Electronic Supplementary Information

A Theoretical Insight on Ethylene Polymerization Catalyzed by Carborane-Containing Metal Complexes: the Role of Carborane

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Detailed illustration about corrected Gibbs activation energies ($\Delta G^{\circ\ddagger}$)

For the bimolecular reactions, it is difficult to accurately estimate the activation entropy because it is a solution-based reaction, we corrected the activation Gibbs free energy ($\Delta G^{\circ\ddagger}$, kcal/mol at 298 K) based on the free volume theory. This provides a rate of a solution based bimolecular reaction that is about 80 times faster than the corresponding reaction in the gas phase. This means that the activation free energy for solution reaction should be about 2.8 kcal/mol smaller than the value calculated in the gas phase.
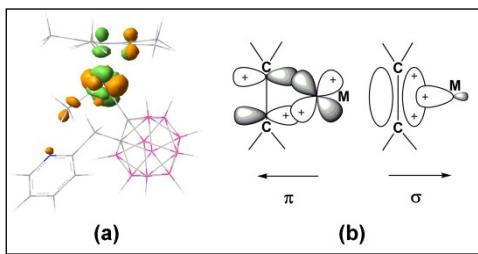
**Fig. S1** (a) Fukui dual descriptors of **1M**; (b) **C2H4** interact with metal.

1TS1　　　　**2TS1**　　　　**3TS1**
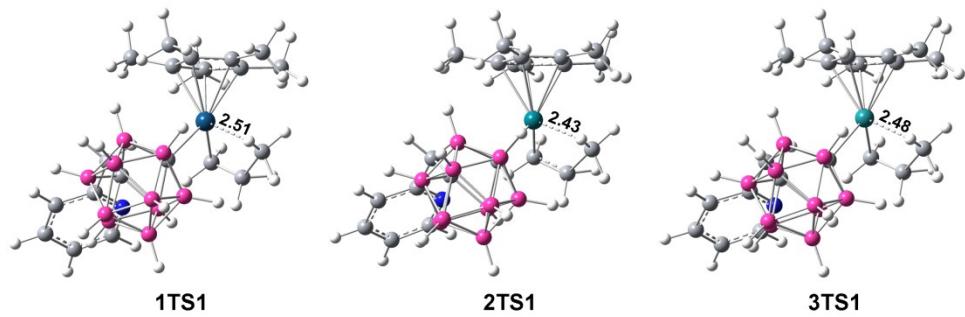
Fig. S2 The Ir···H$_{\alpha}$ distances of transition states for the **1V**(Ir^{III}), **2V**(Rh^{III}) and **3V**(Ru^{II}).
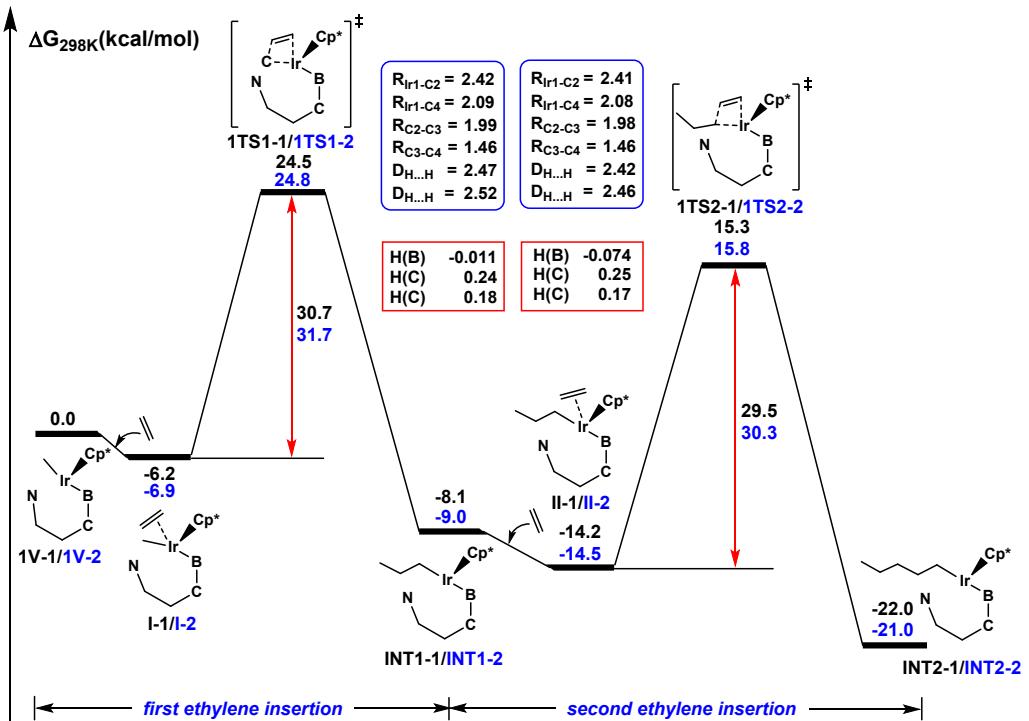
Fig. S3 Energy profile of the ethylene insertion step in the polymerization process catalyzed by the **1V-1** and **1V-2**.
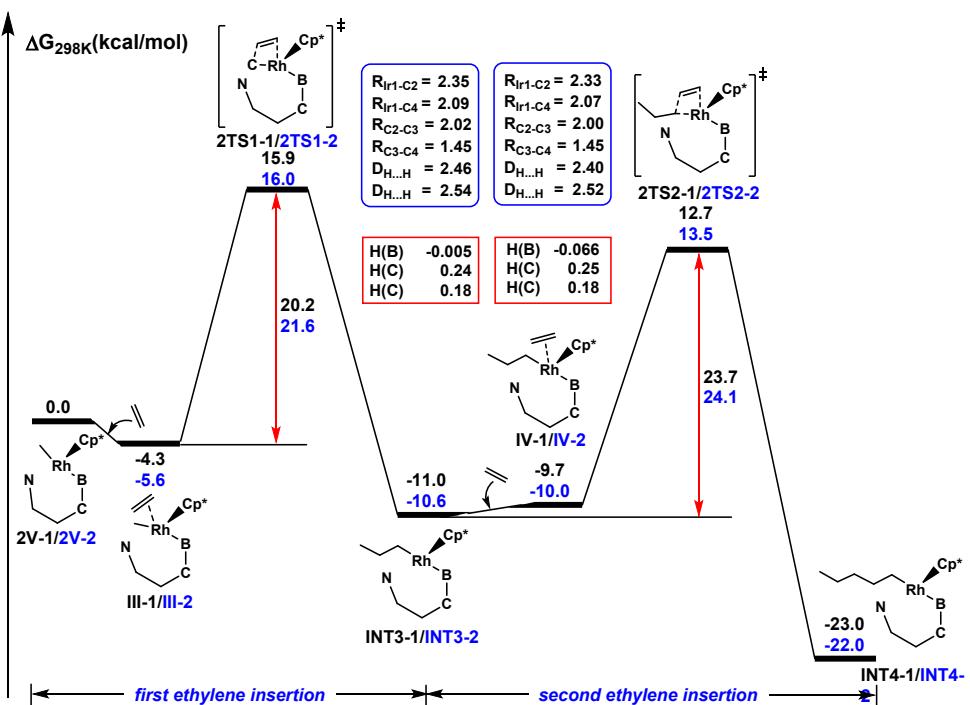
Fig. S4 Energy profile of the ethylene insertion step in the polymerization process catalyzed by the **2V-1** and **2V-2**.
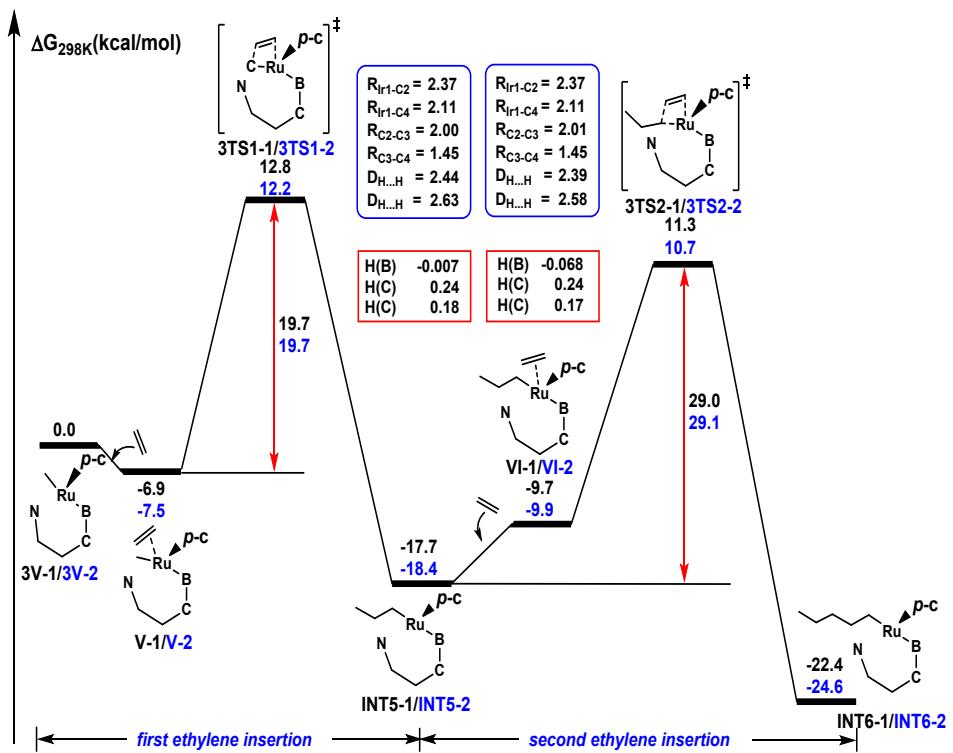
Fig. S5 Energy profile of the ethylene insertion step in the polymerization process catalyzed by the **3V-1** and **3V-2**.
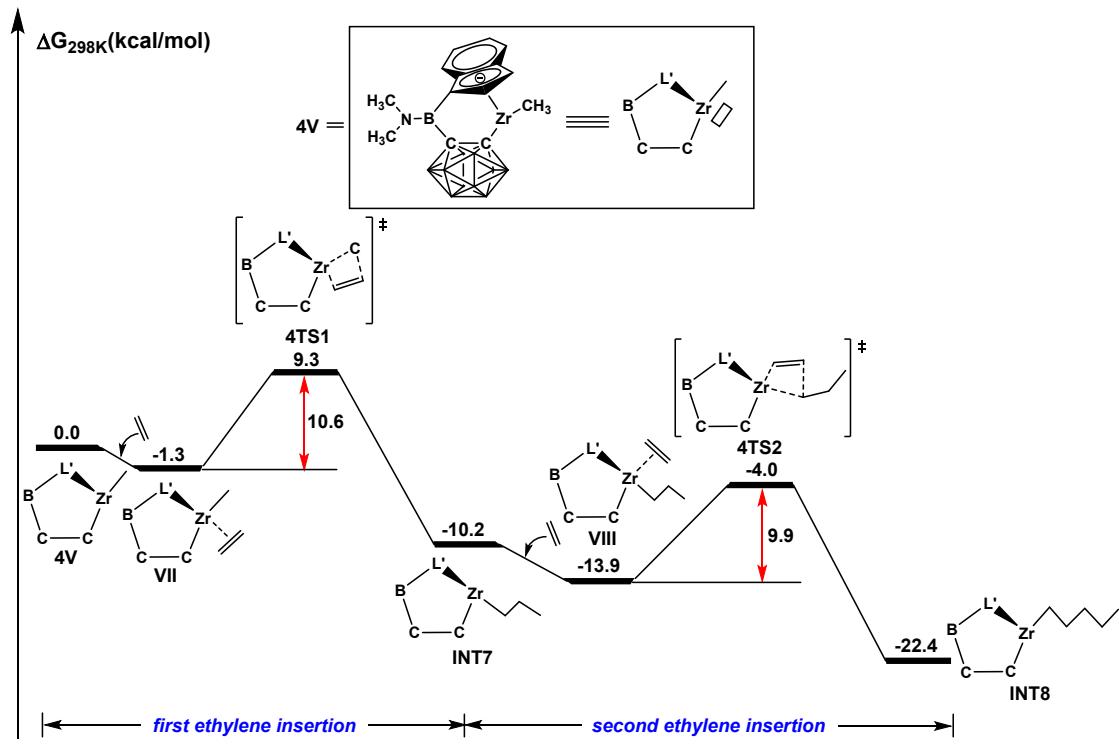
**Fig. S6** Energy profile of the ethylene insertion step in the polymerization process catalyzed by the **4V**.

Table S1. charge decomposition analysis (CDA) of π-complex and translate state for the first ethylene insertion step.
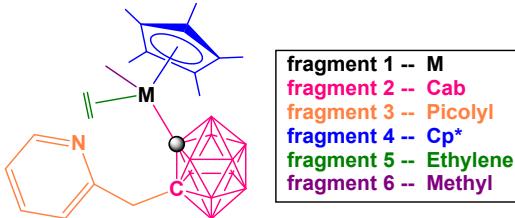
	Ir-CCB$_{10}$/π-complex **I**				Ir-CCB$_{10}$/**1TS1**			
	d	b	d-b	r	d	b	d-b	r
1-2	0.004574	0.191086	-0.186512	0.004667	0.003809	0.197680	-0.193871	-0.018047
1-3	0.001750	0.011001	-0.009251	-0.001874	0.001792	0.014364	-0.012572	-0.002171
1-4	0.037893	0.340601	-0.302708	-0.026330	0.040567	0.319276	-0.278708	-0.064304
1-5	0.040857	0.198527	-0.157670	-0.049068	0.040512	0.146105	-0.105593	-0.009733
1-6	0.005709	0.238051	-0.232343	0.058173	0.004349	0.137946	-0.133597	-0.000865
2-3	0.238183	0.017055	0.221128	-0.276255	0.238699	0.018907	0.219792	-0.272726
2-4	0.013980	0.013026	0.000954	-0.047726	0.019621	0.016580	0.003041	-0.066620
2-5	0.015781	0.007567	0.008214	-0.095271	0.014835	0.006675	0.008160	-0.088858
2-6	0.023722	0.007611	0.016111	-0.110376	0.012606	0.002930	0.009676	-0.061572
3-4	0.004938	0.006583	-0.001645	-0.020246	0.002221	0.003174	-0.000953	-0.010033
3-5	0.018315	0.002708	0.015607	-0.024492	0.017526	0.002902	0.014624	-0.024232
3-6	0.000005	-0.000063	0.000068	-0.000037	0.000001	-0.000031	0.000032	-0.000014
4-5	0.017918	0.001505	0.016413	-0.027968	0.015879	-0.000203	0.016083	-0.014129
4-6	0.006291	0.003578	0.002713	-0.039745	0.009141	0.007463	0.001678	-0.031465
5-6	0.001199	0.002052	-0.000853	-0.068815	-0.011121	0.084266	-0.095387	-0.154025

	Ir-BC$_2$B$_9$/π-complex **I-1**				Ir-BC$_2$B$_9$/**1TS-1**			
	d	b	d-b	r	d	b	d-b	r
1-2	0.006551	0.091547	-0.084996	-0.072919	0.002840	0.104501	-0.101660	-0.116192
1-3	0.000970	0.008921	-0.007951	-0.001109	0.001202	0.012543	-0.011341	-0.001119
1-4	0.034525	0.320631	-0.286106	-0.030737	0.040902	0.303870	-0.262969	-0.075295
1-5	0.034728	0.205449	-0.170721	-0.027523	0.037519	0.164566	-0.127047	-0.000977
1-6	0.006729	0.243259	-0.236530	0.061541	0.005526	0.143455	-0.137929	-0.003820
2-3	0.241212	0.027311	0.213902	-0.270167	0.242597	0.028603	0.213994	-0.267239
2-4	0.011786	0.020569	-0.008783	-0.019941	0.015956	0.020087	-0.004131	-0.032344
2-5	0.009724	-0.000011	0.009735	-0.093419	0.012977	0.000225	0.012752	-0.088345
2-6	0.021646	0.003120	0.018526	-0.092232	0.008895	-0.002690	0.011585	-0.048897
3-4	0.003716	0.006039	-0.002323	-0.012756	0.001504	0.003026	-0.001522	-0.006207
3-5	0.012264	0.003938	0.008326	-0.016641	0.013234	0.004539	0.008695	-0.018657
3-6	0.000003	-0.000055	0.000058	-0.000026	0.000001	-0.000031	0.000032	-0.000013
4-5	0.016874	0.000799	0.016076	-0.026464	0.013008	-0.000309	0.013317	-0.013934
4-6	0.006070	0.004549	0.001521	-0.037826	0.007494	0.005883	0.001611	-0.024485
5-6	0.000942	0.002841	-0.001899	-0.068575	-0.012192	0.089731	-0.101923	-0.167997

	Ir-BCB$_{10}^-$/π-complex **I-2**				Ir-BCB$_{10}^-$/**1TS-2**			
	d	b	d-b	r	d	b	d-b	r
1-2	0.011365	0.164445	-0.153080	-0.014296	0.006793	0.181433	-0.174640	-0.066076
1-3	0.001185	0.008465	-0.007280	-0.001387	0.001273	0.014120	-0.012847	-0.001304
1-4	0.034577	0.309496	-0.274919	-0.059226	0.039737	0.281138	-0.241401	-0.084436
1-5	0.046887	0.217018	-0.170131	-0.052389	0.040720	0.164027	-0.123307	-0.003849
1-6	0.007428	0.265590	-0.258162	0.034911	0.006260	0.137034	-0.130774	0.001299
2-3	0.234423	0.009482	0.224941	-0.226253	0.236138	0.010448	0.225690	-0.222405

	d	b	d-b	r	d	b	d-b	r
2-4	0.021626	0.017530	0.004096	-0.032023	0.027813	0.018152	0.009661	-0.046255
2-5	0.017576	-0.001300	0.018876	-0.097135	0.020785	-0.001746	0.022531	-0.093079
2-6	0.026821	-0.002607	0.029428	-0.100443	0.011675	-0.003269	0.014944	-0.054972
3-4	0.005319	0.005534	-0.000214	-0.018441	0.002027	0.002667	-0.000641	-0.008656
3-5	0.010075	0.003022	0.007053	-0.016643	0.011619	0.003367	0.008252	-0.019310
3-6	0.000005	-0.000071	0.000076	-0.000038	0.000001	-0.000038	0.000039	-0.000017
4-5	0.015287	0.001102	0.014185	-0.025449	0.011798	-0.000736	0.012534	-0.014518
4-6	0.005439	0.006152	-0.000713	-0.038417	0.006649	0.006511	0.000138	-0.024473
5-6	0.000611	0.002430	-0.001819	-0.070738	-0.013110	0.089933	-0.103043	-0.171292

	Rh-CCB$_{10}$/π-complex **III**				Rh-CCB$_{10}$/**2TS1**			
	d	b	d-b	r	d	b	d-b	r
1-2	0.003573	0.206671	-0.203098	0.000462	0.003451	0.214130	-0.210678	-0.015243
1-3	0.001356	0.013206	-0.011850	-0.001217	0.001135	0.016078	-0.014943	-0.001104
1-4	0.024295	0.333922	-0.309627	-0.031391	0.022507	0.330244	-0.307737	-0.056927
1-5	0.022095	0.185640	-0.163545	-0.040558	0.031572	0.124821	-0.093249	-0.020385
1-6	0.004405	0.208760	-0.204355	0.040564	0.003636	0.134027	-0.130390	0.001717
2-3	0.237945	0.015974	0.221972	-0.278876	0.238393	0.017111	0.221282	-0.277043
2-4	0.015618	0.012835	0.002782	-0.043215	0.020711	0.016600	0.004112	-0.054098
2-5	0.016126	0.007772	0.008354	-0.071293	0.015634	0.007108	0.008525	-0.070010
2-6	0.023100	0.006612	0.016488	-0.089452	0.012406	0.002710	0.009696	-0.055136
3-4	0.004281	0.006690	-0.002409	-0.020037	0.002332	0.003898	-0.001566	-0.010819
3-5	0.020748	0.002743	0.018005	-0.024565	0.019107	0.003530	0.015577	-0.024459
3-6	0.000003	-0.000034	0.000037	-0.000035	0.000000	-0.000016	0.000016	-0.000013
4-5	0.016333	0.002422	0.013911	-0.024998	0.016661	0.000570	-0.016091	-0.013058
4-6	0.005398	0.004250	0.001147	-0.026171	0.009479	0.008347	0.001132	-0.032174
5-6	0.001469	0.003487	-0.002017	-0.053534	-0.010643	0.074108	-0.084751	-0.114016

	Rh-BC$_2$B$_9$/π-complex **III-1**				Rh-BC$_2$B$_9$/**2TS1-1**			
	d	b	d-b	r	d	b	d-b	r
1-2	0.009321	0.173270	-0.163949	-0.055441	0.011089	0.193343	-0.182254	-0.066322
1-3	0.000761	0.014091	-0.013330	-0.000696	0.000623	0.016245	-0.015622	-0.000512
1-4	0.021736	0.325314	-0.303578	-0.041875	0.021008	0.321875	-0.300868	-0.071410
1-5	0.023100	0.192441	-0.169341	-0.045691	0.028611	0.138574	-0.109963	-0.020321
1-6	0.005484	0.229647	-0.224162	0.019384	0.004611	0.141691	-0.137080	-0.003685
2-3	0.241042	0.027689	0.213353	-0.277893	0.241986	0.028504	0.213482	-0.275415
2-4	0.012089	0.019837	-0.007747	-0.011217	0.015365	0.020698	-0.005333	-0.010415
2-5	0.010217	0.004982	0.005235	-0.053855	0.013086	0.003193	0.009893	-0.055475
2-6	0.020060	0.003396	0.016663	-0.063446	0.008597	-0.001771	0.010368	-0.041944
3-4	0.003196	0.007147	-0.003951	-0.013580	0.001558	0.003892	-0.002335	-0.007160
3-5	0.014286	0.003615	0.010671	-0.017356	0.013448	0.005148	0.008300	-0.018316
3-6	0.000002	-0.000027	0.000030	-0.000029	0.000000	-0.000019	0.000019	-0.000012
4-5	0.015408	0.001839	0.013568	-0.023032	0.013830	0.000407	0.013423	-0.012897
4-6	0.005765	0.005713	0.000052	-0.025902	0.007472	0.006047	0.001425	-0.023997
5-6	0.001038	0.003704	-0.002666	-0.054155	-0.011593	0.081168	-0.092761	-0.129889

	Rh-BCB$_{10}^{-}$/π-complex **III-2**				Rh-BCB$_{10}^{-}$/**2TS1-2**			
	d	b	d-b	r	d	b	d-b	r
1-2	0.010085	0.196801	-0.186716	-0.027551	0.011307	0.217106	-0.205799	-0.042991
1-3	0.000897	0.013534	-0.012637	-0.000008	0.000702	0.017697	-0.016995	-0.000598
1-4	0.019168	0.309011	-0.259843	-0.047533	0.017985	0.301426	-0.283441	-0.069645
1-5	0.029801	0.196775	-0.166974	-0.055716	0.032502	0.137098	-0.104596	-0.024240
1-6	0.006044	0.239711	-0.233668	0.013667	0.005391	0.136215	-0.130823	0.000522
2-3	0.234822	0.009533	0.225289	-0.231736	0.236807	0.010433	0.226373	-0.229182
2-4	0.019958	0.015949	0.004009	-0.021868	0.025768	0.017360	0.008408	-0.023545

2-5	0.018232	0.002292	0.015940	-0.059073	0.020664	-0.000221	0.020885	-0.058643
2-6	0.024668	-0.003229	0.027897	-0.068988	0.011289	-0.003215	0.014504	-0.046280
3-4	0.004681	0.006762	-0.002081	-0.018657	0.002097	0.003619	-0.001522	-0.009599
3-5	0.012843	0.003171	0.009672	-0.017897	0.012029	0.003980	0.008050	-0.018901
3-6	0.000003	-0.000033	0.000036	-0.000043	0.000000	-0.000021	0.000020	-0.000018
4-5	0.013604	0.002512	0.011092	-0.021154	0.012369	0.000339	0.012029	-0.013247
4-6	0.005287	0.008034	-0.002747	-0.027018	0.006811	0.006877	-0.000067	-0.023885
5-6	0.000734	0.002936	-0.002203	-0.054728	-0.012566	0.080858	-0.093424	-0.129173

	Ru-CCB$_{10}$/π-complex **V**				Ru-CCB$_{10}$/**3TS1**			
	d	b	d-b	r	d	b	d-b	r
1-2	0.005265	0.173987	-0.168722	0.015162	0.003974	0.188258	-0.184284	0.002573
1-3	0.000989	0.016059	-0.015070	-0.001610	0.000760	0.016097	-0.015337	-0.001572
1-4	0.039698	0.269700	-0.230002	-0.076971	0.079775	0.281470	-0.201695	-0.163664
1-5	0.027631	0.152265	-0.124633	-0.038405	0.025129	0.106714	-0.081585	-0.021487
1-6	0.004318	0.172233	-0.167915	0.099682	0.002519	0.145570	-0.143051	-0.027217
2-3	0.238599	0.014252	0.224347	-0.274246	0.238706	0.015645	0.223061	-0.277168
2-4	0.012413	0.008783	0.003631	-0.038483	0.016363	0.011417	0.004946	-0.051305
2-5	0.014653	0.006955	0.007698	-0.061637	0.016800	0.008416	0.008383	-0.066346
2-6	0.020223	0.006905	0.013318	-0.084005	0.013344	0.003625	0.009719	-0.054507
3-4	0.003129	0.003978	-0.000849	-0.014064	0.003578	0.003941	-0.000363	-0.013159
3-5	0.017915	0.004361	0.013554	-0.027117	0.013649	0.003269	0.010380	-0.017403
3-6	0.000002	-0.000017	0.000019	-0.000036	0.000000	-0.000013	0.000013	-0.000012
4-5	0.011810	0.000347	0.011463	-0.028559	0.013536	-0.001533	0.015069	-0.015816
4-6	0.005859	0.004438	0.001421	-0.038602	0.004035	0.000181	0.003853	-0.026656
5-6	0.001828	0.005672	-0.003844	-0.062249	-0.010158	0.080217	-0.090976	-0.126463

	Ru-BC$_2$B$_9$/π-complex **V-1**				Ru-BC$_2$B$_9$/**3TS1-1**			
	d	b	d-b	r	d	b	d-b	r
1-2	0.013125	0.163398	-0.150273	-0.026333	0.009795	0.171870	-0.162075	-0.056883
1-3	0.000182	0.013431	-0.013249	-0.000846	0.000073	0.014850	-0.014777	-0.000589
1-4	0.050485	0.230983	-0.180499	-0.114554	0.075109	0.239210	-0.164101	-0.162343
1-5	0.027870	0.149330	-0.121460	-0.041125	0.043088	0.131619	-0.088531	-0.045777
1-6	0.004834	0.183496	-0.178661	0.071519	0.003750	0.119259	-0.115509	0.025818
2-3	0.240842	0.024926	0.215196	-0.274267	0.242480	0.026277	0.216203	-0.276311
2-4	0.015216	0.079136	-0.003920	-0.008299	0.014895	0.019195	-0.004299	0.002612
2-5	0.013043	0.005624	0.007419	-0.037896	0.015673	0.005585	0.010088	-0.052680
2-6	0.017137	0.005540	0.011597	-0.054464	0.008654	-0.000710	0.009364	-0.033227
3-4	0.002388	0.004105	-0.001716	-0.007366	0.003274	0.004430	-0.001156	-0.009994
3-5	0.009092	0.006674	0.002418	-0.018454	0.008120	0.004748	0.003372	-0.011839
3-6	0.000001	-0.000020	0.000022	-0.000023	0.000000	-0.000015	0.000015	-0.000011
4-5	0.012682	-0.001747	0.014429	-0.029180	0.011770	-0.001394	0.013163	-0.015551
4-6	0.006135	0.004175	0.001960	-0.033162	0.003758	-0.000130	0.003889	-0.022393
5-6	0.002728	0.007193	-0.004465	-0.054542	-0.010883	0.086638	-0.097521	-0.139418

	Ru-BCB$_{10}^{-}$/π-complex **V-2**				Ru-BCB$_{10}^{-}$/**3TS1-2**			
	d	b	d-b	r	d	b	d-b	r
1-2	0.010896	0.192921	-0.182025	0.006309	0.008642	0.199616	-0.190974	-0.033861
1-3	0.000100	0.013059	-0.012960	-0.000923	0.000498	0.016458	-0.015960	-0.001126
1-4	0.058863	0.205827	-0.149664	-0.151366	0.080867	0.219690	-0.138823	-0.188436
1-5	0.030733	0.143258	-0.112525	-0.064104	0.039761	0.130007	-0.090246	-0.040531
1-6	0.004467	0.190678	-0.186211	0.059435	0.005387	0.122981	-0.117594	0.015180
2-3	0.236236	0.008558	0.227678	-0.227493	0.236535	0.007960	0.228576	-0.229397
2-4	0.028244	0.016332	0.011912	-0.035727	0.025419	0.015634	0.009785	-0.008259
2-5	0.027220	0.004585	0.022635	-0.047784	0.023298	0.002919	0.020379	-0.054308

2-6	0.020302	0.000105	0.020196	-0.062252	0.011542	-0.001419	0.012961	-0.037294
3-4	0.003456	0.003099	0.000357	-0.009924	0.005379	0.003997	0.001382	-0.014660
3-5	0.004271	0.005745	-0.014740	-0.015564	0.006956	0.004147	0.002809	-0.012208
3-6	0.000002	-0.000035	0.000037	-0.000040	0.000000	-0.000020	0.000019	-0.000013
4-5	0.013021	-0.003009	0.016030	-0.031040	0.011289	-0.002126	0.013415	-0.018135
4-6	0.005288	0.002389	0.002899	-0.026940	0.003680	-0.000035	0.003715	-0.022874
5-6	0.003909	0.007138	-0.003229	-0.045130	-0.011357	0.088333	-0.099690	-0.142233

fragment 1 -- Zr
fragment 2 -- Cab
fragment 3 -- BN ligand
fragment 4 -- $C_9H_6^-$
fragment 5 -- Ethylene
fragment 6 -- Methyl
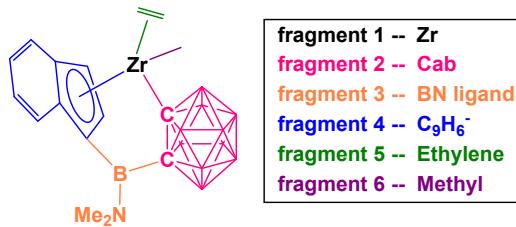
	Zr-CCB$_{10}$/π-complex **VII**				Zr-CCB$_{10}$/**4TS1**			
	d	**b**	**d-b**	**r**	**d**	**b**	**d-b**	**r**
1-2	-0.007712	0.421007	-0.428718	-0.141809	-0.009329	0.450989	-0.460318	-0.149096
1-3	0.001197	-0.008263	0.009459	0.000202	0.001633	-0.005942	0.007575	0.000245
1-4	0.005308	0.353499	-0.348191	-0.114592	0.003929	0.359977	-0.356048	-0.115756
1-5	0.003189	0.193095	-0.189906	-0.019278	-0.005049	0.192332	-0.197381	-0.087321
1-6	-0.001840	0.342062	-0.343902	-0.172743	-0.003381	0.256796	-0.260177	-0.113979
2-3	0.268275	0.010563	0.257712	0.024633	0.262864	0.010415	0.252449	0.024538
2-4	0.021792	0.012624	0.009169	-0.176872	0.022941	0.012850	0.010091	-0.166067
2-5	0.001568	-0.000023	0.001591	-0.032062	-0.002404	-0.001661	-0.000743	-0.037693
2-6	0.002963	0.000168	0.002796	-0.005412	-0.000105	0.000318	-0.000423	-0.007411
3-4	-0.005585	0.237801	-0.243386	0.095703	-0.004519	0.236290	-0.240809	0.083844
3-5	-0.000001	0.000038	-0.000039	0.000002	0.000006	0.000003	0.000003	-0.000001
3-6	-0.000009	0.000188	-0.000198	-0.000049	-0.000007	0.000151	-0.000158	0.000011
4-5	0.000528	-0.000121	0.000649	-0.011192	0.002726	-0.000893	0.003618	-0.018760
4-6	0.012146	-0.002116	0.014261	-0.042625	0.012189	-0.006519	0.018708	-0.044498
5-6	-0.000059	-0.001816	0.001756	-0.010128	0.000940	0.083212	-0.082272	-0.172309

