070000	0.758538000
6	6.652894000	-1.234743000	0.253866000
6	3.172487000	-1.688967000	-0.573114000
6	3.199682000	-0.237373000	-0.162689000
1	4.661781000	2.119451000	0.827683000
1	7.057631000	2.015209000	1.356458000
1	7.212578000	-2.151987000	0.104152000
6	2.047839000	0.589486000	-0.192745000
6	0.666648000	0.265461000	-0.158654000

6	2.116510000	2.089607000	-0.339060000
6	-0.081399000	1.493083000	-0.258763000
6	-0.072529000	-0.932901000	0.019356000
6	-1.451510000	1.544590000	-0.215619000
6	-1.446324000	-0.891874000	0.069714000
1	0.448677000	-1.876310000	0.086716000
6	-2.180982000	0.328250000	-0.051873000
1	-1.965105000	2.494417000	-0.295966000
1	-1.990230000	-1.821631000	0.200747000
8	3.091858000	2.819850000	-0.445917000
8	2.237076000	-2.372358000	-0.964229000
7	0.802751000	2.550774000	-0.381042000
7	4.478288000	-2.158798000	-0.470638000
6	4.863832000	-3.514355000	-0.802629000
1	5.605270000	-3.522994000	-1.608568000
1	5.279916000	-4.028045000	0.070832000
1	3.964598000	-4.034417000	-1.133662000
6	0.454774000	3.948136000	-0.535114000
1	-0.138578000	4.105378000	-1.442020000
1	-0.111385000	4.309306000	0.330289000
1	1.387833000	4.506491000	-0.614271000
6	8.671268000	-0.078933000	1.040712000
6	-3.602389000	0.336671000	-0.004920000
6	-4.473334000	1.449074000	-0.118110000
16	-4.593479000	-1.099878000	0.214031000
1	-4.122554000	2.464974000	-0.263182000
6	-6.044535000	-0.078199000	0.134049000
6	-7.338796000	-0.591402000	0.246752000
6	-7.557188000	-1.982165000	0.435163000
7	-7.709662000	-3.128169000	0.589888000
6	-8.469662000	0.267484000	0.176467000
7	-9.417292000	0.943729000	0.123528000
7	-5.775939000	1.233969000	-0.044726000
1	9.271533000	-0.970444000	0.891590000
1	9.176650000	0.801240000	1.423484000

S2IIDS0-T1 E=-1298.677257 Hartree

6	-1.162105000	1.147425000	-0.151431000
6	-0.328855000	-0.003282000	-0.085183000
6	-0.960117000	-1.244720000	0.075785000
6	-2.350229000	-1.316374000	0.144401000

6	-3.165552000	-0.170992000	0.050554000
6	-2.544024000	1.087559000	-0.098064000
6	0.970977000	1.966483000	-0.209573000
6	1.060631000	0.460182000	-0.116862000
1	-0.369804000	-2.146766000	0.118079000
1	-2.813140000	-2.293392000	0.228756000
1	-3.134788000	1.995845000	-0.123624000
6	2.265776000	-0.232882000	-0.110992000
6	3.628380000	0.201566000	0.098133000
6	2.362414000	-1.721930000	-0.400879000
6	4.482971000	-0.945119000	-0.048274000
6	4.239323000	1.423116000	0.471768000
6	5.840678000	-0.903849000	0.122280000
6	5.603176000	1.485421000	0.655217000
1	3.630566000	2.306333000	0.588106000
6	6.457750000	0.343347000	0.481439000
1	6.453706000	-1.790593000	0.000098000
1	6.060882000	2.429191000	0.936263000
8	1.482330000	-2.525824000	-0.672991000
8	1.860005000	2.805307000	-0.294466000
7	3.706614000	-2.054437000	-0.361867000
7	-0.378079000	2.290355000	-0.242468000
6	-0.863764000	3.649041000	-0.353267000
1	-1.477348000	3.772051000	-1.252305000
1	-1.459497000	3.925641000	0.523719000
1	0.008085000	4.300170000	-0.418737000
6	4.200505000	-3.390800000	-0.616166000
1	4.886192000	-3.396499000	-1.470264000
1	4.722549000	-3.788296000	0.261178000
1	3.337844000	-4.018512000	-0.840055000
6	-4.633508000	-0.279053000	0.104749000
6	-5.460325000	0.636537000	-0.604339000
6	-5.263554000	-1.300295000	0.869834000
6	-6.829653000	0.547106000	-0.562063000
1	-4.991255000	1.398691000	-1.218899000
6	-6.630677000	-1.406494000	0.934315000
1	-4.644132000	-1.985392000	1.439845000
6	-7.494858000	-0.483995000	0.216944000
1	-7.463042000	1.233457000	-1.115055000
1	-7.114663000	-2.173938000	1.529967000
6	7.828333000	0.443944000	0.661428000
8	-8.745309000	-0.572424000	0.266884000
1	8.480147000	-0.413557000	0.532752000
1	8.289595000	1.386028000	0.936584000

S3IIDS0-T1 E=-1784.050723 Hartree

6	5.353522000	-1.127051000	-0.064708000
6	4.593472000	0.077313000	0.138857000
6	5.291032000	1.215838000	0.613003000
6	6.647830000	1.149167000	0.836286000
6	7.409101000	-0.048474000	0.605713000
6	6.703122000	-1.212748000	0.144255000
6	3.188695000	-1.692423000	-0.525436000
6	3.209572000	-0.222552000	-0.134906000
1	4.754053000	2.137819000	0.773989000
1	7.173754000	2.028912000	1.194621000
1	7.244656000	-2.137808000	-0.022720000
6	2.067768000	0.573289000	-0.126531000
6	0.646088000	0.228686000	-0.158078000
6	2.108668000	2.082219000	-0.129498000
6	-0.086710000	1.450228000	-0.175667000
6	-0.088349000	-0.963836000	-0.087648000
6	-1.468486000	1.504915000	-0.159139000
6	-1.479694000	-0.924666000	-0.068079000
1	0.424834000	-1.912692000	-0.078070000
6	-2.191336000	0.291044000	-0.113317000
1	-1.981160000	2.459287000	-0.146132000
1	-2.024494000	-1.863115000	-0.045865000
8	3.066433000	2.845211000	-0.139865000
8	2.250926000	-2.394926000	-0.873574000
7	0.791493000	2.523299000	-0.178393000
7	4.497316000	-2.141861000	-0.474788000
6	4.884591000	-3.497091000	-0.805994000
1	5.595459000	-3.505566000	-1.639004000
1	5.340792000	-3.994717000	0.056674000
1	3.980166000	-4.031796000	-1.096359000
6	0.426482000	3.923703000	-0.218752000
1	-0.146871000	4.151355000	-1.123772000
1	-0.168015000	4.199907000	0.659114000
1	1.352345000	4.499061000	-0.223620000
6	8.775559000	-0.076951000	0.828798000
6	-3.645332000	0.316684000	-0.114225000
6	-4.492334000	1.359892000	-0.508370000
16	-4.628676000	-1.028973000	0.402173000
1	-4.133313000	2.306436000	-0.895621000
6	-6.077247000	-0.070916000	0.036344000
6	-7.384873000	-0.572672000	0.229195000

6	-7.600415000	-1.884504000	0.720107000
7	-7.754981000	-2.968092000	1.125598000
6	-8.515220000	0.231686000	-0.064820000
7	-9.464354000	0.868552000	-0.296905000
7	-5.813407000	1.151494000	-0.427568000
1	9.357996000	-0.976083000	0.658374000
1	9.304219000	0.801865000	1.181212000

S1TIIDS0-CS E=-1768.019941 Hartree

6	5.279039000	-1.202788000	-0.013341000
6	4.499106000	0.013245000	0.198915000
6	5.166727000	1.137151000	0.793408000
6	6.483864000	1.047754000	1.115469000
6	7.269724000	-0.157739000	0.883550000
6	6.595974000	-1.303166000	0.298537000
6	3.145587000	-1.657596000	-0.682243000
6	3.186669000	-0.236956000	-0.195779000
1	4.617768000	2.054439000	0.950065000
1	6.991079000	1.898549000	1.560666000
1	7.155471000	-2.217098000	0.128397000
6	2.040222000	0.623096000	-0.224171000
6	0.677479000	0.326384000	-0.179384000
6	2.143833000	2.116101000	-0.385346000
6	-0.065454000	1.570059000	-0.285348000
6	-0.080183000	-0.873085000	0.001304000
6	-1.427228000	1.634388000	-0.238605000
6	-1.442863000	-0.817217000	0.054397000
1	0.435058000	-1.820692000	0.065124000
6	-2.177007000	0.419529000	-0.066958000
1	-1.934371000	2.587455000	-0.321159000
1	-1.997188000	-1.740523000	0.187710000
8	3.136331000	2.820969000	-0.497395000
8	2.209355000	-2.299890000	-1.137316000
7	0.837018000	2.608169000	-0.418733000
7	4.439948000	-2.161999000	-0.551428000
6	4.811694000	-3.507360000	-0.934539000
1	5.582245000	-3.494165000	-1.712797000
1	5.184721000	-4.071802000	-0.072902000
1	3.915041000	-3.991417000	-1.322802000
6	0.519087000	4.011517000	-0.577322000
1	-0.076172000	4.178607000	-1.481357000
1	-0.033135000	4.390061000	0.289800000
1	1.464275000	4.548143000	-0.664915000

6	8.587511000	-0.199756000	1.214687000
6	-3.576943000	0.439047000	-0.013162000
6	-4.445455000	1.564356000	-0.121225000
16	-4.548694000	-1.031301000	0.214550000
6	-5.779449000	1.274107000	-0.028630000
1	-4.072656000	2.570540000	-0.267017000
6	-6.049252000	-0.117706000	0.161326000
1	-6.579080000	2.002163000	-0.088992000
6	-7.300187000	-0.710651000	0.291192000
6	-8.476102000	0.089995000	0.238727000
7	-9.422849000	0.768805000	0.192465000
6	-7.444537000	-2.112644000	0.478861000
7	-7.534543000	-3.265035000	0.632491000
1	9.085585000	0.657322000	1.655433000
1	9.186813000	-1.089364000	1.050153000

S2TIIDS0-CS E=-1850.500703 Hartree

6	0.747245000	1.690987000	-0.284109000
6	1.412831000	0.405410000	-0.196269000
6	0.583032000	-0.747365000	-0.051303000
6	-0.776991000	-0.610322000	-0.014155000
6	-1.432669000	0.666836000	-0.116938000
6	-0.610595000	1.835567000	-0.252282000
6	2.988364000	2.105917000	-0.343454000
6	2.795379000	0.623291000	-0.217685000
1	1.038692000	-1.725847000	-0.002014000
1	-1.386919000	-1.501723000	0.091723000
1	-1.057880000	2.819515000	-0.320602000
6	3.887785000	-0.304518000	-0.189628000
6	5.208454000	-0.140943000	0.223787000
6	3.768858000	-1.713074000	-0.699257000
6	5.916886000	-1.397902000	0.003427000
6	5.937131000	0.931414000	0.841795000
6	7.220473000	-1.584199000	0.331254000
6	7.241696000	0.756814000	1.180045000
1	5.443338000	1.878964000	1.002505000
6	7.956275000	-0.491391000	0.942379000
1	7.724410000	-2.528947000	0.155292000
1	7.793849000	1.569302000	1.643202000
8	2.803357000	-2.292980000	-1.177658000
8	4.020651000	2.758763000	-0.426950000
7	5.028462000	-2.297310000	-0.559415000

7	1.711893000	2.675661000	-0.383478000
6	1.481318000	4.097646000	-0.514628000
1	0.910555000	4.321267000	-1.422593000
1	0.939662000	4.491200000	0.352857000
1	2.458705000	4.577346000	-0.577113000
6	5.323147000	-3.656412000	-0.957908000
1	6.104180000	-3.679566000	-1.725644000
1	5.649556000	-4.255578000	-0.100576000
1	4.404167000	-4.079127000	-1.365338000
6	-2.835113000	0.771984000	-0.080775000
6	-3.629678000	1.946868000	-0.173588000
16	-3.899044000	-0.630015000	0.099002000
6	-4.983120000	1.733748000	-0.104647000
1	-3.195645000	2.931943000	-0.290956000
6	-5.360957000	0.367070000	0.048560000
1	-5.710674000	2.533038000	-0.161616000
6	9.264228000	-0.620278000	1.290558000
6	-6.649346000	-0.168682000	0.149125000
6	-6.872938000	-1.586342000	0.301890000
6	-7.816950000	0.681735000	0.104481000
6	-8.120920000	-2.109484000	0.401063000
1	-6.011662000	-2.248646000	0.337605000
6	-9.072795000	0.176996000	0.202181000
1	-7.682869000	1.752541000	-0.010134000
6	-9.321366000	-1.262204000	0.358843000
1	-8.282608000	-3.176580000	0.515685000
1	-9.946677000	0.819849000	0.168295000
8	-10.462197000	-1.730387000	0.449326000
1	9.808297000	0.197872000	1.750495000
1	9.809261000	-1.543203000	1.120824000

S3TIIDS0-CS E=-2335.871539 Hartree

6	1.808275000	1.676595000	-0.274927000
6	2.467368000	0.388525000	-0.192790000
6	1.633471000	-0.762267000	-0.064598000
6	0.272954000	-0.620645000	-0.038470000
6	-0.374957000	0.659159000	-0.136920000
6	0.449434000	1.825460000	-0.254348000
6	4.048042000	2.090010000	-0.309969000
6	3.852130000	0.601907000	-0.198502000
1	2.085229000	-1.742567000	-0.018382000
1	-0.340093000	-1.511231000	0.054933000
1	0.005911000	2.811220000	-0.318200000

6	4.940928000	-0.324962000	-0.172374000
6	6.265376000	-0.163455000	0.240000000
6	4.819236000	-1.734158000	-0.682426000
6	6.969271000	-1.421159000	0.014005000
6	6.994716000	0.903946000	0.862812000
6	8.274191000	-1.610494000	0.337234000
6	8.300628000	0.726070000	1.197297000
1	6.503003000	1.850852000	1.031764000
6	9.011679000	-0.521097000	0.950241000
1	8.776478000	-2.554908000	0.155734000
1	8.854237000	1.535159000	1.664339000
8	3.851422000	-2.311858000	-1.157645000
8	5.082456000	2.738418000	-0.380671000
7	6.078699000	-2.317832000	-0.549099000
7	2.774258000	2.661226000	-0.356454000
6	2.545585000	4.085557000	-0.478235000
1	1.983016000	4.315533000	-1.389362000
1	1.997106000	4.471326000	0.388077000
1	3.523246000	4.565755000	-0.528702000
6	6.372342000	-3.676719000	-0.952180000
1	7.150203000	-3.696905000	-1.722927000
1	6.701914000	-4.276915000	-0.097036000
1	5.452236000	-4.099093000	-1.357075000
6	-1.781372000	0.769696000	-0.113140000
6	-2.570216000	1.942820000	-0.203471000
16	-2.845153000	-0.637012000	0.045734000
6	-3.928955000	1.730527000	-0.148332000
1	-2.134667000	2.928442000	-0.308865000
6	-4.296364000	0.366699000	-0.010191000
1	-4.667593000	2.521589000	-0.204076000
6	10.321126000	-0.652274000	1.293777000
6	-5.581936000	-0.163081000	0.074315000
6	-5.957985000	-1.528137000	0.212837000
16	-7.058374000	0.805556000	0.024451000
1	-5.228626000	-2.331930000	0.267537000
6	-8.004288000	-0.697191000	0.192407000
6	-9.393184000	-0.707380000	0.233011000
6	-10.127880000	0.505810000	0.140133000
7	-10.701202000	1.518418000	0.061631000
6	-10.111207000	-1.928439000	0.368628000
7	-10.729316000	-2.909861000	0.479012000
7	-7.239404000	-1.816557000	0.275896000
1	10.867004000	0.163465000	1.755790000
1	10.865118000	-1.574680000	1.118175000

S4TIIDS0-CS E=-2301.899461 Hartree

6	1.280030000	1.766986000	-0.277839000
6	1.921258000	0.466257000	-0.207383000
6	1.068078000	-0.674043000	-0.083973000
6	-0.287614000	-0.512185000	-0.049167000
6	-0.920984000	0.781133000	-0.134056000
6	-0.073239000	1.937059000	-0.248869000
6	3.529636000	2.136606000	-0.322528000
6	3.305083000	0.656740000	-0.220654000
1	1.505307000	-1.661610000	-0.049188000
1	-0.915156000	-1.392935000	0.040094000
1	-0.500908000	2.930531000	-0.302777000
6	4.379441000	-0.294860000	-0.202638000
6	5.696135000	-0.167748000	0.229811000
6	4.237787000	-1.687256000	-0.747544000
6	6.382806000	-1.433770000	-0.011148000
6	6.438530000	0.876631000	0.879955000
6	7.678047000	-1.652926000	0.328136000
6	7.734738000	0.668578000	1.229392000
1	5.961346000	1.830182000	1.055337000
6	8.427627000	-0.588644000	0.972780000
1	8.165834000	-2.603226000	0.137055000
1	8.297503000	1.459401000	1.716709000
8	3.266496000	-2.234668000	-1.251554000
8	4.576139000	2.768196000	-0.390544000
7	5.483508000	-2.301369000	-0.605442000
7	2.265481000	2.733201000	-0.358129000
6	2.064594000	4.161377000	-0.467217000
1	1.502690000	4.411446000	-1.373850000
1	1.526925000	4.551949000	0.404131000
1	3.051884000	4.621909000	-0.517592000
6	5.754799000	-3.656661000	-1.032053000
1	6.544770000	-3.678775000	-1.790684000
1	6.057765000	-4.282482000	-0.185189000
1	4.832278000	-4.050187000	-1.460302000
6	-2.317165000	0.907742000	-0.099839000
6	-3.081426000	2.110458000	-0.181407000
16	-3.405024000	-0.487290000	0.060599000
6	-4.433832000	1.928395000	-0.120031000
1	-2.623677000	3.086208000	-0.285575000
6	-4.833869000	0.557962000	0.016078000
1	-5.159494000	2.732125000	-0.168247000

6	9.727911000	-0.751242000	1.334013000
6	-6.117968000	0.080634000	0.102767000
6	-6.443267000	-1.338887000	0.241499000
16	-7.581129000	1.076201000	0.063147000
6	-8.629648000	-0.398053000	0.230795000
7	-7.831820000	-1.523662000	0.304649000
6	-8.433372000	-2.845476000	0.443248000
1	-9.086145000	-3.052605000	-0.407683000
1	-7.617583000	-3.566789000	0.477761000
1	-9.022665000	-2.896291000	1.361577000
8	-9.836718000	-0.374894000	0.269651000
8	-5.634172000	-2.257639000	0.297312000
1	10.282145000	0.045515000	1.818739000
1	10.256785000	-1.680926000	1.150502000

S5TIIDS0-CS E=-2073.363550 Hartree

6	1.662016000	1.785597000	-0.267500000
6	2.303436000	0.485033000	-0.204667000
6	1.451982000	-0.657793000	-0.093504000
6	0.095884000	-0.498063000	-0.063284000
6	-0.536655000	0.795916000	-0.141650000
6	0.307384000	1.953103000	-0.243642000
6	3.907683000	2.164132000	-0.297918000
6	3.687096000	0.677148000	-0.208131000
1	1.890778000	-1.644690000	-0.063245000
1	-0.531427000	-1.379296000	0.016950000
1	-0.122932000	2.945543000	-0.291382000
6	4.763058000	-0.268029000	-0.196043000
6	6.082927000	-0.136668000	0.233542000
6	4.624626000	-1.660382000	-0.743991000
6	6.771475000	-1.399422000	-0.016332000
6	6.821018000	0.905690000	0.889213000
6	8.069722000	-1.614809000	0.315951000
6	8.120093000	0.700904000	1.232393000
1	6.340850000	1.855385000	1.075567000
6	8.815951000	-0.550873000	0.963017000
1	8.560993000	-2.561517000	0.116951000
1	8.680741000	1.490296000	1.724144000
8	3.653015000	-2.208957000	-1.244606000
8	4.953424000	2.794426000	-0.358044000
7	5.873762000	-2.267691000	-0.611134000

7	2.643678000	2.756328000	-0.334954000
6	2.437063000	4.185696000	-0.434736000
1	1.878073000	4.438249000	-1.342061000
1	1.894325000	4.566276000	0.437447000
1	3.421984000	4.651602000	-0.477844000
6	6.150380000	-3.620434000	-1.045456000
1	6.936078000	-3.633857000	-1.808409000
1	6.461072000	-4.247306000	-0.202456000
1	5.228020000	-4.017559000	-1.470391000
6	-1.937295000	0.921214000	-0.112309000
6	-2.700936000	2.116915000	-0.189945000
16	-3.020589000	-0.477637000	0.036964000
6	-4.056203000	1.920132000	-0.133439000
1	-2.254434000	3.098730000	-0.287669000
6	-4.445218000	0.551060000	-0.006219000
1	-4.774906000	2.728165000	-0.180874000
6	10.119067000	-0.708935000	1.317312000
6	-5.755871000	0.057629000	0.076070000
6	-6.892210000	0.907100000	0.039337000
6	-5.969649000	-1.392131000	0.206205000
6	-8.167918000	0.414518000	0.121392000
1	-6.761423000	1.979121000	-0.056042000
6	-8.431672000	-1.029490000	0.252465000
6	-9.293032000	1.288830000	0.082776000
7	-10.182335000	2.039363000	0.047459000
8	-5.035571000	-2.196308000	0.246157000
8	-9.557373000	-1.499599000	0.328187000
7	-7.284225000	-1.846728000	0.285464000
6	-7.467227000	-3.296813000	0.414149000
1	-7.022383000	-3.803221000	-0.444881000
1	-6.969206000	-3.653655000	1.318009000
1	-8.535970000	-3.489093000	0.462810000
1	10.671325000	0.087633000	1.804544000
1	10.651896000	-1.634675000	1.125683000

S6TIIDS0-CS E=-2434.686688 Hartree

6	2.024017000	1.794470000	-0.263638000
6	2.644069000	0.482027000	-0.207503000
6	1.772814000	-0.648102000	-0.105710000
6	0.420574000	-0.466105000	-0.077227000
6	-0.191725000	0.840283000	-0.147984000
6	0.673501000	1.984690000	-0.241219000

6	4.276356000	2.133154000	-0.288206000
6	4.029021000	0.650384000	-0.207529000
1	2.195515000	-1.642227000	-0.081340000
1	-0.222401000	-1.336494000	-0.003966000
1	0.258988000	2.983966000	-0.283789000
6	5.089146000	-0.314786000	-0.198064000
6	6.406352000	-0.210905000	0.242632000
6	4.930486000	-1.697929000	-0.762206000
6	7.075765000	-1.482907000	-0.014816000
6	7.157595000	0.812818000	0.913708000
6	8.367235000	-1.723573000	0.325439000
6	8.449921000	0.582502000	1.264620000
1	6.692125000	1.768929000	1.104942000
6	9.126714000	-0.678826000	0.988933000
1	8.843994000	-2.676551000	0.120956000
1	9.020412000	1.357494000	1.767894000
8	3.953263000	-2.224070000	-1.275972000
8	5.333655000	2.744836000	-0.341828000
7	6.167801000	-2.329157000	-0.625491000
7	3.023177000	2.747970000	-0.323628000
6	2.841825000	4.181258000	-0.414429000
1	2.289844000	4.449701000	-1.321501000
1	2.302952000	4.565365000	0.458610000
1	3.834891000	4.630130000	-0.451533000
6	6.423546000	-3.682070000	-1.071213000
1	7.214689000	-3.702327000	-1.828449000
1	6.716630000	-4.322916000	-0.232363000
1	5.497427000	-4.058296000	-1.506947000
6	-1.586626000	0.989273000	-0.119782000
6	-2.330814000	2.200351000	-0.187836000
16	-2.694250000	-0.392294000	0.015565000
6	-3.687900000	2.034645000	-0.135435000
1	-1.865162000	3.174412000	-0.275888000
6	-4.104731000	0.665740000	-0.020501000
1	-4.419406000	2.827081000	-0.173346000
6	10.423719000	-0.862803000	1.352000000
6	-5.416319000	0.181274000	0.055910000
6	-6.561294000	1.087521000	0.023358000
6	-5.625816000	-1.251763000	0.169804000
6	-8.066061000	-0.885073000	0.217087000
8	-4.691825000	-2.056257000	0.202420000
7	-6.954754000	-1.708820000	0.243852000
6	-7.150634000	-3.162321000	0.357472000
1	-7.744009000	-3.522161000	-0.484228000

1	-6.164777000	-3.618622000	0.359194000
1	-7.686825000	-3.392295000	1.279280000
7	-7.837637000	0.474862000	0.108531000
6	-8.999596000	1.377227000	0.077174000
1	-9.637884000	1.128440000	-0.771867000
1	-9.583473000	1.259766000	0.991212000
1	-8.616301000	2.389502000	-0.010083000
8	-6.485601000	2.310251000	-0.070091000
16	-9.617491000	-1.511537000	0.312440000
1	10.985701000	-0.080640000	1.851318000
1	10.942042000	-1.795779000	1.155676000

S7TIIDS0-CS E=-2188.615833 Hartree

6	-2.164469000	-1.862820000	-0.451058000
6	-2.754437000	-0.547458000	-0.278887000
6	-1.857400000	0.559855000	-0.162174000
6	-0.508610000	0.354228000	-0.219353000
6	0.070968000	-0.954182000	-0.399183000
6	-0.818016000	-2.076146000	-0.516245000
6	-4.420184000	-2.165547000	-0.366506000
6	-4.141731000	-0.694346000	-0.209399000
1	-2.258093000	1.558365000	-0.062962000
1	0.153352000	1.210500000	-0.144576000
1	-0.425883000	-3.078153000	-0.636399000
6	-5.181583000	0.282766000	-0.079328000
6	-6.476807000	0.169213000	0.422884000
6	-5.027547000	1.698933000	-0.557692000
6	-7.134883000	1.465269000	0.285301000
6	-7.210933000	-0.884818000	1.064783000
6	-8.402706000	1.702231000	0.707914000
6	-8.479185000	-0.658914000	1.497719000
1	-6.754050000	-1.858289000	1.168946000
6	-9.146055000	0.627489000	1.340505000
1	-8.871502000	2.673770000	0.591347000
1	-9.036789000	-1.456891000	1.979025000
8	-4.068965000	2.244478000	-1.085591000
8	-5.489522000	-2.757570000	-0.397702000
7	-6.244597000	2.337107000	-0.314984000
7	-3.182531000	-2.795647000	-0.511193000
6	-3.033299000	-4.222825000	-0.702110000
1	-2.537699000	-4.440965000	-1.654092000
1	-2.454185000	-4.670074000	0.113213000
1	-4.035107000	-4.653306000	-0.711139000

6	-6.498665000	3.720411000	-0.656786000
1	-7.326987000	3.802197000	-1.368711000
1	-6.736989000	4.307921000	0.236653000
1	-5.589574000	4.111574000	-1.114625000
6	1.463195000	-1.134179000	-0.445699000
6	2.185612000	-2.338128000	-0.677011000
16	2.602793000	0.196543000	-0.219637000
6	3.547070000	-2.199882000	-0.664917000
1	1.693493000	-3.284896000	-0.861647000
6	3.998549000	-0.858660000	-0.424280000
1	4.259756000	-2.998508000	-0.811853000
6	-10.419417000	0.806171000	1.782117000
6	5.332055000	-0.488042000	-0.238780000
6	6.378115000	-1.522220000	0.051757000
6	5.940203000	0.812727000	-0.027987000
6	7.518381000	-0.787749000	0.652230000
6	7.244427000	0.591349000	0.657888000
6	8.693628000	-1.316867000	1.166013000
6	8.176526000	1.469996000	1.216664000
6	9.621816000	-0.434835000	1.724723000
1	8.865636000	-2.387749000	1.128224000
6	9.356117000	0.938580000	1.751440000
1	8.007415000	2.537492000	1.254299000
1	10.550089000	-0.812491000	2.142305000
1	10.080551000	1.614357000	2.195787000
8	6.324550000	-2.733370000	-0.116652000
6	5.509444000	2.042632000	-0.508155000
6	4.508941000	2.196759000	-1.513135000
7	3.741597000	2.371083000	-2.372914000
6	6.138346000	3.275469000	-0.153484000
7	6.613792000	4.300991000	0.130380000
1	-10.969174000	0.001039000	2.257987000
1	-10.930107000	1.757598000	1.674324000

S8TIIDS0-CS E=-2623.835400 Hartree

6	-7.536506000	1.426927000	0.282808000
6	-6.854441000	0.144892000	0.432847000
6	-7.567134000	-0.915727000	1.087282000
6	-8.839149000	-0.709279000	1.519434000
6	-9.530205000	0.562250000	1.348725000
6	-8.808398000	1.644208000	0.704172000
6	-5.434702000	1.692528000	-0.564262000
6	-5.561653000	0.277990000	-0.072688000

1	-7.091781000	-1.879046000	1.201987000
1	-9.380802000	-1.512350000	2.010309000
1	-9.295739000	2.605294000	0.577741000
6	-4.504497000	-0.680233000	-0.195452000
6	-3.120385000	-0.508935000	-0.272891000
6	-4.756014000	-2.159316000	-0.335499000
6	-2.507420000	-1.815143000	-0.433109000
6	-2.243583000	0.615886000	-0.172176000
6	-1.157418000	-2.004511000	-0.502459000
6	-0.891529000	0.434276000	-0.233263000
1	-2.662227000	1.607797000	-0.081598000
6	-0.289445000	-0.865156000	-0.401958000
1	-0.747509000	-3.000420000	-0.613097000
1	-0.245413000	1.303489000	-0.169784000
8	-5.814420000	-2.770300000	-0.356011000
8	-4.486790000	2.250951000	-1.097750000
7	-3.507769000	-2.767557000	-0.478322000
7	-6.663535000	2.309323000	-0.327273000
6	-6.944477000	3.684213000	-0.682610000
1	-7.773395000	3.742679000	-1.396068000
1	-7.195250000	4.275137000	0.205084000
1	-6.042835000	4.088884000	-1.143357000
6	-3.332151000	-4.194091000	-0.654143000
1	-2.837570000	-4.413051000	-1.606365000
1	-2.740384000	-4.620505000	0.163106000
1	-4.325429000	-4.643874000	-0.652954000
6	-10.806519000	0.721145000	1.789643000
6	1.105883000	-1.020068000	-0.453829000
6	1.848801000	-2.211627000	-0.677617000
16	2.219797000	0.336431000	-0.250160000
6	3.206890000	-2.046781000	-0.676559000
1	1.375557000	-3.170121000	-0.848743000
6	3.633636000	-0.695215000	-0.449474000
1	3.910417000	-2.852996000	-0.832750000
6	4.951686000	-0.288753000	-0.276323000
6	5.557319000	0.997192000	-0.076441000
6	7.296810000	-0.433934000	0.798882000
6	6.828007000	0.884319000	0.695439000
6	8.472630000	-0.786455000	1.441677000
6	7.592358000	1.891819000	1.302832000
6	9.220133000	0.232234000	2.035549000
1	8.789371000	-1.823007000	1.487438000
6	8.773573000	1.554342000	1.966186000
1	7.278254000	2.925438000	1.278646000

1	10.142740000	-0.005302000	2.555280000
1	9.351788000	2.342032000	2.438725000
6	5.083951000	2.188842000	-0.629324000
6	5.590726000	3.480119000	-0.297328000
7	5.960551000	4.556346000	-0.043552000
6	4.135869000	2.221928000	-1.692261000
7	3.397515000	2.291106000	-2.591838000
16	6.199695000	-1.582333000	-0.005900000
8	5.724314000	-2.590951000	0.955004000
8	6.760764000	-2.046142000	-1.285152000
1	-11.340336000	-0.089291000	2.274550000
1	-11.335506000	1.661346000	1.672125000

S9TIIDS0-CS E=-2609.776026 Hartree

6	6.890318000	-1.516315000	0.002654000
6	6.223962000	-0.239227000	0.239771000
6	6.986097000	0.791735000	0.890322000
6	8.275793000	0.559082000	1.247330000
6	8.947122000	-0.712242000	0.998812000
6	8.178448000	-1.761336000	0.349919000
6	4.744993000	-1.728561000	-0.746938000
6	4.907767000	-0.340225000	-0.197514000
1	6.526389000	1.755509000	1.057884000
1	8.851693000	1.340625000	1.734723000
1	8.647685000	-2.721939000	0.162744000
6	3.849683000	0.632242000	-0.218693000
6	2.459159000	0.462020000	-0.209136000
6	4.098453000	2.100698000	-0.309233000
6	1.838657000	1.771557000	-0.273722000
6	1.586961000	-0.661933000	-0.095337000
6	0.487404000	1.964290000	-0.247606000
6	0.231826000	-0.477212000	-0.064620000
1	2.006287000	-1.657474000	-0.065758000
6	-0.379859000	0.822734000	-0.143302000
1	0.077153000	2.965749000	-0.297284000
1	-0.409092000	-1.350081000	0.016695000
8	5.153543000	2.724022000	-0.368784000
8	3.768280000	-2.260104000	-1.259633000
7	2.841653000	2.719896000	-0.345577000
7	5.977732000	-2.367765000	-0.596672000
6	6.225191000	-3.726605000	-1.022222000
1	7.021264000	-3.764947000	-1.774224000
1	6.509005000	-4.360601000	-0.174386000

1	5.298275000	-4.100654000	-1.458759000
6	2.668043000	4.150556000	-0.445263000
1	2.114220000	4.419713000	-1.352013000
1	2.134241000	4.547228000	0.426355000
1	3.664899000	4.591344000	-0.488512000
6	10.241518000	-0.901803000	1.368196000
6	-1.773705000	0.977853000	-0.115267000
6	-2.529941000	2.185942000	-0.188916000
16	-2.888954000	-0.397258000	0.026746000
6	-3.886940000	2.025238000	-0.135562000
1	-2.055971000	3.154754000	-0.281933000
6	-4.315178000	0.665467000	-0.014566000
1	-4.591405000	2.848362000	-0.180704000
6	-5.599747000	0.193421000	0.061385000
16	-5.982530000	-1.524043000	0.209489000
16	-7.010140000	1.264490000	0.018667000
6	-7.740086000	-1.328107000	0.244214000
6	-8.223881000	-0.014477000	0.154229000
6	-8.628096000	-2.400532000	0.354340000
6	-9.598483000	0.232848000	0.173930000
6	-9.999343000	-2.149322000	0.373680000
1	-8.252743000	-3.416500000	0.423740000
6	-10.481440000	-0.840539000	0.283995000
1	-9.972784000	1.249193000	0.104176000
1	-10.692810000	-2.979591000	0.459022000
1	-11.550100000	-0.652593000	0.299579000
1	10.809466000	-0.116273000	1.855457000
1	10.751852000	-1.842608000	1.188577000

S10TIIDS0-CS E=-2456.117306 Hartree

6	0.733230000	1.671215000	-0.295274000
6	1.425272000	0.399839000	-0.204893000
6	0.617479000	-0.766329000	-0.050738000
6	-0.745530000	-0.654948000	-0.007191000
6	-1.428270000	0.606866000	-0.111402000
6	-0.626357000	1.790632000	-0.256487000
6	2.971153000	2.122133000	-0.368367000
6	2.804498000	0.645502000	-0.236801000
1	1.090973000	-1.736441000	-0.000807000
1	-1.336467000	-1.559123000	0.105123000
1	-1.091414000	2.766598000	-0.326959000
6	3.914406000	-0.266862000	-0.203985000
6	5.228265000	-0.082505000	0.212887000

6	3.821630000	-1.676469000	-0.714330000
6	5.960789000	-1.327242000	0.000833000
6	5.940480000	1.005642000	0.825734000
6	7.264407000	-1.492372000	0.337352000
6	7.245115000	0.853291000	1.171723000
1	5.430655000	1.947177000	0.973666000
6	7.982163000	-0.385844000	0.948071000
1	7.783194000	-2.430800000	0.169402000
1	7.783026000	1.678009000	1.630557000
8	2.869721000	-2.274280000	-1.200072000
8	3.989545000	2.800759000	-0.457369000
7	5.089257000	-2.243171000	-0.563581000
7	1.681743000	2.670592000	-0.404798000
6	1.428706000	4.086390000	-0.539494000
1	0.849515000	4.300373000	-1.445111000
1	0.884989000	4.476910000	0.328799000
1	2.399290000	4.579476000	-0.608345000
6	5.405898000	-3.597515000	-0.956180000
1	6.194199000	-3.612826000	-1.717145000
1	5.733784000	-4.191908000	-0.095630000
1	4.495904000	-4.033187000	-1.370620000
6	-2.828620000	0.686623000	-0.069185000
6	-3.651269000	1.848192000	-0.162926000
16	-3.864736000	-0.743695000	0.121492000
6	-4.997288000	1.613787000	-0.087809000
1	-3.233115000	2.839084000	-0.285980000
6	-5.347387000	0.237180000	0.072277000
1	-5.746848000	2.395492000	-0.144073000
6	9.289300000	-0.494625000	1.305092000
6	-6.603092000	-0.305391000	0.176618000
16	-6.898262000	-2.039278000	0.372461000
16	-8.083865000	0.670943000	0.127130000
6	-8.649515000	-1.908278000	0.422089000
6	-9.183660000	-0.685832000	0.311401000
1	-10.243943000	-0.466130000	0.326441000
1	-9.213199000	-2.825271000	0.540029000
1	9.819110000	0.333572000	1.763826000
1	9.848209000	-1.410790000	1.143593000

S1TIIDS0-OS E=-1768.020964 Hartree

6	-5.295350000	-1.194354000	0.016060000
6	-4.532365000	0.027737000	-0.172793000
6	-5.222518000	1.161497000	-0.704384000

6	-6.553915000	1.075183000	-0.990473000
6	-7.321642000	-0.137527000	-0.777170000
6	-6.624714000	-1.294399000	-0.257891000
6	-3.142576000	-1.682108000	0.595350000
6	-3.191633000	-0.236282000	0.169748000
1	-4.685713000	2.087554000	-0.847481000
1	-7.076295000	1.939340000	-1.389919000
1	-7.170090000	-2.219559000	-0.103678000
6	-2.052182000	0.610711000	0.197014000
6	-0.667093000	0.308105000	0.165831000
6	-2.145786000	2.108090000	0.333718000
6	0.062690000	1.547822000	0.258859000
6	0.091802000	-0.879697000	-0.003170000
6	1.431442000	1.619995000	0.216554000
6	1.464290000	-0.817589000	-0.052663000
1	-0.414385000	-1.831749000	-0.063897000
6	2.181927000	0.414631000	0.061182000
1	1.930739000	2.577994000	0.290903000
1	2.019746000	-1.741593000	-0.176576000
8	-3.132409000	2.824904000	0.434487000
8	-2.198462000	-2.346037000	0.999745000
7	-0.838863000	2.591554000	0.373701000
7	-4.439777000	-2.175706000	0.488568000
6	-4.803919000	-3.534297000	0.830473000
1	-5.550511000	-3.548903000	1.631679000
1	-5.205478000	-4.063454000	-0.040656000
1	-3.897870000	-4.035480000	1.172051000
6	-0.515062000	3.994935000	0.518385000
1	0.075267000	4.169104000	1.424379000
1	0.045291000	4.360662000	-0.349112000
1	-1.457857000	4.537446000	0.593487000
6	-8.657271000	-0.179263000	-1.067473000
6	3.601951000	0.447495000	0.015551000
6	4.454799000	1.570366000	0.123407000
16	4.572951000	-1.017104000	-0.199388000
6	5.799889000	1.282520000	0.039500000
1	4.078170000	2.575943000	0.263076000
6	6.071376000	-0.101025000	-0.141309000
1	6.594968000	2.015497000	0.101917000
6	7.328734000	-0.700351000	-0.261983000
6	8.504098000	0.098338000	-0.206879000
7	9.451774000	0.776317000	-0.158547000
6	7.473251000	-2.101818000	-0.441642000
7	7.565557000	-3.255291000	-0.589019000

1	-9.174935000	0.688956000	-1.460995000
1	-9.243485000	-1.079441000	-0.914549000

S2TIIDS0-OS E=-1850.505066 Hartree

6	0.750942000	1.654371000	-0.240204000
6	1.396516000	0.376384000	-0.180892000
6	0.564828000	-0.758995000	-0.068684000
6	-0.809745000	-0.610940000	-0.041652000
6	-1.439385000	0.658872000	-0.122920000
6	-0.616818000	1.812659000	-0.219038000
6	2.990106000	2.094973000	-0.245459000
6	2.814771000	0.600877000	-0.171583000
1	1.005786000	-1.743767000	-0.032549000
1	-1.422690000	-1.503467000	0.032714000
1	-1.051892000	2.803717000	-0.260108000
6	3.898401000	-0.301481000	-0.149743000
6	5.267259000	-0.117273000	0.183766000
6	3.766876000	-1.748162000	-0.568320000
6	5.948943000	-1.380189000	-0.005488000
6	6.031009000	0.966443000	0.706997000
6	7.273334000	-1.566608000	0.260786000
6	7.360066000	0.795814000	0.986660000
1	5.556386000	1.925146000	0.852749000
6	8.045942000	-0.459439000	0.772146000
1	7.754565000	-2.526512000	0.105039000
1	7.936687000	1.627398000	1.380768000
8	2.787281000	-2.362632000	-0.967362000
8	4.013815000	2.765901000	-0.300481000
7	5.033108000	-2.312817000	-0.468783000
7	1.713846000	2.649665000	-0.295694000
6	1.471330000	4.072487000	-0.393398000
1	0.910892000	4.312938000	-1.303468000
1	0.912395000	4.437420000	0.475644000
1	2.444079000	4.563765000	-0.429052000
6	5.317155000	-3.690377000	-0.808190000
1	6.057951000	-3.749796000	-1.612870000
1	5.693224000	-4.239275000	0.062279000
1	4.382316000	-4.140176000	-1.143613000
6	-2.874704000	0.789162000	-0.104098000
6	-3.644441000	1.948570000	-0.240913000
16	-3.935207000	-0.596847000	0.110915000
6	-5.020498000	1.736860000	-0.178269000
1	-3.208563000	2.928253000	-0.392621000

6	-5.389723000	0.395697000	0.011559000
1	-5.743538000	2.537087000	-0.272950000
6	9.383983000	-0.589013000	1.054169000
6	-6.697891000	-0.158447000	0.118702000
6	-6.907279000	-1.565368000	0.298315000
6	-7.859634000	0.682613000	0.050418000
6	-8.158968000	-2.097167000	0.402185000
1	-6.043512000	-2.222774000	0.351131000
6	-9.119294000	0.170976000	0.152178000
1	-7.730228000	1.751577000	-0.083840000
6	-9.355391000	-1.259752000	0.335988000
1	-8.313583000	-3.162867000	0.537269000
1	-9.995999000	0.808787000	0.100943000
8	-10.501529000	-1.735186000	0.430179000
1	9.959569000	0.244289000	1.442464000
1	9.908117000	-1.526071000	0.897973000

S3TIIDS0-OS E=-2335.876101 Hartree

6	-1.811897000	1.641766000	0.223633000
6	-2.454493000	0.361897000	0.183705000
6	-1.622056000	-0.774711000	0.102951000
6	-0.246865000	-0.625919000	0.087954000
6	0.378869000	0.645746000	0.150772000
6	-0.443484000	1.800806000	0.214142000
6	-4.050259000	2.081746000	0.193608000
6	-3.874273000	0.584795000	0.154112000
1	-2.061954000	-1.760300000	0.082612000
1	0.366960000	-1.519883000	0.042498000
1	-0.009235000	2.792785000	0.234684000
6	-4.955696000	-0.317372000	0.141446000
6	-6.324323000	-0.140026000	-0.202824000
6	-4.825967000	-1.757643000	0.586316000
6	-7.004924000	-1.399863000	0.006955000
6	-7.084817000	0.932813000	-0.750841000
6	-8.328230000	-1.592085000	-0.261806000
6	-8.412846000	0.756013000	-1.033626000
1	-6.610202000	1.888616000	-0.913670000
6	-9.097943000	-0.495075000	-0.797523000
1	-8.809956000	-2.548879000	-0.089967000
1	-8.987842000	1.579263000	-1.446866000
8	-3.847572000	-2.363452000	1.000179000
8	-5.074441000	2.752116000	0.222806000
7	-6.091122000	-2.323394000	0.491897000

7	-2.774910000	2.637414000	0.246672000
6	-2.533198000	4.062752000	0.316862000
1	-1.983413000	4.321909000	1.228094000
1	-1.964737000	4.408571000	-0.553600000
1	-3.505993000	4.554811000	0.331075000
6	-6.377253000	-3.695065000	0.855222000
1	-7.122137000	-3.738897000	1.656914000
1	-6.748619000	-4.259249000	-0.007278000
1	-5.444529000	-4.138996000	1.203801000
6	1.815688000	0.777779000	0.145620000
6	2.582659000	1.933665000	0.311265000
16	2.873851000	-0.607909000	-0.089615000
6	3.961068000	1.722841000	0.256903000
1	2.144782000	2.908899000	0.482525000
6	4.320292000	0.386764000	0.044693000
1	4.694932000	2.512077000	0.373516000
6	-10.435065000	-0.630434000	-1.083155000
6	5.618601000	-0.163919000	-0.061259000
6	5.982035000	-1.513634000	-0.258088000
16	7.087103000	0.795012000	0.038996000
1	5.253680000	-2.313424000	-0.351760000
6	8.031784000	-0.697950000	-0.190567000
6	9.431833000	-0.701899000	-0.222863000
6	10.164775000	0.504144000	-0.070618000
7	10.740568000	1.510810000	0.057141000
6	10.150345000	-1.913393000	-0.409290000
7	10.769181000	-2.889506000	-0.560531000
7	7.275092000	-1.802199000	-0.327637000
1	-11.008982000	0.195115000	-1.489995000
1	-10.959716000	-1.564479000	-0.911549000

S4TIIDS0-OS E=-2301.900692 Hartree

6	1.282830000	1.737802000	-0.250921000
6	1.911456000	0.443796000	-0.192564000
6	1.058461000	-0.683720000	-0.078862000
6	-0.307088000	-0.514846000	-0.046943000
6	-0.923886000	0.771708000	-0.125454000
6	-0.077384000	1.916642000	-0.225759000
6	3.530807000	2.125632000	-0.270031000
6	3.319162000	0.638908000	-0.190808000
1	1.486237000	-1.674823000	-0.046001000
1	-0.935453000	-1.395813000	0.033866000
1	-0.497184000	2.913975000	-0.271006000

