

Electronic Supplementary Material (ESI) for RSC Advances.

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Supporting Information

Experimental and Theoretical Evaluation of Structures of $\text{Pr}_2\text{@C}_{72}$ and Its Functionalized Adduct with Adamantylidene Carbene

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Geometries of stationary points

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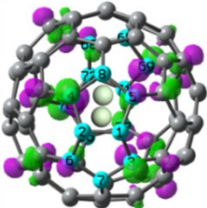
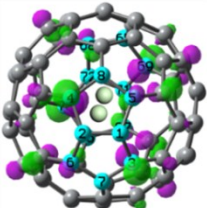
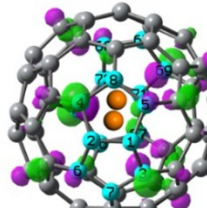
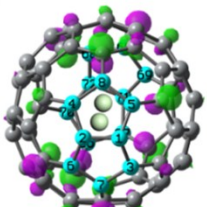
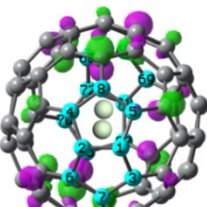
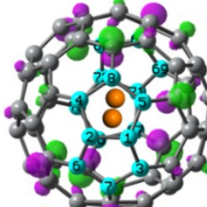
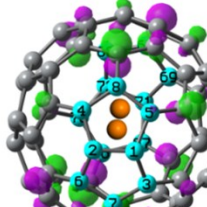
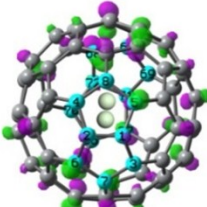
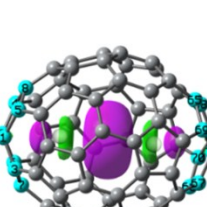
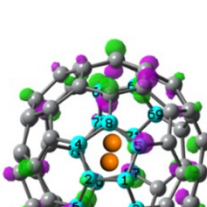
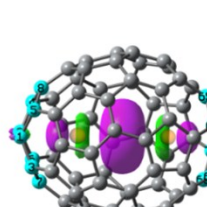
$\text{Pr}_2@\text{D}_2(10611)\text{-C}_{72}$				$\text{La}_2@\text{D}_2(10611)\text{-C}_{72}$			
231 α -2.52 eV ☐		231 β -2.36 eV ☐		231 α -2.53 eV ☐		231 β -2.37 eV ☐	
230 α -2.60 eV ☐		230 β -2.54 eV ☐		230 α -2.61 eV ☐		230 β -2.55 eV ☐	
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Table S1 (Continued)

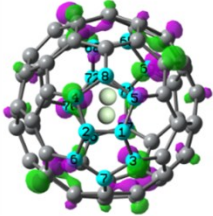
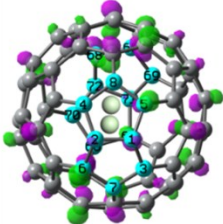
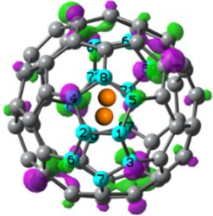
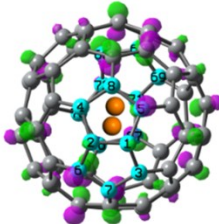
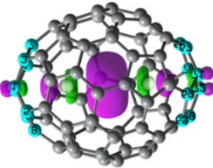
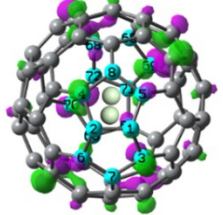
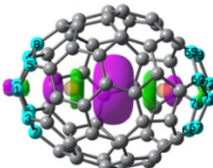
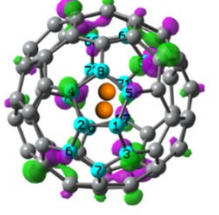
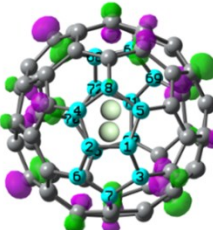
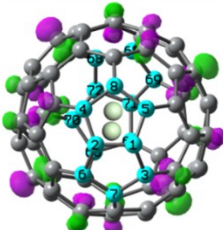
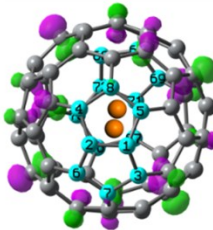
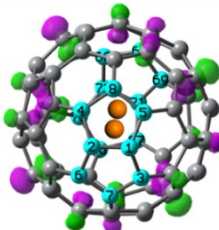
Pr ₂ @D ₂ (10611)-C ₇₂				La ₂ @D ₂ (10611)-C ₇₂			
228α −5.03 eV SOMO 		228β −2.83 eV 		228α −5.05 eV SOMO 		228β −2.85 eV 	
227α −5.18 eV 		227β −4.19 eV LUMO 		227α −5.08 eV 		227β −4.20 eV LUMO 	
226α −5.33 eV 		226β −5.29 eV 		226α −5.36 eV 		226β −5.31 eV 	

Table S2 Computed cage charges in $\text{Pr}_2\text{C}_2@\text{C}_2(7892)\text{-C}_{70}$ and $\text{Sc}_2\text{S}@\text{C}_2(7892)\text{-C}_{70}$ using the B3LYP method and different population analysis methods.

Isomers	Mulliken		Hirshfeld	NPA
	3-21G~SDD	6-31G(d)~SDD	6-31G(d)~SDD	6-31G(d)~SDD
$\text{Pr}_2\text{C}_2@\text{C}_2(7892)\text{-C}_{70}$	-4.43	-2.56	-0.37	-1.58
$\text{Sc}_2\text{S}@\text{C}_2(7892)\text{-C}_{70}$	-4.09	-2.23	-0.59	-1.61

Table S3 Electronic total energies (TEs, in hartree), zero-point vibrational energies (ZPVE, in hartree), electronic energies with ZPVE correction (TE+ZPVE, in hartree), relative energies including ZPVE correction, and the lowest normal modes (ν_1 , cm^{-1}) of the optimized C_{72} isomers at the B3LYP/6-31G(d)~MWB level of theory.

Isomers	TE	ZPVE	TE+ZPVE	RE	ν_1
10611	-2743.415916	0.447279	-2742.968637	42.28	210.3
10610	-2743.416635	0.447225	-2742.969411	41.79	212.3
10616	-2743.407847	0.447388	-2742.960459	47.41	211.0
10528	-2743.433697	0.448116	-2742.985581	31.64	219.4
11188	-2743.485559	0.449550	-2743.036008	0.00	207.5
10557	-2743.427428	0.448776	-2742.978652	35.99	210.2
10626	-2743.422835	0.448675	-2742.974160	38.81	207.9
10612	-2743.456400	0.449327	-2743.007072	18.16	214.2
10693	-2743.431015	0.448366	-2742.982649	33.48	221.5
10615	-2743.427308	0.448777	-2742.978530	36.07	214.7
10538	-2743.445014	0.449153	-2742.995861	25.19	216.4
10849	-2743.426291	0.448323	-2742.977968	36.42	209.9
11029	-2743.442114	0.449637	-2742.992477	27.32	215.1
10554	-2743.431279	0.449039	-2742.982240	33.74	212.1
10689	-2743.435662	0.448855	-2742.986808	30.87	218.6
10629	-2743.419663	0.448463	-2742.971199	40.67	210.2
10530	-2743.420745	0.447762	-2742.972984	39.55	210.3
11037	-2743.437864	0.448835	-2742.989029	29.48	210.4
11078	-2743.441902	0.449561	-2742.992341	27.40	217.2
11097	-2743.444744	0.449339	-2742.995405	25.48	221.3
10784	-2743.441842	0.449121	-2742.992721	27.16	223.4
11032	-2743.424645	0.449341	-2742.975303	38.09	215.7
10534	-2743.411457	0.447309	-2742.964148	45.09	196.3
10981	-2743.438641	0.449857	-2742.988784	29.63	213.5
11158	-2743.440065	0.448778	-2742.991287	28.06	222.8
11184	-2743.434378	0.449635	-2742.984742	32.17	213.4
10780	-2743.433044	0.448905	-2742.984139	32.55	217.5
10848	-2743.414074	0.447709	-2742.966365	43.70	205.0
10962	-2743.435344	0.449634	-2742.985711	31.56	210.3
11163	-2743.439037	0.449309	-2742.989728	29.04	217.8
11030	-2743.455785	0.450108	-2743.005677	19.03	214.5
10958	-2743.430230	0.449526	-2742.980704	34.70	207.1
10627	-2743.418549	0.448690	-2742.969859	41.51	209.4
10797	-2743.426997	0.449041	-2742.977956	36.43	207.2
11026	-2743.428103	0.449595	-2742.978509	36.08	217.2
10730	-2743.398784	0.448036	-2742.950748	53.50	203.9
11185	-2743.441273	0.449818	-2742.991455	27.96	213.5

10978	-2743.414409	0.449523	-2742.964886	44.63	211.2
10777	-2743.406271	0.448815	-2742.957456	49.29	217.9
11190	-2743.467523	0.450475	-2743.017049	11.90	212.4
11105	-2743.388034	0.449126	-2742.938908	60.93	209.2