Cartesian coordinates of all the optimized structures

1   **HF =** -1572.2779202 hartree

77	0.675113	-0.212684	-0.153473
17	0.728223	0.165596	-2.584823
6	-1.427974	-0.518838	-0.232124
6	-2.364571	0.525492	0.678130
5	-2.207737	-1.081849	1.214213
1	-1.548403	-1.261347	2.179131
5	-2.222827	-2.053396	-0.245836
1	-1.557663	-3.030541	-0.315827
5	-2.351914	-0.972319	-1.631754
1	-1.778928	-1.208469	-2.636081
5	-2.407260	0.680091	-1.027921
1	-1.877813	1.603487	-1.533020
5	-3.753427	-0.224031	1.348726
1	-4.091612	0.141082	2.427910
5	-3.697143	-1.889882	0.747331
1	-4.108056	-2.795646	1.400139
5	-3.799205	-1.817438	-1.030213
1	-4.294434	-2.689978	-1.669036
5	-3.907477	-0.106359	-1.517168
1	-4.477122	0.266006	-2.491840
5	-3.874942	0.871387	-0.040603
1	-4.306692	1.968479	0.109864
5	-4.746861	-0.676168	-0.044708
1	-5.932816	-0.710363	0.039724
6	-1.616529	1.565178	1.516172
1	-2.357863	2.176445	2.036374
1	-1.035823	1.040670	2.281789
6	-0.695487	2.468013	0.741635
6	-0.846604	3.855162	0.806060
1	-1.648582	4.267632	1.409096
6	0.013251	4.687770	0.096196
1	-0.100235	5.766873	0.141225
6	1.008231	4.102185	-0.681555
1	1.697021	4.697267	-1.271589
6	1.102762	2.716404	-0.715234
1	1.825716	2.214794	-1.343828
7	0.284021	1.907978	-0.007923
6	1.308499	-2.064256	1.001693
6	1.622671	-0.873532	1.761368
6	2.651139	-0.146436	1.018248
6	2.892472	-0.821251	-0.202320
6	2.000747	-1.986919	-0.252348
6	0.561010	-3.254616	1.517456
1	1.251351	-3.855386	2.126405
1	0.190537	-3.887195	0.710350
1	-0.284642	-2.978601	2.148447
6	1.261744	-0.624777	3.197609
1	1.992179	-1.097645	3.869405
1	0.277694	-1.033070	3.440769
1	1.250890	0.444761	3.430683
6	3.346669	1.084413	1.520300
1	4.136797	0.807916	2.230879
1	2.656127	1.752173	2.044200

1	3.813261	1.650078	0.709925
6	3.889507	-0.474798	-1.265585
1	4.687803	-1.227824	-1.294821
1	4.357295	0.496919	-1.083679
1	3.411393	-0.443558	-2.249568
6	2.010017	-3.017211	-1.341536
1	2.860615	-3.702102	-1.219696
1	2.087360	-2.540063	-2.321804
1	1.091647	-3.609203	-1.335952

1M   **HF =** -1151.939489 hartree

77	0.688089	-0.167011	-0.285336
6	-1.406192	-0.519272	-0.301150
6	-2.338302	0.488229	0.673723
5	-2.103910	-1.115837	1.181318
1	-1.394245	-1.282934	2.110413
5	-2.163119	-2.073611	-0.286285
1	-1.476287	-3.034634	-0.398069
5	-2.397014	-0.979483	-1.646489
1	-1.877682	-1.182745	-2.690147
5	-2.474010	0.658774	-1.016970
1	-2.010792	1.613122	-1.535892
5	-3.668568	-0.310014	1.402618
1	-3.964660	0.030296	2.502045
5	-3.591164	-1.965831	0.777877
1	-3.942138	-2.891823	1.437238
5	-3.785604	-1.878926	-0.990787
1	-4.286188	-2.758114	-1.616582
5	-3.971923	-0.166294	-1.448096
1	-4.597941	0.199347	-2.390838
5	-3.896016	0.796147	0.037479
1	-4.352253	1.878511	0.219776
5	-4.717978	-0.778602	0.055298
1	-5.896665	-0.851777	0.197932
6	-1.573983	1.537842	1.483945
1	-2.300667	2.123477	2.052458
1	-0.938384	1.015742	2.207368
6	-0.711684	2.471468	0.679149
6	-0.897092	3.853926	0.764275
1	-1.692276	4.237603	1.394891
6	-0.076590	4.719034	0.047517
1	-0.215731	5.794144	0.110449
6	0.919022	4.167981	-0.755472
1	1.586448	4.788005	-1.344718
6	1.045424	2.785799	-0.807040
1	1.791337	2.316299	-1.434039
7	0.261035	1.940611	-0.103204
6	1.443540	-1.925319	1.165071
6	1.992290	-0.724853	1.670779
6	2.810055	-0.132206	0.611941
6	2.782302	-0.996841	-0.518047
6	1.834138	-2.065270	-0.231535
6	0.699328	-2.973377	1.935323
1	1.368486	-3.825114	2.121060
1	-0.165230	-3.350545	1.384246
1	0.350343	-2.607633	2.903413
6	1.889464	-0.193915	3.072500
1	2.774743	-0.459528	3.667761

1	1.014129	-0.594328	3.591991
1	1.812588	0.899087	3.084443
6	3.681308	1.077799	0.796204
1	4.577762	0.823374	1.378000
1	3.160383	1.875279	1.336536
1	4.019158	1.486233	-0.160554
6	3.631692	-0.898444	-1.750541
1	4.521683	-1.533912	-1.646845
1	3.978048	0.123595	-1.932415
1	3.092379	-1.229745	-2.641986
6	1.639584	-3.298820	-1.067254
1	2.411620	-4.051196	-0.850037
1	1.694152	-3.068048	-2.135247
1	0.664504	-3.756358	-0.881737
6	0.575066	0.136397	-2.370704
1	0.417529	-0.818534	-2.880790
1	-0.240420	0.808116	-2.650278
1	1.516492	0.567758	-2.738462
1V	**HF =** -1151.9134062 hartree		
77	-1.186439	-0.337100	-0.312702
6	0.358402	1.117079	-0.283905
6	1.921539	0.917049	0.392110
5	0.761838	1.865719	1.213874
1	0.307288	1.423765	2.214702
5	-0.122979	2.748701	-0.024083
1	-1.278663	2.962980	0.134666
5	0.490568	2.212647	-1.592348
1	-0.232374	2.058217	-2.522832
5	1.771523	1.026564	-1.298618
1	1.962872	0.066829	-1.953970
5	2.464691	2.364526	1.128280
1	3.121559	2.245843	2.111892
5	1.184455	3.555181	0.859760
1	0.954218	4.406977	1.657911
5	1.020347	3.775027	-0.905783
1	0.666837	4.802857	-1.389548
5	2.199727	2.698857	-1.707192
1	2.699925	2.945859	-2.757225
5	3.093885	1.847593	-0.442434
1	4.185987	1.400004	-0.541127
5	2.628969	3.540933	-0.187553
1	3.456945	4.394106	-0.144292
6	2.236417	-0.428122	1.074198
1	2.364861	-0.225679	2.141995
1	1.359618	-1.069540	0.960639
6	3.448859	-1.182711	0.564897
6	4.726937	-0.935771	1.083722
1	4.865551	-0.176290	1.847499
6	5.808150	-1.668180	0.599433
1	6.808950	-1.491873	0.984276
6	5.581027	-2.629045	-0.385728
1	6.391656	-3.224976	-0.794065
6	4.273700	-2.810999	-0.835761
1	4.050133	-3.553874	-1.599573
7	3.227861	-2.114358	-0.375554
6	-3.333750	0.465822	0.110121
6	-2.736642	0.342030	1.378184

6	-2.213211	-1.017430	1.459569
6	-2.737847	-1.794843	0.331731
6	-3.336182	-0.859911	-0.548800
6	-3.970281	1.688567	-0.475113
1	-5.064207	1.621957	-0.395633
1	-3.723579	1.798151	-1.535583
1	-3.647179	2.596492	0.038191
6	-2.645950	1.389158	2.446785
1	-2.539849	2.392644	2.027480
1	-1.794194	1.218367	3.108537
1	-3.553166	1.377095	3.066614
6	-1.529442	-1.603385	2.657495
1	-2.273666	-1.902669	3.408978
1	-0.854243	-0.880482	3.123213
1	-0.947757	-2.489863	2.391261
6	-2.645286	-3.281986	0.172164
1	-3.444597	-3.779505	0.737740
1	-1.688436	-3.666647	0.537494
1	-2.743024	-3.582389	-0.874379
6	-4.005448	-1.147021	-1.859217
1	-5.093249	-1.226383	-1.726874
1	-3.650551	-2.084308	-2.294911
1	-3.817162	-0.348696	-2.583401
6	-0.146740	-1.574699	-1.597586
1	-0.706652	-2.495851	-1.799094
1	0.862268	-1.831565	-1.258499
1	-0.035968	-1.016709	-2.540504

I	**HF =** -1230.4632448 hartree		
77	-1.287602	-0.007177	-0.434067
6	0.398448	1.351443	-0.274648
6	1.943177	0.866213	0.468365
5	0.853082	1.861118	1.316371
1	0.284230	1.416603	2.248882
5	0.162585	2.998651	0.167923
1	-0.950374	3.370160	0.328768
5	0.814755	2.572950	-1.414902
1	0.198805	2.658091	-2.422662
5	1.879192	1.187676	-1.194870
1	2.006585	0.312922	-1.974860
5	2.611566	2.134145	1.390991
1	3.172234	1.817328	2.390631
5	1.511654	3.506301	1.204407
1	1.339525	4.279687	2.091889
5	1.498662	3.951249	-0.520217
1	1.315350	5.065719	-0.893881
5	2.568385	2.817404	-1.384575
1	3.157127	3.101754	-2.378012
5	3.262574	1.717012	-0.196052
1	4.287117	1.134164	-0.312528
5	3.010457	3.417266	0.238513
1	3.939330	4.136941	0.424669
6	2.073905	-0.574653	0.982498
1	2.137285	-0.525536	2.073167
1	1.152749	-1.102677	0.725249
6	3.248252	-1.376578	0.456466
6	4.475871	-1.389833	1.131781
1	4.604523	-0.799872	2.034396

S15

6	5.522341	-2.154136	0.621400
1	6.484573	-2.176662	1.125688
6	5.311736	-2.885732	-0.547385
1	6.096938	-3.495327	-0.984045
6	4.054472	-2.817896	-1.146336
1	3.845552	-3.377059	-2.056820
7	3.040666	-2.090217	-0.661789
6	-3.386888	-0.382945	0.452298
6	-2.522446	0.085628	1.518810
6	-1.583134	-0.977857	1.806185
6	-1.774395	-2.010307	0.850442
6	-2.884555	-1.634664	-0.013653
6	-4.681125	0.253899	0.044042
1	-5.480201	-0.096961	0.711268
1	-4.967731	-0.007322	-0.977909
1	-4.647677	1.343047	0.116725
6	-2.796313	1.275070	2.394070
1	-3.184315	2.118732	1.815887
1	-1.891156	1.616818	2.901121
1	-3.541593	1.031526	3.164364
6	-0.729123	-1.082786	3.035150
1	-1.338980	-1.461661	3.867536
1	-0.321576	-0.118889	3.343773
1	0.102813	-1.778331	2.900170
6	-1.091030	-3.347616	0.850110
1	-1.598962	-4.033843	1.542175
1	-0.045667	-3.277795	1.163591
1	-1.110317	-3.816998	-0.137162
6	-3.523840	-2.518781	-1.047033
1	-4.193589	-3.252253	-0.577812
1	-2.780538	-3.082017	-1.620734
1	-4.117802	-1.938271	-1.758571
6	-0.861501	-0.380350	-2.549318
6	-0.162984	-1.339707	-1.791336
1	-0.327508	0.457913	-2.984363
1	-1.783866	-0.649132	-3.058936
1	-0.585970	-2.335406	-1.692673
1	0.909041	-1.297989	-1.644876
6	-2.308555	1.616375	-1.383872
1	-2.704052	2.283538	-0.613945
1	-1.665092	2.193004	-2.040525
1	-3.134572	1.202631	-1.970095

1TS1   **HF =** -1230.4182879 hartree $v^{\ddagger} = -452.8138\ icm^{-1}$

77	-1.224165	-0.212082	-0.335118
6	0.401250	1.214655	-0.262557
6	1.985936	0.885588	0.449545
5	0.863705	1.846396	1.282986
1	0.382122	1.403102	2.264108
5	0.046913	2.857914	0.096018
1	-1.096598	3.139874	0.255060
5	0.681938	2.399284	-1.480229
1	0.011480	2.385452	-2.455158
5	1.854031	1.105919	-1.224187
1	2.024652	0.190287	-1.948287
5	2.593273	2.251636	1.276855
1	3.208971	2.037264	2.271209
5	1.386211	3.526537	1.057069

S16

1	1.185588	4.335310	1.906496
5	1.286512	3.870050	-0.687405
1	1.008089	4.944854	-1.115562
5	2.411961	2.769510	-1.527496
1	2.946120	3.041069	-2.555167
5	3.222933	1.789868	-0.305494
1	4.284983	1.277919	-0.422922
5	2.858217	3.492742	0.043832
1	3.735324	4.288479	0.157255
6	2.213210	-0.513871	1.041158
1	2.288326	-0.400098	2.126654
1	1.318981	-1.105179	0.828640
6	3.427740	-1.268680	0.538729
6	4.664444	-1.163831	1.189244
1	4.768322	-0.516754	2.055208
6	5.750520	-1.888103	0.703877
1	6.719692	-1.819685	1.190558
6	5.569781	-2.699418	-0.416129
1	6.385777	-3.283074	-0.831421
6	4.301411	-2.746583	-0.993676
1	4.114942	-3.371118	-1.865876
7	3.250357	-2.057743	-0.533186
6	-3.458687	0.089681	0.556298
6	-2.546247	0.349805	1.596051
6	-1.690050	-0.834377	1.751168
6	-2.190437	-1.851975	0.850266
6	-3.218554	-1.262361	0.052293
6	-4.531078	1.003061	0.045628
1	-5.525361	0.586259	0.252902
1	-4.464481	1.146695	-1.040021
1	-4.478533	1.989356	0.512583
6	-2.543781	1.548182	2.497934
1	-2.984819	2.424149	2.015836
1	-1.536456	1.820527	2.815104
1	-3.128639	1.334659	3.403890
6	-0.823697	-1.117368	2.946210
1	-1.446688	-1.449718	3.789077
1	-0.271620	-0.234714	3.274217
1	-0.099010	-1.910028	2.741131
6	-1.770676	-3.293047	0.845972
1	-2.319149	-3.846310	1.620476
1	-0.702349	-3.406398	1.049568
1	-1.980765	-3.777347	-0.111752
6	-4.087970	-1.967410	-0.950063
1	-5.007730	-2.338331	-0.476711
1	-3.579300	-2.827589	-1.394939
1	-4.393787	-1.302851	-1.764716
6	-0.658290	-0.663606	-2.621725
6	-0.128677	-1.508435	-1.558688
1	0.063105	-0.011141	-3.101335
1	-1.349078	-1.134003	-3.317907
1	-0.546200	-2.515330	-1.507708
1	0.948486	-1.507761	-1.415015
6	-2.033498	0.777758	-2.382488
1	-2.127503	1.662756	-1.753040
1	-1.686942	1.131955	-3.351439
1	-2.986078	0.264714	-2.498647

INT1   **HF =** -1230.4764875 hartree

77	1.097718	-0.237552	0.117313
6	-0.457973	1.220114	0.263450
6	-1.981873	1.012886	-0.501564
5	-0.835459	2.057951	-1.208876
1	-0.317691	1.704905	-2.213162
5	-0.035249	2.881763	0.125384
1	1.116696	3.152781	0.042065
5	-0.695808	2.233316	1.624428
1	-0.002738	2.069638	2.571868
5	-1.901901	1.014346	1.198860
1	-2.082231	-0.000583	1.770884
5	-2.557784	2.486219	-1.168617
1	-3.169498	2.402273	-2.184139
5	-1.338101	3.699873	-0.765565
1	-1.107035	4.611246	-1.494628
5	-1.259820	3.808561	1.015070
1	-0.968965	4.814774	1.579027
5	-2.426346	2.638368	1.692493
1	-2.983323	2.795824	2.731178
5	-3.225001	1.835002	0.336001
1	-4.299468	1.335755	0.358123
5	-2.825371	3.560799	0.213475
1	-3.685975	4.381830	0.188511
6	-2.226717	-0.294598	-1.281436
1	-2.508158	-0.008359	-2.299730
1	-1.275012	-0.829825	-1.338478
6	-3.264680	-1.251024	-0.728187
6	-4.619574	-1.126360	-1.062833
1	-4.947113	-0.318274	-1.709773
6	-5.532021	-2.046700	-0.551864
1	-6.587863	-1.968287	-0.796319
6	-5.064078	-3.067813	0.274456
1	-5.736248	-3.809052	0.695964
6	-3.696799	-3.118529	0.544769
1	-3.287990	-3.903047	1.179177
7	-2.811007	-2.241417	0.057259
6	3.170964	0.276797	-0.268620
6	2.611998	0.609297	-1.576358
6	1.980917	-0.550060	-2.050960
6	2.259424	-1.660583	-1.110642
6	3.105980	-1.172018	-0.079613
6	3.970800	1.225619	0.570717
1	5.000090	1.286499	0.189028
1	4.018451	0.899888	1.612474
1	3.543809	2.231828	0.548184
6	2.710093	1.945008	-2.248261
1	2.531014	2.767050	-1.550738
1	1.989474	2.042613	-3.063453
1	3.714365	2.082446	-2.672513
6	1.235376	-0.719256	-3.338955
1	1.892214	-1.162587	-4.100246
1	0.868214	0.234033	-3.725368
1	0.378846	-1.389712	-3.220934
6	1.866076	-3.087063	-1.351694
1	2.519465	-3.544398	-2.107512
1	0.835643	-3.160507	-1.712340
1	1.941317	-3.681791	-0.438050

6	3.834157	-1.967611	0.961087
1	4.823108	-2.267202	0.588015
1	3.292436	-2.878790	1.229880
1	3.984319	-1.390780	1.876980
6	0.383645	-0.852772	3.170236
6	0.435953	-1.389387	1.731230
1	-0.291147	0.003292	3.237133
1	-0.063314	-1.637850	3.800909
1	1.051301	-2.301100	1.725601
1	-0.577726	-1.685675	1.420847
6	1.740833	-0.466483	3.764529
1	2.193229	0.358067	3.200386
1	1.638497	-0.141188	4.806775
1	2.440946	-1.312082	3.750257

II	**HF =** -1309.0246997 hartree		
77	-1.122946	-0.210837	-0.230523
6	0.417085	1.312560	0.010794
6	2.084958	0.929365	0.525322
5	0.985464	1.623259	1.619960
1	0.576838	0.965939	2.509017
5	0.045103	2.822554	0.747774
1	-1.078332	3.008708	1.073540
5	0.564136	2.740240	-0.938711
1	-0.161740	2.891366	-1.862902
5	1.801852	1.492529	-1.047536
1	1.948380	0.779234	-1.974628
5	2.697147	2.117326	1.583401
1	3.396670	1.727808	2.462653
5	1.429882	3.339834	1.728280
1	1.264678	3.936113	2.744538
5	1.173492	4.042155	0.110985
1	0.819556	5.166278	-0.051618
5	2.268204	3.209631	-1.022963
1	2.706571	3.720546	-2.003345
5	3.214407	2.042563	-0.102180
1	4.280696	1.626620	-0.407222
5	2.812013	3.606424	0.631530
1	3.664343	4.406315	0.852682
6	2.447649	-0.539709	0.786555
1	2.604667	-0.646498	1.863479
1	1.584667	-1.150412	0.513432
6	3.665668	-1.074297	0.059161
6	4.935751	-1.031481	0.649103
1	5.062274	-0.587519	1.632020
6	6.024518	-1.550459	-0.047377
1	7.019536	-1.525100	0.388561
6	5.812753	-2.099508	-1.311956
1	6.629868	-2.515350	-1.893501
6	4.512606	-2.104419	-1.816002
1	4.302214	-2.526957	-2.797028
7	3.458709	-1.612839	-1.153083
6	-3.051176	-1.052237	0.759417
6	-2.169224	-0.582601	1.811048
6	-1.055408	-1.501847	1.878323
6	-1.170624	-2.418747	0.802011
6	-2.402566	-2.127282	0.082460
6	-4.479970	-0.629858	0.591591

1	-5.081410	-1.094624	1.384886
1	-4.897534	-0.948518	-0.365688
1	-4.612204	0.451326	0.678226
6	-2.532303	0.429630	2.859640
1	-3.167311	1.220223	2.449405
1	-1.643738	0.909458	3.277559
1	-3.084206	-0.039298	3.686545
6	-0.096359	-1.633359	3.024495
1	-0.520944	-2.324150	3.767064
1	0.082512	-0.683426	3.529576
1	0.868143	-2.043916	2.716369
6	-0.298132	-3.619380	0.574298
1	-0.654104	-4.465837	1.178623
1	0.742923	-3.433253	0.853035
1	-0.309674	-3.945280	-0.469295
6	-2.981773	-2.972504	-1.017073
1	-3.454509	-3.877575	-0.611937
1	-2.213541	-3.299961	-1.725556
1	-3.741015	-2.428205	-1.585619
6	-2.426843	1.442001	-0.776991
1	-2.964136	1.648649	0.155018
1	-1.817672	2.315445	-0.978377
6	-3.417474	1.277211	-1.932469
6	-4.468712	2.400732	-1.941204
1	-3.931267	0.308263	-1.903217
1	-2.880775	1.307122	-2.887446
1	-5.140758	2.308770	-2.803446
1	-5.084615	2.382385	-1.033213
1	-3.990141	3.385885	-1.992827
6	-0.832234	-0.252594	-2.398926
6	0.057897	-1.177189	-1.817806
1	-0.461873	0.701099	-2.761685
1	-1.734989	-0.609414	-2.885639
1	-0.209569	-2.229767	-1.829603
1	1.122404	-0.994965	-1.749769

1TS2	**HF =** -1308.9781293 hartree		$v^{\ddagger} = -409.4409\ icm^{-1}$
77	1.061716	-0.304414	0.054268
6	-0.492642	1.216214	-0.073544
6	-2.180547	0.831294	-0.486087
5	-1.165681	1.538124	-1.643993
1	-0.843420	0.878621	-2.564816
5	-0.167448	2.732476	-0.826058
1	0.945574	2.924880	-1.192302
5	-0.586663	2.653752	0.877006
1	0.198736	2.857411	1.734240
5	-1.797986	1.387097	1.072316
1	-1.870805	0.661723	2.001086
5	-2.869292	2.023271	-1.495880
1	-3.620960	1.632281	-2.330314
5	-1.617964	3.251344	-1.719883
1	-1.523916	3.850681	-2.743902
5	-1.267422	3.948731	-0.123805
1	-0.907428	5.073243	0.024513
5	-2.281923	3.104170	1.079180
1	-2.656596	3.613256	2.086998
5	-3.275126	1.931582	0.219952
1	-4.319983	1.509338	0.585401

5	-2.933172	3.504446	-0.534462
1	-3.802014	4.300750	-0.697315
6	-2.537979	-0.639309	-0.753309
1	-2.730709	-0.734588	-1.825761
1	-1.655709	-1.240286	-0.522266
6	-3.729689	-1.185161	0.007819
6	-5.011041	-1.175963	-0.559488
1	-5.162865	-0.755914	-1.549377
6	-6.078958	-1.697593	0.166772
1	-7.081683	-1.697764	-0.252121
6	-5.836198	-2.216133	1.438420
1	-6.635826	-2.633069	2.043183
6	-4.527102	-2.188261	1.918708
1	-4.292605	-2.586530	2.904623
7	-3.493646	-1.693169	1.227869
6	3.173677	-0.289681	-1.120912
6	2.149534	-0.084425	-2.068592
6	1.223890	-1.220468	-1.987005
6	1.769578	-2.153601	-1.028117
6	2.925125	-1.557062	-0.438008
6	4.360219	0.594882	-0.878496
1	5.244534	0.209755	-1.404417
1	4.620221	0.649892	0.184094
1	4.184385	1.614477	-1.231924
6	2.105237	0.996475	-3.107011
1	2.669100	1.880729	-2.800110
1	1.085015	1.315091	-3.325015
1	2.545673	0.628639	-4.044717
6	0.220850	-1.602189	-3.039303
1	0.716902	-2.190444	-3.824941
1	-0.229845	-0.731754	-3.516950
1	-0.585452	-2.217003	-2.629853
6	1.272294	-3.550456	-0.796638
1	1.710139	-4.232808	-1.538147
1	0.184401	-3.615454	-0.889303
1	1.547804	-3.925224	0.193366
6	3.872428	-2.238678	0.508908
1	4.574345	-2.880467	-0.041765
1	3.345432	-2.874856	1.227024
1	4.469778	-1.519560	1.074716
6	2.107990	0.962820	1.949011
1	2.575810	1.356293	1.047002
1	1.424104	1.717937	2.312391
6	3.191810	0.658222	2.979821
6	4.068382	1.894691	3.241109
1	3.828755	-0.172055	2.649322
1	2.740462	0.343020	3.929382
1	4.826508	1.678091	4.003086
1	4.588017	2.220543	2.332321
1	3.465809	2.738073	3.597274
6	0.893065	-0.637930	2.402084
6	0.003719	-1.371590	1.513583
1	0.414572	0.027335	3.116296
1	1.709137	-1.214855	2.823574
1	0.219637	-2.436148	1.413462
1	-1.060126	-1.182775	1.608016

INT2   **HF =** -1309.0443344 hartree

77	-1.011675	-0.231280	-0.328877
6	0.569767	-0.486350	1.071440
6	2.233621	-0.682801	0.683568
5	1.324467	-2.037841	1.179205
1	1.081423	-2.856499	0.359951
5	0.236557	-1.474396	2.441297
1	-0.849203	-1.945372	2.527548
5	0.480876	0.267250	2.601880
1	-0.431958	0.999731	2.805972
5	1.737356	0.748050	1.449967
1	1.756166	1.748188	0.829078
5	2.991823	-1.798154	1.739256
1	3.833883	-2.489535	1.263941
5	1.741549	-2.304371	2.884030
1	1.725876	-3.404564	3.336698
5	1.216369	-0.851343	3.781095
1	0.817366	-0.903624	4.900580
5	2.146959	0.543204	3.163678
1	2.424519	1.488685	3.829076
5	3.247718	-0.057912	1.918513
1	4.269114	0.444563	1.591187
5	2.928116	-1.054997	3.349140
1	3.785005	-1.257820	4.148899
6	2.616914	-0.675003	-0.808257
1	2.938305	-1.688637	-1.066971
1	1.712291	-0.455627	-1.380393
6	3.691517	0.308320	-1.226137
6	5.047598	-0.042427	-1.188903
1	5.344523	-1.025683	-0.836018
6	5.999414	0.888169	-1.598708
1	7.057225	0.640528	-1.575760
6	5.568055	2.139771	-2.037559
1	6.271797	2.898249	-2.366867
6	4.196929	2.395417	-2.048423
1	3.817265	3.356919	-2.389912
7	3.273594	1.508075	-1.659545
6	-2.930314	-1.492494	-0.097851
6	-1.966647	-2.425455	-0.546408
6	-1.376657	-1.854993	-1.738769
6	-2.183748	-0.695515	-2.157748
6	-3.111988	-0.446025	-1.121573
6	-3.760516	-1.602764	1.143846
1	-4.741340	-2.038340	0.906688
1	-3.937667	-0.622107	1.595534
1	-3.280438	-2.236952	1.892292
6	-1.636115	-3.743010	0.088307
1	-1.571165	-3.670385	1.177308
1	-0.685392	-4.140354	-0.272070
1	-2.413968	-4.481095	-0.151301
6	-0.339760	-2.511642	-2.598130
1	-0.822061	-3.213729	-3.292863
1	0.381394	-3.073575	-2.000155
1	0.208899	-1.778497	-3.195511
6	-2.058269	0.017980	-3.469650
1	-2.543590	-0.560573	-4.267272
1	-1.010752	0.161913	-3.751799
1	-2.530718	1.003024	-3.438872
6	-4.218211	0.565091	-1.116563

1	-5.146369	0.109431	-1.489030
1	-3.987584	1.421703	-1.753996
1	-4.416383	0.944048	-0.111044
6	-2.236207	3.050274	0.589474
1	-2.836293	3.205893	-0.320265
1	-2.623459	2.134957	1.062296
6	-2.451411	4.235296	1.540717
6	-3.917761	4.439918	1.936079
1	-2.069004	5.151279	1.067938
1	-1.846362	4.084916	2.445594
1	-4.036330	5.296194	2.610117
1	-4.545909	4.621599	1.054525
1	-4.316578	3.556367	2.450707
6	-0.765263	2.840475	0.212181
6	-0.479637	1.734664	-0.827556
1	-0.192733	2.663615	1.127228
1	-0.376853	3.785049	-0.203076
1	-1.025144	1.979605	-1.749922
1	0.589225	1.759721	-1.070250

1V-1   HF = -1151.9065907 hartree

77	-1.325366	-0.309813	-0.324813
6	1.912703	0.724554	0.379951
5	0.945748	1.812920	1.254275
1	0.563602	1.461674	2.322001
5	0.158940	2.832006	0.045510
1	-0.909215	3.320004	0.236155
5	0.661166	2.241392	-1.558527
1	-0.019182	2.298124	-2.532789
5	1.758561	0.885654	-1.307158
1	2.008422	-0.045622	-1.984630
5	2.694120	2.083286	1.130836
1	3.461633	1.839664	2.000004
5	1.601653	3.440615	0.904767
1	1.557988	4.309033	1.715720
5	1.421987	3.706044	-0.853447
1	1.250408	4.787486	-1.316952
5	2.417528	2.498420	-1.688853
1	3.043249	2.616074	-2.689589
1	4.022410	1.057969	-0.562640
5	2.996126	3.241201	-0.176423
1	4.014871	3.848849	-0.156634
6	2.259812	-0.646237	0.997215
1	2.292570	-0.517676	2.083121
1	1.425352	-1.310388	0.764321
6	3.543345	-1.301263	0.527132
6	4.754572	-1.105427	1.205935
1	4.789306	-0.471362	2.087092
6	5.905408	-1.738066	0.736299
1	6.854980	-1.602183	1.246850
6	5.811797	-2.549681	-0.393107
1	6.679130	-3.065132	-0.794198
6	4.562002	-2.690474	-0.998964
1	4.442408	-3.319608	-1.879326
7	3.452458	-2.088464	-0.557908
6	-3.374311	0.605308	0.077868
6	-2.744930	0.481388	1.338548
6	-2.361411	-0.917728	1.457801

S23

6	-3.046447	-1.684733	0.403091
6	-3.606474	-0.747256	-0.477245
6	-3.901995	1.866479	-0.537526
1	-4.969719	1.992008	-0.308482
1	-3.797644	1.851469	-1.626672
1	-3.369263	2.744614	-0.164662
6	-2.529946	1.555081	2.361433
1	-2.395720	2.536410	1.899982
1	-1.647343	1.358481	2.974512
1	-3.394945	1.616383	3.037089
6	-1.692579	-1.533018	2.650298
1	-2.436522	-1.788690	3.418444
1	-0.969772	-0.845390	3.097509
1	-1.164205	-2.451445	2.378217
6	-3.054166	-3.179231	0.291488
1	-3.778109	-3.621250	0.989700
1	-2.071443	-3.602486	0.524098
1	-3.323694	-3.507527	-0.716133
6	-4.353759	-1.015046	-1.748894
1	-5.435881	-0.898924	-1.597561
1	-4.174374	-2.028265	-2.118070
1	-4.056983	-0.315476	-2.536867
6	-0.316423	-1.583132	-1.610836
1	-0.891619	-2.503458	-1.783380
1	0.704086	-1.857628	-1.322596
1	-0.228405	-1.050211	-2.572693
5	0.294466	1.052473	-0.248366
6	3.075819	1.570025	-0.445156

I-1   **HF =** -1230.4684931 hartree

77	-1.360877	-0.026282	-0.448420
6	1.927319	0.738460	0.455032
5	0.976832	1.826262	1.335188
1	0.486089	1.453365	2.345133
5	0.362702	3.004218	0.177441
1	-0.669492	3.567265	0.351528
5	0.957968	2.518139	-1.428830
1	0.406689	2.732341	-2.457770
5	1.900182	1.056155	-1.215852
1	2.152995	0.183147	-1.967786
5	2.746860	1.964180	1.376182
1	3.415878	1.584174	2.277898
5	1.775703	3.414730	1.192849
1	1.726990	4.209424	2.075857
5	1.763452	3.845468	-0.538380
1	1.712644	4.971611	-0.916024
5	2.724565	2.631922	-1.401744
1	3.434750	2.775070	-2.341051
1	4.114808	0.972213	-0.304664
5	3.235790	3.196997	0.205668
1	4.295100	3.710736	0.351650
6	2.139500	-0.700983	0.962643
1	2.158650	-0.666317	2.055173
1	1.254866	-1.266633	0.660839
6	3.371728	-1.429009	0.463250
6	4.574049	-1.403449	1.184277
1	4.637431	-0.850423	2.117001
6	5.677632	-2.097653	0.689103