6	4.388663000	-0.294863000	-0.173407000
6	5.740454000	-0.148655000	0.198947000
6	4.235425000	-1.718497000	-0.645900000
6	6.408613000	-1.420353000	-0.014023000
6	6.509322000	0.909647000	0.775568000
6	7.720094000	-1.635269000	0.280569000
6	7.824015000	0.708569000	1.082633000
1	6.045302000	1.871612000	0.936013000
6	8.497572000	-0.554701000	0.847518000
1	8.192187000	-2.596893000	0.107980000
1	8.405308000	1.516858000	1.516481000
8	3.251786000	-2.294978000	-1.089494000
8	4.571237000	2.769701000	-0.328501000
7	5.487630000	-2.316819000	-0.531426000
7	2.265981000	2.711167000	-0.313068000
6	2.055866000	4.138967000	-0.410448000
1	1.498024000	4.392624000	-1.318571000
1	1.508914000	4.517289000	0.460530000
1	3.039780000	4.607398000	-0.449813000
6	5.749964000	-3.688435000	-0.909291000
1	6.509496000	-3.739136000	-1.697003000
1	6.090957000	-4.274586000	-0.048654000
1	4.814018000	-4.105038000	-1.282692000
6	-2.341424000	0.914792000	-0.098615000
6	-3.090370000	2.110155000	-0.185848000
16	-3.425891000	-0.473628000	0.059067000
6	-4.455240000	1.930371000	-0.130381000
1	-2.630756000	3.084987000	-0.290946000
6	-4.852795000	0.570480000	0.005410000
1	-5.176909000	2.737348000	-0.184531000
6	9.820178000	-0.713187000	1.160456000
6	-6.144481000	0.084732000	0.087906000
6	-6.471667000	-1.332346000	0.227343000
16	-7.601903000	1.082123000	0.039531000
6	-8.657113000	-0.389972000	0.204766000
7	-7.862173000	-1.515600000	0.284253000
6	-8.465466000	-2.836681000	0.422299000
1	-9.113687000	-3.045331000	-0.431755000
1	-7.650303000	-3.558412000	0.462686000
1	-9.059650000	-2.885340000	1.337596000
8	-9.864255000	-0.361697000	0.237444000
8	-5.665055000	-2.253431000	0.288684000
1	10.397945000	0.098470000	1.589475000
1	10.334880000	-1.653169000	0.990440000

S5TIIDS0-OS E=-2073.364569 Hartree

6	1.664436000	1.758961000	-0.243574000
6	2.296390000	0.465053000	-0.192039000
6	1.447007000	-0.667476000	-0.088476000
6	0.081900000	-0.503453000	-0.059993000
6	-0.538196000	0.783432000	-0.132389000
6	0.303801000	1.932449000	-0.222198000
6	3.909342000	2.154408000	-0.252601000
6	3.701409000	0.663142000	-0.183928000
1	1.878711000	-1.656976000	-0.060494000
1	-0.544599000	-1.385991000	0.013147000
1	-0.120549000	2.927912000	-0.262120000
6	4.773285000	-0.266835000	-0.172301000
6	6.123130000	-0.118977000	0.205778000
6	4.625965000	-1.686462000	-0.659851000
6	6.796171000	-1.386407000	-0.020424000
6	6.884159000	0.936231000	0.798058000
6	8.108105000	-1.598085000	0.274114000
6	8.198925000	0.737672000	1.105451000
1	6.415334000	1.893650000	0.970446000
6	8.878038000	-0.519767000	0.855233000
1	8.585876000	-2.554818000	0.091056000
1	8.775498000	1.542697000	1.551202000
8	3.644463000	-2.260102000	-1.110240000
8	4.948877000	2.797956000	-0.303672000
7	5.880302000	-2.280222000	-0.550060000
7	2.643753000	2.736062000	-0.295667000
6	2.428442000	4.164671000	-0.384583000
1	1.872677000	4.420955000	-1.292926000
1	1.877725000	4.534290000	0.487423000
1	3.410303000	4.637576000	-0.418035000
6	6.149583000	-3.647116000	-0.942869000
1	6.909925000	-3.684889000	-1.730274000
1	6.492032000	-4.240339000	-0.087911000
1	5.216213000	-4.064213000	-1.321856000
6	-1.956409000	0.920961000	-0.108914000
6	-2.707698000	2.112707000	-0.192037000
16	-3.036446000	-0.471084000	0.038831000
6	-4.071939000	1.918747000	-0.140313000
1	-2.258353000	3.092994000	-0.291284000
6	-4.461622000	0.558053000	-0.012310000
1	-4.786606000	2.730227000	-0.193172000

6	10.200279000	-0.674461000	1.168810000
6	-5.778624000	0.062957000	0.066312000
6	-6.910472000	0.913263000	0.023537000
6	-5.996622000	-1.387774000	0.198498000
6	-8.189654000	0.422605000	0.101398000
1	-6.777249000	1.984788000	-0.073161000
6	-8.457279000	-1.020453000	0.233981000
6	-9.312251000	1.298801000	0.056622000
7	-10.200038000	2.051061000	0.016291000
8	-5.065350000	-2.193679000	0.244024000
8	-9.585136000	-1.486423000	0.305865000
7	-7.312669000	-1.839706000	0.273197000
6	-7.498779000	-3.289433000	0.404010000
1	-7.051017000	-3.798114000	-0.452096000
1	-7.005361000	-3.645103000	1.310801000
1	-8.568005000	-3.479956000	0.448368000
1	10.772712000	0.135230000	1.608558000
1	10.720675000	-1.609438000	0.988876000

S6TIIDS0-OS E=-2434.686971 Hartree

6	2.025022000	1.777673000	-0.250750000
6	2.639629000	0.469564000	-0.199741000
6	1.770025000	-0.654269000	-0.099951000
6	0.412404000	-0.469816000	-0.072008000
6	-0.192759000	0.831925000	-0.141282000
6	0.670875000	1.971354000	-0.229486000
6	4.276835000	2.126791000	-0.264207000
6	4.037215000	0.641411000	-0.193488000
1	2.188604000	-1.649789000	-0.075390000
1	-0.229922000	-1.340882000	-0.000614000
1	0.259849000	2.972254000	-0.269101000
6	5.095242000	-0.314440000	-0.183230000
6	6.431225000	-0.199323000	0.225790000
6	4.930231000	-1.715386000	-0.708919000
6	7.091178000	-1.474505000	-0.015944000
6	7.196925000	0.833617000	0.857288000
6	8.391607000	-1.711758000	0.301159000
6	8.499286000	0.608140000	1.186388000
1	6.738273000	1.794476000	1.039309000
6	9.166075000	-0.656704000	0.923140000
1	8.860159000	-2.670934000	0.107117000
1	9.079871000	1.393595000	1.661013000
8	3.946206000	-2.257808000	-1.191662000

8	5.330586000	2.746310000	-0.314450000
7	6.171308000	-2.337764000	-0.585791000
7	3.022561000	2.735132000	-0.303613000
6	2.835709000	4.167902000	-0.390330000
1	2.285740000	4.436930000	-1.298490000
1	2.291831000	4.546851000	0.481909000
1	3.826913000	4.621129000	-0.422341000
6	6.422304000	-3.700042000	-1.005106000
1	7.196849000	-3.735120000	-1.778760000
1	6.736525000	-4.319596000	-0.157971000
1	5.488512000	-4.089832000	-1.411378000
6	-1.597708000	0.987797000	-0.116264000
6	-2.334745000	2.197084000	-0.186346000
16	-2.703481000	-0.390596000	0.016876000
6	-3.696270000	2.033709000	-0.136808000
1	-1.867160000	3.170214000	-0.274042000
6	-4.114592000	0.668553000	-0.022561000
1	-4.425009000	2.828596000	-0.176880000
6	10.475227000	-0.837338000	1.261129000
6	-5.427988000	0.183468000	0.051353000
6	-6.572395000	1.090822000	0.016071000
6	-5.639814000	-1.249816000	0.165293000
6	-8.079943000	-0.879568000	0.207164000
8	-4.707259000	-2.055477000	0.200151000
7	-6.969632000	-1.704678000	0.236594000
6	-7.167724000	-3.157974000	0.350334000
1	-7.759760000	-3.517242000	-0.492532000
1	-6.182542000	-3.615676000	0.354343000
1	-7.706166000	-3.386795000	1.271099000
7	-7.849554000	0.480034000	0.098616000
6	-9.010231000	1.384062000	0.064411000
1	-9.647005000	1.135768000	-0.785891000
1	-9.596125000	1.267820000	0.977297000
1	-8.625414000	2.395785000	-0.022479000
8	-6.494278000	2.313292000	-0.077608000
16	-9.632266000	-1.503954000	0.299373000
1	11.049898000	-0.046077000	1.730630000
1	10.986151000	-1.775884000	1.072493000

S7TIIDS0-OS E=-2188.616515 Hartree

6	-2.164484000	-1.839881000	-0.430548000
6	-2.747634000	-0.530293000	-0.270587000
6	-1.854039000	0.569023000	-0.162029000

6	-0.497315000	0.360534000	-0.222255000
6	0.072427000	-0.941223000	-0.395857000
6	-0.812851000	-2.057628000	-0.498956000
6	-4.418501000	-2.160353000	-0.325639000
6	-4.153222000	-0.683403000	-0.188445000
1	-2.249300000	1.569414000	-0.065250000
1	0.163218000	1.218747000	-0.156894000
1	-0.424554000	-3.062531000	-0.607900000
6	-5.190507000	0.279441000	-0.059962000
6	-6.515414000	0.154079000	0.398365000
6	-5.025419000	1.716410000	-0.485009000
6	-7.158993000	1.452281000	0.280520000
6	-7.272714000	-0.907520000	0.986147000
6	-8.441056000	1.687773000	0.670926000
6	-8.556905000	-0.685334000	1.388661000
1	-6.826282000	-1.886504000	1.078790000
6	-9.208407000	0.604180000	1.247025000
1	-8.897324000	2.666716000	0.567702000
1	-9.130884000	-1.494402000	1.830488000
8	-4.055195000	2.281584000	-0.968858000
8	-5.481909000	-2.765386000	-0.348503000
7	-6.249086000	2.343210000	-0.263044000
7	-3.179077000	-2.780136000	-0.474968000
6	-3.020496000	-4.207616000	-0.654853000
1	-2.527694000	-4.429647000	-1.607440000
1	-2.433738000	-4.643901000	0.161032000
1	-4.018991000	-4.645614000	-0.655365000
6	-6.495085000	3.736367000	-0.569162000
1	-7.302592000	3.838869000	-1.301965000
1	-6.760901000	4.295358000	0.334750000
1	-5.573916000	4.142611000	-0.987806000
6	1.479504000	-1.130405000	-0.452119000
6	2.190460000	-2.324808000	-0.714275000
16	2.616201000	0.189457000	-0.194369000
6	3.559448000	-2.189908000	-0.701982000
1	1.695057000	-3.264453000	-0.924606000
6	4.011001000	-0.861248000	-0.433187000
1	4.267898000	-2.988187000	-0.869971000
6	-10.500899000	0.782015000	1.654225000
6	5.347807000	-0.490444000	-0.241198000
6	6.392684000	-1.527161000	0.047779000
6	5.958036000	0.807984000	-0.032902000
6	7.536434000	-0.794807000	0.643741000
6	7.265019000	0.584872000	0.648321000

6	8.712227000	-1.325461000	1.154576000
6	8.200189000	1.462384000	1.203210000
6	9.643880000	-0.444377000	1.709166000
1	8.882128000	-2.396721000	1.117973000
6	9.380693000	0.929434000	1.734867000
1	8.033261000	2.530236000	1.240242000
1	10.572710000	-0.823199000	2.124389000
1	10.107723000	1.604539000	2.175963000
8	6.333218000	-2.737585000	-0.121098000
6	5.526960000	2.038611000	-0.512984000
6	4.518853000	2.195220000	-1.510294000
7	3.745737000	2.374861000	-2.363694000
6	6.162173000	3.269966000	-0.165311000
7	6.642993000	4.294594000	0.112841000
1	-11.070772000	-0.031815000	2.089662000
1	-11.000254000	1.740340000	1.556004000

S8TIIDS0-OS E=-2623.836375 Hartree

6	-7.575577000	1.406660000	0.300210000
6	-6.908182000	0.120782000	0.402322000
6	-7.646322000	-0.962646000	0.970984000
6	-8.937801000	-0.771515000	1.370093000
6	-9.612990000	0.505647000	1.242497000
6	-8.864856000	1.611655000	0.686753000
6	-5.443903000	1.728670000	-0.448235000
6	-5.580365000	0.280205000	-0.047578000
1	-7.181380000	-1.933745000	1.053244000
1	-9.497239000	-1.598172000	1.797659000
1	-9.339268000	2.583015000	0.594845000
6	-4.524798000	-0.656216000	-0.186079000
6	-3.118905000	-0.472318000	-0.274602000
6	-4.756864000	-2.139462000	-0.330056000
6	-2.511534000	-1.767317000	-0.445111000
6	-2.248816000	0.642720000	-0.161836000
6	-1.154607000	-1.957377000	-0.521229000
6	-0.886579000	0.461994000	-0.229355000
1	-2.663207000	1.634316000	-0.056529000
6	-0.294196000	-0.824916000	-0.414800000
1	-0.746209000	-2.953846000	-0.634039000
1	-0.243994000	1.333727000	-0.163460000
8	-5.806277000	-2.768086000	-0.352265000
8	-4.483751000	2.322094000	-0.917692000
7	-3.505261000	-2.729700000	-0.489674000

7	-6.681425000	2.324863000	-0.224493000
6	-6.955844000	3.717240000	-0.510512000
1	-7.761079000	3.813335000	-1.246592000
1	-7.239041000	4.255757000	0.400454000
1	-6.041444000	4.150008000	-0.917100000
6	-3.315183000	-4.152569000	-0.678616000
1	-2.823040000	-4.357533000	-1.635269000
1	-2.713913000	-4.579388000	0.131549000
1	-4.303254000	-4.613431000	-0.676022000
6	-10.912483000	0.652507000	1.644819000
6	1.120370000	-0.987390000	-0.479950000
6	1.849405000	-2.154835000	-0.791342000
16	2.228391000	0.343059000	-0.169885000
6	3.217416000	-1.991015000	-0.778496000
1	1.372558000	-3.092798000	-1.045657000
6	3.639715000	-0.669475000	-0.455775000
1	3.921870000	-2.776162000	-1.020693000
6	4.966737000	-0.279024000	-0.250253000
6	5.601618000	0.987620000	-0.076010000
6	7.335942000	-0.471378000	0.772769000
6	6.903783000	0.856866000	0.641590000
6	8.533201000	-0.839622000	1.365656000
6	7.734200000	1.859013000	1.165331000
6	9.345899000	0.174164000	1.875843000
1	8.818832000	-1.883897000	1.434983000
6	8.938867000	1.506902000	1.776991000
1	7.455857000	2.901700000	1.114820000
1	10.288169000	-0.075007000	2.353044000
1	9.567934000	2.292315000	2.183796000
6	5.129518000	2.189562000	-0.621736000
6	5.664403000	3.473384000	-0.311662000
7	6.054465000	4.546901000	-0.075353000
6	4.147851000	2.237473000	-1.652484000
7	3.382832000	2.323753000	-2.528257000
16	6.151613000	-1.613568000	0.095681000
8	5.642744000	-2.502082000	1.152113000
8	6.636924000	-2.220971000	-1.154721000
1	-11.468484000	-0.178544000	2.065349000
1	-11.429860000	1.602213000	1.556975000

S9TIIDS0-OS E=-2609.776553 Hartree

6	6.906569000	-1.507754000	0.000636000
6	6.252706000	-0.226931000	0.219508000

6	7.032386000	0.812945000	0.822443000
6	8.334942000	0.585274000	1.151198000
6	8.993835000	-0.689244000	0.915584000
6	8.206254000	-1.749301000	0.318012000
6	4.740612000	-1.750088000	-0.678968000
6	4.912722000	-0.341232000	-0.178588000
1	6.581229000	1.781658000	0.981889000
1	8.923233000	1.378180000	1.604103000
1	8.665262000	-2.716946000	0.142444000
6	3.857217000	0.619318000	-0.199119000
6	2.452578000	0.447990000	-0.199124000
6	4.098551000	2.093670000	-0.278658000
6	1.840535000	1.753544000	-0.257756000
6	1.579391000	-0.667419000	-0.090100000
6	0.485278000	1.953114000	-0.233761000
6	0.218779000	-0.477324000	-0.060764000
1	1.992362000	-1.665227000	-0.060617000
6	-0.382086000	0.819419000	-0.136679000
1	0.080637000	2.957036000	-0.279296000
1	-0.423564000	-1.349325000	0.016774000
8	5.150463000	2.722745000	-0.334797000
8	3.754361000	-2.301518000	-1.150766000
7	2.842141000	2.706350000	-0.319792000
7	5.978674000	-2.378318000	-0.547772000
6	6.219668000	-3.748107000	-0.941358000
1	6.994181000	-3.804536000	-1.714369000
1	6.530812000	-4.355932000	-0.084058000
1	5.282537000	-4.138217000	-1.340130000
6	2.662702000	4.136943000	-0.414474000
1	2.111349000	4.406470000	-1.322506000
1	2.122948000	4.527041000	0.456336000
1	3.657315000	4.583009000	-0.451677000
6	10.303648000	-0.875339000	1.252620000
6	-1.788632000	0.985359000	-0.112358000
6	-2.535434000	2.187456000	-0.187188000
16	-2.902849000	-0.387139000	0.026471000
6	-3.900761000	2.029437000	-0.137025000
1	-2.060732000	3.156274000	-0.279172000
6	-4.326431000	0.674685000	-0.017921000
1	-4.603047000	2.854104000	-0.183870000
6	-5.615550000	0.196922000	0.055547000
16	-5.995946000	-1.520783000	0.202336000
16	-7.024714000	1.268114000	0.009998000
6	-7.753647000	-1.325368000	0.232755000

6	-8.237930000	-0.011773000	0.142087000
6	-8.641622000	-2.398174000	0.340337000
6	-9.612826000	0.234524000	0.158596000
6	-10.013031000	-2.147808000	0.356487000
1	-8.265895000	-3.413983000	0.410256000
6	-10.495604000	-0.839226000	0.266130000
1	-9.987435000	1.250735000	0.088313000
1	-10.706258000	-2.978503000	0.439855000
1	-11.564408000	-0.651814000	0.279212000
1	10.887476000	-0.079786000	1.703268000
1	10.804930000	-1.822408000	1.081215000

S10TIIDS0-OS E=-2456.117888 Hartree

6	0.735487000	1.653238000	-0.275328000
6	1.418083000	0.384985000	-0.192700000
6	0.608242000	-0.772574000	-0.046292000
6	-0.760738000	-0.655673000	-0.005090000
6	-1.431617000	0.603938000	-0.105012000
6	-0.628609000	1.779779000	-0.239759000
6	2.971340000	2.115322000	-0.331169000
6	2.812052000	0.632403000	-0.213714000
1	1.074939000	-1.745624000	0.002472000
1	-1.353640000	-1.559106000	0.101392000
1	-1.087639000	2.758980000	-0.304640000
6	3.918320000	-0.268197000	-0.182928000
6	5.255622000	-0.070804000	0.193135000
6	3.817466000	-1.697351000	-0.644313000
6	5.975338000	-1.319488000	-0.001455000
6	5.985172000	1.025145000	0.757685000
6	7.290338000	-1.482005000	0.303546000
6	7.302520000	0.877117000	1.073753000
1	5.484110000	1.971963000	0.898477000
6	8.026691000	-0.365492000	0.861858000
1	7.798774000	-2.427909000	0.146675000
1	7.852370000	1.712522000	1.497632000
8	2.857211000	-2.314301000	-1.087801000
8	3.986317000	2.799599000	-0.415798000
7	5.089405000	-2.253672000	-0.513623000
7	1.682820000	2.657331000	-0.372415000
6	1.424354000	4.073013000	-0.501190000
1	0.848412000	4.288126000	-1.408502000
1	0.874341000	4.456096000	0.366335000

1	2.392621000	4.571319000	-0.562889000
6	5.400222000	-3.618098000	-0.875458000
1	6.167388000	-3.652360000	-1.657060000
1	5.754392000	-4.185649000	-0.007299000
1	4.481109000	-4.068831000	-1.251658000
6	-2.845768000	0.694445000	-0.067987000
6	-3.657684000	1.850693000	-0.162201000
16	-3.881746000	-0.733017000	0.116444000
6	-5.012796000	1.618952000	-0.092184000
1	-3.238248000	2.841673000	-0.282544000
6	-5.361143000	0.247612000	0.063504000
1	-5.759814000	2.402711000	-0.150205000
6	9.349300000	-0.471380000	1.184595000
6	-6.621733000	-0.300978000	0.163128000
16	-6.915469000	-2.035025000	0.354214000
16	-8.100452000	0.676645000	0.110443000
6	-8.666790000	-1.903672000	0.397602000
6	-9.200606000	-0.680792000	0.287621000
1	-10.261101000	-0.461890000	0.299358000
1	-9.231324000	-2.820664000	0.511472000
1	9.894681000	0.366356000	1.606004000
1	9.899124000	-1.394185000	1.030546000

S1TIIDS0-T1 E=-1768.013146 Hartree

6	5.333601000	-1.156239000	-0.066067000
6	4.589401000	0.056185000	0.145411000
6	5.299629000	1.178468000	0.638038000
6	6.653828000	1.089568000	0.871043000
6	7.399671000	-0.115933000	0.632666000
6	6.680359000	-1.264074000	0.152406000
6	3.164274000	-1.685439000	-0.550185000
6	3.202574000	-0.221103000	-0.142427000
1	4.774880000	2.106291000	0.805649000
1	7.189377000	1.957586000	1.243556000
1	7.209459000	-2.195156000	-0.021006000
6	2.072057000	0.589676000	-0.132095000
6	0.645350000	0.266111000	-0.178729000
6	2.134220000	2.098288000	-0.114097000
6	-0.069734000	1.497534000	-0.184055000
6	-0.107322000	-0.915861000	-0.130648000
6	-1.450716000	1.572222000	-0.175535000
6	-1.498412000	-0.856284000	-0.119684000
1	0.391452000	-1.872426000	-0.132176000

6	-2.192571000	0.369724000	-0.151185000
1	-1.950213000	2.533423000	-0.151493000
1	-2.055693000	-1.787630000	-0.117923000
8	3.102810000	2.847879000	-0.108026000
8	2.220053000	-2.371033000	-0.914541000
7	0.824208000	2.558443000	-0.165713000
7	4.466251000	-2.153956000	-0.494460000
6	4.836831000	-3.510415000	-0.838602000
1	5.554416000	-3.519461000	-1.665898000
1	5.278892000	-4.024836000	0.021631000
1	3.927200000	-4.028549000	-1.142516000
6	0.479454000	3.963923000	-0.187912000
1	-0.084499000	4.213117000	-1.093286000
1	-0.117427000	4.235830000	0.689783000
1	1.413360000	4.526146000	-0.178074000
6	8.764170000	-0.166988000	0.866002000
6	-3.648060000	0.417064000	-0.157415000
6	-4.473755000	1.471145000	-0.549517000
16	-4.610708000	-0.951929000	0.374281000
6	-5.838736000	1.199182000	-0.440735000
1	-4.083692000	2.405104000	-0.934989000
6	-6.109053000	-0.091668000	0.047898000
1	-6.628628000	1.889845000	-0.710520000
6	-7.376726000	-0.672368000	0.272406000
6	-8.554142000	0.073696000	0.004969000
7	-9.506150000	0.708787000	-0.223174000
6	-7.517281000	-1.994373000	0.763866000
7	-7.610220000	-3.085098000	1.169351000
1	9.302727000	0.699902000	1.232683000
1	9.334730000	-1.072578000	0.689702000

S2TIIDS0-T1 E=-1850.501163 Hartree

6	0.736130000	1.613775000	-0.212336000
6	1.384953000	0.346185000	-0.225984000
6	0.566691000	-0.794059000	-0.233183000
6	-0.818394000	-0.658396000	-0.255336000
6	-1.444449000	0.603621000	-0.264506000
6	-0.638980000	1.762763000	-0.232808000
6	2.965990000	2.090775000	-0.072438000
6	2.821224000	0.588584000	-0.133897000
1	1.013464000	-1.775990000	-0.252914000
1	-1.427431000	-1.555667000	-0.298033000
1	-1.089261000	2.747546000	-0.189063000

6	3.908951000	-0.283758000	-0.137497000
6	5.294953000	-0.091910000	0.203976000
6	3.804940000	-1.726892000	-0.597012000
6	5.982616000	-1.335742000	-0.025446000
6	6.047765000	0.973988000	0.758701000
6	7.312883000	-1.522901000	0.232452000
6	7.385366000	0.804618000	1.031983000
1	5.567394000	1.922954000	0.940862000
6	8.076154000	-0.431508000	0.776057000
1	7.797920000	-2.474871000	0.043768000
1	7.953182000	1.629553000	1.451879000
8	2.838512000	-2.348799000	-1.014944000
8	3.974644000	2.784633000	-0.023326000
7	5.078287000	-2.269016000	-0.516282000
7	1.685222000	2.624211000	-0.140408000
6	1.418154000	4.046151000	-0.130491000
1	0.891445000	4.351098000	-1.041329000
1	0.814496000	4.326827000	0.739874000
1	2.380773000	4.555648000	-0.082247000
6	5.385902000	-3.631072000	-0.896067000
1	6.128381000	-3.652951000	-1.701038000
1	5.771615000	-4.198035000	-0.041590000
1	4.459558000	-4.087416000	-1.245462000
6	-2.898608000	0.734394000	-0.305812000
6	-3.652767000	1.813631000	-0.737303000
16	-3.951071000	-0.555169000	0.235919000
6	-5.042316000	1.612772000	-0.646556000
1	-3.207660000	2.714781000	-1.141807000
6	-5.404088000	0.367435000	-0.139134000
1	-5.765403000	2.353994000	-0.963348000
6	9.425330000	-0.563215000	1.051329000
6	-6.722490000	-0.165696000	0.083078000
6	-6.921803000	-1.505231000	0.538126000
6	-7.882094000	0.640512000	-0.146836000
6	-8.174354000	-2.012227000	0.749990000
1	-6.055639000	-2.137552000	0.713159000
6	-9.142778000	0.153736000	0.058282000
1	-7.756063000	1.663970000	-0.484434000
6	-9.369813000	-1.209940000	0.521762000
1	-8.323531000	-3.030996000	1.092991000
1	-10.021884000	0.766628000	-0.113627000
8	-10.517998000	-1.662658000	0.711814000
1	9.996058000	0.260796000	1.465314000
1	9.953479000	-1.491731000	0.862246000

S3TIIDS0-T1 E=-2335.872612 Hartree

6	1.799149000	1.610297000	-0.166431000
6	2.445203000	0.341076000	-0.212039000
6	1.625793000	-0.797593000	-0.251308000
6	0.241204000	-0.659160000	-0.272973000
6	-0.381745000	0.604343000	-0.250683000
6	0.424356000	1.761956000	-0.187383000
6	4.029905000	2.076176000	-0.009536000
6	3.881282000	0.577753000	-0.111226000
1	2.071356000	-1.779207000	-0.296929000
1	-0.368385000	-1.554537000	-0.342386000
1	-0.024125000	2.746106000	-0.119157000
6	4.966544000	-0.298690000	-0.136727000
6	6.350142000	-0.121350000	0.214641000
6	4.859621000	-1.727578000	-0.640194000
6	7.035597000	-1.360237000	-0.049720000
6	7.103220000	0.926620000	0.803658000
6	8.364090000	-1.557875000	0.207052000
6	8.438884000	0.746016000	1.076278000
1	6.624211000	1.870880000	1.012018000
6	9.127491000	-0.484225000	0.785720000
1	8.848183000	-2.504642000	-0.008059000
1	9.007440000	1.556398000	1.522514000
8	3.891906000	-2.332204000	-1.079536000
8	5.039810000	2.765833000	0.060425000
7	6.130517000	-2.275803000	-0.571336000
7	2.749709000	2.615173000	-0.065994000
6	2.486813000	4.037560000	-0.019079000
1	1.964065000	4.368208000	-0.923119000
1	1.882010000	4.296845000	0.857018000
1	3.450885000	4.542431000	0.045282000
6	6.435840000	-3.627081000	-0.990958000
1	7.180937000	-3.626475000	-1.793665000
1	6.816801000	-4.220226000	-0.152402000
1	5.509662000	-4.070286000	-1.357154000
6	-1.834462000	0.738112000	-0.291496000
6	-2.587282000	1.831773000	-0.692582000
16	-2.885547000	-0.569644000	0.210749000
6	-3.976545000	1.629479000	-0.612770000
1	-2.139744000	2.744084000	-1.067110000
6	-4.330640000	0.369105000	-0.144175000
1	-4.708961000	2.374596000	-0.902308000

6	10.474580000	-0.626879000	1.061562000
6	-5.635012000	-0.169699000	0.056345000
6	-5.989707000	-1.458876000	0.493388000
16	-7.100356000	0.745835000	-0.226452000
1	-5.260297000	-2.225009000	0.735799000
6	-8.042382000	-0.683231000	0.264871000
6	-9.448523000	-0.683747000	0.285953000
6	-10.182434000	0.470379000	-0.090076000
7	-10.761398000	1.433625000	-0.404280000
6	-10.165662000	-1.841853000	0.685572000
7	-10.783503000	-2.776297000	1.008674000
7	-7.288527000	-1.736041000	0.605927000
1	11.045586000	0.183179000	1.501862000
1	11.001598000	-1.550451000	0.846860000

S4TIIDS0-T1 E=-2301.893804 Hartree

6	1.269383000	1.681222000	-0.160669000
6	1.894360000	0.403843000	-0.220449000
6	1.055594000	-0.719522000	-0.271777000
6	-0.327131000	-0.557854000	-0.292067000
6	-0.930721000	0.715208000	-0.257123000
6	-0.102274000	1.856985000	-0.180446000
6	3.507231000	2.113911000	0.004981000
6	3.337028000	0.617005000	-0.115362000
1	1.483629000	-1.708400000	-0.325396000
1	-0.951519000	-1.442194000	-0.367166000
1	-0.532597000	2.848465000	-0.102232000
6	4.407768000	-0.271603000	-0.150237000
6	5.800901000	-0.115889000	0.194325000
6	4.278157000	-1.697650000	-0.656446000
6	6.463737000	-1.363176000	-0.077151000
6	6.574035000	0.916114000	0.780910000
6	7.791481000	-1.584013000	0.171264000
6	7.909957000	0.712725000	1.045257000
1	6.112132000	1.867383000	0.995646000
6	8.575895000	-0.526238000	0.747771000
1	8.257563000	-2.538501000	-0.049688000
1	8.493696000	1.513111000	1.490094000
8	3.300828000	-2.288474000	-1.093255000
8	4.527478000	2.787669000	0.084808000
7	5.541726000	-2.263939000	-0.595992000
7	2.236891000	2.671342000	-0.047718000
6	1.994335000	4.096227000	0.015532000

1	1.476639000	4.444597000	-0.884863000
1	1.391735000	4.353806000	0.893756000
1	2.965273000	4.586878000	0.086679000
6	5.824581000	-3.618139000	-1.020395000
1	6.565415000	-3.626914000	-1.827152000
1	6.201551000	-4.219176000	-0.185520000
1	4.889783000	-4.046536000	-1.382414000
6	-2.380934000	0.871215000	-0.296068000
6	-3.105652000	1.999577000	-0.670453000
16	-3.453513000	-0.440308000	0.161523000
6	-4.491026000	1.827679000	-0.605331000
1	-2.635856000	2.913612000	-1.013180000
6	-4.880498000	0.547756000	-0.171062000
1	-5.209473000	2.593997000	-0.873178000
6	9.924667000	-0.692849000	1.015350000
6	-6.184083000	0.067700000	-0.001168000
6	-6.508840000	-1.280121000	0.448891000
16	-7.634523000	1.015774000	-0.306200000
6	-8.696911000	-0.388881000	0.164188000
7	-7.902478000	-1.458438000	0.514550000
6	-8.503265000	-2.719088000	0.936697000
1	-9.129784000	-3.123441000	0.138488000
1	-7.685963000	-3.404477000	1.158737000
1	-9.118718000	-2.563928000	1.825726000
8	-9.904361000	-0.357244000	0.160286000
8	-5.702766000	-2.158566000	0.737874000
1	10.511736000	0.106271000	1.454442000
1	10.434279000	-1.624716000	0.794689000

S5TIIDS0-T1 E=-2073.357171 Hartree

6	1.652184000	1.702428000	-0.119798000
6	2.281215000	0.427847000	-0.208907000
6	1.447984000	-0.698136000	-0.282609000
6	0.064753000	-0.542009000	-0.295862000
6	-0.543479000	0.728494000	-0.233270000
6	0.280061000	1.872836000	-0.135305000
6	3.889326000	2.137381000	0.051196000
6	3.723850000	0.644234000	-0.102998000
1	1.880232000	-1.683612000	-0.358957000
1	-0.555916000	-1.427232000	-0.387655000
1	-0.153680000	2.860945000	-0.037113000
6	4.796467000	-0.240965000	-0.161698000
6	6.189001000	-0.089986000	0.183154000

6	4.669871000	-1.655368000	-0.704078000
6	6.854820000	-1.328404000	-0.121007000
6	6.959492000	0.930345000	0.793737000
6	8.183621000	-1.550681000	0.118989000
6	8.296445000	0.724983000	1.049980000
1	6.494651000	1.874315000	1.032945000
6	8.965178000	-0.504316000	0.719994000
1	8.652815000	-2.497550000	-0.126476000
1	8.878744000	1.515764000	1.513303000
8	3.692618000	-2.236051000	-1.153626000
8	4.907066000	2.812547000	0.145190000
7	5.934520000	-2.218980000	-0.660195000
7	2.616315000	2.691963000	0.012704000
6	2.369643000	4.114703000	0.108538000
1	1.850456000	4.481849000	-0.783414000
1	1.767492000	4.350250000	0.993149000
1	3.339237000	4.606316000	0.189949000
6	6.221090000	-3.561466000	-1.119493000
1	6.960557000	-3.546811000	-1.927260000
1	6.601083000	-4.181948000	-0.300515000
1	5.287312000	-3.983769000	-1.491003000
6	-1.992787000	0.877007000	-0.265748000
6	-2.721551000	2.018536000	-0.601085000
16	-3.060247000	-0.450588000	0.144584000
6	-4.101866000	1.833116000	-0.541129000
1	-2.259503000	2.947441000	-0.912278000
6	-4.489788000	0.536803000	-0.151131000
1	-4.811826000	2.613147000	-0.786630000
6	10.314834000	-0.672779000	0.980423000
6	-5.817626000	0.055446000	0.001011000
6	-6.943226000	0.875403000	-0.225679000
6	-6.040584000	-1.346472000	0.409194000
6	-8.227836000	0.401688000	-0.081694000
1	-6.808075000	1.909413000	-0.521376000
6	-8.499275000	-0.990668000	0.318214000
6	-9.348216000	1.247706000	-0.315948000
7	-10.235482000	1.974630000	-0.517552000
8	-5.112102000	-2.123004000	0.632405000
8	-9.630287000	-1.435419000	0.451499000
7	-7.358046000	-1.781830000	0.539478000
6	-7.546500000	-3.180445000	0.943979000
1	-7.078020000	-3.842169000	0.212827000
1	-7.074784000	-3.350948000	1.913720000
1	-8.616250000	-3.364804000	0.999294000

1	10.900121000	0.117212000	1.437993000
1	10.827200000	-1.597041000	0.735559000

S6TIIDS0-T1 E=-2434.677464 Hartree

6	2.014603000	1.708873000	-0.110528000
6	2.620189000	0.422776000	-0.191755000
6	1.766736000	-0.688275000	-0.254777000
6	0.386579000	-0.507117000	-0.265552000
6	-0.199978000	0.775026000	-0.212248000
6	0.646447000	1.904814000	-0.125153000
6	4.259769000	2.106486000	0.053072000
6	4.068422000	0.614475000	-0.090629000
1	2.180555000	-1.682104000	-0.323411000
1	-0.249766000	-1.382104000	-0.345782000
1	0.232573000	2.902081000	-0.036738000
6	5.124291000	-0.288049000	-0.146163000
6	6.524075000	-0.157210000	0.188122000
6	4.970758000	-1.706795000	-0.671394000
6	7.165221000	-1.409520000	-0.106919000
6	7.316081000	0.855106000	0.781883000
6	8.492147000	-1.653011000	0.126424000
6	8.651957000	0.628811000	1.031271000
1	6.869735000	1.809560000	1.014457000
6	9.295929000	-0.614812000	0.710265000
1	8.942413000	-2.610802000	-0.112020000
1	9.251032000	1.414401000	1.481857000
8	3.981143000	-2.276501000	-1.107573000
8	5.289412000	2.764242000	0.140501000
7	6.226080000	-2.290422000	-0.630038000
7	2.997171000	2.682246000	0.012688000
6	2.775097000	4.109870000	0.096439000
1	2.259874000	4.477555000	-0.797546000
1	2.178949000	4.363251000	0.980156000
1	3.753048000	4.585649000	0.171385000
6	6.487072000	-3.642584000	-1.075869000
1	7.222300000	-3.649390000	-1.887603000
1	6.860986000	-4.260447000	-0.252101000
1	5.544203000	-4.052933000	-1.437685000
6	-1.643889000	0.948179000	-0.242157000
6	-2.353434000	2.118591000	-0.533616000
16	-2.736355000	-0.379122000	0.110689000
6	-3.732297000	1.965685000	-0.488102000
1	-1.872177000	3.051032000	-0.802883000

6	-4.153491000	0.652070000	-0.149283000
1	-4.452606000	2.742477000	-0.694011000
6	10.645673000	-0.804847000	0.963295000
6	-5.473178000	0.175913000	-0.018140000
6	-6.617928000	1.061879000	-0.227716000
6	-5.691942000	-1.220863000	0.330908000
6	-8.132412000	-0.853397000	0.244378000
8	-4.763094000	-2.006058000	0.526277000
7	-7.024167000	-1.658834000	0.441020000
6	-7.228436000	-3.073747000	0.790756000
1	-7.795533000	-3.570631000	0.002501000
1	-6.244984000	-3.521648000	0.900853000
1	-7.794449000	-3.146134000	1.720403000
7	-7.896819000	0.470624000	-0.079573000
6	-9.054448000	1.354704000	-0.292513000
1	-9.667957000	0.969503000	-1.108114000
1	-9.664826000	1.387666000	0.610976000
1	-8.665504000	2.339642000	-0.532846000
8	-6.531750000	2.252500000	-0.516309000
16	-9.687063000	-1.458521000	0.394158000
1	11.248077000	-0.020509000	1.408143000
1	11.139517000	-1.740763000	0.724825000

S7TIIDS0-T1 E=-2188.608894 Hartree

6	-2.135162000	-1.785426000	-0.322364000
6	-2.727700000	-0.491035000	-0.278541000
6	-1.865308000	0.614619000	-0.313079000
6	-0.489696000	0.423234000	-0.412344000
6	0.079231000	-0.864840000	-0.477051000
6	-0.771731000	-1.991661000	-0.423939000
6	-4.372685000	-2.172607000	-0.064940000
6	-4.169570000	-0.676597000	-0.110911000
1	-2.270204000	1.614341000	-0.294184000
1	0.153221000	1.294790000	-0.480860000
1	-0.362419000	-2.994973000	-0.424727000
6	-5.216036000	0.237988000	-0.040262000
6	-6.593649000	0.095954000	0.365624000
6	-5.074445000	1.688820000	-0.472060000
6	-7.235848000	1.372126000	0.197859000
6	-7.362869000	-0.949948000	0.932550000
6	-8.543468000	1.608942000	0.525391000
6	-8.678258000	-0.731022000	1.275482000
1	-6.915605000	-1.922225000	1.070185000

6	-9.324956000	0.538140000	1.081262000
1	-8.995256000	2.584775000	0.381868000
1	-9.260002000	-1.541473000	1.704252000
8	-4.104271000	2.279247000	-0.923495000
8	-5.404500000	-2.825853000	0.031030000
7	-6.317774000	2.279502000	-0.316054000
7	-3.121322000	-2.756045000	-0.214844000
6	-2.913916000	-4.187968000	-0.245486000
1	-2.452605000	-4.495224000	-1.190276000
1	-2.274507000	-4.510010000	0.583988000
1	-3.892687000	-4.658661000	-0.151410000
6	-6.586247000	3.662216000	-0.649964000
1	-7.365317000	3.733110000	-1.416473000
1	-6.905825000	4.223032000	0.235176000
1	-5.659912000	4.089123000	-1.034631000
6	1.518397000	-1.053099000	-0.594332000
6	2.202339000	-2.165057000	-1.090504000
16	2.642486000	0.183907000	-0.092351000
6	3.588635000	-2.033902000	-1.068871000
1	1.691787000	-3.033573000	-1.488294000
6	4.036544000	-0.791968000	-0.563897000
1	4.289146000	-2.786102000	-1.402304000
6	-10.654078000	0.720299000	1.426002000
6	5.380537000	-0.442735000	-0.317142000
6	6.428738000	-1.507871000	-0.161668000
6	5.991627000	0.819805000	0.028286000
6	7.584156000	-0.847350000	0.490864000
6	7.313622000	0.523357000	0.653529000
6	8.768496000	-1.430030000	0.918088000
6	8.258669000	1.334463000	1.285620000
6	9.711155000	-0.614596000	1.549744000
1	8.937017000	-2.490480000	0.760465000
6	9.449171000	0.747162000	1.732434000
1	8.093722000	2.391333000	1.444705000
1	10.647067000	-1.035951000	1.903290000
1	10.184696000	1.370419000	2.231825000
8	6.353976000	-2.688765000	-0.468419000
6	5.545958000	2.097724000	-0.297634000
6	4.505541000	2.368472000	-1.236312000
7	3.705675000	2.655330000	-2.033801000
6	6.193420000	3.281979000	0.167956000
7	6.685054000	4.269326000	0.545106000
1	-11.239112000	-0.088769000	1.849284000
1	-11.149744000	1.674646000	1.283625000

S8TIIDS0-T1 E=-2623.829744 Hartree

6	-7.646025000	1.335544000	0.239833000
6	-6.978066000	0.067759000	0.372891000
6	-7.725636000	-1.008637000	0.912685000
6	-9.044073000	-0.825306000	1.262241000
6	-9.716533000	0.435913000	1.102228000
6	-8.957295000	1.537123000	0.574452000
6	-5.492256000	1.711568000	-0.422771000
6	-5.605726000	0.247315000	-0.029857000
1	-7.258765000	-1.975100000	1.023759000
1	-9.609138000	-1.658115000	1.669902000
1	-9.429015000	2.507045000	0.457517000
6	-4.541715000	-0.646079000	-0.126631000
6	-3.104668000	-0.428245000	-0.285940000
6	-4.716995000	-2.145772000	-0.126644000
6	-2.487248000	-1.709715000	-0.368294000
6	-2.264198000	0.694918000	-0.285441000
6	-1.119880000	-1.885988000	-0.474086000
6	-0.885275000	0.533279000	-0.388241000
1	-2.689002000	1.685406000	-0.237742000
6	-0.292261000	-0.741258000	-0.490833000
1	-0.690137000	-2.880292000	-0.503167000
1	-0.259201000	1.418652000	-0.430850000
8	-5.736620000	-2.820438000	-0.052593000
8	-4.533658000	2.332157000	-0.858187000
7	-3.454334000	-2.701208000	-0.291886000
7	-6.746520000	2.273914000	-0.250275000
6	-7.042134000	3.659720000	-0.546801000
1	-7.823486000	3.735928000	-1.310424000
1	-7.371101000	4.190340000	0.353362000
1	-6.124812000	4.114619000	-0.920813000
6	-3.219869000	-4.127723000	-0.364627000
1	-2.753025000	-4.398208000	-1.317845000
1	-2.574675000	-4.461734000	0.455469000
1	-4.189610000	-4.619271000	-0.285079000
6	-11.047717000	0.581762000	1.452485000
6	1.150788000	-0.898431000	-0.610358000
6	1.854604000	-1.973001000	-1.154888000
16	2.248152000	0.328863000	-0.034879000
6	3.239513000	-1.817088000	-1.115176000
1	1.362280000	-2.827402000	-1.602111000
6	3.656109000	-0.598387000	-0.547334000

1	3.944929000	-2.533540000	-1.518314000
6	4.993389000	-0.239430000	-0.272802000
6	5.641264000	0.991382000	-0.005050000
6	7.383147000	-0.547649000	0.679358000
6	6.971602000	0.793560000	0.645604000
6	8.600275000	-0.970880000	1.188815000
6	7.848518000	1.748152000	1.180683000
6	9.458366000	-0.002975000	1.714074000
1	8.868253000	-2.022105000	1.182731000
6	9.074769000	1.339889000	1.710061000
1	7.593031000	2.797639000	1.200597000
1	10.417602000	-0.296081000	2.128149000
1	9.739925000	2.089914000	2.126070000
6	5.151738000	2.245877000	-0.425252000
6	5.691737000	3.493498000	-0.005644000
7	6.084539000	4.541551000	0.324650000
6	4.144194000	2.393689000	-1.421075000
7	3.361270000	2.578691000	-2.265320000
16	6.139929000	-1.624984000	0.002901000
8	5.616846000	-2.519529000	1.045406000
8	6.561686000	-2.207946000	-1.281651000
1	-11.615829000	-0.249949000	1.854423000
1	-11.562883000	1.529293000	1.336063000

S9TIIDS0-T1 E=-2609.767442 Hartree

6	6.964506000	-1.459750000	-0.046216000
6	6.334671000	-0.189484000	0.187787000
6	7.141455000	0.843536000	0.722092000
6	8.477870000	0.618629000	0.972650000
6	9.110508000	-0.644575000	0.712099000
6	8.291845000	-1.702885000	0.189084000
6	4.760985000	-1.766168000	-0.575952000
6	4.929764000	-0.327295000	-0.129876000
1	6.706149000	1.812999000	0.908963000
1	9.086595000	1.421840000	1.377399000
1	8.731056000	-2.676197000	-0.003520000
6	3.878806000	0.584712000	-0.112346000
6	2.432379000	0.404505000	-0.193803000
6	4.085462000	2.082388000	-0.042832000
6	1.836081000	1.696795000	-0.164834000
6	1.562534000	-0.697528000	-0.203928000
6	0.470625000	1.907379000	-0.171708000
6	0.185508000	-0.501609000	-0.213177000

1	1.965078000	-1.698191000	-0.232825000
6	-0.392015000	0.786211000	-0.207008000
1	0.070128000	2.912866000	-0.120272000
1	-0.459031000	-1.374070000	-0.252657000
8	5.122123000	2.734291000	0.000506000
8	3.764453000	-2.355640000	-0.972059000
7	2.828752000	2.667641000	-0.094404000
7	6.013820000	-2.358198000	-0.515072000
6	6.258744000	-3.733361000	-0.890070000
1	6.985005000	-3.791572000	-1.708199000
1	6.637354000	-4.310446000	-0.038921000
1	5.308065000	-4.153639000	-1.218989000
6	2.620648000	4.098578000	-0.074369000
1	2.096825000	4.429994000	-0.977765000
1	2.037544000	4.399250000	0.803495000
1	3.603777000	4.568119000	-0.033664000
6	10.461311000	-0.833521000	0.964192000
6	-1.832647000	0.976855000	-0.231794000
6	-2.553384000	2.134171000	-0.503858000
16	-2.942397000	-0.353123000	0.110354000
6	-3.943479000	1.986789000	-0.452849000
1	-2.072739000	3.070409000	-0.762517000
6	-4.360288000	0.678993000	-0.131709000
1	-4.641480000	2.791391000	-0.652475000
6	-5.662164000	0.195056000	-0.002581000
16	-6.034539000	-1.484236000	0.392548000
16	-7.069460000	1.243072000	-0.224353000
6	-7.792762000	-1.299469000	0.345913000
6	-8.279828000	-0.015542000	0.054428000
6	-8.680068000	-2.352149000	0.583012000
6	-9.656103000	0.218449000	-0.000681000
6	-10.052488000	-2.113372000	0.527101000
1	-8.302270000	-3.344508000	0.807839000
6	-10.537695000	-0.835190000	0.236860000
1	-10.032630000	1.211074000	-0.226551000
1	-10.744298000	-2.929120000	0.710664000
1	-11.607246000	-0.656130000	0.194512000
1	11.074109000	-0.032699000	1.363188000
1	10.945040000	-1.784976000	0.770496000