Table S4 Computed electronic total energies (TE, in hartree), zero-point vibrational energies (ZPVE, in hartree), electronic energies with ZPVE correction (TE+ZPVE, in hartree), relative energies with ZPVE correction (RE, in kcal/mol), and the lowest vibrational modes (ν_1 , cm^{-1}) of $\text{Pr}_2@\text{C}_{72}$ and $\text{Pr}_2\text{C}_2@\text{C}_{70}$ with different multiplicities (m) at the B3LYP/6-31G(d)~MWB48 level of theory

	m	TE	ZPVE	TE+ZPVE	RE	ν_1
$\text{Pr}_2@\text{D}_2(10611)\text{-C}_{72}$	1	-2809.237775	0.446112	-2808.791664	1.55	40.0
	3	-2809.240044	0.445911	-2808.794133	0.00	60.2
$\text{Pr}_2@\text{C}_s(10528)\text{-C}_{72}$	1	-2809.213248	0.445895	-2808.767353	16.80	86.9
	3	-2809.223219	0.445647	-2808.777572	10.39	75.1
$\text{Pr}_2@\text{C}_1(10610)\text{-C}_{72}$	1	-2809.206623	0.445036	-2808.761588	20.42	48.7
	3	-2809.218765	0.445391	-2808.773374	13.03	54.9
$\text{Pr}_2@\text{C}_s(10616)\text{-C}_{72}$	1	-2809.203295	0.445040	-2808.758255	22.51	48.0
	3	-2809.219063	0.445544	-2808.773519	12.94	60.7
$\text{Pr}_2@\text{C}_2(10626)\text{-C}_{72}$	1	-2809.197620	0.444838	-2808.752782	25.95	56.0
	3	-2809.209477	0.445325	-2808.764152	18.81	51.7
$\text{Pr}_2@\text{C}_1(10557)\text{-C}_{72}$	1	-2809.193931	0.444726	-2808.749205	28.19	46.3
	3	-2809.201427	0.444867	-2808.756559	23.58	61.9
$\text{Pr}_2@\text{C}_2(10612)\text{-C}_{72}$	1	-2809.162234	0.443923	-2808.718311	47.58	46.5
	3	-2809.164849	0.443103	-2808.721745	45.42	24.2
$\text{Pr}_2@\text{C}_{2v}(11188)\text{-C}_{72}$	1	-2809.153180	0.441821	-2808.711359	51.94	36.3
	3	-2809.157549	0.442532	-2808.715017	49.65	56.2
$\text{Pr}_2@\text{D}_{6d}(11190)\text{-C}_{72}$	1	-2809.124515	0.439970	-2808.684546	68.77	40.6
	3	-2809.132815	0.440012	-2808.692803	63.59	39.6
$\text{Pr}_2\text{C}_2@\text{C}_2(7892)\text{-C}_{70}$	1	-2809.066150	0.440816	-2808.625334	105.92	78.0
	3	-2809.033126	0.438275	-2808.594851	125.05	75.7
$\text{Pr}_2\text{C}_2@\text{C}_2(7957)\text{-C}_{70}$	1	-2809.048109	0.439698	-2808.608411	116.54	49.9
	3	-2809.013913	0.436384	-2808.577530	135.92	67.6
$\text{Pr}_2\text{C}_2@\text{D}_{5h}(8149)\text{-C}_{70}$	1	-2809.040128	0.436992	-2808.603136	119.85	46.0
	3	-2809.027330	0.435304	-2808.592026	126.82	12.3

Table S5 Computed Mulliken and NBO charges of the metal atoms in $\text{Pr}_2@D_2(10611)\text{-C}_{72}$, $\text{La}_2@D_2(10611)\text{-C}_{72}$, $\text{Ce}_2@D_2(10611)\text{-C}_{72}$, $\text{La}_2@C_s(17490)\text{-C}_{76}$, $\text{Pr}_2@I_h\text{-C}_{80}$, and $\text{La}_2@I_h\text{-C}_{80}$ using the B3LYP and M06-2X functionals with the basis sets of 3-21G and 6-31G(d) (for Cl, C, H), MWB46 (for La), MWB47 (for Ce), MWB48 (for Pr), and SDD (for Pr, La, Ce)

Methods	Population analysis	Basis sets	$\text{Pr}_2@D_2(10611)\text{-C}_{72}$	$\text{La}_2@D_2(10611)\text{-C}_{72}$	$\text{Ce}_2@D_2(10611)\text{-C}_{72}$	$\text{La}_2@C_s(17490)\text{-C}_{76}$	$\text{Pr}_2@I_h\text{-C}_{80}$	$\text{La}_2@I_h\text{-C}_{80}$
B3LYP	Mulliken	3-21G~MWB	5.24	5.42	5.28	5.40	5.56	5.74
		3-21G~SDD	4.80	5.18	5.00	5.06	4.58	4.98
		6-31G(d)~MWB	1.17	1.24	1.20	1.38	1.68	1.74
		6-31G(d)~SDD	1.20	0.94	1.19	1.00	1.40	1.28
	NBO	3-21G~SDD	1.84	1.76	2.11	1.95	2.62	2.40
		6-31G(d)~SDD	1.95	1.86	2.13	2.03	2.71	2.46
M06-2X	Mulliken	3-21G~MWB	4.96	5.14	5.00	5.12	5.32	5.50
		3-21G~SDD	4.14	4.48	4.20	4.42	4.14	4.42
		6-31G(d)~MWB	1.32	1.42	1.38	1.54	1.82	1.90
		6-31G(d)~SDD	0.88	0.62	0.72	0.74	1.26	1.04
	NBO	3-21G~SDD	1.48	1.80	1.78	1.98	2.43	2.37
		6-31G(d)~SDD	1.89	1.93	2.15	2.10	2.50	2.49

Table S6 Computed relative energies (RE, kcal/mol), HOMO-LUMO energy gaps (E_{gap} , eV), the number of pyracylenes (Pyras), and energy gap (E'_{gap} , eV) between LUMO+3 and LUMO+2. The computed relative energies include ZPVE correction.

Isomers	C_{72}	C_{72}^{6-}			
	RE	RE	E_{gap}	Pyras	E'_{gap}
10611	42.28	0.00	1.97	6	1.39
10610	41.79	17.39	1.53	9	0.84
10616	47.41	17.93	1.32	8	0.63
10528	31.64	17.88	1.19	8	0.36
11188	0.00	20.39	1.41	14	0.74
10557	35.99	25.61	1.58	10	0.80
10626	38.81	27.49	1.46	10	0.60
10612	18.16	27.67	1.48	15	0.24
10693	33.48	28.94	1.46	11	0.45
10615	36.07	32.08	1.37	11	0.60
10538	25.19	32.88	1.22	11	0.37
10849	36.42	54.85	1.46	12	0.67
11029	27.32	33.52	1.43	12	0.69
10554	33.74	33.67	1.37	11	0.64
10689	30.87	34.85	1.38	12	0.56
10629	40.67	35.83	1.54	12	0.86
10530	39.55	37.80	1.14	11	0.05
11037	29.48	39.17	1.24	12	0.08
11078	27.40	39.74	1.39	13	0.38
11097	25.48	41.47	1.35	13	0.26
10784	27.16	41.19	1.14	12	0.18
11032	38.09	42.68	1.19	12	0.26
10534	45.09	42.97	1.25	12	0.12
10981	29.63	44.31	1.62	14	0.99
11158	28.06	45.08	1.33	13	0.14
11184	32.17	48.72	1.51	14	0.72
10780	32.55	48.30	1.20	13	0.08
10848	43.70	51.03	1.35	14	0.37
10962	31.56	52.87	1.21	14	0.34
11163	29.04	52.68	1.30	14	0.23
11030	19.03	52.60	1.14	18	0.06
10958	34.70	55.81	1.30	14	0.38
10627	41.51	57.80	1.08	14	0.13
10797	36.43	58.11	1.32	15	0.13
11026	36.08	58.43	1.10	10	0.12
10730	53.50	58.90	1.24	14	0.33
11185	27.96	58.93	1.24	15	0.28
10978	44.63	68.48	1.31	16	0.12
10777	49.29	69.40	1.05	14	0.05
11190	11.90	66.78	1.03	24	0.65

11105	60.93	92.76	1.17	18	0.43
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Table S7 Electronic total energies (TEs, in hartree), zero-point vibrational energies (ZPVE, in hartree), electronic energies with ZPVE correction (TE+ZPVE, in hartree), relative energies including ZPVE correction, and the lowest normal modes of the optimized C_{72}^{6-} isomers at the B3LYP/6-31G(d)~MWB level of theory.

Isomers	TE	ZPVE	TE+ZPVE	RE	ν_1
10611	-2742.423189	0.433612	-2741.989577	0.00	211.7
10610	-2742.394281	0.432408	-2741.961872	17.39	210.2
10616	-2742.393346	0.432340	-2741.961006	17.93	211.5
10528	-2742.392755	0.431674	-2741.961082	17.88	212.7
11188	-2742.387427	0.430339	-2741.957088	20.39	219.8
10557	-2742.380911	0.432142	-2741.948769	25.61	208.4
10626	-2742.377853	0.432077	-2741.945776	27.49	203.9
10612	-2742.376417	0.430932	-2741.945485	27.67	203.1
10693	-2742.375192	0.431733	-2741.943459	28.94	216.0
10615	-2742.37014	0.431690	-2741.938450	32.08	211.3
10538	-2742.368104	0.430918	-2741.937186	32.88	211.1
10849	-2742.333440	0.431275	-2741.902165	54.85	205.0
11029	-2742.367808	0.431642	-2741.936166	33.52	209.4
10554	-2742.367205	0.431278	-2741.935927	33.67	208.1
10689	-2742.365279	0.431231	-2741.934048	34.85	213.6
10629	-2742.364234	0.431757	-2741.932478	35.83	205.1
10530	-2742.359784	0.430451	-2741.929333	37.80	171.3
11037	-2742.357748	0.430585	-2741.927162	39.17	179.1
11078	-2742.357287	0.431034	-2741.926252	39.74	211.4
11097	-2742.354176	0.430687	-2741.923489	41.47	207.2
10784	-2742.354095	0.430153	-2741.923942	41.19	193.4
11032	-2742.352738	0.431174	-2741.921564	42.68	208.9
10534	-2742.351694	0.430595	-2741.921100	42.97	195.8
10981	-2742.350220	0.431249	-2741.918970	44.31	206.0
11158	-2742.347656	0.429924	-2741.917732	45.08	203.6
11184	-2742.342629	0.430695	-2741.911934	48.72	207.8
10780	-2742.342398	0.429787	-2741.912607	48.30	167.9
10848	-2742.338422	0.430158	-2741.908263	51.03	204.7
10962	-2742.335603	0.430277	-2741.905326	52.87	203.1
11163	-2742.335233	0.429610	-2741.905622	52.68	201.8
11030	-2742.334952	0.429203	-2741.905749	52.60	186.4
10958	-2742.330824	0.430182	-2741.900642	55.81	198.7
10627	-2742.326845	0.429383	-2741.897462	57.80	154.0
10797	-2742.326537	0.429562	-2741.896976	58.11	184.4
11026	-2742.326401	0.429940	-2741.896460	58.43	188.7
10730	-2742.325822	0.430107	-2741.895715	58.90	194.4
11185	-2742.325139	0.429469	-2741.895670	58.93	204.1

10978	-2742.310618	0.430162	-2741.880449	68.48	198.1
10777	-2742.307430	0.428455	-2741.878975	69.40	169.5
11190	-2742.306652	0.423496	-2741.883156	66.78	173.6
11105	-2742.270117	0.428357	-2741.841760	92.76	196.7

Table S8 Computed spin densities (spin), charges, and POAV values of all C atoms in the triplet $\text{Pr}_2@\text{D}_2(10611)\text{-C}_{72}$ using the B3LYP/6-31G(d)~MWB48-optimized geometries.