1	6.619175	-2.093075	1.231458
6	5.546806	-2.799358	-0.508261
1	6.376271	-3.357064	-0.932091
6	4.309330	-2.772974	-1.153361
1	4.162076	-3.312058	-2.087565
7	3.244459	-2.110740	-0.687939
6	-3.552848	-0.206754	0.471405
6	-2.594832	0.253586	1.466872
6	-1.723271	-0.857590	1.767943
6	-2.060467	-1.924593	0.880536
6	-3.204114	-1.527540	0.088381
6	-4.768621	0.553276	0.032489
1	-5.581505	0.408401	0.757198
1	-5.133591	0.217010	-0.942382
1	-4.578331	1.627253	-0.034818
6	-2.731509	1.513214	2.274533
1	-1.775011	1.814463	2.707902
1	-3.449165	1.381680	3.096892
1	-3.085039	2.346471	1.659723
6	-0.844370	-0.991707	2.977833
1	-1.430798	-1.394829	3.816208
1	-0.434325	-0.033920	3.300436
1	-0.010376	-1.679048	2.810224
6	-1.477778	-3.308717	0.919099
1	-2.030269	-3.938392	1.630703
1	-0.429262	-3.302890	1.231073
1	-1.532958	-3.804925	-0.054743
6	-3.923303	-2.403395	-0.898304
1	-4.608332	-3.099555	-0.394745
1	-3.223991	-3.009465	-1.485226
1	-4.516802	-1.812802	-1.602370
6	-0.973211	-0.532338	-2.513563
6	-0.225352	-1.416607	-1.696404
1	-0.463123	0.268059	-3.041593
1	-1.890756	-0.871834	-2.992451
1	-0.610219	-2.418569	-1.520116
1	0.853226	-1.350704	-1.630802
6	-2.193803	1.670176	-1.448375
1	-2.479289	2.415454	-0.700424
1	-1.520752	2.139034	-2.160802
1	-3.085541	1.328937	-1.985949
6	3.205207	1.550359	-0.203015
5	0.343757	1.245302	-0.272980

1TS1-1   **HF =** -1230.4160976 hartree $v^{\ddagger} = -473.8487\ icm^{-1}$

77	-1.317492	-0.193523	-0.337997
6	1.965333	0.751086	0.454406
5	1.005079	1.825128	1.329208
1	0.602775	1.459520	2.381632
5	0.270079	2.914752	0.148865
1	-0.787569	3.429194	0.332609
5	0.813772	2.380933	-1.456728
1	0.184448	2.513556	-2.455915
5	1.848005	0.981124	-1.220332
1	2.107845	0.079161	-1.935886
5	2.762486	2.061139	1.273932
1	3.494245	1.763552	2.157434
5	1.705526	3.448664	1.072736

1	1.658068	4.283326	1.918329
5	1.588909	3.790388	-0.675412
1	1.459380	4.892568	-1.102757
5	2.573885	2.586926	-1.527525
1	3.228534	2.720669	-2.507991
1	4.104319	1.058965	-0.421357
5	3.128668	3.257966	0.024444
1	4.162936	3.835019	0.094695
6	2.259604	-0.646934	1.029841
1	2.308227	-0.551621	2.118244
1	1.389061	-1.260758	0.787956
6	3.510304	-1.343350	0.532891
6	4.727420	-1.228155	1.219958
1	4.787470	-0.628388	2.123588
6	5.849903	-1.895842	0.731181
1	6.802545	-1.822123	1.248701
6	5.723805	-2.661850	-0.426608
1	6.567769	-3.202894	-0.843496
6	4.471612	-2.722305	-1.040214
1	4.327264	-3.313551	-1.942925
7	3.388758	-2.085897	-0.580757
6	-3.502712	0.263569	0.534102
6	-2.532322	0.455589	1.546976
6	-1.818934	-0.812006	1.719504
6	-2.486409	-1.797475	0.878864
6	-3.484632	-1.135577	0.125729
6	-4.471706	1.286281	0.019711
1	-5.495436	1.054834	0.343595
1	-4.483065	1.325050	-1.076713
1	-4.227482	2.287929	0.382640
6	-2.403737	1.668212	2.421925
1	-1.403365	1.763405	2.845175
1	-3.112534	1.601857	3.259884
1	-2.616246	2.592039	1.877376
6	-0.935471	-1.156698	2.885816
1	-1.541055	-1.417627	3.766100
1	-0.291167	-0.320591	3.165093
1	-0.293419	-2.014576	2.663824
6	-2.177890	-3.266461	0.869322
1	-2.727661	-3.782439	1.668531
1	-1.111825	-3.452640	1.029611
1	-2.458122	-3.738109	-0.077527
6	-4.443356	-1.751386	-0.852651
1	-5.423010	-1.931315	-0.387793
1	-4.080239	-2.712829	-1.228446
1	-4.618323	-1.100025	-1.716469
6	-0.708933	-0.725812	-2.591030
6	-0.215888	-1.550946	-1.488752
1	0.048318	-0.132525	-3.094150
1	-1.396267	-1.209123	-3.283210
1	-0.662601	-2.545899	-1.414733
1	0.863280	-1.590087	-1.361206
6	-2.007185	0.771242	-2.453195
1	-2.060148	1.684136	-1.861612
1	-1.635614	1.068147	-3.433102
1	-2.988239	0.310716	-2.561927
6	3.170219	1.593832	-0.303902
5	0.325253	1.140166	-0.219187

INT1-1 **HF =** -1230.4710699 hartree

77	1.308374	-0.233502	0.107879
6	-1.986585	0.782176	-0.322053
5	-1.068513	1.998963	-1.062738
1	-0.707631	1.798783	-2.174980
5	-0.269522	2.866341	0.250742
1	0.784774	3.397636	0.103839
5	-0.719641	2.059100	1.773341
1	-0.016796	2.005428	2.731449
5	-1.797842	0.723092	1.365622
1	-2.021361	-0.298410	1.909074
5	-2.815296	2.209934	-0.868736
1	-3.597574	2.066230	-1.747007
5	-1.744324	3.550046	-0.490110
1	-1.736522	4.518377	-1.179954
5	-1.525478	3.587381	1.283242
1	-1.363754	4.601952	1.881623
5	-2.477016	2.257757	1.974732
1	-3.081003	2.228254	2.995074
1	-4.080352	0.941804	0.704722
5	-3.106856	3.179416	0.586192
1	-4.137446	3.761262	0.669101
6	-2.319289	-0.507477	-1.100818
1	-2.320011	-0.255223	-2.165291
1	-1.495529	-1.200986	-0.922023
6	-3.618738	-1.203176	-0.747809
6	-4.805047	-0.927888	-1.442823
1	-4.807817	-0.198750	-2.247594
6	-5.971659	-1.604289	-1.087582
1	-6.902486	-1.409073	-1.613180
6	-5.917600	-2.537196	-0.053188
1	-6.798255	-3.091599	0.256498
6	-4.690277	-2.748474	0.577780
1	-4.602578	-3.472159	1.386350
7	-3.565399	-2.105518	0.246391
6	3.341500	0.690432	-0.381707
6	2.554377	0.852765	-1.549063
6	2.080178	-0.474231	-1.891189
6	2.845861	-1.462575	-1.103688
6	3.593766	-0.747261	-0.159477
6	3.996612	1.787930	0.402061
1	5.025660	1.951192	0.051604
1	4.047563	1.542485	1.467319
1	3.451427	2.729724	0.301222
6	2.303926	2.125635	-2.298810
1	1.369108	2.089745	-2.861470
1	3.115939	2.308830	-3.017036
1	2.249533	2.988440	-1.630335
6	1.253552	-0.817420	-3.094004
1	1.900307	-0.968094	-3.970366
1	0.547067	-0.017997	-3.332231
1	0.685782	-1.739320	-2.937378
6	2.787201	-2.946421	-1.303414
1	3.397884	-3.248662	-2.165325
1	1.762629	-3.283780	-1.491581
1	3.157130	-3.487447	-0.428128
6	4.545423	-1.294305	0.861284

1	5.582339	-1.205572	0.507654
1	4.354478	-2.350583	1.068606
1	4.476190	-0.753235	1.809032
6	0.500833	-1.505225	2.829927
6	0.461902	-1.738627	1.300930
1	-0.072084	-0.610208	3.094436
1	-0.018900	-2.348220	3.312492
1	1.015489	-2.667032	1.085125
1	-0.582088	-1.930490	1.023819
6	1.900781	-1.389175	3.441237
1	2.412217	-0.485075	3.089153
1	1.851272	-1.338599	4.536091
1	2.525938	-2.251861	3.176400
6	-3.147535	1.486831	0.634461
5	-0.358033	1.061638	0.311604

II-1   **HF =** -1309.0315787 hartree

77	-1.197454	-0.209800	-0.259061
6	2.093255	0.735451	0.531376
5	1.124986	1.533902	1.664152
1	0.768863	0.930922	2.617429
5	0.295120	2.822604	0.792328
1	-0.769028	3.222709	1.138539
5	0.791588	2.699170	-0.914965
1	0.136714	3.028481	-1.848987
5	1.885635	1.339208	-1.042835
1	2.156750	0.651548	-1.961728
5	2.868609	1.863678	1.605132
1	3.650209	1.407479	2.370294
5	1.746130	3.204157	1.764371
1	1.697202	3.818472	2.781083
5	1.536549	3.930740	0.147800
1	1.340655	5.092770	-0.009496
5	2.531948	3.005628	-0.990182
1	3.136209	3.392392	-1.934773
1	4.169971	1.346901	-0.322652
5	3.126400	3.331963	0.654879
1	4.138545	3.928719	0.818623
6	2.499110	-0.735184	0.747047
1	2.590103	-0.898485	1.823831
1	1.665731	-1.341782	0.387616
6	3.768680	-1.200578	0.062401
6	5.004962	-1.165525	0.723189
1	5.066266	-0.796745	1.742906
6	6.144957	-1.609935	0.054151
1	7.113573	-1.592359	0.546284
6	6.015862	-2.079887	-1.251980
1	6.873695	-2.438214	-1.812676
6	4.743608	-2.084026	-1.826124
1	4.597256	-2.448176	-2.841478
7	3.643431	-1.659886	-1.194340
6	-3.240385	-0.775994	0.895095
6	-2.168878	-0.461354	1.821198
6	-1.199390	-1.528174	1.733478
6	-1.616647	-2.402891	0.682194
6	-2.884525	-1.942199	0.166940
6	-4.567513	-0.078153	0.883728
1	-5.120286	-0.334173	1.798213

1	-5.185704	-0.374699	0.033277
1	-4.465048	1.010658	0.866245
6	-2.276201	0.558201	2.920244
1	-2.687840	1.503304	2.552673
1	-1.302633	0.778836	3.362305
1	-2.935937	0.201068	3.724229
6	-0.143920	-1.849537	2.752562
1	-0.595054	-2.396383	3.593228
1	0.324183	-0.953640	3.163332
1	0.643478	-2.487416	2.341348
6	-0.968482	-3.709340	0.322198
1	-1.351549	-4.515686	0.963367
1	0.117902	-3.679200	0.446574
1	-1.178181	-3.998794	-0.712211
6	-3.707340	-2.648292	-0.873880
1	-4.251894	-3.502196	-0.447170
1	-3.084085	-3.039117	-1.686115
1	-4.445789	-1.979384	-1.324477
6	-2.290479	1.572150	-0.835692
1	-2.710769	1.935261	0.110398
1	-1.610780	2.345773	-1.179544
6	-3.402887	1.429612	-1.882479
6	-4.272599	2.695900	-1.967129
1	-4.049391	0.568019	-1.677982
1	-2.963855	1.249719	-2.870552
1	-5.031984	2.606883	-2.754456
1	-4.793223	2.888440	-1.020500
1	-3.660959	3.578698	-2.189232
6	-0.935833	-0.319095	-2.404049
6	-0.018779	-1.212658	-1.795494
1	-0.577441	0.615044	-2.827492
1	-1.834317	-0.710887	-2.876101
1	-0.257829	-2.273248	-1.779151
1	1.044505	-1.012331	-1.789387
5	0.402068	1.181983	0.027945
6	3.221177	1.791416	-0.050747

1TS2-1　　　　**HF =** -1308.9 792731 hartree　　$v^{\ddagger} = -438.1918\ icm^{-1}$

77	1.166316	-0.293373	0.060759
6	-2.159690	0.629998	-0.532385
5	-1.297805	1.371799	-1.773119
1	-1.039131	0.709891	-2.719771
5	-0.398678	2.701958	-1.041188
1	0.631543	3.097002	-1.485032
5	-0.742558	2.663629	0.696267
1	-0.001353	3.067773	1.528273
5	-1.812310	1.299190	0.991601
1	-1.988546	0.646770	1.960101
5	-3.029321	1.708037	-1.583633
1	-3.872188	1.216027	-2.255695
5	-1.931831	3.036657	-1.902534
1	-1.977437	3.602823	-2.947387
5	-1.590040	3.838468	-0.347528
1	-1.384876	5.006496	-0.259227
5	-2.474731	2.962900	0.918604
1	-2.995132	3.395513	1.893177
1	-4.156023	1.274681	0.472992
5	-3.212286	3.214684	-0.681312

1	-4.237308	3.803435	-0.783918
6	-2.573649	-0.847091	-0.688019
1	-2.712286	-1.034760	-1.756112
1	-1.722300	-1.444861	-0.358046
6	-3.818093	-1.283482	0.057663
6	-5.061283	-1.350924	-0.587485
1	-5.143987	-1.086548	-1.637594
6	-6.181184	-1.760522	0.135365
1	-7.154087	-1.820515	-0.344961
6	-6.026860	-2.093614	1.480023
1	-6.868206	-2.420022	2.083681
6	-4.750007	-2.000670	2.036728
1	-4.584034	-2.256132	3.081991
7	-3.669299	-1.608791	1.353403
6	3.235701	-0.073821	-1.092392
6	2.158113	-0.063785	-2.016886
6	1.441224	-1.332138	-1.877549
6	2.195844	-2.147896	-0.939261
6	3.265706	-1.372100	-0.433499
6	4.258468	1.009418	-0.910738
1	5.166967	0.798927	-1.492275
1	4.564388	1.109742	0.136649
1	3.874871	1.980053	-1.237390
6	1.956140	0.946995	-3.106872
1	2.281471	1.945157	-2.804170
1	0.912537	1.021159	-3.413289
1	2.542500	0.656728	-3.990696
6	0.435665	-1.882024	-2.850353
1	0.942595	-2.334019	-3.715631
1	-0.230893	-1.104298	-3.227798
1	-0.182517	-2.659258	-2.390035
6	1.903634	-3.583424	-0.613051
1	2.367136	-4.251721	-1.352011
1	0.828643	-3.787356	-0.617990
1	2.292202	-3.865560	0.370600
6	4.329804	-1.838700	0.519210
1	5.153727	-2.326027	-0.021125
1	3.943685	-2.563933	1.243065
1	4.763610	-1.006541	1.081077
6	1.945582	1.080846	2.013463
1	2.383555	1.553183	1.134317
1	1.167075	1.743481	2.374805
6	3.042845	0.871330	3.054597
6	3.788884	2.179836	3.361157
1	3.761060	0.118316	2.704318
1	2.617913	0.480979	3.989012
1	4.556824	2.021536	4.128138
1	4.283250	2.579110	2.467552
1	3.100912	2.949970	3.729074
6	0.943458	-0.650013	2.393338
6	0.077229	-1.390552	1.479920
1	0.437610	-0.075913	3.167203
1	1.799904	-1.198896	2.773969
1	0.313797	-2.451810	1.372839
1	-0.989902	-1.230367	1.598976
5	-0.429950	1.095053	-0.184376
6	-3.236069	1.707198	0.100724

INT2-1   **HF =** -1309.0400697 hartree

77	-1.199967	-0.383993	-0.136949
6	2.169725	0.367167	0.433606
5	1.766947	-0.767602	1.634754
1	1.804005	-1.916485	1.333734
5	0.675467	0.077156	2.739971
1	-0.162077	-0.498593	3.354803
5	0.407017	1.710990	2.088891
1	-0.602655	2.325051	2.226074
5	1.352649	1.856206	0.616477
1	1.198206	2.521172	-0.347928
5	3.330441	0.062740	1.689530
1	4.357244	-0.430998	1.378219
5	2.397550	-0.095096	3.166627
1	2.785634	-0.804965	4.038090
5	1.550770	1.452071	3.449560
1	1.327427	1.860852	4.543636
5	1.975502	2.555058	2.126442
1	2.149738	3.727731	2.164008
1	3.728777	2.072797	0.475360
5	3.198662	1.446306	2.789713
1	4.196816	1.871818	3.269095
6	2.549130	-0.057867	-0.999039
1	2.025755	-0.997358	-1.191698
1	2.137976	0.680311	-1.691319
6	4.024524	-0.216399	-1.306066
6	4.581786	-1.473262	-1.568358
1	3.962176	-2.363802	-1.520424
6	5.936563	-1.562249	-1.885059
1	6.390781	-2.527343	-2.092616
6	6.694318	-0.393309	-1.928880
1	7.752298	-0.411722	-2.171551
6	6.053722	0.815097	-1.651100
1	6.608386	1.751616	-1.674003
7	4.753610	0.912803	-1.353023
6	-2.833420	-1.334806	1.200374
6	-1.800256	-2.284070	1.076137
6	-1.594635	-2.475546	-0.358863
6	-2.726980	-1.872638	-1.076310
6	-3.429153	-1.103925	-0.135175
6	-3.388686	-0.761147	2.469660
1	-4.298561	-1.298248	2.772811
1	-3.655573	0.293071	2.346473
1	-2.667207	-0.825444	3.287135
6	-1.079591	-3.017578	2.165376
1	-1.209722	-2.532039	3.134312
1	-0.005673	-3.085476	1.974749
1	-1.468773	-4.042367	2.247770
6	-0.637766	-3.462548	-0.958338
1	-1.093168	-4.463036	-0.991598
1	0.279540	-3.533525	-0.367496
1	-0.366768	-3.185730	-1.981408
6	-3.003825	-2.031102	-2.541046
1	-3.464156	-3.006781	-2.748860
1	-2.084417	-1.971319	-3.132922
1	-3.683334	-1.258562	-2.910991
6	-4.645781	-0.258762	-0.364855
1	-5.542576	-0.762601	0.021640

1	-4.807574	-0.058408	-1.426896
1	-4.567256	0.704320	0.149553
6	-2.172402	2.869610	-1.233059
1	-2.425235	2.437082	-0.252796
1	-1.233414	3.421242	-1.081075
6	-3.271655	3.851785	-1.658057
6	-3.494416	4.986046	-0.651570
1	-4.213709	3.302646	-1.804587
1	-3.015689	4.278494	-2.638783
1	-4.285027	5.669558	-0.983154
1	-3.783505	4.592998	0.331224
1	-2.580001	5.575615	-0.512271
6	-1.934057	1.736537	-2.240927
6	-0.796029	0.765739	-1.857164
1	-1.698810	2.188731	-3.219490
1	-2.872647	1.183323	-2.387896
1	-0.667818	0.042894	-2.678749
1	0.132065	1.342558	-1.812489
5	0.481444	0.299723	0.955410
6	2.975297	1.633393	1.118985

1V-2　　　　**HF =** -1138.8246004 hartree

77	-1.277736	-0.315439	-0.338645
6	1.985075	0.837727	0.322551
5	0.943140	1.825778	1.256250
1	0.585588	1.403528	2.314554
5	0.045311	2.820849	0.110021
1	-1.059054	3.213287	0.346689
5	0.549593	2.326126	-1.526181
1	-0.185886	2.361699	-2.469744
5	1.771125	1.050364	-1.352010
1	1.949058	0.132134	-2.083310
5	2.668083	2.217258	1.096056
1	3.388744	2.024721	2.030152
5	1.460106	3.502587	0.952304
1	1.351019	4.337018	1.802212
5	1.218235	3.814896	-0.785191
1	0.929234	4.899669	-1.198715
5	2.285984	2.715727	-1.697565
1	2.766917	2.996235	-2.755433
5	3.183040	1.746548	-0.530015
1	4.256504	1.265668	-0.704336
5	2.847470	3.445679	-0.164608
1	3.736418	4.244496	-0.123681
6	2.303436	-0.540718	0.949620
1	2.382662	-0.391881	2.032808
1	1.450787	-1.198062	0.771350
6	3.544956	-1.270961	0.482561
6	4.825210	-0.893916	0.923396
1	4.932821	-0.030619	1.572397
6	5.933402	-1.624164	0.509325
1	6.931399	-1.344624	0.839162
6	5.741691	-2.717699	-0.338168
1	6.576120	-3.318640	-0.690025
6	4.437421	-3.020987	-0.722087
1	4.239332	-3.867108	-1.380294
7	3.362209	-2.329747	-0.324287
6	-3.357774	0.534527	0.086889

6	-2.699234	0.437739	1.334630
6	-2.266271	-0.949831	1.443181
6	-2.982311	-1.742080	0.424603
6	-3.589707	-0.827505	-0.442153
6	-3.917651	1.781790	-0.531606
1	-4.970392	1.928470	-0.246595
1	-3.873323	1.733978	-1.624253
1	-3.349365	2.661669	-0.220737
6	-2.504752	1.512741	2.359216
1	-2.550473	2.507218	1.910487
1	-1.533620	1.430935	2.852600
1	-3.285602	1.450682	3.133113
6	-1.560000	-1.535617	2.630890
1	-2.273376	-1.760722	3.438539
1	-0.812876	-0.838877	3.020806
1	-1.046762	-2.465313	2.366643
6	-2.934889	-3.236204	0.314332
1	-3.558267	-3.715068	1.083452
1	-1.912290	-3.609221	0.439339
1	-3.290969	-3.580632	-0.661479
6	-4.355242	-1.118945	-1.698564
1	-5.435155	-0.968978	-1.553192
1	-4.203277	-2.149048	-2.034091
1	-4.040798	-0.456978	-2.512642
6	-0.214876	-1.572627	-1.592517
1	-0.768391	-2.508277	-1.772987
1	0.802076	-1.823808	-1.275126
1	-0.112723	-1.040135	-2.552432
5	0.328557	1.084991	-0.256286

I-2	**HF =** -1217.3879783 hartree		
77	-1.330978	-0.000226	-0.459712
6	1.995597	0.828108	0.425595
5	0.995775	1.876581	1.329255
1	0.487649	1.477147	2.327429
5	0.332963	3.052140	0.199858
1	-0.725082	3.571729	0.391795
5	0.940696	2.617888	-1.415188
1	0.349915	2.829579	-2.431087
5	1.953283	1.184739	-1.235741
1	2.113492	0.320128	-2.035599
5	2.764920	2.054984	1.360067
1	3.359406	1.704336	2.336125
5	1.736396	3.485950	1.212923
1	1.641593	4.263165	2.116967
5	1.707982	3.949078	-0.503275
1	1.592651	5.087506	-0.851723
5	2.711830	2.788302	-1.401523
1	3.320286	3.069091	-2.391547
5	3.365577	1.633752	-0.245520
1	4.381435	1.029517	-0.373891
5	3.210712	3.331351	0.223750
1	4.183736	4.001897	0.406319
6	2.127142	-0.619003	0.950038
1	2.197367	-0.565070	2.041556
1	1.205314	-1.150039	0.703569
6	3.284970	-1.453445	0.444223
6	4.568295	-1.333543	1.004068

1	4.743381	-0.597849	1.782783
6	5.596621	-2.144865	0.538135
1	6.596652	-2.061755	0.957429
6	5.323311	-3.061337	-0.479735
1	6.093926	-3.714965	-0.879581
6	4.021710	-3.115467	-0.972667
1	3.761569	-3.817072	-1.765328
7	3.021492	-2.345507	-0.525981
6	-3.510865	-0.289513	0.523891
6	-2.536086	0.179661	1.499251
6	-1.627577	-0.910125	1.752279
6	-1.958398	-1.965643	0.849827
6	-3.143423	-1.593434	0.111411
6	-4.749517	0.455663	0.122429
1	-5.538646	0.323730	0.876737
1	-5.146756	0.103165	-0.834957
1	-4.563764	1.528727	0.026989
6	-2.677871	1.415373	2.342436
1	-3.137414	2.232733	1.778141
1	-1.703099	1.770655	2.684234
1	-3.307292	1.229758	3.226660
6	-0.717731	-1.039479	2.939446
1	-1.294356	-1.375471	3.815310
1	-0.242672	-0.092115	3.198178
1	0.073596	-1.775092	2.771050
6	-1.317219	-3.324718	0.821387
1	-1.805936	-4.005862	1.534140
1	-0.255540	-3.278751	1.080474
1	-1.391901	-3.789007	-0.167585
6	-3.850867	-2.462975	-0.889383
1	-4.483886	-3.220915	-0.403999
1	-3.140668	-3.002154	-1.528151
1	-4.496589	-1.873153	-1.547936
6	-0.935315	-0.384583	-2.536693
6	-0.182096	-1.301831	-1.759094
1	-0.427628	0.448327	-3.014022
1	-1.844421	-0.713102	-3.042343
1	-0.556766	-2.317676	-1.639592
1	0.892791	-1.219804	-1.672027
6	-2.217110	1.710686	-1.364452
1	-2.525876	2.405577	-0.577158
1	-1.557857	2.244480	-2.043109
1	-3.100449	1.369642	-1.922033
5	0.404915	1.316779	-0.282376

1TS1-2   **HF =** -1217.3332489 hartree $v^{\ddagger} = -478.9147\ icm^{-1}$

77	-1.283193	-0.194893	-0.352391
6	2.036836	0.845630	0.418703
5	1.011913	1.849270	1.328934
1	0.614088	1.434673	2.372365
5	0.197192	2.922401	0.186991
1	-0.896933	3.361962	0.394978
5	0.761420	2.465940	-1.434504
1	0.095321	2.590299	-2.418714
5	1.891258	1.120666	-1.247615
1	2.078230	0.225044	-2.008016
5	2.756501	2.167753	1.259897
1	3.423086	1.910308	2.218352

S34

5	1.611689	3.508080	1.109518
1	1.503137	4.316326	1.984581
5	1.464736	3.889749	-0.621430
1	1.245590	4.999566	-1.011269
5	2.513265	2.767242	-1.522563
1	3.048382	3.050223	-2.554019
5	3.310637	1.717562	-0.353960
1	4.363304	1.185501	-0.507417
5	3.045757	3.421304	0.050342
1	3.970371	4.172416	0.154818
6	2.274730	-0.564520	1.002661
1	2.363216	-0.455738	2.089351
1	1.381033	-1.159510	0.802900
6	3.475720	-1.341402	0.507615
6	4.760613	-1.099815	1.023669
1	4.900083	-0.313070	1.758399
6	5.834040	-1.859393	0.572797
1	6.835101	-1.682178	0.959309
6	5.603873	-2.848177	-0.386461
1	6.410022	-3.466931	-0.771686
6	4.298089	-3.021480	-0.839351
1	4.070619	-3.782846	-1.585753
7	3.255653	-2.300983	-0.407477
6	-3.491388	0.190237	0.583271
6	-2.504077	0.397248	1.575071
6	-1.745309	-0.846984	1.703867
6	-2.403357	-1.838563	0.860277
6	-3.448215	-1.200151	0.154192
6	-4.486823	1.196706	0.085948
1	-5.511028	0.925848	0.379988
1	-4.476201	1.272968	-1.009662
1	-4.278378	2.193677	0.483047
6	-2.370994	1.597849	2.463663
1	-2.772419	2.499287	1.993194
1	-1.328240	1.802071	2.707741
1	-2.916454	1.437296	3.406792
6	-0.836673	-1.183431	2.853324
1	-1.420474	-1.460075	3.745703
1	-0.201250	-0.336211	3.117690
1	-0.181403	-2.026811	2.613911
6	-2.041811	-3.295318	0.812538
1	-2.551639	-3.855152	1.610433
1	-0.965265	-3.440324	0.943146
1	-2.322161	-3.755336	-0.140980
6	-4.398311	-1.821848	-0.828962
1	-5.377986	-2.033221	-0.373494
1	-4.012243	-2.768971	-1.220522
1	-4.584989	-1.162650	-1.685755
6	-0.662547	-0.615655	-2.613884
6	-0.155147	-1.476081	-1.544985
1	0.082583	0.027746	-3.070492
1	-1.325708	-1.088977	-3.338415
1	-0.575745	-2.487005	-1.517988
1	0.922206	-1.487492	-1.403727
6	-2.007734	0.818996	-2.414226
1	-2.069136	1.707719	-1.786980
1	-1.657052	1.167317	-3.385441
1	-2.978866	0.334936	-2.528721

| 5 | 0.380516 | 1.181598 | -0.229519 |

INT1-2 **HF =** -1217.3892998 hartree

77	1.262732	-0.222070	0.123924
6	-2.054353	0.880502	-0.309002
5	-1.059254	2.017372	-1.112479
1	-0.700113	1.742579	-2.215918
5	-0.184327	2.885134	0.147947
1	0.905345	3.344068	-0.035678
5	-0.656655	2.166958	1.710102
1	0.084516	2.108872	2.647935
5	-1.837627	0.884526	1.374848
1	-1.990307	-0.128390	1.974022
5	-2.793029	2.323329	-0.897904
1	-3.513051	2.226813	-1.847072
5	-1.629854	3.620706	-0.593051
1	-1.554469	4.561285	-1.328063
5	-1.381941	3.714567	1.169385
1	-1.125491	4.746877	1.716514
5	-2.404455	2.471505	1.936772
1	-2.886151	2.596695	3.023497
5	-3.276866	1.631207	0.657140
1	-4.330649	1.093274	0.773606
5	-3.004002	3.372069	0.513211
1	-3.919278	4.138559	0.578705
6	-2.339232	-0.426311	-1.087225
1	-2.407397	-0.165571	-2.149706
1	-1.478854	-1.086669	-0.964058
6	-3.575464	-1.213865	-0.709000
6	-4.851113	-0.829306	-1.155855
1	-4.958358	0.072385	-1.750633
6	-5.956769	-1.598117	-0.810511
1	-6.951944	-1.312246	-1.143451
6	-5.766042	-2.737194	-0.025334
1	-6.598742	-3.368243	0.273886
6	-4.465283	-3.045986	0.366724
1	-4.268801	-3.927544	0.977084
7	-3.392112	-2.317906	0.034440
6	3.290500	0.653658	-0.468802
6	2.476131	0.725071	-1.625547
6	1.998231	-0.630119	-1.845837
6	2.815642	-1.550392	-1.027504
6	3.578583	-0.761717	-0.161344
6	3.945272	1.817477	0.215626
1	4.936144	2.023945	-0.216435
1	4.084393	1.623552	1.283876
1	3.334116	2.718751	0.120447
6	2.215561	1.931169	-2.474920
1	2.123375	2.838858	-1.873400
1	1.289784	1.831712	-3.044376
1	3.038567	2.078482	-3.191729
6	1.136848	-1.063847	-2.995929
1	1.743509	-1.209217	-3.902915
1	0.371766	-0.313788	-3.213753
1	0.629033	-2.008231	-2.777350
6	2.740854	-3.045719	-1.098133
1	3.184603	-3.424716	-2.029863
1	1.701263	-3.390906	-1.062422

1	3.269453	-3.515496	-0.263285
6	4.544978	-1.219734	0.889935
1	5.584647	-1.113101	0.545903
1	4.387952	-2.269418	1.154812
1	4.444684	-0.633095	1.808338
6	0.444651	-1.375961	2.892704
6	0.387146	-1.660255	1.374408
1	-0.090814	-0.449381	3.120062
1	-0.102966	-2.178796	3.414757
1	0.915833	-2.612404	1.187344
1	-0.661759	-1.828164	1.106258
6	1.854048	-1.292198	3.489843
1	2.393392	-0.420268	3.100667
1	1.818927	-1.201611	4.584142
1	2.446931	-2.185888	3.248618
5	-0.403158	1.108269	0.290153

II-2	**HF =** -1295.9510211 hartree		
77	-1.167650	-0.209657	-0.267865
6	2.141454	0.888485	0.476194
5	1.116631	1.646979	1.608762
1	0.763821	1.034002	2.564399
5	0.209602	2.878243	0.736706
1	-0.881934	3.212643	1.087756
5	0.708601	2.772246	-0.970673
1	0.004444	3.048639	-1.894911
5	1.896370	1.476440	-1.097815
1	2.082795	0.772664	-2.037282
5	2.844836	2.056675	1.531500
1	3.567292	1.650375	2.392802
5	1.642137	3.342009	1.693352
1	1.541686	3.957340	2.713920
5	1.391075	4.045393	0.079305
1	1.105811	5.196675	-0.074712
5	2.436475	3.173679	-1.065784
1	2.907086	3.676023	-2.043047
5	3.333118	1.960017	-0.161636
1	4.395837	1.520517	-0.463067
5	3.021232	3.535227	0.581161
1	3.920095	4.294587	0.792457
6	2.501216	-0.586983	0.756147
1	2.633264	-0.690284	1.837931
1	1.647193	-1.203034	0.469511
6	3.727687	-1.159548	0.078204
6	5.012606	-0.956672	0.609737
1	5.131930	-0.341120	1.495942
6	6.111262	-1.531683	-0.018475
1	7.113038	-1.381405	0.377307
6	5.904733	-2.299415	-1.166739
1	6.731173	-2.767406	-1.694842
6	4.596422	-2.451987	-1.620047
1	4.387842	-3.045526	-2.510149
7	3.529693	-1.909808	-1.019023
6	-3.182196	-0.898437	0.931975
6	-2.116890	-0.503483	1.835824
6	-1.090186	-1.510903	1.752545
6	-1.468588	-2.423957	0.719763
6	-2.775031	-2.059633	0.228955