S10TIIDS0-T1 E=-2456.108883 Hartree

6	0.733272000	1.597751000	-0.196328000
6	1.397040000	0.338378000	-0.187716000

6	0.586475000	-0.807426000	-0.145887000
6	-0.798866000	-0.684464000	-0.141943000
6	-1.444008000	0.570649000	-0.173280000
6	-0.641310000	1.736019000	-0.190713000
6	2.960426000	2.105030000	-0.121716000
6	2.832457000	0.596987000	-0.134127000
1	1.041081000	-1.785979000	-0.145012000
1	-1.396627000	-1.590498000	-0.140669000
1	-1.093674000	2.720394000	-0.169668000
6	3.930149000	-0.258782000	-0.133995000
6	5.329527000	-0.035704000	0.158077000
6	3.832284000	-1.719807000	-0.525233000
6	6.023020000	-1.278846000	-0.039020000
6	6.087175000	1.057331000	0.642750000
6	7.364303000	-1.442928000	0.185293000
6	7.436722000	0.912490000	0.881481000
1	5.603394000	2.008757000	0.800889000
6	8.132309000	-0.324422000	0.657491000
1	7.852076000	-2.398244000	0.021550000
1	8.007034000	1.761031000	1.247893000
8	2.863579000	-2.375245000	-0.885269000
8	3.961544000	2.811664000	-0.117344000
7	5.115491000	-2.242639000	-0.461145000
7	1.673918000	2.621303000	-0.175419000
6	1.390557000	4.039079000	-0.203416000
1	0.838511000	4.309510000	-1.110328000
1	0.803422000	4.340424000	0.671534000
1	2.347850000	4.560783000	-0.193757000
6	5.428269000	-3.615836000	-0.789880000
1	6.146532000	-3.665810000	-1.615596000
1	5.847333000	-4.140749000	0.075972000
1	4.497211000	-4.097182000	-1.089985000
6	-2.892701000	0.684253000	-0.183756000
6	-3.677947000	1.791393000	-0.482335000
16	-3.926360000	-0.690830000	0.216490000
6	-5.058041000	1.571789000	-0.406707000
1	-3.251891000	2.743182000	-0.777407000
6	-5.399630000	0.255941000	-0.037837000
1	-5.800613000	2.331419000	-0.621518000
6	9.494310000	-0.432560000	0.896238000
6	-6.672554000	-0.293790000	0.126168000
16	-6.960734000	-1.978089000	0.581330000
16	-8.147754000	0.658428000	-0.110329000
6	-8.712509000	-1.852048000	0.557732000

6	-9.246986000	-0.664137000	0.245511000
1	-10.308648000	-0.455966000	0.196990000
1	-9.278912000	-2.743139000	0.798158000
1	10.068775000	0.413596000	1.256870000
1	10.025405000	-1.363732000	0.729977000

S2IIDS1-CS E=-1483.164593 Hartree

6	-2.075780000	1.162768000	-0.358069000
6	-1.216257000	0.005217000	-0.191519000
6	-1.850322000	-1.224137000	0.162423000
6	-3.206447000	-1.275516000	0.314892000
6	-4.069609000	-0.130047000	0.122002000
6	-3.432830000	1.112784000	-0.223629000
6	0.061762000	1.892403000	-0.656428000
6	0.110043000	0.416962000	-0.362390000
1	-1.253319000	-2.117031000	0.276913000
1	-3.647222000	-2.232494000	0.558937000
1	-4.012844000	2.017695000	-0.341495000
6	1.329174000	-0.326898000	-0.337041000
6	2.640867000	0.072771000	-0.088737000
6	1.391060000	-1.801850000	-0.671667000
6	3.506754000	-1.088841000	-0.237669000
6	3.252480000	1.302756000	0.323066000
6	4.851969000	-1.048850000	-0.029298000
6	4.595462000	1.355908000	0.541141000
1	2.642182000	2.187543000	0.431094000
6	5.447287000	0.197099000	0.369916000
1	5.474563000	-1.927688000	-0.149051000
1	5.056532000	2.287555000	0.849583000
8	0.487671000	-2.561301000	-0.981261000
8	0.974507000	2.668209000	-0.896249000
7	2.731228000	-2.173728000	-0.597117000
7	-1.285190000	2.258887000	-0.644165000
6	-1.744461000	3.607753000	-0.906291000
1	-2.403830000	3.632875000	-1.780116000
1	-2.279090000	4.014244000	-0.041169000
1	-0.861859000	4.216691000	-1.103499000
6	3.207154000	-3.516795000	-0.867763000
1	3.914478000	-3.517073000	-1.702986000
1	3.695366000	-3.941935000	0.015042000
1	2.338702000	-4.121731000	-1.128850000
6	6.823656000	0.289765000	0.598626000

6	7.441966000	1.507191000	1.004089000
7	7.942329000	2.505884000	1.337259000
6	7.678796000	-0.838350000	0.438794000
7	8.357232000	-1.776460000	0.302037000
6	-5.473954000	-0.230136000	0.270453000
6	-6.109075000	-1.427749000	0.781278000
6	-6.355751000	0.864694000	-0.079426000
6	-7.452516000	-1.525937000	0.936315000
1	-5.493414000	-2.267564000	1.078813000
6	-7.702168000	0.784024000	0.055486000
1	-5.932042000	1.772107000	-0.492831000
6	-8.356485000	-0.423118000	0.581281000
1	-7.913659000	-2.423605000	1.335551000
1	-8.352324000	1.606119000	-0.226360000
8	-9.580686000	-0.503285000	0.714426000

S2IIDS3-CS E=-2051.014759 Hartree

6	-3.688157000	-1.112011000	0.428203000
6	-2.909035000	0.088257000	0.205886000
6	-3.614199000	1.233927000	-0.264841000
6	-4.967888000	1.177732000	-0.452418000
6	-5.750961000	-0.011155000	-0.208760000
6	-5.039161000	-1.176582000	0.238024000
6	-1.522395000	-1.661858000	0.872356000
6	-1.559029000	-0.211157000	0.461245000
1	-3.075880000	2.151530000	-0.450089000
1	-5.458753000	2.064978000	-0.828772000
1	-5.562911000	-2.098204000	0.451413000
6	-0.398716000	0.609947000	0.428965000
6	0.963242000	0.282577000	0.312200000
6	-0.455306000	2.111037000	0.591879000
6	1.730802000	1.508965000	0.381893000
6	1.685808000	-0.925432000	0.081502000
6	3.091576000	1.550197000	0.265037000
6	3.047864000	-0.894347000	-0.043128000
1	1.152300000	-1.863213000	0.033266000
6	3.805982000	0.324896000	0.049821000
1	3.617208000	2.494626000	0.326317000
1	3.578246000	-1.825279000	-0.214347000
8	-1.421998000	2.839843000	0.754600000
8	-0.572606000	-2.352392000	1.210567000
7	0.860576000	2.567908000	0.563938000
7	-2.838143000	-2.120943000	0.841820000

6	-3.216282000	-3.474949000	1.191929000
1	-3.909280000	-3.479853000	2.039697000
1	-3.685335000	-3.982209000	0.342097000
1	-2.304204000	-4.003771000	1.469424000
6	1.222284000	3.963535000	0.708570000
1	1.864931000	4.111378000	1.582653000
1	1.740981000	4.328097000	-0.184476000
1	0.297440000	4.524887000	0.842914000
6	5.206877000	0.316281000	-0.074504000
6	6.096905000	1.430943000	-0.005070000
16	6.182149000	-1.125439000	-0.353234000
1	5.756654000	2.447411000	0.162295000
6	7.640595000	-0.107651000	-0.349378000
6	8.918663000	-0.616725000	-0.533135000
6	9.123836000	-2.008727000	-0.739165000
7	9.262715000	-3.154147000	-0.906433000
6	10.054705000	0.240918000	-0.520827000
7	11.005031000	0.914493000	-0.516716000
7	7.383630000	1.213343000	-0.149652000
6	-7.155104000	-0.027569000	-0.412370000
6	-7.901607000	1.179771000	-0.694465000
6	-7.919109000	-1.254841000	-0.345776000
6	-9.245408000	1.174285000	-0.880949000
1	-7.380144000	2.128487000	-0.727512000
6	-9.260919000	-1.286226000	-0.541584000
1	-7.402530000	-2.189545000	-0.162946000
6	-10.030496000	-0.065927000	-0.822243000
1	-9.795219000	2.089737000	-1.074605000
1	-9.819326000	-2.216197000	-0.505398000
8	-11.252573000	-0.083585000	-0.996951000

S2IIDS4-CS E=-2017.042434 Hartree

6	-2.281773000	-1.123070000	0.399466000
6	-1.424681000	0.041166000	0.254975000
6	-2.055862000	1.275171000	-0.107452000
6	-3.405659000	1.321367000	-0.280410000
6	-4.259142000	0.159279000	-0.112967000
6	-3.632951000	-1.094345000	0.235503000
6	-0.147187000	-1.838189000	0.751447000
6	-0.102083000	-0.358887000	0.454556000
1	-1.456106000	2.167429000	-0.213528000
1	-3.864497000	2.266636000	-0.551539000
1	-4.248234000	-1.975041000	0.352113000

6	1.113572000	0.392586000	0.456787000
6	2.436618000	-0.006312000	0.239514000
6	1.163139000	1.863452000	0.775991000
6	3.294351000	1.152800000	0.397652000
6	3.068916000	-1.226028000	-0.150679000
6	4.646449000	1.115628000	0.218409000
6	4.419890000	-1.265275000	-0.347091000
1	2.473509000	-2.121332000	-0.255622000
6	5.281289000	-0.116749000	-0.166895000
1	5.223656000	2.023177000	0.330724000
1	4.859808000	-2.215825000	-0.617055000
8	0.254771000	2.630918000	1.059387000
8	0.768777000	-2.604546000	1.013600000
7	2.506180000	2.239933000	0.726184000
7	-1.486611000	-2.213402000	0.708377000
6	-1.947949000	-3.563790000	0.959180000
1	-2.630383000	-3.589303000	1.814770000
1	-2.463330000	-3.969063000	0.082226000
1	-1.068974000	-4.170671000	1.177624000
6	2.965241000	3.586442000	0.995987000
1	3.653825000	3.601789000	1.847418000
1	3.468588000	4.012103000	0.121140000
1	2.085763000	4.185685000	1.233216000
6	-5.630976000	0.267798000	-0.293517000
6	-6.614803000	-0.831211000	-0.160727000
16	-6.450726000	1.774209000	-0.724787000
6	-8.070843000	0.967187000	-0.732306000
7	-7.911475000	-0.368489000	-0.413683000
8	-9.107344000	1.535395000	-0.979988000
8	-6.400636000	-2.002041000	0.125169000
6	-9.052616000	-1.276260000	-0.342624000
1	-8.936850000	-2.077628000	-1.075759000
1	-9.111430000	-1.718963000	0.653925000
1	-9.949653000	-0.696608000	-0.554365000
6	6.681213000	-0.202319000	-0.363769000
6	7.308783000	-1.384827000	-0.914633000
6	7.566324000	0.892439000	-0.026575000
6	8.647702000	-1.469354000	-1.116501000
1	6.690107000	-2.225170000	-1.205144000
6	8.908749000	0.825061000	-0.208359000
1	7.150566000	1.789979000	0.416034000
6	9.555071000	-0.366386000	-0.775183000
1	9.101090000	-2.357221000	-1.545686000
1	9.560871000	1.648536000	0.065175000

	8	10.775924000	-0.434273000	-0.951156000
S2IIDS5-CS	E=-1788.495327 Hartree			
	6	1.900795000	1.198845000	0.270580000
	6	1.055505000	0.020741000	0.257728000
	6	1.704521000	-1.232417000	0.041065000
	6	3.059383000	-1.292660000	-0.128652000
	6	3.907761000	-0.119675000	-0.077182000
	6	3.255415000	1.150153000	0.124164000
	6	-0.236034000	1.944571000	0.503887000
	6	-0.274360000	0.434615000	0.392245000
	1	1.118525000	-2.139912000	0.039311000
	1	3.535773000	-2.245932000	-0.295497000
	1	3.815693000	2.074758000	0.112560000
	6	-1.483551000	-0.312486000	0.475576000
	6	-2.812002000	0.054810000	0.214051000
	6	-1.527455000	-1.738987000	0.960111000
	6	-3.661231000	-1.085229000	0.499310000
	6	-3.449704000	1.219092000	-0.307524000
	6	-5.014937000	-1.074310000	0.321002000
	6	-4.804976000	1.237571000	-0.482977000
	1	-2.857597000	2.091847000	-0.540276000
	6	-5.657970000	0.110969000	-0.176937000
	1	-5.592526000	-1.950509000	0.581394000
	1	-5.244432000	2.134404000	-0.898003000
	8	-0.616831000	-2.463259000	1.330087000
	8	-1.155987000	2.731007000	0.662299000
	7	-2.869814000	-2.121240000	0.956612000
	7	1.102253000	2.318440000	0.427653000
	6	1.554366000	3.692507000	0.518152000
	1	2.227832000	3.825534000	1.371017000
	1	2.071904000	3.994954000	-0.398289000
	1	0.670882000	4.316100000	0.656054000
	6	-3.324046000	-3.430819000	1.378011000
	1	-4.007197000	-3.351961000	2.230155000
	1	-3.830805000	-3.951403000	0.558453000
	1	-2.441787000	-3.998239000	1.675194000
	6	5.320310000	-0.192750000	-0.207443000
	6	6.022546000	-1.438657000	-0.635571000
	6	6.137409000	0.939719000	0.073512000
	6	7.500641000	0.930581000	-0.030910000
	1	5.678051000	1.854945000	0.423162000
	6	8.231560000	-0.274003000	-0.460124000

6	8.265091000	2.090584000	0.287393000
7	8.848329000	3.061890000	0.555026000
8	5.465685000	-2.492903000	-0.928790000
8	9.448008000	-0.308973000	-0.571155000
7	7.421748000	-1.387138000	-0.728627000
6	8.080269000	-2.625769000	-1.163668000
1	7.843804000	-3.433456000	-0.468512000
1	7.717714000	-2.909851000	-2.153456000
1	9.150466000	-2.437757000	-1.185589000
6	-7.060715000	0.172492000	-0.370801000
6	-7.733585000	1.408240000	-0.712709000
6	-7.899987000	-0.999480000	-0.233977000
6	-9.076401000	1.477259000	-0.890335000
1	-7.154483000	2.319216000	-0.800348000
6	-9.242508000	-0.956530000	-0.419281000
1	-7.441370000	-1.953711000	-0.003963000
6	-9.936976000	0.293508000	-0.760253000
1	-9.569874000	2.413748000	-1.129721000
1	-9.857859000	-1.846052000	-0.329510000
8	-11.159016000	0.343463000	-0.926122000

S2IIDS6-CS E=-2149.814907 Hartree

6	3.948676000	-1.122956000	-0.481741000
6	3.124767000	0.045965000	-0.235079000
6	3.791816000	1.219640000	0.229276000
6	5.145819000	1.211842000	0.407853000
6	5.974371000	0.056995000	0.136124000
6	5.303949000	-1.130751000	-0.320830000
6	1.794224000	-1.751538000	-0.877349000
6	1.788669000	-0.304497000	-0.460158000
1	3.221729000	2.119926000	0.406385000
1	5.613035000	2.129916000	0.737279000
1	5.856064000	-2.042459000	-0.502998000
6	0.594238000	0.473083000	-0.385925000
6	-0.732540000	0.098082000	-0.184961000
6	0.582047000	1.976283000	-0.590000000
6	-1.558181000	1.290574000	-0.239196000
6	-1.404955000	-1.131346000	0.107372000
6	-2.906158000	1.291984000	-0.047863000
6	-2.749663000	-1.147178000	0.322879000
1	-0.842070000	-2.053321000	0.125599000
6	-3.580577000	0.052683000	0.262732000
1	-3.478553000	2.204569000	-0.089618000

1	-3.231501000	-2.084421000	0.548399000
8	1.516093000	2.727038000	-0.823743000
8	0.862907000	-2.471460000	-1.201614000
7	-0.743083000	2.381347000	-0.494640000
7	3.128608000	-2.164182000	-0.870593000
6	3.548715000	-3.500922000	-1.237775000
1	4.222978000	-3.475778000	-2.100274000
1	4.053971000	-3.996083000	-0.401637000
1	2.650446000	-4.060982000	-1.498959000
6	-1.176706000	3.756520000	-0.646840000
1	-1.873277000	3.852850000	-1.485438000
1	-1.667741000	4.111418000	0.264767000
1	-0.288454000	4.357892000	-0.841077000
6	-4.980388000	-0.012423000	0.442088000
6	-5.845032000	1.158719000	0.207610000
6	-5.639767000	-1.257416000	0.880074000
6	-7.823882000	-0.338868000	0.153596000
8	-5.066016000	-2.188342000	1.435707000
7	-7.027715000	-1.362754000	0.628220000
6	-7.656433000	-2.660373000	0.926620000
1	-6.878578000	-3.314194000	1.309111000
1	-8.445819000	-2.527899000	1.668049000
1	-8.101714000	-3.069598000	0.019038000
8	-5.452485000	2.320976000	0.144152000
7	-7.221949000	0.898108000	0.013484000
6	-8.063833000	2.044986000	-0.366776000
1	-8.860721000	2.176794000	0.366454000
1	-7.422166000	2.920056000	-0.397462000
1	-8.519491000	1.860250000	-1.340397000
16	-9.445508000	-0.571929000	-0.189560000
6	7.378454000	0.096339000	0.316110000
6	8.230391000	-0.996526000	-0.105255000
6	8.042751000	1.226389000	0.932044000
6	9.576025000	-0.973472000	0.058750000
1	7.785306000	-1.853174000	-0.597144000
6	9.385636000	1.265551000	1.117113000
1	7.449627000	2.060816000	1.285422000
6	10.259563000	0.164295000	0.690523000
1	10.203830000	-1.792750000	-0.276927000
1	9.868016000	2.112400000	1.594660000
8	11.483275000	0.191415000	0.850290000

S2IIDS7-CS

E=-1903.755998 Hartree

6	-4.173639000	-1.030489000	0.657438000
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6	-3.275545000	0.004262000	0.181230000
6	-3.860235000	1.074612000	-0.559669000
6	-5.208579000	1.099803000	-0.778660000
6	-6.110748000	0.084995000	-0.280415000
6	-5.523608000	-1.001237000	0.456422000
6	-2.070794000	-1.672110000	1.257192000
6	-1.966692000	-0.358245000	0.526628000
1	-3.233934000	1.878851000	-0.916811000
1	-5.611999000	1.942722000	-1.323141000
1	-6.133556000	-1.816125000	0.821320000
6	-0.728102000	0.318152000	0.326893000
6	0.583534000	-0.159470000	0.282151000
6	-0.635633000	1.823574000	0.169724000
6	1.469008000	0.973392000	0.076413000
6	1.182480000	-1.459632000	0.299571000
6	2.819714000	0.850997000	-0.056893000
6	2.532939000	-1.594681000	0.164441000
1	0.559203000	-2.328709000	0.451794000
6	3.418917000	-0.450790000	0.035229000
1	3.428658000	1.719568000	-0.261461000
1	2.983182000	-2.577038000	0.179573000
8	-1.527964000	2.655727000	0.199172000
8	-1.193108000	-2.352951000	1.763580000
7	0.711978000	2.128402000	0.016535000
7	-3.427547000	-1.999615000	1.299366000
6	-3.936907000	-3.192487000	1.944305000
1	-4.626753000	-2.934193000	2.754538000
1	-4.453482000	-3.836574000	1.224623000
1	-3.080677000	-3.726734000	2.356831000
6	1.227915000	3.483147000	-0.055417000
1	1.935378000	3.662005000	0.759885000
1	1.725996000	3.661124000	-1.014306000
1	0.378395000	4.159761000	0.038370000
6	4.807372000	-0.642095000	-0.063179000
6	5.432766000	-1.930291000	-0.521022000
6	5.882728000	0.337019000	0.029313000
6	6.810657000	-1.583585000	-0.947276000
6	7.070547000	-0.230919000	-0.665411000
6	7.746173000	-2.412619000	-1.550448000
6	8.306508000	0.316646000	-1.022046000
6	8.980071000	-1.861794000	-1.902872000
1	7.504639000	-3.454144000	-1.736297000
6	9.246177000	-0.511714000	-1.645522000
1	8.548671000	1.354686000	-0.839541000

1	9.735632000	-2.477828000	-2.380545000
1	10.205118000	-0.092097000	-1.933772000
8	4.935791000	-3.045482000	-0.590335000
6	5.910952000	1.499971000	0.787701000
6	4.895939000	1.888251000	1.714559000
7	4.111180000	2.250839000	2.496046000
6	7.032569000	2.386042000	0.801113000
7	7.917919000	3.143342000	0.823700000
6	-7.506497000	0.158391000	-0.512392000
6	-8.087180000	1.148480000	-1.395192000
6	-8.431730000	-0.757929000	0.120953000
6	-9.421081000	1.216285000	-1.631011000
1	-7.436712000	1.843972000	-1.911088000
6	-9.769859000	-0.700612000	-0.090418000
1	-8.049950000	-1.498517000	0.813559000
6	-10.369142000	0.293573000	-0.992151000
1	-9.840781000	1.953501000	-2.307956000
1	-10.453396000	-1.383312000	0.404280000
8	-11.585256000	0.348573000	-1.197051000

S2IIDS8-CS E=-2338.976461 Hartree

6	-4.478366000	-0.952360000	0.715986000
6	-3.597533000	0.081061000	0.206261000
6	-4.195175000	1.103521000	-0.589182000
6	-5.540828000	1.088260000	-0.826383000
6	-6.426654000	0.076721000	-0.294170000
6	-5.826113000	-0.962313000	0.497319000
6	-2.370431000	-1.520809000	1.368333000
6	-2.284961000	-0.236818000	0.584067000
1	-3.582446000	1.904919000	-0.974782000
1	-5.955114000	1.896752000	-1.413237000
1	-6.422662000	-1.774148000	0.890056000
6	-1.059855000	0.457816000	0.370332000
6	0.263987000	0.010429000	0.363221000
6	-0.999839000	1.956628000	0.144480000
6	1.124621000	1.153183000	0.114287000
6	0.891640000	-1.271971000	0.459779000
6	2.479545000	1.058154000	-0.003985000
6	2.244908000	-1.380572000	0.336265000
1	0.290057000	-2.143840000	0.670469000
6	3.101696000	-0.226646000	0.135668000
1	3.073729000	1.929258000	-0.240876000
1	2.702239000	-2.354668000	0.456762000

8	-1.910647000	2.768243000	0.124881000
8	-1.485047000	-2.159751000	1.914218000
7	0.342517000	2.285615000	-0.006934000
7	-3.719981000	-1.875758000	1.408410000
6	-4.211644000	-3.051925000	2.096975000
1	-4.917566000	-2.775130000	2.886919000
1	-4.704098000	-3.736834000	1.398490000
1	-3.349596000	-3.549143000	2.542268000
6	0.827258000	3.646522000	-0.144821000
1	1.515750000	3.887914000	0.670670000
1	1.337453000	3.784064000	-1.103886000
1	-0.039435000	4.306199000	-0.101318000
6	4.487026000	-0.395585000	0.021464000
6	5.577270000	0.538982000	0.094578000
6	6.694577000	-1.324283000	-0.962348000
6	6.781065000	0.034874000	-0.626950000
6	7.699380000	-2.022581000	-1.613084000
6	7.946265000	0.721633000	-1.000447000
6	8.855889000	-1.323723000	-1.963095000
1	7.580318000	-3.075118000	-1.847188000
6	8.965969000	0.036776000	-1.663253000
1	8.066506000	1.775966000	-0.797125000
1	9.663846000	-1.835895000	-2.475514000
1	9.860112000	0.579936000	-1.951999000
6	5.575306000	1.698690000	0.872663000
6	4.548218000	2.023815000	1.807858000
7	3.746602000	2.337583000	2.593758000
6	6.649690000	2.637331000	0.904966000
7	7.489501000	3.444299000	0.956041000
16	5.128678000	-2.020999000	-0.479990000
8	4.420638000	-2.518501000	-1.669252000
8	5.271670000	-2.914387000	0.681207000
6	-7.820659000	0.108883000	-0.546182000
6	-8.410077000	1.043838000	-1.481930000
6	-8.734168000	-0.796761000	0.119018000
6	-9.741827000	1.071747000	-1.736549000
1	-7.767475000	1.727508000	-2.022799000
6	-10.070306000	-0.778109000	-0.110402000
1	-8.345576000	-1.495264000	0.850400000
6	-10.678359000	0.159893000	-1.065340000
1	-10.168313000	1.766620000	-2.452844000
1	-10.745922000	-1.451006000	0.407969000
8	-11.892390000	0.179385000	-1.286542000

S2IIDS9-CS

E=-2324.927673 Hartree

6	3.774345000	-1.134164000	-0.409133000
6	2.938506000	0.038796000	-0.257314000
6	3.594921000	1.242814000	0.141042000
6	4.944358000	1.251965000	0.357218000
6	5.782397000	0.086129000	0.189732000
6	5.124245000	-1.129232000	-0.209256000
6	1.635149000	-1.802297000	-0.817790000
6	1.608095000	-0.331471000	-0.489265000
1	3.018079000	2.151472000	0.236394000
1	5.402664000	2.192819000	0.631699000
1	5.682311000	-2.049924000	-0.313459000
6	0.406232000	0.441576000	-0.495690000
6	-0.933754000	0.054217000	-0.322863000
6	0.390779000	1.914893000	-0.754768000
6	-1.767397000	1.234721000	-0.454088000
6	-1.591232000	-1.169301000	0.001415000
6	-3.123635000	1.215678000	-0.308425000
6	-2.949537000	-1.201146000	0.154878000
1	-1.010240000	-2.075118000	0.094295000
6	-3.776209000	-0.029664000	0.001495000
1	-3.699522000	2.128219000	-0.418026000
1	-3.420191000	-2.149022000	0.396834000
8	1.312607000	2.687918000	-0.984995000
8	0.717068000	-2.553061000	-1.120410000
7	-0.951025000	2.314627000	-0.725246000
7	2.968082000	-2.206243000	-0.751678000
6	3.403825000	-3.559412000	-1.020164000
1	4.107509000	-3.585484000	-1.859205000
1	3.883962000	-4.000738000	-0.139693000
1	2.516390000	-4.139192000	-1.275959000
6	-1.375649000	3.678429000	-0.950113000
1	-2.042077000	3.745516000	-1.817264000
1	-1.893104000	4.080940000	-0.071799000
1	-0.477040000	4.266420000	-1.140250000
6	-5.158152000	-0.102204000	0.152596000
6	-7.632649000	-0.907949000	0.572554000
6	-7.729153000	0.464986000	0.304925000
6	-8.780585000	-1.656435000	0.846073000
6	-8.973437000	1.100600000	0.308615000
6	-10.019695000	-1.019049000	0.848832000
1	-8.705787000	-2.719078000	1.053197000
6	-10.115643000	0.350578000	0.581868000

1	-9.047228000	2.163316000	0.101449000
1	-10.914930000	-1.594510000	1.060509000
1	-11.085223000	0.837699000	0.586439000
16	-6.209646000	1.299958000	-0.027734000
16	-6.007984000	-1.597197000	0.537487000
6	7.182655000	0.136453000	0.409917000
6	8.048348000	-0.971211000	0.074165000
6	7.828486000	1.294593000	0.985059000
6	9.390410000	-0.936793000	0.278775000
1	7.620549000	-1.853639000	-0.388090000
6	9.167025000	1.345896000	1.210035000
1	7.224090000	2.145081000	1.277820000
6	10.05557000	0.229517000	0.870549000
1	10.026745000	-1.772424000	0.004105000
1	9.631652000	2.218396000	1.658805000
8	11.276878000	0.267309000	1.067827000

S2IIDS10-CS E=-2171.269408 Hartree

6	2.790318000	-1.158157000	-0.343470000
6	1.939142000	0.008232000	-0.202552000
6	2.572893000	1.229995000	0.169742000
6	3.927062000	1.273935000	0.357962000
6	4.770828000	0.117352000	0.194868000
6	4.142723000	-1.126619000	-0.163340000
6	0.648927000	-1.855961000	-0.716030000
6	0.608091000	-0.390710000	-0.419361000
1	1.978633000	2.126184000	0.271555000
1	4.379726000	2.220828000	0.636034000
1	4.732647000	-2.029087000	-0.282436000
6	-0.603020000	0.367238000	-0.423206000
6	-1.934748000	-0.025176000	-0.237515000
6	-0.640092000	1.846556000	-0.710520000
6	-2.780705000	1.141629000	-0.378302000
6	-2.586597000	-1.247479000	0.108846000
6	-4.135288000	1.115473000	-0.214649000
6	-3.941163000	-1.278455000	0.288706000
1	-2.001383000	-2.151803000	0.193699000
6	-4.788717000	-0.118217000	0.132132000
1	-4.701671000	2.032322000	-0.307335000
1	-4.394924000	-2.232087000	0.523880000
8	0.276031000	2.616733000	-0.967254000
8	-0.256236000	-2.634582000	-0.989745000

7	-1.979113000	2.232613000	-0.668687000
7	1.995014000	-2.240141000	-0.663036000
6	2.442119000	-3.592387000	-0.912423000
1	3.130516000	-3.629005000	-1.764130000
1	2.942658000	-4.011763000	-0.032167000
1	1.555839000	-4.185722000	-1.140149000
6	-2.424675000	3.587619000	-0.910300000
1	-3.106578000	3.629271000	-1.766525000
1	-2.933131000	3.997961000	-0.030734000
1	-1.538259000	4.184939000	-1.126150000
6	6.148741000	0.202331000	0.382248000
6	8.591367000	0.995936000	0.872032000
6	8.706508000	-0.307573000	0.584806000
16	6.984190000	1.691650000	0.827880000
16	7.234860000	-1.175741000	0.195666000
1	9.634068000	-0.866102000	0.572571000
1	9.412292000	1.654147000	1.127945000
6	-6.193722000	-0.190803000	0.313575000
6	-6.839991000	-1.371508000	0.839976000
6	-7.063857000	0.915350000	-0.015102000
6	-8.183293000	-1.444487000	1.027984000
1	-6.232940000	-2.222479000	1.125834000
6	-8.410371000	0.859749000	0.152813000
1	-6.635001000	1.814895000	-0.442102000
6	-9.076356000	-0.329778000	0.695218000
1	-8.648643000	-2.334208000	1.440765000
1	-9.049533000	1.695072000	-0.116197000
8	-10.301940000	-0.387117000	0.859016000

S2IIDS1-OS E=-1483.167414 Hartree

6	2.079117000	1.137380000	0.274322000
6	1.248279000	-0.025526000	0.157372000
6	1.894087000	-1.252566000	-0.114969000
6	3.268736000	-1.297644000	-0.242108000
6	4.091365000	-0.143977000	-0.093626000
6	3.450614000	1.098137000	0.169981000
6	-0.060061000	1.900415000	0.468994000
6	-0.118092000	0.399399000	0.268803000
1	1.312142000	-2.158186000	-0.192315000
1	3.732407000	-2.261657000	-0.410990000
1	4.024471000	2.013788000	0.234472000
6	-1.320181000	-0.323366000	0.259125000
6	-2.674410000	0.092193000	0.071091000

6	-1.385643000	-1.816267000	0.526453000
6	-3.515463000	-1.072524000	0.203837000
6	-3.304659000	1.315147000	-0.278094000
6	-4.875099000	-1.042220000	0.044359000
6	-4.667593000	1.363698000	-0.450031000
1	-2.711242000	2.210397000	-0.382976000
6	-5.492180000	0.202444000	-0.286975000
1	-5.479517000	-1.934756000	0.155900000
1	-5.140779000	2.303488000	-0.712342000
8	-0.484679000	-2.601758000	0.775461000
8	-0.968422000	2.698411000	0.647331000
7	-2.726966000	-2.173022000	0.491880000
7	1.282580000	2.254398000	0.472284000
6	1.745593000	3.614008000	0.663494000
1	2.388612000	3.685297000	1.546859000
1	2.300581000	3.964962000	-0.213045000
1	0.864420000	4.239384000	0.807296000
6	-3.200704000	-3.523424000	0.726163000
1	-3.880215000	-3.552172000	1.583791000
1	-3.721145000	-3.911478000	-0.155480000
1	-2.327776000	-4.141984000	0.934277000
6	-6.895331000	0.286816000	-0.461222000
6	-7.537876000	1.507654000	-0.799685000
7	-8.057942000	2.514018000	-1.078747000
6	-7.727615000	-0.854129000	-0.306864000
7	-8.387963000	-1.807018000	-0.174867000
6	5.532894000	-0.230019000	-0.208283000
6	6.163320000	-1.329125000	-0.878934000
6	6.383719000	0.783693000	0.342494000
6	7.520446000	-1.412526000	-1.004295000
1	5.544369000	-2.092269000	-1.337384000
6	7.743836000	0.713937000	0.245083000
1	5.936859000	1.605669000	0.891262000
6	8.402934000	-0.392675000	-0.443998000
1	7.993266000	-2.233729000	-1.533286000
1	8.385944000	1.470618000	0.684371000
8	9.641780000	-0.461604000	-0.546438000

S2IIDS3- OS E=-2051.022975 Hartree

6	-3.706350000	-1.086215000	0.311688000
6	-2.965882000	0.119871000	0.126732000
6	-3.695587000	1.271032000	-0.224558000
6	-5.076302000	1.209943000	-0.343969000

6	-5.804578000	0.012197000	-0.137899000
6	-5.078125000	-1.160225000	0.190134000
6	-1.525267000	-1.688840000	0.601448000
6	-1.558108000	-0.199255000	0.292573000
1	-3.179845000	2.204213000	-0.387376000
1	-5.603533000	2.107631000	-0.644247000
1	-5.591652000	-2.093964000	0.382931000
6	-0.416458000	0.589284000	0.251138000
6	0.996629000	0.249352000	0.202200000
6	-0.455674000	2.106742000	0.301514000
6	1.735234000	1.472130000	0.219859000
6	1.731808000	-0.942956000	0.068888000
6	3.110174000	1.529288000	0.146264000
6	3.115381000	-0.901112000	-0.012666000
1	1.218044000	-1.891175000	0.052526000
6	3.837685000	0.315746000	0.032896000
1	3.616838000	2.486048000	0.162630000
1	3.654476000	-1.838402000	-0.104993000
8	-1.411885000	2.863844000	0.377884000
8	-0.573128000	-2.414979000	0.846781000
7	0.859803000	2.545423000	0.299367000
7	-2.838298000	-2.127418000	0.614252000
6	-3.215147000	-3.498232000	0.893216000
1	-3.867699000	-3.550990000	1.770903000
1	-3.732024000	-3.942908000	0.036061000
1	-2.298339000	-4.053556000	1.090835000
6	1.229321000	3.944840000	0.362021000
1	1.843100000	4.145840000	1.246316000
1	1.783564000	4.243349000	-0.534348000
1	0.306411000	4.521288000	0.424731000
6	5.276615000	0.334414000	-0.039262000
6	6.138514000	1.445593000	0.040047000
16	6.257317000	-1.101057000	-0.247795000
1	5.791284000	2.463421000	0.175870000
6	7.708712000	-0.080778000	-0.208903000
6	9.006685000	-0.605153000	-0.334073000
6	9.218392000	-1.998397000	-0.498638000
7	9.366662000	-3.147810000	-0.633266000
6	10.138676000	0.251246000	-0.299186000
7	11.087893000	0.927593000	-0.274692000
7	7.448192000	1.226134000	-0.050771000
6	-7.257133000	-0.019501000	-0.269177000
6	-8.039529000	1.163209000	-0.091784000
6	-7.945146000	-1.233482000	-0.577216000

6	-9.403445000	1.144746000	-0.201726000
1	-7.541167000	2.087846000	0.178989000
6	-9.306783000	-1.274818000	-0.707229000
1	-7.368652000	-2.135393000	-0.754798000
6	-10.123477000	-0.081613000	-0.521394000
1	-9.999043000	2.038262000	-0.044657000
1	-9.827150000	-2.192140000	-0.963329000
8	-11.367047000	-0.109395000	-0.630312000

S2IIDS4-OS E=-2017.045651 Hartree

6	-2.285121000	-1.091793000	0.319979000
6	-1.453524000	0.073959000	0.194314000
6	-2.101757000	1.298048000	-0.108640000
6	-3.469688000	1.336793000	-0.243371000
6	-4.293749000	0.172239000	-0.088689000
6	-3.649856000	-1.075312000	0.196688000
6	-0.144230000	-1.838311000	0.573025000
6	-0.089401000	-0.339754000	0.338346000
1	-1.518954000	2.200834000	-0.208501000
1	-3.939516000	2.288084000	-0.471461000
1	-4.247254000	-1.969688000	0.302337000
6	1.108784000	0.386726000	0.330154000
6	2.478222000	-0.032244000	0.187119000
6	1.166137000	1.885629000	0.537595000
6	3.305208000	1.132458000	0.293005000
6	3.125060000	-1.252956000	-0.103918000
6	4.674865000	1.102309000	0.158876000
6	4.498485000	-1.290022000	-0.260066000
1	2.545883000	-2.161061000	-0.172595000
6	5.317114000	-0.133946000	-0.124671000
1	5.244786000	2.021125000	0.215804000
1	4.963817000	-2.251024000	-0.442277000
8	0.260883000	2.683096000	0.739858000
8	0.765727000	-2.627871000	0.782638000
7	2.507269000	2.245143000	0.514049000
7	-1.482656000	-2.197847000	0.562779000
6	-1.946900000	-3.553674000	0.776508000
1	-2.604952000	-3.605245000	1.649848000
1	-2.491395000	-3.921449000	-0.099423000
1	-1.067423000	-4.174799000	0.946427000
6	2.968533000	3.604502000	0.704088000
1	3.629372000	3.673811000	1.574637000
1	3.505154000	3.963549000	-0.180824000

1	2.087747000	4.225253000	0.869232000
6	-5.693404000	0.265626000	-0.223296000
6	-6.654260000	-0.845621000	-0.097317000
16	-6.534607000	1.771798000	-0.576365000
6	-8.151520000	0.948348000	-0.562019000
7	-7.967127000	-0.392536000	-0.294121000
8	-9.198622000	1.517148000	-0.758732000
8	-6.416257000	-2.023456000	0.142710000
6	-9.093584000	-1.317989000	-0.218121000
1	-8.992634000	-2.091237000	-0.982982000
1	-9.113608000	-1.796401000	0.763329000
1	-10.004616000	-0.743839000	-0.379289000
6	6.758008000	-0.210242000	-0.271120000
6	7.379952000	-1.295704000	-0.969184000
6	7.615057000	0.799652000	0.274263000
6	8.735297000	-1.370007000	-1.124428000
1	6.754920000	-2.056214000	-1.424161000
6	8.973903000	0.738957000	0.146263000
1	7.175501000	1.611881000	0.843411000
6	9.624245000	-0.353650000	-0.570663000
1	9.200407000	-2.181968000	-1.674272000
1	9.620708000	1.493956000	0.581740000
8	10.862283000	-0.414155000	-0.701025000

S2IIDS5-OS E=-1788.500096 Hartree

6	-1.907843000	1.175170000	-0.072047000
6	-1.091184000	0.000609000	-0.162411000
6	-1.750927000	-1.243213000	-0.089457000
6	-3.127710000	-1.301403000	0.040641000
6	-3.937547000	-0.127873000	0.085118000
6	-3.276580000	1.135947000	0.032433000
6	0.238828000	1.945154000	-0.142450000
6	0.287595000	0.428281000	-0.212415000
1	-1.181695000	-2.156770000	-0.161392000
1	-3.612349000	-2.264057000	0.095223000
1	-3.831478000	2.059791000	0.134704000
6	1.475148000	-0.288006000	-0.340435000
6	2.855973000	0.090740000	-0.140063000
6	1.521998000	-1.731238000	-0.814252000
6	3.666891000	-1.044947000	-0.452108000
6	3.517415000	1.239850000	0.338243000
6	5.039865000	-1.049268000	-0.333504000
6	4.897308000	1.248305000	0.454295000

1	2.946736000	2.117697000	0.598577000
6	5.697472000	0.123201000	0.121987000
1	5.606827000	-1.924563000	-0.624627000
1	5.370677000	2.137527000	0.852669000
8	0.609778000	-2.472471000	-1.146579000
8	1.150537000	2.757614000	-0.180069000
7	2.859434000	-2.093522000	-0.869077000
7	-1.099154000	2.302868000	-0.077973000
6	-1.552604000	3.678075000	-0.027699000
1	-2.199782000	3.905089000	-0.881280000
1	-2.101247000	3.874738000	0.899599000
1	-0.667867000	4.313499000	-0.065935000
6	3.310803000	-3.401320000	-1.299059000
1	3.960936000	-3.319695000	-2.176369000
1	3.855179000	-3.909893000	-0.496188000
1	2.424985000	-3.980939000	-1.558899000
6	-5.379357000	-0.184162000	0.152488000
6	-6.091405000	-1.395863000	0.644986000
6	-6.162997000	0.917067000	-0.246905000
6	-7.540652000	0.907285000	-0.206440000
1	-5.678066000	1.799839000	-0.645894000
6	-8.288303000	-0.268657000	0.272618000
6	-8.291229000	2.031961000	-0.647147000
7	-8.864549000	2.977120000	-1.014479000
8	-5.528709000	-2.407852000	1.051546000
8	-9.509695000	-0.299221000	0.323738000
7	-7.493120000	-1.355012000	0.661629000
6	-8.166671000	-2.561454000	1.159778000
1	-7.888761000	-3.419225000	0.544607000
1	-7.855695000	-2.761459000	2.186975000
1	-9.237778000	-2.383853000	1.110551000
6	7.145737000	0.164898000	0.254483000
6	7.854303000	1.408024000	0.243002000
6	7.911859000	-1.034901000	0.398291000
6	9.216026000	1.459863000	0.354679000
1	7.299673000	2.328584000	0.097426000
6	9.272655000	-1.008293000	0.527947000
1	7.395019000	-1.987317000	0.450119000
6	10.013764000	0.248349000	0.508831000
1	9.754038000	2.401793000	0.322085000
1	9.850279000	-1.917483000	0.660423000
8	11.255628000	0.283611000	0.618407000

S2IIDS6-OS E=-2149.817086 Hartree

6	-3.957331000	-1.099885000	0.418203000
6	-3.162246000	0.073627000	0.193276000
6	-3.843088000	1.244897000	-0.211496000
6	-5.215262000	1.230271000	-0.359964000
6	-6.003881000	0.069718000	-0.104832000
6	-5.327115000	-1.117249000	0.292968000
6	-1.796471000	-1.760713000	0.722136000
6	-1.787306000	-0.289340000	0.364814000
1	-3.288526000	2.156945000	-0.372291000
1	-5.706772000	2.155971000	-0.632365000
1	-5.871830000	-2.040493000	0.443656000
6	-0.608441000	0.470199000	0.288553000
6	0.754119000	0.085022000	0.138992000
6	-0.592587000	1.985869000	0.410208000
6	1.559762000	1.280014000	0.155688000
6	1.438526000	-1.137189000	-0.088894000
6	2.917559000	1.291342000	-0.001488000
6	2.798512000	-1.147547000	-0.275018000
1	0.889770000	-2.066543000	-0.085903000
6	3.608348000	0.053491000	-0.238000000
1	3.476898000	2.212587000	0.019950000
1	3.289477000	-2.091612000	-0.446942000
8	-1.523262000	2.757320000	0.586393000
8	-0.865187000	-2.500838000	1.000275000
7	0.733301000	2.380266000	0.334560000
7	-3.127653000	-2.161481000	0.740482000
6	-3.547147000	-3.508617000	1.068712000
1	-4.199950000	-3.510199000	1.947909000
1	-4.077318000	-3.969039000	0.228163000
1	-2.647138000	-4.083833000	1.286670000
6	1.165513000	3.760302000	0.437119000
1	1.845495000	3.890258000	1.284775000
1	1.676512000	4.075327000	-0.478313000
1	0.274728000	4.370276000	0.586834000
6	5.024972000	-0.008231000	-0.375788000
6	5.881402000	1.149308000	-0.068304000
6	5.686855000	-1.237042000	-0.847557000
6	7.868399000	-0.339608000	-0.089526000
8	5.110123000	-2.149955000	-1.430247000
7	7.075693000	-1.346329000	-0.604940000
6	7.708926000	-2.627390000	-0.960114000
1	6.932128000	-3.268276000	-1.365997000
1	8.494232000	-2.460162000	-1.698788000

1	8.160161000	-3.072258000	-0.072462000
8	5.480082000	2.302633000	0.067382000
7	7.259212000	0.884629000	0.115594000
6	8.093476000	2.013560000	0.561165000
1	8.886042000	2.196113000	-0.165883000
1	7.444978000	2.879842000	0.647244000
1	8.554680000	1.773949000	1.520018000
16	9.494174000	-0.577586000	0.230891000
6	-7.443576000	0.095567000	-0.246071000
6	-8.270901000	-0.892838000	0.382997000
6	-8.100174000	1.107225000	-1.022483000
6	-9.630308000	-0.878826000	0.261431000
1	-7.806981000	-1.646215000	1.010321000
6	-9.456609000	1.132112000	-1.173186000
1	-7.499991000	1.846866000	-1.540377000
6	-10.314877000	0.137545000	-0.534384000
1	-10.254069000	-1.614328000	0.759272000
1	-9.947205000	1.885400000	-1.781191000
8	-11.553037000	0.154295000	-0.659226000

S2IIDS7-OS E=-1903.758983 Hartree

6	-4.178388000	-1.034027000	0.570563000
6	-3.313981000	0.017493000	0.123696000
6	-3.918176000	1.109627000	-0.536161000
6	-5.288823000	1.139287000	-0.713970000
6	-6.144984000	0.105976000	-0.239866000
6	-5.546263000	-1.003222000	0.416859000
6	-2.066577000	-1.742689000	1.059775000
6	-1.959570000	-0.378741000	0.404755000
1	-3.309702000	1.934925000	-0.872769000
1	-5.721746000	2.011528000	-1.188189000
1	-6.147088000	-1.841685000	0.745625000
6	-0.740965000	0.279304000	0.208168000
6	0.610804000	-0.198060000	0.213107000
6	-0.640450000	1.778914000	-0.022769000
6	1.473173000	0.929895000	-0.021613000
6	1.222381000	-1.473071000	0.292763000
6	2.834999000	0.827941000	-0.126691000
6	2.590446000	-1.593618000	0.185805000
1	0.615087000	-2.347710000	0.467281000
6	3.447892000	-0.452749000	0.018029000
1	3.431728000	1.700713000	-0.351610000
1	3.048048000	-2.570532000	0.249096000