No.	Spin	Charge	POA V	No.	Spin	Charge	POAV
1	0.00	0.00	15.89	37	0.06	-0.03	10.07
2	0.00	0.00	15.89	38	0.06	-0.03	10.07
3	0.06	-0.00	12.37	39	0.02	-0.01	10.96
4	0.06	-0.00	12.37	40	0.02	-0.01	10.96
5	0.05	-0.03	12.48	41	0.01	0.05	8.74
6	0.05	-0.03	12.48	42	0.01	0.05	8.74
7	-0.01	-0.06	11.48	43	-0.03	-0.03	10.79
8	-0.01	-0.06	11.48	44	-0.03	-0.03	10.79
9	-0.02	-0.04	10.80	45	0.02	-0.04	10.01
10	-0.02	-0.04	10.80	46	0.02	-0.04	10.01
11	-0.03	0.01	9.38	47	-0.01	-0.03	10.62
12	-0.03	0.01	9.38	48	-0.01	-0.03	10.62
13	0.01	-0.04	11.28	49	-0.01	0.03	8.66
14	0.01	-0.04	11.28	50	-0.01	0.03	8.66
15	0.02	-0.00	8.52	51	-0.03	-0.02	10.66
16	0.02	-0.00	8.52	52	-0.03	-0.02	10.66
17	0.02	-0.03	10.57	53	0.12	-0.03	9.67
18	0.02	-0.03	10.57	54	0.12	-0.03	9.67
19	0.12	-0.03	9.65	55	0.02	-0.03	10.56
20	0.12	-0.03	9.65	56	0.02	-0.03	10.56
21	-0.03	-0.02	10.66	57	0.02	-0.00	8.52
22	-0.03	-0.02	10.66	58	0.02	-0.00	8.52
23	-0.01	0.03	8.68	59	0.01	-0.04	11.27
24	-0.01	0.03	8.68	60	0.01	-0.04	11.27
25	-0.01	-0.03	10.61	61	-0.03	0.01	9.37
26	-0.01	-0.03	10.61	62	-0.03	0.01	9.37
27	0.02	-0.04	10.00	63	-0.02	-0.04	10.80
28	0.02	-0.04	10.00	64	-0.02	-0.04	10.80
29	-0.03	-0.03	10.79	65	-0.01	-0.06	11.49
30	-0.03	-0.03	10.79	66	-0.01	-0.06	11.49
31	0.01	0.05	8.74	67	0.05	-0.03	12.48
32	0.01	0.05	8.74	68	0.05	-0.03	12.48
33	0.02	-0.01	10.95	69	0.06	-0.00	12.37
34	0.02	-0.01	10.95	70	0.06	-0.00	12.37
35	0.06	-0.03	10.07	71	0.00	0.00	15.90
36	0.06	-0.03	10.07	72	0.00	0.00	15.90

Table S9 Computed electronic total energies (TE, kcal/mol), zero-point vibrational energies (ZPVE, hartree), Gibbs free energies (G, kcal/mol, 298.15 K), and the lowest normal mode (ν , cm^{-1}) of the mono-adduct $\text{Pr}_2\text{@D}_2(10611)\text{-C}_{72}(\text{Ad})$ at different addition positions with various spin multiplicity (m) at the B3LYP/6-31G(d)~MWB48 level of theory.

Isomers ^a	Addition positions	m	TE	ZPVE	G	ν
^S A	C5-C8	1	-3198.752344	0.666470	-3198.145086	44.9
^T A	C5-C8	3	-3198.751226	0.666039	-3198.145598	44.4
^S B	C14-C12	1	-3198.750049	0.666735	-3198.142514	51.9
^T C	C5-C1	3	-3198.747187	0.665546	-3198.142107	46.7
^T B	C14-C12	3	-3198.746753	0.666362	-3198.140705	50.7
^T D	C8-C4	3	-3198.745931	0.665992	-3198.140482	43.6
^S C	C5-C1	1	-3198.745288	0.665861	-3198.138744	44.5
^S D	C8-C4	1	-3198.745127	0.666088	-3198.138471	43.7
^T E	C4-C2	3	-3198.738100	0.665897	-3198.132155	56.6
^S F	C5-C11	1	-3198.736440	0.665707	-3198.130399	40.8
^S G	C10-C14	1	-3198.736153	0.666089	-3198.129777	36.8
^S E	C4-C2	1	-3198.736119	0.665975	-3198.129066	53.3
^T F	C5-C11	3	-3198.735980	0.665445	-3198.131401	43.3
^T G	C10-C14	3	-3198.733345	0.665540	-3198.128660	36.3
^T H	C8-C16	3	-3198.729105	0.665758	-3198.122803	53.7
^S H	C8-C16	1	-3198.728660	0.666072	-3198.122304	47.4
^T I	C4-C10	3	-3198.725761	0.665214	-3198.121261	32.4
^T J	C14-C26	3	-3198.723381	0.665515	-3198.118229	25.4
^S I	C4-C10	1	-3198.721197	0.664842	-3198.116822	32.5
^S J	C14-C26	1	-3198.716527	0.665398	-3198.111444	27.9
^S K	C10-C18	1	-3198.714383	0.665408	-3198.109034	40.8
^T K	C10-C18	3	-3198.714104	0.665054	-3198.110226	37.1

^a The superscripts S and T represent the singlet and triplet structures, respectively.

Table S10 Computed relative energies (REs, kcal/mol) with zero-point energy correction, relative Gibbs free energies (ΔG , kcal/mol) at 298.15 K, HOMO-LUMO energy gap (E_{gap} , eV), and equilibrium concentration distribution (ECD, 298.15 K) of the mono-adduct $\text{Pr}_2\text{@D}_2(10611)\text{-C}_{72}(\text{Ad})$ at different addition positions with various spin multiplicity (m) at the B3LYP/6-31G(d)~MWB48 level of theory.

Isomers ^a	Addition positions	m	REs	ΔG	E_{gap}	ECD ^b
^S A	C5-C8	1	0.00	0.00	1.12	35.22%
^T A	C5-C8	3	0.43	-0.32	0.84	60.07%
^S B	C14-C12	1	1.61	1.61	1.23	2.41%
^T C	C5-C1	3	2.66	1.87	0.84	1.58%
^T B	C14-C12	3	3.44	2.75	0.76	0.37%
^T D	C8-C4	3	3.72	2.89	0.84	0.29%
^S C	C5-C1	1	4.05	3.98	1.08	0.05%
^S D	C8-C4	1	4.29	4.15	1.09	0.01%
^T E	C4-C2	3	8.58	8.11	0.82	\
^S F	C5-C11	1	9.50	9.22	1.15	\
^S G	C10-C14	1	9.92	9.61	1.18	\
^S E	C4-C2	1	9.87	10.05	1.08	\
^T F	C5-C11	3	9.63	8.59	0.83	\
^T G	C10-C14	3	11.34	10.31	0.80	\
^T H	C8-C16	3	14.14	13.98	0.84	\
^S H	C8-C16	1	14.61	14.30	1.10	\
^T I	C4-C10	3	15.89	14.95	0.85	\
^T J	C14-C26	3	17.58	16.85	0.97	\
^S I	C4-C10	1	18.52	17.74	1.09	\
^S J	C14-C26	1	21.80	21.11	0.87	\
^S K	C10-C18	1	23.15	22.62	1.14	\
^T K	C10-C18	3	23.11	21.87	0.85	\

^a The superscripts S and T represent the singlet and triplet structures, respectively.

^b For a mixture consisting of n molecules, the mole fraction (x_i) of the isomer i can be computed through the partition function (q_i) and the ground-state energies (ΔE_i , 0 K), and the expression can be written as follows:

$$x_i = \frac{q_i \exp\left[\frac{-\Delta E_i}{RT}\right]}{\sum_{j=1}^n q_j \exp\left[\frac{-\Delta E_j}{RT}\right]}$$

where R is the gas constant, and T corresponds to the absolute temperature.

Geometries of stationary points

1. $\text{Pr}_2@D_2(10611)\text{-C}_{72}$ (B3LYP/6-31G(d)~MWB48)

singlet state:

C	-0.55678000	0.45925800	-4.45301200
C	0.55678000	-0.45925800	-4.45301200
C	-1.72111100	-0.24947000	-3.95616200
C	1.72111100	0.24947000	-3.95616200
C	-0.11762700	1.74723300	-3.92135400
C	0.11762700	-1.74723300	-3.92135400
C	-1.32361000	-1.61080000	-3.60951400
C	1.32361000	1.61080000	-3.60951400
C	-2.59171100	0.46802800	-3.09012800
C	2.59171100	-0.46802800	-3.09012800
C	-0.99441800	2.44330500	-2.99980100
C	0.99441800	-2.44330500	-2.99980100
C	-2.26969300	1.82700700	-2.67214600
C	2.26969300	-1.82700700	-2.67214600
C	-1.89943000	-2.26160100	-2.43376700
C	1.89943000	2.26160100	-2.43376700
C	-3.25292400	-0.19588900	-2.00354400
C	3.25292400	0.19588900	-2.00354400
C	-0.38193100	3.24151700	-1.98314000
C	0.38193100	-3.24151700	-1.98314000
C	1.05645500	3.18506600	-1.73934500
C	-1.05645500	-3.18506600	-1.73934500
C	-2.93499900	-1.55792000	-1.65690200
C	2.93499900	1.55792000	-1.65690200
C	-2.86350200	2.01648200	-1.37529200
C	2.86350200	-2.01648200	-1.37529200
C	-3.50645800	0.79076500	-0.98131500
C	3.50645800	-0.79076500	-0.98131500
C	-1.02369700	3.49360100	-0.72227000
C	1.02369700	-3.49360100	-0.72227000
C	-2.26096800	2.86824800	-0.39321100
C	2.26096800	-2.86824800	-0.39321100
C	1.26456800	3.49856500	-0.35413700
C	-1.26456800	-3.49856500	-0.35413700
C	-3.14097200	-1.92299700	-0.28711200
C	3.14097200	1.92299700	-0.28711200
C	0.00000000	3.68226200	0.28658400
C	0.00000000	-3.68226200	0.28658400
C	-2.32373200	-2.90533300	0.35362900
C	2.32373200	2.90533300	0.35362900