6	-4.540951	-0.262452	0.911738
1	-5.074881	-0.492327	1.845129
1	-5.155698	-0.626459	0.083784
1	-4.485384	0.827636	0.835323
6	-2.258049	0.532051	2.915738
1	-2.779001	1.422548	2.549533
1	-1.282838	0.860511	3.280718
1	-2.830795	0.142074	3.771912
6	-0.012313	-1.756852	2.768978
1	-0.438266	-2.265116	3.648032
1	0.449046	-0.830114	3.113848
1	0.779062	-2.400545	2.375019
6	-0.734351	-3.683022	0.351947
1	0.350722	-3.555198	0.407991
1	-0.974887	-4.008522	-0.665701
1	-1.008251	-4.508376	1.026006
6	-3.548083	-2.814484	-0.816238
1	-4.393445	-2.228771	-1.190241
1	-3.950274	-3.762668	-0.429497
1	-2.919866	-3.062138	-1.681243
6	-2.329343	1.521446	-0.808525
1	-2.759636	1.850481	0.146610
1	-1.684294	2.328284	-1.142350
6	-3.444872	1.338860	-1.846324
6	-4.381764	2.558209	-1.907583
1	-4.043458	0.439528	-1.649557
1	-3.006335	1.197300	-2.841300
1	-5.144056	2.445382	-2.691322
1	-4.903484	2.710300	-0.953471
1	-3.815692	3.473956	-2.117458
6	-0.901332	-0.275220	-2.401301
6	0.033739	-1.157033	-1.798995
1	-0.558298	0.673483	-2.804708
1	-1.785194	-0.684124	-2.890128
1	-0.182478	-2.224154	-1.801707
1	1.089740	-0.926549	-1.774769
5	0.437269	1.260571	-0.020237

1TS2-2	**HF =** -1295.895414 hartree		$v^{\ddagger} = - 447.7705\ icm^{-1}$
77	1.132272	-0.296363	0.063350
6	-2.214938	0.780654	-0.457859
5	-1.303208	1.514485	-1.687303
1	-1.063248	0.866903	-2.656539
5	-0.318589	2.764032	-0.927579
1	0.741497	3.103674	-1.365301
5	-0.664151	2.703051	0.808433
1	0.120860	3.045328	1.637673
5	-1.826432	1.398004	1.080192
1	-1.914594	0.703996	2.044008
5	-3.015623	1.927904	-1.464512
1	-3.811360	1.503372	-2.249005
5	-1.836083	3.208232	-1.764692
1	-1.832980	3.801208	-2.803728
5	-1.446132	3.946104	-0.198233
1	-1.149992	5.100398	-0.091398
5	-2.378536	3.094872	1.060360
1	-2.757844	3.621000	2.065142
5	-3.347666	1.859037	0.268819

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1	-4.379126	1.424121	0.670490
5	-3.112113	3.422023	-0.533263
1	-4.028183	4.176902	-0.678070
6	-2.586751	-0.699133	-0.710554
1	-2.761909	-0.805941	-1.786457
1	-1.721855	-1.315027	-0.459893
6	-3.793315	-1.253624	0.016439
6	-5.092956	-1.049170	-0.478721
1	-5.233508	-0.448529	-1.371950
6	-6.177119	-1.600498	0.194167
1	-7.189285	-1.447896	-0.173576
6	-5.942479	-2.347562	1.350694
1	-6.756340	-2.797495	1.913138
6	-4.622020	-2.502363	1.766672
1	-4.391485	-3.079757	2.662266
7	-3.569624	-1.982132	1.123235
6	3.196800	-0.130665	-1.160824
6	2.089821	-0.060318	-2.045263
6	1.328112	-1.299351	-1.897375
6	2.091497	-2.163985	-1.006222
6	3.211784	-1.444854	-0.536204
6	4.253676	0.919935	-0.977901
1	5.149965	0.703408	-1.578303
1	4.578866	0.991029	0.067321
1	3.886715	1.907037	-1.273603
6	1.884906	0.977966	-3.107983
1	2.294357	1.947480	-2.814166
1	0.828942	1.129760	-3.330104
1	2.388023	0.664810	-4.036262
6	0.277997	-1.797318	-2.851227
1	0.742003	-2.254723	-3.739636
1	-0.369423	-0.987083	-3.190286
1	-0.358653	-2.556000	-2.384433
6	1.745014	-3.589746	-0.689096
1	0.661591	-3.732289	-0.629798
1	2.173492	-3.910465	0.266702
1	2.124133	-4.272111	-1.464178
6	4.287237	-1.958001	0.379477
1	4.720370	-1.154985	0.984786
1	5.114958	-2.413691	-0.185460
1	3.907967	-2.721272	1.067789
6	1.994762	1.012443	2.007575
1	2.459440	1.448878	1.123160
1	1.269715	1.735017	2.363545
6	3.081615	0.741700	3.045947
6	3.916402	1.999452	3.336976
1	3.749371	-0.063043	2.707376
1	2.634637	0.393661	3.987927
1	4.676568	1.802323	4.104791
1	4.431447	2.354466	2.436053
1	3.280818	2.818444	3.693948
6	0.880196	-0.629742	2.388859
6	0.014235	-1.361969	1.467098
1	0.365020	-0.014945	3.124796
1	1.694494	-1.209407	2.815875
1	0.232168	-2.430390	1.376021
1	-1.050115	-1.176720	1.557334
5	-0.471847	1.158323	-0.113555

INT2-2　　　　　**HF =** -1295.9570904 hartree

77	-1.193156	-0.097095	-0.305566
6	2.202927	-0.890613	0.303551
5	1.347208	-2.375600	0.391746
1	1.124827	-2.944604	-0.635075
5	0.341386	-2.281055	1.835354
1	-0.697323	-2.864112	1.917751
5	0.576470	-0.663963	2.541604
1	-0.285863	-0.082455	3.132835
5	1.757604	0.198880	1.533182
1	1.792068	1.366878	1.321058
5	3.046576	-2.268923	0.898734
1	3.884867	-2.751808	0.197849
5	1.888863	-3.157354	1.898399
1	1.940041	-4.349504	1.979860
5	1.411266	-2.088775	3.240390
1	1.110212	-2.519202	4.315156
5	2.284056	-0.545022	3.056537
1	2.617080	0.135037	3.981304
5	3.301764	-0.672966	1.621158
1	4.316372	-0.083051	1.430131
5	3.095377	-2.089076	2.659294
1	4.014123	-2.512874	3.296342
6	2.565526	-0.413850	-1.123850
1	2.667444	-1.308857	-1.748024
1	1.730153	0.166554	-1.517211
6	3.818924	0.421265	-1.280887
6	5.087934	-0.177845	-1.355725
1	5.175579	-1.255101	-1.256935
6	6.212248	0.620823	-1.532056
1	7.202241	0.173776	-1.587853
6	6.046405	2.003765	-1.631485
1	6.893628	2.670607	-1.768298
6	4.750588	2.509889	-1.550819
1	4.573643	3.583016	-1.626335
7	3.660252	1.751164	-1.387816
6	-3.167340	-1.265456	0.091196
6	-2.372323	-2.049503	-0.765868
6	-2.048577	-1.194743	-1.911054
6	-2.947846	-0.029124	-1.881675
6	-3.553935	-0.027258	-0.619190
6	-3.694204	-1.655182	1.440605
1	-4.728369	-2.025575	1.373767
1	-3.692327	-0.800744	2.125129
1	-3.075871	-2.433301	1.893885
6	-1.969815	-3.483720	-0.608954
1	-2.143112	-3.839491	0.408332
1	-0.910135	-3.636559	-0.826681
1	-2.553534	-4.116437	-1.295203
6	-1.275887	-1.654822	-3.112808
1	-1.917078	-2.239052	-3.790891
1	-0.436627	-2.286964	-2.809444
1	-0.873558	-0.807557	-3.676376
6	-3.071017	0.990110	-2.974375
1	-2.088242	1.278768	-3.363944
1	-3.562666	1.902208	-2.622322
1	-3.657275	0.601085	-3.819664

6	-4.494996	0.994282	-0.052671
1	-4.229870	1.245919	0.979672
1	-5.528295	0.617426	-0.040829
1	-4.484025	1.921551	-0.632581
6	-1.054183	3.073441	1.310912
1	-1.552797	2.188434	1.732674
1	-0.020078	3.030451	1.677444
6	-1.732521	4.343891	1.840099
6	-1.732175	4.439229	3.370352
1	-2.769508	4.386423	1.472157
1	-1.227679	5.227014	1.419953
1	-2.220360	5.357785	3.721453
1	-2.258415	3.587202	3.818515
1	-0.708540	4.430891	3.764047
6	-1.050398	2.970674	-0.220835
6	-0.293933	1.746389	-0.784474
1	-0.587863	3.889338	-0.624529
1	-2.091837	2.979061	-0.579270
1	-0.310690	1.820654	-1.884652
1	0.754597	1.830722	-0.491468
5	0.492204	-0.845183	0.759932

2V   **HF =** -1156.7310178 hartree

6	0.224822	1.048354	-0.299508
6	1.788665	0.896720	0.357436
5	0.612931	1.813199	1.184067
1	0.189730	1.363177	2.196089
5	-0.313339	2.663475	-0.045368
1	-1.475353	2.835086	0.127673
5	0.299486	2.134465	-1.614200
1	-0.433858	1.944311	-2.532860
5	1.617988	0.987756	-1.331403
1	1.828897	0.029307	-1.984501
5	2.299287	2.364998	1.077579
1	2.972534	2.274065	2.053067
5	0.978786	3.514939	0.818074
1	0.734182	4.364518	1.614286
5	0.787154	3.719612	-0.948489
1	0.399325	4.733497	-1.435267
5	1.989628	2.671642	-1.758016
1	2.470028	2.926202	-2.815502
5	2.925384	1.856152	-0.497518
1	4.030128	1.442819	-0.605162
5	2.410521	3.535432	-0.248266
1	3.212652	4.413744	-0.220830
6	2.141138	-0.434456	1.048003
1	2.262215	-0.221746	2.114669
1	1.283742	-1.101291	0.936504
6	3.376110	-1.157320	0.547831
6	4.646474	-0.857348	1.057684
1	4.760714	-0.077594	1.804855
6	5.750006	-1.564584	0.587034
1	6.745144	-1.348056	0.966000
6	5.552170	-2.553614	-0.376481
1	6.380889	-3.132341	-0.773070
6	4.250775	-2.787096	-0.819813
1	4.050533	-3.553260	-1.566921
7	3.183252	-2.115074	-0.372350

6	-3.660554	0.270545	0.112052
6	-2.940774	0.267784	1.304081
6	-2.248221	-1.025046	1.381807
6	-2.780036	-1.889409	0.326463
6	-3.542246	-1.062861	-0.519972
6	-4.460130	1.393006	-0.475347
1	-5.536038	1.180429	-0.410989
1	-4.223348	1.536230	-1.535625
1	-4.270132	2.338661	0.036926
6	-2.877280	1.344068	2.344449
1	-3.296989	2.284339	1.979477
1	-1.852900	1.544596	2.667675
1	-3.450456	1.045390	3.233146
6	-1.470620	-1.496224	2.572470
1	-2.158762	-1.817331	3.368374
1	-0.843884	-0.698387	2.979573
1	-0.828371	-2.345629	2.324963
6	-2.563193	-3.368691	0.219213
1	-3.263063	-3.901680	0.877336
1	-1.548873	-3.653745	0.513138
1	-2.728295	-3.731167	-0.798958
6	-4.273943	-1.465967	-1.765835
1	-5.335508	-1.652791	-1.551089
1	-3.857303	-2.377810	-2.201865
1	-4.231261	-0.680832	-2.527844
6	-0.246905	-1.662061	-1.545978
1	-0.787407	-2.606288	-1.665303
1	0.764409	-1.851234	-1.183441
1	-0.180772	-1.149410	-2.518576
45	-1.380044	-0.338520	-0.452785

III **HF =** -1235.2786173 hartree

6	0.284588	1.373211	-0.314680
6	1.788634	0.868490	0.444727
5	0.706303	1.883764	1.278115
1	0.119476	1.448865	2.204952
5	0.052921	3.023656	0.111134
1	-1.058902	3.410988	0.248455
5	0.721663	2.582511	-1.458328
1	0.114475	2.670256	-2.472091
5	1.759552	1.180980	-1.221021
1	1.876923	0.295064	-1.991714
5	2.469127	2.127753	1.374372
1	3.013464	1.804728	2.380911
5	1.393997	3.517672	1.166360
1	1.223008	4.299044	2.046973
5	1.413714	3.954306	-0.561198
1	1.254291	5.069878	-0.942446
5	2.478837	2.800063	-1.406137
1	3.087012	3.071146	-2.391592
5	3.136208	1.692856	-0.202573
1	4.152987	1.092505	-0.297027
5	2.905072	3.397954	0.222251
1	3.842652	4.103512	0.419202
6	1.886714	-0.573847	0.966668
1	1.940412	-0.521538	2.057588
1	0.959125	-1.087650	0.704808
6	3.049796	-1.401230	0.455936

6	4.268461	-1.440774	1.146073
1	4.398989	-0.852750	2.049638
6	5.303604	-2.229381	0.649758
1	6.258732	-2.272826	1.166017
6	5.090788	-2.958460	-0.520161
1	5.867197	-3.586731	-0.945869
6	3.842879	-2.863589	-1.134719
1	3.632520	-3.420045	-2.046481
7	2.839941	-2.112103	-0.663853
6	-3.553345	-0.338733	0.371646
6	-2.685813	0.103969	1.436155
6	-1.773750	-0.982339	1.734285
6	-1.978107	-2.002658	0.780349
6	-3.066058	-1.589693	-0.098271
6	-4.828583	0.331366	-0.042809
1	-5.636499	0.035177	0.640480
1	-5.136201	0.048377	-1.053186
1	-4.755990	1.421315	-0.007070
6	-2.932285	1.301739	2.307047
1	-3.316479	2.148015	1.729752
1	-2.019016	1.633363	2.806196
1	-3.673670	1.071943	3.085896
6	-0.931684	-1.094145	2.971021
1	-1.562621	-1.397151	3.818814
1	-0.461302	-0.146968	3.242691
1	-0.146659	-1.847710	2.866550
6	-1.332964	-3.359469	0.782436
1	-1.867015	-4.039094	1.461558
1	-0.290455	-3.320350	1.111927
1	-1.348948	-3.823673	-0.207903
6	-3.711021	-2.456335	-1.143012
1	-4.396513	-3.182083	-0.683891
1	-2.974321	-3.031127	-1.714324
1	-4.291559	-1.863629	-1.855846
6	-0.953852	-0.421935	-2.667518
6	-0.315125	-1.391773	-1.915146
1	-0.403275	0.428749	-3.052538
1	-1.907781	-0.625311	-3.145986
1	-0.788454	-2.357987	-1.773585
1	0.743526	-1.358261	-1.686562
6	-2.410876	1.597418	-1.508346
1	-2.772153	2.282030	-0.738892
1	-1.746918	2.128255	-2.182052
1	-3.248041	1.169982	-2.065711
45	-1.422235	0.005508	-0.508093

2TS1   **HF =** -1235.2478211 hartree $v^{\ddagger} = -428.9979 \ icm^{-1}$

6	0.293461	1.219634	-0.287246
6	1.840856	0.878842	0.444446
5	0.711864	1.838106	1.269507
1	0.209076	1.389397	2.238398
5	-0.077191	2.857436	0.072604
1	-1.223996	3.137727	0.213581
5	0.582892	2.409294	-1.494881
1	-0.076356	2.400218	-2.478328
5	1.744565	1.109456	-1.231849
1	1.918514	0.194103	-1.957306
5	2.444616	2.234668	1.294687

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1	3.045143	2.008266	2.295632
5	1.246738	3.517164	1.062609
1	1.035285	4.321598	1.913438
5	1.178888	3.872691	-0.682393
1	0.913583	4.952134	-1.106988
5	2.315538	2.773497	-1.511110
1	2.870463	3.050577	-2.526202
5	3.099267	1.779859	-0.281091
1	4.161046	1.263406	-0.380474
5	2.735935	3.481775	0.074198
1	3.614591	4.272502	0.209256
6	2.047971	-0.527694	1.030050
1	2.124175	-0.419805	2.115972
1	1.146354	-1.106586	0.815704
6	3.249834	-1.300159	0.524509
6	4.489305	-1.216342	1.172358
1	4.605423	-0.572783	2.039361
6	5.562224	-1.957560	0.683222
1	6.533415	-1.906066	1.167889
6	5.365595	-2.763946	-0.437649
1	6.171014	-3.360121	-0.855709
6	4.095389	-2.789771	-1.012479
1	3.896881	-3.409770	-1.885179
7	3.056743	-2.084595	-0.548244
6	-3.624833	-0.000565	0.492345
6	-2.725306	0.270431	1.536584
6	-1.861189	-0.901915	1.699881
6	-2.314363	-1.910293	0.787053
6	-3.334329	-1.331879	-0.026888
6	-4.723206	0.884060	-0.014486
1	-5.701323	0.400805	0.107400
1	-4.611593	1.109957	-1.083459
1	-4.754372	1.836552	0.519979
6	-2.746447	1.458674	2.451966
1	-3.284654	2.302386	2.012490
1	-1.741037	1.804205	2.699070
1	-3.245517	1.200868	3.397013
6	-0.989480	-1.161144	2.895480
1	-1.607830	-1.480737	3.747126
1	-0.441405	-0.270272	3.208845
1	-0.262651	-1.955842	2.705253
6	-1.864551	-3.342979	0.772012
1	-2.416630	-3.922170	1.525221
1	-0.798723	-3.442137	0.997759
1	-2.045631	-3.820030	-0.195648
6	-4.162144	-2.042313	-1.060561
1	-5.085750	-2.441600	-0.618216
1	-3.624745	-2.885436	-1.505384
1	-4.463327	-1.372559	-1.873220
6	-0.789333	-0.653067	-2.671692
6	-0.280166	-1.514968	-1.635465
1	-0.069378	0.016391	-3.128859
1	-1.495427	-1.088427	-3.374759
1	-0.730906	-2.502797	-1.553082
1	0.785935	-1.509228	-1.429991
6	-2.181029	0.813656	-2.382123
1	-2.291227	1.659040	-1.701939
1	-1.808482	1.210534	-3.322958

1	-3.123213	0.292023	-2.537234
45	-1.367312	-0.195513	-0.426801
INT3	**HF =** -1235.2970539 hartree		
6	-0.315304	1.066413	0.356350
6	-1.889700	1.000504	-0.308881
5	-0.752683	2.094440	-0.949432
1	-0.334210	1.867388	-2.032531
5	0.166106	2.717225	0.416100
1	1.320610	2.957184	0.274465
5	-0.411971	1.879063	1.855370
1	0.340069	1.544597	2.715737
5	-1.697112	0.768791	1.360780
1	-1.883326	-0.303375	1.811483
5	-2.452548	2.564284	-0.725349
1	-3.134606	2.645878	-1.695449
5	-1.161989	3.680315	-0.255719
1	-0.951914	4.675423	-0.873146
5	-0.954405	3.545090	1.514475
1	-0.588269	4.456454	2.185695
5	-2.114181	2.323067	2.112865
1	-2.587655	2.351006	3.203290
5	-3.041591	1.740543	0.723999
1	-4.130674	1.276121	0.760084
5	-2.580531	3.450999	0.804177
1	-3.407126	4.293295	0.954219
6	-2.223508	-0.188448	-1.230019
1	-2.362813	0.211957	-2.238971
1	-1.352815	-0.846875	-1.249367
6	-3.437415	-1.014565	-0.853511
6	-4.715446	-0.679391	-1.320058
1	-4.852263	0.197019	-1.946639
6	-5.798936	-1.477478	-0.960728
1	-6.799847	-1.235616	-1.307796
6	-5.573528	-2.589402	-0.149618
1	-6.385798	-3.241551	0.156831
6	-4.265645	-2.849609	0.258676
1	-4.044246	-3.711228	0.886340
7	-3.217207	-2.091227	-0.082887
6	3.562741	0.594342	-0.508836
6	2.705476	0.710783	-1.595268
6	2.070473	-0.604943	-1.786415
6	2.774607	-1.566936	-0.938202
6	3.589402	-0.816997	-0.071997
6	4.377134	1.679776	0.126003
1	5.444740	1.551380	-0.100421
1	4.277142	1.668547	1.217431
1	4.074912	2.668512	-0.227240
6	2.494948	1.927548	-2.446962
1	2.400248	2.838561	-1.848688
1	1.596842	1.844080	-3.060730
1	3.346851	2.062421	-3.127572
6	1.202801	-0.968274	-2.953453
1	1.820086	-1.124641	-3.850452
1	0.484049	-0.176908	-3.180893
1	0.646001	-1.890666	-2.768079
6	2.680446	-3.058584	-1.044177
1	3.376508	-3.426599	-1.810611

1	1.676213	-3.384880	-1.329220
1	2.936001	-3.551608	-0.102132
6	4.531102	-1.341982	0.970527
1	5.552801	-1.395967	0.568274
1	4.251678	-2.343167	1.306589
1	4.565423	-0.690785	1.849802
6	0.371423	-1.809410	2.587785
6	0.316080	-1.846738	1.052336
1	-0.028232	-0.863565	2.969834
1	-0.326210	-2.582876	2.949719
1	0.793830	-2.764257	0.690255
1	-0.721995	-1.851474	0.717613
6	1.744866	-2.065587	3.218524
1	2.449914	-1.255733	2.998177
1	1.665952	-2.143146	4.309411
1	2.185593	-3.001850	2.851345
45	1.355542	-0.246882	0.205662

IV **HF =** -1313.8353489 hartree

6	0.228593	1.263280	-0.034127
6	1.902726	0.939786	0.497214
5	0.781196	1.601222	1.578414
1	0.401390	0.935808	2.475337
5	-0.200837	2.752738	0.700040
1	-1.321391	2.892669	1.049783
5	0.310354	2.677901	-0.987574
1	-0.437298	2.791204	-1.899821
5	1.594716	1.467878	-1.085586
1	1.763566	0.737135	-1.997796
5	2.475528	2.161610	1.534831
1	3.191280	1.807854	2.416122
5	1.165633	3.335819	1.669291
1	0.979891	3.938762	2.678094
5	0.879141	4.010732	0.045301
1	0.485718	5.120020	-0.129417
5	1.999875	3.204168	-1.085594
1	2.419792	3.720631	-2.071357
5	2.990731	2.081264	-0.152458
1	4.071012	1.701277	-0.456052
5	2.533702	3.639642	0.563113
1	3.356243	4.473325	0.772947
6	2.311026	-0.509716	0.808065
1	2.418960	-0.585094	1.893632
1	1.488759	-1.166496	0.517118
6	3.588287	-1.001038	0.156482
6	4.822079	-0.881230	0.809423
1	4.874018	-0.412334	1.787393
6	5.970509	-1.355701	0.180620
1	6.938984	-1.270306	0.665898
6	5.853057	-1.939168	-1.080907
1	6.719501	-2.322890	-1.610783
6	4.583034	-2.021902	-1.650412
1	4.445615	-2.474137	-2.631066
7	3.472802	-1.572008	-1.052896
6	-3.233595	-1.115346	0.575966
6	-2.393659	-0.625448	1.640180
6	-1.297684	-1.565421	1.794730
6	-1.392863	-2.524905	0.767619

6	-2.570489	-2.218935	-0.031441
6	-4.641980	-0.692174	0.279289
1	-5.338093	-1.424945	0.710100
1	-4.850757	-0.643263	-0.793870
1	-4.883976	0.279057	0.713303
6	-2.762870	0.420574	2.652648
1	-1.879585	0.943169	3.028956
1	-3.272232	-0.034912	3.514127
1	-3.433548	1.175147	2.234097
6	-0.386577	-1.662008	2.983536
1	-0.849488	-2.300620	3.750084
1	-0.196544	-0.691428	3.443781
1	0.577407	-2.112201	2.729897
6	-0.552655	-3.763944	0.645358
1	-0.909355	-4.534623	1.343399
1	0.500143	-3.577730	0.880300
1	-0.601215	-4.199446	-0.356866
6	-3.124845	-3.083777	-1.128671
1	-3.647822	-3.959232	-0.718639
1	-2.339549	-3.462493	-1.792275
1	-3.843297	-2.535981	-1.745652
6	-0.676059	-0.668102	-2.557459
6	0.141807	-1.497772	-1.824320
1	-0.295514	0.272436	-2.938233
1	-1.591440	-1.033955	-3.012762
1	-0.134498	-2.535200	-1.673535
1	1.181757	-1.259353	-1.636551
6	-2.517523	1.015314	-1.481928
1	-1.933413	1.411258	-2.310010
1	-3.235594	0.294271	-1.888415
45	-1.220539	-0.341438	-0.358079
6	-3.244000	2.174300	-0.809161
1	-3.659939	1.897167	0.164504
1	-2.545196	2.989809	-0.618822
6	-4.379627	2.702663	-1.707068
1	-5.148291	1.938494	-1.879276
1	-4.866388	3.572973	-1.250015
1	-3.995318	3.012093	-2.686549

2TS2   **HF =** -1313.8015209 hartree $v^{\ddagger} = -332.5478\ icm^{-1}$

6	0.333634	1.216453	0.007566
6	1.973121	0.900911	0.561948
5	0.834245	1.580978	1.621005
1	0.434799	0.930207	2.520372
5	-0.125276	2.723084	0.695627
1	-1.266737	2.869298	0.984394
5	0.439492	2.622534	-0.970093
1	-0.275639	2.718690	-1.910019
5	1.721588	1.419674	-1.027640
1	1.914820	0.681285	-1.928049
5	2.528866	2.129033	1.610721
1	3.223311	1.782275	2.511443
5	1.217528	3.313269	1.699544
1	1.009581	3.927276	2.697351
5	0.976917	3.970702	0.060201
1	0.590577	5.078975	-0.136673
5	2.128273	3.152866	-1.030089
1	2.572558	3.658772	-2.010790

5	3.089333	2.036123	-0.060468
1	4.176939	1.650055	-0.327630
5	2.616999	3.600391	0.628755
1	3.435157	4.434873	0.852400
6	2.353126	-0.559817	0.850255
1	2.493299	-0.653410	1.930938
1	1.499745	-1.180252	0.569221
6	3.584165	-1.094141	0.146196
6	4.855102	-0.984034	0.726107
1	4.972069	-0.485078	1.683504
6	5.955273	-1.510461	0.053898
1	6.950759	-1.434450	0.482895
6	5.753846	-2.134798	-1.177098
1	6.579849	-2.560837	-1.738462
6	4.452473	-2.203466	-1.673062
1	4.250386	-2.686964	-2.627384
7	3.387371	-1.704359	-1.033726
6	-3.335235	-0.904915	0.869228
6	-2.394279	-0.590642	1.858305
6	-1.269717	-1.520872	1.711103
6	-1.588240	-2.435851	0.654458
6	-2.806689	-1.997458	0.059479
6	-4.699496	-0.311400	0.684977
1	-5.471509	-1.033903	0.984120
1	-4.901821	-0.049743	-0.359869
1	-4.840984	0.588805	1.288212
6	-2.544861	0.399886	2.975634
1	-1.632847	0.983391	3.127450
1	-2.766558	-0.111914	3.922973
1	-3.358979	1.104650	2.784829
6	-0.259484	-1.797097	2.788007
1	-0.735488	-2.381245	3.589529
1	0.131464	-0.884722	3.241192
1	0.584798	-2.383875	2.417593
6	-0.831114	-3.690860	0.325322
1	-1.107410	-4.494281	1.022488
1	0.251901	-3.551829	0.395354
1	-1.054640	-4.050162	-0.683179
6	-3.570113	-2.710778	-1.021433
1	-4.225966	-3.484397	-0.597636
1	-2.902428	-3.206769	-1.733634
1	-4.210306	-2.026438	-1.587588
6	-0.820063	-0.251903	-2.623570
6	-0.094843	-1.212512	-1.819614
1	-0.266511	0.619229	-2.956697
1	-1.463073	-0.681291	-3.387513
1	-0.392707	-2.253652	-1.940979
1	0.976830	-1.093554	-1.701239
6	-2.512903	0.764600	-2.063611
1	-2.402983	1.131271	-3.084631
1	-3.255102	-0.035263	-2.079191
45	-1.183510	-0.364932	-0.273934
6	-2.975387	1.966370	-1.232871
1	-3.185584	1.694163	-0.197487
1	-2.196712	2.726648	-1.201510
6	-4.234678	2.582013	-1.874519
1	-5.064022	1.865140	-1.921137
1	-4.572099	3.448009	-1.292949

1	-4.034030	2.924814	-2.896967
INT4	**HF =** -1313.8644263 hartree		
6	-0.493284	1.065102	0.386714
6	-2.145502	1.032887	-0.091964
5	-1.126942	2.263841	-0.669757
1	-0.847852	2.233671	-1.818853
5	-0.059749	2.707034	0.657135
1	1.059965	3.022952	0.417927
5	-0.434912	1.622562	1.997203
1	0.420511	1.192629	2.701189
5	-1.739290	0.546307	1.477289
1	-1.845830	-0.592198	1.759910
5	-2.797773	2.615948	-0.175524
1	-3.593315	2.818895	-1.035277
5	-1.487880	3.700802	0.314505
1	-1.381985	4.789887	-0.152607
5	-1.059248	3.293778	2.001512
1	-0.638641	4.101361	2.767137
5	-2.103074	1.938393	2.521558
1	-2.437804	1.768049	3.649922
5	-3.179671	1.544006	1.176183
1	-4.242717	1.028623	1.264797
5	-2.757401	3.239926	1.482880
1	-3.582277	4.007325	1.865148
6	-2.552393	-0.006215	-1.152809
1	-2.850633	0.546680	-2.049102
1	-1.663370	-0.589140	-1.400834
6	-3.658951	-0.972247	-0.778348
6	-5.006936	-0.642774	-0.973442
1	-5.275611	0.330167	-1.374034
6	-5.987531	-1.574324	-0.641181
1	-7.039262	-1.340375	-0.782251
6	-5.593392	-2.809585	-0.127226
1	-6.320642	-3.568506	0.145032
6	-4.228490	-3.051288	0.025403
1	-3.876763	-4.004357	0.416975
7	-3.277905	-2.164655	-0.293508
6	3.302590	0.800160	-1.074920
6	2.287787	1.169656	-1.951183
6	1.557637	-0.057278	-2.304563
6	2.329165	-1.194479	-1.803704
6	3.323026	-0.672149	-0.958600
6	4.272042	1.699602	-0.369594
1	5.279491	1.599276	-0.796519
1	4.347833	1.448086	0.694110
1	3.979128	2.749402	-0.443285
6	2.014376	2.538531	-2.497150
1	0.947170	2.726355	-2.626336
1	2.489154	2.654499	-3.481978
1	2.408962	3.322591	-1.845794
6	0.519180	-0.143236	-3.382248
1	1.002614	-0.108086	-4.369890
1	-0.185623	0.690228	-3.331194
1	-0.047093	-1.076576	-3.324068
6	2.131517	-2.623686	-2.208183
1	2.605961	-2.806258	-3.182382
1	1.072675	-2.880807	-2.304452

1	2.579109	-3.316100	-1.489903
6	4.402837	-1.443042	-0.257710
1	5.291609	-1.528805	-0.899286
1	4.080747	-2.456650	-0.004116
1	4.717897	-0.951855	0.666497
6	0.471565	-2.124429	2.044080
6	0.326328	-1.895596	0.528069
1	-0.037060	-1.337138	2.610630
1	-0.102880	-3.042404	2.252740
1	0.834304	-2.707999	-0.003627
1	-0.731813	-1.927828	0.261074
6	1.888345	-2.311764	2.616065
1	1.813957	-2.893922	3.545930
1	2.493013	-2.922159	1.927997
45	1.186950	-0.131571	-0.179999
6	2.622504	-1.005044	2.938256
1	2.716715	-0.398573	2.021438
1	2.004864	-0.408462	3.622022
6	4.005596	-1.217529	3.563110
1	4.659296	-1.808711	2.909655
1	4.506399	-0.263760	3.767407
1	3.924005	-1.757359	4.514611

2V-1 **HF =** -1156.7213032 hartree

6	1.746047	0.696818	0.347898
5	0.742811	1.757276	1.211667
1	0.371503	1.398396	2.281766
5	-0.070574	2.751555	-0.003494
1	-1.156093	3.200287	0.182511
5	0.458424	2.171790	-1.601974
1	-0.219686	2.203914	-2.580147
5	1.592717	0.846047	-1.342356
1	1.873350	-0.077334	-2.019008
5	2.482957	2.082302	1.096250
1	3.252899	1.864460	1.969921
5	1.349309	3.404931	0.861466
1	1.276557	4.272802	1.670716
5	1.172292	3.661146	-0.898937
1	0.971594	4.735248	-1.367414
5	2.206357	2.478547	-1.725940
1	2.833191	2.610686	-2.724041
1	3.848223	1.090295	-0.587621
5	2.755063	3.243219	-0.213391
1	3.755352	3.880646	-0.191029
6	2.132818	-0.656827	0.978570
1	2.158907	-0.516735	2.063002
1	1.319678	-1.347941	0.750251
6	3.440210	-1.271107	0.518669
6	4.635598	-1.046320	1.216232
1	4.638912	-0.422008	2.104932
6	5.811731	-1.636775	0.754218
1	6.749924	-1.477646	1.278859
6	5.758297	-2.436114	-0.386490
1	6.646600	-2.918582	-0.782658
6	4.521525	-2.607978	-1.010830
1	4.433208	-3.228794	-1.900728
7	3.388194	-2.046273	-0.577249
6	-3.759295	0.405161	0.093406