8	-1.526071000	2.619488000	-0.052831000
8	-1.188267000	-2.465289000	1.505188000
7	0.706976000	2.077568000	-0.145886000
7	-3.419231000	-2.049558000	1.130808000
6	-3.926122000	-3.270981000	1.722200000
1	-4.590183000	-3.049222000	2.564158000
1	-4.472134000	-3.866494000	0.982667000
1	-3.066955000	-3.838495000	2.080037000
6	1.220088000	3.429132000	-0.267811000
1	1.903831000	3.649185000	0.557824000
1	1.745559000	3.563098000	-1.219370000
1	0.366512000	4.105832000	-0.230350000
6	4.856275000	-0.624677000	-0.065763000
6	5.496756000	-1.894054000	-0.552893000
6	5.915766000	0.351700000	0.094421000
6	6.897059000	-1.541528000	-0.890278000
6	7.143246000	-0.200462000	-0.547603000
6	7.862099000	-2.353289000	-1.469135000
6	8.398310000	0.352925000	-0.814595000
6	9.116028000	-1.796641000	-1.731729000
1	7.628326000	-3.386303000	-1.705668000
6	9.370468000	-0.458328000	-1.411826000
1	8.633831000	1.382565000	-0.582916000
1	9.895483000	-2.399178000	-2.187637000
1	10.345551000	-0.033259000	-1.629209000
8	4.989330000	-2.997068000	-0.695604000
6	5.893106000	1.513686000	0.860402000
6	4.826622000	1.894743000	1.730331000
7	4.003493000	2.257858000	2.471093000
6	7.004837000	2.407289000	0.939629000
7	7.881315000	3.171737000	1.015944000
6	-7.582354000	0.179051000	-0.420626000
6	-8.164405000	1.012446000	-1.430257000
6	-8.473505000	-0.583159000	0.402304000
6	-9.515908000	1.077366000	-1.618246000
1	-7.512571000	1.572719000	-2.091365000
6	-9.829054000	-0.522171000	0.244984000
1	-8.062457000	-1.190397000	1.201631000
6	-10.439524000	0.312539000	-0.785796000
1	-9.952486000	1.691367000	-2.399392000
1	-10.502535000	-1.082153000	0.885848000
8	-11.673968000	0.368271000	-0.944304000

S2IIDS8-OS E=-2338.980408 Hartree

6	-4.485155000	-0.956045000	0.626507000
6	-3.645322000	0.093001000	0.134803000
6	-4.271576000	1.137369000	-0.576590000
6	-5.643327000	1.126197000	-0.760176000
6	-6.474309000	0.096657000	-0.241666000
6	-5.853564000	-0.965793000	0.466937000
6	-2.361818000	-1.595982000	1.158056000
6	-2.279068000	-0.259005000	0.440331000
1	-3.681626000	1.959626000	-0.950781000
1	-6.095262000	1.964738000	-1.275885000
1	-6.436163000	-1.802264000	0.831858000
6	-1.077304000	0.412481000	0.219051000
6	0.292969000	-0.031063000	0.272262000
6	-1.007394000	1.895080000	-0.110891000
6	1.126095000	1.099976000	-0.025016000
6	0.932258000	-1.278466000	0.449103000
6	2.493977000	1.028206000	-0.112038000
6	2.306433000	-1.369360000	0.361294000
1	0.347321000	-2.153299000	0.685776000
6	3.127819000	-0.225504000	0.110115000
1	3.075298000	1.898837000	-0.383777000
1	2.779015000	-2.327284000	0.543602000
8	-1.909695000	2.712094000	-0.210925000
8	-1.471320000	-2.277632000	1.641228000
7	0.334606000	2.217480000	-0.233405000
7	-3.706394000	-1.927923000	1.236649000
6	-4.190404000	-3.132166000	1.880894000
1	-4.863383000	-2.886261000	2.708877000
1	-4.719695000	-3.771606000	1.166442000
1	-3.321559000	-3.664626000	2.267841000
6	0.816233000	3.567991000	-0.452167000
1	1.476270000	3.872162000	0.366173000
1	1.358240000	3.640388000	-1.401043000
1	-0.054542000	4.222628000	-0.484162000
6	4.542046000	-0.374860000	0.018819000
6	5.613228000	0.546071000	0.182433000
6	6.802186000	-1.283591000	-0.865859000
6	6.878120000	0.051289000	-0.442273000
6	7.855198000	-1.971220000	-1.447595000
6	8.091917000	0.723655000	-0.646661000
6	9.057065000	-1.285607000	-1.632525000
1	7.740227000	-3.005939000	-1.752562000
6	9.162443000	0.050434000	-1.239035000

1	8.217146000	1.758843000	-0.364851000
1	9.903903000	-1.789175000	-2.087316000
1	10.094087000	0.584826000	-1.395149000
6	5.538120000	1.715547000	0.961544000
6	4.447316000	2.026439000	1.825055000
7	3.600111000	2.337416000	2.563272000
6	6.585816000	2.675106000	1.063797000
7	7.399769000	3.503871000	1.171193000
16	5.182114000	-1.963464000	-0.586718000
8	4.551105000	-2.312472000	-1.867816000
8	5.202224000	-2.965969000	0.491520000
6	-7.915248000	0.126815000	-0.429542000
6	-8.509726000	0.879419000	-1.492344000
6	-8.790478000	-0.598314000	0.440576000
6	-9.862505000	0.903852000	-1.686001000
1	-7.866640000	1.408056000	-2.187349000
6	-10.147320000	-0.576451000	0.277596000
1	-8.367732000	-1.142910000	1.278136000
6	-10.771142000	0.176128000	-0.806175000
1	-10.309901000	1.455996000	-2.506198000
1	-10.810900000	-1.107441000	0.952521000
8	-12.006821000	0.195795000	-0.969551000

S2IIDS9-OS E=-2324.929206 Hartree

6	-3.781570000	-1.126551000	0.343404000
6	-2.964159000	0.048783000	0.224568000
6	-3.626311000	1.254325000	-0.113475000
6	-4.991482000	1.265312000	-0.304823000
6	-5.803504000	0.098169000	-0.162693000
6	-5.144367000	-1.121309000	0.172075000
6	-1.634651000	-1.824359000	0.667527000
6	-1.603668000	-0.338952000	0.412676000
1	-3.058971000	2.170117000	-0.187271000
1	-5.464770000	2.214576000	-0.523406000
1	-5.699372000	-2.048329000	0.239603000
6	-0.410486000	0.419364000	0.424715000
6	0.949036000	0.029446000	0.280549000
6	-0.389411000	1.905409000	0.659781000
6	1.769898000	1.210344000	0.405219000
6	1.617440000	-1.188360000	-0.016497000
6	3.131906000	1.201061000	0.279818000
6	2.983192000	-1.214730000	-0.151100000
1	1.044621000	-2.098981000	-0.107981000

6	3.796199000	-0.039919000	-0.001705000
1	3.697424000	2.120555000	0.383965000
1	3.461084000	-2.163657000	-0.373447000
8	-1.308963000	2.685702000	0.869585000
8	-0.718323000	-2.598633000	0.917538000
7	0.949689000	2.297894000	0.645995000
7	-2.969349000	-2.215874000	0.617713000
6	-3.406315000	-3.577547000	0.835905000
1	-4.090607000	-3.637320000	1.689239000
1	-3.910060000	-3.976560000	-0.051619000
1	-2.516716000	-4.172524000	1.044481000
6	1.376667000	3.663414000	0.857479000
1	2.032280000	3.738706000	1.732051000
1	1.907671000	4.050654000	-0.019506000
1	0.478787000	4.258276000	1.027713000
6	5.188737000	-0.102939000	-0.130520000
6	7.672512000	-0.895374000	-0.501367000
6	7.754927000	0.481857000	-0.250128000
6	8.830325000	-1.638290000	-0.747418000
6	8.994713000	1.126306000	-0.243131000
6	10.064773000	-0.991981000	-0.739526000
1	8.766444000	-2.704066000	-0.941829000
6	10.146591000	0.381638000	-0.489014000
1	9.057510000	2.192159000	-0.048727000
1	10.967308000	-1.563497000	-0.929949000
1	11.112519000	0.876023000	-0.485063000
16	6.224709000	1.310462000	0.048813000
16	6.052751000	-1.597251000	-0.482457000
6	-7.232397000	0.147420000	-0.350864000
6	-8.089111000	-0.898230000	0.131301000
6	-7.864618000	1.241551000	-1.031601000
6	-9.442741000	-0.863130000	-0.037770000
1	-7.653018000	-1.721948000	0.686397000
6	-9.214363000	1.290666000	-1.226733000
1	-7.247718000	2.033652000	-1.441429000
6	-10.100394000	0.237700000	-0.737577000
1	-10.083546000	-1.648065000	0.351742000
1	-9.679421000	2.111678000	-1.763433000
8	-11.333638000	0.274991000	-0.905077000

S2IIDS10-OS E=-2171.271013 Hartree

6	-2.793065000	-1.141366000	0.308735000
6	-1.956755000	0.027151000	0.175979000

6	-2.605027000	1.244891000	-0.160680000
6	-3.967933000	1.283211000	-0.324215000
6	-4.796051000	0.121360000	-0.166742000
6	-4.152590000	-1.119865000	0.154805000
6	-0.647652000	-1.854885000	0.623151000
6	-0.604127000	-0.374735000	0.357070000
1	-2.020314000	2.147122000	-0.259701000
1	-4.430419000	2.232459000	-0.576402000
1	-4.730512000	-2.030785000	0.267022000
6	0.597402000	0.369384000	0.354125000
6	1.958016000	-0.037806000	0.206901000
6	0.639936000	1.860264000	0.573157000
6	2.785548000	1.131006000	0.316051000
6	2.614128000	-1.257977000	-0.086489000
6	4.151881000	1.107183000	0.176327000
6	3.983364000	-1.288209000	-0.245992000
1	2.038515000	-2.169245000	-0.151339000
6	4.804696000	-0.126880000	-0.113519000
1	4.715605000	2.029616000	0.234075000
1	4.450903000	-2.247539000	-0.430502000
8	-0.272682000	2.650915000	0.782819000
8	0.257566000	-2.641439000	0.868943000
7	1.979723000	2.235621000	0.544997000
7	-1.990950000	-2.232523000	0.589720000
6	-2.437866000	-3.588346000	0.821126000
1	-3.112178000	-3.637780000	1.683265000
1	-2.955031000	-3.988548000	-0.058334000
1	-1.550540000	-4.189245000	1.022643000
6	2.427328000	3.597345000	0.739843000
1	3.093112000	3.670499000	1.606672000
1	2.955335000	3.968952000	-0.145488000
1	1.540216000	4.206988000	0.913776000
6	-6.186102000	0.196635000	-0.325779000
6	-8.641133000	0.977623000	-0.753108000
6	-8.740003000	-0.331800000	-0.486425000
16	-7.039464000	1.687292000	-0.728663000
16	-7.254417000	-1.195042000	-0.141047000
1	-9.663113000	-0.897437000	-0.465986000
1	-9.473096000	1.632204000	-0.981232000
6	6.237262000	-0.195762000	-0.267311000
6	6.872360000	-1.311358000	-0.909009000
6	7.094243000	0.850930000	0.211555000
6	8.225708000	-1.379340000	-1.071697000
1	6.255990000	-2.105576000	-1.315567000

6	8.451038000	0.797532000	0.074669000
1	6.654727000	1.691354000	0.738223000
6	9.112033000	-0.325460000	-0.585395000
1	8.693622000	-2.217016000	-1.579378000
1	9.091523000	1.583968000	0.461665000
8	10.348431000	-0.379731000	-0.723493000

S2IIDS1-T1 E=-1483.162554 Hartree

6	-2.083138000	1.119834000	-0.197741000
6	-1.272399000	-0.045836000	-0.112767000
6	-1.925771000	-1.270664000	0.092975000
6	-3.314321000	-1.311793000	0.185866000
6	-4.107756000	-0.152025000	0.072692000
6	-3.463690000	1.089861000	-0.120945000
6	0.057668000	1.902528000	-0.315519000
6	0.123999000	0.385784000	-0.182222000
1	-1.352655000	-2.182350000	0.153599000
1	-3.795082000	-2.276044000	0.305763000
1	-4.036619000	2.008581000	-0.162218000
6	1.311966000	-0.321365000	-0.183396000
6	2.699696000	0.105647000	-0.045517000
6	1.382039000	-1.825219000	-0.396931000
6	3.522307000	-1.061147000	-0.169892000
6	3.342636000	1.324554000	0.244437000
6	4.892101000	-1.038114000	-0.057026000
6	4.721094000	1.369744000	0.369763000
1	2.761180000	2.226916000	0.347157000
6	5.524586000	0.205812000	0.214498000
1	5.483207000	-1.940187000	-0.163047000
1	5.204001000	2.316145000	0.587171000
8	0.483613000	-2.630440000	-0.586557000
8	0.962819000	2.714534000	-0.437898000
7	2.723841000	-2.171390000	-0.396956000
7	-1.281229000	2.247511000	-0.333714000
6	-1.747677000	3.612390000	-0.472499000
1	-2.374787000	3.719079000	-1.363692000
1	-2.322091000	3.919779000	0.407848000
1	-0.868158000	4.248487000	-0.571006000
6	3.195732000	-3.527517000	-0.598502000
1	3.846859000	-3.583919000	-1.476653000
1	3.747761000	-3.880958000	0.278587000
1	2.319666000	-4.156570000	-0.754744000
6	6.947974000	0.284890000	0.338415000

6	7.607265000	1.508390000	0.616823000
7	8.141066000	2.520854000	0.847069000
6	7.763308000	-0.865013000	0.189301000
7	8.410010000	-1.828901000	0.062073000
6	-5.575200000	-0.227658000	0.154190000
6	-6.211360000	-1.221613000	0.950157000
6	-6.393918000	0.692355000	-0.559318000
6	-7.578608000	-1.297304000	1.040577000
1	-5.596875000	-1.908306000	1.523411000
6	-7.763398000	0.631656000	-0.493303000
1	-5.920517000	1.432330000	-1.197091000
6	-8.435347000	-0.370613000	0.318265000
1	-8.068326000	-2.041945000	1.659781000
1	-8.392416000	1.319304000	-1.049406000
8	-9.685145000	-0.431875000	0.390822000

S2IIDS3-T1 E=-2051.020992 Hartree

6	-3.714283000	-1.071018000	0.322094000
6	-2.978279000	0.127752000	0.108728000
6	-3.707512000	1.270554000	-0.255039000
6	-5.093530000	1.207907000	-0.363418000
6	-5.813880000	0.017513000	-0.129379000
6	-5.089821000	-1.147210000	0.214442000
6	-1.532918000	-1.680950000	0.606402000
6	-1.558816000	-0.193465000	0.272630000
1	-3.193184000	2.200212000	-0.439181000
1	-5.625840000	2.100077000	-0.672703000
1	-5.604959000	-2.076327000	0.426495000
6	-0.420051000	0.583278000	0.210144000
6	1.005029000	0.237138000	0.198260000
6	-0.451572000	2.103017000	0.183033000
6	1.739363000	1.457292000	0.171270000
6	1.739722000	-0.955947000	0.131473000
6	3.118060000	1.513254000	0.114804000
6	3.128990000	-0.916972000	0.070171000
1	1.227406000	-1.904535000	0.151075000
6	3.844074000	0.298734000	0.070947000
1	3.625667000	2.469138000	0.074719000
1	3.670720000	-1.856995000	0.044574000
8	-1.403668000	2.868803000	0.202852000
8	-0.583616000	-2.409321000	0.855978000
7	0.864803000	2.535363000	0.181949000
7	-2.846195000	-2.111244000	0.635584000

6	-3.228022000	-3.475274000	0.939753000
1	-3.874006000	-3.509942000	1.823200000
1	-3.754686000	-3.930336000	0.094082000
1	-2.312898000	-4.032746000	1.138820000
6	1.239111000	3.934865000	0.179075000
1	1.841147000	4.177841000	1.060927000
1	1.807848000	4.185491000	-0.722896000
1	0.317944000	4.517047000	0.198828000
6	5.292803000	0.321876000	0.025417000
6	6.150949000	1.404562000	0.272241000
16	6.267390000	-1.076173000	-0.358296000
1	5.802757000	2.391889000	0.552988000
6	7.722028000	-0.082075000	-0.148252000
6	9.023309000	-0.598784000	-0.318990000
6	9.230337000	-1.958837000	-0.662073000
7	9.375860000	-3.081742000	-0.944526000
6	10.158131000	0.236128000	-0.151488000
7	11.110157000	0.896702000	-0.020983000
7	7.466313000	1.188705000	0.179640000
6	-7.276476000	-0.017815000	-0.248500000
6	-8.058952000	1.146330000	0.003547000
6	-7.953892000	-1.215951000	-0.617630000
6	-9.426345000	1.125095000	-0.096098000
1	-7.559558000	2.056725000	0.318590000
6	-9.319326000	-1.260094000	-0.735388000
1	-7.369703000	-2.101173000	-0.848332000
6	-10.138517000	-0.085663000	-0.475811000
1	-10.026301000	2.004640000	0.114201000
1	-9.836780000	-2.165666000	-1.035414000
8	-11.386298000	-0.116043000	-0.574212000

S2IIDS4-T1 E=-2017.041250 Hartree

6	2.287300000	-1.072567000	-0.250994000
6	1.472249000	0.093864000	-0.135790000
6	2.130468000	1.313101000	0.115647000
6	3.510821000	1.347476000	0.214762000
6	4.315185000	0.180894000	0.071776000
6	3.660461000	-1.063491000	-0.162815000
6	0.142444000	-1.838739000	-0.429599000
6	0.079656000	-0.328679000	-0.240163000
1	1.558112000	2.222156000	0.210948000
1	3.988239000	2.303570000	0.403985000
1	4.246805000	-1.966083000	-0.260641000

6	-1.106078000	0.381571000	-0.226556000
6	-2.505355000	-0.047033000	-0.132364000
6	-1.170312000	1.894174000	-0.364051000
6	-3.314038000	1.120121000	-0.209798000
6	-3.160364000	-1.267604000	0.086612000
6	-4.693417000	1.096030000	-0.112466000
6	-4.548281000	-1.303459000	0.200747000
1	-2.589337000	-2.180961000	0.141085000
6	-5.340379000	-0.142346000	0.095682000
1	-5.262419000	2.017489000	-0.148434000
1	-5.029517000	-2.266335000	0.330317000
8	-0.267724000	2.708179000	-0.502214000
8	-0.763416000	-2.643906000	-0.591303000
7	-2.509777000	2.243708000	-0.362570000
7	1.479813000	-2.188113000	-0.443484000
6	1.946359000	-3.547639000	-0.626793000
1	2.584959000	-3.621524000	-1.512901000
1	2.513455000	-3.885144000	0.247013000
1	1.067196000	-4.178389000	-0.757350000
6	-2.973028000	3.608780000	-0.499572000
1	-3.613973000	3.715188000	-1.381199000
1	-3.533083000	3.922756000	0.387973000
1	-2.092325000	4.240677000	-0.614170000
6	5.734165000	0.264618000	0.168379000
6	6.679442000	-0.853821000	0.047858000
16	6.587992000	1.770652000	0.457935000
6	8.203639000	0.937452000	0.423915000
7	8.003063000	-0.406655000	0.197924000
8	9.257001000	1.507948000	0.578301000
8	6.426289000	-2.036794000	-0.154113000
6	9.119573000	-1.343598000	0.117372000
1	9.032011000	-2.096012000	0.904333000
1	9.110845000	-1.847265000	-0.851543000
1	10.039210000	-0.773682000	0.240434000
6	-6.805721000	-0.212549000	0.198891000
6	-7.435772000	-1.210419000	0.995696000
6	-7.632874000	0.716853000	-0.493298000
6	-8.801511000	-1.280821000	1.106596000
1	-6.816037000	-1.904907000	1.553689000
6	-9.001175000	0.661738000	-0.406358000
1	-7.166545000	1.460318000	-1.132211000
6	-9.666065000	-0.344287000	0.406487000
1	-9.284577000	-2.028825000	1.727093000
1	-9.635268000	1.357153000	-0.946964000

	8	-10.914858000	-0.400542000	0.498037000
S2IIDS5-T1	E=-1788.496991 Hartree			
	6	1.910812000	1.160507000	-0.016961000
	6	1.106367000	-0.010720000	0.112566000
	6	1.769850000	-1.246434000	0.104228000
	6	3.156245000	-1.300640000	-0.001084000
	6	3.948976000	-0.128545000	-0.086123000
	6	3.285384000	1.128077000	-0.099960000
	6	-0.240487000	1.931671000	-0.018232000
	6	-0.293834000	0.418962000	0.126320000
	1	1.206366000	-2.160470000	0.202242000
	1	3.645768000	-2.262913000	-0.003290000
	1	3.839994000	2.048920000	-0.232636000
	6	-1.471727000	-0.284112000	0.273672000
	6	-2.873652000	0.100450000	0.099154000
	6	-1.520859000	-1.733805000	0.744311000
	6	-3.670109000	-1.031446000	0.427934000
	6	-3.542746000	1.245255000	-0.360154000
	6	-5.049793000	-1.038819000	0.341136000
	6	-4.931862000	1.251500000	-0.448521000
	1	-2.979794000	2.123965000	-0.632270000
	6	-5.711831000	0.129245000	-0.099846000
	1	-5.613442000	-1.914125000	0.640907000
	1	-5.419906000	2.140546000	-0.831331000
	8	-0.608275000	-2.484202000	1.054746000
	8	-1.148805000	2.748924000	-0.040027000
	7	-2.855803000	-2.086080000	0.825416000
	7	1.097398000	2.285119000	-0.074149000
	6	1.550787000	3.656502000	-0.185629000
	1	2.185760000	3.925533000	0.665005000
	1	2.113286000	3.807482000	-1.113294000
	1	0.665493000	4.292138000	-0.191801000
	6	-3.306599000	-3.392584000	1.259783000
	1	-3.939090000	-3.309427000	2.149765000
	1	-3.870752000	-3.894034000	0.466120000
	1	-2.419960000	-3.979248000	1.499852000
	6	5.402787000	-0.176247000	-0.120845000
	6	6.121201000	-1.367118000	-0.649288000
	6	6.167899000	0.905694000	0.338207000
	6	7.551617000	0.896532000	0.322450000
	1	5.669528000	1.770562000	0.760590000
	6	8.308294000	-0.260901000	-0.188376000

6	8.293635000	2.001229000	0.819314000
7	8.860660000	2.931291000	1.233265000
8	5.557738000	-2.356919000	-1.105321000
8	9.530842000	-0.288558000	-0.214711000
7	7.522593000	-1.330622000	-0.636161000
6	8.204888000	-2.517445000	-1.168707000
1	7.913823000	-3.398423000	-0.593755000
1	7.914334000	-2.675328000	-2.209115000
1	9.275062000	-2.344269000	-1.091217000
6	-7.177352000	0.165901000	-0.200684000
6	-7.890685000	1.386678000	-0.027724000
6	-7.922861000	-1.016991000	-0.472247000
6	-9.259018000	1.433575000	-0.111244000
1	-7.337224000	2.288670000	0.212466000
6	-9.290761000	-0.994450000	-0.571592000
1	-7.390130000	-1.947401000	-0.641840000
6	-10.040562000	0.239197000	-0.391753000
1	-9.807386000	2.357999000	0.038739000
1	-9.861003000	-1.889842000	-0.797249000
8	-11.290090000	0.270430000	-0.474328000

S2IIDS6-T1 E=-2149.812043 Hartree

6	3.972909000	-1.074794000	-0.370420000
6	3.198184000	0.095439000	-0.138408000
6	3.885985000	1.259585000	0.236401000
6	5.273669000	1.242194000	0.348663000
6	6.032091000	0.082170000	0.090060000
6	5.352522000	-1.100836000	-0.275103000
6	1.809602000	-1.761001000	-0.620236000
6	1.789918000	-0.276270000	-0.279438000
1	3.339680000	2.173151000	0.411503000
1	5.782630000	2.165519000	0.601191000
1	5.896979000	-2.024289000	-0.432758000
6	0.625266000	0.462253000	-0.190218000
6	-0.774778000	0.064497000	-0.112787000
6	0.601602000	1.984325000	-0.194436000
6	-1.562845000	1.258946000	-0.075323000
6	-1.465926000	-1.154047000	0.008498000
6	-2.931086000	1.275338000	0.032604000
6	-2.844010000	-1.163649000	0.145673000
1	-0.926543000	-2.086824000	-0.031621000
6	-3.631361000	0.036680000	0.155520000
1	-3.479546000	2.203236000	0.043897000

1	-3.345831000	-2.114862000	0.226362000
8	1.527967000	2.777404000	-0.275927000
8	0.882179000	-2.516431000	-0.868558000
7	-0.726310000	2.366587000	-0.142907000
7	3.138132000	-2.146038000	-0.666592000
6	3.562929000	-3.493377000	-0.987330000
1	4.199950000	-3.498026000	-1.878014000
1	4.113768000	-3.938469000	-0.151831000
1	2.664917000	-4.079627000	-1.181996000
6	-1.158342000	3.750125000	-0.163508000
1	-1.816487000	3.934926000	-1.018224000
1	-1.694676000	4.002170000	0.757197000
1	-0.265526000	4.369387000	-0.247163000
6	-5.065606000	-0.025159000	0.243785000
6	-5.903634000	1.096983000	-0.197210000
6	-5.724316000	-1.215723000	0.797950000
6	-7.922442000	-0.321506000	0.082873000
8	-5.129375000	-2.110827000	1.391756000
7	-7.126003000	-1.305338000	0.636148000
6	-7.767617000	-2.537713000	1.124197000
1	-6.984027000	-3.166039000	1.536666000
1	-8.507233000	-2.292418000	1.887629000
1	-8.276665000	-3.038234000	0.299616000
8	-5.470693000	2.201633000	-0.518406000
7	-7.294401000	0.854097000	-0.285715000
6	-8.119873000	1.949126000	-0.822971000
1	-8.865305000	2.245806000	-0.083794000
1	-7.452284000	2.774859000	-1.048890000
1	-8.640047000	1.611673000	-1.720151000
16	-9.572794000	-0.531868000	-0.106806000
6	7.499538000	0.097732000	0.196675000
6	8.299827000	-0.748176000	-0.621960000
6	8.155195000	0.957613000	1.122543000
6	9.669296000	-0.742540000	-0.533547000
1	7.812939000	-1.382457000	-1.356165000
6	9.522564000	0.974997000	1.237019000
1	7.554153000	1.584053000	1.773778000
6	10.360573000	0.122155000	0.409385000
1	10.284464000	-1.372530000	-1.167975000
1	10.026144000	1.615832000	1.953617000
8	11.610461000	0.131435000	0.503108000

S2IIDS7-T1 E=-1903.754895 Hartree

6	-4.180060000	-1.037084000	0.510101000
6	-3.339198000	0.019827000	0.063685000
6	-3.959486000	1.120945000	-0.545922000
6	-5.345093000	1.155486000	-0.676729000
6	-6.169506000	0.112871000	-0.205763000
6	-5.558047000	-1.008026000	0.398976000
6	-2.060311000	-1.778539000	0.923617000
6	-1.954008000	-0.391317000	0.300710000
1	-3.363061000	1.951598000	-0.888911000
1	-5.799288000	2.036553000	-1.115668000
1	-6.153108000	-1.851737000	0.727581000
6	-0.751157000	0.253467000	0.092105000
6	0.631223000	-0.219680000	0.135189000
6	-0.647773000	1.741380000	-0.211860000
6	1.474462000	0.902763000	-0.136165000
6	1.252695000	-1.471128000	0.285389000
6	2.844159000	0.817921000	-0.219235000
6	2.634109000	-1.577528000	0.203194000
1	0.657438000	-2.346746000	0.488985000
6	3.467069000	-0.441798000	-0.014063000
1	3.432357000	1.690395000	-0.469494000
1	3.099010000	-2.545711000	0.323257000
8	-1.530042000	2.581921000	-0.302216000
8	-1.179658000	-2.524515000	1.323915000
7	0.698836000	2.038272000	-0.321570000
7	-3.408609000	-2.071941000	1.026027000
6	-3.910750000	-3.305011000	1.596897000
1	-4.552570000	-3.099830000	2.460050000
1	-4.480663000	-3.875140000	0.855383000
1	-3.048536000	-3.889282000	1.918108000
6	1.206588000	3.384147000	-0.505508000
1	1.872912000	3.652096000	0.320487000
1	1.750827000	3.470173000	-1.452170000
1	0.349066000	4.056515000	-0.520837000
6	4.891745000	-0.599625000	-0.081803000
6	5.538831000	-1.850150000	-0.607285000
6	5.940142000	0.360894000	0.154232000
6	6.961580000	-1.508070000	-0.843597000
6	7.201916000	-0.186296000	-0.428915000
6	7.949994000	-2.309161000	-1.396472000
6	8.478064000	0.357357000	-0.591633000
6	9.225871000	-1.762027000	-1.554898000
1	7.718163000	-3.327013000	-1.693141000
6	9.476561000	-0.443741000	-1.160266000

1	8.713351000	1.371864000	-0.300818000
1	10.024530000	-2.356699000	-1.987163000
1	10.469232000	-0.025243000	-1.295097000
8	5.012811000	-2.929001000	-0.836477000
6	5.872319000	1.521687000	0.926073000
6	4.755100000	1.905458000	1.727557000
7	3.893187000	2.276883000	2.418566000
6	6.977363000	2.412607000	1.077089000
7	7.848407000	3.175633000	1.211816000
6	-7.631915000	0.185075000	-0.338366000
6	-8.233911000	0.889686000	-1.419648000
6	-8.483937000	-0.449816000	0.609571000
6	-9.597034000	0.956172000	-1.559294000
1	-7.595541000	1.350792000	-2.166331000
6	-9.850025000	-0.389395000	0.497944000
1	-8.038347000	-0.959375000	1.458178000
6	-10.486798000	0.318005000	-0.601940000
1	-10.059588000	1.476584000	-2.391764000
1	-10.503091000	-0.856135000	1.228351000
8	-11.733179000	0.374131000	-0.717805000

S2IIDS8-T1 E=-2338.977120 Hartree

6	-4.488191000	-0.958074000	0.584625000
6	-3.666795000	0.087067000	0.077443000
6	-4.306636000	1.134550000	-0.603147000
6	-5.691363000	1.130800000	-0.743156000
6	-6.497138000	0.102062000	-0.211798000
6	-5.865333000	-0.965654000	0.465172000
6	-2.356894000	-1.626990000	1.055336000
6	-2.275346000	-0.277514000	0.347570000
1	-3.725710000	1.954499000	-0.994777000
1	-6.160849000	1.972780000	-1.238831000
1	-6.443993000	-1.800099000	0.842773000
6	-1.085506000	0.378784000	0.107937000
6	0.308941000	-0.060033000	0.196267000
6	-1.010838000	1.843769000	-0.293914000
6	1.128236000	1.061329000	-0.136119000
6	0.952712000	-1.284583000	0.433781000
6	2.502585000	1.002361000	-0.200993000
6	2.337912000	-1.365537000	0.369949000
1	0.374706000	-2.157577000	0.690704000
6	3.140250000	-0.230595000	0.081320000
1	3.080079000	1.869114000	-0.494931000

1	2.818307000	-2.311941000	0.589536000
8	-1.908764000	2.656436000	-0.455661000
8	-1.463087000	-2.327053000	1.505131000
7	0.331236000	2.164216000	-0.404003000
7	-3.698664000	-1.942253000	1.168151000
6	-4.178599000	-3.149221000	1.810186000
1	-4.830452000	-2.905674000	2.655589000
1	-4.730989000	-3.775114000	1.101201000
1	-3.306614000	-3.694412000	2.171168000
6	0.809736000	3.502278000	-0.690882000
1	1.449801000	3.859460000	0.122164000
1	1.372924000	3.522506000	-1.630036000
1	-0.063708000	4.147857000	-0.780194000
6	4.571928000	-0.365650000	0.012106000
6	5.625523000	0.542879000	0.253422000
6	6.867328000	-1.240453000	-0.817216000
6	6.927457000	0.065928000	-0.310234000
6	7.950973000	-1.909964000	-1.362133000
6	8.161788000	0.726816000	-0.381975000
6	9.171388000	-1.234201000	-1.419890000
1	7.846374000	-2.923644000	-1.734160000
6	9.264485000	0.072461000	-0.936486000
1	8.282118000	1.738842000	-0.024366000
1	10.042451000	-1.723368000	-1.843468000
1	10.212142000	0.598838000	-0.989115000
6	5.495241000	1.707699000	1.045426000
6	4.362410000	1.989997000	1.861812000
7	3.483742000	2.282222000	2.570682000
6	6.515575000	2.687078000	1.197999000
7	7.305466000	3.533660000	1.344582000
16	5.226108000	-1.912213000	-0.678649000
8	4.652057000	-2.149784000	-2.010346000
8	5.178024000	-2.990208000	0.323023000
6	-7.958852000	0.134576000	-0.355778000
6	-8.569523000	0.767604000	-1.476374000
6	-8.803418000	-0.467966000	0.620215000
6	-9.932515000	0.796388000	-1.626527000
1	-7.936977000	1.202063000	-2.243626000
6	-10.169449000	-0.443078000	0.498740000
1	-8.352786000	-0.921842000	1.497224000
6	-10.814641000	0.190919000	-0.640764000
1	-10.400896000	1.261149000	-2.488134000
1	-10.816885000	-0.884227000	1.249751000
8	-12.060707000	0.213900000	-0.765585000

S2IIDS9-T1 E=-2324.922373 Hartree

6	3.794262000	-1.116910000	-0.239760000
6	2.999931000	0.060889000	-0.157650000
6	3.669102000	1.267055000	0.094119000
6	5.055403000	1.280387000	0.235237000
6	5.833363000	0.110032000	0.125894000
6	5.172522000	-1.114323000	-0.115564000
6	1.636911000	-1.845197000	-0.446598000
6	1.597981000	-0.346734000	-0.284859000
1	3.111854000	2.188932000	0.151537000
1	5.548124000	2.234055000	0.389534000
1	5.728563000	-2.043744000	-0.156507000
6	0.418180000	0.390439000	-0.303496000
6	-0.969653000	-0.003332000	-0.203269000
6	0.387737000	1.896025000	-0.496871000
6	-1.772643000	1.177574000	-0.316951000
6	-1.652323000	-1.215026000	0.042840000
6	-3.142350000	1.181187000	-0.226667000
6	-3.029135000	-1.234880000	0.142527000
1	-1.090204000	-2.131969000	0.130918000
6	-3.823200000	-0.055160000	0.004434000
1	-3.693889000	2.110028000	-0.320419000
1	-3.517217000	-2.186719000	0.326163000
8	1.304948000	2.687590000	-0.663577000
8	0.724858000	-2.647736000	-0.615786000
7	-0.946814000	2.277035000	-0.506832000
7	2.974032000	-2.221341000	-0.426675000
6	3.412862000	-3.591181000	-0.578786000
1	4.068347000	-3.697281000	-1.450197000
1	3.950714000	-3.933260000	0.312615000
1	2.521251000	-4.202366000	-0.720307000
6	-1.378243000	3.645562000	-0.691076000
1	-2.014793000	3.738382000	-1.577797000
1	-1.932883000	4.003421000	0.183577000
1	-0.482187000	4.252064000	-0.824304000
6	-5.230690000	-0.105061000	0.096316000
6	-7.727155000	-0.880250000	0.382834000
6	-7.789720000	0.503696000	0.160887000
6	-8.898955000	-1.615839000	0.580639000
6	-9.023235000	1.159842000	0.135523000
6	-10.126861000	-0.957539000	0.554503000
1	-8.850449000	-2.686366000	0.752346000

6	-10.188776000	0.422032000	0.333313000
1	-9.070516000	2.230437000	-0.036171000
1	-11.039534000	-1.524255000	0.707608000
1	-11.149423000	0.926396000	0.314691000
16	-6.244872000	1.324969000	-0.078321000
16	-6.114815000	-1.599678000	0.392327000
6	7.297601000	0.157979000	0.257377000
6	8.125994000	-0.770739000	-0.433992000
6	7.927916000	1.132690000	1.081993000
6	9.493281000	-0.737201000	-0.319640000
1	7.661320000	-1.497014000	-1.093635000
6	9.292471000	1.182151000	1.218959000
1	7.307428000	1.826877000	1.639676000
6	10.157575000	0.245298000	0.521026000
1	10.127226000	-1.433462000	-0.859565000
1	9.773695000	1.913621000	1.860449000
8	11.405960000	0.282259000	0.636961000

S2IIDS10-T1 E=-2171.264240 Hartree

6	2.796152000	-1.118917000	-0.249258000
6	1.979645000	0.051724000	-0.128309000
6	2.646386000	1.265563000	0.148262000
6	4.021443000	1.297243000	0.269583000
6	4.828833000	0.128155000	0.124373000
6	4.164610000	-1.110440000	-0.137745000
6	0.646242000	-1.855382000	-0.474986000
6	0.597542000	-0.353837000	-0.256754000
1	2.073750000	2.175369000	0.242758000
1	4.497167000	2.250747000	0.476268000
1	4.726924000	-2.032172000	-0.238551000
6	-0.589932000	0.371236000	-0.244180000
6	-1.989495000	-0.052393000	-0.146337000
6	-0.641367000	1.871506000	-0.380317000
6	-2.794409000	1.118784000	-0.220722000
6	-2.650497000	-1.269231000	0.073787000
6	-4.174324000	1.100541000	-0.118626000
6	-4.038619000	-1.298588000	0.192618000
1	-2.085070000	-2.186528000	0.124079000
6	-4.826684000	-0.134228000	0.091128000
1	-4.738884000	2.025105000	-0.152319000
1	-4.523994000	-2.259639000	0.322483000
8	0.265024000	2.686137000	-0.520686000
8	-0.259875000	-2.653382000	-0.669371000

7	-1.982442000	2.234221000	-0.375294000
7	1.984829000	-2.223126000	-0.470356000
6	2.432662000	-3.584046000	-0.670614000
1	3.083730000	-3.655915000	-1.548725000
1	2.977184000	-3.951358000	0.206502000
1	1.544820000	-4.196836000	-0.827959000
6	-2.432482000	3.602160000	-0.510321000
1	-3.075148000	3.717370000	-1.390099000
1	-2.987802000	3.923198000	0.378207000
1	-1.544875000	4.224370000	-0.626785000
6	6.234873000	0.190230000	0.238961000
6	8.705862000	0.954623000	0.566768000
6	8.782661000	-0.362984000	0.333367000
16	7.112448000	1.683679000	0.574567000
16	7.278931000	-1.220859000	0.058965000
1	9.699841000	-0.937623000	0.299755000
1	9.552886000	1.604014000	0.750058000
6	-6.292086000	-0.198847000	0.198355000
6	-6.925691000	-1.195076000	0.994350000
6	-7.118890000	0.734737000	-0.488479000
6	-8.291629000	-1.260320000	1.108642000
1	-6.307217000	-1.893664000	1.548762000
6	-8.487367000	0.685749000	-0.396595000
1	-6.651244000	1.477886000	-1.126889000
6	-9.155053000	-0.318879000	0.414762000
1	-8.775522000	-2.008430000	1.728579000
1	-9.119640000	1.385932000	-0.933410000
8	-10.404649000	-0.370144000	0.510065000

S2TIIDTS1-CS E=-2586.797553 Hartree

6	-1.888669000	1.637160000	-0.591529000
6	-1.228062000	0.356624000	-0.493443000
6	-2.046230000	-0.773037000	-0.218155000
6	-3.403134000	-0.621871000	-0.080130000
6	-4.054404000	0.648514000	-0.202433000
6	-3.242174000	1.797546000	-0.461215000
6	0.339818000	2.050630000	-0.838324000
6	0.164559000	0.568940000	-0.634088000
1	-1.595866000	-1.751678000	-0.145867000
1	-4.003724000	-1.502212000	0.124906000
1	-3.685683000	2.781718000	-0.546369000
6	1.250148000	-0.342580000	-0.650080000
6	2.632986000	-0.147277000	-0.441467000

6	1.084437000	-1.806230000	-0.983910000
6	3.299781000	-1.417619000	-0.618713000
6	3.440377000	0.956400000	-0.044302000
6	4.645307000	-1.591990000	-0.450111000
6	4.788827000	0.792265000	0.134060000
1	2.985666000	1.926751000	0.088494000
6	5.448314000	-0.468309000	-0.065676000
1	5.093129000	-2.566817000	-0.596588000
1	5.380402000	1.651600000	0.432655000
8	0.074626000	-2.433774000	-1.269232000
8	1.357407000	2.701481000	-1.031701000
7	2.356578000	-2.372418000	-0.956091000
7	-0.935623000	2.614225000	-0.813758000
6	-1.181048000	4.029363000	-0.994320000
1	-1.820060000	4.207709000	-1.865826000
1	-1.656527000	4.462144000	-0.107224000
1	-0.213745000	4.506518000	-1.153757000
6	2.611865000	-3.768406000	-1.243118000
1	3.284353000	-3.874431000	-2.100977000
1	3.054266000	-4.272638000	-0.377034000
1	1.652753000	-4.230371000	-1.478380000
6	-5.457176000	0.770714000	-0.066408000
6	-6.245274000	1.946122000	-0.160290000
16	-6.506645000	-0.608060000	0.262088000
6	-7.593445000	1.748884000	0.020156000
1	-5.815468000	2.919656000	-0.359397000
6	-7.963102000	0.397107000	0.269564000
1	-8.318531000	2.551224000	-0.023258000
6	6.838722000	-0.602609000	0.115979000
6	7.635641000	-1.768680000	-0.045929000
16	7.870701000	0.752744000	0.607841000
6	8.972411000	-1.592689000	0.205326000
1	7.215666000	-2.720596000	-0.346143000
6	9.308702000	-0.258466000	0.585090000
1	9.724946000	-2.368210000	0.132088000
6	10.575787000	0.224467000	0.902104000
6	11.699209000	-0.647937000	0.863750000
7	12.602435000	-1.384319000	0.824600000
6	10.785723000	1.581287000	1.269188000
7	10.929890000	2.699451000	1.567642000
6	-9.243672000	-0.125286000	0.492119000
6	-10.407542000	0.731529000	0.490619000
6	-9.457103000	-1.532639000	0.731357000
6	-11.654065000	0.240819000	0.705128000

1	-10.277970000	1.794064000	0.313402000
6	-10.695544000	-2.042311000	0.947668000
1	-8.597180000	-2.197291000	0.736685000
6	-11.892923000	-1.188370000	0.950928000
1	-12.526702000	0.886008000	0.703785000
1	-10.852433000	-3.101041000	1.126974000
8	-13.024462000	-1.643710000	1.147165000

S2TIIDTS3-CS E=-3154.650772 Hartree

6	-1.509572000	-1.538772000	0.707142000
6	-0.878628000	-0.251629000	0.582450000
6	-1.721918000	0.852357000	0.299408000
6	-3.080524000	0.670212000	0.177236000
6	-3.699659000	-0.607230000	0.326100000
6	-2.863124000	-1.731316000	0.593736000
6	0.726173000	-1.919622000	0.932951000
6	0.529053000	-0.436620000	0.709090000
1	-1.294305000	1.838988000	0.205424000
1	-3.699861000	1.535875000	-0.034457000
1	-3.283649000	-2.723650000	0.698227000
6	1.595580000	0.482951000	0.700258000
6	2.999353000	0.298498000	0.525584000
6	1.406250000	1.959526000	0.952803000
6	3.635368000	1.583566000	0.652993000
6	3.831418000	-0.800853000	0.195827000
6	4.984749000	1.776758000	0.501919000
6	5.185744000	-0.618116000	0.035282000
1	3.399750000	-1.785156000	0.096911000
6	5.812021000	0.656173000	0.188701000
1	5.409212000	2.766868000	0.611554000
1	5.797080000	-1.480060000	-0.211794000
8	0.385759000	2.592328000	1.185843000
8	1.754232000	-2.553176000	1.126111000
7	2.671577000	2.539344000	0.924817000
7	-0.537997000	-2.499639000	0.932574000
6	-0.762529000	-3.915293000	1.137588000
1	-1.389731000	-4.087598000	2.018687000
1	-1.242504000	-4.367176000	0.262660000
1	0.212225000	-4.377931000	1.293511000
6	2.901985000	3.951319000	1.146126000
1	3.554767000	4.110005000	2.011166000
1	3.355777000	4.417994000	0.264894000
1	1.931990000	4.410465000	1.338118000

6	-5.110111000	-0.766090000	0.206877000
6	-5.869412000	-1.945770000	0.331871000
16	-6.184937000	0.589946000	-0.139937000
6	-7.231646000	-1.776288000	0.159664000
1	-5.421372000	-2.907617000	0.547196000
6	-7.613588000	-0.444321000	-0.111050000
1	-7.953315000	-2.582240000	0.224111000
6	7.215512000	0.814099000	0.029997000
6	7.979542000	1.997764000	0.153396000
16	8.281074000	-0.529183000	-0.370713000
6	9.330583000	1.833510000	-0.061071000
1	7.535933000	2.954526000	0.398343000
6	9.717976000	0.502336000	-0.368382000
1	10.041070000	2.647748000	-0.000846000
6	-8.903723000	0.052282000	-0.332547000
6	-9.290154000	1.390581000	-0.603917000
16	-10.357514000	-0.943652000	-0.314456000
1	-8.574242000	2.205320000	-0.668308000
6	-11.317328000	0.518066000	-0.668041000
6	-12.702169000	0.486808000	-0.809536000
6	-13.415649000	-0.734148000	-0.674793000
7	-13.972266000	-1.752664000	-0.558426000
6	-13.432974000	1.673622000	-1.091971000
7	-14.060868000	2.627642000	-1.323412000
7	-10.571968000	1.642720000	-0.782937000
6	11.005053000	0.009530000	-0.637069000
6	11.235964000	-1.382745000	-0.933978000
6	12.152685000	0.885894000	-0.625989000
6	12.478578000	-1.862537000	-1.194905000
1	10.387482000	-2.061765000	-0.947481000
6	13.403274000	0.425692000	-0.884400000
1	12.008723000	1.938392000	-0.405452000
6	13.660580000	-0.988349000	-1.189543000
1	12.649165000	-2.910781000	-1.417841000
1	14.264673000	1.085721000	-0.875844000
8	14.795685000	-1.415977000	-1.426236000

S2TIIDTS4-CS E=-3120.677991 Hartree

6	-1.993020000	1.683345000	-0.707219000
6	-1.368678000	0.384252000	-0.610602000
6	-2.218453000	-0.719211000	-0.319052000
6	-3.567130000	-0.526957000	-0.162648000
6	-4.184200000	0.763517000	-0.282203000