C	-3.62697500	0.43030300	0.39279600
C	3.62697500	-0.43030300	0.39279600
C	-3.51473900	-0.95150100	0.72190200
C	3.51473900	0.95150100	0.72190200
C	-2.50603200	2.57764000	0.98092400
C	2.50603200	-2.57764000	0.98092400
C	-3.21582600	1.38926600	1.37486300
C	3.21582600	-1.38926600	1.37486300
C	-0.20370300	3.31583000	1.65624700
C	0.20370300	-3.31583000	1.65624700
C	-2.16519300	-2.56388900	1.73891500
C	2.16519300	2.56388900	1.73891500
C	-2.96489700	-1.36708300	1.98298000
C	2.96489700	1.36708300	1.98298000
C	-1.53134700	2.87592000	2.00277300
C	1.53134700	-2.87592000	2.00277300
C	0.93732700	2.80040400	2.43330100
C	-0.93732700	-2.80040400	2.43330100
C	-2.74389300	0.98161800	2.67171700
C	2.74389300	-0.98161800	2.67171700
C	-2.60318400	-0.42759500	2.99923200
C	2.60318400	0.42759500	2.99923200
C	-1.75243100	1.96556700	3.08940200
C	1.75243100	-1.96556700	3.08940200
C	0.68285500	1.96995100	3.60929500
C	-0.68285500	-1.96995100	3.60929500
C	-1.55190000	-0.81189700	3.92099500
C	1.55190000	0.81189700	3.92099500
C	-0.68592700	1.59812900	3.95593400
C	0.68592700	-1.59812900	3.95593400
C	-0.68244900	0.23503300	4.45289800
C	0.68244900	-0.23503300	4.45289800
Pr	0.00000000	0.00000000	2.06324600
Pr	0.00000000	0.00000000	-2.06166700

triplet state:

C	-0.55164200	0.45889300	-4.46723800
C	0.55164200	-0.45889300	-4.46723800
C	-1.70621600	-0.23269200	-3.94077000
C	1.70621600	0.23269200	-3.94077000
C	-0.11090200	1.73387100	-3.90488600
C	0.11090200	-1.73387100	-3.90488600
C	-1.32043800	-1.60165900	-3.59499000
C	1.32043800	1.60165900	-3.59499000
C	-2.58423600	0.47988500	-3.08605500

C	2.58423600	-0.47988500	-3.08605500
C	-0.98798800	2.43958900	-2.99464800
C	0.98798800	-2.43958900	-2.99464800
C	-2.27009700	1.83929900	-2.66974400
C	2.27009700	-1.83929900	-2.66974400
C	-1.90219400	-2.25514900	-2.43154900
C	1.90219400	2.25514900	-2.43154900
C	-3.24938500	-0.18511400	-1.99881800
C	3.24938500	0.18511400	-1.99881800
C	-0.37089200	3.23190700	-1.97355400
C	0.37089200	-3.23190700	-1.97355400
C	1.06510200	3.18651800	-1.73823500
C	-1.06510200	-3.18651800	-1.73823500
C	-2.94051400	-1.55290900	-1.65642600
C	2.94051400	1.55290900	-1.65642600
C	-2.86844200	2.03240100	-1.37724200
C	2.86844200	-2.03240100	-1.37724200
C	-3.50588000	0.79903600	-0.98203100
C	3.50588000	-0.79903600	-0.98203100
C	-1.02167300	3.50019800	-0.71580600
C	1.02167300	-3.50019800	-0.71580600
C	-2.26153300	2.87584900	-0.39357800
C	2.26153300	-2.87584900	-0.39357800
C	1.27210200	3.49737100	-0.35331000
C	-1.27210200	-3.49737100	-0.35331000
C	-3.14488800	-1.91570000	-0.29145300
C	3.14488800	1.91570000	-0.29145300
C	0.00000000	3.68307600	0.29105700
C	0.00000000	-3.68307600	0.29105700
C	-2.32425000	-2.90539000	0.35299300
C	2.32425000	2.90539000	0.35299300
C	-3.63193600	0.43541500	0.39314900
C	3.63193600	-0.43541500	0.39314900
C	-3.52003800	-0.94810600	0.71542200
C	3.52003800	0.94810600	0.71542200
C	-2.50576700	2.57826200	0.98167100
C	2.50576700	-2.57826200	0.98167100
C	-3.22700100	1.39218100	1.37695300
C	3.22700100	-1.39218100	1.37695300
C	-0.20345200	3.31931600	1.65603300
C	0.20345200	-3.31931600	1.65603300
C	-2.16677000	-2.56723700	1.73794800
C	2.16677000	2.56723700	1.73794800
C	-2.95289600	-1.36470500	1.97337100

C	2.95289600	1.36470500	1.97337100
C	-1.53204900	2.87110500	1.99846100
C	1.53204900	-2.87110500	1.99846100
C	0.93614400	2.79786600	2.43148500
C	-0.93614400	-2.79786600	2.43148500
C	-2.75141800	0.98181100	2.66969300
C	2.75141800	-0.98181100	2.66969300
C	-2.59723600	-0.42559500	2.99455100
C	2.59723600	0.42559500	2.99455100
C	-1.75410200	1.95735600	3.08606800
C	1.75410200	-1.95735600	3.08606800
C	0.68073700	1.96080200	3.59498300
C	-0.68073700	-1.96080200	3.59498300
C	-1.53836200	-0.80742700	3.90513700
C	1.53836200	0.80742700	3.90513700
C	-0.68899800	1.57822700	3.94099400
C	0.68899800	-1.57822700	3.94099400
C	-0.67900500	0.23245300	4.46776300
C	0.67900500	-0.23245300	4.46776300
Pr	0.00000000	0.00000000	1.94359300
Pr	0.00000000	0.00000000	-1.94306400

2. $\text{Pr}_2@C_s(10528)\text{-C}_{72}$ (B3LYP/6-31G(d)~MWB48)

singlet state:

C	-4.22178600	-1.37214400	-0.01832100
C	-4.16789800	-0.53234700	1.18166700
C	-4.12771000	-0.49138800	-1.19046800
C	-4.05023700	0.87012900	0.80563700
C	-4.02103200	0.90932400	-0.70199600
C	-3.32667200	-2.52431200	0.17780200
C	-3.25455000	-1.15061000	2.13727500
C	-3.25846600	-0.92537700	-2.26237900
C	-3.16682400	1.89365800	-1.39402500
C	-3.14744400	1.71892800	1.57069600
C	-2.77447500	-2.41447300	1.54057200
C	-2.46527200	-2.17389600	-2.14219000
C	-2.43732000	-2.95666300	-0.90886700
C	-2.63124800	2.95163400	-0.59811500
C	-2.61531200	2.87376300	0.89102200
C	-2.43340200	0.05022000	-2.97045500
C	-2.36775900	-0.33437600	2.93764400
C	-2.38071700	1.45426800	-2.59535800
C	-2.35215200	1.14185000	2.70779200
C	-1.46411400	-2.94242900	1.87448500

C	-1.23459000	-1.98426000	-2.90662400
C	-1.22873100	-0.62934800	-3.42539100
C	-1.44279400	3.69090400	-1.00387500
C	-1.43364800	3.55491100	1.35259200
C	-1.18168400	-3.56769800	-0.54616300
C	-1.18406700	-0.98595900	3.44342000
C	-1.18731400	2.17111800	-2.94902900
C	-1.18556900	1.86160500	3.13426500
C	-0.70339900	4.07839300	0.19110800
C	-0.72527400	-3.63659300	0.84351200
C	-0.73135200	-2.26930400	2.90581700
C	-0.73147900	3.29892800	-2.15640000
C	-0.72871900	3.08888700	2.48451800
C	-0.00000600	1.49619800	-3.49064100
C	0.00000400	1.16487100	3.61658600
C	-0.00000500	0.08553800	-3.65599100
C	0.00000500	-0.22525100	3.77516100
C	-0.00000200	-2.65714900	-2.56916800
C	0.00000000	-3.49024500	-1.39891600
C	0.72872200	3.08888800	2.48451700
C	0.73146900	3.29892900	-2.15640200
C	0.73136200	-2.26930300	2.90581400
C	0.72527900	-3.63659300	0.84351000
C	0.70339500	4.07839400	0.19110600
C	1.18557500	1.86160600	3.13426200
C	1.18730300	2.17112000	-2.94903200
C	1.18407700	-0.98595700	3.44341600
C	1.18168600	-3.56769700	-0.54616600
C	1.43364700	3.55491200	1.35258900
C	1.44278700	3.69090600	-1.00387800
C	1.22872100	-0.62934700	-3.42539500
C	1.23458300	-1.98425900	-2.90662800
C	1.46412100	-2.94242700	1.87448000
C	2.35215800	1.14185300	2.70778600
C	2.38070800	1.45427000	-2.59536400
C	2.36776700	-0.33437300	2.93763700
C	2.43339300	0.05022300	-2.97046100
C	2.61531100	2.87376600	0.89101500
C	2.63124200	2.95163700	-0.59812200
C	2.43732100	-2.95666000	-0.90887400
C	2.46526800	-2.17389300	-2.14219600
C	2.77448200	-2.41447000	1.54056400
C	3.14744700	1.71893100	1.57068700
C	3.16681800	1.89366200	-1.39403400