6	-2.949895	0.427481	1.233349
6	-2.361586	-0.908353	1.356346
6	-3.063474	-1.793084	0.409358
6	-3.850263	-0.979960	-0.405488
6	-4.518004	1.553132	-0.503799
1	-5.587790	1.486393	-0.260233
1	-4.437599	1.560352	-1.596621
1	-4.149907	2.514714	-0.137586
6	-2.767474	1.557072	2.201140
1	-3.014564	2.521569	1.750571
1	-1.741413	1.620992	2.568924
1	-3.423021	1.419301	3.073205
6	-1.581757	-1.389710	2.544314
1	-2.261990	-1.654259	3.368004
1	-0.900753	-0.617999	2.912557
1	-0.992244	-2.279665	2.305303
6	-2.912161	-3.283602	0.359256
1	-3.513949	-3.762772	1.144022
1	-1.871864	-3.588019	0.512191
1	-3.237441	-3.694098	-0.601177
6	-4.707134	-1.394715	-1.565426
1	-5.773116	-1.369700	-1.299010
1	-4.474235	-2.409604	-1.899344
1	-4.576504	-0.724196	-2.422591
6	-0.372367	-1.697091	-1.497918
1	-0.907582	-2.654724	-1.502220
1	0.667371	-1.871395	-1.216793
1	-0.371451	-1.287102	-2.524314
5	0.130183	0.978123	-0.290400
6	2.886154	1.573932	-0.475676
45	-1.522999	-0.304445	-0.505571

III-1 **HF =** -1235.2811625 hartree

6	1.750037	0.750523	0.440763
5	0.792531	1.854512	1.295457
1	0.274878	1.492716	2.295880
5	0.221137	3.033497	0.115569
1	-0.809137	3.607525	0.261811
5	0.845750	2.530983	-1.474304
1	0.315773	2.743978	-2.514839
5	1.763196	1.056884	-1.234411
1	2.016017	0.172668	-1.973659
5	2.565129	1.970032	1.373032
1	3.209415	1.586014	2.290660
5	1.616319	3.432568	1.160046
1	1.559300	4.233200	2.036883
5	1.648677	3.853361	-0.573755
1	1.620938	4.977439	-0.959292
5	2.613307	2.621140	-1.409325
1	3.345678	2.749892	-2.333466
1	3.956883	0.949590	-0.271444
5	3.094958	3.189333	0.206268
1	4.157138	3.690586	0.372988
6	1.928512	-0.689187	0.960934
1	1.950102	-0.646082	2.052933
1	1.028176	-1.233898	0.667098
6	3.141915	-1.450086	0.464745
6	4.344014	-1.451950	1.186403

1	4.420037	-0.898992	2.118252
6	5.430977	-2.173339	0.693095
1	6.372192	-2.190037	1.235722
6	5.283788	-2.874415	-0.502690
1	6.099879	-3.452532	-0.925050
6	4.047510	-2.820384	-1.148293
1	3.887618	-3.358234	-2.081052
7	2.998805	-2.131409	-0.684875
6	-3.707872	-0.213279	0.369274
6	-2.767564	0.245072	1.378391
6	-1.908500	-0.864526	1.703953
6	-2.218844	-1.925884	0.811146
6	-3.343495	-1.524058	-0.009857
6	-4.915518	0.550423	-0.085950
1	-5.725196	0.454877	0.650829
1	-5.299078	0.180991	-1.041893
1	-4.707885	1.618071	-0.201900
6	-2.918000	1.509154	2.175935
1	-1.974650	1.803853	2.642083
1	-3.663486	1.388554	2.975487
1	-3.245778	2.343912	1.547971
6	-1.050648	-0.988636	2.930604
1	-1.658516	-1.337292	3.778362
1	-0.604512	-0.037314	3.226091
1	-0.243177	-1.715130	2.798466
6	-1.645119	-3.314082	0.861380
1	-2.218542	-3.948194	1.552828
1	-0.605358	-3.317440	1.203170
1	-1.674827	-3.806566	-0.116102
6	-4.036080	-2.404107	-1.012421
1	-4.691977	-3.137666	-0.522891
1	-3.320612	-2.972954	-1.618564
1	-4.656521	-1.821338	-1.699971
6	-1.060165	-0.522415	-2.628680
6	-0.382779	-1.443144	-1.832489
1	-0.523050	0.293705	-3.099598
1	-2.015073	-0.775262	-3.083402
1	-0.832334	-2.410956	-1.629290
1	0.689025	-1.402037	-1.683644
6	-2.301241	1.672334	-1.541896
1	-2.585141	2.406246	-0.783911
1	-1.625513	2.136385	-2.254407
1	-3.188906	1.307382	-2.068063
6	3.053212	1.540727	-0.193810
5	0.208410	1.275540	-0.321217
45	-1.493718	-0.011056	-0.530244

2TS1-1   **HF =** -1235.2435204 hartree $\nu^{\ddagger} = -450.1092\ icm^{-1}$

6	1.797218	0.738962	0.443666
5	0.809940	1.799818	1.308483
1	0.386764	1.423676	2.348141
5	0.091422	2.889618	0.115976
1	-0.977279	3.387625	0.279642
5	0.673458	2.372468	-1.481325
1	0.059923	2.502889	-2.490112
5	1.714498	0.978857	-1.236848
1	1.992437	0.081532	-1.951824
5	2.567332	2.049416	1.288541

S52

1	3.283834	1.750603	2.183825
5	1.502135	3.430561	1.074328
1	1.430702	4.259099	1.923811
5	1.420251	3.783343	-0.674349
1	1.290790	4.887072	-1.096974
5	2.433239	2.593789	-1.514664
1	3.107958	2.739368	-2.479472
1	3.951519	1.068475	-0.385228
5	2.948606	3.256714	0.054182
1	3.976494	3.841289	0.150057
6	2.090646	-0.662462	1.013003
1	2.127732	-0.574517	2.102270
1	1.226174	-1.279357	0.758669
6	3.347818	-1.351309	0.521848
6	4.558918	-1.237212	1.219145
1	4.610259	-0.644503	2.127986
6	5.687043	-1.898087	0.733780
1	6.635560	-1.825424	1.258896
6	5.571659	-2.656119	-0.430276
1	6.420335	-3.191604	-0.844672
6	4.324236	-2.716410	-1.053712
1	4.188349	-3.301905	-1.961359
7	3.236184	-2.086239	-0.597812
6	-3.683432	0.183130	0.497742
6	-2.711582	0.373017	1.505410
6	-1.985583	-0.880952	1.657589
6	-2.621056	-1.855674	0.796074
6	-3.627503	-1.197879	0.053653
6	-4.675428	1.195695	0.006789
1	-5.701630	0.904551	0.268904
1	-4.645899	1.305250	-1.085820
1	-4.490911	2.182118	0.440766
6	-2.602380	1.574400	2.400858
1	-1.619778	1.649267	2.868545
1	-3.345939	1.515811	3.208886
1	-2.775888	2.508997	1.859378
6	-1.090050	-1.229496	2.814111
1	-1.685072	-1.512037	3.695400
1	-0.455898	-0.389466	3.106321
1	-0.437576	-2.076773	2.580316
6	-2.295117	-3.321525	0.761893
1	-2.857728	-3.865791	1.533487
1	-1.231686	-3.504429	0.944833
1	-2.548178	-3.775894	-0.201618
6	-4.569217	-1.812410	-0.942938
1	-5.544776	-2.035737	-0.487823
1	-4.179467	-2.751880	-1.348139
1	-4.763338	-1.140889	-1.787823
6	-0.845216	-0.723175	-2.646818
6	-0.356894	-1.558030	-1.568873
1	-0.095562	-0.115963	-3.144319
1	-1.549414	-1.180952	-3.339032
1	-0.830181	-2.534245	-1.456532
1	0.715434	-1.589469	-1.399065
6	-2.160897	0.792015	-2.455554
1	-2.237821	1.666207	-1.807787
1	-1.767312	1.142682	-3.407406
1	-3.130933	0.318845	-2.603778

6	3.010843	1.595369	-0.284862
5	0.193998	1.123508	-0.257552
45	-1.465419	-0.194275	-0.440349

INT3-1   **HF =** -1235.2882145 hartree

6	-1.862428	0.796702	-0.296523
5	-0.917495	2.022991	-0.977213
1	-0.592414	1.880299	-2.109231
5	-0.067757	2.789678	0.369107
1	1.002210	3.290039	0.230325
5	-0.520552	1.905408	1.848089
1	0.196756	1.766828	2.788771
5	-1.648169	0.628769	1.381541
1	-1.895649	-0.412152	1.874931
5	-2.654849	2.281343	-0.738067
1	-3.456006	2.217308	-1.608453
5	-1.532640	3.560797	-0.301775
1	-1.505545	4.566629	-0.934961
5	-1.283203	3.486409	1.467657
1	-1.079513	4.456935	2.123274
5	-2.265888	2.145932	2.095353
1	-2.852615	2.071513	3.123347
1	-3.932674	0.959409	0.778403
5	-2.888408	3.168761	0.776826
1	-3.898177	3.776490	0.912992
6	-2.248724	-0.423938	-1.156545
1	-2.276113	-0.092569	-2.198551
1	-1.435600	-1.145395	-1.058310
6	-3.555566	-1.112303	-0.816420
6	-4.742223	-0.790390	-1.490087
1	-4.738872	-0.031802	-2.267206
6	-5.917649	-1.459988	-1.151047
1	-6.848853	-1.229284	-1.661330
6	-5.871880	-2.431820	-0.152904
1	-6.759578	-2.982453	0.143039
6	-4.643546	-2.687487	0.459582
1	-4.562300	-3.442395	1.239764
7	-3.510345	-2.051986	0.142829
6	3.664066	0.690668	-0.441532
6	2.740334	0.850935	-1.476178
6	2.188812	-0.479331	-1.759992
6	3.017420	-1.461467	-1.040394
6	3.856362	-0.746930	-0.186221
6	4.437146	1.769495	0.257678
1	5.478841	1.799542	-0.092249
1	4.468095	1.601970	1.340347
1	3.998373	2.755716	0.086481
6	2.448533	2.109511	-2.236331
1	1.426109	2.134873	-2.616094
1	3.122178	2.191975	-3.101825
1	2.591835	3.001642	-1.621056
6	1.328608	-0.811119	-2.944311
1	1.944430	-0.915611	-3.850491
1	0.590877	-0.027073	-3.134816
1	0.793832	-1.754470	-2.799293
6	2.948322	-2.945684	-1.237302
1	3.513577	-3.244853	-2.131168
1	1.917716	-3.287681	-1.375861

1	3.366141	-3.491415	-0.386059
6	4.866311	-1.295420	0.778186
1	5.887054	-1.178432	0.387559
1	4.706057	-2.359348	0.972224
1	4.831902	-0.774369	1.741431
6	0.562091	-1.869451	2.552316
6	0.452208	-1.863205	1.015475
1	0.086904	-0.975372	2.975240
1	-0.028691	-2.720236	2.930898
1	0.951958	-2.755654	0.613583
1	-0.601042	-1.928118	0.734033
6	1.986466	-1.987247	3.111371
1	2.591608	-1.105091	2.866488
1	1.975554	-2.086867	4.203695
1	2.502459	-2.864823	2.700904
6	-2.984255	1.478726	0.722859
5	-0.224037	0.988877	0.325750
45	1.490758	-0.226182	0.241623

IV-1	**HF =** -1313.8385299 hartree		
6	1.885523	0.740940	0.518857
5	0.899937	1.515402	1.645509
1	0.565225	0.908513	2.603529
5	0.044075	2.781999	0.781097
1	-1.011712	3.166156	1.160276
5	0.524337	2.671491	-0.930684
1	-0.157684	2.984305	-1.849521
5	1.654184	1.330523	-1.063791
1	1.930251	0.643053	-1.982640
5	2.639924	1.891988	1.579175
1	3.436067	1.455882	2.340697
5	1.489537	3.202219	1.740637
1	1.429022	3.818977	2.755092
5	1.253278	3.919869	0.123719
1	1.027763	5.076204	-0.035521
5	2.261345	3.014633	-1.019534
1	2.852251	3.411475	-1.968413
1	3.941508	1.394179	-0.356199
5	2.858850	3.359907	0.620896
1	3.857358	3.980870	0.778761
6	2.333806	-0.710482	0.786135
1	2.411589	-0.830466	1.869771
1	1.525211	-1.358806	0.444110
6	3.633623	-1.152423	0.143813
6	4.838674	-1.135906	0.859829
1	4.853536	-0.798929	1.892006
6	6.008772	-1.557776	0.228865
1	6.954128	-1.554703	0.764500
6	5.940405	-1.985810	-1.095981
1	6.823524	-2.325347	-1.628352
6	4.695842	-1.971730	-1.727751
1	4.596294	-2.301808	-2.760234
7	3.568022	-1.569213	-1.132231
6	-3.452920	-0.948567	0.531743
6	-2.562640	-0.460800	1.568789
6	-1.534839	-1.457430	1.752602
6	-1.725989	-2.465993	0.771666
6	-2.909460	-2.145568	0.009248

6	-4.801446	-0.396285	0.166089
1	-5.578945	-1.143519	0.371916
1	-4.879298	-0.135189	-0.896176
1	-5.048018	0.495715	0.745582
6	-2.869843	0.635056	2.551922
1	-3.458886	0.248155	3.396491
1	-3.442884	1.446575	2.097233
1	-1.957157	1.076049	2.961890
6	-0.629404	-1.587699	2.944611
1	-1.090577	-2.246791	3.695064
1	-0.444291	-0.628299	3.429038
1	0.339812	-2.027438	2.687732
6	-0.965809	-3.759113	0.692556
1	-1.397640	-4.502835	1.377708
1	0.086137	-3.637164	0.970531
1	-1.000075	-4.198774	-0.309708
6	-3.526764	-3.000089	-1.062055
1	-4.164555	-3.787976	-0.635942
1	-2.768606	-3.502651	-1.673956
1	-4.153291	-2.405994	-1.735328
6	-0.796325	-0.774340	-2.509788
6	0.067438	-1.529451	-1.730318
1	-0.434068	0.124040	-2.996761
1	-1.700388	-1.204766	-2.933103
1	-0.164777	-2.565608	-1.507042
1	1.112877	-1.265984	-1.639717
6	-2.377122	1.186877	-1.510493
1	-1.725284	1.585855	-2.287098
1	-3.126752	0.551825	-2.002328
6	2.984974	1.818869	-0.079378
5	0.192427	1.150121	-0.002687
45	-1.302361	-0.335720	-0.385116
6	-3.066557	2.355860	-0.814610
1	-3.664540	2.023333	0.038776
1	-2.324085	3.048956	-0.416747
6	-3.980672	3.122218	-1.789367
1	-4.779642	2.479291	-2.180885
1	-4.452591	3.981206	-1.295619
1	-3.411777	3.501417	-2.647173

2TS2-1   **HF =** -1313.7988204 hartree $v^{\ddagger} = -341.8466\ icm^{-1}$

6	1.942025	0.683270	0.560087
5	0.944505	1.441288	1.693956
1	0.610664	0.823738	2.646192
5	0.080298	2.710604	0.824668
1	-0.999704	3.073475	1.165209
5	0.592501	2.613667	-0.878608
1	-0.068489	2.916996	-1.816726
5	1.734654	1.291813	-1.007988
1	2.030155	0.613014	-1.926726
5	2.678147	1.823730	1.647727
1	3.468333	1.387947	2.415827
5	1.514171	3.130555	1.809820
1	1.440331	3.735700	2.830472
5	1.292268	3.862917	0.196537
1	1.061729	5.019737	0.046742
5	2.325179	2.978359	-0.940950
1	2.922359	3.390573	-1.879388

1	4.009959	1.364443	-0.272871
5	2.896751	3.308955	0.711234
1	3.887683	3.936674	0.889026
6	2.373452	-0.783354	0.752793
1	2.429626	-0.973442	1.827650
1	1.564176	-1.393949	0.347293
6	3.673628	-1.205914	0.099007
6	4.888740	-1.155786	0.797093
1	4.911393	-0.803757	1.824257
6	6.057345	-1.565734	0.156032
1	7.010135	-1.537306	0.677671
6	5.977129	-2.017044	-1.160546
1	6.858438	-2.349752	-1.700302
6	4.723016	-2.037326	-1.773018
1	4.614907	-2.388226	-2.797837
7	3.595700	-1.646191	-1.168509
6	-3.471625	-0.763604	0.890327
6	-2.436204	-0.529516	1.816149
6	-1.417226	-1.550733	1.597256
6	-1.914651	-2.449793	0.577925
6	-3.142394	-1.940052	0.106207
6	-4.768943	-0.019907	0.767703
1	-5.603281	-0.634915	1.133048
1	-5.000709	0.236068	-0.273610
1	-4.768663	0.907888	1.345801
6	-2.449210	0.455438	2.950088
1	-2.771674	-0.027165	3.884635
1	-3.135517	1.286026	2.759587
1	-1.460853	0.884815	3.129359
6	-0.379065	-1.942589	2.612638
1	-0.845187	-2.529140	3.418716
1	0.094675	-1.075929	3.077011
1	0.406397	-2.566559	2.176124
6	-1.262394	-3.741690	0.175227
1	-1.546157	-4.552939	0.860675
1	-0.170364	-3.668409	0.190673
1	-1.557530	-4.054236	-0.831532
6	-4.038355	-2.556424	-0.931388
1	-4.836681	-3.156304	-0.470975
1	-3.485186	-3.219216	-1.604879
1	-4.533348	-1.797156	-1.548402
6	-0.921719	-0.147663	-2.639871
6	-0.211772	-1.155445	-1.867390
1	-0.335675	0.702369	-2.977663
1	-1.579946	-0.544469	-3.409913
1	-0.546901	-2.183650	-2.013804
1	0.869321	-1.081883	-1.804456
6	-2.537419	0.924077	-2.039167
1	-2.471739	1.274484	-3.070566
1	-3.337206	0.180329	-2.004799
6	3.046192	1.778806	-0.005580
5	0.259207	1.084145	0.050757
45	-1.297359	-0.333590	-0.314838
6	-2.864110	2.162162	-1.195417
1	-3.067767	1.901149	-0.155268
1	-2.014471	2.844220	-1.181445
6	-4.077446	2.903317	-1.790689
1	-4.974142	2.271133	-1.809235

1	-4.310092	3.795774	-1.197260
1	-3.880128	3.229575	-2.819601

INT4-1 **HF =** -1313.8590535 hartree

6	-2.039627	0.825085	-0.319436
5	-1.154591	2.042471	-1.088303
1	-0.896416	1.879082	-2.233565
5	-0.236311	2.856763	0.181150
1	0.814606	3.370532	-0.036870
5	-0.593118	2.016091	1.709040
1	0.172551	1.927068	2.613803
5	-1.720793	0.709562	1.343536
1	-1.931590	-0.319509	1.877722
5	-2.878645	2.286802	-0.757510
1	-3.726580	2.185770	-1.579064
5	-1.749953	3.591066	-0.424708
1	-1.772640	4.577701	-1.087592
5	-1.399726	3.571747	1.327281
1	-1.171840	4.563494	1.942074
5	-2.323822	2.238425	2.049023
1	-2.847324	2.186443	3.112109
1	-4.045095	0.991529	0.867521
5	-3.036497	3.214566	0.741321
1	-4.045633	3.812566	0.919305
6	-2.459174	-0.428948	-1.112013
1	-2.602523	-0.126486	-2.153319
1	-1.609471	-1.112941	-1.076396
6	-3.693439	-1.165182	-0.629455
6	-4.966006	-0.859952	-1.133370
1	-5.083156	-0.080364	-1.880475
6	-6.069781	-1.572708	-0.665956
1	-7.065299	-1.354687	-1.042990
6	-5.869540	-2.571375	0.285813
1	-6.696802	-3.155576	0.677156
6	-4.565592	-2.809564	0.723506
1	-4.363433	-3.584787	1.460622
7	-3.500089	-2.131517	0.283621
6	3.439609	0.531386	-1.124706
6	2.361885	0.798936	-1.975417
6	1.646512	-0.465760	-2.164671
6	2.479959	-1.529921	-1.585823
6	3.530895	-0.918170	-0.900575
6	4.432346	1.527279	-0.600344
1	5.359192	1.505510	-1.191304
1	4.709636	1.314935	0.437619
1	4.037803	2.546019	-0.639035
6	2.074950	2.101446	-2.662398
1	2.657908	2.178009	-3.591905
1	2.337771	2.959703	-2.037271
1	1.022389	2.203830	-2.928626
6	0.601176	-0.708245	-3.215098
1	1.075312	-0.860284	-4.196509
1	-0.082355	0.138965	-3.306875
1	0.009101	-1.601764	-2.995841
6	2.234888	-2.998160	-1.761111
1	2.613306	-3.338670	-2.735255
1	1.168026	-3.240042	-1.723266
1	2.736513	-3.590733	-0.990078

6	4.641523	-1.596878	-0.152182
1	5.522295	-1.742584	-0.794091
1	4.339041	-2.581765	0.216334
1	4.969499	-1.007011	0.709154
6	0.544869	-1.762222	2.447070
6	0.390341	-1.779651	0.912810
1	-0.086016	-0.981854	2.889858
1	0.135633	-2.716357	2.818992
1	0.909037	-2.665749	0.521544
1	-0.669893	-1.897595	0.675099
6	1.971902	-1.606254	2.998382
1	1.991108	-1.949247	4.043164
1	2.658002	-2.266445	2.446199
6	-3.109890	1.522211	0.741044
5	-0.357859	1.052899	0.200156
45	1.336985	-0.180502	-0.049600
6	2.493997	-0.166735	2.960970
1	2.462408	0.217226	1.917978
1	1.810204	0.480139	3.524218
6	3.915901	-0.004301	3.505202
1	4.633634	-0.622489	2.952108
1	4.252245	1.037611	3.448638
1	3.965493	-0.311856	4.557369

2V-2	**HF =** -1143.6417161 hartree		
6	1.845575	0.813504	0.296038
5	0.777181	1.767222	1.234654
1	0.472745	1.347923	2.309852
5	-0.201093	2.690118	0.091929
1	-1.321166	3.020681	0.344872
5	0.291058	2.184060	-1.548119
1	-0.471549	2.155119	-2.472754
5	1.586664	0.977221	-1.380311
1	1.791948	0.053661	-2.096876
5	2.474507	2.244723	1.021370
1	3.226358	2.112837	1.940728
5	1.195788	3.462113	0.882603
1	1.064548	4.307739	1.717483
5	0.894682	3.723803	-0.856018
1	0.539823	4.781822	-1.285685
5	1.998780	2.660691	-1.773299
1	2.438383	2.942194	-2.848229
5	2.975447	1.765470	-0.606765
1	4.068151	1.337130	-0.795887
5	2.555991	3.451036	-0.269389
1	3.400837	4.296871	-0.268271
6	2.240401	-0.532138	0.949129
1	2.318349	-0.354633	2.027855
1	1.422455	-1.237074	0.792914
6	3.517304	-1.203749	0.489600
6	4.776149	-0.744884	0.913813
1	4.838446	0.137390	1.543003
6	5.921551	-1.421095	0.509133
1	6.903851	-1.078678	0.826495
6	5.787078	-2.542930	-0.311788
1	6.652173	-3.104220	-0.654816
6	4.499919	-2.927871	-0.680353
1	4.346515	-3.798978	-1.317465

7	3.389476	-2.289080	-0.291685
6	-3.709504	0.400931	0.271010
6	-2.833462	0.233399	1.347722
6	-2.298790	-1.126370	1.254606
6	-3.102170	-1.840949	0.247468
6	-3.898122	-0.895623	-0.394468
6	-4.436821	1.656197	-0.117088
1	-5.479122	1.648424	0.236926
1	-4.468226	1.776896	-1.206325
1	-3.947046	2.542841	0.294315
6	-2.554182	1.208386	2.450502
1	-2.734466	2.239577	2.136309
1	-1.517616	1.153529	2.787496
1	-3.202093	1.001778	3.316821
6	-1.482604	-1.797488	2.322396
1	-2.122322	-2.179111	3.134813
1	-0.763685	-1.100203	2.761495
1	-0.919444	-2.642986	1.915705
6	-3.030534	-3.316233	-0.011558
1	-3.636997	-3.876556	0.715814
1	-2.003712	-3.687074	0.068239
1	-3.395227	-3.574421	-1.011441
6	-4.824585	-1.112513	-1.556169
1	-5.879567	-1.030099	-1.254710
1	-4.686983	-2.101868	-2.003529
1	-4.661335	-0.367962	-2.345292
6	-0.287850	-1.679243	-1.498544
1	-0.832288	-2.632699	-1.555573
1	0.723560	-1.870234	-1.136748
1	-0.202944	-1.257561	-2.513993
5	0.182143	0.972204	-0.246462
45	-1.469345	-0.299106	-0.526698

III-2   **HF =** -1222.2029287 hartree

6	1.820891	0.821718	0.410313
5	0.818160	1.884690	1.299048
1	0.281060	1.488289	2.282375
5	0.200513	3.074193	0.156358
1	-0.854455	3.607040	0.324663
5	0.836741	2.635008	-1.447817
1	0.265338	2.856175	-2.472869
5	1.820941	1.181789	-1.253034
1	1.972198	0.311485	-2.048723
5	2.590843	2.031823	1.364540
1	3.159787	1.669141	2.350809
5	1.589738	3.481424	1.200132
1	1.490637	4.258496	2.103314
5	1.606128	3.949474	-0.515474
1	1.517428	5.090108	-0.863399
5	2.609645	2.773785	-1.397047
1	3.243664	3.047178	-2.372707
5	3.218997	1.604204	-0.230117
1	4.226272	0.981329	-0.335710
5	3.081445	3.302691	0.240903
1	4.061044	3.956390	0.446442
6	1.916625	-0.630116	0.929745
1	1.967177	-0.584247	2.022283
1	0.990803	-1.144772	0.664344

6	3.070745	-1.476082	0.436400
6	4.328434	-1.424380	1.060018
1	4.486769	-0.735915	1.884299
6	5.354667	-2.241555	0.599214
1	6.335625	-2.211162	1.067722
6	5.103719	-3.095372	-0.476903
1	5.873377	-3.751171	-0.874837
6	3.825786	-3.084210	-1.031477
1	3.583809	-3.735904	-1.870918
7	2.828036	-2.307840	-0.591019
6	-3.682417	-0.308124	0.409328
6	-2.738688	0.163505	1.408756
6	-1.834909	-0.915824	1.690776
6	-2.122103	-1.967341	0.778599
6	-3.285725	-1.598464	0.002640
6	-4.914059	0.434466	-0.018985
1	-5.691094	0.383204	0.757722
1	-5.342868	0.019454	-0.937381
1	-4.709774	1.494207	-0.202738
6	-2.907560	1.404149	2.239725
1	-3.376015	2.209866	1.665065
1	-1.942642	1.778188	2.591480
1	-3.543084	1.219156	3.120301
6	-0.952788	-1.028701	2.901105
1	-1.545023	-1.352051	3.771710
1	-0.482445	-0.078055	3.159601
1	-0.157504	-1.767088	2.762236
6	-1.479017	-3.326398	0.765895
1	-1.999187	-4.022573	1.441883
1	-0.431576	-3.285643	1.080183
1	-1.501853	-3.778074	-0.232253
6	-3.950607	-2.478988	-1.018417
1	-4.517323	-3.299406	-0.552589
1	-3.220237	-2.945245	-1.692950
1	-4.652159	-1.915065	-1.642021
6	-1.001822	-0.317531	-2.655976
6	-0.355436	-1.302863	-1.909369
1	-0.441185	0.523913	-3.048055
1	-1.946936	-0.527728	-3.153918
1	-0.822705	-2.278097	-1.790266
1	0.710344	-1.280140	-1.721894
6	-2.327244	1.730751	-1.454126
1	-2.630888	2.405312	-0.649109
1	-1.669685	2.265655	-2.133209
1	-3.206791	1.365259	-1.998893
5	0.273109	1.345463	-0.325270
45	-1.460409	0.032063	-0.547323

2TS1-2   **HF =** -1222.1639075 hartree $v^{\ddagger} = -452.0303\ icm^{-1}$

6	1.874524	0.829700	0.410835
5	0.818466	1.818441	1.307726
1	0.392187	1.387866	2.331679
5	0.026531	2.896321	0.151477
1	-1.078033	3.319094	0.334991
5	0.637794	2.461435	-1.461041
1	-0.008222	2.585729	-2.458018
5	1.772708	1.120262	-1.260641
1	1.977805	0.230701	-2.023691

S61

5	2.562898	2.147515	1.284385
1	3.207193	1.883920	2.255762
5	1.412403	3.482565	1.117129
1	1.275776	4.281251	1.996317
5	1.308888	3.881102	-0.614352
1	1.092760	4.992985	-0.998477
5	2.389368	2.774534	-1.499334
1	2.950342	3.071864	-2.512409
5	3.162136	1.716346	-0.319856
1	4.221432	1.191536	-0.449080
5	2.874191	3.414070	0.094447
1	3.790294	4.169905	0.231172
6	2.104530	-0.586145	0.984658
1	2.175058	-0.488611	2.073312
1	1.216090	-1.181878	0.765171
6	3.314219	-1.353912	0.497341
6	4.585710	-1.135412	1.054171
1	4.709527	-0.374150	1.818098
6	5.667295	-1.885334	0.606133
1	6.658668	-1.726468	1.024165
6	5.457528	-2.840511	-0.390840
1	6.270638	-3.450521	-0.775163
6	4.163248	-2.992092	-0.883385
1	3.952171	-3.726994	-1.660284
7	3.113156	-2.280927	-0.454816
6	-3.686331	0.091134	0.552751
6	-2.697304	0.298815	1.539566
6	-1.919976	-0.923879	1.643765
6	-2.534903	-1.902265	0.770666
6	-3.591809	-1.274096	0.078220
6	-4.712091	1.079669	0.079732
1	-5.734282	0.722544	0.270229
1	-4.636633	1.263630	-1.002284
1	-4.599941	2.045468	0.580435
6	-2.591027	1.485012	2.453748
1	-2.997229	2.390888	1.994172
1	-1.554575	1.699992	2.717304
1	-3.145087	1.307880	3.389242
6	-0.999995	-1.263726	2.784089
1	-1.572356	-1.573293	3.673691
1	-0.382840	-0.409417	3.070442
1	-0.326242	-2.088554	2.529764
6	-2.141388	-3.350307	0.687092
1	-2.655735	-3.949950	1.453307
1	-1.065379	-3.483077	0.837642
1	-2.392334	-3.787718	-0.285847
6	-4.514202	-1.892934	-0.934373
1	-5.494174	-2.147012	-0.501376
1	-4.097987	-2.817104	-1.350773
1	-4.710966	-1.214116	-1.774686
6	-0.790765	-0.585231	-2.681498
6	-0.297840	-1.467544	-1.642915
1	-0.049300	0.075392	-3.118718
1	-1.464514	-1.025994	-3.416467
1	-0.753269	-2.459261	-1.588342
1	0.771206	-1.482091	-1.454061
6	-2.159153	0.847118	-2.416824
1	-2.242795	1.689697	-1.728121

1	-1.798046	1.257651	-3.358065
1	-3.118251	0.348175	-2.565496
5	0.257530	1.171223	-0.273516
45	-1.419361	-0.178909	-0.465145

INT3-2 **HF =** -1222.2091269 hartree

6	-1.962428	0.905715	-0.259435
5	-0.953678	2.077880	-0.993789
1	-0.665939	1.910292	-2.137325
5	0.025257	2.771585	0.300027
1	1.126447	3.192226	0.101085
5	-0.402448	1.907804	1.804081
1	0.386105	1.708302	2.685756
5	-1.664934	0.718868	1.405781
1	-1.829125	-0.342117	1.909692
5	-2.659124	2.433585	-0.648193
1	-3.432175	2.475269	-1.557844
5	-1.418324	3.639682	-0.276927
1	-1.337173	4.648654	-0.913123
5	-1.075858	3.536099	1.471125
1	-0.743173	4.490686	2.109512
5	-2.118407	2.260198	2.160306
1	-2.536287	2.288110	3.279418
5	-3.098516	1.599472	0.848424
1	-4.170266	1.098483	0.964448
5	-2.743006	3.332141	0.873880
1	-3.613561	4.126525	1.073188
6	-2.337018	-0.294062	-1.161444
1	-2.431479	0.086707	-2.184680
1	-1.505661	-1.001485	-1.150460
6	-3.598853	-1.056831	-0.818416
6	-4.863764	-0.572602	-1.192574
1	-4.940229	0.382454	-1.702900
6	-5.998086	-1.315500	-0.885483
1	-6.985313	-0.953574	-1.163447
6	-5.845818	-2.529013	-0.211433
1	-6.701549	-3.144512	0.052982
6	-4.553006	-2.933451	0.114972
1	-4.386184	-3.875024	0.638241
7	-3.453146	-2.230258	-0.181043
6	3.568863	0.801820	-0.595898
6	2.611676	0.684033	-1.605827
6	2.209024	-0.725484	-1.656856
6	3.160815	-1.473688	-0.819684
6	3.924699	-0.539792	-0.124227
6	4.229092	2.066505	-0.127276
1	5.229217	2.192084	-0.570916
1	4.358280	2.073368	0.961558
1	3.633023	2.944605	-0.390121
6	2.166813	1.766764	-2.543046
1	1.976557	2.709427	-2.022073
1	1.246330	1.497273	-3.062840
1	2.939455	1.950338	-3.305665
6	1.396096	-1.345868	-2.759032
1	2.016565	-1.550556	-3.646793
1	0.579036	-0.688308	-3.069025
1	0.953231	-2.294281	-2.439475
6	3.270997	-2.968890	-0.775142