6	-3.337530000	1.886184000	-0.559577000
6	0.244014000	2.028355000	-0.984656000
6	0.026806000	0.552987000	-0.769296000
1	-1.796518000	-1.710713000	-0.249206000
1	-4.191351000	-1.387573000	0.054530000
1	-3.751084000	2.883492000	-0.643082000
6	1.084516000	-0.391093000	-0.793046000
6	2.478190000	-0.234550000	-0.601013000
6	0.871877000	-1.847822000	-1.112181000
6	3.103621000	-1.524141000	-0.774683000
6	3.322600000	0.845294000	-0.223397000
6	4.446906000	-1.737584000	-0.618926000
6	4.669715000	0.640917000	-0.058961000
1	2.899656000	1.830439000	-0.094385000
6	5.286282000	-0.637601000	-0.254167000
1	4.862627000	-2.727233000	-0.762205000
1	5.290632000	1.484610000	0.224688000
8	-0.157994000	-2.451015000	-1.382591000
8	1.278342000	2.647999000	-1.194551000
7	2.128358000	-2.452388000	-1.093550000
7	-1.012564000	2.630489000	-0.946964000
6	-1.217670000	4.050673000	-1.132517000
1	-1.862855000	4.243870000	-1.996448000
1	-1.668737000	4.502906000	-0.242192000
1	-0.238579000	4.497585000	-1.307319000
6	2.336720000	-3.857063000	-1.371156000
1	2.996117000	-3.992269000	-2.235379000
1	2.772783000	-4.368903000	-0.506000000
1	1.360650000	-4.290028000	-1.591958000
6	-5.576971000	0.925451000	-0.126296000
6	-6.323449000	2.133290000	-0.223130000
16	-6.659746000	-0.429159000	0.233632000
6	-7.669744000	1.984787000	-0.022794000
1	-5.863311000	3.089290000	-0.439197000
6	-8.072675000	0.638551000	0.247172000
1	-8.384249000	2.798953000	-0.060920000
6	6.679958000	-0.815862000	-0.087511000
6	7.435563000	-2.003452000	-0.248081000
16	7.760781000	0.499927000	0.377414000
6	8.783850000	-1.863890000	-0.013579000
1	6.984044000	-2.945040000	-0.534532000
6	9.185724000	-0.548797000	0.349982000
1	9.485762000	-2.683470000	-0.097653000
6	-9.350359000	0.190705000	0.486833000

6	-9.676913000	-1.210842000	0.756392000
16	-10.796405000	1.205630000	0.511281000
6	-11.843217000	-0.235215000	0.880765000
7	-11.054744000	-1.366539000	0.961159000
6	-11.655379000	-2.664919000	1.249469000
1	-12.383721000	-2.921808000	0.477129000
1	-10.847502000	-3.395676000	1.264542000
1	-12.160234000	-2.638536000	2.217654000
8	-13.040381000	-0.185536000	1.028918000
8	-8.875191000	-2.136324000	0.802016000
6	10.474734000	-0.085385000	0.650704000
6	10.722980000	1.290188000	1.005622000
6	11.612011000	-0.974577000	0.616723000
6	11.969246000	1.741894000	1.298179000
1	9.883695000	1.980215000	1.037952000
6	12.865861000	-0.541898000	0.906081000
1	11.457439000	-2.015710000	0.352609000
6	13.140079000	0.854184000	1.270327000
1	12.150451000	2.778256000	1.564621000
1	13.718034000	-1.213523000	0.879441000
8	14.278928000	1.256784000	1.535734000

S2TIIDTS5-CS E=-2892.141597 Hartree

6	1.602149000	-1.685542000	-0.718590000
6	0.979795000	-0.386176000	-0.628148000
6	1.831821000	0.720029000	-0.356405000
6	3.182597000	0.529334000	-0.212363000
6	3.796597000	-0.762300000	-0.326437000
6	2.949161000	-1.886637000	-0.583480000
6	-0.634831000	-2.039934000	-0.967370000
6	-0.418429000	-0.557030000	-0.768677000
1	1.410650000	1.711991000	-0.290505000
1	3.809361000	1.391223000	-0.010079000
1	3.363219000	-2.884059000	-0.661278000
6	-1.476659000	0.381570000	-0.792512000
6	-2.872495000	0.221954000	-0.595000000
6	-1.269303000	1.838688000	-1.117066000
6	-3.499329000	1.509231000	-0.773995000
6	-3.711917000	-0.856301000	-0.206926000
6	-4.843678000	1.720544000	-0.616992000
6	-5.059989000	-0.653796000	-0.040728000
1	-3.287187000	-1.839398000	-0.070235000
6	-5.678400000	0.621125000	-0.244226000

1	-5.261591000	2.708272000	-0.766169000
1	-5.677524000	-1.497125000	0.251137000
8	-0.242323000	2.443484000	-1.391474000
8	-1.670871000	-2.659885000	-1.160685000
7	-2.527874000	2.438209000	-1.100041000
7	0.621446000	-2.638019000	-0.937730000
6	0.829447000	-4.060202000	-1.112181000
1	1.466205000	-4.258109000	-1.980943000
1	1.291327000	-4.501305000	-0.222148000
1	-0.149359000	-4.512766000	-1.272595000
6	-2.741504000	3.841515000	-1.383999000
1	-3.402271000	3.969793000	-2.248055000
1	-3.177813000	4.355228000	-0.520258000
1	-1.767413000	4.276993000	-1.608139000
6	5.195384000	-0.924009000	-0.183071000
6	5.938839000	-2.126077000	-0.276964000
16	6.279183000	0.434692000	0.154962000
6	7.290532000	-1.963960000	-0.089191000
1	5.486548000	-3.088786000	-0.480527000
6	7.687519000	-0.618802000	0.164461000
1	7.996463000	-2.783587000	-0.129999000
6	-7.073850000	0.796972000	-0.076669000
6	-7.830920000	1.983386000	-0.243271000
16	-8.148868000	-0.517843000	0.395567000
6	-9.178319000	1.842098000	-0.006714000
1	-7.381245000	2.924037000	-0.535023000
6	-9.576095000	0.527599000	0.364133000
1	-9.881990000	2.659749000	-0.094387000
6	8.995186000	-0.157430000	0.393079000
6	10.116341000	-1.025279000	0.396014000
6	9.218631000	1.276387000	0.639375000
6	11.388381000	-0.565444000	0.619859000
1	9.978311000	-2.085699000	0.217546000
6	11.661446000	0.860838000	0.870105000
6	12.498971000	-1.458196000	0.618156000
7	13.376710000	-2.223111000	0.607927000
8	8.296637000	2.095068000	0.654076000
8	12.783553000	1.301214000	1.072683000
7	10.527907000	1.697521000	0.860735000
6	10.720606000	3.131981000	1.102378000
1	10.357426000	3.703036000	0.245524000
1	10.153247000	3.437985000	1.983720000
1	11.784077000	3.298954000	1.252948000
6	-10.863029000	0.062873000	0.668173000

6	-11.105981000	-1.312787000	1.030269000
6	-12.002513000	0.950581000	0.630234000
6	-12.350082000	-1.766222000	1.325866000
1	-10.264507000	-1.999760000	1.065214000
6	-13.254300000	0.516253000	0.922553000
1	-11.850193000	1.990470000	0.360832000
6	-13.523211000	-0.879996000	1.294046000
1	-12.529378000	-2.801413000	1.597688000
1	-14.108867000	1.184555000	0.893558000
8	-14.659653000	-1.284016000	1.561791000

S2TIIDTS6-CS E=-3253.464394 Hartree

6	-1.223662000	1.742179000	-0.738740000
6	-0.608476000	0.435601000	-0.672056000
6	-1.468243000	-0.672066000	-0.421188000
6	-2.815988000	-0.476052000	-0.274139000
6	-3.424241000	0.823712000	-0.363907000
6	-2.567882000	1.948893000	-0.600311000
6	1.016273000	2.081895000	-0.981906000
6	0.786991000	0.598757000	-0.809480000
1	-1.052330000	-1.667472000	-0.374701000
1	-3.449328000	-1.336682000	-0.088122000
1	-2.977049000	2.949491000	-0.659496000
6	1.839455000	-0.350351000	-0.849818000
6	3.230754000	-0.207513000	-0.633142000
6	1.622999000	-1.794207000	-1.219273000
6	3.851651000	-1.494767000	-0.841847000
6	4.073854000	0.854921000	-0.206458000
6	5.192053000	-1.719299000	-0.676220000
6	5.417543000	0.638522000	-0.031812000
1	3.653746000	1.836904000	-0.048050000
6	6.030560000	-0.635803000	-0.263671000
1	5.605501000	-2.705215000	-0.848251000
1	6.038109000	1.468779000	0.289631000
8	0.593596000	-2.381241000	-1.522219000
8	2.058243000	2.695657000	-1.163429000
7	2.876654000	-2.405773000	-1.204713000
7	-0.235277000	2.690242000	-0.940670000
6	-0.431707000	4.116976000	-1.089062000
1	-1.066313000	4.336069000	-1.954307000
1	-0.890850000	4.545284000	-0.191408000
1	0.550909000	4.564418000	-1.240486000

6	3.081416000	-3.802100000	-1.526261000
1	3.750574000	-3.911905000	-2.386444000
1	3.503700000	-4.344229000	-0.672937000
1	2.106066000	-4.222231000	-1.773261000
6	-4.816977000	0.990483000	-0.217626000
6	-5.554652000	2.201842000	-0.287878000
16	-5.910319000	-0.368451000	0.094036000
6	-6.904760000	2.053450000	-0.104478000
1	-5.093517000	3.164386000	-0.472692000
6	-7.315622000	0.699343000	0.124391000
1	-7.631946000	2.850591000	-0.122028000
6	7.420956000	-0.825217000	-0.085584000
6	8.172897000	-2.012391000	-0.276031000
16	8.500641000	0.468980000	0.434852000
6	9.517708000	-1.887262000	-0.020793000
1	7.720178000	-2.941555000	-0.598379000
6	9.920936000	-0.585702000	0.390599000
1	10.216823000	-2.707151000	-0.122873000
6	-8.617207000	0.230275000	0.344505000
6	-9.757343000	1.143629000	0.363128000
6	-8.821693000	-1.192869000	0.556549000
6	-11.246700000	-0.801691000	0.797133000
8	-7.891431000	-2.002244000	0.551627000
7	-10.140473000	-1.632681000	0.772323000
6	-10.331552000	-3.076083000	0.983703000
1	-10.997386000	-3.476657000	0.218078000
1	-9.351196000	-3.540378000	0.925364000
1	-10.786172000	-3.249698000	1.960025000
7	-11.023215000	0.548236000	0.593990000
6	-12.179771000	1.458168000	0.614973000
1	-12.891348000	1.169083000	-0.159743000
1	-12.681033000	1.396192000	1.581925000
1	-11.801511000	2.460655000	0.438538000
8	-9.683923000	2.358549000	0.195829000
16	-12.785982000	-1.408146000	1.062098000
6	11.207235000	-0.139699000	0.721260000
6	11.456747000	1.223506000	1.124078000
6	12.340911000	-1.034389000	0.671269000
6	12.700809000	1.658997000	1.445554000
1	10.620029000	1.915745000	1.169038000
6	13.592507000	-0.617790000	0.989032000
1	12.184185000	-2.065329000	0.371525000
6	13.867843000	0.765414000	1.401858000
1	12.884513000	2.684920000	1.747943000

1	14.442340000	-1.291677000	0.950745000
8	15.004303000	1.153215000	1.693185000

S2TIIDTS7-CS E=-3007.393930 Hartree

6	1.038687000	-1.780742000	-1.033775000
6	0.443652000	-0.475774000	-0.864411000
6	1.325425000	0.604077000	-0.579344000
6	2.675925000	0.383866000	-0.488704000
6	3.260406000	-0.913137000	-0.675098000
6	2.384994000	-2.011059000	-0.953883000
6	-1.211831000	-2.084875000	-1.217835000
6	-0.960883000	-0.616733000	-0.962402000
1	0.926100000	1.600785000	-0.465995000
1	3.327126000	1.227982000	-0.287597000
1	2.778021000	-3.011912000	-1.080430000
6	-2.002756000	0.339975000	-0.905740000
6	-3.391875000	0.194800000	-0.662041000
6	-1.781438000	1.806190000	-1.175413000
6	-4.002479000	1.498884000	-0.762046000
6	-4.235580000	-0.885808000	-0.288398000
6	-5.335869000	1.724664000	-0.544955000
6	-5.572286000	-0.668972000	-0.062167000
1	-3.823454000	-1.880647000	-0.210437000
6	-6.175560000	0.623683000	-0.187349000
1	-5.741536000	2.724540000	-0.635695000
1	-6.193516000	-1.513935000	0.216886000
8	-0.754651000	2.405411000	-1.461724000
8	-2.265461000	-2.677924000	-1.400914000
7	-3.027643000	2.425114000	-1.084949000
7	0.033333000	-2.705521000	-1.258208000
6	0.208729000	-4.121724000	-1.502926000
1	0.811695000	-4.290983000	-2.401320000
1	0.692549000	-4.610362000	-0.650142000
1	-0.783310000	-4.549703000	-1.648910000
6	-3.226233000	3.842610000	-1.301245000
1	-3.916705000	4.018528000	-2.133087000
1	-3.620185000	4.326235000	-0.400549000
1	-2.253518000	4.271001000	-1.544293000
6	4.655785000	-1.112372000	-0.575017000
6	5.387827000	-2.305716000	-0.806166000
16	5.765451000	0.181509000	-0.129347000
6	6.743161000	-2.188265000	-0.629596000
1	4.913677000	-3.229826000	-1.112399000

6	7.171051000	-0.875509000	-0.249319000
1	7.462008000	-2.985855000	-0.749860000
6	-7.559823000	0.814400000	0.041111000
6	-8.302136000	2.018538000	-0.046969000
16	-8.639445000	-0.501921000	0.500488000
6	-9.641731000	1.888958000	0.235706000
1	-7.847533000	2.963239000	-0.317304000
6	-10.048232000	0.566587000	0.567461000
1	-10.333935000	2.720549000	0.208980000
6	8.477226000	-0.532551000	0.111974000
6	9.476919000	-1.596260000	0.457684000
6	9.066700000	0.745065000	0.463209000
6	10.547812000	-0.912568000	1.222286000
6	10.284794000	0.467837000	1.275919000
6	11.654072000	-1.485480000	1.833055000
6	11.154332000	1.301096000	1.984496000
6	12.520012000	-0.648577000	2.541300000
1	11.821629000	-2.554791000	1.753882000
6	12.262769000	0.724616000	2.616402000
1	10.989855000	2.367010000	2.063972000
1	13.392786000	-1.061437000	3.037716000
1	12.937600000	1.364704000	3.176556000
8	9.431549000	-2.794567000	0.213584000
6	8.700482000	2.006168000	0.009348000
6	7.817449000	2.230765000	-1.088161000
7	7.149500000	2.465216000	-2.014093000
6	9.295778000	3.208193000	0.500522000
7	9.744727000	4.209709000	0.892768000
6	-11.330625000	0.110355000	0.902214000
6	-11.584173000	-1.274967000	1.216517000
6	-12.454823000	1.016872000	0.945792000
6	-12.823922000	-1.720184000	1.541896000
1	-10.754405000	-1.976449000	1.189935000
6	-13.702022000	0.590938000	1.268986000
1	-12.294660000	2.064608000	0.713774000
6	-13.981431000	-0.814849000	1.592960000
1	-13.010812000	-2.762887000	1.777579000
1	-14.544922000	1.273790000	1.301156000
8	-15.113905000	-1.211336000	1.888482000

S2TIIDTS8-CS E=-3442.613433 Hartree

6	-4.464231000	1.541415000	-0.738664000
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6	-3.837927000	0.243742000	-0.659300000
6	-4.666943000	-0.852205000	-0.299340000
6	-6.006055000	-0.655190000	-0.067387000
6	-6.625075000	0.631274000	-0.173099000
6	-5.800140000	1.747550000	-0.515940000
6	-2.248114000	1.883278000	-1.151111000
6	-2.450237000	0.409999000	-0.904062000
1	-4.242592000	-1.842852000	-0.235941000
1	-6.615894000	-1.511790000	0.201053000
1	-6.218201000	2.743515000	-0.591805000
6	-1.397427000	-0.531885000	-0.978342000
6	0.006494000	-0.375199000	-0.886944000
6	-1.631342000	-2.001018000	-1.251301000
6	0.615635000	-1.670308000	-1.076967000
6	0.876613000	0.711232000	-0.593003000
6	1.965465000	-1.885401000	-1.008568000
6	2.230441000	0.506054000	-0.513378000
1	0.466140000	1.701443000	-0.464097000
6	2.828384000	-0.780840000	-0.720935000
1	2.369618000	-2.879916000	-1.148916000
1	2.872372000	1.355606000	-0.305452000
8	-2.678665000	-2.604008000	-1.436097000
8	-1.229663000	2.499923000	-1.429476000
7	-0.379210000	-2.604965000	-1.306996000
7	-3.501878000	2.484527000	-1.049535000
6	-3.718954000	3.902691000	-1.243668000
1	-4.412083000	4.082453000	-2.072425000
1	-4.118506000	4.366846000	-0.335275000
1	-2.752080000	4.347455000	-1.480425000
6	-0.186962000	-4.015945000	-1.570728000
1	0.411921000	-4.165653000	-2.475204000
1	0.308996000	-4.508326000	-0.727258000
1	-1.174160000	-4.455261000	-1.715500000
6	-8.011727000	0.801503000	0.060243000
6	-8.768319000	1.998086000	-0.008427000
16	-9.073915000	-0.534490000	0.500267000
6	-10.105744000	1.847900000	0.274001000
1	-8.325441000	2.952208000	-0.264570000
6	-10.495406000	0.515644000	0.585799000
1	-10.807960000	2.671372000	0.261176000
6	4.227682000	-0.964920000	-0.632642000
6	4.972745000	-2.141127000	-0.897569000
16	5.320993000	0.335132000	-0.164520000
6	6.327855000	-2.007026000	-0.729575000

1	4.511196000	-3.063830000	-1.225401000
6	6.738179000	-0.699546000	-0.318434000
1	7.037939000	-2.803936000	-0.905311000
6	8.035749000	-0.342475000	0.042377000
6	8.646856000	0.904883000	0.389482000
6	10.260657000	-0.633115000	1.327311000
6	9.841657000	0.704147000	1.259549000
6	11.367590000	-1.060308000	2.043148000
6	10.584086000	1.650228000	1.982137000
6	12.094372000	-0.101500000	2.751237000
1	11.648235000	-2.108136000	2.056125000
6	11.695403000	1.237078000	2.719343000
1	10.306272000	2.694337000	1.989487000
1	12.963348000	-0.398336000	3.329573000
1	12.256474000	1.978266000	3.279627000
6	8.251497000	2.147494000	-0.117527000
6	8.747073000	3.397920000	0.354608000
7	9.108769000	4.444707000	0.719947000
6	7.410158000	2.282529000	-1.258713000
7	6.761810000	2.437742000	-2.215385000
16	9.195168000	-1.700352000	0.382310000
8	8.581343000	-2.711087000	1.258260000
8	9.849462000	-2.154336000	-0.855779000
6	-11.771495000	0.038727000	0.915067000
6	-12.007187000	-1.354583000	1.208403000
6	-12.906584000	0.931075000	0.973839000
6	-13.240738000	-1.819902000	1.528405000
1	-11.168848000	-2.045165000	1.170043000
6	-14.147838000	0.485012000	1.291939000
1	-12.759447000	1.984040000	0.757710000
6	-14.409165000	-0.929261000	1.594531000
1	-13.414761000	-2.868210000	1.748408000
1	-14.999163000	1.156620000	1.335722000
8	-15.535935000	-1.343957000	1.885437000

S2TIIDTS9-CS E=-3428.556892 Hartree

6	3.617271000	-1.511673000	-0.801873000
6	2.999739000	-0.220599000	-0.620735000
6	3.852166000	0.847986000	-0.229434000
6	5.196567000	0.630495000	-0.055695000
6	5.804450000	-0.651097000	-0.255214000
6	4.956982000	-1.739293000	-0.636959000

6	1.385673000	-1.816075000	-1.159552000
6	1.605452000	-0.363773000	-0.822820000
1	3.436520000	1.835961000	-0.097284000
1	5.822890000	1.466714000	0.238179000
1	5.364812000	-2.731736000	-0.784695000
6	0.553714000	0.587173000	-0.794660000
6	-0.849104000	0.422449000	-0.651644000
6	0.780809000	2.059256000	-0.976003000
6	-1.464116000	1.725500000	-0.727416000
6	-1.708484000	-0.678129000	-0.392079000
6	-2.810086000	1.935043000	-0.588260000
6	-3.059938000	-0.479265000	-0.245560000
1	-1.294703000	-1.674098000	-0.339214000
6	-3.665858000	0.813684000	-0.343518000
1	-3.215423000	2.937273000	-0.655819000
1	-3.690624000	-1.342016000	-0.053192000
8	1.818244000	2.684379000	-1.163083000
8	0.353931000	-2.411420000	-1.445165000
7	-0.475090000	2.669524000	-0.938268000
7	2.636416000	-2.430555000	-1.136528000
6	2.836704000	-3.832970000	-1.426263000
1	3.503763000	-3.965161000	-2.285303000
1	3.261333000	-4.357656000	-0.562835000
1	1.859409000	-4.256116000	-1.660719000
6	-0.666944000	4.093630000	-1.095312000
1	-1.301665000	4.312226000	-1.961433000
1	-1.123631000	4.532137000	-0.200514000
1	0.318156000	4.534992000	-1.250425000
6	7.195368000	-0.845147000	-0.077763000
6	7.942763000	-2.034138000	-0.244260000
16	8.285132000	0.456385000	0.413645000
6	9.291784000	-1.908963000	0.005216000
1	7.487023000	-2.968978000	-0.546674000
6	9.701520000	-0.603638000	0.387827000
1	9.987479000	-2.733581000	-0.081984000
6	-5.060484000	0.987802000	-0.200084000
6	-5.809207000	2.193395000	-0.272009000
16	-6.158795000	-0.365145000	0.112664000
6	-7.161199000	2.047427000	-0.089533000
1	-5.341754000	3.151817000	-0.458198000
6	-7.577737000	0.702996000	0.140738000
1	-7.862953000	2.873536000	-0.116147000
6	-8.855850000	0.241040000	0.355600000
16	-9.224424000	-1.459894000	0.627302000

16	-10.257599000	1.316129000	0.379171000
6	-10.971298000	-1.253624000	0.806528000
6	-11.458541000	0.056507000	0.689414000
6	-11.847371000	-2.313638000	1.051740000
6	-12.825533000	0.314664000	0.816922000
6	-13.210479000	-2.051670000	1.178291000
1	-11.469514000	-3.326941000	1.142071000
6	-13.696258000	-0.745883000	1.061618000
1	-13.202752000	1.328189000	0.726310000
1	-13.895675000	-2.871157000	1.368769000
1	-14.758995000	-0.550882000	1.161484000
6	10.993220000	-0.153093000	0.707624000
6	11.250864000	1.214008000	1.080292000
6	12.122942000	-1.048947000	0.675951000
6	12.499120000	1.652126000	1.391260000
1	10.417728000	1.911848000	1.111854000
6	13.378640000	-0.629957000	0.983564000
1	11.963325000	-2.086181000	0.398527000
6	13.662634000	0.757502000	1.366401000
1	12.684561000	2.684396000	1.671004000
1	14.224404000	-1.309952000	0.957681000
8	14.803901000	1.147830000	1.648696000

S2TIIDTS10-CS E=-3274.898293 Hartree

6	2.529835000	-1.525747000	-0.695934000
6	1.881926000	-0.245064000	-0.549570000
6	2.708847000	0.855640000	-0.201486000
6	4.061777000	0.678770000	-0.039043000
6	4.700607000	-0.590552000	-0.206935000
6	3.877653000	-1.712863000	-0.541759000
6	0.299052000	-1.894703000	-1.013081000
6	0.486208000	-0.432652000	-0.732649000
1	2.270041000	1.836330000	-0.093563000
1	4.667200000	1.541660000	0.221837000
1	4.308495000	-2.699067000	-0.664824000
6	-0.587672000	0.493206000	-0.721596000
6	-1.982159000	0.304791000	-0.559946000
6	-0.396904000	1.969400000	-0.957403000
6	-2.627157000	1.590334000	-0.669354000
6	-2.816064000	-0.806527000	-0.258430000
6	-3.975119000	1.775790000	-0.519073000
6	-4.168720000	-0.631951000	-0.100239000

1	-2.379306000	-1.791281000	-0.182242000
6	-4.803412000	0.645628000	-0.228295000
1	-4.403927000	2.766177000	-0.610539000
1	-4.780250000	-1.499964000	0.124459000
8	0.625454000	2.606181000	-1.180750000
8	-0.718677000	-2.530568000	-1.262107000
7	-1.662505000	2.551810000	-0.921577000
7	1.568625000	-2.476793000	-0.988056000
6	1.798264000	-3.882926000	-1.232094000
1	2.454779000	-4.030413000	-2.097008000
1	2.248108000	-4.367688000	-0.357921000
1	0.827414000	-4.335982000	-1.435748000
6	-1.891392000	3.965205000	-1.123325000
1	-2.544366000	4.138033000	-1.985966000
1	-2.345862000	4.421969000	-0.236788000
1	-0.920342000	4.425447000	-1.308699000
6	6.096372000	-0.741854000	-0.044682000
6	6.876071000	-1.921315000	-0.178402000
16	7.154469000	0.613053000	0.380140000
6	8.220745000	-1.755441000	0.043397000
1	6.436916000	-2.876269000	-0.437178000
6	8.597956000	-0.420687000	0.369926000
1	8.943318000	-2.561363000	-0.021509000
6	-6.202144000	0.795571000	-0.069097000
6	-6.974443000	1.975682000	-0.171569000
16	-7.269977000	-0.560849000	0.308803000
6	-8.325023000	1.803142000	0.038817000
1	-6.535319000	2.939104000	-0.399773000
6	-8.710817000	0.465897000	0.323022000
1	-9.038531000	2.615734000	-0.008009000
6	9.859748000	0.058294000	0.643653000
16	10.191135000	1.747077000	1.036350000
16	11.299997000	-0.969666000	0.632461000
6	11.923069000	1.540063000	1.233250000
6	12.423831000	0.311470000	1.050528000
1	13.469542000	0.044911000	1.140435000
1	12.502528000	2.417065000	1.493175000
6	-9.997663000	-0.034840000	0.582589000
6	-10.229900000	-1.429840000	0.854804000
6	-11.147693000	0.835251000	0.587597000
6	-11.473377000	-1.916525000	1.107430000
1	-9.381072000	-2.109242000	0.856543000
6	-12.398987000	0.367742000	0.838120000
1	-11.007456000	1.892563000	0.385769000

6	-12.657307000	-1.048879000	1.118500000
1	-11.639567000	-2.969614000	1.311430000
1	-13.260124000	1.028668000	0.840484000
8	-13.794414000	-1.483461000	1.348231000

S2TIIDTS1-OS E=-2586.808548 Hartree

6	-1.904507000	1.583528000	-0.483267000
6	-1.268077000	0.308459000	-0.436671000
6	-2.098591000	-0.815067000	-0.280134000
6	-3.476283000	-0.658349000	-0.202580000
6	-4.094313000	0.609443000	-0.273806000
6	-3.271880000	1.753853000	-0.410290000
6	0.329501000	2.042522000	-0.570354000
6	0.170097000	0.532501000	-0.487232000
1	-1.664626000	-1.801906000	-0.245807000
1	-4.091609000	-1.547347000	-0.109743000
1	-3.702082000	2.747828000	-0.425907000
6	1.245949000	-0.341918000	-0.506392000
6	2.678465000	-0.127261000	-0.350869000
6	1.097086000	-1.830386000	-0.765047000
6	3.322786000	-1.391837000	-0.504567000
6	3.494288000	0.970874000	-0.025288000
6	4.683790000	-1.571475000	-0.380620000
6	4.865215000	0.804606000	0.108879000
1	3.054615000	1.947887000	0.098396000
6	5.495474000	-0.449604000	-0.071164000
1	5.116525000	-2.556649000	-0.502025000
1	5.465947000	1.676370000	0.347541000
8	0.093122000	-2.492841000	-0.984203000
8	1.343579000	2.719394000	-0.661431000
7	2.374071000	-2.370653000	-0.766781000
7	-0.945263000	2.583839000	-0.579439000
6	-1.202230000	4.006004000	-0.670906000
1	-1.800204000	4.236893000	-1.558876000
1	-1.729896000	4.366434000	0.218849000
1	-0.236638000	4.506180000	-0.745676000
6	2.640061000	-3.774354000	-1.002580000
1	3.283166000	-3.907038000	-1.879094000
1	3.122428000	-4.232922000	-0.132433000
1	1.680929000	-4.260235000	-1.181782000
6	-5.536731000	0.756185000	-0.206558000
6	-6.306234000	1.873510000	-0.517408000

16	-6.576740000	-0.555511000	0.315666000
6	-7.683415000	1.685203000	-0.351000000
1	-5.878210000	2.798318000	-0.884508000
6	-8.035259000	0.408823000	0.099138000
1	-8.412605000	2.455808000	-0.566788000
6	6.924776000	-0.598746000	0.059194000
6	7.702745000	-1.744114000	-0.167664000
16	7.954303000	0.741521000	0.558168000
6	9.063073000	-1.565970000	0.043730000
1	7.277981000	-2.686077000	-0.491230000
6	9.397655000	-0.254940000	0.450138000
1	9.814209000	-2.335697000	-0.085913000
6	10.680373000	0.240407000	0.742288000
6	11.810117000	-0.615044000	0.641701000
7	12.720611000	-1.338612000	0.551093000
6	10.888378000	1.586071000	1.140856000
7	11.034523000	2.696888000	1.467006000
6	-9.340278000	-0.114343000	0.371477000
6	-10.501746000	0.715777000	0.240848000
6	-9.533553000	-1.472008000	0.781902000
6	-11.753798000	0.236482000	0.496897000
1	-10.380972000	1.750102000	-0.063666000
6	-10.777268000	-1.971607000	1.043151000
1	-8.667645000	-2.120684000	0.882883000
6	-11.974194000	-1.144681000	0.916731000
1	-12.632869000	0.865492000	0.399746000
1	-10.922369000	-3.001737000	1.352107000
8	-13.113391000	-1.590635000	1.152409000

S2TIIDTS3-OS E=-3154.665980 Hartree

6	-1.522485000	-1.507270000	0.268966000
6	-0.914385000	-0.224148000	0.156360000
6	-1.765733000	0.868678000	-0.069420000
6	-3.140981000	0.677263000	-0.152771000
6	-3.729268000	-0.596193000	-0.015366000
6	-2.886902000	-1.711550000	0.198214000
6	0.719321000	-1.912443000	0.424851000
6	0.533947000	-0.415083000	0.246331000
1	-1.352530000	1.859880000	-0.166939000
1	-3.770559000	1.539346000	-0.348785000
1	-3.301228000	-2.704152000	0.327418000
6	1.589755000	0.478053000	0.228100000
6	3.035541000	0.286340000	0.136648000

6	1.403809000	1.983369000	0.357486000
6	3.643820000	1.572648000	0.200251000
6	3.888147000	-0.813277000	-0.055402000
6	5.006534000	1.775981000	0.112706000
6	5.261656000	-0.623170000	-0.154935000
1	3.475779000	-1.807904000	-0.114271000
6	5.851077000	0.655305000	-0.067630000
1	5.419312000	2.773588000	0.201211000
1	5.891570000	-1.491061000	-0.320912000
8	0.380104000	2.638907000	0.488951000
8	1.742091000	-2.566427000	0.570547000
7	2.666704000	2.549309000	0.352019000
7	-0.545795000	-2.477617000	0.448454000
6	-0.776462000	-3.896231000	0.624371000
1	-1.378535000	-4.085081000	1.519544000
1	-1.288459000	-4.320068000	-0.246449000
1	0.197850000	-4.371546000	0.737763000
6	2.898125000	3.973115000	0.478097000
1	3.506879000	4.191861000	1.361836000
1	3.403954000	4.366882000	-0.410212000
1	1.924762000	4.452404000	0.582440000
6	-5.170170000	-0.781024000	-0.095310000
6	-5.878957000	-1.956093000	-0.315497000
16	-6.278217000	0.564589000	0.094344000
6	-7.271251000	-1.788187000	-0.344688000
1	-5.394994000	-2.910322000	-0.482580000
6	-7.680382000	-0.471211000	-0.143815000
1	-7.970124000	-2.598079000	-0.520423000
6	7.290220000	0.838309000	-0.164372000
6	7.997499000	2.013104000	-0.392985000
16	8.404001000	-0.503797000	0.008916000
6	9.388237000	1.844891000	-0.437724000
1	7.513795000	2.968989000	-0.553290000
6	9.809948000	0.527522000	-0.241996000
1	10.073672000	2.662105000	-0.623560000
6	-9.003635000	0.047733000	-0.113039000
6	-9.413329000	1.385459000	0.051062000
16	-10.431255000	-0.954265000	-0.284322000
1	-8.715914000	2.207723000	0.176414000
6	-11.431256000	0.510329000	-0.122517000
6	-12.833872000	0.470188000	-0.169619000
6	-13.520086000	-0.758263000	-0.352241000
7	-14.057802000	-1.782654000	-0.503575000
6	-13.597495000	1.659869000	-0.035222000

7	-14.252528000	2.618223000	0.071730000
7	-10.719897000	1.635295000	0.045962000
6	11.146551000	0.008607000	-0.225513000
6	11.406212000	-1.389217000	-0.064671000
6	12.271209000	0.884764000	-0.369845000
6	12.679174000	-1.884541000	-0.048060000
1	10.568120000	-2.072582000	0.042002000
6	13.551530000	0.410687000	-0.356281000
1	12.100348000	1.949757000	-0.487141000
6	13.839667000	-1.011163000	-0.193920000
1	12.874454000	-2.945279000	0.071870000
1	14.403385000	1.074512000	-0.463740000
8	15.005212000	-1.452751000	-0.180869000

S2TIIDTS4-OS E=-3120.689517 Hartree

6	-2.012784000	1.638150000	-0.600752000
6	-1.408658000	0.347799000	-0.534934000
6	-2.265408000	-0.747065000	-0.323166000
6	-3.634875000	-0.550305000	-0.211191000
6	-4.224066000	0.732444000	-0.302389000
6	-3.371223000	1.848943000	-0.496600000
6	0.230853000	2.031424000	-0.764914000
6	0.033585000	0.530932000	-0.632935000
1	-1.857679000	-1.744192000	-0.270608000
1	-4.268375000	-1.419379000	-0.067001000
1	-3.771785000	2.854290000	-0.539223000
6	1.084651000	-0.372446000	-0.654678000
6	2.528547000	-0.193956000	-0.546894000
6	0.888018000	-1.864058000	-0.859536000
6	3.131383000	-1.479039000	-0.675315000
6	3.383939000	0.888421000	-0.280543000
6	4.491311000	-1.694836000	-0.577693000
6	4.754897000	0.685916000	-0.177532000
1	2.976096000	1.882015000	-0.181662000
6	5.339857000	-0.589449000	-0.329925000
1	4.894787000	-2.697023000	-0.657638000
1	5.391275000	1.546890000	-0.000034000
8	-0.139407000	-2.505032000	-1.031575000
8	1.258954000	2.679430000	-0.903702000
7	2.148643000	-2.440113000	-0.875707000
7	-1.029106000	2.607591000	-0.754784000
6	-1.249717000	4.032379000	-0.881902000
1	-1.866021000	4.254493000	-1.759725000

1	-1.742597000	4.433871000	0.010434000
1	-0.273118000	4.502585000	-0.997811000
6	2.369416000	-3.857273000	-1.070524000
1	2.987593000	-4.037125000	-1.956656000
1	2.860221000	-4.301336000	-0.197435000
1	1.392961000	-4.321057000	-1.210984000
6	-5.654837000	0.915163000	-0.196385000
6	-6.388291000	2.087888000	-0.418835000
16	-6.725157000	-0.407707000	0.255418000
6	-7.757919000	1.941887000	-0.241062000
1	-5.931535000	3.022042000	-0.721415000
6	-8.146736000	0.635368000	0.133153000
1	-8.475698000	2.742352000	-0.378908000
6	6.776043000	-0.783994000	-0.235012000
6	7.525315000	-1.888941000	-0.626126000
16	7.832794000	0.442698000	0.438458000
6	8.901659000	-1.756808000	-0.402407000
1	7.084551000	-2.762152000	-1.091506000
6	9.272438000	-0.538825000	0.174778000
1	9.617114000	-2.524490000	-0.668979000
6	-9.437777000	0.180095000	0.384668000
6	-9.758786000	-1.193290000	0.763853000
16	-10.885383000	1.179016000	0.286014000
6	-11.936363000	-0.235261000	0.749416000
7	-11.142842000	-1.346052000	0.945498000
6	-11.739145000	-2.621791000	1.328081000
1	-12.444462000	-2.951972000	0.562212000
1	-10.925194000	-3.339333000	1.425905000
1	-12.269343000	-2.519259000	2.277497000
8	-13.137353000	-0.180269000	0.860717000
8	-8.952777000	-2.105401000	0.910283000
6	10.581618000	-0.080406000	0.532154000
6	10.798337000	1.229595000	1.066194000
6	11.724116000	-0.929626000	0.364912000
6	12.046060000	1.667372000	1.408174000
1	9.947467000	1.892740000	1.196960000
6	12.979699000	-0.511811000	0.700283000
1	11.585577000	-1.929808000	-0.032257000
6	13.223815000	0.820023000	1.246301000
1	12.208247000	2.662113000	1.810608000
1	13.843993000	-1.156266000	0.575252000
8	14.366725000	1.209794000	1.554948000

S2TIIDTS5-OS E=-2892.152355 Hartree

6	1.622673000	-1.647520000	-0.603589000
6	1.015825000	-0.356807000	-0.557022000
6	1.869084000	0.745071000	-0.369094000
6	3.239714000	0.555024000	-0.262631000
6	3.831833000	-0.728102000	-0.336598000
6	2.982670000	-1.851344000	-0.505763000
6	-0.620940000	-2.048807000	-0.743672000
6	-0.426634000	-0.545973000	-0.642751000
1	1.458118000	1.741462000	-0.331228000
1	3.871511000	1.428034000	-0.137466000
1	3.387229000	-2.855545000	-0.533218000
6	-1.479263000	0.354964000	-0.677411000
6	-2.920329000	0.176947000	-0.556811000
6	-1.286657000	1.843682000	-0.919879000
6	-3.526891000	1.457686000	-0.712664000
6	-3.771345000	-0.901278000	-0.258338000
6	-4.886387000	1.672343000	-0.612215000
6	-5.141426000	-0.699509000	-0.151814000
1	-3.360277000	-1.891103000	-0.137412000
6	-5.730690000	0.570923000	-0.332194000
1	-5.292878000	2.671099000	-0.715106000
1	-5.774361000	-1.557132000	0.051798000
8	-0.260801000	2.479867000	-1.113557000
8	-1.648248000	-2.701384000	-0.861456000
7	-2.547843000	2.416122000	-0.942481000
7	0.641189000	-2.621457000	-0.732818000
6	0.864854000	-4.048318000	-0.834726000
1	1.474579000	-4.285034000	-1.713190000
1	1.365525000	-4.431162000	0.061332000
1	-0.111238000	-4.523234000	-0.933986000
6	-2.773532000	3.828159000	-1.170192000
1	-3.396892000	3.984508000	-2.056986000
1	-3.260510000	4.291292000	-0.305076000
1	-1.799351000	4.291247000	-1.327290000
6	5.263808000	-0.903055000	-0.237935000
6	5.998476000	-2.076164000	-0.456313000
16	6.332283000	0.424519000	0.196676000
6	7.366711000	-1.916832000	-0.286897000
1	5.548048000	-3.016066000	-0.750197000
6	7.753761000	-0.606816000	0.075677000
1	8.075757000	-2.723004000	-0.427288000
6	-7.166105000	0.763649000	-0.233047000
6	-7.919191000	1.863208000	-0.633833000

16	-8.217705000	-0.457311000	0.458269000
6	-9.293770000	1.731219000	-0.402987000
1	-7.482416000	2.732428000	-1.110227000
6	-9.659689000	0.518863000	0.189885000
1	-10.011722000	2.494669000	-0.674724000
6	9.071122000	-0.149421000	0.318809000
6	10.193690000	-1.003052000	0.223791000
6	9.291894000	1.263544000	0.683946000
6	11.470253000	-0.550562000	0.458073000
1	10.059181000	-2.045788000	-0.039973000
6	11.739861000	0.852485000	0.822210000
6	12.586552000	-1.428722000	0.356308000
7	13.469969000	-2.181434000	0.261988000
8	8.365899000	2.067914000	0.791329000
8	12.865065000	1.279632000	1.034872000
7	10.603035000	1.676595000	0.910218000
6	10.790814000	3.087402000	1.270225000
1	10.403660000	3.726006000	0.473832000
1	10.241962000	3.310548000	2.187276000
1	11.856113000	3.251242000	1.410603000
6	-10.966336000	0.062566000	0.558319000
6	-11.177550000	-1.241001000	1.110568000
6	-12.111117000	0.907592000	0.383927000
6	-12.422750000	-1.676892000	1.463128000
1	-10.324674000	-1.900372000	1.246897000
6	-13.364319000	0.491649000	0.729649000
1	-11.976215000	1.902535000	-0.027206000
6	-13.602890000	-0.833691000	1.294347000
1	-12.581572000	-2.666408000	1.879418000
1	-14.230692000	1.132197000	0.599482000
8	-14.743326000	-1.221680000	1.612506000

S2TIIDTS6-OS E=-3253.473747 Hartree

6	-1.239460000	1.688537000	-0.610541000
6	-0.643164000	0.391746000	-0.544492000
6	-1.506467000	-0.699725000	-0.330736000
6	-2.872497000	-0.494971000	-0.218256000
6	-3.456404000	0.794386000	-0.310908000
6	-2.595102000	1.907117000	-0.507470000
6	1.006798000	2.062200000	-0.778006000
6	0.796825000	0.564322000	-0.643863000
1	-1.103911000	-1.698846000	-0.276071000
1	-3.510705000	-1.358145000	-0.062548000

1	-2.990863000	2.913340000	-0.564034000
6	1.841222000	-0.349843000	-0.666246000
6	3.281826000	-0.184526000	-0.546625000
6	1.632881000	-1.838330000	-0.888699000
6	3.876660000	-1.473838000	-0.682491000
6	4.143112000	0.890214000	-0.262488000
6	5.233621000	-1.699745000	-0.576369000
6	5.510316000	0.676801000	-0.150128000
1	3.741212000	1.885734000	-0.157722000
6	6.088319000	-0.602296000	-0.310563000
1	5.630379000	-2.703729000	-0.665129000
1	6.150932000	1.531121000	0.043144000
8	0.600610000	-2.466005000	-1.076680000
8	2.040714000	2.699905000	-0.918117000
7	2.888453000	-2.425012000	-0.900386000
7	-0.248883000	2.648867000	-0.768769000
6	-0.458444000	4.075637000	-0.898574000
1	-1.071728000	4.300715000	-1.777589000
1	-0.949168000	4.481783000	-0.007317000
1	0.521831000	4.538127000	-1.014040000
6	3.099233000	-3.842182000	-1.108936000
1	3.722317000	-4.017241000	-1.992459000
1	3.579583000	-4.299269000	-0.236888000
1	2.120257000	-4.296591000	-1.261723000
6	-4.879814000	0.981547000	-0.203721000
6	-5.597066000	2.186736000	-0.313343000
16	-5.975018000	-0.365556000	0.098956000
6	-6.962993000	2.046296000	-0.163473000
1	-5.126844000	3.143551000	-0.504208000
6	-7.382554000	0.704767000	0.074741000
1	-7.682867000	2.848585000	-0.215678000
6	7.520604000	-0.806627000	-0.205040000
6	8.262589000	-1.927130000	-0.569397000
16	8.586114000	0.425199000	0.445820000
6	9.637852000	-1.802651000	-0.342793000
1	7.816691000	-2.807486000	-1.015860000
6	10.017457000	-0.575086000	0.210294000
1	10.347292000	-2.582715000	-0.588420000
6	-8.693616000	0.237817000	0.268954000
6	-9.833220000	1.154713000	0.245184000
6	-8.910272000	-1.183748000	0.496774000
6	-11.339612000	-0.778917000	0.667596000
8	-7.983796000	-1.995317000	0.528232000
7	-10.235727000	-1.614186000	0.683455000

6	-10.438523000	-3.054144000	0.910329000
1	-11.086021000	-3.462557000	0.133314000
1	-9.459281000	-3.523538000	0.884064000
1	-10.918742000	-3.211633000	1.877008000
7	-11.105674000	0.567675000	0.451519000
6	-12.259141000	1.482176000	0.429858000
1	-12.950757000	1.185364000	-0.359789000
1	-12.785706000	1.434562000	1.384002000
1	-11.872902000	2.481046000	0.250444000
8	-9.748298000	2.366064000	0.062147000
16	-12.886673000	-1.375817000	0.900225000
6	11.328489000	-0.121957000	0.563459000
6	11.554143000	1.195167000	1.077216000
6	12.464701000	-0.983365000	0.412511000
6	12.804086000	1.628268000	1.415340000
1	10.708180000	1.866827000	1.195574000
6	13.722424000	-0.570417000	0.744384000
1	12.319160000	-1.988331000	0.030366000
6	13.975599000	0.768456000	1.269915000
1	12.973607000	2.627811000	1.802464000
1	14.582030000	-1.223309000	0.631770000
8	15.120223000	1.153823000	1.575191000

S2TIIDTS7-OS E=-3007.404330 Hartree

6	1.064227000	-1.730858000	-0.917866000
6	0.480572000	-0.434758000	-0.788613000
6	1.357573000	0.645514000	-0.584682000
6	2.728122000	0.431297000	-0.536617000
6	3.293856000	-0.856444000	-0.687900000
6	2.423233000	-1.959328000	-0.878435000
6	-1.188939000	-2.092845000	-0.992640000
6	-0.967263000	-0.599264000	-0.828927000
1	0.964647000	1.645601000	-0.492628000
1	3.380942000	1.289072000	-0.412451000
1	2.813126000	-2.966659000	-0.958097000
6	-2.006524000	0.316545000	-0.780760000
6	-3.445241000	0.152457000	-0.616251000
6	-1.800035000	1.812900000	-0.955691000
6	-4.037123000	1.447564000	-0.687091000
6	-4.301841000	-0.927277000	-0.340256000
6	-5.388823000	1.675566000	-0.526990000
6	-5.664045000	-0.712257000	-0.174133000
1	-3.902169000	-1.927409000	-0.282916000