C	3.25845900	-0.92537300	-2.26238700
C	3.25455800	-1.15060600	2.13726700
C	3.32667600	-2.52430900	0.17779300
C	4.02102800	0.90932800	-0.70200700
C	4.05023900	0.87013400	0.80562700
C	4.12770600	-0.49138300	-1.19047900
C	4.16790300	-0.53234300	1.18165600
C	4.22178800	-1.37214000	-0.01833300
Pr	1.86501000	-0.29535900	-0.05578600
Pr	-1.86500900	-0.29535800	-0.05579100
triplet state:			
C	-4.23270400	-1.36303900	-0.02530800
C	-4.17555300	-0.53258500	1.17769800
C	-4.13597900	-0.48175500	-1.19503900
C	-4.03376800	0.86869200	0.79728500
C	-4.02152500	0.91591700	-0.70729800
C	-3.32688600	-2.51573400	0.16830800
C	-3.26422800	-1.15135500	2.13336700
C	-3.25431700	-0.91136800	-2.26229800
C	-3.16118900	1.89462400	-1.39246500
C	-3.14160900	1.72243300	1.56910000
C	-2.77902000	-2.41484200	1.53444900
C	-2.46824600	-2.16283200	-2.15247400
C	-2.44203800	-2.94572000	-0.91809000
C	-2.62595200	2.95473700	-0.59510500
C	-2.62173700	2.88382500	0.89613300
C	-2.43347200	0.06145800	-2.97577900
C	-2.37013600	-0.33558100	2.92963600
C	-2.38060400	1.46470200	-2.59535100
C	-2.35006100	1.14198400	2.70781800
C	-1.46762900	-2.94166800	1.87049600
C	-1.23876600	-1.97493600	-2.92310700
C	-1.23305200	-0.62175600	-3.44348900
C	-1.43923300	3.69116900	-0.99769500
C	-1.43871100	3.56526500	1.35964800
C	-1.18205100	-3.55393900	-0.55442600
C	-1.18231500	-0.98525700	3.42473900
C	-1.18702600	2.18434300	-2.94378000
C	-1.18666800	1.86160300	3.14383600
C	-0.70338800	4.08129400	0.19945200
C	-0.72660900	-3.61980100	0.83259700
C	-0.73110800	-2.28068600	2.90920800
C	-0.73058700	3.32081600	-2.16212100
C	-0.72953500	3.07848100	2.47785300

C	-0.00002500	1.50020700	-3.46378900
C	0.00001200	1.17214500	3.63810100
C	-0.00001900	0.08924000	-3.65299900
C	0.00001900	-0.22176700	3.75377000
C	-0.00000100	-2.63267300	-2.57393800
C	0.00000800	-3.46632700	-1.40254800
C	0.72952900	3.07848800	2.47784500
C	0.73053300	3.32082200	-2.16212800
C	0.73115600	-2.28067800	2.90920000
C	0.72664900	-3.61979400	0.83259000
C	0.70335000	4.08130000	0.19944500
C	1.18668100	1.86161400	3.14382500
C	1.18697400	2.18435300	-2.94379000
C	1.18235700	-0.98524500	3.42472500
C	1.18207700	-3.55392700	-0.55443800
C	1.43868900	3.56527700	1.35963400
C	1.43918700	3.69118200	-0.99770900
C	1.23302200	-0.62174600	-3.44350300
C	1.23875300	-1.97492600	-2.92312100
C	1.46767200	-2.94165400	1.87048100
C	2.35007800	1.14200700	2.70779600
C	2.38056100	1.46472200	-2.59537200
C	2.37016900	-0.33555800	2.92961300
C	2.43343900	0.06148000	-2.97580300
C	2.62171800	2.88384900	0.89610700
C	2.62591600	2.95476100	-0.59513000
C	2.44205600	-2.94569800	-0.91811600
C	2.46824200	-2.16280900	-2.15249900
C	2.77905800	-2.41481800	1.53442200
C	3.14160900	1.72246300	1.56907000
C	3.16115200	1.89465000	-1.39249400
C	3.25429700	-0.91133600	-2.26232800
C	3.26426300	-1.15132600	2.13333800
C	3.32691400	-2.51570600	0.16827400
C	4.02150300	0.91595300	-0.70733600
C	4.03376800	0.86872900	0.79724500
C	4.13596400	-0.48171600	-1.19507900
C	4.17557600	-0.53254700	1.17765900
C	4.23272000	-1.36300200	-0.02535000
Pr	1.84886900	-0.31721400	-0.04440500
Pr	-1.84886100	-0.31720800	-0.04442200

3. Pr₂@C₁(10610)-C₇₂ (B3LYP/6-31G(d)~MWB48)

singlet state:

C	-4.53624000	0.17669300	-0.32536600
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C	-4.31940400	-1.23357200	-0.40473200
C	-4.13198600	0.63832900	1.00984400
C	-3.95299500	0.78930500	-1.51152900
C	-3.76500800	-0.55293200	1.75848500
C	-3.79489500	-1.71424900	0.87945400
C	-3.60087300	-1.51226600	-1.64834700
C	-3.38158400	1.86987800	1.16867500
C	-3.33694100	-0.25505700	-2.34433100
C	-3.28665600	2.00752900	-1.35081000
C	-3.12880000	2.63673500	-0.03801500
C	-2.77542900	-0.46345300	2.76590300
C	-2.70872800	-2.68632800	0.92427500
C	-2.39286800	1.96326200	2.26146400
C	-2.60843900	-2.51586400	-1.60254800
C	-2.15002900	0.79279000	3.06536300
C	-2.13060200	2.33714400	-2.16990900
C	-2.24212300	-3.18961100	-0.35454500
C	-1.98274900	3.49128500	-0.14301500
C	-2.04005500	-0.01725100	-3.00804700
C	-1.81646200	-1.51594100	2.94992700
C	-1.72781400	-2.61230500	2.02261100
C	-1.40612900	3.35208400	-1.46944000
C	-1.45830500	1.32437500	-2.95090100
C	-1.31817600	2.90506100	2.15692800
C	-1.42144500	-2.38611600	-2.40826800
C	-1.12304300	3.67105300	0.95011600
C	-0.83688200	0.50067900	3.58334500
C	-1.12918600	-1.16517200	-3.10790500
C	-0.63256700	-0.92180000	3.52593300
C	-0.88662600	-3.62824800	-0.51938800
C	-0.37557400	-3.15973900	-1.77858900
C	-0.42755900	-3.20597100	1.85492300
C	-0.01357400	2.62748900	2.70619200
C	-0.02886900	3.52044200	-1.66930300
C	0.29351700	3.83796100	0.73839100
C	0.24376400	1.40644200	3.37708900
C	-0.01447700	-3.71405000	0.57885800
C	-0.01014200	1.51886500	-3.16374400
C	0.65885600	-1.47361600	3.28681500
C	0.24942500	-0.94129500	-3.36867300
C	0.98953800	3.19231600	1.81301800
C	0.83583300	3.82112200	-0.55994500
C	0.65884200	2.62643400	-2.55209500
C	0.74343700	-2.65491000	2.49414800

C	0.79664500	0.37942400	-3.44880700
C	1.01259000	-2.88265000	-1.97996800
C	1.38923100	-3.47173500	0.39823900
C	1.55840500	0.85112700	3.26070500
C	1.29397900	-1.83732300	-2.91423500
C	1.77521400	-0.56954000	3.25302200
C	1.87991500	-2.86224500	1.62420700
C	2.10745100	3.19185500	-0.78814300
C	2.02070500	2.50203600	-2.06996000
C	2.27375700	2.60209900	1.61896300
C	1.94435500	-3.11958300	-0.87247400
C	2.20099800	0.31037700	-3.11588200
C	2.58792800	1.47608800	2.47569700
C	2.50564500	-1.07710700	-2.83682200
C	2.89162400	2.65491100	0.28093600
C	2.97500700	-0.84449400	2.50524900
C	2.83027900	1.37679100	-2.36774100
C	3.03581500	-2.01741900	1.63643900
C	3.52128700	0.44911800	2.08681800
C	3.19979500	-2.39271400	-0.85132200
C	3.49409800	-1.41282300	-1.87816100
C	3.87934600	1.63510000	-0.07944300
C	3.79745500	-1.90984600	0.40862600
C	3.88639300	1.04197800	-1.42820500
C	4.23972300	0.56612500	0.85815100
C	4.27316500	-0.34450200	-1.28723700
C	4.48361600	-0.65498900	0.10178100
Pr	-1.94683100	-0.22024100	-0.20120300
Pr	1.98401100	-0.09781900	-0.00348300

triplet state:

C	-4.51864200	0.13871400	-0.43523700
C	-4.28721000	-1.26977900	-0.50226200
C	-4.17943300	0.61643500	0.90540100
C	-3.90094000	0.74469500	-1.60719000
C	-3.81997800	-0.57332700	1.67494400
C	-3.80561100	-1.74073200	0.79650600
C	-3.52987400	-1.54916900	-1.71389300
C	-3.42983900	1.86016600	1.06860900
C	-3.25390300	-0.29553700	-2.40901200
C	-3.26261200	1.97356600	-1.45270700
C	-3.13717300	2.61103700	-0.13765600
C	-2.83230500	-0.46384300	2.68988300
C	-2.70922900	-2.70673800	0.86676200
C	-2.45522200	1.96550800	2.17747900

C	-2.54200200	-2.54469600	-1.65363600
C	-2.21852300	0.80036600	2.99450700
C	-2.09749800	2.30686400	-2.25002800
C	-2.20213400	-3.20997400	-0.39502400
C	-1.99860000	3.48079100	-0.22560300
C	-1.95709300	-0.05853000	-3.03472600
C	-1.86669200	-1.50805300	2.90165100
C	-1.75146900	-2.61328700	1.98516200
C	-1.39790200	3.33831700	-1.53989500
C	-1.39423500	1.29342700	-2.99860400
C	-1.37920000	2.90353100	2.08064900
C	-1.34705200	-2.42478300	-2.44546000
C	-1.16411900	3.67807900	0.88530500
C	-0.91379300	0.52053100	3.54113500
C	-1.04469900	-1.20615900	-3.13988200
C	-0.69879500	-0.89880500	3.49532100
C	-0.84523300	-3.65293700	-0.53500800
C	-0.31293600	-3.20091200	-1.79485600
C	-0.44307000	-3.18299500	1.84025400
C	-0.07838900	2.63711700	2.66028500
C	-0.01805300	3.48753800	-1.69828300
C	0.25704400	3.86003600	0.71166900
C	0.17168700	1.42903500	3.35860400
C	0.00278400	-3.70801000	0.58211000
C	0.05258800	1.49227800	-3.19379500
C	0.60586200	-1.43840700	3.29223700
C	0.33296400	-0.97049400	-3.39650000
C	0.93548300	3.22092900	1.80426400
C	0.82321200	3.80851200	-0.57349700
C	0.70090000	2.60632600	-2.57266900
C	0.71503000	-2.62175400	2.50383600
C	0.86922900	0.35657100	-3.46922400
C	1.06853300	-2.88912600	-1.95409500
C	1.41001600	-3.46464800	0.43882400
C	1.49316800	0.88746200	3.29022600
C	1.36829700	-1.84950600	-2.89363800
C	1.71756300	-0.53255600	3.29293000
C	1.86904200	-2.84312700	1.67272300
C	2.10411700	3.19498200	-0.77918100
C	2.05136100	2.50618400	-2.06523100
C	2.22390700	2.62586500	1.63650000
C	1.98411500	-3.10597000	-0.81957200
C	2.26230200	0.30228600	-3.08428700
C	2.52732800	1.51098100	2.50605000