1	3.854134	-3.348944	-1.627793
1	2.288123	-3.449655	-0.820114
1	3.761964	-3.316187	0.139823
6	4.978270	-0.803924	0.912407
1	5.981773	-0.548956	0.540608
1	4.996453	-1.854941	1.215775
1	4.813708	-0.202133	1.815321
6	0.489230	-1.972621	2.476712
6	0.351902	-1.855431	0.948065
1	0.174564	-1.036534	2.956041
1	-0.223068	-2.735352	2.836856
1	0.791376	-2.746780	0.474641
1	-0.705637	-1.840181	0.683416
6	1.889227	-2.351926	2.978969
1	2.629817	-1.588974	2.710882
1	1.906142	-2.466715	4.071197
1	2.222690	-3.302032	2.538915
5	-0.291026	1.007053	0.270817
45	1.421950	-0.204714	0.262728

IV-2　　　　**HF =** -1300.7588676 hartree

6	1.939744	0.880531	0.472791
5	0.895093	1.611569	1.597961
1	0.558913	0.994148	2.555864
5	-0.036580	2.820373	0.732617
1	-1.117554	3.135338	1.121464
5	0.450987	2.731933	-0.980169
1	-0.272515	2.992816	-1.892636
5	1.675643	1.458214	-1.109851
1	1.868959	0.750840	-2.046739
5	2.616368	2.068664	1.517557
1	3.350078	1.682275	2.377995
5	1.386097	3.320892	1.680774
1	1.270515	3.935731	2.699646
5	1.112325	4.017479	0.067309
1	0.797800	5.160959	-0.086233
5	2.173643	3.169291	-1.082086
1	2.630691	3.681466	-2.060586
5	3.102678	1.977092	-0.177386
1	4.173580	1.560424	-0.482462
5	2.755041	3.546801	0.562279
1	3.634637	4.328674	0.771621
6	2.343726	-0.576763	0.797774
1	2.454216	-0.641853	1.884853
1	1.519904	-1.235988	0.518892
6	3.611261	-1.109694	0.163208
6	4.866803	-0.885866	0.752582
1	4.933343	-0.288817	1.656694
6	6.006141	-1.414524	0.156321
1	6.986226	-1.246677	0.596715
6	5.869164	-2.158087	-1.017690
1	6.729442	-2.589640	-1.522119
6	4.585589	-2.333695	-1.529587
1	4.429958	-2.908609	-2.442340
7	3.481413	-1.835231	-0.960112
6	-3.392373	-1.046482	0.606963
6	-2.475382	-0.545736	1.611676
6	-1.416887	-1.511313	1.739022

S64

6	-1.628639	-2.521594	0.760296
6	-2.852514	-2.234742	0.063078
6	-4.761117	-0.511487	0.288527
1	-5.518936	-1.291665	0.443397
1	-4.855876	-0.171907	-0.750852
1	-5.025886	0.330105	0.933360
6	-2.757869	0.545274	2.608079
1	-3.269736	0.149981	3.499983
1	-3.391301	1.331011	2.186881
1	-1.834223	1.026955	2.939711
6	-0.460478	-1.623717	2.892374
1	-0.911063	-2.215130	3.705551
1	-0.196778	-0.648224	3.302890
1	0.470863	-2.124725	2.609910
6	-0.826015	-3.784709	0.622853
1	-1.193285	-4.563294	1.308847
1	0.232703	-3.625045	0.851146
1	-0.887186	-4.202542	-0.388511
6	-3.483627	-3.082176	-1.006791
1	-4.091472	-3.900091	-0.589197
1	-2.731213	-3.548444	-1.655111
1	-4.143128	-2.487725	-1.649173
6	-0.715319	-0.648135	-2.523934
6	0.117858	-1.445934	-1.750799
1	-0.330412	0.272996	-2.946202
1	-1.603881	-1.055188	-3.002320
1	-0.127901	-2.491208	-1.587362
1	1.157121	-1.189943	-1.600362
6	-2.427161	1.135071	-1.496616
1	-1.819461	1.573033	-2.287150
1	-3.164372	0.466924	-1.969863
5	0.232690	1.220497	-0.044246
45	-1.263592	-0.325264	-0.408942
6	-3.144322	2.268561	-0.770394
1	-3.692519	1.907865	0.105163
1	-2.413524	2.987673	-0.400341
6	-4.129885	2.998739	-1.702503
1	-4.915920	2.323797	-2.069364
1	-4.620604	3.835593	-1.186715
1	-3.610573	3.406455	-2.578946

2TS2-2	**HF =** -1300.7186481 hartree		$v^{\ddagger} = -346.4976 \; icm^{-1}$
6	2.010376	0.824862	0.531952
5	0.944116	1.544540	1.650817
1	0.605392	0.917512	2.602402
5	0.007674	2.745803	0.761058
1	-1.101867	3.042131	1.092354
5	0.542882	2.660329	-0.937051
1	-0.151377	2.907917	-1.876445
5	1.780278	1.406932	-1.043880
1	2.000823	0.701900	-1.975753
5	2.658473	2.011888	1.601469
1	3.379607	1.630671	2.474638
5	1.409514	3.256923	1.743890
1	1.271461	3.868241	2.762163
5	1.162430	3.954582	0.125570
1	0.841157	5.095882	-0.032159
5	2.259601	3.121749	-1.001947

1	2.728306	3.642257	-1.970683
5	3.181222	1.936379	-0.082443
1	4.263346	1.533077	-0.364648
5	2.800141	3.498037	0.655889
1	3.666056	4.289612	0.885193
6	2.393001	-0.646984	0.802057
1	2.503746	-0.764210	1.885079
1	1.554716	-1.271338	0.487833
6	3.642052	-1.182722	0.136221
6	4.913662	-0.964902	0.692898
1	5.006070	-0.366614	1.594086
6	6.034307	-1.503392	0.070776
1	7.026263	-1.341061	0.486090
6	5.862336	-2.250526	-1.096427
1	6.706681	-2.690356	-1.620433
6	4.564795	-2.419980	-1.574544
1	4.383018	-2.998652	-2.480178
7	3.477675	-1.912320	-0.980479
6	-3.451386	-0.820692	0.946175
6	-2.403907	-0.534346	1.841479
6	-1.355815	-1.518926	1.616001
6	-1.848862	-2.452671	0.623642
6	-3.108193	-2.003217	0.183729
6	-4.766316	-0.106492	0.820699
1	-5.592172	-0.726213	1.201093
1	-5.008093	0.129518	-0.224313
1	-4.777663	0.832751	1.381188
6	-2.414446	0.479632	2.949481
1	-2.660065	0.010445	3.915553
1	-3.154753	1.266923	2.773140
1	-1.442866	0.967132	3.057415
6	-0.300886	-1.870854	2.630325
1	-0.746149	-2.442136	3.461250
1	0.169788	-0.983316	3.056836
1	0.489107	-2.492910	2.198894
6	-1.153453	-3.723364	0.221840
1	-1.377243	-4.539842	0.925199
1	-0.066024	-3.599265	0.200296
1	-1.462899	-4.063049	-0.772928
6	-3.998598	-2.646599	-0.842155
1	-4.827159	-3.206429	-0.380961
1	-3.446467	-3.352884	-1.472088
1	-4.458559	-1.904774	-1.508618
6	-0.823650	-0.156417	-2.639740
6	-0.124714	-1.151020	-1.838063
1	-0.239369	0.705463	-2.947030
1	-1.438246	-0.568116	-3.439712
1	-0.444123	-2.185840	-1.987530
1	0.951747	-1.058416	-1.738784
6	-2.477839	0.838226	-2.089982
1	-2.406175	1.211646	-3.114433
1	-3.250703	0.062707	-2.085552
5	0.320219	1.146096	0.009567
45	-1.240749	-0.322402	-0.329855
6	-2.885412	2.052327	-1.243017
1	-3.101427	1.772561	-0.210456
1	-2.065233	2.767643	-1.200486
6	-4.118225	2.742074	-1.859095

1	-4.982468	2.066079	-1.912165
1	-4.411723	3.613686	-1.260305
1	-3.910211	3.093591	-2.878431

INT4-2 **HF =** -1300.7769235 hartree

6	-2.201785	0.940672	-0.059771
5	-1.300413	2.279395	-0.623576
1	-1.134250	2.366741	-1.798556
5	-0.205039	2.731950	0.685154
1	0.861415	3.229317	0.471979
5	-0.460018	1.558094	2.007861
1	0.417870	1.216698	2.748203
5	-1.730803	0.426009	1.489799
1	-1.826044	-0.722452	1.768221
5	-2.966916	2.486918	-0.046972
1	-3.829457	2.683226	-0.850043
5	-1.718381	3.640476	0.446838
1	-1.723831	4.761641	0.031849
5	-1.195093	3.189858	2.091771
1	-0.817557	4.003358	2.882466
5	-2.135312	1.756903	2.594660
1	-2.434932	1.533714	3.729662
5	-3.232497	1.343544	1.274852
1	-4.276318	0.785950	1.387179
5	-2.910848	3.046099	1.630264
1	-3.772655	3.744649	2.075160
6	-2.643004	-0.056675	-1.156672
1	-2.874800	0.530287	-2.052657
1	-1.793790	-0.698996	-1.397074
6	-3.824568	-0.954405	-0.857108
6	-5.142365	-0.476192	-0.951579
1	-5.315160	0.565488	-1.203357
6	-6.202302	-1.341032	-0.703552
1	-7.228622	-0.987136	-0.768635
6	-5.924138	-2.667306	-0.366147
1	-6.717773	-3.380834	-0.161108
6	-4.587403	-3.054886	-0.300526
1	-4.323263	-4.080813	-0.043908
7	-3.558829	-2.233368	-0.543920
6	3.250575	1.177235	-1.045404
6	2.157750	1.184569	-1.914280
6	1.799097	-0.214492	-2.171332
6	2.894212	-1.039506	-1.634699
6	3.723250	-0.201619	-0.895555
6	3.929078	2.380163	-0.455382
1	4.817925	2.673413	-1.036016
1	4.265256	2.191477	0.570948
1	3.251541	3.237928	-0.424099
6	1.559762	2.394226	-2.569166
1	2.249260	2.788493	-3.331534
1	1.357426	3.195479	-1.852596
1	0.616807	2.161627	-3.065690
6	0.852266	-0.675690	-3.244388
1	1.340090	-0.691469	-4.232697
1	-0.017998	-0.017134	-3.311707
1	0.484906	-1.686367	-3.039982
6	3.069918	-2.506901	-1.890259
1	3.545950	-2.685130	-2.866578

1	2.111104	-3.035471	-1.901884
1	3.696640	-2.983192	-1.128397
6	4.947273	-0.583693	-0.114903
1	5.867483	-0.273175	-0.632415
1	5.008261	-1.665028	0.042029
1	4.963017	-0.105592	0.871407
6	0.474590	-2.403932	1.765390
6	0.325946	-1.909091	0.312108
1	-0.062701	-1.734321	2.447756
1	-0.055435	-3.370252	1.829451
1	0.805398	-2.643979	-0.352427
1	-0.737807	-1.905514	0.065960
6	1.903373	-2.615618	2.305856
1	1.870880	-3.367774	3.109964
1	2.542575	-3.042838	1.516910
5	-0.482420	0.999578	0.318546
45	1.260608	-0.094032	-0.102170
6	2.563159	-1.352276	2.872500
1	2.632833	-0.588611	2.081783
1	1.908113	-0.921550	3.641444
6	3.952225	-1.604882	3.468593
1	4.642677	-2.010055	2.717843
1	4.394941	-0.682841	3.865763
1	3.901718	-2.330096	4.292137

3V **HF =** -1140.4766668 hartree

7	-2.996749	-1.902244	-0.367138
6	-1.605234	1.275212	-0.554839
6	-2.094883	0.097195	-1.418559
1	-2.326724	0.506971	-2.407167
1	-1.258681	-0.592827	-1.530504
6	-3.278447	-0.710458	-0.921660
6	-4.595628	-0.261891	-1.088427
1	-4.787969	0.695307	-1.561724
6	-5.646678	-1.058311	-0.640034
1	-6.675060	-0.727559	-0.756927
6	-5.354350	-2.285392	-0.045619
1	-6.139466	-2.940815	0.318788
6	-4.015467	-2.658826	0.060810
1	-3.742747	-3.614199	0.505758
6	3.370167	-0.466542	-0.423845
6	3.240012	-1.355534	0.716382
1	3.908273	-1.209757	1.560970
6	2.403505	-2.493302	0.706352
1	2.427654	-3.195296	1.532798
6	1.382789	-2.588600	-0.283059
6	1.346723	-1.547036	-1.272907
1	0.565780	-1.577053	-2.025339
6	2.419092	-0.597679	-1.424164
1	2.396680	0.087476	-2.262629
6	4.493529	0.557611	-0.429228
1	4.484173	1.037011	0.560807
6	5.854179	-0.157902	-0.584806
1	6.672832	0.566009	-0.506919
1	5.925567	-0.646639	-1.563785
1	6.006757	-0.922519	0.184719
6	4.336691	1.659022	-1.484741
1	3.384785	2.188228	-1.380766

1	4.400523	1.252493	-2.501662
1	5.142586	2.392597	-1.377043
6	0.383667	-3.712938	-0.317010
1	0.679899	-4.454235	-1.071070
1	-0.613283	-3.336693	-0.569639
1	0.322048	-4.220093	0.649700
5	-0.123996	1.947470	-1.060446
1	0.408738	1.465561	-2.003310
5	0.684067	2.494864	0.406287
1	1.867787	2.406963	0.480720
5	-0.342757	2.060493	1.772477
1	0.133036	1.677023	2.792597
5	-1.775000	1.250176	1.139935
1	-2.326196	0.337630	1.644237
1	-3.831432	2.266708	-0.004011
5	-1.634065	2.861488	-1.227110
1	-2.100102	2.969786	-2.314582
5	-0.184982	3.664084	-0.610018
1	0.398989	4.471779	-1.259446
5	-0.329890	3.736517	1.172078
1	0.155112	4.612583	1.814160
5	-1.871906	2.955779	1.631907
1	-2.502342	3.264580	2.591447
5	-1.771424	3.958468	0.155753
1	-2.346784	4.994832	0.054622
6	-0.216585	-1.438306	2.073861
1	0.113083	-2.427292	2.410942
1	-0.186793	-0.734737	2.919165
1	-1.240577	-1.502995	1.703444
5	-2.665754	2.423203	0.142029
6	-0.229372	1.034599	0.404094
44	1.104031	-0.642804	0.679354

V	**HF =** -1219.0297636 hartree		
6	-1.715686	0.989343	-0.513670
5	-0.384048	1.729045	-1.259272
1	0.161070	1.149224	-2.136018
5	0.402938	2.737430	-0.051213
1	1.578404	2.889727	-0.096540
5	-0.465472	2.493050	1.463852
1	0.060114	2.485652	2.524760
5	-1.747133	1.326751	1.147700
1	-2.112917	0.506920	1.914518
5	-2.039044	2.337898	-1.504993
1	-2.553804	2.109538	-2.552664
5	-0.714974	3.473490	-1.221026
1	-0.311590	4.177991	-2.091257
5	-0.779791	3.952871	0.494035
1	-0.419945	5.021323	0.874387
5	-2.127366	3.067673	1.257801
1	-2.743120	3.487518	2.184848
1	-4.028741	1.716850	0.033063
5	-2.287880	3.700931	-0.404220
1	-3.037677	4.581013	-0.685630
6	-2.070710	-0.409081	-1.044777
1	-1.993935	-0.370323	-2.136014
1	-1.312858	-1.105829	-0.682710
6	-3.434389	-0.951629	-0.665086

6	-4.551230	-0.744171	-1.485190
1	-4.452853	-0.165467	-2.398778
6	-5.780398	-1.276652	-1.103515
1	-6.661305	-1.126332	-1.721705
6	-5.858194	-2.002120	0.085318
1	-6.794089	-2.435118	0.425152
6	-4.692389	-2.163048	0.833272
1	-4.706948	-2.726319	1.764875
7	-3.505379	-1.660815	0.472636
6	0.504246	-0.858306	2.704865
6	-0.277854	-1.608996	1.820226
1	0.096106	0.046693	3.142074
1	1.304104	-1.324481	3.275989
1	-0.064067	-2.667177	1.687628
1	-1.296687	-1.328260	1.581978
6	2.332269	0.868850	1.925853
1	2.850715	1.564311	1.259405
1	1.728558	1.449326	2.617497
1	3.062888	0.284300	2.495944
6	3.409370	-0.540266	-0.592530
6	3.264447	-1.602019	0.357451
1	3.985946	-1.699563	1.162422
6	2.235106	-2.549651	0.235031
1	2.179715	-3.367785	0.947685
6	1.305753	-2.501196	-0.853017
6	1.361358	-1.376761	-1.680604
1	0.631646	-1.253830	-2.473782
6	2.397406	-0.401552	-1.547949
1	2.407397	0.434004	-2.236141
6	4.633177	0.358048	-0.526720
1	4.779079	0.621233	0.529431
6	5.876414	-0.439716	-0.982313
1	6.775927	0.176331	-0.875206
1	5.789151	-0.730729	-2.035799
1	6.019019	-1.350606	-0.390724
6	4.507329	1.661964	-1.325702
1	3.624064	2.239173	-1.035120
1	4.452686	1.470425	-2.404423
1	5.389908	2.286199	-1.151575
6	0.321777	-3.618316	-1.083787
1	-0.131715	-3.963239	-0.149146
1	0.830946	-4.479160	-1.536697
1	-0.481394	-3.312249	-1.759773
5	-2.904339	2.089624	0.014581
6	-0.185741	1.186624	0.385763
44	1.219933	-0.462216	0.669906

3TS1   **HF =** -1219.0007889 hartree $v^{\ddagger} = -442.5156 \ icm^{-1}$

6	-1.748791	0.994634	-0.509064
5	-0.432723	1.720568	-1.299229
1	0.032606	1.175203	-2.240563
5	0.464661	2.606000	-0.074927
1	1.646848	2.684058	-0.158677
5	-0.329372	2.319447	1.466210
1	0.276567	2.216838	2.478053
5	-1.689764	1.241909	1.167911
1	-2.056907	0.389121	1.897490
5	-2.066120	2.414818	-1.408340

1	-2.655090	2.274383	-2.431717
5	-0.671236	3.470169	-1.136568
1	-0.280499	4.206115	-1.986196
5	-0.616768	3.847646	0.603829
1	-0.179896	4.872018	1.023297
5	-1.966385	2.988228	1.394989
1	-2.509112	3.383101	2.377177
1	-3.998694	1.804780	0.198193
5	-2.183628	3.721019	-0.219701
1	-2.900475	4.651973	-0.408001
6	-2.184902	-0.367202	-1.074513
1	-2.146788	-0.296175	-2.166374
1	-1.443728	-1.103255	-0.757122
6	-3.554508	-0.864587	-0.658966
6	-4.697832	-0.545971	-1.403930
1	-4.613629	0.087962	-2.281693
6	-5.933289	-1.041515	-0.994705
1	-6.834202	-0.805749	-1.554726
6	-5.990298	-1.843178	0.145335
1	-6.929824	-2.252926	0.503634
6	-4.799200	-2.112489	0.818778
1	-4.798421	-2.738263	1.709747
7	-3.605825	-1.645457	0.432064
6	0.512157	-0.869779	2.756226
6	-0.138161	-1.658082	1.736692
1	-0.091864	-0.077962	3.186625
1	1.109259	-1.405481	3.491454
1	0.096405	-2.723598	1.723604
1	-1.184706	-1.453715	1.530046
6	2.110162	0.332388	2.466205
1	2.357390	1.139567	1.774211
1	1.786242	0.815572	3.384920
1	2.974445	-0.297538	2.672201
6	3.462905	-0.415478	-0.623268
6	3.308013	-1.573608	0.223423
1	4.013162	-1.721414	1.036704
6	2.335958	-2.561223	-0.007385
1	2.307329	-3.449166	0.617061
6	1.332331	-2.360356	-1.008035
6	1.380948	-1.142051	-1.724804
1	0.617113	-0.934056	-2.464285
6	2.461497	-0.207215	-1.569026
1	2.455410	0.688669	-2.177884
6	4.653899	0.502581	-0.404258
1	4.671820	0.745188	0.670378
6	5.967808	-0.242379	-0.729632
1	6.829815	0.393383	-0.498793
1	6.012429	-0.500435	-1.794386
1	6.070591	-1.169121	-0.154842
6	4.583978	1.823638	-1.180725
1	3.676588	2.388921	-0.948785
1	4.616392	1.653354	-2.263944
1	5.444925	2.449418	-0.922919
6	0.318290	-3.430238	-1.318681
1	-0.032343	-3.931272	-0.411158
1	0.766882	-4.193831	-1.967888
1	-0.550999	-3.019836	-1.839459
5	-2.858418	2.121405	0.143593

6	-0.200078	1.063408	0.293756
44	1.212481	-0.626624	0.489564

INT5   **HF =** -1219.0539562 hartree

6	-1.796522	1.088532	-0.435967
5	-0.525640	1.912704	-1.206453
1	-0.123149	1.490388	-2.237360
5	0.452841	2.625880	0.065810
1	1.624680	2.711535	-0.085087
5	-0.236553	2.127838	1.603731
1	0.454347	1.870515	2.535348
5	-1.635935	1.111142	1.254209
1	-1.970115	0.169220	1.881591
5	-2.155410	2.618977	-1.113245
1	-2.811724	2.620635	-2.104639
5	-0.737457	3.625740	-0.792773
1	-0.393766	4.469827	-1.557930
5	-0.565672	3.761772	0.977650
1	-0.090817	4.719105	1.501142
5	-1.871068	2.808346	1.731542
1	-2.346988	3.068636	2.790298
1	-3.990986	1.802118	0.515339
5	-2.184395	3.753359	0.247184
1	-2.901116	4.702964	0.232875
6	-2.272125	-0.184247	-1.157550
1	-2.312314	0.043490	-2.227380
1	-1.506144	-0.947939	-1.003350
6	-3.609129	-0.750593	-0.723184
6	-4.800059	-0.352869	-1.345396
1	-4.776574	0.391113	-2.136146
6	-6.004012	-0.915904	-0.929211
1	-6.940057	-0.621195	-1.395895
6	-5.983671	-1.862778	0.094649
1	-6.895781	-2.330677	0.452576
6	-4.750332	-2.200983	0.650698
1	-4.688680	-2.939309	1.448575
7	-3.587303	-1.668834	0.256311
6	0.567096	-1.173369	2.494982
6	-0.121494	-1.827643	1.337211
1	1.286421	-0.320520	2.112519
1	-0.116829	-0.546385	3.075508
1	0.107457	-2.890883	1.217932
1	-1.187497	-1.642016	1.236625
6	1.428690	-2.064936	3.391585
1	2.105983	-2.688392	2.797212
1	2.031988	-1.476989	4.092439
1	0.785634	-2.732372	3.976121
6	3.530912	-0.160858	-0.535516
6	3.316704	-1.450039	0.080913
1	3.933178	-1.725485	0.932534
6	2.422515	-2.406165	-0.441141
1	2.359425	-3.391632	0.009806
6	1.512412	-2.039792	-1.481041
6	1.588747	-0.702187	-1.951552
1	0.883436	-0.369641	-2.703591
6	2.639018	0.194745	-1.545046
1	2.672376	1.182447	-1.988907
6	4.703977	0.688955	-0.068863

1	4.687559	0.678011	1.030517
6	6.027956	0.029874	-0.517756
1	6.882462	0.593575	-0.126856
1	6.102582	0.016817	-1.611719
1	6.114691	-1.002934	-0.162556
6	4.653930	2.151756	-0.525506
1	3.733519	2.647783	-0.205575
1	4.728894	2.234763	-1.616820
1	5.500495	2.700561	-0.099222
6	0.545820	-3.035053	-2.066212
1	0.154252	-3.711499	-1.300759
1	1.047486	-3.644544	-2.829640
1	-0.300226	-2.532280	-2.542790
5	-2.852904	2.121149	0.432723
6	-0.214594	1.049174	0.263692
44	1.193476	-0.629664	0.244602

VI	**HF =** -1297.5807825 hartree		
6	-1.933851	0.918115	-0.658615
5	-0.616729	1.414396	-1.593559
1	-0.188267	0.666300	-2.406492
5	0.346599	2.525251	-0.636369
1	1.514233	2.559521	-0.830334
5	-0.393256	2.591117	0.968006
1	0.226967	2.686027	1.972376
5	-1.781125	1.498282	0.931095
1	-2.138368	0.835735	1.841837
5	-2.237211	2.129012	-1.813354
1	-2.855387	1.793630	-2.772575
5	-0.814530	3.170482	-1.811909
1	-0.435829	3.698461	-2.809045
5	-0.688007	3.908709	-0.194454
1	-0.218615	4.987680	-0.016353
5	-2.022258	3.264573	0.801898
1	-2.522525	3.870432	1.694986
1	-4.120592	1.918995	-0.041850
5	-2.284640	3.656749	-0.920950
1	-2.989485	4.546454	-1.278109
6	-2.437157	-0.500506	-0.969631
1	-2.436550	-0.607281	-2.058821
1	-1.713696	-1.213379	-0.571191
6	-3.813727	-0.860045	-0.444689
6	-4.959613	-0.662335	-1.226344
1	-4.872474	-0.225080	-2.216465
6	-6.202421	-1.020957	-0.709953
1	-7.105144	-0.873903	-1.296674
6	-6.265159	-1.569220	0.571005
1	-7.210652	-1.863520	1.016275
6	-5.071574	-1.734928	1.272612
1	-5.073700	-2.162931	2.273653
7	-3.872195	-1.397755	0.783662
6	0.216012	-0.729612	2.651850
6	-0.592224	-1.500043	1.814713
1	-0.154093	0.225305	3.007573
1	0.979749	-1.187997	3.276089
1	-0.445138	-2.575752	1.772167
1	-1.593355	-1.177196	1.556121
6	2.225004	0.749552	1.903243

1	1.626886	1.184683	2.703236
1	2.882752	0.002051	2.368431
6	3.164844	-1.008757	-0.825203
6	2.983865	-1.871053	0.303511
1	3.750789	-1.909875	1.071073
6	1.890037	-2.746943	0.381578
1	1.827214	-3.450754	1.206860
6	0.900674	-2.781097	-0.649067
6	0.971806	-1.784515	-1.625858
1	0.195775	-1.714060	-2.380431
6	2.094746	-0.909455	-1.716496
1	2.128170	-0.200308	-2.534480
6	4.509638	-0.334521	-1.049597
1	4.836656	0.080263	-0.087965
6	5.543833	-1.411011	-1.456754
1	6.532813	-0.954059	-1.573255
1	5.269678	-1.873757	-2.412171
1	5.625509	-2.205787	-0.707512
6	4.490213	0.797332	-2.086243
1	3.743878	1.562667	-1.851594
1	4.282623	0.413778	-3.092426
1	5.470917	1.283173	-2.119942
6	-0.150880	-3.858898	-0.692033
1	0.265571	-4.764037	-1.153613
1	-1.016956	-3.552596	-1.285589
1	-0.500566	-4.136772	0.306586
5	-2.977813	2.182808	-0.211241
6	-0.296968	1.125911	0.107316
44	0.996597	-0.535729	0.604791
6	3.075884	1.877477	1.310979
1	3.484094	1.626800	0.328616
1	2.458131	2.764851	1.158299
6	4.237356	2.244372	2.253020
1	4.928171	1.401341	2.388689
1	4.813261	3.091583	1.859999
1	3.865452	2.525636	3.245736

3TS2 **HF =** -1297.5520429 hartree $\nu^\ddagger = -329.7913\ icm^{-1}$

6	-1.946126	0.927006	-0.689411
5	-0.627245	1.465446	-1.610332
1	-0.214242	0.769044	-2.473548
5	0.348977	2.489877	-0.568122
1	1.525702	2.506788	-0.719285
5	-0.404482	2.465544	1.024777
1	0.211071	2.481841	2.036103
5	-1.812768	1.417352	0.925524
1	-2.188322	0.706161	1.789676
5	-2.234117	2.209702	-1.780345
1	-2.859076	1.944738	-2.756944
5	-0.792919	3.230595	-1.711155
1	-0.403094	3.812698	-2.673162
5	-0.662193	3.861911	-0.048921
1	-0.173313	4.918526	0.198343
5	-2.015688	3.188212	0.898050
1	-2.506552	3.747037	1.826448
1	-4.132166	1.930713	-0.042537
5	-2.260216	3.684154	-0.799296
1	-2.946562	4.606809	-1.105052

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6	-2.461112	-0.479393	-1.031693
1	-2.473246	-0.568432	-2.122824
1	-1.734916	-1.194229	-0.642427
6	-3.826060	-0.853880	-0.488772
6	-4.992952	-0.609869	-1.224914
1	-4.931564	-0.122111	-2.193247
6	-6.222456	-0.989268	-0.691897
1	-7.141047	-0.807700	-1.243292
6	-6.250718	-1.603681	0.559958
1	-7.184553	-1.916882	1.016909
6	-5.037873	-1.812354	1.215878
1	-5.013926	-2.293711	2.192168
7	-3.850483	-1.456408	0.710955
6	0.337461	-0.519246	2.759624
6	-0.362517	-1.401485	1.850584
1	-0.180288	0.394203	3.034292
1	0.824049	-1.008152	3.600322
1	-0.201936	-2.468325	2.019204
1	-1.399537	-1.174482	1.620285
6	2.164023	0.338006	2.469391
1	1.919470	0.745621	3.451463
1	2.819274	-0.520963	2.631764
6	3.197790	-0.863854	-0.974954
6	3.057082	-1.771224	0.137326
1	3.852022	-1.806352	0.878329
6	2.012668	-2.708596	0.226702
1	2.012733	-3.452160	1.017901
6	0.912945	-2.631084	-0.683032
6	0.934002	-1.573846	-1.625601
1	0.098083	-1.454345	-2.303818
6	2.092640	-0.745612	-1.807542
1	2.075082	-0.007832	-2.601201
6	4.515453	-0.138506	-1.191441
1	4.886324	0.165808	-0.202221
6	5.554163	-1.121008	-1.779331
1	6.531320	-0.632729	-1.869142
1	5.249005	-1.456851	-2.777440
1	5.676043	-2.008412	-1.148239
6	4.406335	1.119922	-2.063448
1	3.661344	1.822229	-1.675934
1	4.134025	0.870186	-3.095919
1	5.373154	1.633187	-2.098820
6	-0.173260	-3.674789	-0.684072
1	0.165744	-4.558085	-1.241308
1	-1.084313	-3.308689	-1.164329
1	-0.428194	-3.999473	0.328716
5	-2.983873	2.186065	-0.182503
6	-0.347827	1.050777	0.057804
44	1.007109	-0.656593	0.457391
6	2.897364	1.470777	1.737168
1	3.248210	1.161717	0.752843
1	2.227878	2.315319	1.575275
6	4.097532	1.943070	2.580619
1	4.816965	1.132425	2.754672
1	4.626569	2.757991	2.071926
1	3.774648	2.316332	3.560088

INT6   **HF =** -1297.6134668 hartree

6	-1.978595	1.211551	-0.259227
5	-0.710807	2.184172	-0.844756
1	-0.339933	2.005185	-1.956461
5	0.311781	2.545063	0.539506
1	1.486673	2.633731	0.388701
5	-0.360131	1.693555	1.926856
1	0.342122	1.198436	2.744962
5	-1.791370	0.816625	1.381809
1	-2.126686	-0.251153	1.753142
5	-2.319931	2.869297	-0.537279
1	-3.000527	3.121587	-1.478879
5	-0.873962	3.745461	-0.017283
1	-0.528191	4.746391	-0.559907
5	-0.659648	3.437827	1.729869
1	-0.153452	4.230187	2.458978
5	-1.974533	2.352514	2.262508
1	-2.422859	2.358796	3.364039
1	-4.139251	1.714454	0.889845
5	-2.293296	3.636493	1.060727
1	-2.987960	4.572797	1.298005
6	-2.496346	0.154195	-1.251071
1	-2.603720	0.644750	-2.224021
1	-1.723997	-0.612045	-1.341124
6	-3.796526	-0.541134	-0.899453
6	-5.035396	0.015742	-1.243727
1	-5.077430	0.976281	-1.748579
6	-6.201359	-0.674449	-0.922113
1	-7.173570	-0.261245	-1.176764
6	-6.096024	-1.902847	-0.269707
1	-6.976244	-2.478080	0.001031
6	-4.820030	-2.382058	0.025097
1	-4.692126	-3.339304	0.527728
7	-3.692653	-1.728847	-0.282166
6	0.115190	-2.007333	2.466782
6	-0.077257	-2.002847	0.938597
1	-0.275291	-1.084885	2.910835
1	-0.526431	-2.814883	2.855373
1	0.228876	-2.982817	0.549790
1	-1.137858	-1.878527	0.706538
6	1.550164	-2.241544	2.969829
1	1.516144	-2.622603	4.000195
1	2.026931	-3.032584	2.370240
6	3.186368	0.204748	-1.297192
6	3.209301	-1.092422	-0.646945
1	3.994080	-1.290276	0.077814
6	2.369098	-2.155512	-1.034204
1	2.510399	-3.145766	-0.614359
6	1.226483	-1.873976	-1.839827
6	1.048957	-0.511255	-2.248867
1	0.171117	-0.253048	-2.831321
6	2.095414	0.470374	-2.107671
1	1.958711	1.446524	-2.556245
6	4.327529	1.175627	-1.036688
1	4.472719	1.209214	0.053157
6	5.631095	0.627341	-1.659992
1	6.473521	1.282271	-1.411541
1	5.548185	0.581316	-2.752424
1	5.869136	-0.378782	-1.297990