6	-6.239494000	0.573446000	-0.270637000
1	-5.783097000	2.683720000	-0.566037000
1	-6.302569000	-1.570155000	0.009995000
8	-0.772363000	2.444557000	-1.153131000
8	-2.230047000	-2.724661000	-1.102720000
7	-3.052531000	2.402749000	-0.904825000
7	0.063269000	-2.683423000	-1.054518000
6	0.260630000	-4.106856000	-1.231728000
1	0.834806000	-4.309696000	-2.141997000
1	0.787193000	-4.538872000	-0.373698000
1	-0.725746000	-4.562743000	-1.317510000
6	-3.264166000	3.827328000	-1.054750000
1	-3.916462000	4.035860000	-1.909409000
1	-3.712406000	4.253896000	-0.150749000
1	-2.289139000	4.284074000	-1.224699000
6	4.722797000	-1.062589000	-0.643726000
6	5.445202000	-2.198295000	-1.039015000
16	5.813962000	0.174039000	-0.056138000
6	6.817086000	-2.085289000	-0.875965000
1	4.970894000	-3.074171000	-1.464119000
6	7.232141000	-0.833740000	-0.350117000
1	7.538233000	-2.853417000	-1.115695000
6	-7.667414000	0.780915000	-0.110116000
6	-8.417424000	1.908166000	-0.431528000
16	-8.712074000	-0.456715000	0.561966000
6	-9.784769000	1.784248000	-0.156822000
1	-7.984728000	2.792687000	-0.882819000
6	-10.147697000	0.550590000	0.392215000
1	-10.500121000	2.569481000	-0.366216000
6	8.545952000	-0.505292000	0.027179000
6	9.559641000	-1.585039000	0.279533000
6	9.134625000	0.747608000	0.450708000
6	10.643823000	-0.947162000	1.063449000
6	10.374187000	0.425030000	1.214229000
6	11.766847000	-1.551310000	1.610312000
6	11.253978000	1.215484000	1.957687000
6	12.643874000	-0.756737000	2.352821000
1	11.938706000	-2.611904000	1.457512000
6	12.380201000	0.606411000	2.524641000
1	11.085226000	2.272427000	2.112284000
1	13.529991000	-1.195135000	2.801222000
1	13.063827000	1.212976000	3.110752000
8	9.508248000	-2.761807000	-0.048066000
6	8.748406000	2.033463000	0.089337000

6	7.823206000	2.325993000	-0.957136000
7	7.120629000	2.625657000	-1.837223000
6	9.358350000	3.204332000	0.634159000
7	9.819722000	4.180914000	1.072141000
6	-11.447103000	0.095515000	0.786861000
6	-11.658061000	-1.228448000	1.288231000
6	-12.584769000	0.962403000	0.691288000
6	-12.896349000	-1.663086000	1.665918000
1	-10.810710000	-1.904423000	1.364710000
6	-13.831005000	0.548079000	1.063249000
1	-12.449858000	1.972720000	0.319475000
6	-14.069148000	-0.797759000	1.577240000
1	-13.054882000	-2.668011000	2.043667000
1	-14.691841000	1.205232000	0.992543000
8	-15.203275000	-1.184456000	1.918993000

S2TIIDTS8-OS E=-3442.624511 Hartree

6	-4.508449000	1.505206000	-0.644660000
6	-3.898112000	0.217387000	-0.614447000
6	-4.738612000	-0.882618000	-0.371606000
6	-6.103762000	-0.692563000	-0.198205000
6	-6.697422000	0.586989000	-0.254532000
6	-5.863156000	1.708697000	-0.476837000
6	-2.277513000	1.912532000	-0.902503000
6	-2.461578000	0.407326000	-0.775054000
1	-4.324518000	-1.878121000	-0.345172000
1	-6.729789000	-1.564851000	-0.040847000
1	-6.272134000	2.711707000	-0.483688000
6	-1.409833000	-0.490356000	-0.854006000
6	0.037334000	-0.305284000	-0.815591000
6	-1.609556000	-1.981973000	-1.059526000
6	0.638124000	-1.588065000	-0.986597000
6	0.898498000	0.781017000	-0.583844000
6	2.001365000	-1.797381000	-0.961211000
6	2.273164000	0.585804000	-0.549783000
1	0.491422000	1.771914000	-0.460097000
6	2.854401000	-0.687787000	-0.742614000
1	2.406976000	-2.795944000	-1.068955000
1	2.914739000	1.449175000	-0.406871000
8	-2.641380000	-2.626332000	-1.181764000
8	-1.259360000	2.564996000	-1.079550000

7	-0.348822000	-2.551120000	-1.145552000
7	-3.538158000	2.481404000	-0.832798000
6	-3.771416000	3.906822000	-0.937277000
1	-4.427860000	4.132227000	-1.784386000
1	-4.224922000	4.297446000	-0.019802000
1	-2.803706000	4.383560000	-1.093391000
6	-0.130655000	-3.966145000	-1.363632000
1	0.441235000	-4.134311000	-2.282296000
1	0.407305000	-4.413479000	-0.520759000
1	-1.110355000	-4.434674000	-1.456957000
6	-8.128358000	0.769115000	-0.087015000
6	-8.895434000	1.891958000	-0.381390000
16	-9.152591000	-0.499155000	0.558041000
6	-10.260457000	1.741062000	-0.107479000
1	-8.476832000	2.792732000	-0.813440000
6	-10.603362000	0.489941000	0.413661000
1	-10.988025000	2.519876000	-0.297831000
6	4.288881000	-0.875753000	-0.713446000
6	5.025281000	-1.964912000	-1.195222000
16	5.356405000	0.325724000	-0.024328000
6	6.397128000	-1.840410000	-1.021118000
1	4.565171000	-2.808246000	-1.694469000
6	6.786133000	-0.631937000	-0.399090000
1	7.121410000	-2.569559000	-1.362497000
6	8.094534000	-0.314299000	0.006823000
6	8.734622000	0.891323000	0.403740000
6	10.366817000	-0.720750000	1.181127000
6	9.979018000	0.627817000	1.186370000
6	11.510942000	-1.198833000	1.799844000
6	10.798144000	1.529788000	1.881136000
6	12.313761000	-0.282474000	2.481398000
1	11.764358000	-2.252840000	1.758209000
6	11.949235000	1.065319000	2.520843000
1	10.552948000	2.580204000	1.941076000
1	13.214784000	-0.619571000	2.983438000
1	12.569851000	1.774191000	3.059661000
6	8.324407000	2.172741000	-0.005702000
6	8.856602000	3.386175000	0.515464000
7	9.245119000	4.407545000	0.923947000
6	7.422195000	2.391377000	-1.086095000
7	6.727184000	2.628873000	-1.991742000
16	9.197001000	-1.731390000	0.301368000
8	8.564186000	-2.691996000	1.216972000
8	9.749875000	-2.229018000	-0.969139000

6	-11.895230000	0.006156000	0.800205000
6	-12.085052000	-1.332330000	1.270268000
6	-13.045628000	0.858203000	0.727653000
6	-13.315859000	-1.794241000	1.640135000
1	-11.227612000	-1.997258000	1.328780000
6	-14.284717000	0.416661000	1.092281000
1	-12.926573000	1.878965000	0.379793000
6	-14.501409000	-0.944435000	1.574515000
1	-13.458625000	-2.810089000	1.994166000
1	-15.155398000	1.062372000	1.039130000
8	-15.628852000	-1.355954000	1.909359000

S2TIIDTS9-OS E=-3428.565678 Hartree

6	-3.637096000	-1.497988000	0.653015000
6	-3.042527000	-0.206062000	0.539796000
6	-3.906608000	0.871206000	0.275265000
6	-5.273851000	0.657595000	0.158691000
6	-5.851249000	-0.624452000	0.295708000
6	-4.993747000	-1.724382000	0.542638000
6	-1.389923000	-1.857331000	0.851968000
6	-1.601264000	-0.372520000	0.657483000
1	-3.506702000	1.869430000	0.189373000
1	-5.915693000	1.514557000	-0.019394000
1	-5.388433000	-2.730786000	0.614161000
6	-0.556340000	0.547062000	0.649010000
6	0.879598000	0.382146000	0.541582000
6	-0.771257000	2.039530000	0.811691000
6	1.475837000	1.678233000	0.623638000
6	1.749461000	-0.702328000	0.311831000
6	2.829421000	1.903874000	0.516524000
6	3.113494000	-0.490888000	0.196570000
1	1.349562000	-1.702277000	0.247024000
6	3.696025000	0.797610000	0.301515000
1	3.220618000	2.911525000	0.585918000
1	3.753291000	-1.351419000	0.027586000
8	-1.805673000	2.673947000	0.971688000
8	-0.357373000	-2.492586000	1.026757000
7	0.482500000	2.633032000	0.801551000
7	-2.646203000	-2.449219000	0.854079000
6	-2.851566000	-3.869306000	1.036166000
1	-3.473813000	-4.064778000	1.916434000
1	-3.331156000	-4.313540000	0.156610000
1	-1.870168000	-4.321870000	1.179869000

6	0.685314000	4.057068000	0.953333000
1	1.303482000	4.272565000	1.831791000
1	1.168276000	4.482040000	0.066189000
1	-0.297054000	4.511799000	1.082820000
6	-7.282390000	-0.829319000	0.186034000
6	-8.023590000	-1.958847000	0.523823000
16	-8.352089000	0.415132000	-0.437119000
6	-9.399001000	-1.832195000	0.299916000
1	-7.575650000	-2.848389000	0.949691000
6	-9.782847000	-0.593159000	-0.224574000
1	-10.106741000	-2.619456000	0.527336000
6	5.115241000	0.994978000	0.191687000
6	5.844669000	2.188949000	0.294387000
16	6.221547000	-0.350070000	-0.111983000
6	7.216255000	2.051712000	0.140750000
1	5.371455000	3.144746000	0.483154000
6	7.634962000	0.718980000	-0.093702000
1	7.912873000	2.880344000	0.194980000
6	8.925764000	0.250326000	-0.286862000
16	9.299270000	-1.449892000	-0.568119000
16	10.325910000	1.329320000	-0.267959000
6	11.049845000	-1.238100000	-0.704428000
6	11.533314000	0.071499000	-0.562807000
6	11.933230000	-2.294274000	-0.940060000
6	12.902964000	0.330368000	-0.656284000
6	13.299023000	-2.031168000	-1.032610000
1	11.558219000	-3.306855000	-1.049337000
6	13.780880000	-0.726601000	-0.891534000
1	13.277000000	1.343291000	-0.546699000
1	13.988801000	-2.848652000	-1.215537000
1	14.845497000	-0.529565000	-0.964775000
6	-11.094168000	-0.135249000	-0.566180000
6	-11.324799000	1.191744000	-1.051111000
6	-12.229660000	-1.000510000	-0.433541000
6	-12.576216000	1.629374000	-1.378739000
1	-10.480427000	1.867843000	-1.155882000
6	-13.488611000	-0.582856000	-0.755400000
1	-12.082312000	-2.013384000	-0.073041000
6	-13.746612000	0.765820000	-1.251728000
1	-12.747137000	2.637029000	-1.743924000
1	-14.346358000	-1.240492000	-0.655740000
8	-14.892901000	1.155457000	-1.547934000

S2TIIDTS10-OS E=-3274.907139 Hartree

6	-2.542696000	-1.493530000	0.592136000
6	-1.914096000	-0.218118000	0.450346000
6	-2.753587000	0.871627000	0.145237000
6	-4.120148000	0.685526000	0.016184000
6	-4.735172000	-0.581338000	0.180606000
6	-3.899269000	-1.693567000	0.472171000
6	-0.308599000	-1.895552000	0.842240000
6	-0.484587000	-0.409851000	0.593765000
1	-2.328723000	1.856993000	0.033120000
1	-4.735949000	1.549927000	-0.211990000
1	-4.315722000	-2.686538000	0.589734000
6	0.581896000	0.484398000	0.571479000
6	2.020710000	0.278399000	0.491014000
6	0.402981000	1.982135000	0.679323000
6	2.644118000	1.560543000	0.544195000
6	2.863245000	-0.831491000	0.303014000
6	4.007604000	1.749130000	0.447701000
6	4.237144000	-0.656269000	0.201160000
1	2.441087000	-1.823486000	0.264654000
6	4.842668000	0.617737000	0.278353000
1	4.425100000	2.748594000	0.470840000
1	4.861313000	-1.536377000	0.083264000
8	-0.616892000	2.650006000	0.798439000
8	0.707206000	-2.543934000	1.056483000
7	1.672950000	2.544086000	0.673104000
7	-1.575899000	-2.459692000	0.840878000
6	-1.815465000	-3.868043000	1.066995000
1	-2.453787000	-4.020270000	1.944293000
1	-2.293009000	-4.330366000	0.195730000
1	-0.846671000	-4.337342000	1.239613000
6	1.909181000	3.966982000	0.780260000
1	2.519940000	4.196887000	1.660263000
1	2.415212000	4.350279000	-0.113047000
1	0.936535000	4.449378000	0.879590000
6	-6.156800000	-0.751972000	0.055173000
6	-6.916540000	-1.920744000	0.206341000
16	-7.225564000	0.600516000	-0.338799000
6	-8.282355000	-1.759503000	0.020006000
1	-6.470254000	-2.876276000	0.453187000
6	-8.663754000	-0.432646000	-0.291148000
1	-8.999669000	-2.567837000	0.104185000
6	6.280068000	0.783283000	0.185075000
6	7.042252000	1.911379000	0.477791000

16	7.330137000	-0.516409000	-0.352846000
6	8.417944000	1.741353000	0.286519000
1	6.608465000	2.831920000	0.848920000
6	8.780906000	0.468135000	-0.165967000
1	9.140406000	2.522754000	0.486164000
6	-9.939861000	0.057395000	-0.532992000
16	-10.278209000	1.749765000	-0.911109000
16	-11.378046000	-0.974306000	-0.486945000
6	-12.015243000	1.540177000	-1.061957000
6	-12.511022000	0.310846000	-0.870414000
1	-13.559351000	0.046877000	-0.934001000
1	-12.603062000	2.416992000	-1.303224000
6	10.086568000	-0.037152000	-0.459108000
6	10.293541000	-1.392169000	-0.871810000
6	11.240200000	0.807037000	-0.349145000
6	11.539565000	-1.874918000	-1.153457000
1	9.435041000	-2.052917000	-0.958093000
6	12.494126000	0.344320000	-0.625852000
1	11.111155000	1.840110000	-0.043047000
6	12.728097000	-1.033506000	-1.048476000
1	11.692413000	-2.903586000	-1.463975000
1	13.365653000	0.986038000	-0.543470000
8	13.869649000	-1.464296000	-1.303163000

S2TIIDTS1-T1 E=-2586.807293 Hartree

6	-1.912305000	1.561792000	-0.512696000
6	-1.274609000	0.290530000	-0.463192000
6	-2.101198000	-0.834364000	-0.317490000
6	-3.482857000	-0.682195000	-0.253864000
6	-4.100098000	0.582293000	-0.326811000
6	-3.282401000	1.728580000	-0.450717000
6	0.320258000	2.035220000	-0.576458000
6	0.169982000	0.521536000	-0.501025000
1	-1.664845000	-1.819846000	-0.280075000
1	-4.097894000	-1.572666000	-0.174459000
1	-3.717805000	2.720556000	-0.462045000
6	1.247183000	-0.342762000	-0.514395000
6	2.687154000	-0.118237000	-0.369663000
6	1.107222000	-1.837068000	-0.750510000
6	3.332928000	-1.380175000	-0.513359000
6	3.498877000	0.984707000	-0.062490000
6	4.697103000	-1.554153000	-0.395707000
6	4.874321000	0.825175000	0.063814000

1	3.056943000	1.961516000	0.052799000
6	5.504128000	-0.426747000	-0.106174000
1	5.133019000	-2.540549000	-0.495523000
1	5.475239000	1.703281000	0.277532000
8	0.106876000	-2.510362000	-0.951786000
8	1.330703000	2.718919000	-0.653742000
7	2.387165000	-2.368101000	-0.754540000
7	-0.956472000	2.567887000	-0.596383000
6	-1.221471000	3.988984000	-0.683079000
1	-1.814344000	4.219902000	-1.574413000
1	-1.758460000	4.341561000	0.204205000
1	-0.258660000	4.495743000	-0.748047000
6	2.660638000	-3.773396000	-0.971887000
1	3.300481000	-3.914044000	-1.849535000
1	3.150272000	-4.216553000	-0.097826000
1	1.703790000	-4.267778000	-1.139434000
6	-5.549165000	0.728341000	-0.275456000
6	-6.319990000	1.806899000	-0.685346000
16	-6.579364000	-0.536159000	0.362437000
6	-7.700492000	1.625266000	-0.502924000
1	-5.894471000	2.694500000	-1.137852000
6	-8.042796000	0.395156000	0.058218000
1	-8.434347000	2.367615000	-0.790422000
6	6.940553000	-0.572541000	0.013779000
6	7.730000000	-1.675628000	-0.331761000
16	7.947592000	0.718339000	0.658176000
6	9.090735000	-1.502125000	-0.099650000
1	7.316979000	-2.577930000	-0.765248000
6	9.405508000	-0.239577000	0.444264000
1	9.852715000	-2.241762000	-0.313872000
6	10.682410000	0.241965000	0.791662000
6	11.824303000	-0.582006000	0.607275000
7	12.745534000	-1.279242000	0.445313000
6	10.870265000	1.541339000	1.328177000
7	11.000414000	2.614356000	1.768266000
6	-9.348296000	-0.113936000	0.377111000
6	-10.512075000	0.699620000	0.193207000
6	-9.532377000	-1.437320000	0.885728000
6	-11.761901000	0.234885000	0.490360000
1	-10.396894000	1.710311000	-0.184161000
6	-10.773704000	-1.922202000	1.189713000
1	-8.663381000	-2.074076000	1.027499000
6	-11.973387000	-1.111974000	1.009852000
1	-12.643959000	0.852207000	0.353406000

1	-10.912363000	-2.927903000	1.573129000
8	-13.110934000	-1.544625000	1.283641000

S2TIIDTS3- T1 E=-3154.665448 Hartree

6	-1.525417000	-1.502418000	0.221601000
6	-0.917536000	-0.220383000	0.109270000
6	-1.767861000	0.872928000	-0.111359000
6	-3.144699000	0.682734000	-0.191278000
6	-3.731864000	-0.589767000	-0.054388000
6	-2.890986000	-1.705725000	0.155143000
6	0.716366000	-1.912306000	0.371268000
6	0.533933000	-0.413640000	0.196105000
1	-1.354284000	1.863875000	-0.208944000
1	-3.774580000	1.545012000	-0.385419000
1	-3.306935000	-2.697548000	0.285797000
6	1.589897000	0.475956000	0.176791000
6	3.038809000	0.281917000	0.091970000
6	1.406508000	1.983391000	0.295414000
6	3.646670000	1.567431000	0.150069000
6	3.890965000	-0.818854000	-0.087898000
6	5.010650000	1.769691000	0.068350000
6	5.266158000	-0.630086000	-0.182628000
1	3.478451000	-1.813561000	-0.142675000
6	5.854264000	0.647881000	-0.101103000
1	5.424899000	2.766960000	0.154770000
1	5.896772000	-1.498774000	-0.341568000
8	0.383615000	2.641871000	0.417710000
8	1.737866000	-2.569170000	0.512473000
7	2.669962000	2.546639000	0.291383000
7	-0.549531000	-2.474691000	0.396984000
6	-0.782556000	-3.893215000	0.570609000
1	-1.382605000	-4.082626000	1.467018000
1	-1.297952000	-4.314053000	-0.299657000
1	0.191055000	-4.370802000	0.680253000
6	2.903561000	3.970857000	0.408876000
1	3.508899000	4.194284000	1.293777000
1	3.414276000	4.357421000	-0.479787000
1	1.930754000	4.452831000	0.505562000
6	-5.175313000	-0.775113000	-0.131812000
6	-5.882014000	-1.940949000	-0.394216000
16	-6.282619000	0.559088000	0.121458000
6	-7.276352000	-1.774268000	-0.405826000

1	-5.396599000	-2.885784000	-0.605091000
6	-7.684876000	-0.468423000	-0.148454000
1	-7.975202000	-2.577620000	-0.609601000
6	7.296138000	0.831299000	-0.193691000
6	8.000941000	1.995171000	-0.470029000
16	8.410124000	-0.497939000	0.052808000
6	9.394251000	1.828385000	-0.493938000
1	7.515423000	2.940277000	-0.681247000
6	9.815859000	0.523944000	-0.233361000
1	10.079616000	2.637493000	-0.712764000
6	-9.009606000	0.048759000	-0.086546000
6	-9.418659000	1.377640000	0.134512000
16	-10.436500000	-0.947165000	-0.287521000
1	-8.721426000	2.195194000	0.287858000
6	-11.436981000	0.508029000	-0.059256000
6	-12.840772000	0.467121000	-0.097655000
6	-13.526629000	-0.753917000	-0.324686000
7	-14.064372000	-1.772126000	-0.513319000
6	-13.604897000	1.648946000	0.090384000
7	-14.260383000	2.601177000	0.240890000
7	-10.726491000	1.625601000	0.149229000
6	11.154862000	0.007818000	-0.180412000
6	11.414216000	-1.381506000	0.037510000
6	12.279014000	0.879801000	-0.344978000
6	12.688178000	-1.873547000	0.088450000
1	10.576000000	-2.062072000	0.159817000
6	13.560337000	0.409016000	-0.297869000
1	12.107854000	1.939267000	-0.504391000
6	13.848349000	-1.004408000	-0.077348000
1	12.883457000	-2.928522000	0.251458000
1	14.412330000	1.070057000	-0.420366000
8	15.015015000	-1.442999000	-0.033237000

S2TIIDTS4-T1 E=-3120.688433 Hartree

6	-2.022283000	1.630913000	-0.608946000
6	-1.415677000	0.343531000	-0.564761000
6	-2.268117000	-0.757431000	-0.384878000
6	-3.642032000	-0.568362000	-0.283054000
6	-4.231793000	0.712088000	-0.352622000
6	-3.384012000	1.834930000	-0.512902000
6	0.221051000	2.042606000	-0.739134000
6	0.032929000	0.536290000	-0.645533000
1	-1.857342000	-1.753870000	-0.349144000

1	-4.275058000	-1.442549000	-0.171369000
1	-3.789667000	2.839216000	-0.528416000
6	1.086296000	-0.356570000	-0.679563000
6	2.536117000	-0.171100000	-0.576085000
6	0.899259000	-1.849389000	-0.896914000
6	3.141693000	-1.450446000	-0.721567000
6	3.386515000	0.910734000	-0.303078000
6	4.504441000	-1.662219000	-0.632809000
6	4.761445000	0.713246000	-0.211041000
1	2.975246000	1.901186000	-0.189784000
6	5.347410000	-0.556454000	-0.379771000
1	4.913671000	-2.661556000	-0.720961000
1	5.396616000	1.574848000	-0.032378000
8	-0.124375000	-2.496384000	-1.067817000
8	1.245886000	2.700774000	-0.849968000
7	2.162868000	-2.415722000	-0.926020000
7	-1.041937000	2.609472000	-0.729716000
6	-1.270728000	4.035638000	-0.823925000
1	-1.880475000	4.274899000	-1.701786000
1	-1.774834000	4.411601000	0.073215000
1	-0.296381000	4.515020000	-0.918907000
6	2.392289000	-3.829716000	-1.134165000
1	3.007298000	-3.997320000	-2.024863000
1	2.890906000	-4.277500000	-0.267468000
1	1.418471000	-4.299229000	-1.273567000
6	-5.669336000	0.890971000	-0.258761000
6	-6.410379000	2.033492000	-0.572008000
16	-6.723077000	-0.401423000	0.298422000
6	-7.781951000	1.887510000	-0.382518000
1	-5.961296000	2.941641000	-0.955092000
6	-8.155627000	0.612902000	0.092982000
1	-8.507946000	2.666223000	-0.586291000
6	6.789842000	-0.748916000	-0.297865000
6	7.545999000	-1.805759000	-0.784584000
16	7.830653000	0.418608000	0.490378000
6	8.923833000	-1.682682000	-0.542537000
1	7.112615000	-2.633352000	-1.333170000
6	9.279510000	-0.521718000	0.143819000
1	9.647402000	-2.415384000	-0.877211000
6	-9.443776000	0.162489000	0.381897000
6	-9.750028000	-1.180109000	0.866056000
16	-10.900337000	1.135661000	0.207838000
6	-11.937809000	-0.249595000	0.779349000
7	-11.132962000	-1.333250000	1.059723000

6	-11.715542000	-2.582044000	1.539853000
1	-12.417999000	-2.977232000	0.802673000
1	-10.893987000	-3.281457000	1.690952000
1	-12.245952000	-2.412763000	2.479560000
8	-13.139344000	-0.197749000	0.886462000
8	-8.934701000	-2.070022000	1.082504000
6	10.586006000	-0.083405000	0.549495000
6	10.788459000	1.181422000	1.184615000
6	11.733684000	-0.910538000	0.327934000
6	12.031207000	1.598969000	1.571476000
1	9.932486000	1.828173000	1.357149000
6	12.984492000	-0.512574000	0.706553000
1	11.604497000	-1.878466000	-0.145029000
6	13.214456000	0.773715000	1.355444000
1	12.183268000	2.560670000	2.050803000
1	13.853792000	-1.140917000	0.540870000
8	14.353284000	1.145201000	1.704243000

S2TIIDTS5- T1 E=-2892.151204 Hartree

6	1.632562000	-1.644303000	-0.599687000
6	1.023090000	-0.356858000	-0.584377000
6	1.871620000	0.751545000	-0.436940000
6	3.246799000	0.569804000	-0.338983000
6	3.839535000	-0.710832000	-0.381534000
6	2.995872000	-1.840831000	-0.508853000
6	-0.610754000	-2.063945000	-0.702843000
6	-0.426201000	-0.556303000	-0.651552000
1	1.457501000	1.747068000	-0.423637000
1	3.877757000	1.448179000	-0.252848000
1	3.405612000	-2.843513000	-0.502440000
6	-1.481266000	0.333243000	-0.704834000
6	-2.928456000	0.148869000	-0.588302000
6	-1.298392000	1.821666000	-0.968804000
6	-3.537705000	1.422200000	-0.769216000
6	-3.774881000	-0.926651000	-0.277608000
6	-4.900127000	1.633366000	-0.679612000
6	-5.149147000	-0.729482000	-0.184155000
1	-3.360476000	-1.912182000	-0.136199000
6	-5.739162000	0.533621000	-0.388534000
1	-5.312257000	2.628504000	-0.796155000
1	-5.781228000	-1.586441000	0.024754000
8	-0.276193000	2.462755000	-1.164891000
8	-1.634168000	-2.727545000	-0.787488000

7	-2.562433000	2.383622000	-1.008181000
7	0.654721000	-2.627228000	-0.688529000
6	0.886620000	-4.055275000	-0.746369000
1	1.489910000	-4.316246000	-1.622400000
1	1.398255000	-4.405626000	0.156762000
1	-0.087153000	-4.539302000	-0.820940000
6	-2.796969000	3.790555000	-1.257982000
1	-3.417137000	3.928825000	-2.149976000
1	-3.291999000	4.262595000	-0.402339000
1	-1.825502000	4.258557000	-1.417009000
6	5.278044000	-0.881134000	-0.293555000
6	6.019560000	-2.028081000	-0.594257000
16	6.330529000	0.420299000	0.236528000
6	7.389027000	-1.868055000	-0.413992000
1	5.575334000	-2.944874000	-0.961786000
6	7.762889000	-0.585457000	0.040527000
1	8.105594000	-2.654482000	-0.615385000
6	-7.181234000	0.724961000	-0.304477000
6	-7.941514000	1.769484000	-0.811248000
16	-8.216415000	-0.427456000	0.512807000
6	-9.317951000	1.648834000	-0.561175000
1	-7.512557000	2.586228000	-1.379221000
6	-9.668004000	0.502344000	0.151974000
1	-10.044396000	2.372703000	-0.908431000
6	9.077521000	-0.133023000	0.317048000
6	10.207029000	-0.967531000	0.165358000
6	9.285394000	1.254122000	0.778949000
6	11.479999000	-0.519813000	0.430875000
1	10.082230000	-1.991254000	-0.168282000
6	11.736690000	0.857762000	0.889662000
6	12.604279000	-1.378430000	0.270620000
7	13.494801000	-2.114692000	0.126078000
8	8.352011000	2.040094000	0.941358000
8	12.858213000	1.279221000	1.131164000
7	10.592616000	1.663242000	1.033161000
6	10.767112000	3.047910000	1.489074000
1	10.372778000	3.735696000	0.738518000
1	10.217273000	3.202138000	2.419596000
1	11.830917000	3.212205000	1.639784000
6	-10.972101000	0.070438000	0.573073000
6	-11.168448000	-1.179653000	1.238523000
6	-12.122360000	0.889641000	0.336279000
6	-12.408574000	-1.591038000	1.639988000
1	-10.310171000	-1.819999000	1.423008000

6	-13.370720000	0.497718000	0.729004000
1	-11.997398000	1.846309000	-0.160060000
6	-13.594549000	-0.773607000	1.408957000
1	-12.556594000	-2.541441000	2.142486000
1	-14.242335000	1.119654000	0.551927000
8	-14.730926000	-1.139539000	1.770744000

S2TIIDTS6- T1 E=-3253.472244 Hartree

6	-1.249169000	1.692221000	-0.597655000
6	-0.651347000	0.398422000	-0.566483000
6	-1.510762000	-0.699792000	-0.397753000
6	-2.882017000	-0.502785000	-0.294178000
6	-3.465789000	0.784330000	-0.352402000
6	-2.608487000	1.904045000	-0.502583000
6	0.997502000	2.086632000	-0.724751000
6	0.797695000	0.581858000	-0.645824000
1	-1.106237000	-1.698979000	-0.370470000
1	-3.519427000	-1.373368000	-0.182364000
1	-3.006634000	2.910887000	-0.519939000
6	1.843915000	-0.319740000	-0.688890000
6	3.293141000	-0.147911000	-0.578770000
6	1.645365000	-1.809497000	-0.929166000
6	3.889114000	-1.430092000	-0.740247000
6	4.150727000	0.924010000	-0.287145000
6	5.249792000	-1.653305000	-0.649604000
6	5.523289000	0.714676000	-0.193231000
1	3.746359000	1.915848000	-0.161364000
6	6.099913000	-0.557419000	-0.378147000
1	5.651991000	-2.654237000	-0.750398000
1	6.164530000	1.568507000	-0.000006000
8	0.616419000	-2.443195000	-1.114035000
8	2.027524000	2.737151000	-0.828964000
7	2.903832000	-2.385147000	-0.961783000
7	-0.261585000	2.663206000	-0.710563000
6	-0.479519000	4.092315000	-0.792368000
1	-1.085512000	4.343820000	-1.669276000
1	-0.982368000	4.463427000	0.107368000
1	0.498562000	4.565118000	-0.881135000
6	3.123354000	-3.798059000	-1.190056000
1	3.740057000	-3.956733000	-2.081082000
1	3.615421000	-4.261874000	-0.328203000
1	2.146727000	-4.258377000	-1.339748000
6	-4.896944000	0.967037000	-0.256712000

6	-5.621680000	2.154222000	-0.446955000
16	-5.976390000	-0.365872000	0.136028000
6	-6.989126000	2.010915000	-0.290753000
1	-5.159301000	3.097361000	-0.711184000
6	-7.395689000	0.686205000	0.036544000
1	-7.716201000	2.800556000	-0.402337000
6	7.540757000	-0.761926000	-0.294031000
6	8.290218000	-1.817584000	-0.792812000
16	8.587320000	0.387088000	0.513021000
6	9.668373000	-1.707884000	-0.544800000
1	7.852727000	-2.634534000	-1.353947000
6	10.029739000	-0.559138000	0.158333000
1	10.387697000	-2.441231000	-0.886996000
6	-8.703079000	0.219520000	0.261671000
6	-9.851543000	1.122403000	0.179359000
6	-8.907082000	-1.186832000	0.580643000
6	-11.340708000	-0.794911000	0.719477000
8	-7.973041000	-1.985399000	0.667005000
7	-10.228914000	-1.616843000	0.791149000
6	-10.418858000	-3.041356000	1.109132000
1	-11.059873000	-3.504748000	0.358039000
1	-9.435188000	-3.502070000	1.115626000
1	-10.900723000	-3.141253000	2.082615000
7	-11.118768000	0.537605000	0.419518000
6	-12.280651000	1.438132000	0.337991000
1	-12.967191000	1.085894000	-0.433062000
1	-12.809356000	1.445491000	1.292091000
1	-11.903218000	2.427401000	0.097186000
8	-9.776713000	2.320680000	-0.078382000
16	-12.882646000	-1.390695000	0.985277000
6	11.338609000	-0.135670000	0.574671000
6	11.547591000	1.119162000	1.226870000
6	12.480448000	-0.968605000	0.346161000
6	12.792034000	1.522477000	1.623577000
1	10.695818000	1.769961000	1.404788000
6	13.732920000	-0.584951000	0.734335000
1	12.345732000	-1.929280000	-0.139791000
6	13.969678000	0.691090000	1.400705000
1	12.949613000	2.476626000	2.115982000
1	14.598195000	-1.217437000	0.563600000
8	15.109929000	1.049496000	1.758331000

S2TIIDTS7- T1 E=-3007.403170 Hartree

6	1.073746000	-1.724299000	-0.906668000
6	0.487409000	-0.430711000	-0.793278000
6	1.359272000	0.654537000	-0.612595000
6	2.733821000	0.446798000	-0.572173000
6	3.300506000	-0.838836000	-0.707370000
6	2.435503000	-1.947280000	-0.873264000
6	-1.178319000	-2.103100000	-0.959667000
6	-0.966884000	-0.604139000	-0.822785000
1	0.963277000	1.654133000	-0.531221000
1	3.384508000	1.309095000	-0.469737000
1	2.830241000	-2.954024000	-0.936994000
6	-2.008519000	0.301923000	-0.784025000
6	-3.454563000	0.131046000	-0.632209000
6	-1.810113000	1.801803000	-0.956115000
6	-4.048238000	1.422093000	-0.710953000
6	-4.308602000	-0.949916000	-0.364513000
6	-5.403672000	1.646532000	-0.564026000
6	-5.675955000	-0.739500000	-0.214249000
1	-3.906325000	-1.948401000	-0.300329000
6	-6.251086000	0.542504000	-0.317551000
1	-5.802707000	2.653015000	-0.602802000
1	-6.315256000	-1.599066000	-0.040989000
8	-0.784643000	2.440520000	-1.141122000
8	-2.214926000	-2.745134000	-1.050577000
7	-3.065706000	2.382940000	-0.918655000
7	0.076977000	-2.685132000	-1.020860000
6	0.283010000	-4.110092000	-1.174648000
1	0.853046000	-4.324533000	-2.084864000
1	0.818152000	-4.523323000	-0.312688000
1	-0.700601000	-4.574250000	-1.246153000
6	-3.284725000	3.806431000	-1.069199000
1	-3.930469000	4.011341000	-1.929659000
1	-3.744472000	4.228923000	-0.169107000
1	-2.311175000	4.269689000	-1.229422000
6	4.735693000	-1.040775000	-0.673965000
6	5.460588000	-2.152843000	-1.118934000
16	5.817295000	0.174236000	-0.033443000
6	6.834674000	-2.038942000	-0.952117000
1	4.988843000	-3.009873000	-1.583649000
6	7.241736000	-0.810280000	-0.374953000
1	7.559423000	-2.791979000	-1.226488000
6	-7.686603000	0.748845000	-0.174824000
6	-8.445363000	1.833801000	-0.590617000
16	-8.713975000	-0.437507000	0.602730000

6	-9.814993000	1.717501000	-0.303568000
1	-8.021207000	2.678157000	-1.120536000
6	-10.160973000	0.533806000	0.348081000
1	-10.540153000	2.472030000	-0.581338000
6	8.554894000	-0.487013000	0.014960000
6	9.574094000	-1.569512000	0.233520000
6	9.138067000	0.754891000	0.474059000
6	10.657540000	-0.949945000	1.032698000
6	10.381841000	0.416063000	1.224031000
6	11.784952000	-1.564338000	1.558684000
6	11.259918000	1.188715000	1.987738000
6	12.660438000	-0.787422000	2.321485000
1	11.961388000	-2.619230000	1.374801000
6	12.390802000	0.568831000	2.533518000
1	11.086698000	2.239887000	2.173562000
1	13.549905000	-1.234392000	2.754489000
1	13.073294000	1.161450000	3.135003000
8	9.525431000	-2.735861000	-0.129103000
6	8.743396000	2.049157000	0.152344000
6	7.811202000	2.368314000	-0.880159000
7	7.102471000	2.692233000	-1.746595000
6	9.350195000	3.206348000	0.728647000
7	9.808993000	4.171899000	1.193055000
6	-11.457881000	0.095206000	0.784079000
6	-11.653717000	-1.191475000	1.375843000
6	-12.601385000	0.944421000	0.637509000
6	-12.887025000	-1.609231000	1.791530000
1	-10.800782000	-1.854748000	1.491149000
6	-13.842862000	0.546721000	1.045972000
1	-12.476472000	1.928747000	0.198536000
6	-14.066029000	-0.761632000	1.651794000
1	-13.034611000	-2.587310000	2.237930000
1	-14.709157000	1.191406000	0.937299000
8	-15.196162000	-1.133031000	2.027502000

S2TIIDTS8-T1 E=-3442.623504 Hartree

6	-4.517805000	1.487183000	-0.658726000
6	-3.906133000	0.202469000	-0.626925000
6	-4.744658000	-0.899191000	-0.395954000
6	-6.114179000	-0.713166000	-0.235586000
6	-6.707353000	0.563728000	-0.292487000
6	-5.875649000	1.687502000	-0.501507000
6	-2.286077000	1.906918000	-0.894279000

6	-2.463376000	0.398326000	-0.775609000
1	-4.328512000	-1.893630000	-0.367747000
1	-6.740993000	-1.587120000	-0.091233000
1	-6.288525000	2.689100000	-0.504101000
6	-1.409815000	-0.491200000	-0.849623000
6	0.042887000	-0.298464000	-0.819111000
6	-1.600811000	-1.987036000	-1.038003000
6	0.645775000	-1.579102000	-0.980576000
6	0.899605000	0.791765000	-0.603364000
6	2.011234000	-1.783932000	-0.960271000
6	2.277599000	0.601973000	-0.575948000
1	0.489986000	1.782156000	-0.485508000
6	2.859392000	-0.669822000	-0.758593000
1	2.420978000	-2.781959000	-1.058207000
1	2.917350000	1.469095000	-0.448178000
8	-2.628598000	-2.640063000	-1.147173000
8	-1.269728000	2.565610000	-1.057569000
7	-0.337557000	-2.548916000	-1.124512000
7	-3.549139000	2.468573000	-0.834026000
6	-3.788503000	3.893447000	-0.932859000
1	-4.439248000	4.119805000	-1.784078000
1	-4.251817000	4.276627000	-0.017175000
1	-2.822058000	4.375997000	-1.078335000
6	-0.112164000	-3.965019000	-1.327772000
1	0.456617000	-4.139973000	-2.247111000
1	0.432479000	-4.399576000	-0.482508000
1	-1.089449000	-4.440341000	-1.411215000
6	-8.144825000	0.744899000	-0.139584000
6	-8.918722000	1.835644000	-0.510661000
16	-9.155183000	-0.485275000	0.590898000
6	-10.285963000	1.689793000	-0.227005000
1	-8.506877000	2.706321000	-1.006592000
6	-10.615160000	0.476307000	0.377260000
1	-11.021408000	2.445339000	-0.473072000
6	4.299130000	-0.854206000	-0.738453000
6	5.036878000	-1.919380000	-1.262903000
16	5.358910000	0.321697000	-0.000764000
6	6.410644000	-1.796527000	-1.082567000
1	4.578385000	-2.742437000	-1.796439000
6	6.792980000	-0.613300000	-0.415283000
1	7.138576000	-2.508621000	-1.451480000
6	8.101182000	-0.303068000	0.003941000
6	8.739167000	0.893494000	0.425079000
6	10.376391000	-0.731354000	1.165594000

6	9.987714000	0.616693000	1.196840000
6	11.524262000	-1.219499000	1.769254000
6	10.810326000	1.506736000	1.902575000
6	12.330384000	-0.314768000	2.462428000
1	11.778244000	-2.272376000	1.707406000
6	11.965336000	1.031818000	2.527539000
1	10.565341000	2.555886000	1.982175000
1	13.234384000	-0.660076000	2.953381000
1	12.588668000	1.731594000	3.075025000
6	8.322829000	2.183288000	0.044681000
6	8.851585000	3.386417000	0.591737000
7	9.236939000	4.399996000	1.022244000
6	7.417376000	2.423277000	-1.028512000
7	6.720221000	2.681135000	-1.926920000
16	9.201826000	-1.726634000	0.274806000
8	8.568095000	-2.698137000	1.177831000
8	9.748761000	-2.205827000	-1.005253000
6	-11.905303000	0.003785000	0.797065000
6	-12.082544000	-1.306546000	1.341049000
6	-13.060735000	0.841775000	0.682049000
6	-13.309488000	-1.756593000	1.741339000
1	-11.220268000	-1.961479000	1.431928000
6	-14.296162000	0.411914000	1.075789000
1	-12.950084000	1.843107000	0.279234000
6	-14.500404000	-0.920933000	1.633145000
1	-13.443057000	-2.752366000	2.151540000
1	-15.171566000	1.047792000	0.990940000
8	-15.624817000	-1.321742000	1.995115000

S2TIIDTS9-T1 E=-3428.563934 Hartree

6	3.646740000	-1.469072000	-0.658096000
6	3.054231000	-0.179049000	-0.555206000
6	3.917295000	0.901929000	-0.322860000
6	5.290881000	0.693224000	-0.228406000
6	5.863184000	-0.587281000	-0.354615000
6	5.008100000	-1.691861000	-0.566435000
6	1.397278000	-1.844518000	-0.810591000
6	1.601966000	-0.353928000	-0.647552000
1	3.517290000	1.900371000	-0.243931000
1	5.935920000	1.553919000	-0.082863000
1	5.406746000	-2.698051000	-0.620859000
6	0.556481000	0.554994000	-0.638736000
6	-0.886683000	0.385298000	-0.536094000

6	0.763210000	2.053674000	-0.794137000
6	-1.482882000	1.678020000	-0.616300000
6	-1.754733000	-0.699114000	-0.314800000
6	-2.838528000	1.902685000	-0.514138000
6	-3.122198000	-0.489607000	-0.205417000
1	-1.354582000	-1.698719000	-0.249918000
6	-3.703830000	0.796286000	-0.308067000
1	-3.229930000	2.910604000	-0.578120000
1	-3.761313000	-1.352331000	-0.045816000
8	1.794643000	2.693846000	-0.946774000
8	0.366661000	-2.490412000	-0.953987000
7	-0.491800000	2.638962000	-0.785897000
7	2.656344000	-2.428136000	-0.825168000
6	2.866905000	-3.850386000	-0.983993000
1	3.475682000	-4.058533000	-1.870726000
1	3.364093000	-4.274864000	-0.104495000
1	1.886055000	-4.311223000	-1.102492000
6	-0.702277000	4.062704000	-0.932002000
1	-1.319290000	4.277849000	-1.811279000
1	-1.190815000	4.480244000	-0.044475000
1	0.277505000	4.524218000	-1.056345000
6	7.304337000	-0.791951000	-0.271440000
6	8.049758000	-1.866422000	-0.735181000
16	8.357732000	0.382215000	0.490051000
6	9.429402000	-1.751346000	-0.497416000
1	7.606802000	-2.701099000	-1.265070000
6	9.797920000	-0.579087000	0.161936000
1	10.145444000	-2.498158000	-0.817064000
6	-5.129066000	0.994167000	-0.204479000
6	-5.860298000	2.179270000	-0.335788000
16	-6.229507000	-0.348116000	0.128762000
6	-7.235373000	2.040203000	-0.181793000
1	-5.391264000	3.132235000	-0.548751000
6	-7.647104000	0.713063000	0.081778000
1	-7.935210000	2.864234000	-0.258277000
6	-8.937804000	0.239888000	0.283150000
16	-9.303252000	-1.456349000	0.599925000
16	-10.342839000	1.312234000	0.239287000
6	-11.055382000	-1.250087000	0.724478000
6	-11.544832000	0.054064000	0.554215000
6	-11.934766000	-2.305482000	0.978045000
6	-12.916225000	0.307455000	0.636936000
6	-13.302312000	-2.047699000	1.059782000
1	-11.555139000	-3.313736000	1.109387000

6	-13.790067000	-0.748796000	0.890180000
1	-13.294815000	1.316055000	0.505135000
1	-13.988687000	-2.864866000	1.256553000
1	-14.855956000	-0.555600000	0.955047000
6	11.109183000	-0.143955000	0.554721000
6	11.325702000	1.133011000	1.160037000
6	12.249021000	-0.986199000	0.350532000
6	12.573361000	1.547553000	1.534701000
1	10.476248000	1.791713000	1.319209000
6	13.504403000	-0.591339000	0.717447000
1	12.109805000	-1.963656000	-0.099599000
6	13.748533000	0.707034000	1.335929000
1	12.735101000	2.518739000	1.991321000
1	14.367215000	-1.231850000	0.564530000
8	14.891939000	1.075680000	1.674012000

S2TIIDTS10-T1 E=-3274.905399 Hartree

6	2.550717000	-1.488512000	-0.595104000
6	1.921625000	-0.217091000	-0.450835000
6	2.758857000	0.872291000	-0.149467000
6	4.128777000	0.688594000	-0.025703000
6	4.743507000	-0.575057000	-0.192029000
6	3.909346000	-1.687147000	-0.479698000
6	0.318032000	-1.905228000	-0.838229000
6	0.485296000	-0.414014000	-0.591037000
1	2.333244000	1.856729000	-0.034082000
1	4.743596000	1.555103000	0.196646000
1	4.326373000	-2.680154000	-0.594823000
6	-0.581881000	0.469224000	-0.566431000
6	-2.030774000	0.255170000	-0.511447000
6	-0.410906000	1.970945000	-0.638229000
6	-2.652877000	1.534788000	-0.549693000
6	-2.870948000	-0.857535000	-0.358551000
6	-4.020647000	1.719809000	-0.470110000
6	-4.250627000	-0.687013000	-0.277044000
1	-2.448046000	-1.849264000	-0.330929000
6	-4.851870000	0.584956000	-0.338616000
1	-4.442844000	2.717837000	-0.472892000
1	-4.876821000	-1.569637000	-0.193823000
8	0.605906000	2.648255000	-0.724422000
8	-0.694548000	-2.559131000	-1.048268000

7	-1.683512000	2.524874000	-0.642166000
7	1.586633000	-2.460622000	-0.840023000
6	1.834265000	-3.867945000	-1.065220000
1	2.472108000	-4.016464000	-1.943421000
1	2.316684000	-4.325798000	-0.194371000
1	0.868371000	-4.343873000	-1.235457000
6	-1.925932000	3.948685000	-0.721288000
1	-2.524884000	4.194484000	-1.605077000
1	-2.447724000	4.309044000	0.172469000
1	-0.954723000	4.438384000	-0.795059000
6	6.171006000	-0.745609000	-0.071878000
6	6.933884000	-1.902279000	-0.258358000
16	7.232063000	0.599853000	0.363100000
6	8.302655000	-1.739767000	-0.068156000
1	6.493096000	-2.851751000	-0.537179000
6	8.675467000	-0.422459000	0.282064000
1	9.024152000	-2.540980000	-0.179149000
6	-6.298744000	0.750639000	-0.269508000
6	-7.062509000	1.832001000	-0.684910000
16	-7.335405000	-0.489162000	0.406063000
6	-8.442588000	1.671378000	-0.478226000
1	-6.631409000	2.705517000	-1.159034000
6	-8.793127000	0.455293000	0.107510000
1	-9.171301000	2.418291000	-0.767570000
6	9.950467000	0.070349000	0.538354000
16	10.278615000	1.753846000	0.964414000
16	11.394239000	-0.952395000	0.462934000
6	12.017069000	1.549411000	1.107291000
6	12.519763000	0.328788000	0.880856000
1	13.569835000	0.069890000	0.936207000
1	12.600565000	2.422205000	1.372507000
6	-10.099553000	-0.031870000	0.452204000
6	-10.294479000	-1.344762000	0.983505000
6	-11.256445000	0.792689000	0.273157000
6	-11.537580000	-1.808846000	1.312396000
1	-9.431690000	-1.990578000	1.122499000
6	-12.507632000	0.348454000	0.595153000
1	-11.134107000	1.796221000	-0.121029000
6	-12.729830000	-0.987163000	1.137970000
1	-11.682758000	-2.807044000	1.712883000
1	-13.383414000	0.975484000	0.461257000
8	-13.869239000	-1.400963000	1.434740000