C	2.57314100	-1.08024400	-2.78918800
C	2.86657800	2.66618600	0.30919600
C	2.92723600	-0.80422000	2.55577500
C	2.87187100	1.37739600	-2.33372600
C	3.01610700	-1.97993900	1.70022500
C	3.47022200	0.48612200	2.13464600
C	3.23635600	-2.37932800	-0.77845700
C	3.54665800	-1.40009900	-1.80815800
C	3.86810000	1.65587900	-0.02305200
C	3.79650700	-1.87535800	0.48771700
C	3.90012900	1.05440900	-1.36549200
C	4.22321000	0.59887200	0.92733500
C	4.30356400	-0.32775900	-1.20960700
C	4.48497400	-0.61886300	0.18629100
Pr	-1.91819800	-0.19501500	-0.07821100
Pr	1.93470100	-0.11081500	-0.01094300

4. $\text{Pr}_2@C_8(10616)\text{-}C_{72}$ (B3LYP/3-21G~MWB48)

singlet state:

C	4.37459600	-0.38506400	-1.13808400
C	4.27524900	-1.42718700	-0.12136500
C	4.23994500	0.92832600	-0.47838800
C	4.14140500	-0.79390100	1.18837000
C	4.10425200	0.67757100	0.98840900
C	3.51933900	-0.77257400	-2.26326400
C	3.33520200	-2.46726600	-0.59202000
C	3.40724400	1.94591300	-1.12614200
C	3.21914200	-1.39020100	2.10609300
C	3.20337600	1.51075400	1.80868400
C	2.85745900	-2.05451500	-1.94039000
C	2.75407500	0.23811000	-2.90242400
C	2.75560700	1.61841400	-2.39310500
C	2.71950800	2.87356600	-0.27619600
C	2.67816700	2.69824900	1.18841800
C	2.40615200	-3.05316000	0.35599000
C	2.42877800	-2.57758800	1.73421200
C	2.41550400	-0.57416700	3.00141300
C	2.38887300	0.87389700	2.88579200
C	1.46928000	-2.29781000	-2.34924300
C	1.43655900	-0.05281000	-3.46452500
C	1.47015100	2.21309700	-2.76320900
C	1.46577400	3.51133100	-0.68374000
C	1.45648500	3.33123500	1.66458600
C	1.20559000	-2.54612800	2.52468200
C	1.21277500	-1.32768900	3.32294300

C	1.14506600	-3.53176800	-0.16016500
C	1.19434800	1.53675900	3.34730200
C	0.73892900	-1.29294300	-3.14907600
C	0.72591600	1.20636600	-3.50221400
C	0.77853800	3.12422100	-1.88757700
C	0.73077100	3.85834700	0.51823100
C	0.70250000	-3.17994200	-1.51147400
C	0.74738600	2.78273800	2.75507800
C	-0.00322500	0.77008900	3.70257100
C	-0.01400000	-0.65320300	3.64195700
C	-0.02975500	-3.08766500	2.01961200
C	-0.03059300	-3.63601400	0.68019600
C	-0.71553600	2.78641500	2.72917600
C	-0.74393700	-3.16287800	-1.52039500
C	-0.68181100	3.90391800	0.51175800
C	-0.71605200	3.14457100	-1.88442200
C	-0.67255300	1.20584200	-3.46792500
C	-0.74702500	-1.29803100	-3.17098900
C	-1.18587400	1.54046300	3.30420300
C	-1.20178100	-3.48244200	-0.16639100
C	-1.25140900	-1.29923200	3.29130600
C	-1.26279700	-2.52460900	2.50527100
C	-1.41497500	3.36474100	1.65016600
C	-1.40764100	3.56535000	-0.69889700
C	-1.41153500	2.22178100	-2.74723000
C	-1.41342600	-0.03851800	-3.45165700
C	-1.49547600	-2.28827100	-2.37477300
C	-2.39939300	0.90967200	2.85932700
C	-2.44647300	-0.53819700	2.97474000
C	-2.49001400	-2.54868700	1.71987400
C	-2.47016000	-3.01721900	0.33554000
C	-2.63399000	2.73163300	1.15908000
C	-2.66148700	2.90684000	-0.29572900
C	-2.71607300	1.65948200	-2.41212500
C	-2.73141400	0.27409900	-2.91832900
C	-2.88061100	-2.00980000	-1.95847200
C	-3.19556900	1.55796300	1.78270000
C	-3.26251400	-1.34865000	2.08121800
C	-3.36111300	1.98559700	-1.14904200
C	-3.39119100	-2.42064800	-0.61889400
C	-3.50501500	-0.72101900	-2.27249000
C	-4.09323600	0.73302800	0.95255700
C	-4.15455400	-0.73544100	1.14461000
C	-4.21880400	0.98050800	-0.51237900

C	-4.34625200	-1.38251700	-0.16448700
C	-4.39675600	-0.32779500	-1.16706600
Pr	-1.94069600	-0.25250000	-0.12199000
Pr	1.94578900	-0.24838200	-0.16090200
triplet state:			
C	4.38560100	-0.34824400	-1.15511400
C	4.31305300	-1.40151300	-0.15211600
C	4.22397300	0.95681500	-0.49300100
C	4.14709000	-0.76811700	1.15936500
C	4.09393400	0.70179600	0.97033100
C	3.50903100	-0.73077900	-2.26959100
C	3.36342200	-2.43794800	-0.61928000
C	3.38033000	1.97129900	-1.12962400
C	3.23975500	-1.37779800	2.08404300
C	3.19645800	1.52789000	1.79919100
C	2.86830800	-2.01997700	-1.96036400
C	2.74237600	0.27216100	-2.91160500
C	2.73420500	1.65413700	-2.39698800
C	2.68900800	2.89478000	-0.27459800
C	2.65582200	2.71348000	1.18566000
C	2.43891900	-3.03567000	0.32867600
C	2.45884200	-2.57008400	1.71244100
C	2.42933600	-0.56853000	2.98194700
C	2.39195200	0.88018800	2.87448300
C	1.48328700	-2.27907800	-2.37514400
C	1.42612000	-0.02702800	-3.46104400
C	1.44218000	2.23504800	-2.74797300
C	1.43774100	3.54500800	-0.67737200
C	1.43581700	3.34341900	1.67224400
C	1.23262800	-2.54591600	2.49993500
C	1.23019200	-1.32722200	3.29684100
C	1.17312300	-3.50345200	-0.18290600
C	1.18873500	1.52479700	3.33108300
C	0.74383100	-1.27757700	-3.17026900
C	0.69994100	1.22613200	-3.48391000
C	0.74832000	3.14738200	-1.87432100
C	0.70601100	3.88202500	0.53164200
C	0.72323700	-3.16185200	-1.53420400
C	0.73055400	2.77468300	2.75323300
C	-0.00153800	0.75495600	3.70516400
C	-0.00167400	-0.66789100	3.63383600
C	-0.00133000	-3.09562000	2.00154600
C	-0.00083100	-3.63767900	0.65965400
C	-0.73216000	2.77497900	2.75271300

C	-0.72289000	-3.16157400	-1.53479700
C	-0.70526600	3.88207500	0.53102400
C	-0.74578700	3.14755800	-1.87501200
C	-0.69661400	1.22636500	-3.48469400
C	-0.74157600	-1.27731800	-3.17098900
C	-1.19127100	1.52523500	3.33032600
C	-1.17403900	-3.50300600	-0.18389800
C	-1.23348000	-1.32684600	3.29574800
C	-1.23561800	-2.54552800	2.49882600
C	-1.43625500	3.34375300	1.67101300
C	-1.43605200	3.54524300	-0.67855600
C	-1.43917100	2.23552900	-2.74933500
C	-1.42319000	-0.02660600	-3.46246300
C	-1.48195000	-2.27845100	-2.37625200
C	-2.39428500	0.88098500	2.87254600
C	-2.43216100	-0.56779600	2.97986300
C	-2.46123800	-2.56945200	1.71042900
C	-2.44032000	-3.03515000	0.32662700
C	-2.65611600	2.71428300	1.18340800
C	-2.68785000	2.89549600	-0.27685400
C	-2.73156900	1.65490300	-2.39930300
C	-2.73975900	0.27297200	-2.91393200
C	-2.86712300	-2.01903500	-1.96259100
C	-3.19775900	1.52890900	1.79660000
C	-3.24233800	-1.37695300	2.08148900
C	-3.37848800	1.97204700	-1.13246700
C	-3.36371800	-2.43703500	-0.62211100
C	-3.50691400	-0.72956700	-2.27219800
C	-4.09487100	0.70300900	0.96703100
C	-4.14899200	-0.76701900	1.15607800
C	-4.22293100	0.95790600	-0.49650200
C	-4.31352300	-1.40030400	-0.15565400
C	-4.38423100	-0.34693400	-1.15860500
Pr	-1.91988200	-0.26044500	-0.12920300
Pr	1.92006000	-0.25989700	-0.13107500

5. Pr₂@C₂(10626)-C₇₂ (B3LYP/3-21G~MWB48)

singlet state:

C	-4.66003700	0.08458100	0.02393700
C	-4.33453300	-0.15982500	-1.38723800
C	-4.34264400	-1.12805600	0.77694800
C	-4.16202500	1.43132100	0.38947900
C	-3.79515800	-2.11510500	-0.18119400
C	-3.72348300	-1.50003500	-1.52369200
C	-3.71210600	1.02892900	-1.92966600