6	4.060453	2.606016	-1.521131
1	3.149450	3.021557	-1.080708
1	3.967495	2.647338	-2.613446
1	4.897122	3.254523	-1.240677
6	0.274829	-2.951583	-2.283712
1	0.597664	-3.351024	-3.254350
1	-0.741478	-2.564277	-2.400496
1	0.240752	-3.782035	-1.573688
5	-2.995081	2.019289	0.859604
6	-0.398974	0.986377	0.367436
44	1.070221	-0.558676	-0.075919
6	2.422279	-0.981891	2.957621
1	2.357917	-0.491707	1.964123
1	2.009726	-0.248645	3.661627
6	3.895286	-1.242204	3.283752
1	4.348673	-1.937615	2.565066
1	4.481518	-0.315981	3.274980
1	4.000185	-1.691321	4.279067

3V-1   **HF =** -1140.4678297 hartree

7	3.960434	-1.245820	-1.047366
6	1.730591	0.637309	0.393799
6	2.356094	-0.735935	0.711798
1	2.301549	-0.869426	1.796081
1	1.714778	-1.489717	0.252254
6	3.783381	-0.956156	0.253284
6	4.855707	-0.874635	1.151669
1	4.674332	-0.639353	2.196136
6	6.150435	-1.100275	0.684770
1	6.997248	-1.044839	1.363453
6	6.334833	-1.399255	-0.663931
1	7.323084	-1.584653	-1.073564
6	5.206270	-1.458011	-1.484258
1	5.304865	-1.689992	-2.543427
6	-3.771486	-0.286442	0.037314
6	-3.692198	-1.621770	-0.510890
1	-4.299569	-1.864187	-1.378574
6	-2.826101	-2.577658	0.011196
1	-2.758332	-3.559937	-0.446986
6	-1.894590	-2.212645	1.043503
6	-2.032712	-0.909362	1.635996
1	-1.383509	-0.636520	2.460471
6	-3.022326	0.013343	1.188953
1	-3.077130	0.992708	1.646721
6	-4.769022	0.682683	-0.582615
1	-4.793985	0.458160	-1.658388
6	-6.180744	0.407164	-0.020548
1	-6.921070	1.043678	-0.518793
1	-6.218458	0.621165	1.054281
1	-6.478814	-0.637313	-0.165954
6	-4.393932	2.162505	-0.427524
1	-3.384022	2.362319	-0.798004
1	-4.440564	2.487240	0.618433
1	-5.098007	2.784556	-0.991351
6	-0.932054	-3.222589	1.611914
1	-1.431365	-3.844747	2.367749
1	-0.083726	-2.727360	2.092992
1	-0.544515	-3.885202	0.832378

5	0.681652	1.349876	1.521545
1	0.458417	0.746188	2.521564
5	-0.366806	2.422966	0.598449
1	-1.475361	2.666610	0.954169
5	0.069402	2.242832	-1.118860
1	-0.702151	2.357850	-2.019914
5	1.393586	1.081738	-1.216793
1	1.726963	0.361250	-2.087775
1	3.656433	1.513675	-0.593271
5	2.345217	1.946384	1.353625
1	3.221472	1.685872	2.106984
5	1.030935	3.104438	1.473098
1	0.921793	3.781293	2.444572
5	0.644351	3.663642	-0.180267
1	0.254490	4.764241	-0.405010
5	1.738857	2.830485	-1.303817
1	2.239913	3.244577	-2.295803
5	2.329379	3.364833	0.290690
1	3.231677	4.130968	0.371268
6	-0.162951	-1.751391	-1.687118
1	-0.407499	-2.820771	-1.735930
1	-0.481801	-1.285055	-2.644511
1	0.922014	-1.643355	-1.639344
5	0.036040	0.777506	-0.065827
6	2.656001	1.818056	-0.314740
44	-1.467646	-0.697098	-0.447863

V-1   **HF =** -1219.0304166 hartree

6	-1.699214	0.825083	-0.443561
5	-0.506315	1.672542	-1.281346
1	-0.038797	1.173116	-2.252380
5	0.248237	2.752596	-0.107815
1	1.378606	3.106209	-0.219694
5	-0.527283	2.450821	1.463210
1	-0.008841	2.602583	2.518866
5	-1.716406	1.184308	1.218356
1	-2.185996	0.405036	1.970435
5	-2.208875	2.152165	-1.449635
1	-2.880483	1.872626	-2.385591
5	-0.988741	3.392310	-1.231660
1	-0.727085	4.130788	-2.126456
5	-1.005118	3.874136	0.487292
1	-0.761053	4.982800	0.841083
5	-2.236343	2.895734	1.308078
1	-2.965025	3.206460	2.191092
1	-3.845106	1.496349	0.153469
5	-2.523323	3.494437	-0.343662
1	-3.452157	4.195944	-0.574188
6	-2.154977	-0.559900	-0.945218
1	-2.040035	-0.569372	-2.033272
1	-1.454961	-1.284524	-0.525934
6	-3.565075	-0.986625	-0.588945
6	-4.636758	-0.763437	-1.465193
1	-4.466838	-0.269929	-2.417539
6	-5.914242	-1.183451	-1.095794
1	-6.759584	-1.022508	-1.759315
6	-6.082832	-1.815942	0.135001
1	-7.057179	-2.162839	0.465245

6	-4.956640	-1.999090	0.939198
1	-5.042786	-2.492451	1.905801
7	-3.726940	-1.601347	0.595090
6	0.808732	-1.298331	2.608046
6	-0.164263	-1.741376	1.695334
1	0.565371	-0.495619	3.296393
1	1.591543	-1.968292	2.961989
1	-0.118470	-2.761623	1.316114
1	-1.164955	-1.331179	1.715076
6	2.243837	0.884771	1.951862
1	2.622528	1.726161	1.363630
1	1.581528	1.281832	2.717580
1	3.081622	0.377792	2.447605
6	-2.836854	1.887273	0.103310
5	-0.100728	1.039650	0.392289
6	3.513473	-0.359008	-0.563237
6	3.499845	-1.564272	0.200647
1	4.263209	-1.728209	0.955092
6	2.528517	-2.556858	-0.028556
1	2.553857	-3.472390	0.556859
6	1.532732	-2.401298	-1.034284
6	1.466120	-1.159321	-1.688562
1	0.696166	-0.982118	-2.430972
6	2.448123	-0.145613	-1.457569
1	2.374464	0.781582	-2.010778
6	4.665691	0.619898	-0.384646
1	4.780772	0.780271	0.695854
6	5.972162	-0.020661	-0.905012
1	6.818243	0.652248	-0.725919
1	5.912189	-0.207956	-1.983921
1	6.189160	-0.973232	-0.410028
6	4.445082	1.988363	-1.041666
1	3.524238	2.466389	-0.695412
1	4.400141	1.906660	-2.134855
1	5.281798	2.651973	-0.798454
6	0.593883	-3.530247	-1.373918
1	0.265105	-4.067783	-0.478044
1	1.095233	-4.258752	-2.024439
1	-0.293816	-3.169252	-1.901328
44	1.362645	-0.559832	0.628903

3TS1-1   **HF =** -1218.9949925 hartree $v^{\ddagger} = -460.4794 \ icm^{-1}$

6	-1.720049	0.824717	-0.478708
5	-0.541674	1.684180	-1.328666
1	-0.127574	1.217243	-2.339443
5	0.288944	2.682853	-0.132848
1	1.425599	3.009635	-0.265637
5	-0.425153	2.316936	1.450127
1	0.160436	2.385061	2.482170
5	-1.666111	1.100152	1.194498
1	-2.117766	0.283136	1.917609
5	-2.235718	2.210524	-1.394732
1	-2.956292	2.002357	-2.312560
5	-0.975787	3.410696	-1.167409
1	-0.735137	4.189661	-2.033154
5	-0.905940	3.803524	0.573254
1	-0.616120	4.886218	0.970687
5	-2.126841	2.816950	1.398771

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1	-2.808428	3.100770	2.327503
1	-3.824411	1.520065	0.243120
5	-2.468390	3.503974	-0.208612
1	-3.385080	4.240942	-0.364590
6	-2.214037	-0.536160	-1.004082
1	-2.120165	-0.523708	-2.094328
1	-1.516380	-1.278345	-0.611481
6	-3.622908	-0.946607	-0.626542
6	-4.715627	-0.643321	-1.451494
1	-4.562324	-0.098690	-2.378464
6	-5.991778	-1.051336	-1.065101
1	-6.853060	-0.829169	-1.689303
6	-6.138267	-1.752671	0.130803
1	-7.110728	-2.094205	0.472076
6	-4.992378	-2.013478	0.884034
1	-5.061340	-2.563011	1.821282
7	-3.763468	-1.627253	0.523736
6	0.665366	-0.853442	2.765288
6	0.027829	-1.682608	1.764827
1	0.032643	-0.086892	3.202162
1	1.280949	-1.361325	3.506353
1	0.300944	-2.740321	1.771776
1	-1.037053	-1.534683	1.603129
6	2.197153	0.401889	2.455486
1	2.395280	1.208386	1.746931
1	1.870354	0.886504	3.373492
1	3.096596	-0.181439	2.652228
6	-2.808320	1.886713	0.171237
5	-0.099511	0.958050	0.285127
6	3.543159	-0.319190	-0.631268
6	3.543503	-1.556492	0.107499
1	4.317242	-1.716990	0.853948
6	2.602190	-2.563581	-0.115418
1	2.654277	-3.490887	0.447882
6	1.501660	-2.334851	-1.005262
6	1.462750	-1.097806	-1.700520
1	0.666368	-0.911420	-2.411648
6	2.492234	-0.114353	-1.533406
1	2.417714	0.810846	-2.091541
6	4.674911	0.670778	-0.397397
1	4.741245	0.823741	0.691538
6	6.020109	0.068347	-0.859692
1	6.844748	0.749890	-0.621016
1	6.018135	-0.094340	-1.944277
1	6.229152	-0.892836	-0.377822
6	4.457914	2.043778	-1.045829
1	3.517266	2.502505	-0.727747
1	4.451051	1.972236	-2.140545
1	5.274897	2.718576	-0.768053
6	0.510578	-3.434315	-1.293203
1	0.231871	-3.973649	-0.382214
1	0.942742	-4.163523	-1.991662
1	-0.402690	-3.040138	-1.747680
44	1.352597	-0.635380	0.494729

INT5-1   **HF =** -1219.0474968 hartree

6	-1.850770	0.617113	0.062743
5	-1.047879	1.148938	-1.327199

1	-0.920251	0.385579	-2.228687
5	0.034579	2.438354	-0.798840
1	1.047250	2.675759	-1.374084
5	-0.128610	2.587096	0.963322
1	0.752852	2.928629	1.687211
5	-1.307557	1.396091	1.479953
1	-1.454093	0.831080	2.509785
5	-2.711946	1.675555	-1.014023
1	-3.662369	1.239345	-1.563919
5	-1.530888	2.854267	-1.549859
1	-1.623746	3.332597	-2.634656
5	-0.960642	3.751567	-0.115859
1	-0.640689	4.895764	-0.169941
5	-1.798058	3.098803	1.302469
1	-2.183223	3.668382	2.269385
1	-3.673727	1.521952	1.162310
5	-2.662680	3.267477	-0.241270
1	-3.631137	3.948672	-0.316602
6	-2.376361	-0.823146	0.211939
1	-1.725429	-1.452250	-0.398391
1	-2.231671	-1.131266	1.250075
6	-3.825021	-1.075121	-0.153939
6	-4.169771	-1.823403	-1.285696
1	-3.393911	-2.207030	-1.941669
6	-5.516062	-2.061147	-1.558353
1	-5.807042	-2.639754	-2.430903
6	-6.477872	-1.542604	-0.693143
1	-7.538280	-1.701515	-0.862955
6	-6.041001	-0.806846	0.409282
1	-6.759138	-0.384014	1.109817
7	-4.752060	-0.578773	0.684323
6	1.489424	-0.019368	2.806951
6	0.657366	-1.145472	2.276181
1	1.958392	0.608612	1.913626
1	0.878688	0.780126	3.239350
1	1.015276	-2.141154	2.557038
1	-0.413056	-1.055962	2.447970
6	2.666104	-0.383167	3.715499
1	3.258154	-1.196971	3.282960
1	3.331542	0.471550	3.884152
1	2.293493	-0.718924	4.690268
6	-2.757610	1.847904	0.683253
5	-0.100879	0.932670	0.213078
6	3.476894	-0.252885	-0.940898
6	3.680608	-1.340001	-0.017932
1	4.559600	-1.319694	0.621296
6	2.795460	-2.419967	0.075258
1	2.990442	-3.221419	0.782017
6	1.575875	-2.420977	-0.676881
6	1.355049	-1.336161	-1.569043
1	0.454685	-1.319450	-2.171534
6	2.318204	-0.286312	-1.732200
1	2.099125	0.517906	-2.423649
6	4.573960	0.795318	-1.073914
1	4.943739	0.994310	-0.057967
6	5.750913	0.211317	-1.886714
1	6.580871	0.926400	-1.924820
1	5.441447	-0.003131	-2.916805

1	6.126690	-0.720211	-1.448747
6	4.115270	2.130154	-1.672599
1	3.275850	2.556018	-1.116504
1	3.807620	2.018714	-2.719368
1	4.942075	2.848840	-1.653154
6	0.631098	-3.593004	-0.603998
1	0.533112	-3.962863	0.421536
1	0.998172	-4.421599	-1.224937
1	-0.365804	-3.324318	-0.965191
44	1.514572	-0.490107	0.479813

VI-1   **HF =** -1297.5847347 hartree

6	-1.880979	0.698719	-0.627803
5	-0.679110	1.263524	-1.660740
1	-0.318851	0.552853	-2.541042
5	0.229589	2.473541	-0.761680
1	1.368802	2.703060	-1.010024
5	-0.465305	2.547766	0.874119
1	0.127341	2.849649	1.854601
5	-1.762187	1.365339	0.934077
1	-2.244959	0.791103	1.845419
5	-2.344365	1.857232	-1.842613
1	-3.091573	1.468006	-2.676207
5	-1.020642	2.998737	-1.926151
1	-0.756050	3.527092	-2.958172
5	-0.891483	3.796663	-0.335565
1	-0.536825	4.924983	-0.213454
5	-2.140335	3.103575	0.716262
1	-2.784185	3.638397	1.556825
1	-3.923174	1.661142	-0.066526
5	-2.483406	3.404732	-1.003594
1	-3.366460	4.130298	-1.322474
6	-2.488880	-0.699079	-0.863928
1	-2.444809	-0.895356	-1.939156
1	-1.832217	-1.413602	-0.368875
6	-3.908127	-0.916543	-0.377552
6	-5.000110	-0.789424	-1.247729
1	-4.838608	-0.528221	-2.289483
6	-6.287928	-1.001901	-0.756375
1	-7.149184	-0.909088	-1.412417
6	-6.446476	-1.337996	0.587028
1	-7.428396	-1.514945	1.015137
6	-5.300140	-1.447449	1.376431
1	-5.378169	-1.712973	2.429347
7	-4.060708	-1.246037	0.916386
6	0.598248	-1.568858	2.513431
6	-0.511725	-1.639456	1.653847
1	0.602550	-0.847533	3.322784
1	1.218197	-2.444975	2.699541
1	-0.757660	-2.582451	1.168181
1	-1.371591	-1.010060	1.835094
6	1.952977	0.704267	2.060971
1	1.115929	1.093111	2.646584
1	2.538949	0.063100	2.735385
6	-2.892925	1.943690	-0.241270
5	-0.208738	0.925409	0.091172
6	3.331912	-0.718194	-0.821202
6	3.334898	-1.752069	0.164816

1	4.150172	-1.804628	0.880583
6	2.365666	-2.772179	0.143510
1	2.435443	-3.587813	0.858582
6	1.300520	-2.762793	-0.792851
6	1.185835	-1.632024	-1.625302
1	0.364343	-1.562543	-2.328980
6	2.209088	-0.637654	-1.656098
1	2.120094	0.173218	-2.368760
6	4.574773	0.139111	-1.010481
1	4.961933	0.380330	-0.012745
6	5.654410	-0.708238	-1.724374
1	6.582367	-0.132890	-1.819788
1	5.325243	-0.989439	-2.731957
1	5.880696	-1.628274	-1.174553
6	4.341916	1.452275	-1.768071
1	3.552452	2.053127	-1.309683
1	4.070509	1.268624	-2.814692
1	5.263348	2.044575	-1.772632
6	0.342858	-3.921752	-0.896060
1	0.165051	-4.388984	0.078280
1	0.751652	-4.695088	-1.559349
1	-0.621660	-3.609763	-1.308255
44	1.174194	-0.708823	0.590792
6	2.851035	1.872485	1.647387
1	3.761629	1.503985	1.160399
1	2.354336	2.524899	0.925580
6	3.271683	2.717217	2.864110
1	3.798376	2.106873	3.609430
1	3.938444	3.538543	2.570647
1	2.395666	3.156620	3.356221

3TS2-1 **HF =** -1297.547506 hartree $v^{\ddagger} = -343.6371 \ icm^{-1}$

6	-1.895707	0.743649	-0.615348
5	-0.701961	1.404281	-1.611083
1	-0.334559	0.766923	-2.543217
5	0.197988	2.543390	-0.609418
1	1.341613	2.794675	-0.821276
5	-0.499221	2.468874	1.024698
1	0.091582	2.673820	2.034509
5	-1.788485	1.284253	0.989101
1	-2.257244	0.623135	1.847393
5	-2.374416	1.986739	-1.734734
1	-3.122081	1.662462	-2.595264
5	-1.060643	3.150475	-1.726152
1	-0.807588	3.767307	-2.710754
5	-0.935491	3.815264	-0.073457
1	-0.592439	4.933844	0.139659
5	-2.177521	3.030430	0.918137
1	-2.823476	3.488904	1.801362
1	-3.950989	1.639867	0.019394
5	-2.527010	3.463241	-0.771846
1	-3.415996	4.205369	-1.030428
6	-2.472222	-0.654067	-0.911098
1	-2.407946	-0.816185	-1.991459
1	-1.806336	-1.366931	-0.421896
6	-3.890141	-0.922384	-0.448031
6	-4.986660	-0.711386	-1.296304
1	-4.830722	-0.346270	-2.307195

6	-6.271315	-0.977303	-0.823518
1	-7.135893	-0.821676	-1.463110
6	-6.422572	-1.449494	0.479370
1	-7.402009	-1.672724	0.891235
6	-5.272331	-1.636306	1.247887
1	-5.344628	-2.009682	2.267954
7	-4.035376	-1.384730	0.805525
6	0.542376	-0.532637	2.796330
6	-0.200608	-1.418174	1.917904
1	0.029700	0.371146	3.114863
1	1.064895	-1.029344	3.611899
1	-0.031612	-2.484658	2.088019
1	-1.253980	-1.199098	1.765752
6	2.313801	0.372369	2.424680
1	2.158487	0.691535	3.456981
1	3.042293	-0.442227	2.459501
6	-2.923090	1.944646	-0.129847
5	-0.237807	0.926924	0.092440
6	3.243914	-0.780579	-1.008149
6	3.286014	-1.812332	-0.007884
1	4.159763	-1.872394	0.637259
6	2.286459	-2.781248	0.118814
1	2.387106	-3.578999	0.849083
6	1.081664	-2.664607	-0.643926
6	0.980934	-1.585895	-1.564007
1	0.099049	-1.493026	-2.186182
6	2.067505	-0.674019	-1.754586
1	1.953916	0.116591	-2.486267
6	4.483725	0.067825	-1.252321
1	4.877057	0.361786	-0.268256
6	5.573122	-0.786160	-1.939843
1	6.495820	-0.206035	-2.058461
1	5.242717	-1.105887	-2.935468
1	5.811680	-1.685512	-1.361414
6	4.224813	1.348486	-2.057339
1	3.444532	1.967753	-1.603851
1	3.921077	1.118837	-3.085901
1	5.142255	1.944279	-2.115265
6	0.031155	-3.744615	-0.581011
1	-0.108017	-4.114378	0.439480
1	0.330747	-4.597068	-1.205134
1	-0.935519	-3.388827	-0.947447
44	1.150778	-0.699902	0.491158
6	2.874036	1.606583	1.706035
1	3.146337	1.383643	0.674617
1	2.117535	2.390926	1.661382
6	4.106413	2.145394	2.457218
1	4.909052	1.397882	2.506889
1	4.507792	3.034658	1.955860
1	3.854570	2.428544	3.486933

INT6-1   **HF =** -1297.6054078 hartree

6	-2.009934	0.575696	-0.213248
5	-1.206036	0.671998	-1.702634
1	-1.092485	-0.322048	-2.344847
5	-0.096565	2.034635	-1.557344
1	0.924079	2.075448	-2.165668
5	-0.251107	2.683638	0.090185

1	0.636445	3.206141	0.683447
5	-1.451725	1.717224	0.926052
1	-1.608272	1.464400	2.069672
5	-2.857197	1.295108	-1.549911
1	-3.819602	0.736258	-1.948138
5	-1.657779	2.250932	-2.399652
1	-1.745719	2.401781	-3.575940
5	-1.060851	3.508815	-1.281219
1	-0.718182	4.583048	-1.659124
5	-1.906732	3.306228	0.263947
1	-2.276497	4.137242	1.025560
1	-3.808451	1.794295	0.582010
5	-2.774383	3.041615	-1.265319
1	-3.729112	3.692971	-1.533257
6	-2.567202	-0.750106	0.341082
1	-2.001590	-1.549566	-0.141028
1	-2.334344	-0.793908	1.408164
6	-4.050688	-1.014330	0.171394
6	-4.514541	-2.028481	-0.675048
1	-3.811222	-2.615253	-1.258540
6	-5.885188	-2.268278	-0.760261
1	-6.267297	-3.050945	-1.409964
6	-6.752472	-1.486198	0.000404
1	-7.827214	-1.635931	-0.031299
6	-6.200597	-0.494495	0.812244
1	-6.841642	0.140592	1.421240
7	-4.886904	-0.261075	0.907175
6	1.042322	0.783485	3.268518
6	0.599086	-0.413750	2.403986
1	0.515519	1.695366	2.961465
1	0.726208	0.591084	4.307055
1	0.992842	-1.331071	2.867948
1	-0.491751	-0.488689	2.453949
6	2.552015	1.066895	3.263410
1	2.807819	1.723407	4.107590
1	3.105246	0.128926	3.423985
6	-2.890865	1.951013	0.027083
5	-0.265743	0.885783	-0.161136
6	3.087958	-1.000549	-1.266620
6	3.438116	-1.556984	0.020537
1	4.414399	-1.320401	0.435166
6	2.586571	-2.406823	0.728480
1	2.900405	-2.827539	1.678862
6	1.241974	-2.602133	0.272622
6	0.868297	-1.993594	-0.968338
1	-0.125401	-2.168366	-1.364567
6	1.813983	-1.271572	-1.769884
1	1.491940	-0.858678	-2.717807
6	4.156556	-0.224374	-2.025597
1	4.646527	0.435736	-1.295542
6	5.229545	-1.202269	-2.555003
1	6.043233	-0.649453	-3.038318
1	4.797256	-1.885686	-3.295754
1	5.663213	-1.808520	-1.752060
6	3.622087	0.652094	-3.164851
1	2.849996	1.344712	-2.818075
1	3.198291	0.045287	-3.974453
1	4.440222	1.239715	-3.595634

6	0.309458	-3.534190	1.001245
1	0.402076	-3.428069	2.086317
1	0.541072	-4.576827	0.744807
1	-0.733770	-3.348381	0.730612
44	1.371067	-0.404911	0.427323
6	3.033318	1.738718	1.975959
1	2.669197	1.170965	1.084057
1	2.565216	2.725128	1.878944
6	4.553516	1.863353	1.860265
1	5.038009	0.879455	1.894582
1	4.848801	2.355754	0.926510
1	4.956610	2.456563	2.690532

3V-2   **HF =** -1127.3869833 hartree

7	-3.066528	-2.003570	-0.364692
6	-1.682377	1.195454	-0.558573
6	-2.205288	0.019285	-1.417686
1	-2.487175	0.425412	-2.395771
1	-1.378197	-0.674445	-1.571413
6	-3.363103	-0.798637	-0.883005
6	-4.691123	-0.351539	-0.981198
1	-4.899524	0.616861	-1.422027
6	-5.721071	-1.153102	-0.499831
1	-6.753493	-0.817176	-0.562785
6	-5.406332	-2.390798	0.063248
1	-6.175291	-3.050135	0.456616
6	-4.064671	-2.764631	0.099073
1	-3.770808	-3.727327	0.516669
6	3.477843	-0.477009	-0.377467
6	3.461613	-1.571815	0.568711
1	4.230079	-1.605075	1.337133
6	2.504443	-2.583349	0.511670
1	2.522474	-3.393909	1.234762
6	1.376908	-2.450430	-0.370371
6	1.382974	-1.347198	-1.295401
1	0.588913	-1.267888	-2.029882
6	2.481797	-0.429172	-1.356167
1	2.447112	0.380024	-2.074735
6	4.635277	0.512238	-0.305903
1	4.742510	0.797067	0.751379
6	5.950970	-0.175907	-0.732541
1	6.801760	0.505868	-0.607493
1	5.905467	-0.470042	-1.788726
1	6.150797	-1.078174	-0.143596
6	4.422576	1.799004	-1.113523
1	3.489447	2.296909	-0.836381
1	4.398121	1.594529	-2.191512
1	5.251050	2.494512	-0.932805
6	0.310061	-3.512585	-0.440828
1	0.544359	-4.246501	-1.226615
1	-0.670406	-3.073334	-0.649739
1	0.233407	-4.051538	0.509340
5	-0.250311	1.939575	-1.120361
1	0.258037	1.513735	-2.114152
5	0.565231	2.561246	0.320198
1	1.756499	2.654475	0.380876
5	-0.424176	2.112460	1.733560
1	0.056115	1.879944	2.805124

5	-1.834417	1.222601	1.140999
1	-2.407796	0.335229	1.684225
1	-3.959103	2.145036	-0.000421
5	-1.805666	2.773112	-1.275466
1	-2.318308	2.846289	-2.351518
5	-0.393469	3.664167	-0.707468
1	0.123723	4.497259	-1.391839
5	-0.505008	3.772058	1.073139
1	-0.065958	4.707424	1.675516
5	-1.999855	2.941135	1.580450
1	-2.642787	3.264442	2.534702
5	-1.976613	3.899529	0.075647
1	-2.608755	4.907295	-0.044871
6	-0.102238	-1.360589	2.112373
1	0.285936	-2.320133	2.488389
1	-0.121369	-0.633466	2.938310
1	-1.128383	-1.507845	1.769338
5	-2.789560	2.326080	0.126363
44	1.242452	-0.583892	0.704872
5	-0.228203	0.951155	0.384319

V-2	**HF =** -1205.9481362 hartree		
6	-1.758162	0.959382	-0.381277
5	-0.509683	1.716241	-1.256053
1	-0.077380	1.177750	-2.228366
5	0.351378	2.745499	-0.119382
1	1.510015	3.006677	-0.262281
5	-0.411119	2.530129	1.470806
1	0.168299	2.655174	2.504287
5	-1.715764	1.356993	1.272113
1	-2.121820	0.587859	2.083812
5	-2.184314	2.294478	-1.387558
1	-2.792427	2.055478	-2.389027
5	-0.863385	3.455910	-1.221105
1	-0.545928	4.154837	-2.138772
5	-0.808709	3.964752	0.480561
1	-0.450012	5.059023	0.804772
5	-2.093638	3.098497	1.352890
1	-2.668075	3.548061	2.300170
1	-4.071078	1.724213	0.281228
5	-2.378231	3.679831	-0.309831
1	-3.161307	4.547416	-0.563185
6	-2.182539	-0.441906	-0.878016
1	-2.075757	-0.445561	-1.969635
1	-1.477447	-1.167706	-0.472412
6	-3.575712	-0.930967	-0.541597
6	-4.699508	-0.485664	-1.258644
1	-4.574016	0.261141	-2.036234
6	-5.954885	-0.995050	-0.947501
1	-6.835475	-0.658618	-1.490003
6	-6.063994	-1.940002	0.075305
1	-7.023410	-2.365609	0.357268
6	-4.896472	-2.326712	0.729326
1	-4.933423	-3.063771	1.531765
7	-3.680638	-1.850144	0.433175
6	0.943592	-1.600446	2.524937
6	-0.236989	-1.629276	1.755602
1	1.017377	-0.923772	3.370465

1	1.570738	-2.489318	2.615550
1	-0.517709	-2.540758	1.227125
1	-1.076632	-1.004630	2.022848
6	2.196232	0.775720	2.009657
1	2.511712	1.683451	1.486016
1	1.522726	1.072419	2.812592
1	3.075200	0.280835	2.451236
5	-0.136751	1.094144	0.414679
6	3.454163	-0.406072	-0.597265
6	3.407074	-1.639879	0.112683
1	4.173205	-1.867004	0.848588
6	2.385077	-2.587516	-0.144458
1	2.381608	-3.526053	0.405409
6	1.388056	-2.358586	-1.129448
6	1.354585	-1.081455	-1.715648
1	0.566672	-0.827484	-2.414000
6	2.379071	-0.114437	-1.458813
1	2.309847	0.847352	-1.949628
6	4.636120	0.530285	-0.381132
1	4.750397	0.646950	0.705424
6	5.927473	-0.121757	-0.922112
1	6.792974	0.520012	-0.716262
1	5.864627	-0.264300	-2.008370
1	6.115667	-1.100274	-0.466797
6	4.455756	1.929257	-0.983272
1	3.547545	2.415942	-0.617739
1	4.404622	1.889030	-2.078897
1	5.313054	2.558995	-0.717378
6	0.384712	-3.425878	-1.484560
1	0.060552	-3.980597	-0.596579
1	0.818078	-4.152409	-2.185782
1	-0.503569	-2.994610	-1.954826
5	-2.939600	2.078937	0.193828
44	1.349595	-0.615919	0.628592

3TS1-2 **HF =** -1205.914001 hartree $v^{\ddagger} = -460.1923\ icm^{-1}$

6	-1.758824	0.945170	-0.425765
5	-0.520668	1.721361	-1.301817
1	-0.122465	1.210992	-2.305228
5	0.394045	2.669998	-0.133195
1	1.556065	2.912643	-0.285182
5	-0.322212	2.378610	1.463945
1	0.305045	2.415838	2.480371
5	-1.661116	1.246313	1.243716
1	-2.039920	0.421945	2.014313
5	-2.187214	2.338661	-1.344006
1	-2.835438	2.173588	-2.334803
5	-0.837375	3.464565	-1.154647
1	-0.537372	4.212532	-2.038792
5	-0.718898	3.875268	0.572251
1	-0.327358	4.942979	0.944127
5	-1.995258	2.986391	1.437851
1	-2.531300	3.395358	2.425529
1	-4.035746	1.713959	0.349409
5	-2.318752	3.664843	-0.182029
1	-3.088850	4.562028	-0.361106
6	-2.214729	-0.429206	-0.962277
1	-2.117874	-0.405709	-2.054315

1	-1.516009	-1.174972	-0.580455
6	-3.612952	-0.895790	-0.620195
6	-4.731393	-0.435879	-1.336035
1	-4.595579	0.303239	-2.119397
6	-5.994492	-0.920318	-1.016213
1	-6.871186	-0.572661	-1.557975
6	-6.116109	-1.855389	0.014138
1	-7.081633	-2.262433	0.302546
6	-4.953099	-2.257065	0.667499
1	-5.000135	-2.986812	1.476004
7	-3.730416	-1.804459	0.363112
6	0.641531	-0.785519	2.789190
6	-0.032653	-1.618304	1.818884
1	0.044965	0.027152	3.190957
1	1.238937	-1.294254	3.546720
1	0.198212	-2.687010	1.854550
1	-1.086416	-1.421471	1.643944
6	2.229507	0.389843	2.433925
1	2.429422	1.181725	1.708973
1	1.937260	0.899862	3.350043
1	3.114743	-0.221317	2.619966
5	-0.126003	1.005391	0.312853
6	3.469279	-0.395579	-0.687737
6	3.485689	-1.628338	0.062385
1	4.287118	-1.791455	0.779442
6	2.519357	-2.621303	-0.108178
1	2.575608	-3.542587	0.465941
6	1.374820	-2.370429	-0.937853
6	1.330730	-1.145863	-1.660050
1	0.500076	-0.941079	-2.324192
6	2.385503	-0.180688	-1.548803
1	2.290590	0.746243	-2.100049
6	4.616297	0.586451	-0.495620
1	4.684808	0.787579	0.586280
6	5.956963	-0.045929	-0.929589
1	6.789929	0.636519	-0.718223
1	5.953942	-0.252108	-2.007433
1	6.156494	-0.990182	-0.410977
6	4.419750	1.933953	-1.201508
1	3.486593	2.417353	-0.900067
1	4.405803	1.812926	-2.292383
1	5.249427	2.607700	-0.955906
6	0.344007	-3.449963	-1.156300
1	0.115925	-3.978671	-0.224825
1	0.709404	-4.192209	-1.880823
1	-0.590800	-3.035385	-1.542605
5	-2.899544	2.050673	0.249449
44	1.324330	-0.657503	0.515741