S9TIIDTS1-CS E=-3346.077355 Hartree

6	0.791192000	1.794010000	0.617198000
6	0.158145000	0.497404000	0.572561000
6	1.003710000	-0.624446000	0.363479000
6	2.360361000	-0.450869000	0.236195000
6	2.984008000	0.835432000	0.304673000
6	2.142902000	1.977576000	0.496872000
6	-1.452683000	2.167088000	0.812860000
6	-1.243370000	0.688120000	0.684819000
1	0.575700000	-1.615297000	0.333790000
1	2.980611000	-1.328801000	0.082542000
1	2.563148000	2.974923000	0.540127000
6	-2.309788000	-0.247073000	0.725193000
6	-3.692264000	-0.094722000	0.486345000
6	-2.117597000	-1.690337000	1.128122000
6	-4.333986000	-1.370481000	0.705610000
6	-4.520128000	0.971446000	0.031567000
6	-5.670817000	-1.585838000	0.518696000
6	-5.860627000	0.766825000	-0.165395000
1	-4.085686000	1.946981000	-0.129867000
6	-6.494344000	-0.500342000	0.071648000
1	-6.097690000	-2.565107000	0.696074000
1	-6.467503000	1.598741000	-0.507886000
8	-1.099762000	-2.282127000	1.461566000
8	-2.484542000	2.811339000	0.958777000
7	-3.374707000	-2.288428000	1.100561000
7	-0.186666000	2.757908000	0.779190000
6	0.023099000	4.184114000	0.892291000
1	0.643772000	4.422660000	1.763197000
1	0.503061000	4.585303000	-0.007690000
1	-0.958197000	4.644252000	1.012885000
6	-3.602912000	-3.675529000	1.442625000
1	-4.290987000	-3.761890000	2.290563000
1	-4.015839000	-4.228096000	0.591296000
1	-2.638105000	-4.103227000	1.716766000
6	4.383873000	0.982814000	0.182029000
6	5.149433000	2.179741000	0.228695000
16	5.464935000	-0.395149000	-0.065363000
6	6.501739000	2.006447000	0.076264000
1	4.693819000	3.150600000	0.374518000
6	6.900207000	0.649524000	-0.102105000
1	7.215948000	2.822195000	0.088790000
6	-7.877164000	-0.679235000	-0.132295000

6	-8.649564000	-1.852825000	0.063741000
16	-8.933333000	0.626924000	-0.707161000
6	-9.986541000	-1.721751000	-0.223896000
1	-8.214649000	-2.780279000	0.415767000
6	-10.346847000	-0.417179000	-0.669850000
1	-10.721041000	-2.512288000	-0.131416000
6	-11.620131000	0.021330000	-1.036884000
6	-12.721569000	-0.876508000	-0.983794000
7	-13.607215000	-1.633978000	-0.931176000
6	-11.854363000	1.353762000	-1.469091000
7	-12.020867000	2.453556000	-1.821384000
6	8.175523000	0.161273000	-0.278450000
16	9.592611000	1.212682000	-0.310996000
16	8.520733000	-1.551442000	-0.487906000
6	10.779317000	-0.073763000	-0.559313000
6	10.273503000	-1.379203000	-0.642831000
6	12.152152000	0.159797000	-0.670759000
6	11.136163000	-2.460387000	-0.838284000
6	13.009427000	-0.921577000	-0.865738000
1	12.543915000	1.169744000	-0.606170000
6	12.504968000	-2.223067000	-0.948956000
1	10.743972000	-3.470170000	-0.902738000
1	14.076679000	-0.746506000	-0.953043000
1	13.180407000	-3.058492000	-1.100841000

S9TIIDTS3-CS E=-3913.931013 Hartree

6	-2.574914000	-1.445858000	0.866703000
6	-1.957942000	-0.157797000	0.689678000
6	-2.813440000	0.918852000	0.339761000
6	-4.165954000	0.710264000	0.200492000
6	-4.771054000	-0.568505000	0.397220000
6	-3.922031000	-1.664903000	0.736439000
6	-0.338566000	-1.779607000	1.153767000
6	-0.553034000	-0.314040000	0.848821000
1	-2.397563000	1.906581000	0.208940000
1	-4.794369000	1.555117000	-0.062452000
1	-4.330400000	-2.657631000	0.879713000
6	0.502408000	0.621938000	0.808545000
6	1.910477000	0.446141000	0.655052000
6	0.290727000	2.099669000	0.984775000
6	2.530635000	1.743971000	0.723706000
6	2.759388000	-0.657037000	0.388970000

6	3.878700000	1.946473000	0.574987000
6	4.113341000	-0.465625000	0.232076000
1	2.340724000	-1.650637000	0.337107000
6	4.723912000	0.821576000	0.325983000
1	4.289206000	2.946683000	0.639248000
1	4.736361000	-1.332691000	0.034511000
8	-0.738722000	2.734927000	1.176037000
8	0.695117000	-2.387208000	1.399969000
7	1.551080000	2.696818000	0.939268000
7	-1.593134000	-2.379907000	1.157584000
6	-1.800451000	-3.785899000	1.429542000
1	-2.443241000	-3.924456000	2.305584000
1	-2.256281000	-4.289754000	0.569972000
1	-0.822027000	-4.224236000	1.627755000
6	1.757303000	4.120289000	1.090765000
1	2.399203000	4.334587000	1.952428000
1	2.212321000	4.550871000	0.191496000
1	0.777719000	4.571789000	1.250580000
6	-6.174792000	-0.756094000	0.256262000
6	-6.920923000	-1.936711000	0.426241000
16	-7.263678000	0.563870000	-0.187147000
6	-8.282305000	-1.797779000	0.214555000
1	-6.465150000	-2.879253000	0.703162000
6	-8.677667000	-0.489377000	-0.135296000
1	-8.993799000	-2.610090000	0.305847000
6	6.123625000	0.989503000	0.173242000
6	6.876314000	2.189810000	0.238757000
16	7.208347000	-0.368375000	-0.143440000
6	8.228364000	2.034617000	0.047429000
1	6.415951000	3.151263000	0.426156000
6	8.632242000	0.689415000	-0.182654000
1	8.934988000	2.856711000	0.068052000
6	-9.970801000	-0.025547000	-0.413075000
6	-10.375008000	1.283833000	-0.763387000
16	-11.409328000	-1.048299000	-0.375393000
1	-9.673208000	2.108371000	-0.854852000
6	-12.386648000	0.374152000	-0.829039000
6	-13.769218000	0.305553000	-1.000552000
6	-14.461077000	-0.920569000	-0.817083000
7	-15.001696000	-1.942717000	-0.659451000
6	-14.516395000	1.459514000	-1.362923000
7	-15.157955000	2.386428000	-1.659804000
7	-11.659310000	1.503281000	-0.986114000
6	9.908863000	0.216454000	-0.405825000

16	11.314020000	1.280271000	-0.439972000
16	10.261368000	-1.484241000	-0.676548000
6	12.505230000	0.013700000	-0.756905000
6	12.008090000	-1.293025000	-0.868696000
6	13.873016000	0.263092000	-0.894309000
6	12.874142000	-2.360320000	-1.118588000
6	14.733505000	-0.804279000	-1.143561000
1	14.258153000	1.273922000	-0.807892000
6	14.237616000	-2.107183000	-1.254957000
1	12.488762000	-3.371063000	-1.204868000
1	15.796849000	-0.617429000	-1.251316000
1	14.916036000	-2.931319000	-1.449118000

S9TIIDTS4-CS E=-3879.954632 Hartree

6	3.040814000	-1.608872000	-0.869689000
6	2.429250000	-0.307742000	-0.720808000
6	3.289195000	0.768302000	-0.356962000
6	4.629758000	0.548647000	-0.177677000
6	5.233845000	-0.744592000	-0.343993000
6	4.377080000	-1.839181000	-0.699272000
6	0.806721000	-1.903196000	-1.219929000
6	1.039567000	-0.445893000	-0.918654000
1	2.878108000	1.761609000	-0.251788000
1	5.261421000	1.387985000	0.094515000
1	4.779227000	-2.837367000	-0.821302000
6	-0.006835000	0.517041000	-0.913819000
6	-1.403957000	0.367836000	-0.743090000
6	0.229290000	1.976545000	-1.158730000
6	-2.013972000	1.672128000	-0.861057000
6	-2.265684000	-0.718327000	-0.427970000
6	-3.355694000	1.893988000	-0.709653000
6	-3.612301000	-0.506112000	-0.269169000
1	-1.855867000	-1.713958000	-0.343689000
6	-4.214080000	0.786977000	-0.407864000
1	-3.757494000	2.894920000	-0.810038000
1	-4.245178000	-1.356614000	-0.034076000
8	1.269060000	2.583997000	-1.387063000
8	-0.231077000	-2.495266000	-1.489477000
7	-1.022006000	2.598999000	-1.124708000
7	2.052599000	-2.527908000	-1.181275000
6	2.241211000	-3.938591000	-1.435798000
1	2.906316000	-4.097988000	-2.291775000
1	2.662438000	-4.444979000	-0.559834000

1	1.260195000	-4.359458000	-1.658757000
6	-1.205104000	4.017162000	-1.335339000
1	-1.851363000	4.206996000	-2.199775000
1	-1.644301000	4.494918000	-0.451908000
1	-0.218900000	4.443422000	-1.522745000
6	6.617628000	-0.936023000	-0.159927000
6	7.351938000	-2.145062000	-0.299512000
16	7.712028000	0.382792000	0.301928000
6	8.695201000	-2.027523000	-0.054783000
1	6.886259000	-3.082047000	-0.579100000
6	9.108890000	-0.704699000	0.297313000
1	9.399522000	-2.849038000	-0.116935000
6	-5.602976000	0.973412000	-0.249489000
6	-6.347717000	2.180723000	-0.356671000
16	-6.704579000	-0.360222000	0.133576000
6	-7.696206000	2.050111000	-0.147458000
1	-5.878035000	3.128248000	-0.587630000
6	-8.117351000	0.717481000	0.142148000
1	-8.393981000	2.878666000	-0.195299000
6	10.386259000	-0.288078000	0.596448000
6	10.727836000	1.084848000	0.948211000
16	11.817173000	-1.332189000	0.605904000
6	12.876429000	0.064152000	1.079634000
7	12.105775000	1.203051000	1.198654000
6	12.718446000	2.472212000	1.571769000
1	13.474212000	2.757059000	0.836096000
1	11.921922000	3.215097000	1.601613000
1	13.194291000	2.387896000	2.551571000
8	14.069882000	-0.013362000	1.258317000
8	9.946113000	2.027498000	1.023902000
6	-9.393475000	0.273363000	0.394853000
16	-10.789520000	1.357852000	0.398373000
16	-9.768145000	-1.414007000	0.739319000
6	-11.992334000	0.118511000	0.776555000
6	-11.510848000	-1.189097000	0.937402000
6	-13.355625000	0.389963000	0.915115000
6	-12.389177000	-2.232909000	1.237613000
6	-14.228708000	-0.654532000	1.214768000
1	-13.728347000	1.401579000	0.790658000
6	-13.748712000	-1.957721000	1.375024000
1	-12.015729000	-3.244290000	1.361717000
1	-15.288592000	-0.448868000	1.323384000
1	-14.435431000	-2.764843000	1.608144000

S9TIIDTS5-CS E=-3651.421736 Hartree

6	-2.653770000	-1.603904000	0.868469000
6	-2.046724000	-0.302197000	0.733054000
6	-2.911233000	0.778203000	0.401175000
6	-4.256067000	0.560815000	0.238735000
6	-4.854056000	-0.733843000	0.393141000
6	-3.994266000	-1.832018000	0.715403000
6	-0.417381000	-1.915101000	1.174523000
6	-0.649689000	-0.445386000	0.903871000
1	-2.502726000	1.773147000	0.304323000
1	-4.891941000	1.403886000	-0.009426000
1	-4.394999000	-2.831952000	0.825923000
6	0.396694000	0.508515000	0.901248000
6	1.799913000	0.355543000	0.730166000
6	0.166862000	1.970667000	1.148642000
6	2.409118000	1.657086000	0.853892000
6	2.657861000	-0.727913000	0.407779000
6	3.753060000	1.878170000	0.704778000
6	4.006958000	-0.516501000	0.250406000
1	2.247766000	-1.722294000	0.314773000
6	4.607582000	0.772708000	0.398250000
1	4.155482000	2.878067000	0.811420000
1	4.637367000	-1.367037000	0.009115000
8	-0.869611000	2.581680000	1.377315000
8	0.623042000	-2.512030000	1.416606000
7	1.420592000	2.586367000	1.120556000
7	-1.663541000	-2.532821000	1.146851000
6	-1.855273000	-3.947970000	1.379302000
1	-2.507510000	-4.117917000	2.242734000
1	-2.293126000	-4.435171000	0.500983000
1	-0.873629000	-4.378454000	1.579079000
6	1.609776000	4.003666000	1.336727000
1	2.254872000	4.186592000	2.203295000
1	2.052673000	4.481741000	0.455534000
1	0.625422000	4.434075000	1.523645000
6	-6.247427000	-0.925961000	0.226999000
6	-6.975265000	-2.129947000	0.361300000
16	-7.345120000	0.397533000	-0.201433000
6	-8.327127000	-1.997994000	0.134759000
1	-6.515088000	-3.075237000	0.622255000
6	-8.736862000	-0.676159000	-0.192367000
1	-9.021746000	-2.825813000	0.199518000
6	6.001299000	0.959327000	0.242514000

6	6.744674000	2.164358000	0.356897000
16	7.097716000	-0.372215000	-0.144791000
6	8.094882000	2.031550000	0.148134000
1	6.276439000	3.111457000	0.591737000
6	8.511187000	0.701485000	-0.146885000
1	8.793844000	2.858809000	0.200681000
6	-10.048532000	-0.243289000	-0.475396000
6	-11.155180000	-1.124880000	-0.463203000
6	-10.285542000	1.169504000	-0.795814000
6	-12.431469000	-0.699423000	-0.739919000
1	-11.005545000	-2.173186000	-0.229608000
6	-12.719692000	0.705086000	-1.065734000
6	-13.525115000	-1.612174000	-0.720183000
7	-14.388683000	-2.393190000	-0.692747000
8	-9.378116000	2.005658000	-0.829762000
8	-13.842606000	1.121916000	-1.317781000
7	-11.597275000	1.557898000	-1.069400000
6	-11.804042000	2.974652000	-1.385220000
1	-11.472144000	3.593143000	-0.548568000
1	-11.217391000	3.247852000	-2.264941000
1	-12.865601000	3.116729000	-1.571423000
6	9.789353000	0.253922000	-0.401375000
16	11.184466000	1.333266000	-0.397819000
16	10.157543000	-1.429531000	-0.753278000
6	12.385501000	0.094612000	-0.782125000
6	11.900739000	-1.210684000	-0.950039000
6	13.749474000	0.364249000	-0.918608000
6	12.775570000	-2.256045000	-1.255542000
6	14.618877000	-0.681362000	-1.223444000
1	14.125008000	1.374063000	-0.788763000
6	14.135357000	-1.982804000	-1.390817000
1	12.399703000	-3.265751000	-1.385205000
1	15.679337000	-0.478458000	-1.330751000
1	14.820369000	-2.790078000	-1.628002000

S9TIIDTS6-CS E=-4012.743789 Hartree

6	-2.272872000	-1.659442000	0.905386000
6	-1.671025000	-0.350891000	0.792924000
6	-2.541542000	0.732947000	0.480277000
6	-3.883447000	0.512404000	0.313595000
6	-4.477395000	-0.790111000	0.443886000
6	-3.610708000	-1.891085000	0.747643000
6	-0.034702000	-1.960404000	1.208454000

6	-0.277086000	-0.488869000	0.961771000
1	-2.136809000	1.731249000	0.402621000
1	-4.524414000	1.355761000	0.080350000
1	-4.008012000	-2.894099000	0.840155000
6	0.765064000	0.473861000	0.974963000
6	2.164049000	0.333328000	0.785679000
6	0.528290000	1.925893000	1.264006000
6	2.769305000	1.635207000	0.937269000
6	3.024337000	-0.738347000	0.426907000
6	4.109881000	1.866183000	0.779992000
6	4.369711000	-0.516421000	0.261373000
1	2.617603000	-1.732137000	0.313506000
6	4.966942000	0.772531000	0.435805000
1	4.509175000	2.864883000	0.907838000
1	5.002048000	-1.357126000	-0.007797000
8	-0.510008000	2.523566000	1.519313000
8	1.010173000	-2.553314000	1.441140000
7	1.778279000	2.550903000	1.238433000
7	-1.276879000	-2.586386000	1.168558000
6	-1.459703000	-4.006377000	1.377251000
1	-2.111566000	-4.194904000	2.237098000
1	-1.893935000	-4.481664000	0.490662000
1	-0.475381000	-4.433745000	1.570612000
6	1.960720000	3.963015000	1.490060000
1	2.614171000	4.127592000	2.354104000
1	2.390752000	4.467500000	0.617194000
1	0.975603000	4.381509000	1.698999000
6	-5.864980000	-0.985213000	0.273060000
6	-6.588494000	-2.198009000	0.381451000
16	-6.970035000	0.341546000	-0.128740000
6	-7.938533000	-2.076759000	0.157936000
1	-6.121047000	-3.145179000	0.622932000
6	-8.359477000	-0.744667000	-0.143595000
1	-8.655033000	-2.882696000	0.195516000
6	6.356117000	0.969125000	0.269816000
6	7.096215000	2.175026000	0.408098000
16	7.455457000	-0.346543000	-0.165664000
6	8.443705000	2.054837000	0.180855000
1	6.626065000	3.113028000	0.673707000
6	8.863951000	0.734645000	-0.154809000
1	9.139404000	2.883824000	0.247786000
6	-9.665463000	-0.300958000	-0.419646000
6	-10.788675000	-1.227946000	-0.424360000
6	-9.880498000	1.103730000	-0.702209000

6	-12.295107000	0.671990000	-0.988000000
8	-8.964090000	1.930189000	-0.712836000
7	-11.202094000	1.516939000	-0.972910000
6	-11.404105000	2.945334000	-1.255547000
1	-12.095933000	3.372555000	-0.528056000
1	-10.430691000	3.423605000	-1.191915000
1	-11.834022000	3.069088000	-2.250701000
7	-12.059761000	-0.661725000	-0.716300000
6	-13.201466000	-1.588381000	-0.724249000
1	-13.938282000	-1.274659000	0.016832000
1	-13.678635000	-1.579784000	-1.705457000
1	-12.812798000	-2.575255000	-0.490789000
8	-10.709211000	-2.434240000	-0.198782000
16	-13.837728000	1.244797000	-1.322306000
6	10.140367000	0.301732000	-0.435592000
16	11.530943000	1.388685000	-0.419177000
16	10.513848000	-1.370488000	-0.837319000
6	12.733465000	0.166890000	-0.850638000
6	12.253551000	-1.136074000	-1.048089000
6	14.094329000	0.447359000	-0.995594000
6	13.130376000	-2.167769000	-1.391744000
6	14.965820000	-0.584745000	-1.338559000
1	14.466043000	1.455408000	-0.842877000
6	14.487194000	-1.883746000	-1.535368000
1	12.758213000	-3.175679000	-1.544233000
1	16.023878000	-0.373022000	-1.452553000
1	15.173465000	-2.680677000	-1.802135000

S9TIIDTS7-CS E=-3766.673474 Hartree

6	2.077348000	-1.678136000	-1.203659000
6	1.494868000	-0.376202000	-0.983757000
6	2.386673000	0.675401000	-0.630514000
6	3.731743000	0.430855000	-0.519524000
6	4.302809000	-0.864164000	-0.752057000
6	3.417704000	-1.933084000	-1.103491000
6	-0.171875000	-1.941998000	-1.453059000
6	0.091545000	-0.491458000	-1.116415000
1	1.998142000	1.671841000	-0.481141000
1	4.390426000	1.254721000	-0.265673000
1	3.799507000	-2.933027000	-1.267325000
6	-0.940402000	0.475210000	-1.030606000
6	-2.338678000	0.332220000	-0.820414000

6	-0.697067000	1.945059000	-1.210818000
6	-2.932681000	1.646553000	-0.857462000
6	-3.201902000	-0.755180000	-0.524883000
6	-4.267497000	1.877081000	-0.652705000
6	-4.541622000	-0.534557000	-0.312190000
1	-2.803630000	-1.758271000	-0.496220000
6	-5.128030000	0.768511000	-0.374415000
1	-4.658437000	2.886272000	-0.695277000
1	-5.176388000	-1.387934000	-0.093362000
8	0.340215000	2.553222000	-1.442151000
8	-1.228522000	-2.511318000	-1.691636000
7	-1.939976000	2.575120000	-1.109409000
7	1.064634000	-2.577982000	-1.495198000
6	1.227488000	-3.981762000	-1.805756000
1	1.851210000	-4.115569000	-2.696142000
1	1.683723000	-4.519814000	-0.967383000
1	0.233787000	-4.387587000	-1.997356000
6	-2.114749000	4.004026000	-1.247375000
1	-2.785777000	4.239299000	-2.080980000
1	-2.520395000	4.442683000	-0.328539000
1	-1.130820000	4.430076000	-1.446199000
6	5.693269000	-1.092262000	-0.627336000
6	6.414046000	-2.278855000	-0.901861000
16	6.811272000	0.158930000	-0.086053000
6	7.769310000	-2.190260000	-0.686452000
1	5.936528000	-3.179056000	-1.269003000
6	8.203553000	-0.909971000	-0.227601000
1	8.478902000	-2.992160000	-0.829350000
6	-6.512507000	0.964870000	-0.163452000
6	-7.241439000	2.184121000	-0.190933000
16	-7.616121000	-0.370601000	0.190564000
6	-8.585787000	2.058715000	0.055040000
1	-6.766783000	3.135830000	-0.391850000
6	-9.012642000	0.720473000	0.294626000
1	-9.273618000	2.896796000	0.068293000
6	9.508366000	-0.603595000	0.191189000
6	10.472424000	-1.696370000	0.523590000
6	10.106275000	0.645747000	0.603730000
6	11.548674000	-1.061361000	1.325839000
6	11.312153000	0.320770000	1.420960000
6	12.635257000	-1.675790000	1.929877000
6	12.190751000	1.112969000	2.163772000
6	13.510222000	-0.880143000	2.675047000
1	12.781755000	-2.745325000	1.817309000

6	13.280465000	0.494357000	2.790037000
1	12.047736000	2.179281000	2.273876000
1	14.368302000	-1.326952000	3.168075000
1	13.961556000	1.103098000	3.377214000
8	10.408003000	-2.888242000	0.246389000
6	9.760529000	1.935115000	0.207176000
6	8.911665000	2.223778000	-0.901293000
7	8.273682000	2.512299000	-1.833560000
6	10.348252000	3.105036000	0.776506000
7	10.791022000	4.082659000	1.232394000
6	-10.288202000	0.277689000	0.567344000
16	-11.666634000	1.374687000	0.665803000
16	-10.670784000	-1.417208000	0.843249000
6	-12.873249000	0.133680000	1.024351000
6	-12.403270000	-1.185093000	1.108111000
6	-14.227893000	0.414055000	1.219399000
6	-13.283794000	-2.233011000	1.387286000
6	-15.103037000	-0.634205000	1.497769000
1	-14.591948000	1.434301000	1.154635000
6	-14.634300000	-1.949015000	1.581159000
1	-12.919344000	-3.253125000	1.451786000
1	-16.156300000	-0.422810000	1.650205000
1	-15.323531000	-2.758351000	1.798299000

S9TIIDTS8-CS E=-4201.894063 Hartree

6	-3.410355000	1.718708000	-0.801271000
6	-2.801885000	0.411561000	-0.804945000
6	-3.651246000	-0.693599000	-0.541986000
6	-4.994199000	-0.495246000	-0.322318000
6	-5.594834000	0.801313000	-0.345389000
6	-4.748370000	1.927413000	-0.589487000
6	-1.178913000	2.057208000	-1.144382000
6	-1.402962000	0.578321000	-1.011181000
1	-3.241498000	-1.692331000	-0.542820000
1	-5.618198000	-1.362537000	-0.128783000
1	-5.150917000	2.932820000	-0.601626000
6	-0.360394000	-0.369963000	-1.127734000
6	1.044689000	-0.240149000	-1.003380000
6	-0.606918000	-1.817497000	-1.497258000
6	1.639844000	-1.528256000	-1.259523000
6	1.926010000	0.812264000	-0.631007000
6	2.984715000	-1.769718000	-1.176134000
6	3.275584000	0.580806000	-0.535837000

1	1.527469000	1.800044000	-0.453876000
6	3.858230000	-0.699908000	-0.805368000
1	3.376761000	-2.761344000	-1.364268000
1	3.926184000	1.406500000	-0.267545000
8	-1.657853000	-2.394217000	-1.741660000
8	-0.150055000	2.685819000	-1.356132000
7	0.636725000	-2.434711000	-1.564571000
7	-2.429647000	2.667187000	-1.024264000
6	-2.623026000	4.097570000	-1.117373000
1	-3.296912000	4.349861000	-1.943588000
1	-3.034377000	4.501505000	-0.185315000
1	-1.644823000	4.542565000	-1.302207000
6	0.816546000	-3.828853000	-1.909450000
1	1.434830000	-3.932423000	-2.807495000
1	1.286991000	-4.379360000	-1.087343000
1	-0.172742000	-4.244270000	-2.102921000
6	-6.983203000	0.975388000	-0.128697000
6	-7.725125000	2.186004000	-0.117454000
16	-8.069909000	-0.382870000	0.181334000
6	-9.068612000	2.036735000	0.124062000
1	-7.261609000	3.149149000	-0.287199000
6	-9.478676000	0.687251000	0.320057000
1	-9.766139000	2.865893000	0.164214000
6	5.254972000	-0.916036000	-0.697238000
6	5.987946000	-2.075779000	-1.033605000
16	6.355073000	0.326373000	-0.104508000
6	7.344958000	-1.972768000	-0.826623000
1	5.523563000	-2.962293000	-1.446961000
6	7.758567000	-0.713223000	-0.306379000
1	8.053809000	-2.756295000	-1.060807000
6	9.058952000	-0.408705000	0.120015000
6	9.699883000	0.797911000	0.517155000
6	11.270734000	-0.820553000	1.396671000
6	10.909655000	0.533821000	1.352472000
6	12.381249000	-1.304037000	2.069946000
6	11.724205000	1.438855000	2.049556000
6	13.176586000	-0.386211000	2.758156000
1	12.614516000	-2.363564000	2.063091000
6	12.840183000	0.969512000	2.745371000
1	11.500615000	2.495711000	2.066770000
1	14.050877000	-0.727261000	3.303395000
1	13.456266000	1.681044000	3.286303000
6	9.320094000	2.080774000	0.085795000
6	9.806594000	3.293223000	0.651917000

7	10.160946000	4.312285000	1.096877000
6	8.498820000	2.294752000	-1.055787000
7	7.866651000	2.513988000	-2.011667000
16	10.123223000	-1.829074000	0.484777000
8	9.448553000	-2.773908000	1.390824000
8	10.739010000	-2.368182000	-0.741132000
6	-10.749880000	0.219974000	0.578165000
16	-12.140175000	1.295990000	0.711130000
16	-11.111130000	-1.486332000	0.799000000
6	-13.332030000	0.030267000	1.029647000
6	-12.846127000	-1.284691000	1.071080000
6	-14.689880000	0.288169000	1.233496000
6	-13.713535000	-2.351894000	1.316425000
6	-15.551830000	-0.779141000	1.478012000
1	-15.066337000	1.305439000	1.201515000
6	-15.067137000	-2.090321000	1.519190000
1	-13.336807000	-3.369062000	1.348225000
1	-16.607521000	-0.585697000	1.637140000
1	-15.746561000	-2.914357000	1.710239000

S9TIIDTS10-CS E=-4034.170013 Hartree

6	-3.572048000	-1.453796000	0.869434000
6	-2.936486000	-0.172199000	0.658354000
6	-3.772896000	0.892730000	0.218134000
6	-5.114173000	0.682186000	0.026929000
6	-5.741756000	-0.588619000	0.253523000
6	-4.908669000	-1.674000000	0.686217000
6	-1.345549000	-1.750364000	1.281241000
6	-1.552910000	-0.318684000	0.893900000
1	-3.344989000	1.872974000	0.066190000
1	-5.726901000	1.515566000	-0.303825000
1	-5.328427000	-2.657956000	0.857778000
6	-0.491865000	0.634000000	0.849040000
6	0.900124000	0.460039000	0.699398000
6	-0.711940000	2.106135000	1.017513000
6	1.529733000	1.760828000	0.753081000
6	1.752301000	-0.654414000	0.454581000
6	2.873748000	1.957000000	0.600722000
6	3.101309000	-0.469135000	0.296098000
1	1.328436000	-1.647679000	0.425503000
6	3.722376000	0.823382000	0.366341000
1	3.288520000	2.956723000	0.648603000
1	3.725777000	-1.339167000	0.116180000

8	-1.746409000	2.738060000	1.206509000
8	-0.322759000	-2.345877000	1.604643000
7	0.546515000	2.712803000	0.958207000
7	-2.602239000	-2.363356000	1.252732000
6	-2.810896000	-3.753916000	1.582804000
1	-3.493058000	-3.860029000	2.434188000
1	-3.221713000	-4.306926000	0.729826000
1	-1.837800000	-4.169760000	1.847201000
6	0.744894000	4.136859000	1.095661000
1	1.388996000	4.365135000	1.952666000
1	1.195040000	4.563884000	0.191693000
1	-0.237551000	4.583242000	1.254654000
6	-7.122698000	-0.773414000	0.056695000
6	-7.891813000	-1.956384000	0.242061000
16	-8.192501000	0.533739000	-0.493138000
6	-9.228457000	-1.831510000	-0.033160000
1	-7.446002000	-2.884027000	0.578268000
6	-9.620122000	-0.525898000	-0.461048000
1	-9.939932000	-2.644354000	0.061656000
6	5.110937000	0.982207000	0.208537000
6	5.874314000	2.183094000	0.256038000
16	6.201019000	-0.386959000	-0.095500000
6	7.221253000	2.025423000	0.064653000
1	5.415766000	3.147862000	0.432947000
6	7.629482000	0.671842000	-0.150550000
1	7.929808000	2.846116000	0.073739000
6	-10.876229000	-0.092912000	-0.805856000
16	-11.225998000	1.564107000	-1.322252000
16	-12.302704000	-1.148950000	-0.773915000
6	-12.947458000	1.306140000	-1.560421000
6	-13.432332000	0.083056000	-1.313145000
1	-14.470001000	-0.207832000	-1.419690000
1	-13.534781000	2.151463000	-1.896650000
6	8.898667000	0.200537000	-0.368598000
16	10.312431000	1.268124000	-0.420623000
16	9.257691000	-1.511105000	-0.619343000
6	11.501183000	-0.006249000	-0.719709000
6	11.004649000	-1.315212000	-0.813366000
6	12.868956000	0.239590000	-0.860970000
6	11.873549000	-2.383216000	-1.048502000
6	13.732697000	-0.829552000	-1.095705000
1	13.252950000	1.252150000	-0.788356000
6	13.238078000	-2.133279000	-1.188921000
1	11.488410000	-3.395366000	-1.120530000

1	14.795918000	-0.642125000	-1.205880000
1	13.916217000	-2.960552000	-1.371613000

S9TIIDTS1-OS E=-3346.081340 Hartree

6	0.796511000	1.747261000	0.508765000
6	0.181504000	0.454169000	0.464940000
6	1.039102000	-0.653431000	0.289207000
6	2.405006000	-0.466681000	0.189348000
6	3.006695000	0.818797000	0.257060000
6	2.153748000	1.947264000	0.416559000
6	-1.448662000	2.136183000	0.644387000
6	-1.245535000	0.640541000	0.540444000
1	0.624267000	-1.649082000	0.256517000
1	3.034934000	-1.341541000	0.061721000
1	2.560121000	2.950449000	0.455956000
6	-2.304079000	-0.273456000	0.566404000
6	-3.725493000	-0.101216000	0.384347000
6	-2.114731000	-1.743330000	0.866480000
6	-4.346611000	-1.380415000	0.554384000
6	-4.564924000	0.972791000	0.019801000
6	-5.697591000	-1.594452000	0.408490000
6	-5.924161000	0.770956000	-0.136618000
1	-4.144922000	1.957768000	-0.113347000
6	-6.532995000	-0.497778000	0.057587000
1	-6.110669000	-2.585700000	0.548590000
1	-6.541701000	1.620654000	-0.409794000
8	-1.095022000	-2.370499000	1.122786000
8	-2.479689000	2.784898000	0.762866000
7	-3.376866000	-2.324707000	0.857325000
7	-0.186772000	2.717767000	0.634310000
6	0.027944000	4.144751000	0.736728000
1	0.632082000	4.387298000	1.617828000
1	0.530131000	4.531947000	-0.156956000
1	-0.952088000	4.612953000	0.831507000
6	-3.604815000	-3.728237000	1.124734000
1	-4.259915000	-3.859650000	1.992819000
1	-4.057012000	-4.224980000	0.259024000
1	-2.634379000	-4.179004000	1.333643000
6	4.425411000	0.988231000	0.164117000
6	5.171988000	2.179385000	0.227678000
16	5.517400000	-0.382584000	-0.061010000
6	6.540141000	2.016420000	0.104074000
1	4.708780000	3.148392000	0.365581000

6	6.944827000	0.667934000	-0.065293000
1	7.247640000	2.837145000	0.133688000
6	-7.946685000	-0.681564000	-0.098467000
6	-8.699007000	-1.855429000	0.083230000
16	-9.013475000	0.642677000	-0.577400000
6	-10.057549000	-1.712141000	-0.146466000
1	-8.251564000	-2.795003000	0.382845000
6	-10.427553000	-0.399422000	-0.523328000
1	-10.787167000	-2.507353000	-0.053446000
6	-11.718980000	0.063159000	-0.823493000
6	-12.822435000	-0.829664000	-0.763234000
7	-13.710887000	-1.583795000	-0.706236000
6	-11.963066000	1.411554000	-1.191282000
7	-12.140055000	2.525265000	-1.491937000
6	8.231537000	0.177296000	-0.215663000
16	9.643977000	1.236848000	-0.218505000
16	8.586230000	-1.535965000	-0.417469000
6	10.839915000	-0.046336000	-0.440583000
6	10.341349000	-1.354250000	-0.534528000
6	12.214065000	0.191835000	-0.522631000
6	11.213384000	-2.431219000	-0.711007000
6	13.080602000	-0.885562000	-0.698741000
1	12.599978000	1.203553000	-0.449929000
6	12.583523000	-2.188958000	-0.792364000
1	10.826765000	-3.442670000	-0.783520000
1	14.148763000	-0.705720000	-0.763048000
1	13.265316000	-3.021882000	-0.929398000

S9TIIDTS3-OS E=-3913.937971 Hartree

6	-2.584028000	-1.449318000	0.616714000
6	-1.985473000	-0.164974000	0.442096000
6	-2.845207000	0.899874000	0.116747000
6	-4.210871000	0.682999000	0.000311000
6	-4.792894000	-0.589742000	0.198933000
6	-3.940311000	-1.677331000	0.511775000
6	-0.341193000	-1.798041000	0.865831000
6	-0.548129000	-0.325957000	0.585446000
1	-2.441283000	1.889925000	-0.025762000
1	-4.843939000	1.524461000	-0.263108000
1	-4.341916000	-2.669248000	0.679569000
6	0.498477000	0.591997000	0.539820000
6	1.933478000	0.419723000	0.457639000
6	0.284143000	2.091146000	0.622392000

6	2.532003000	1.718097000	0.481166000
6	2.802865000	-0.677613000	0.292660000
6	3.887138000	1.934640000	0.379343000
6	4.167983000	-0.475316000	0.183236000
1	2.400796000	-1.678591000	0.273693000
6	4.752627000	0.816241000	0.230771000
1	4.280456000	2.943513000	0.402089000
1	4.807364000	-1.344618000	0.065411000
8	-0.751130000	2.733607000	0.735230000
8	0.688483000	-2.422453000	1.087305000
7	1.539246000	2.681840000	0.598188000
7	-1.598491000	-2.387790000	0.886902000
6	-1.808530000	-3.795517000	1.147054000
1	-2.436231000	-3.940155000	2.033110000
1	-2.283452000	-4.286651000	0.290361000
1	-0.829243000	-4.241439000	1.322050000
6	1.742926000	4.111985000	0.678912000
1	2.350354000	4.371397000	1.552848000
1	2.237224000	4.489815000	-0.223085000
1	0.759992000	4.574096000	0.772634000
6	-6.221816000	-0.795869000	0.084260000
6	-6.926471000	-1.997695000	0.063185000
16	-7.340689000	0.552505000	-0.054430000
6	-8.311708000	-1.851127000	-0.067948000
1	-6.440886000	-2.963778000	0.121060000
6	-8.731809000	-0.521938000	-0.151608000
1	-9.002716000	-2.685229000	-0.111516000
6	6.172471000	1.003947000	0.128484000
6	6.903870000	2.201475000	0.184147000
16	7.277508000	-0.355066000	-0.099277000
6	8.275504000	2.053667000	0.053157000
1	6.430994000	3.165750000	0.323163000
6	8.692850000	0.710477000	-0.114250000
1	8.973821000	2.882322000	0.077119000
6	-10.051827000	-0.023667000	-0.289840000
6	-10.473678000	1.315455000	-0.401907000
16	-11.470545000	-1.057284000	-0.348192000
1	-9.784744000	2.154540000	-0.394435000
6	-12.479566000	0.401651000	-0.517713000
6	-13.876118000	0.336972000	-0.632078000
6	-14.548967000	-0.912088000	-0.618004000
7	-15.076185000	-1.953119000	-0.603565000
6	-14.648528000	1.521462000	-0.764755000
7	-15.310900000	2.474513000	-0.875103000

7	-11.777312000	1.546582000	-0.524548000
6	9.985187000	0.231329000	-0.270751000
16	11.385599000	1.306212000	-0.286287000
16	10.356516000	-1.478765000	-0.468221000
6	12.593887000	0.035010000	-0.510075000
6	12.108843000	-1.278620000	-0.596074000
6	13.964963000	0.287441000	-0.600996000
6	12.991461000	-2.346829000	-0.773415000
6	14.842023000	-0.781252000	-0.777936000
1	14.340399000	1.303518000	-0.534427000
6	14.358427000	-2.090265000	-0.863635000
1	12.615317000	-3.362649000	-0.839755000
1	15.907809000	-0.590228000	-0.849100000
1	15.048324000	-2.916378000	-1.001375000

S9TIIDTS4-OS E=-3879.960008 Hartree

6	3.051618000	-1.599313000	-0.651840000
6	2.465205000	-0.299443000	-0.548753000
6	3.338695000	0.773172000	-0.279064000
6	4.699137000	0.548388000	-0.147513000
6	5.272409000	-0.742649000	-0.274853000
6	4.402353000	-1.836816000	-0.529366000
6	0.803382000	-1.932325000	-0.876751000
6	1.030981000	-0.450657000	-0.679967000
1	2.946016000	1.774904000	-0.198595000
1	5.343619000	1.398961000	0.049527000
1	4.787170000	-2.845824000	-0.612704000
6	-0.006289000	0.484184000	-0.683051000
6	-1.438780000	0.334915000	-0.567051000
6	0.224974000	1.968124000	-0.872887000
6	-2.024994000	1.636298000	-0.667782000
6	-2.317254000	-0.739308000	-0.314339000
6	-3.375477000	1.874433000	-0.557652000
6	-3.677420000	-0.514485000	-0.195887000
1	-1.925031000	-1.741513000	-0.236057000
6	-4.250613000	0.778321000	-0.319618000
1	-3.759080000	2.883801000	-0.642971000
1	-4.323979000	-1.366110000	-0.008261000
8	1.265739000	2.587852000	-1.049831000
8	-0.235556000	-2.553826000	-1.063000000
7	-1.023411000	2.576737000	-0.866779000
7	2.052655000	-2.539490000	-0.864556000
6	2.243446000	-3.961661000	-1.044906000

1	2.871155000	-4.164625000	-1.919623000
1	2.709979000	-4.411417000	-0.161104000
1	1.258196000	-4.402937000	-1.197426000
6	-1.210620000	3.999951000	-1.042758000
1	-1.830036000	4.207567000	-1.922303000
1	-1.684420000	4.446458000	-0.161200000
1	-0.223451000	4.440577000	-1.184445000
6	6.691427000	-0.951077000	-0.146661000
6	7.402714000	-2.151530000	-0.301739000
16	7.793959000	0.368326000	0.248752000
6	8.770835000	-2.030241000	-0.115480000
1	6.926362000	-3.091069000	-0.553123000
6	9.190504000	-0.714561000	0.197399000
1	9.469755000	-2.854448000	-0.200374000
6	-5.665003000	0.988047000	-0.206129000
6	-6.385100000	2.189369000	-0.315711000
16	-6.783299000	-0.344185000	0.112504000
6	-7.755579000	2.066140000	-0.155628000
1	-5.903369000	3.139099000	-0.512993000
6	-8.186888000	0.738562000	0.091370000
1	-8.444720000	2.900838000	-0.213209000
6	10.488282000	-0.281005000	0.438660000
6	10.842649000	1.097321000	0.754387000
16	11.913011000	-1.322771000	0.401544000
6	12.995552000	0.081700000	0.807805000
7	12.230563000	1.220955000	0.942859000
6	12.856976000	2.496724000	1.269807000
1	13.579084000	2.770994000	0.497344000
1	12.061409000	3.239250000	1.323280000
1	13.374925000	2.427446000	2.229126000
8	14.194853000	0.002554000	0.934246000
8	10.063331000	2.039890000	0.849826000
6	-9.480447000	0.285276000	0.292907000
16	-10.870556000	1.377408000	0.269745000
16	-9.869743000	-1.408811000	0.589826000
6	-12.088999000	0.133917000	0.579548000
6	-11.617680000	-1.179012000	0.730479000
6	-13.455717000	0.406861000	0.675635000
6	-12.510302000	-2.224618000	0.978045000
6	-14.342916000	-0.639596000	0.922825000
1	-13.820370000	1.422393000	0.558844000
6	-13.873162000	-1.947531000	1.073151000
1	-12.144685000	-3.239829000	1.094485000
1	-15.405314000	-0.431671000	0.998124000

1	-14.570130000	-2.756749000	1.265324000
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S9TIIDTS5- OS E=-3651.425280 Hartree

6	-2.662250000	-1.596119000	0.699035000
6	-2.071260000	-0.296187000	0.595209000
6	-2.941921000	0.781357000	0.325507000
6	-4.301069000	0.561598000	0.194859000
6	-4.879588000	-0.729839000	0.323257000
6	-4.012777000	-1.828113000	0.577950000
6	-0.415963000	-1.933342000	0.921801000
6	-0.642138000	-0.450061000	0.724152000
1	-2.545084000	1.781502000	0.244939000
1	-4.943466000	1.412987000	-0.003849000
1	-4.402450000	-2.834933000	0.663513000
6	0.397725000	0.484618000	0.727746000
6	1.825613000	0.332539000	0.598692000
6	0.170424000	1.965787000	0.935661000
6	2.417456000	1.632311000	0.709490000
6	2.697491000	-0.743398000	0.325556000
6	3.767562000	1.865469000	0.591500000
6	4.056257000	-0.522777000	0.198880000
1	2.300242000	-1.742977000	0.239145000
6	4.635705000	0.767387000	0.333741000
1	4.156375000	2.871933000	0.685912000
1	4.697889000	-1.374441000	-0.004785000
8	-0.867877000	2.584440000	1.126868000
8	0.623200000	-2.553524000	1.106870000
7	1.420922000	2.572210000	0.927262000
7	-1.665912000	-2.538423000	0.911435000
6	-1.859926000	-3.960694000	1.092687000
1	-2.486590000	-4.161237000	1.968490000
1	-2.328623000	-4.409058000	0.209539000
1	-0.875728000	-4.404573000	1.243989000
6	1.612383000	3.993486000	1.117489000
1	2.237874000	4.190095000	1.995142000
1	2.080486000	4.448470000	0.237340000
1	0.627125000	4.434408000	1.270856000
6	-6.296567000	-0.931661000	0.195350000
6	-7.009085000	-2.133444000	0.335930000
16	-7.399320000	0.392448000	-0.180386000
6	-8.375561000	-1.999858000	0.151852000
1	-6.539699000	-3.080321000	0.572662000
6	-8.793070000	-0.680566000	-0.143282000

1	-9.065255000	-2.830972000	0.228823000
6	6.047937000	0.971144000	0.211696000
6	6.773337000	2.171497000	0.326820000
16	7.158101000	-0.360709000	-0.126238000
6	8.140161000	2.044183000	0.155572000
1	6.296038000	3.120749000	0.535556000
6	8.564807000	0.716967000	-0.106340000
1	8.832663000	2.876012000	0.215086000
6	-10.117715000	-0.242936000	-0.380875000
6	-11.219940000	-1.126423000	-0.347514000
6	-10.368338000	1.177510000	-0.673703000
6	-12.505753000	-0.697287000	-0.578167000
1	-11.061895000	-2.177736000	-0.134909000
6	-12.806415000	0.712727000	-0.873580000
6	-13.597906000	-1.610372000	-0.538516000
7	-14.460537000	-2.391699000	-0.496296000
8	-9.464050000	2.013839000	-0.723394000
8	-13.938459000	1.126926000	-1.083024000
7	-11.688049000	1.567816000	-0.899986000
6	-11.906660000	2.989462000	-1.188129000
1	-11.549284000	3.595398000	-0.352968000
1	-11.348633000	3.275958000	-2.081957000
1	-12.973626000	3.132931000	-1.338509000
6	9.855820000	0.262261000	-0.321279000
16	11.247374000	1.348019000	-0.298131000
16	10.235981000	-1.427740000	-0.636061000
6	12.460318000	0.105007000	-0.629155000
6	11.983496000	-1.204633000	-0.788688000
6	13.827046000	0.375266000	-0.733227000
6	12.869806000	-2.251552000	-1.053094000
6	14.707851000	-0.672140000	-0.997145000
1	14.196208000	1.388309000	-0.609829000
6	14.232390000	-1.977342000	-1.156099000
1	12.499984000	-3.264376000	-1.176222000
1	15.770326000	-0.467495000	-1.078908000
1	14.925366000	-2.786678000	-1.361312000

S9TIIDTS6-OS E=-4012.746559 Hartree

6	-2.280556000	-1.642484000	0.734482000
6	-1.694788000	-0.336920000	0.642068000
6	-2.571468000	0.740088000	0.378779000
6	-3.927024000	0.514906000	0.243206000
6	-4.501945000	-0.783122000	0.359636000