C	-3.64290000	-0.95501300	2.02977300
C	-3.58755300	2.03911000	-0.85610400
C	-3.43218500	1.59032100	1.65992800
C	-3.23316300	0.38450300	2.48433200
C	-2.75994700	-3.01261300	0.21417800
C	-2.59916600	-1.89749400	2.43026200
C	-2.52717300	-1.65969100	-2.35109700
C	-2.64796800	0.84669900	-2.85169600
C	-2.19329500	-2.95564300	1.57723300
C	-2.40386900	2.90802800	-0.82646000
C	-2.37959200	2.57465500	1.68647900
C	-1.98913800	0.21507500	3.24588900
C	-2.10279300	-0.50332900	-3.11588700
C	-1.59266200	-1.18302900	3.19805300
C	-1.68393100	-3.33813700	-0.69776400
C	-1.93212300	3.30081300	0.47276900
C	-1.47933700	-2.64808500	-1.95790900
C	-1.56932500	1.80118600	-2.94173200
C	-1.41772700	2.84608700	-1.94227000
C	-1.22188500	2.45302800	2.55683600
C	-0.80124600	-3.36411900	1.52639800
C	-0.99913700	1.24905500	3.30889500
C	-0.72658100	-0.32754800	-3.51686600
C	-0.53526100	-3.70931200	0.13955200
C	-0.55504000	3.69717200	0.68624200
C	-0.40887900	1.09750800	-3.45905900
C	-0.19705200	-1.55710700	3.14855800
C	-0.10141300	3.17394100	1.95850100
C	-0.10342300	-2.51415200	-2.47812400
C	0.23275100	-2.65349300	2.26261400
C	-0.08057800	3.32851500	-1.71631000
C	0.26680700	-1.32968500	-3.26133500
C	0.35616300	0.85672100	3.54915600
C	0.34464700	3.76214300	-0.40243900
C	0.73823000	-3.64022300	-0.37833400
C	0.75124700	-0.54731600	3.50542800
C	0.92004400	1.55833500	-3.19306000
C	0.97331700	-3.15028500	-1.72584700
C	1.08109800	2.72586300	-2.37607800
C	1.26342900	2.77032100	2.16961000
C	1.47239200	1.66194300	3.08270900
C	1.62579800	-2.67800900	1.76180200
C	1.73815400	3.41617900	-0.21312100
C	1.88330100	-3.30193400	0.47661100

C	1.63653000	-0.85725300	-3.23448200
C	2.13903200	-0.61974900	3.10205300
C	1.95827500	0.56397200	-3.18025900
C	2.22091800	2.81735000	-1.47368900
C	2.22762400	2.94897200	1.05419300
C	2.34903500	-2.70196400	-1.75947300
C	2.60203000	0.77336600	2.93103200
C	2.63335800	-1.68709800	2.25606500
C	2.69437100	-1.56646700	-2.54025900
C	2.94021900	-2.85661800	-0.40668500
C	3.20038900	0.74382200	-2.43280600
C	3.31277500	1.87987900	-1.50335900
C	3.43048400	2.12847300	1.01883100
C	3.70673300	-0.60208600	-2.08841900
C	3.63274500	1.06814000	2.01368200
C	3.83336400	-1.40655600	1.44699700
C	3.93111700	-1.92587900	0.05798000
C	4.03752900	1.65646600	-0.24865400
C	4.38666900	-0.82122200	-0.82868800
C	4.37310300	-0.02588100	1.40742500
C	4.66652300	0.34783500	0.02362700
Pr	-2.07434300	0.03545200	-0.07361000
Pr	2.08188200	-0.11988900	0.00710200
triplet state:			
C	-4.66949700	-0.20393600	-0.01703400
C	-4.36246700	0.10701400	1.38031400
C	-4.35214000	0.97902300	-0.81872300
C	-4.10108000	-1.52993900	-0.33343400
C	-3.85063100	2.02667400	0.10156400
C	-3.77273700	1.46226000	1.46525800
C	-3.67881300	-1.03267700	1.95750100
C	-3.66192900	0.78744400	-2.06660800
C	-3.51241500	-2.07136400	0.92554300
C	-3.36887900	-1.72276000	-1.59324700
C	-3.20877200	-0.55501700	-2.47234800
C	-2.84466400	2.94142500	-0.32686800
C	-2.64108400	1.74485600	-2.49883800
C	-2.58248900	1.68805200	2.28978700
C	-2.62900500	-0.79171600	2.87915400
C	-2.27038000	2.84171600	-1.68094600
C	-2.31872500	-2.91673000	0.93273000
C	-2.29606200	-2.68599400	-1.58810600
C	-1.96885300	-0.38029800	-3.22883500
C	-2.12522200	0.57702900	3.10261400

C	-1.61031400	1.03445600	-3.23318300
C	-1.78132600	3.33894000	0.57922700
C	-1.83396900	-3.34968900	-0.34918200
C	-1.55606700	2.67749900	1.84729700
C	-1.52586200	-1.71713800	3.00789400
C	-1.34517900	-2.79610300	2.05296100
C	-1.14576700	-2.57784100	-2.47112400
C	-0.88292500	3.27058900	-1.63355900
C	-0.95342300	-1.39218900	-3.25974400
C	-0.74491000	0.45234300	3.51720600
C	-0.63651700	3.69752700	-0.26079100
C	-0.44751300	-3.72245900	-0.54619400
C	-0.38933000	-0.96455100	3.51028500
C	-0.22844500	1.45603200	-3.21366200
C	-0.00578900	-3.24162100	-1.83833900
C	-0.16943900	2.59802300	2.36650200
C	0.16914700	2.59742100	-2.36717900
C	0.00639000	-3.24107700	1.83923200
C	0.22832900	1.45694500	3.21333500
C	0.38955200	-0.96542900	-3.50991900
C	0.44816300	-3.72224000	0.54722300
C	0.63604400	3.69764800	0.25983100
C	0.74495200	0.45149500	-3.51723600
C	0.95372000	-1.39113300	3.26014700
C	0.88253100	3.27119000	1.63273300
C	1.14626400	-2.57695400	2.47183500
C	1.34570900	-2.79643200	-2.05215200
C	1.52621100	-1.71768600	-3.00734100
C	1.55576000	2.67722400	-1.84797400
C	1.83457100	-3.34924900	0.35009400
C	1.78089600	3.33900100	-0.58008200
C	1.61027100	1.03560100	3.23296000
C	2.12524700	0.57649900	-3.10265500
C	1.96898500	-0.37910600	3.22893200
C	2.29654400	-2.68511100	1.58880700
C	2.31929700	-2.91657900	-0.93192300
C	2.27005900	2.84251400	1.68020800
C	2.62925800	-0.79209300	-2.87889800
C	2.58237600	1.68786100	-2.29018300
C	2.64093300	1.74594800	2.49838500
C	2.84423800	2.94176600	0.32608500
C	3.20891800	-0.55382400	2.47243900
C	3.36929800	-1.72176400	1.59371500
C	3.51301800	-2.07113400	-0.92499800

C	3.66183400	0.78856700	2.06632500
C	3.67917900	-1.03262700	-1.95720400
C	3.77259400	1.46240000	-1.46558200
C	3.85045500	2.02722800	-0.10208900
C	4.10154000	-1.52918100	0.33385700
C	4.35209100	0.97986500	0.81844200
C	4.36263600	0.10731900	-1.38033900
C	4.66972000	-0.20320500	0.01708400
Pr	-2.01341900	-0.00331200	0.06735500
Pr	2.01300100	-0.00386200	-0.06745500

6. Pr₂@C₁(10557)-C₇₂ (B3LYP/3-21G~MWB48)

singlet state :

C	4.41218900	0.42337600	0.37025700
C	4.45009600	-0.04977400	-1.00961600
C	3.88510900	1.76759800	0.64055200
C	4.09764500	-1.45522900	-1.21778000
C	3.95218400	-0.48261900	1.48406300
C	3.70661800	0.72932500	-2.03212700
C	3.58703900	-2.35351600	-0.15944400
C	3.36100300	2.60426600	-0.40828300
C	3.50736100	-1.87368700	1.23743200
C	3.18612300	1.73531400	1.91981500
C	3.20282300	2.03155900	-1.74518500
C	3.18450200	-1.53997900	-2.35530100
C	3.16250900	0.36973100	2.41419800
C	2.85525900	-0.20325200	-2.82007400
C	2.42330600	-3.05157600	-0.73411000
C	2.20665600	3.45978900	-0.15934700
C	2.15457000	-2.48447900	-2.06632600
C	2.11000600	2.61974400	2.17921600
C	2.36249700	-2.33195100	1.99843200
C	1.92166800	2.45083100	-2.27463000
C	1.99982300	-0.10765100	3.13725800
C	1.62110000	3.50004100	1.13167400
C	1.48443800	0.12040800	-3.15030300
C	1.69093100	-1.50397400	3.01837100
C	1.32835800	3.40949800	-1.32034000
C	1.34467000	-3.24657900	1.46764500
C	1.31984300	-3.53280800	0.06408500
C	1.06846300	1.53324600	-2.99789100
C	0.97783700	2.18992900	2.98394900
C	0.89583000	0.83892100	3.46450100
C	0.80495100	-2.26687700	-2.53320500
C	0.18311700	3.64221600	1.29917400

C	0.44372000	-0.94605900	-3.08846500
C	0.33771500	-1.99198700	3.17371400
C	0.09503100	-3.03273300	2.19697500
C	-0.20606600	2.89749300	2.50605000
C	-0.08764600	3.52866500	-1.19094200
C	0.05048200	-3.66537200	-0.57884200
C	-0.20027500	-3.05338500	-1.89110200
C	-0.31377900	1.84131400	-3.04777100
C	-0.42214700	0.30097800	3.69346300
C	-0.68254700	3.69364300	0.16479000
C	-0.70123200	-1.11241500	3.55450100
C	-0.89159800	2.88926800	-2.20296800
C	-0.98995200	-0.57384700	-3.14588000
C	-1.19418800	-3.17400900	1.56256000
C	-1.49882100	2.30230000	2.60720100
C	-1.19245500	-3.61234500	0.17979300
C	-1.33002200	0.82123000	-3.25405400
C	-1.61091900	1.02734700	3.26519400
C	-1.59374200	-2.70880600	-1.97215500
C	-2.02746200	-1.28074200	3.00267500
C	-2.05760000	3.29245000	0.36230000
C	-2.29024200	2.57830100	-2.00527000
C	-2.04225900	-1.51642300	-2.65955100
C	-2.22776100	-3.17414400	-0.72533200
C	-2.46613200	2.59372600	1.57728900
C	-2.30723200	-2.29561500	2.02372200
C	-2.62868600	0.06726000	2.87388200
C	-2.59079700	1.34592400	-2.71242500
C	-2.89710700	2.82383300	-0.72052600
C	-3.58078500	1.70416900	1.26960400
C	-3.66419800	0.37727200	1.91710200
C	-3.38463200	-2.51854800	-0.24684700
C	-3.43794000	-2.03673800	1.13779300
C	-3.37132900	-0.99779500	-2.29463900
C	-3.61278300	0.45639300	-2.23967900
C	-3.89122800	1.89993600	-0.18022600
C	-4.19325700	-0.74511500	1.13292700
C	-4.06033800	-1.57645400	-1.11201500
C	-4.33429600	0.77689500	-0.97171900
C	-4.59326700	-0.50042700	-0.27774700
Pr	1.98075900	-0.29617700	-0.15902400
Pr	-2.06219100	-0.07473200	-0.19792900
triplet state :			
C	4.39945600	0.41178400	0.42748600