INT5-2   **HF = -1205.966589 hartree**

6	-1.829073	0.982869	-0.388370
5	-0.677563	1.836033	-1.310166
1	-0.386433	1.415190	-2.389417
5	0.354198	2.682125	-0.163566
1	1.491619	2.938382	-0.423745
5	-0.194970	2.245138	1.468463
1	0.544853	2.174357	2.407999
5	-1.567911	1.139681	1.284630

1	-1.880777	0.250655	2.011584
5	-2.335215	2.452460	-1.130423
1	-3.081056	2.374844	-2.061335
5	-0.966124	3.559901	-0.980095
1	-0.749546	4.382983	-1.820719
5	-0.669942	3.816534	0.756368
1	-0.234923	4.848117	1.178644
5	-1.860870	2.854845	1.664328
1	-2.293113	3.174159	2.732676
1	-4.012590	1.683897	0.678170
5	-2.339664	3.672667	0.150624
1	-3.117098	4.581081	0.128752
6	-2.341056	-0.335981	-1.011473
1	-2.344224	-0.201045	-2.099616
1	-1.617279	-1.118635	-0.776446
6	-3.708523	-0.832038	-0.593297
6	-4.880918	-0.286911	-1.144445
1	-4.805583	0.537308	-1.846688
6	-6.116901	-0.797995	-0.765855
1	-7.033846	-0.385599	-1.180770
6	-6.158495	-1.844618	0.158085
1	-7.099800	-2.277344	0.486487
6	-4.946988	-2.323959	0.651160
1	-4.931293	-3.141062	1.372703
7	-3.750309	-1.845495	0.288447
6	0.695841	-1.077093	2.495298
6	-0.006540	-1.794548	1.381622
1	1.392180	-0.228231	2.069275
1	0.012214	-0.434905	3.059662
1	0.227742	-2.864773	1.322452
1	-1.078818	-1.626367	1.320461
6	1.580731	-1.919161	3.417943
1	2.249784	-2.562534	2.834522
1	2.198513	-1.295235	4.076553
1	0.958728	-2.564841	4.050537
5	-0.138706	0.984655	0.190323
6	3.579978	-0.181402	-0.512220
6	3.517362	-1.564121	-0.106640
1	4.218238	-1.917445	0.646498
6	2.581111	-2.454701	-0.641190
1	2.554035	-3.485761	-0.297902
6	1.566451	-1.981755	-1.539818
6	1.629395	-0.619266	-1.949086
1	0.893030	-0.236752	-2.644623
6	2.659777	0.259566	-1.477386
1	2.645613	1.294020	-1.796943
6	4.715332	0.675198	0.035836
1	4.832001	0.402269	1.094938
6	6.036422	0.314194	-0.678829
1	6.878682	0.863560	-0.239046
1	5.980628	0.575525	-1.742995
1	6.255859	-0.757574	-0.609023
6	4.467994	2.187455	-0.027740
1	3.524217	2.464565	0.448378
1	4.435668	2.545917	-1.063824
1	5.284482	2.719748	0.475705
6	0.555149	-2.932036	-2.129041
1	0.197065	-3.644314	-1.378492

1	0.994702	-3.507025	-2.957591
1	-0.311265	-2.389681	-2.517530
5	-2.888844	2.027508	0.493948
44	1.325130	-0.656112	0.233230

VI-2   **HF =** -1284.5039455 hartree

6	-1.907025	0.917374	-0.578760
5	-0.650898	1.414758	-1.604241
1	-0.323534	0.699427	-2.500593
5	0.357536	2.521865	-0.685804
1	1.517292	2.653919	-0.939958
5	-0.327617	2.620687	0.952696
1	0.310672	2.845325	1.932572
5	-1.734011	1.551147	0.992538
1	-2.156992	0.956452	1.932650
5	-2.274228	2.125656	-1.754577
1	-2.956879	1.793403	-2.678130
5	-0.853033	3.167790	-1.827380
1	-0.526730	3.687458	-2.854230
5	-0.658097	3.920076	-0.229644
1	-0.188555	5.011654	-0.092939
5	-1.959546	3.313914	0.821214
1	-2.438647	3.950234	1.712593
1	-4.101812	1.986459	0.066471
5	-2.288095	3.667350	-0.896035
1	-3.008715	4.555366	-1.244963
6	-2.482798	-0.486007	-0.880983
1	-2.473895	-0.602936	-1.971277
1	-1.803567	-1.229930	-0.467743
6	-3.877147	-0.821562	-0.392080
6	-5.017507	-0.326370	-1.048059
1	-4.897329	0.350144	-1.888124
6	-6.279509	-0.698927	-0.600240
1	-7.172084	-0.322072	-1.094325
6	-6.379004	-1.560269	0.494854
1	-7.342848	-1.878281	0.883388
6	-5.196164	-2.007001	1.079022
1	-5.225161	-2.683871	1.933086
7	-3.974657	-1.661430	0.652283
6	0.588290	-1.697644	2.475873
6	-0.581150	-1.504644	1.716788
1	0.781934	-1.065353	3.335833
1	1.051480	-2.683036	2.543720
1	-1.028760	-2.343547	1.188351
1	-1.287898	-0.740209	2.002200
6	1.993429	0.585331	2.077531
1	1.171785	0.994331	2.672228
1	2.566387	-0.087569	2.735311
6	3.222994	-0.827045	-0.885345
6	3.186608	-1.906629	0.050830
1	4.019796	-2.053538	0.732511
6	2.138388	-2.850951	0.016953
1	2.167329	-3.700165	0.695860
6	1.044340	-2.718522	-0.873966
6	0.983696	-1.538403	-1.643060
1	0.135590	-1.355739	-2.290863
6	2.082485	-0.623119	-1.673324
1	2.014504	0.235967	-2.328822

6	4.513452	-0.039762	-1.061554
1	4.924029	0.140172	-0.059709
6	5.536917	-0.914309	-1.822016
1	6.496410	-0.389439	-1.909546
1	5.179190	-1.136384	-2.835106
1	5.715263	-1.867924	-1.312552
6	4.350001	1.315217	-1.761296
1	3.591203	1.933840	-1.276221
1	4.064087	1.190205	-2.813069
1	5.302508	1.858137	-1.745093
6	-0.014953	-3.786553	-0.973260
1	0.295886	-4.579761	-1.666997
1	-0.960079	-3.375150	-1.339298
1	-0.204629	-4.255271	-0.001217
5	-2.951737	2.215449	-0.129271
44	1.141789	-0.755032	0.590707
6	2.933825	1.723675	1.676565
1	3.828966	1.321193	1.183679
1	2.456323	2.397166	0.962922
6	3.392792	2.544009	2.895914
1	3.893845	1.908618	3.640139
1	4.093862	3.340390	2.608059
1	2.533667	3.016240	3.387083
5	-0.224626	1.022945	0.133053

3TS2-2　　　　**HF =** -1284.4657935 hartree　　　　$v^{\ddagger} = -346.9146 \ icm^{-1}$

6	-1.942156	0.888977	-0.573016
5	-0.690873	1.474246	-1.569021
1	-0.348406	0.815030	-2.503383
5	0.302131	2.526662	-0.561980
1	1.467853	2.686704	-0.776008
5	-0.394681	2.490295	1.073742
1	0.237060	2.633128	2.077609
5	-1.786885	1.410607	1.034328
1	-2.186871	0.726233	1.922058
5	-2.324070	2.166038	-1.665417
1	-3.003802	1.898363	-2.611840
5	-0.916242	3.235377	-1.659355
1	-0.600353	3.836670	-2.643926
5	-0.735458	3.871761	-0.007673
1	-0.282557	4.957969	0.208284
5	-2.033661	3.176453	0.992113
1	-2.520806	3.742895	1.925670
1	-4.158327	1.878471	0.131009
5	-2.361379	3.645108	-0.697739
1	-3.091440	4.547687	-0.984455
6	-2.487262	-0.514591	-0.914536
1	-2.430419	-0.632853	-2.003199
1	-1.817211	-1.247951	-0.464032
6	-3.894568	-0.856281	-0.473550
6	-5.014774	-0.410180	-1.195282
1	-4.871245	0.227343	-2.062026
6	-6.288451	-0.774609	-0.774487
1	-7.166544	-0.433645	-1.318160
6	-6.418605	-1.579123	0.359790
1	-7.392579	-1.887874	0.730088
6	-5.253218	-1.980232	1.009050
1	-5.306675	-2.611674	1.896029

7	-4.020796	-1.642134	0.609314
6	0.467101	-0.535362	2.792998
6	-0.277660	-1.403621	1.901275
1	-0.022009	0.393144	3.072946
1	0.945543	-1.038378	3.633411
1	-0.141895	-2.475333	2.077571
1	-1.316883	-1.148559	1.715522
6	2.287939	0.276564	2.465068
1	2.118037	0.629448	3.485345
1	2.973742	-0.574273	2.537607
5	-0.276059	0.965826	0.122182
6	3.185150	-0.822419	-1.064733
6	3.245433	-1.868866	-0.077221
1	4.141631	-1.950366	0.535450
6	2.232538	-2.816850	0.074543
1	2.338173	-3.624482	0.794244
6	0.992716	-2.645879	-0.623659
6	0.884924	-1.562652	-1.544600
1	-0.018280	-1.434892	-2.127294
6	1.989293	-0.681861	-1.771262
1	1.862724	0.122690	-2.485134
6	4.434813	0.000370	-1.343461
1	4.879226	0.261635	-0.371141
6	5.475678	-0.858793	-2.096421
1	6.409931	-0.300405	-2.239270
1	5.095887	-1.143590	-3.085572
1	5.711036	-1.780375	-1.551762
6	4.173893	1.307747	-2.103637
1	3.419392	1.923718	-1.605333
1	3.825016	1.110820	-3.124900
1	5.100911	1.888458	-2.181495
6	-0.081272	-3.702139	-0.533230
1	0.134980	-4.525557	-1.229002
1	-1.065091	-3.298709	-0.786407
1	-0.143152	-4.126528	0.474098
5	-3.010060	2.136565	-0.037993
44	1.114351	-0.716427	0.501908
6	2.936309	1.465443	1.741744
1	3.273922	1.190119	0.742410
1	2.205813	2.263841	1.609278
6	4.131408	2.004842	2.551291
1	4.905909	1.238052	2.694039
1	4.595939	2.858137	2.039956
1	3.816758	2.345003	3.546668

INT6-2   **HF =** -1284.5239099 hartree

6	-2.013785	0.983223	-0.274601
5	-0.883614	1.940654	-1.125346
1	-0.608174	1.631760	-2.246296
5	0.174272	2.650298	0.090383
1	1.311506	2.930284	-0.146740
5	-0.347908	2.031175	1.674874
1	0.404915	1.869469	2.589399
5	-1.725869	0.952191	1.401693
1	-2.019383	-0.019235	2.019585
5	-2.534702	2.524995	-0.844402
1	-3.298897	2.553730	-1.762359
5	-1.163365	3.613919	-0.598388

1	-0.963942	4.526727	-1.344989
5	-0.830623	3.672478	1.150731
1	-0.387262	4.650113	1.678527
5	-2.008372	2.614860	1.970135
1	-2.417772	2.817498	3.074821
1	-4.178676	1.557610	0.898226
5	-2.512744	3.594297	0.565156
1	-3.287109	4.500223	0.661542
6	-2.529776	-0.275814	-1.005748
1	-2.460357	-0.080646	-2.082872
1	-1.849625	-1.095837	-0.771228
6	-3.932145	-0.759421	-0.700959
6	-5.063036	-0.109586	-1.224293
1	-4.934880	0.789545	-1.818288
6	-6.328336	-0.618615	-0.955599
1	-7.214522	-0.126353	-1.349656
6	-6.439615	-1.767852	-0.169717
1	-7.406507	-2.202783	0.069165
6	-5.264428	-2.347784	0.302806
1	-5.302940	-3.247346	0.917414
7	-4.039747	-1.871677	0.045354
6	0.402738	-1.510648	2.859986
6	0.137385	-1.804782	1.369960
1	-0.025986	-0.540146	3.133462
1	-0.145880	-2.260378	3.456182
1	0.461891	-2.839718	1.167240
1	-0.942966	-1.775899	1.206132
6	1.878915	-1.544990	3.293821
1	1.939425	-1.674802	4.385726
1	2.372131	-2.426102	2.852473
5	-0.325435	0.928389	0.261171
6	3.212379	-0.056756	-1.387724
6	3.386526	-1.357420	-0.779870
1	4.289479	-1.542318	-0.202784
6	2.450136	-2.380059	-0.928136
1	2.621654	-3.350297	-0.470278
6	1.180704	-2.095631	-1.535061
6	0.983441	-0.787773	-2.094675
1	0.056124	-0.565262	-2.610106
6	2.033712	0.190333	-2.095654
1	1.845214	1.157092	-2.545172
6	4.367421	0.933633	-1.287846
1	4.702327	0.926501	-0.239971
6	5.553196	0.448143	-2.150945
1	6.417300	1.113306	-2.028525
1	5.277497	0.442873	-3.212931
1	5.866322	-0.567047	-1.882353
6	4.003128	2.378322	-1.649502
1	3.152634	2.737659	-1.064037
1	3.748543	2.472151	-2.712799
1	4.858672	3.037717	-1.459580
6	0.161769	-3.188446	-1.733554
1	0.413781	-3.788730	-2.620011
1	-0.839988	-2.775974	-1.880120
1	0.123014	-3.861962	-0.871824
5	-3.058162	1.920771	0.736341
44	1.235631	-0.578584	0.031985
6	2.660115	-0.281076	2.922837

1	2.530507	-0.061477	1.842344
1	2.226376	0.582088	3.441191
6	4.160908	-0.372620	3.211706
1	4.624063	-1.191234	2.644828
1	4.681232	0.556274	2.947660
1	4.345178	-0.566063	4.277034

4V **HF =** -923.2207069 hartree

40	0.913002	-1.201956	-0.838352
7	-0.972627	3.121927	-0.086579
5	-0.702069	1.762941	-0.119582
5	-1.804571	-0.550072	-1.196906
1	-1.136307	-0.317274	-2.168328
5	-1.780387	-2.146452	-0.460258
1	-1.050442	-2.950664	-1.006157
5	-1.725458	-1.961859	1.295405
1	-1.041180	-2.675128	1.948585
5	-1.688912	-0.205284	1.634130
1	-1.024319	0.291258	2.476305
5	-3.282129	0.292362	-0.734114
1	-3.693522	1.148099	-1.441318
5	-3.297192	-1.470811	-1.098040
1	-3.808577	-1.889056	-2.082255
5	-3.270439	-2.352757	0.478035
1	-3.785122	-3.411201	0.613872
5	-3.206377	-1.125261	1.791707
1	-3.683778	-1.292903	2.863207
5	-3.217019	0.489671	1.031662
1	-3.621647	1.469012	1.555822
5	-4.183585	-0.827971	0.315408
1	-5.368108	-0.796421	0.346852
6	-0.961434	-0.855972	0.254342
6	-1.787562	0.580798	0.096782
6	-2.291624	3.740465	0.094478
1	-3.082573	2.996121	0.095206
6	0.072604	4.144293	-0.230841
1	-0.120588	4.759948	-1.117370
6	0.761985	1.221205	-0.470127
6	1.243851	1.057352	-1.804433
1	0.677934	1.300793	-2.697897
6	2.517501	0.432923	-1.808989
1	3.116375	0.212154	-2.686081
6	4.175222	-0.088349	0.147519
1	5.002712	-0.409279	-0.478332
6	4.292407	-0.052031	1.520680
1	5.226766	-0.345271	1.989283
6	3.209489	0.366716	2.343331
1	3.343243	0.377008	3.420857
6	2.004801	0.772175	1.806041
1	1.197044	1.110379	2.446398
6	1.860435	0.796493	0.391478
6	2.953457	0.332438	-0.438461
6	2.084486	-2.651473	0.316167
1	1.341210	-3.389662	0.664261
1	2.752141	-3.158342	-0.405586
1	2.696415	-2.341849	1.167780
1	1.057201	3.686787	-0.324103

1	0.070923	4.802598	0.645808
1	-2.477396	4.448150	-0.721637
1	-2.323094	4.294787	1.039933

VII   **HF =** -1001.8410966 hartree

40	1.009187	-1.108901	-0.223477
7	-1.320283	3.032109	-0.949086
5	-0.935576	1.762281	-0.542473
5	-1.818244	-0.847822	-0.890911
1	-1.143990	-0.856278	-1.880309
5	-1.735372	-2.154242	0.289585
1	-0.964018	-3.047508	0.035216
5	-1.753094	-1.450483	1.905688
1	-1.057680	-1.890466	2.758643
5	-1.827315	0.321859	1.704661
1	-1.226128	1.088680	2.373995
5	-3.367195	-0.011605	-0.720991
1	-3.804154	0.564629	-1.658721
5	-3.263216	-1.795319	-0.544528
1	-3.718919	-2.519616	-1.366168
5	-3.243127	-2.164863	1.221615
1	-3.699207	-3.167494	1.659700
5	-3.294821	-0.603111	2.110765
1	-3.795899	-0.477616	3.177621
5	-3.375416	0.705794	0.904845
1	-3.850911	1.769572	1.106076
5	-4.238242	-0.824105	0.599168
1	-5.423389	-0.863855	0.600019
6	-1.009085	-0.660756	0.592636
6	-1.926347	0.609529	0.005668
6	-2.691460	3.552800	-1.004388
1	-3.420266	2.780283	-0.778931
6	-0.357132	4.050892	-1.387230
1	-0.555277	4.336188	-2.427487
6	0.587173	1.293517	-0.654200
6	1.180162	0.766142	-1.839798
1	0.659979	0.640100	-2.783321
6	2.508529	0.335801	-1.588849
1	3.196250	-0.073600	-2.320096
6	4.052803	0.676017	0.497047
1	4.952806	0.262750	0.050817
6	4.064328	1.186145	1.777588
1	4.984523	1.173618	2.353619
6	2.892435	1.743640	2.360861
1	2.946828	2.140671	3.370076
6	1.699185	1.803799	1.670906
1	0.819680	2.251081	2.121748
6	1.655088	1.317842	0.336660
6	2.844914	0.736720	-0.245334
6	2.138701	-1.848161	1.512306
1	1.442850	-2.553036	2.000879
1	3.001266	-2.424907	1.137053
1	2.511243	-1.148910	2.265874
1	0.665574	3.683068	-1.309477
1	-0.457433	4.948629	-0.765794
1	-2.893567	3.942611	-2.008918
1	-2.812374	4.375697	-0.289774

6	0.892135	-2.869300	-2.606944
6	1.720760	-3.347923	-1.658097
1	1.249543	-2.215288	-3.398885
1	-0.154370	-3.161550	-2.648449
1	1.379839	-4.076565	-0.923013
1	2.786647	-3.121766	-1.669404

4TS1   **HF =** -1001.8234872 hartree $v^{\ddagger} = -329.4650\ icm^{-1}$

40	1.055419	-0.912806	-0.380892
7	-1.712263	2.950225	-0.747527
5	-1.163736	1.717934	-0.418823
5	-1.653667	-0.976853	-0.929594
1	-0.887444	-0.847641	-1.858943
5	-1.485423	-2.342434	0.160644
1	-0.599734	-3.112451	-0.110363
5	-1.662773	-1.742329	1.805400
1	-0.963196	-2.147231	2.673979
5	-1.944230	0.018812	1.699118
1	-1.484726	0.808864	2.449557
5	-3.302815	-0.342378	-0.830512
1	-3.757935	0.233112	-1.759837
5	-2.992748	-2.110329	-0.748755
1	-3.310551	-2.827576	-1.637828
5	-3.022875	-2.587633	0.995422
1	-3.376660	-3.662338	1.348692
5	-3.307688	-1.102247	1.964526
1	-3.878985	-1.104954	3.003163
5	-3.489241	0.260841	0.836403
1	-4.105735	1.241576	1.072628
5	-4.137870	-1.337036	0.387485
1	-5.307942	-1.515341	0.315914
6	-0.953606	-0.792837	0.589119
6	-2.001069	0.404739	0.020284
6	-3.139558	3.285424	-0.821473
1	-3.762724	2.403328	-0.712747
6	-0.886975	4.122772	-1.068467
1	-1.087702	4.458908	-2.092864
6	0.407741	1.472468	-0.544913
6	1.066011	1.145049	-1.774517
1	0.575751	1.083558	-2.740243
6	2.431698	0.839871	-1.546611
1	3.160991	0.574797	-2.302695
6	3.901355	1.020270	0.612491
1	4.844965	0.768285	0.136938
6	3.838791	1.324514	1.951573
1	4.743410	1.307310	2.551685
6	2.604190	1.683044	2.573700
1	2.602651	1.922752	3.632735
6	1.427772	1.750982	1.861984
1	0.502692	2.046932	2.345070
6	1.449594	1.467971	0.464326
6	2.702054	1.081203	-0.158557
6	2.534065	-2.228169	0.763912
1	1.851557	-2.962398	1.213689
1	3.560856	-2.556387	0.916830
1	2.469562	-1.270623	1.349286
1	0.173816	3.894220	-0.970918

1	-1.133754	4.946376	-0.388053
1	-3.353727	3.746484	-1.792631
1	-3.401585	4.006163	-0.037715
6	1.592516	-2.373425	-2.138716
6	2.636822	-2.835730	-1.302297
1	1.860792	-1.731621	-2.975888
1	0.749050	-3.039140	-2.315756
1	2.589722	-3.840703	-0.894406
1	3.642577	-2.454197	-1.448505

INT7　　　　　**HF =** -1001.8533156 hartree

40	0.977611	-0.879808	-0.187371
7	-1.538725	3.079626	-0.149356
5	-1.133412	1.758926	-0.297384
5	-2.511136	-0.463391	-1.393502
1	-2.287855	-0.019288	-2.467867
5	-2.291448	-2.184975	-0.955982
1	-1.898844	-2.929530	-1.790950
5	-1.623341	-2.228876	0.677888
1	-0.727097	-2.979110	0.948814
5	-1.440323	-0.562935	1.226885
1	-0.448536	-0.199458	1.810912
5	-3.719706	0.225337	-0.270839
1	-4.360865	1.144008	-0.650254
5	-3.901696	-1.443741	-0.859402
1	-4.759345	-1.724506	-1.627803
5	-3.348589	-2.549344	0.444775
1	-3.801904	-3.633126	0.602257
5	-2.785471	-1.534572	1.827348
1	-2.824656	-1.878311	2.961506
5	-3.038070	0.179619	1.373046
1	-3.178984	1.071373	2.138600
5	-4.216282	-1.053134	0.865653
1	-5.309384	-1.061465	1.325010
6	-1.233201	-0.981448	-0.406524
6	-2.052480	0.458237	-0.010538
6	-2.851098	3.555366	0.305797
1	-3.488873	2.734963	0.617455
6	-0.672345	4.215637	-0.494046
1	-1.156558	4.829918	-1.262266
6	0.353402	1.408793	-0.748465
6	0.735708	0.799841	-1.986943
1	0.051708	0.571370	-2.796056
6	2.109636	0.457597	-1.978969
1	2.659736	0.004010	-2.792070
6	3.976053	0.872434	-0.187906
1	4.797253	0.473402	-0.776118
6	4.182449	1.362379	1.083250
1	5.180245	1.349071	1.510912
6	3.107424	1.891566	1.856164
1	3.312275	2.260491	2.856667
6	1.822993	1.964005	1.354645
1	1.018529	2.393999	1.944326
6	1.575020	1.517796	0.022282
6	2.662387	0.928984	-0.738952
6	2.549304	-2.425243	1.435797
1	1.540732	-2.730566	1.759995

1	3.223929	-2.819104	2.202518
1	2.674487	-1.325944	1.555951
1	0.289548	3.875516	-0.875804
1	-0.506418	4.847062	0.387208
1	-3.349595	4.105565	-0.500940
1	-2.719392	4.239595	1.152327
6	1.990788	-2.576716	-1.129363
6	2.944430	-2.969331	0.033193
1	2.489277	-2.607655	-2.098142
1	1.133580	-3.278671	-1.173261
1	3.003532	-4.060853	0.118934
1	3.954637	-2.611778	-0.190478

VIII   **HF =** -1080.4651131 hartree

40	0.981594	-0.687724	0.011300
7	-2.230476	2.765159	-0.813590
5	-1.594141	1.543351	-0.632098
5	-2.414965	-1.059216	-1.353159
1	-2.134107	-0.787647	-2.471330
5	-1.951999	-2.584094	-0.548480
1	-1.325360	-3.375805	-1.170332
5	-1.490941	-2.182077	1.106836
1	-0.511891	-2.679085	1.595667
5	-1.685879	-0.436629	1.321535
1	-0.880711	0.229437	1.903815
5	-3.860673	-0.432011	-0.513023
1	-4.602553	0.252805	-1.129746
5	-3.664197	-2.183195	-0.754958
1	-4.349155	-2.771633	-1.523003
5	-3.087680	-2.888543	0.794989
1	-3.352993	-3.993099	1.134336
5	-2.899082	-1.540493	1.979143
1	-3.024894	-1.669696	3.151662
5	-3.402722	-0.031911	1.157327
1	-3.804503	0.939815	1.702042
5	-4.260718	-1.549941	0.814886
1	-5.383253	-1.695675	1.168712
6	-1.204593	-1.105187	-0.164505
6	-2.305716	0.174599	-0.155254
6	-3.651170	3.058000	-0.588763
1	-4.173580	2.203904	-0.170569
6	-1.530947	3.956910	-1.312656
1	-2.007322	4.306936	-2.236125
6	-0.022849	1.408764	-0.857174
6	0.640427	0.772759	-1.952639
1	0.134728	0.319819	-2.798238
6	2.041898	0.736691	-1.742798
1	2.779424	0.338490	-2.425668
6	3.521200	1.788365	0.146094
1	4.480088	1.511229	-0.282808
6	3.448827	2.520095	1.311474
1	4.362348	2.818245	1.817289
6	2.194097	2.918298	1.861990
1	2.185322	3.508249	2.773846
6	1.003111	2.593156	1.248870
1	0.054402	2.922667	1.662821
6	1.033662	1.864860	0.022465

6	2.310597	1.449334	-0.525082
6	1.873014	-2.323224	-1.118560
1	1.813926	-3.058204	-0.278403
1	0.968999	-2.533792	-1.730785
1	-0.483977	3.740195	-1.521975
1	-1.588847	4.767360	-0.575905
1	-4.129992	3.338773	-1.534332
1	-3.746498	3.902590	0.103980
6	1.633980	-0.689977	2.902367
6	2.670781	-1.162154	2.181147
1	1.562376	0.362703	3.162719
1	0.861967	-1.348597	3.293112
1	2.789288	-2.227158	1.987042
1	3.481523	-0.509242	1.865933
6	3.137758	-2.562434	-1.942732
1	3.134650	-3.589485	-2.333010
1	3.118077	-1.911657	-2.826630
6	4.434322	-2.333355	-1.158561
1	4.509697	-1.297996	-0.799813
1	4.495377	-2.998420	-0.287945
1	5.311627	-2.532398	-1.782326

4TS2   **HF =** -1080.4526326 hartree $v^{\ddagger}$ = -254.2536 icm^{-1}

40	1.031518	-0.319498	-0.071114
7	-2.922769	2.235852	-0.687232
5	-1.991119	1.210078	-0.578457
5	-2.260183	-1.518336	-1.332754
1	-2.163543	-1.180770	-2.464233
5	-1.392284	-2.912507	-0.626527
1	-0.674574	-3.538767	-1.334911
5	-0.874053	-2.443254	0.992207
1	0.235721	-2.694368	1.379409
5	-1.417793	-0.789907	1.262974
1	-0.684834	0.026858	1.765102
5	-3.717433	-1.242226	-0.335004
1	-4.653690	-0.741848	-0.856186
5	-3.164000	-2.899642	-0.650875
1	-3.782220	-3.617531	-1.363503
5	-2.295352	-3.478780	0.812302
1	-2.279324	-4.618540	1.138556
5	-2.287860	-2.132939	2.018288
1	-2.260965	-2.296444	3.192521
5	-3.188536	-0.761791	1.298689
1	-3.737006	0.091495	1.909963
5	-3.723968	-2.431312	0.991903
1	-4.746983	-2.824482	1.444867
6	-0.955352	-1.316619	-0.270037
6	-2.314672	-0.303930	-0.110886
6	-4.357309	2.162526	-0.384341
1	-4.622090	1.213707	0.070351
6	-2.569283	3.574655	-1.179530
1	-3.174799	3.816754	-2.061031
6	-0.447853	1.498050	-0.856236
6	0.329042	1.080667	-1.973085
1	-0.062773	0.538973	-2.827281
6	1.706191	1.388672	-1.767496
1	2.506871	1.224094	-2.478764

6	2.892844	2.781354	0.104632
1	3.882223	2.775016	-0.344085
6	2.652255	3.453707	1.283442
1	3.464696	3.976607	1.779180
6	1.350761	3.494572	1.864568
1	1.206488	4.042137	2.790971
6	0.277686	2.871575	1.265859
1	-0.714700	2.924554	1.703986
6	0.478904	2.190895	0.030626
6	1.804362	2.139780	-0.547388
6	2.679997	-1.731012	-0.752828
1	2.133563	-2.631737	-0.420960
1	2.094961	-1.289574	-1.620070
1	-1.516824	3.627727	-1.455800
1	-2.776585	4.328801	-0.410638
1	-4.942883	2.292425	-1.302227
1	-4.625386	2.970060	0.306999
6	2.250336	-0.183866	1.931696
6	3.254576	-0.864198	1.214063
1	2.367162	0.883648	2.106951
1	1.700112	-0.733494	2.694590
1	3.480565	-1.893791	1.466637
1	4.076986	-0.305095	0.777072
6	4.048780	-2.093593	-1.330646
1	3.887206	-2.449468	-2.357537
1	4.656776	-1.184028	-1.424191
6	4.820010	-3.178544	-0.566618
1	5.153719	-2.847197	0.421166
1	4.211741	-4.081513	-0.439710
1	5.714290	-3.460305	-1.130534

INT8 **HF =** -1080.4802639 hartree

40	1.021283	-0.133727	-0.230854
7	-3.324834	1.771173	-0.980970
5	-2.261699	0.966423	-0.596345
5	-1.431666	-1.653354	-1.030487
1	-0.902105	-1.246478	-2.020852
5	-0.576578	-2.677687	0.126287
1	0.567937	-2.940294	-0.148452
5	-0.993170	-2.156886	1.759704
1	-0.161438	-2.113447	2.604734
5	-2.106462	-0.770455	1.601483
1	-2.068805	0.190778	2.289389
5	-3.173178	-1.900035	-0.834763
1	-3.880458	-1.677017	-1.758230
5	-2.032059	-3.276796	-0.701198
1	-1.979728	-4.114679	-1.538716
5	-1.776147	-3.599453	1.055787
1	-1.544524	-4.686259	1.469067
5	-2.734636	-2.391666	1.981769
1	-3.199953	-2.608655	3.050359
5	-3.588618	-1.361090	0.805152
1	-4.599350	-0.788286	1.027401
5	-3.379592	-3.096848	0.463597
1	-4.309704	-3.832543	0.460059
6	-0.877456	-1.050222	0.468581
6	-2.370513	-0.562332	-0.091995

6	-4.735414	1.371902	-1.053112
1	-4.858488	0.311437	-0.855624
6	-3.157040	3.174524	-1.379272
1	-3.483993	3.315097	-2.416616
6	-0.757708	1.501002	-0.690870
6	0.039718	1.432923	-1.872851
1	-0.291977	1.012443	-2.816268
6	1.355975	1.900683	-1.621857
1	2.150826	1.986654	-2.354209
6	2.367834	3.126971	0.456483
1	3.324940	3.365842	0.001649
6	2.073990	3.522467	1.744538
1	2.808932	4.079393	2.317849
6	0.817852	3.221815	2.340663
1	0.628059	3.548338	3.358684
6	-0.166791	2.544761	1.650223
1	-1.129845	2.346305	2.108631
6	0.079865	2.161801	0.302847
6	1.375473	2.433414	-0.282738
6	3.445927	-1.280883	-0.723284
1	2.865364	-2.188834	-0.482723
1	2.888918	-0.707764	-1.513967
1	-2.116448	3.485379	-1.290649
1	-3.773189	3.818785	-0.740772
1	-5.125162	1.589701	-2.054329
1	-5.327155	1.940665	-0.325959
6	2.449211	-0.068573	1.406001
6	3.700207	-0.428812	0.556335
1	2.627614	0.775751	2.071846
1	2.122893	-0.936773	2.008247
1	4.395862	-1.004750	1.177961
1	4.221827	0.488359	0.259776
6	4.737309	-1.727020	-1.450948
1	4.454234	-2.159227	-2.417525
1	5.337506	-0.834777	-1.669468
6	5.568264	-2.746756	-0.664821
1	5.948550	-2.339381	0.277487
1	4.985280	-3.647132	-0.438123
1	6.434901	-3.054498	-1.258170