6	-3.627841000	-1.880342000	0.608460000
6	-0.032837000	-1.965327000	0.960959000
6	-0.269506000	-0.482797000	0.772185000
1	-2.178541000	1.742643000	0.307820000
1	-4.574263000	1.363220000	0.047797000
1	-4.013893000	-2.888977000	0.687277000
6	0.765898000	0.460952000	0.783633000
6	2.190636000	0.319169000	0.640477000
6	0.530305000	1.935022000	1.018708000
6	2.777464000	1.620990000	0.767423000
6	3.065908000	-0.748495000	0.342023000
6	4.124840000	1.862495000	0.641261000
6	4.421490000	-0.518961000	0.207081000
1	2.672646000	-1.748677000	0.243698000
6	4.996485000	0.772642000	0.357753000
1	4.509855000	2.869137000	0.748753000
1	5.065873000	-1.363603000	-0.016335000
8	-0.510551000	2.543316000	1.229691000
8	1.010936000	-2.578099000	1.144778000
7	1.777406000	2.550510000	1.009395000
7	-1.278485000	-2.579424000	0.942924000
6	-1.463477000	-4.004151000	1.114337000
1	-2.090996000	-4.214597000	1.987166000
1	-1.927215000	-4.449666000	0.227174000
1	-0.476679000	-4.442445000	1.265106000
6	1.960981000	3.969459000	1.222153000
1	2.592746000	4.155721000	2.097618000
1	2.418188000	4.442850000	0.345938000
1	0.974009000	4.400687000	1.391532000
6	-5.911308000	-0.989167000	0.226013000
6	-6.618071000	-2.203083000	0.333726000
16	-7.024857000	0.338669000	-0.115343000
6	-7.980851000	-2.083832000	0.153254000
1	-6.139024000	-3.151810000	0.543378000
6	-8.414704000	-0.751685000	-0.108927000
1	-8.690652000	-2.895372000	0.198232000
6	6.404901000	0.984813000	0.226255000
6	7.125808000	2.188117000	0.351876000
16	7.519857000	-0.336243000	-0.140456000
6	8.490760000	2.070857000	0.166654000
1	6.645093000	3.131632000	0.578018000
6	8.921003000	0.749338000	-0.118014000
1	9.179345000	2.905566000	0.231506000
6	-9.730336000	-0.305451000	-0.336325000

6	-10.852786000	-1.237052000	-0.325080000
6	-9.960604000	1.106167000	-0.584831000
6	-12.381120000	0.667624000	-0.803415000
8	-9.047765000	1.934889000	-0.607218000
7	-11.290575000	1.517276000	-0.805649000
6	-11.507479000	2.950510000	-1.053805000
1	-12.177790000	3.359668000	-0.296540000
1	-10.534925000	3.432698000	-1.011408000
1	-11.968710000	3.091059000	-2.032466000
7	-12.132565000	-0.670955000	-0.565769000
6	-13.271290000	-1.602154000	-0.556862000
1	-13.985298000	-1.306023000	0.213085000
1	-13.778330000	-1.575664000	-1.522542000
1	-12.872870000	-2.592142000	-0.355524000
8	-10.759192000	-2.446316000	-0.125969000
16	-13.934107000	1.239828000	-1.077552000
6	10.211823000	0.306000000	-0.350795000
16	11.597912000	1.399635000	-0.324686000
16	10.599300000	-1.377555000	-0.693105000
6	12.814769000	0.168366000	-0.684348000
6	12.344064000	-1.141668000	-0.858169000
6	14.178902000	0.448027000	-0.796882000
6	13.234051000	-2.179392000	-1.145348000
6	15.063438000	-0.590283000	-1.083558000
1	14.543289000	1.461404000	-0.662430000
6	14.594113000	-1.895833000	-1.256723000
1	12.868952000	-3.192540000	-1.279501000
1	16.123927000	-0.378167000	-1.171944000
1	15.289808000	-2.698144000	-1.479616000

S9TIIDTS7-OS E=-3766.676821 Hartree

6	2.088318000	-1.676516000	-1.042440000
6	1.519499000	-0.374308000	-0.864672000
6	2.413778000	0.681109000	-0.584107000
6	3.773237000	0.439049000	-0.507247000
6	4.326841000	-0.854262000	-0.704493000
6	3.438442000	-1.931036000	-0.975610000
6	-0.168628000	-1.976223000	-1.199114000
6	0.084611000	-0.505232000	-0.949363000
1	2.034614000	1.683380000	-0.458096000
1	4.436933000	1.276038000	-0.316604000
1	3.812256000	-2.939847000	-1.100093000
6	-0.942363000	0.441039000	-0.876720000

6	-2.366835000	0.300629000	-0.703918000
6	-0.702762000	1.927244000	-1.028837000
6	-2.944743000	1.611015000	-0.738590000
6	-3.243300000	-0.775430000	-0.446070000
6	-4.286745000	1.854954000	-0.563460000
6	-4.593756000	-0.544212000	-0.262314000
1	-2.856819000	-1.782473000	-0.416121000
6	-5.160169000	0.757388000	-0.322020000
1	-4.664959000	2.869134000	-0.601528000
1	-5.239362000	-1.396047000	-0.072362000
8	0.336294000	2.541362000	-1.228844000
8	-1.221938000	-2.575398000	-1.373230000
7	-1.944117000	2.547495000	-0.950977000
7	1.072298000	-2.596919000	-1.255991000
6	1.240715000	-4.012604000	-1.503047000
1	1.835935000	-4.183266000	-2.406620000
1	1.731732000	-4.503732000	-0.655507000
1	0.246101000	-4.437431000	-1.640204000
6	-2.122792000	3.977856000	-1.074057000
1	-2.776283000	4.219154000	-1.919553000
1	-2.553075000	4.400583000	-0.159198000
1	-1.137685000	4.412950000	-1.244165000
6	5.740896000	-1.086263000	-0.624006000
6	6.450955000	-2.251923000	-0.961247000
16	6.854995000	0.148314000	-0.061490000
6	7.818792000	-2.162844000	-0.774371000
1	5.967972000	-3.136403000	-1.357932000
6	8.253309000	-0.902143000	-0.283979000
1	8.526969000	-2.955658000	-0.967214000
6	-6.564423000	0.972728000	-0.141896000
6	-7.277142000	2.185440000	-0.180694000
16	-7.680338000	-0.358995000	0.178546000
6	-8.638841000	2.067543000	0.033060000
1	-6.794524000	3.136885000	-0.365973000
6	-9.072220000	0.735546000	0.253612000
1	-9.321678000	2.909429000	0.033018000
6	9.567194000	-0.593615000	0.113936000
6	10.544126000	-1.687246000	0.418795000
6	10.173352000	0.655118000	0.515755000
6	11.634489000	-1.052987000	1.200438000
6	11.396434000	0.328522000	1.306125000
6	12.734789000	-1.667079000	1.780060000
6	12.286802000	1.119746000	2.035692000
6	13.622201000	-0.872055000	2.510604000

1	12.881970000	-2.735746000	1.660767000
6	13.390630000	0.501338000	2.636682000
1	12.142806000	2.184969000	2.154499000
1	14.491256000	-1.318375000	2.984244000
1	14.081599000	1.109260000	3.212929000
8	10.472368000	-2.875118000	0.132041000
6	9.818177000	1.943000000	0.124072000
6	8.930731000	2.231605000	-0.954710000
7	8.261507000	2.524928000	-1.862911000
6	10.429597000	3.113109000	0.667641000
7	10.892249000	4.090537000	1.103335000
6	-10.360885000	0.287859000	0.494606000
16	-11.737719000	1.390713000	0.566823000
16	-10.753202000	-1.409667000	0.750677000
6	-12.955159000	0.149396000	0.887637000
6	-12.491089000	-1.171652000	0.974422000
6	-14.313587000	0.431534000	1.051539000
6	-13.382046000	-2.217921000	1.225396000
6	-15.199073000	-0.615314000	1.301852000
1	-14.672842000	1.453401000	0.984389000
6	-14.736362000	-1.931819000	1.388242000
1	-13.022088000	-3.239551000	1.292208000
1	-16.255131000	-0.401305000	1.429859000
1	-15.432777000	-2.740720000	1.583343000

S9TIIDTS8-OS E=-4201.897606 Hartree

6	-3.426363000	1.684402000	-0.695482000
6	-2.831630000	0.381513000	-0.699128000
6	-3.692905000	-0.712755000	-0.470561000
6	-5.046246000	-0.504742000	-0.278313000
6	-5.629373000	0.790154000	-0.300412000
6	-4.771353000	1.905556000	-0.511650000
6	-1.189577000	2.039927000	-0.979574000
6	-1.408386000	0.545895000	-0.870444000
1	-3.293132000	-1.714973000	-0.469300000
1	-5.679940000	-1.370236000	-0.111484000
1	-5.162909000	2.915306000	-0.520440000
6	-0.369816000	-0.382769000	-0.972630000
6	1.065241000	-0.234287000	-0.893198000
6	-0.603853000	-1.851343000	-1.257883000
6	1.649240000	-1.523216000	-1.108595000
6	1.946264000	0.825076000	-0.590391000
6	3.003815000	-1.761106000	-1.056861000

6	3.310068000	0.599322000	-0.528281000
1	1.554812000	1.818575000	-0.436302000
6	3.877371000	-0.679998000	-0.763270000
1	3.391093000	-2.761658000	-1.204956000
1	3.964314000	1.440373000	-0.323261000
8	-1.649829000	-2.460428000	-1.440231000
8	-0.159553000	2.673696000	-1.162697000
7	0.644952000	-2.452285000	-1.338694000
7	-2.439000000	2.640199000	-0.882362000
6	-2.637675000	4.071094000	-0.963587000
1	-3.295774000	4.327543000	-1.800955000
1	-3.072212000	4.460801000	-0.036215000
1	-1.659049000	4.524688000	-1.122181000
6	0.832126000	-3.859264000	-1.621577000
1	1.423645000	-3.998676000	-2.532811000
1	1.335796000	-4.363382000	-0.789362000
1	-0.157035000	-4.295178000	-1.762895000
6	-7.036615000	0.981872000	-0.112293000
6	-7.764701000	2.185835000	-0.115179000
16	-8.133713000	-0.372640000	0.170833000
6	-9.124503000	2.043673000	0.096967000
1	-7.294929000	3.148465000	-0.273443000
6	-9.539385000	0.700541000	0.279441000
1	-9.818310000	2.876155000	0.122271000
6	5.297462000	-0.896891000	-0.698574000
6	6.021719000	-2.022831000	-1.119176000
16	6.388441000	0.310919000	-0.045929000
6	7.390358000	-1.921065000	-0.928807000
1	5.553503000	-2.880381000	-1.585656000
6	7.799314000	-0.696455000	-0.348711000
1	8.102542000	-2.680691000	-1.225740000
6	9.108527000	-0.397008000	0.070485000
6	9.764942000	0.802370000	0.451455000
6	11.353418000	-0.824103000	1.287096000
6	10.998925000	0.532546000	1.249606000
6	12.482577000	-1.311797000	1.925387000
6	11.840174000	1.434659000	1.917484000
6	13.305526000	-0.396140000	2.583433000
1	12.709553000	-2.372641000	1.915226000
6	12.976092000	0.961163000	2.577594000
1	11.623560000	2.492821000	1.939827000
1	14.195374000	-0.740413000	3.100573000
1	13.613312000	1.670940000	3.095719000
6	9.378421000	2.087908000	0.025688000

6	9.897513000	3.298657000	0.564360000
7	10.277264000	4.317872000	0.987490000
6	8.514676000	2.306347000	-1.084204000
7	7.850598000	2.537762000	-2.014909000
16	10.166446000	-1.829091000	0.423628000
8	9.501032000	-2.747903000	1.360788000
8	10.731001000	-2.387616000	-0.817492000
6	-10.822172000	0.228819000	0.509409000
16	-12.212366000	1.310379000	0.615412000
16	-11.191002000	-1.479601000	0.716745000
6	-13.412887000	0.044876000	0.903124000
6	-12.931250000	-1.271813000	0.950977000
6	-14.774474000	0.304462000	1.077951000
6	-13.807490000	-2.336774000	1.173731000
6	-15.645181000	-0.760876000	1.300007000
1	-15.147374000	1.322950000	1.040953000
6	-15.164906000	-2.073178000	1.347588000
1	-13.433980000	-3.355035000	1.210489000
1	-16.703639000	-0.564773000	1.436409000
1	-15.850189000	-2.896385000	1.520919000

S9TIIDTS10- OS E=-4034.175252 Hartree

6	-3.582558000	-1.460944000	0.632130000
6	-2.975553000	-0.174415000	0.480309000
6	-3.833922000	0.895657000	0.153146000
6	-5.194363000	0.681664000	0.012883000
6	-5.788404000	-0.595559000	0.186691000
6	-4.933412000	-1.688067000	0.500902000
6	-1.341315000	-1.807852000	0.907573000
6	-1.547901000	-0.336080000	0.638758000
1	-3.426874000	1.888107000	0.035064000
1	-5.824917000	1.530910000	-0.231964000
1	-5.332258000	-2.687435000	0.626654000
6	-0.496833000	0.586576000	0.612364000
6	0.935184000	0.412686000	0.519099000
6	-0.710023000	2.076993000	0.731227000
6	1.538772000	1.708870000	0.567268000
6	1.802374000	-0.682525000	0.325619000
6	2.893670000	1.924512000	0.460985000
6	3.167142000	-0.480862000	0.211881000
1	1.397953000	-1.682386000	0.289635000
6	3.757067000	0.808184000	0.282462000
1	3.289644000	2.931992000	0.503329000

1	3.804318000	-1.348650000	0.071606000
8	-1.743946000	2.720987000	0.866721000
8	-0.313722000	-2.434045000	1.139894000
7	0.547187000	2.669760000	0.711730000
7	-2.598079000	-2.401859000	0.902125000
6	-2.807347000	-3.811299000	1.144257000
1	-3.450043000	-3.968348000	2.017835000
1	-3.266404000	-4.296984000	0.275408000
1	-1.829070000	-4.255075000	1.331379000
6	0.750505000	4.096294000	0.824068000
1	1.363248000	4.337700000	1.699925000
1	1.239867000	4.496753000	-0.071295000
1	-0.232812000	4.554521000	0.934031000
6	-7.203086000	-0.794174000	0.048914000
6	-7.943800000	-1.975660000	0.205635000
16	-8.295537000	0.533976000	-0.372107000
6	-9.309641000	-1.843508000	0.003704000
1	-7.481437000	-2.919407000	0.468109000
6	-9.715268000	-0.527062000	-0.327121000
1	-10.012158000	-2.664604000	0.089990000
6	5.175782000	0.994765000	0.174576000
6	5.912515000	2.187694000	0.245439000
16	6.279283000	-0.365200000	-0.083521000
6	7.283464000	2.040154000	0.103209000
1	5.442587000	3.150791000	0.403319000
6	7.698967000	0.698180000	-0.089725000
1	7.983768000	2.866862000	0.136525000
6	-10.996224000	-0.066136000	-0.586959000
16	-11.365133000	1.617091000	-0.988829000
16	-12.416917000	-1.126580000	-0.543255000
6	-13.096676000	1.369709000	-1.153447000
6	-13.570183000	0.133377000	-0.952554000
1	-14.612716000	-0.151038000	-1.023292000
1	-13.699915000	2.231514000	-1.410373000
6	8.986656000	0.219686000	-0.261826000
16	10.394169000	1.293843000	-0.267751000
16	9.356348000	-1.491852000	-0.491195000
6	11.596923000	0.021735000	-0.517618000
6	11.108547000	-1.289734000	-0.622973000
6	12.968269000	0.271254000	-0.610693000
6	11.989451000	-2.355463000	-0.821665000
6	13.843778000	-0.795585000	-0.809084000
1	13.345859000	1.285567000	-0.529076000
6	13.357267000	-2.101518000	-0.913991000

1	11.610606000	-3.369325000	-0.902840000
1	14.909653000	-0.604802000	-0.881736000
1	14.044346000	-2.927242000	-1.068277000

S9TIIDTS1-T1 E=-3346.077132 Hartree

6	0.802655000	1.724952000	0.498572000
6	0.193911000	0.436302000	0.446360000
6	1.053963000	-0.665182000	0.282088000
6	2.425487000	-0.474522000	0.199135000
6	3.019107000	0.808271000	0.273419000
6	2.162792000	1.930838000	0.421831000
6	-1.441365000	2.130622000	0.608535000
6	-1.247324000	0.623755000	0.506373000
1	0.643220000	-1.661841000	0.241057000
1	3.058420000	-1.348800000	0.084759000
1	2.564839000	2.935784000	0.460186000
6	-2.302865000	-0.274182000	0.519143000
6	-3.748582000	-0.085539000	0.377687000
6	-2.120994000	-1.757698000	0.744142000
6	-4.361190000	-1.365210000	0.513467000
6	-4.589387000	0.996806000	0.077527000
6	-5.721133000	-1.574138000	0.394589000
6	-5.960855000	0.801737000	-0.049430000
1	-4.173954000	1.986188000	-0.029903000
6	-6.557059000	-0.466987000	0.112592000
1	-6.131313000	-2.572604000	0.485521000
1	-6.585769000	1.665160000	-0.254767000
8	-1.103060000	-2.409253000	0.940253000
8	-2.470044000	2.783233000	0.716212000
7	-3.388296000	-2.326485000	0.746747000
7	-0.180779000	2.701987000	0.611713000
6	0.042592000	4.127967000	0.716396000
1	0.641255000	4.364636000	1.602632000
1	0.556133000	4.510477000	-0.172634000
1	-0.934227000	4.604119000	0.802552000
6	-3.620110000	-3.739418000	0.955095000
1	-4.254412000	-3.905880000	1.832599000
1	-4.098080000	-4.192478000	0.079280000
1	-2.648287000	-4.205661000	1.118062000
6	4.448701000	0.986975000	0.197448000
6	5.190844000	2.166120000	0.319000000
16	5.539010000	-0.374961000	-0.081652000
6	6.567266000	2.007121000	0.198983000

1	4.729232000	3.128952000	0.501508000
6	6.967473000	0.669854000	-0.026150000
1	7.275456000	2.824123000	0.273411000
6	-7.990312000	-0.650470000	-0.007011000
6	-8.754005000	-1.762741000	0.361992000
16	-9.025968000	0.599714000	-0.685534000
6	-10.118941000	-1.627130000	0.121868000
1	-8.320128000	-2.642942000	0.819949000
6	-10.462314000	-0.386759000	-0.451970000
1	-10.863687000	-2.379271000	0.352695000
6	-11.750140000	0.057072000	-0.813894000
6	-12.872680000	-0.789051000	-0.613781000
7	-13.778206000	-1.503783000	-0.438616000
6	-11.968083000	1.338472000	-1.380542000
7	-12.125235000	2.397338000	-1.845897000
6	8.257124000	0.176600000	-0.188901000
16	9.672730000	1.232743000	-0.138153000
16	8.607636000	-1.529582000	-0.460042000
6	10.865877000	-0.045499000	-0.401002000
6	10.364270000	-1.347199000	-0.553133000
6	12.241628000	0.190310000	-0.460814000
6	11.235528000	-2.418306000	-0.765741000
6	13.107266000	-0.881447000	-0.673133000
1	12.629699000	1.197015000	-0.343069000
6	12.607316000	-2.178074000	-0.824743000
1	10.846528000	-3.424673000	-0.883187000
1	14.176512000	-0.702328000	-0.720199000
1	13.287705000	-3.007166000	-0.989684000

S9TIIDTS3-T1 E=-3913.935667 Hartree

6	-2.591351000	-1.426690000	0.513334000
6	-1.995870000	-0.149149000	0.307904000
6	-2.851511000	0.905015000	-0.044349000
6	-4.221450000	0.685340000	-0.158735000
6	-4.797330000	-0.579285000	0.071332000
6	-3.950814000	-1.657561000	0.413480000
6	-0.348568000	-1.774281000	0.780792000
6	-0.548190000	-0.309923000	0.464511000
1	-2.447586000	1.890386000	-0.214472000
1	-4.854764000	1.515679000	-0.455029000
1	-4.358620000	-2.640421000	0.618061000
6	0.497189000	0.599216000	0.400209000
6	1.940046000	0.425718000	0.358607000

6	0.284752000	2.106098000	0.405328000
6	2.534302000	1.722624000	0.333268000
6	2.814709000	-0.673525000	0.268324000
6	3.891920000	1.939762000	0.251794000
6	4.183857000	-0.471966000	0.180957000
1	2.416076000	-1.675694000	0.287580000
6	4.762906000	0.820295000	0.178442000
1	4.281772000	2.950033000	0.230766000
1	4.827522000	-1.344087000	0.123997000
8	-0.751783000	2.753144000	0.464139000
8	0.676361000	-2.400018000	1.020793000
7	1.538627000	2.692315000	0.379602000
7	-1.608463000	-2.358891000	0.811998000
6	-1.823221000	-3.759126000	1.106019000
1	-2.452972000	-3.880398000	1.994186000
1	-2.298469000	-4.269326000	0.260665000
1	-0.845531000	-4.203475000	1.293346000
6	1.744051000	4.124561000	0.395145000
1	2.333467000	4.424553000	1.268353000
1	2.259332000	4.456603000	-0.513012000
1	0.760895000	4.592836000	0.444728000
6	-6.233513000	-0.794552000	-0.044547000
6	-6.915306000	-1.990933000	-0.226467000
16	-7.367580000	0.538617000	0.044564000
6	-8.309813000	-1.848679000	-0.306259000
1	-6.409214000	-2.942494000	-0.331923000
6	-8.745773000	-0.531829000	-0.185305000
1	-8.989824000	-2.678429000	-0.462984000
6	6.189077000	1.010376000	0.099748000
6	6.916691000	2.205582000	0.142998000
16	7.298553000	-0.353722000	-0.075501000
6	8.294585000	2.056213000	0.043569000
1	6.441674000	3.172798000	0.253507000
6	8.713799000	0.711122000	-0.084516000
1	8.992133000	2.885440000	0.064725000
6	-10.077507000	-0.033004000	-0.223585000
6	-10.512616000	1.303353000	-0.141167000
16	-11.483310000	-1.066085000	-0.389644000
1	-9.832337000	2.142413000	-0.035258000
6	-12.510918000	0.387804000	-0.335256000
6	-13.911201000	0.320151000	-0.425849000
6	-14.571721000	-0.927352000	-0.567758000
7	-15.089570000	-1.966593000	-0.684105000
6	-14.698063000	1.501115000	-0.377252000

7	-15.372301000	2.451517000	-0.340769000
7	-11.823212000	1.530695000	-0.201403000
6	10.009968000	0.225610000	-0.203746000
16	11.412042000	1.301023000	-0.217444000
16	10.384312000	-1.490571000	-0.352929000
6	12.623167000	0.023368000	-0.383339000
6	12.139177000	-1.292167000	-0.447525000
6	13.996182000	0.272550000	-0.450821000
6	13.025351000	-2.363984000	-0.579467000
6	14.876791000	-0.799966000	-0.582481000
1	14.370639000	1.290006000	-0.401053000
6	14.394384000	-2.110442000	-0.646448000
1	12.649973000	-3.381104000	-0.628912000
1	15.943993000	-0.610557000	-0.635185000
1	15.086370000	-2.940008000	-0.748889000

S9TIIDTS4-T1 E=-3879.957048 Hartree

6	3.067491000	-1.567075000	-0.660177000
6	2.484268000	-0.269742000	-0.599753000
6	3.355929000	0.812176000	-0.404168000
6	4.727273000	0.596874000	-0.303553000
6	5.292790000	-0.692210000	-0.389400000
6	4.426356000	-1.796823000	-0.564935000
6	0.814668000	-1.931100000	-0.795344000
6	1.030890000	-0.436842000	-0.683643000
1	2.963665000	1.815661000	-0.356992000
1	5.376934000	1.457712000	-0.182628000
1	4.814848000	-2.807950000	-0.590221000
6	-0.007360000	0.479097000	-0.704371000
6	-1.452512000	0.323924000	-0.591898000
6	0.209890000	1.969782000	-0.913677000
6	-2.038500000	1.617255000	-0.716084000
6	-2.327375000	-0.744847000	-0.328855000
6	-3.392443000	1.855984000	-0.616777000
6	-3.693342000	-0.520930000	-0.222289000
1	-1.934645000	-1.744645000	-0.230124000
6	-4.264807000	0.764604000	-0.368631000
1	-3.776339000	2.864344000	-0.712034000
1	-4.338746000	-1.372697000	-0.032130000
8	1.245503000	2.595824000	-1.093088000
8	-0.221370000	-2.573179000	-0.914171000
7	-1.040844000	2.564231000	-0.922386000
7	2.069024000	-2.523840000	-0.793515000

6	2.268869000	-3.952088000	-0.904754000
1	2.873951000	-4.194422000	-1.785322000
1	2.765273000	-4.350192000	-0.012548000
1	1.284459000	-4.409571000	-1.005376000
6	-1.241270000	3.983427000	-1.118379000
1	-1.860139000	4.171724000	-2.002502000
1	-1.723182000	4.436035000	-0.244524000
1	-0.258554000	4.432759000	-1.262652000
6	6.728947000	-0.899743000	-0.298129000
6	7.453411000	-2.032449000	-0.672659000
16	7.797886000	0.340431000	0.341010000
6	8.827436000	-1.919093000	-0.466415000
1	6.991596000	-2.907672000	-1.113150000
6	9.217097000	-0.681542000	0.084189000
1	9.542890000	-2.695524000	-0.712220000
6	-5.689474000	0.977787000	-0.266927000
6	-6.414113000	2.156807000	-0.462029000
16	-6.794735000	-0.336053000	0.151852000
6	-7.789911000	2.035216000	-0.291243000
1	-5.941335000	3.092307000	-0.735720000
6	-8.206704000	0.728577000	0.051627000
1	-8.485700000	2.857308000	-0.412298000
6	10.510930000	-0.267398000	0.406327000
6	10.836795000	1.037136000	0.969209000
16	11.952926000	-1.254036000	0.182081000
6	13.010432000	0.076051000	0.838082000
7	12.222740000	1.154530000	1.177817000
6	12.822888000	2.362574000	1.732997000
1	13.536651000	2.788532000	1.024220000
1	12.011911000	3.065662000	1.920261000
1	13.344689000	2.130311000	2.664153000
8	14.211055000	-0.002307000	0.947613000
8	10.037649000	1.929018000	1.235254000
6	-9.498970000	0.274556000	0.288768000
16	-10.898404000	1.351071000	0.194077000
16	-9.871140000	-1.398863000	0.704491000
6	-12.105039000	0.119156000	0.585733000
6	-11.621383000	-1.176068000	0.826619000
6	-13.474622000	0.384248000	0.661646000
6	-12.504853000	-2.210541000	1.144177000
6	-14.352530000	-0.651156000	0.978931000
1	-13.848715000	1.385884000	0.475176000
6	-13.870566000	-1.941088000	1.218836000
1	-12.129696000	-3.211873000	1.330053000

1	-15.417009000	-0.448696000	1.038656000
1	-14.560001000	-2.742094000	1.465175000

S9TIIDTS5- T1 E=-3651.420968 Hartree

6	-2.678702000	-1.578940000	0.662227000
6	-2.091767000	-0.280793000	0.624610000
6	-2.959301000	0.808320000	0.449118000
6	-4.330651000	0.599642000	0.345969000
6	-4.900827000	-0.690166000	0.410690000
6	-4.038239000	-1.801591000	0.566684000
6	-0.426010000	-1.947955000	0.785746000
6	-0.639803000	-0.453603000	0.703128000
1	-2.563488000	1.811075000	0.420003000
1	-4.977145000	1.464522000	0.239070000
1	-4.430076000	-2.811564000	0.577275000
6	0.400048000	0.461988000	0.740053000
6	1.840858000	0.308643000	0.614501000
6	0.185464000	1.948167000	0.991179000
6	2.430642000	1.598165000	0.767836000
6	2.711810000	-0.755913000	0.317533000
6	3.783804000	1.836178000	0.665192000
6	4.076279000	-0.532205000	0.206775000
1	2.315559000	-1.751926000	0.196219000
6	4.651974000	0.749033000	0.382233000
1	4.171130000	2.840386000	0.786021000
1	4.718393000	-1.379492000	-0.011995000
8	-0.848933000	2.567692000	1.195527000
8	0.608817000	-2.594287000	0.889690000
7	1.436380000	2.541014000	1.006059000
7	-1.682715000	-2.538785000	0.776365000
6	-1.884653000	-3.968833000	0.862302000
1	-2.486162000	-4.226253000	1.740960000
1	-2.385014000	-4.349526000	-0.035195000
1	-0.900569000	-4.429507000	0.950448000
6	1.640397000	3.954568000	1.238973000
1	2.265088000	4.117731000	2.123858000
1	2.117107000	4.429484000	0.374304000
1	0.659529000	4.401493000	1.401792000
6	-6.335701000	-0.888222000	0.317188000
6	-7.060382000	-2.037409000	0.648157000
16	-7.406261000	0.376281000	-0.263885000
6	-8.431149000	-1.907265000	0.451126000
1	-6.602924000	-2.933299000	1.049472000

6	-8.823619000	-0.647295000	-0.047151000
1	-9.135798000	-2.699245000	0.672275000
6	6.074859000	0.960983000	0.275371000
6	6.801732000	2.139192000	0.474762000
16	7.176991000	-0.350717000	-0.156666000
6	8.175507000	2.017520000	0.296219000
1	6.331095000	3.073843000	0.754691000
6	8.589458000	0.712531000	-0.057415000
1	8.872486000	2.838492000	0.417886000
6	-10.144004000	-0.226685000	-0.348774000
6	-11.259667000	-1.075598000	-0.180338000
6	-10.372915000	1.140142000	-0.855815000
6	-12.539206000	-0.660892000	-0.469930000
1	-11.118971000	-2.085898000	0.186420000
6	-12.817208000	0.695433000	-0.973599000
6	-13.648055000	-1.535800000	-0.291395000
7	-14.525524000	-2.284441000	-0.130678000
8	-9.454021000	1.939469000	-1.036668000
8	-13.944113000	1.089969000	-1.237739000
7	-11.686212000	1.516499000	-1.133029000
6	-11.881597000	2.882315000	-1.633636000
1	-11.506620000	3.600768000	-0.902018000
1	-11.325931000	3.017893000	-2.563677000
1	-12.946851000	3.021940000	-1.798562000
6	9.880455000	0.259771000	-0.304292000
16	11.280080000	1.334025000	-0.207834000
16	10.248730000	-1.409767000	-0.734107000
6	12.483939000	0.105563000	-0.618094000
6	11.998208000	-1.187338000	-0.866432000
6	13.853056000	0.371167000	-0.700796000
6	12.878776000	-2.219790000	-1.198376000
6	14.728034000	-0.662067000	-1.032376000
1	14.228871000	1.371046000	-0.508632000
6	14.243900000	-1.949930000	-1.279726000
1	12.502040000	-3.219397000	-1.390074000
1	15.792173000	-0.459701000	-1.097540000
1	14.931466000	-2.748985000	-1.537204000

S9TIIDTS6-T1 E=-4012.741603 Hartree

6	-2.294698000	-1.626953000	0.653831000
6	-1.716927000	-0.324166000	0.613026000
6	-2.592739000	0.758163000	0.432328000
6	-3.961341000	0.538718000	0.327265000

6	-4.524677000	-0.756164000	0.395911000
6	-3.651243000	-1.860565000	0.557721000
6	-0.039533000	-1.978772000	0.784594000
6	-0.264382000	-0.485660000	0.695497000
1	-2.204351000	1.763656000	0.398995000
1	-4.612876000	1.398234000	0.209904000
1	-4.034160000	-2.873472000	0.578666000
6	0.768376000	0.437396000	0.731242000
6	2.211509000	0.293957000	0.609743000
6	0.542636000	1.923094000	0.975740000
6	2.790944000	1.588079000	0.759555000
6	3.090627000	-0.764897000	0.318502000
6	4.142884000	1.835864000	0.658802000
6	4.454100000	-0.531398000	0.210091000
1	2.702129000	-1.764312000	0.200131000
6	5.019346000	0.754380000	0.382170000
1	4.522370000	2.843667000	0.774633000
1	5.103183000	-1.374937000	-0.002472000
8	-0.496591000	2.536014000	1.175147000
8	1.000304000	-2.616051000	0.893605000
7	1.789299000	2.524771000	0.991422000
7	-1.291197000	-2.578713000	0.774787000
6	-1.483059000	-4.009887000	0.866541000
1	-2.085011000	-4.267533000	1.744773000
1	-1.978694000	-4.397778000	-0.030457000
1	-0.495987000	-4.463214000	0.959045000
6	1.982686000	3.940635000	1.219198000
1	2.604962000	4.111633000	2.104307000
1	2.457180000	4.415762000	0.353412000
1	0.998367000	4.381033000	1.378961000
6	-5.953853000	-0.962857000	0.299785000
6	-6.664308000	-2.147039000	0.546721000
16	-7.047139000	0.332333000	-0.170917000
6	-8.033481000	-2.029813000	0.374318000
1	-6.190935000	-3.067116000	0.867075000
6	-8.454543000	-0.731039000	-0.024638000
1	-8.751023000	-2.821774000	0.524362000
6	6.441996000	0.977027000	0.277934000
6	7.161023000	2.156509000	0.491362000
16	7.551923000	-0.322736000	-0.169551000
6	8.536422000	2.045283000	0.312047000
1	6.684758000	3.084482000	0.783848000
6	8.957953000	0.747400000	-0.056575000
1	9.228442000	2.868734000	0.444644000

6	-9.767533000	-0.292887000	-0.283087000
6	-10.903430000	-1.204466000	-0.160419000
6	-9.987097000	1.090464000	-0.677029000
6	-12.415533000	0.661262000	-0.808520000
8	-9.064444000	1.897603000	-0.801119000
7	-11.314500000	1.491857000	-0.918195000
6	-11.520086000	2.894318000	-1.312974000
1	-12.170311000	3.389816000	-0.590721000
1	-10.541845000	3.365797000	-1.340150000
1	-11.998809000	2.935977000	-2.292292000
7	-12.178322000	-0.649618000	-0.437216000
6	-13.328296000	-1.559730000	-0.313418000
1	-14.024279000	-1.175900000	0.433814000
1	-13.851617000	-1.625663000	-1.268333000
1	-12.938858000	-2.529324000	-0.017755000
8	-10.816781000	-2.387248000	0.159702000
16	-13.964809000	1.222297000	-1.113677000
6	10.252039000	0.304551000	-0.308230000
16	11.645217000	1.386249000	-0.200080000
16	10.630285000	-1.358164000	-0.756156000
6	12.856563000	0.168936000	-0.621382000
6	12.378577000	-1.124124000	-0.883833000
6	14.224244000	0.443165000	-0.699657000
6	13.265573000	-2.147883000	-1.225478000
6	15.105635000	-0.581439000	-1.040974000
1	14.594041000	1.443129000	-0.496535000
6	14.629238000	-1.869391000	-1.302368000
1	12.894825000	-3.147593000	-1.428045000
1	16.168667000	-0.372242000	-1.102691000
1	15.321682000	-2.661769000	-1.567340000

S9TIIDTS7-T1 E=-3766.672638 Hartree

6	2.105828000	-1.648783000	-0.970795000
6	1.539517000	-0.347578000	-0.837336000
6	2.427974000	0.718880000	-0.630101000
6	3.799050000	0.487559000	-0.584145000
6	4.345634000	-0.804271000	-0.739633000
6	3.464129000	-1.894602000	-0.932299000
6	-0.154402000	-1.981893000	-1.043409000
6	0.082805000	-0.497462000	-0.878834000
1	2.048312000	1.723625000	-0.534141000
1	4.463420000	1.336924000	-0.461944000
1	3.842925000	-2.906535000	-1.011620000

6	-0.945146000	0.430476000	-0.826903000
6	-2.384564000	0.286428000	-0.669955000
6	-0.717942000	1.927495000	-0.988035000
6	-2.960692000	1.589889000	-0.725623000
6	-3.261771000	-0.784020000	-0.416422000
6	-4.307473000	1.836983000	-0.571311000
6	-4.619856000	-0.551543000	-0.254526000
1	-2.876139000	-1.790309000	-0.368327000
6	-5.182461000	0.744723000	-0.333799000
1	-4.684028000	2.851394000	-0.618419000
1	-5.267319000	-1.403315000	-0.071874000
8	0.318407000	2.547556000	-1.178811000
8	-1.200880000	-2.608313000	-1.152404000
7	-1.960993000	2.534288000	-0.931307000
7	1.093159000	-2.587632000	-1.108653000
6	1.272412000	-4.012215000	-1.287162000
1	1.843215000	-4.222647000	-2.198159000
1	1.794866000	-4.452641000	-0.430536000
1	0.279799000	-4.454817000	-1.371978000
6	-2.152030000	3.962263000	-1.067536000
1	-2.798510000	4.189216000	-1.922175000
1	-2.598254000	4.386258000	-0.161122000
1	-1.170024000	4.407093000	-1.229223000
6	5.777535000	-1.030595000	-0.700747000
6	6.488436000	-2.140693000	-1.171344000
16	6.873182000	0.145957000	-0.013880000
6	7.863083000	-2.055031000	-0.987720000
1	6.006389000	-2.974918000	-1.666018000
6	8.284930000	-0.851967000	-0.371091000
1	8.577522000	-2.812264000	-1.277151000
6	-6.599462000	0.966559000	-0.176095000
6	-7.315259000	2.163085000	-0.283552000
16	-7.707651000	-0.356362000	0.203277000
6	-8.685780000	2.046795000	-0.076977000
1	-6.839436000	3.107590000	-0.517959000
6	-9.107987000	0.727450000	0.206329000
1	-9.374612000	2.881830000	-0.129929000
6	9.599687000	-0.562685000	0.043580000
6	10.595171000	-1.668041000	0.246100000
6	10.198831000	0.655804000	0.538606000
6	11.684552000	-1.087607000	1.067614000
6	11.431956000	0.278077000	1.288922000
6	12.796836000	-1.734370000	1.586294000
6	12.318753000	1.016625000	2.075691000

6	13.681193000	-0.991609000	2.372947000
1	12.955242000	-2.787759000	1.378652000
6	13.434711000	0.363842000	2.614437000
1	12.163438000	2.066310000	2.284364000
1	14.559343000	-1.464822000	2.801300000
1	14.123590000	0.930115000	3.233863000
8	10.529210000	-2.825572000	-0.142600000
6	9.827507000	1.965717000	0.249785000
6	8.914091000	2.328908000	-0.784701000
7	8.223320000	2.689863000	-1.651151000
6	10.444354000	3.096325000	0.866150000
7	10.912076000	4.041235000	1.363396000
6	-10.398301000	0.275407000	0.458100000
16	-11.785566000	1.370183000	0.464267000
16	-10.778260000	-1.413330000	0.793262000
6	-12.995280000	0.132650000	0.827230000
6	-12.520926000	-1.178884000	0.982616000
6	-14.358353000	0.408620000	0.960397000
6	-13.406973000	-2.219519000	1.271649000
6	-15.238828000	-0.632866000	1.248901000
1	-14.725322000	1.422917000	0.840089000
6	-14.766060000	-1.939241000	1.403638000
1	-13.039059000	-3.233527000	1.391381000
1	-16.298298000	-0.422392000	1.352994000
1	-15.457770000	-2.744684000	1.628032000

S9TIIDTS8-T1 E=-4201.893435 Hartree

6	-3.440335000	1.666501000	-0.679471000
6	-2.847325000	0.368955000	-0.665986000
6	-3.710267000	-0.720317000	-0.442508000
6	-5.069978000	-0.510291000	-0.268666000
6	-5.649544000	0.780980000	-0.305926000
6	-4.789186000	1.891425000	-0.513047000
6	-1.203320000	2.039565000	-0.939707000
6	-1.411767000	0.535434000	-0.823330000
1	-3.311587000	-1.722563000	-0.426840000
1	-5.705767000	-1.375313000	-0.108752000
1	-5.178951000	2.901782000	-0.529118000
6	-0.372541000	-0.378505000	-0.907280000
6	1.081902000	-0.211847000	-0.863378000
6	-0.591991000	-1.859022000	-1.118848000
6	1.663888000	-1.501377000	-1.039403000
6	1.956822000	0.858870000	-0.623696000

6	3.025571000	-1.730878000	-1.010956000
6	3.330839000	0.643530000	-0.587530000
1	1.564481000	1.855188000	-0.496074000
6	3.891964000	-0.635786000	-0.784733000
1	3.417997000	-2.734779000	-1.120699000
1	3.985211000	1.496967000	-0.441718000
8	-1.630900000	-2.494402000	-1.246357000
8	-0.175215000	2.677542000	-1.115168000
7	0.663117000	-2.447381000	-1.205284000
7	-2.453343000	2.629081000	-0.859917000
6	-2.662492000	4.058139000	-0.951925000
1	-3.314871000	4.302882000	-1.797088000
1	-3.110434000	4.448675000	-0.031464000
1	-1.686693000	4.519899000	-1.103327000
6	0.859472000	-3.863607000	-1.428747000
1	1.430528000	-4.038216000	-2.347073000
1	1.389172000	-4.324004000	-0.587301000
1	-0.127840000	-4.315463000	-1.525498000
6	-7.067608000	0.979316000	-0.136249000
6	-7.797377000	2.171849000	-0.191168000
16	-8.160054000	-0.370802000	0.188718000
6	-9.165218000	2.031433000	0.013498000
1	-7.332605000	3.130910000	-0.384943000
6	-9.572099000	0.696323000	0.241592000
1	-9.863402000	2.860231000	-0.001548000
6	5.327453000	-0.845964000	-0.755036000
6	6.051608000	-1.917031000	-1.287382000
16	6.401953000	0.299027000	0.010222000
6	7.425444000	-1.822276000	-1.091466000
1	5.582962000	-2.723491000	-1.837129000
6	7.823321000	-0.656638000	-0.403519000
1	8.143821000	-2.542550000	-1.463326000
6	9.132711000	-0.376713000	0.034385000
6	9.786523000	0.800817000	0.479300000
6	11.389590000	-0.862349000	1.209461000
6	11.025762000	0.492090000	1.254323000
6	12.525468000	-1.378766000	1.812192000
6	11.862723000	1.358519000	1.972532000
6	13.345363000	-0.497595000	2.519433000
1	12.759903000	-2.435453000	1.738728000
6	13.005675000	0.854885000	2.597325000
1	11.638002000	2.411469000	2.061364000
1	14.240320000	-0.865473000	3.010657000
1	13.639937000	1.536913000	3.154690000

6	9.392144000	2.105101000	0.120190000
6	9.923979000	3.288839000	0.704266000
7	10.313401000	4.287300000	1.165927000
6	8.510142000	2.378920000	-0.963969000
7	7.834423000	2.664594000	-1.870509000
16	10.202014000	-1.823925000	0.298883000
8	9.543104000	-2.793376000	1.186498000
8	10.752942000	-2.302236000	-0.980279000
6	-10.856507000	0.220167000	0.477168000
16	-12.255445000	1.298038000	0.532348000
16	-11.216814000	-1.484922000	0.741869000
6	-13.450234000	0.033547000	0.848707000
6	-12.961065000	-1.277952000	0.947724000
6	-14.815590000	0.288937000	0.998526000
6	-13.834410000	-2.339449000	1.196812000
6	-15.683352000	-0.773271000	1.247032000
1	-15.194042000	1.303240000	0.921857000
6	-15.195798000	-2.079708000	1.345594000
1	-13.455049000	-3.353431000	1.273032000
1	-16.744565000	-0.579007000	1.363955000
1	-15.877808000	-2.901249000	1.539128000

S9TIIDTS10-T1 E=-4034.172116 Hartree

6	-3.594355000	-1.438206000	0.627382000
6	-2.993604000	-0.155387000	0.478318000
6	-3.853878000	0.913859000	0.178631000
6	-5.222471000	0.701101000	0.062251000
6	-5.807905000	-0.573198000	0.233552000
6	-4.950621000	-1.665978000	0.517202000
6	-1.350205000	-1.808502000	0.855227000
6	-1.548262000	-0.324916000	0.611591000
1	-3.450751000	1.907356000	0.060599000
1	-5.857880000	1.555404000	-0.149654000
1	-5.345918000	-2.668977000	0.624206000
6	-0.498983000	0.579391000	0.580236000
6	0.950176000	0.398779000	0.519230000
6	-0.702683000	2.080156000	0.649615000
6	1.547612000	1.691471000	0.546155000
6	1.818403000	-0.695459000	0.371840000
6	2.907515000	1.908235000	0.460395000
6	3.190845000	-0.494282000	0.282093000
1	1.417848000	-1.696742000	0.350735000
6	3.772090000	0.792343000	0.331418000

1	3.300799000	2.917671000	0.468815000
1	3.831842000	-1.365556000	0.190099000
8	-1.733921000	2.734313000	0.742219000
8	-0.324287000	-2.445917000	1.057714000
7	0.555968000	2.661625000	0.641027000
7	-2.608762000	-2.389855000	0.865647000
6	-2.825647000	-3.801522000	1.090526000
1	-3.456707000	-3.964795000	1.971232000
1	-3.302416000	-4.269631000	0.221746000
1	-1.848856000	-4.256629000	1.256051000
6	0.767420000	4.089989000	0.715025000
1	1.366611000	4.351589000	1.594276000
1	1.276157000	4.459471000	-0.182688000
1	-0.213813000	4.558679000	0.793490000
6	-7.236522000	-0.776203000	0.121929000
6	-7.982908000	-1.918595000	0.409520000
16	-8.311780000	0.508982000	-0.441330000
6	-9.356161000	-1.792601000	0.200136000
1	-7.530967000	-2.829024000	0.784801000
6	-9.743374000	-0.519101000	-0.269601000
1	-10.068193000	-2.588412000	0.385903000
6	5.204296000	0.984594000	0.249438000
6	5.941727000	2.153599000	0.439106000
16	6.295888000	-0.351453000	-0.133906000
6	7.320675000	2.009237000	0.293563000
1	5.477861000	3.097752000	0.698610000
6	7.722970000	0.692479000	-0.022652000
1	8.026895000	2.821851000	0.418321000
6	-11.023942000	-0.065835000	-0.574447000
16	-11.371493000	1.571026000	-1.147787000
16	-12.455681000	-1.098665000	-0.416865000
6	-13.107130000	1.331703000	-1.274880000
6	-13.595289000	0.128919000	-0.945084000
1	-14.642127000	-0.146200000	-0.980290000
1	-13.701402000	2.170462000	-1.615424000
6	9.012190000	0.214031000	-0.230803000
16	10.427112000	1.272178000	-0.133707000
16	9.366420000	-1.473026000	-0.611660000
6	11.621338000	0.013329000	-0.474632000
6	11.122111000	-1.278951000	-0.700505000
6	12.996319000	0.255028000	-0.527143000
6	11.995895000	-2.332586000	-0.979518000
6	13.864513000	-0.799652000	-0.806088000
1	13.382282000	1.254270000	-0.352101000

6	13.367199000	-2.086250000	-1.031068000
1	11.608688000	-3.331481000	-1.153676000
1	14.933097000	-0.614670000	-0.847386000
1	14.048582000	-2.902714000	-1.247497000