C	4.44564200	-0.11561300	-0.91874000
C	3.89933700	1.77517800	0.65354000
C	4.11982200	-1.52728600	-1.10870300
C	3.90017200	-0.44375500	1.55263600
C	3.73779200	0.64322200	-1.99532900
C	3.56628700	-2.36756100	-0.03008800
C	3.39388200	2.57224000	-0.43070800
C	3.45205400	-1.82689000	1.33842900
C	3.19085600	1.79740300	1.92534900
C	3.24644000	1.95503000	-1.74636300
C	3.21732400	-1.63597300	-2.25652500
C	3.12875400	0.44021800	2.45023500
C	2.90352100	-0.30835600	-2.77453800
C	2.41177500	-3.08541100	-0.59418400
C	2.23688900	3.43663400	-0.22358200
C	2.16977400	-2.56406100	-1.95102100
C	2.11425900	2.69311900	2.14239700
C	2.31458400	-2.26939000	2.11414700
C	1.96509700	2.36553000	-2.30525100
C	1.96506000	-0.00744300	3.18158000
C	1.64119400	3.54336100	1.05239600
C	1.53103000	0.00958000	-3.13211700
C	1.64645700	-1.40778100	3.09623900
C	1.36695100	3.34889200	-1.39721500
C	1.30088400	-3.19951500	1.60073400
C	1.29509500	-3.53382400	0.20836500
C	1.11944300	1.42808600	-3.00841000
C	0.96982300	2.29017000	2.93535600
C	0.86620400	0.95797700	3.46167800
C	0.82355300	-2.35063000	-2.43771100
C	0.19884100	3.69209600	1.18703600
C	0.47957200	-1.04638600	-3.05414700
C	0.28633800	-1.88246700	3.25207100
C	0.04477700	-2.95352800	2.30993100
C	-0.20675800	2.97139500	2.39352200
C	-0.05117500	3.50466300	-1.29969300
C	0.03264200	-3.68679700	-0.44949900
C	-0.19483800	-3.11366600	-1.78667300
C	-0.26013900	1.74567300	-3.07521400
C	-0.46033200	0.43888000	3.68147300
C	-0.65815100	3.72004700	0.04100000
C	-0.74527400	-0.97439300	3.57142400
C	-0.84204900	2.84024300	-2.30328800
C	-0.95054200	-0.66673800	-3.13752900

C	-1.23530400	-3.10163900	1.66109300
C	-1.51212500	2.39783900	2.50671500
C	-1.21428400	-3.57887200	0.29112700
C	-1.28162800	0.72612200	-3.27271500
C	-1.64407300	1.15686800	3.21947100
C	-1.58426200	-2.75717100	-1.89741200
C	-2.07174000	-1.15241200	3.01343500
C	-2.03445700	3.32991600	0.23556200
C	-2.24718800	2.53808200	-2.11024400
C	-2.01564000	-1.58368500	-2.62865000
C	-2.23703100	-3.16076900	-0.64231900
C	-2.46590700	2.67724300	1.46548900
C	-2.35057800	-2.20107700	2.07370000
C	-2.66498000	0.19063300	2.84401900
C	-2.54304400	1.27635600	-2.77305200
C	-2.86000700	2.81864200	-0.84591300
C	-3.57843000	1.77465900	1.16681200
C	-3.68158200	0.47657700	1.85529800
C	-3.40437300	-2.49469300	-0.20370800
C	-3.47444100	-1.96763600	1.16595900
C	-3.33652200	-1.04049400	-2.28461300
C	-3.56899900	0.41170900	-2.27900500
C	-3.85899300	1.90852300	-0.28581300
C	-4.20456400	-0.66669800	1.09390000
C	-4.06352200	-1.57785300	-1.10614100
C	-4.31792400	0.77273700	-1.04381700
C	-4.61192600	-0.47270400	-0.32329300
Pr	1.89484100	-0.32313500	-0.25010600
Pr	-1.99132900	-0.11559300	-0.16240700

7. Pr₂@C₂ (10612)-C₇₂ (B3LYP/3-21G~MWB48)

singlet state :

C	-4.18216500	1.41212900	-0.66431400
C	-3.91619500	2.05234800	0.59122600
C	-2.99872700	3.20972700	0.67852100
C	-4.36971500	-0.05221600	-0.74543800
C	-3.36688400	1.83232700	-1.83868000
C	-3.67999400	1.19949300	1.79042600
C	-2.35618600	3.72297900	-0.49988100
C	-4.28983100	-0.85893900	0.45030000
C	-2.49699500	2.94583800	-1.76322700
C	-3.86122100	-0.20467300	1.71475400
C	-2.20124400	3.06521000	1.92823600
C	-3.65927900	-0.52457700	-1.95992800
C	-2.55264000	1.77616100	2.55618300

C	-2.95632000	0.61403800	-2.57520500
C	-0.97108800	4.23859500	-0.44501400
C	-3.71690000	-2.22314600	0.43174300
C	-1.17308500	2.89304500	-2.42944500
C	-2.90919400	-1.10791100	2.41004400
C	-0.86374200	3.56516900	1.97670600
C	-3.05897900	-1.83159400	-1.98296600
C	-0.27317400	3.77921200	-1.67164700
C	-2.91976900	-2.40036600	1.69088500
C	-1.61478800	0.48621100	-3.13244800
C	-1.52572700	0.91553700	3.12648600
C	-0.24332300	4.21956700	0.79767600
C	-3.13645500	-2.73926500	-0.80865800
C	-0.69740600	1.66742500	-3.06396000
C	-1.70791200	-0.57026300	3.06593600
C	0.17112600	2.78137700	2.66418100
C	-1.76038500	-2.03182000	-2.65776100
C	-0.14124100	1.47184800	3.21688900
C	-1.03077000	-0.89060500	-3.22781900
C	1.21003400	3.93133900	0.83980200
C	-1.89958900	-3.60626800	-0.82506500
C	1.13707700	3.50714900	-1.63871200
C	-1.70930200	-3.23096000	1.69270500
C	1.48375500	3.05116800	2.00268200
C	-1.04387400	-3.17035500	-1.98038200
C	0.78650200	1.44105200	-3.11674700
C	-0.50533500	-1.47219900	3.15994600
C	1.93811600	3.65240600	-0.39487300
C	-1.20933500	-3.93324400	0.45567200
C	1.69631700	2.38891300	-2.42824700
C	-0.52997500	-2.78949100	2.47973300
C	0.97801500	0.55516400	3.33179400
C	0.40928100	-1.05493700	-3.37548100
C	0.80783800	-0.89338300	3.35030800
C	1.29883300	0.09121700	-3.34203000
C	2.58743200	2.06311800	2.00600400
C	0.44849600	-3.20698500	-1.94807800
C	3.08806800	2.68938000	-0.44869000
C	0.29575300	-3.92050600	0.51285100
C	2.96479300	1.94505600	-1.77195700
C	0.69778400	-3.29979500	1.80925600
C	2.33559300	0.85556800	2.82562700
C	1.12929700	-2.21209700	-2.77721400
C	3.50458800	1.91178900	0.78190300

C	1.16752500	-3.67175500	-0.68287000
C	2.07112500	-1.51847900	2.88402800
C	2.61131300	-0.34871800	-2.77457700
C	3.43692800	0.54234200	-1.94212400
C	2.01992200	-2.69519600	2.01325500
C	3.01580200	-0.43306600	2.60828500
C	2.50125600	-1.78878100	-2.47630100
C	4.10991000	0.57356900	0.55372300
C	2.54375600	-3.25060000	-0.43539800
C	4.18685500	-0.07049100	-0.83109400
C	3.00424800	-2.84273700	0.93915100
C	3.96057400	-0.55552600	1.51264100
C	3.24987200	-2.37579100	-1.40066100
C	4.02067600	-1.81491700	0.77820000
C	4.17046200	-1.51156600	-0.65633500
Pr	1.33142100	0.90811800	-0.09992900
Pr	-0.67143900	-1.51261800	0.00692500

triplet state :

C	2.74415000	3.24251500	-0.61378300
C	3.24510300	2.72070000	0.62516100
C	3.96143900	1.46741600	0.69418300
C	1.48397900	3.94454500	-0.67218100
C	2.79414300	2.33472600	-1.77186200
C	2.35476900	2.79153900	1.79693200
C	4.16256700	0.66911300	-0.49211300
C	0.70317200	4.14650400	0.50693300
C	3.47308300	1.11615600	-1.71733100
C	1.14404800	3.47630800	1.74251900
C	3.50191700	0.75080500	1.89697700
C	0.75825000	3.48408500	-1.87829500
C	2.45955900	1.53247800	2.53834700
C	1.53526800	2.43943700	-2.50716500
C	4.20326100	-0.78291200	-0.49167200
C	-0.74628000	4.11562000	0.48848100
C	2.95291000	-0.05940200	-2.41813700
C	-0.03787500	2.95285600	2.43297200
C	3.46201400	-0.67386100	1.92253200
C	-0.65367200	3.43315600	-1.89443900
C	3.47503300	-1.23990600	-1.73200400
C	-1.20173900	3.43005600	1.70783000
C	0.91305400	1.27116400	-3.08553100
C	1.27693600	0.90446600	3.06837700
C	3.87469600	-1.49610000	0.75655700
C	-1.45467500	3.81216200	-0.72774300

C	1.63625100	-0.00961500	-3.05745700
C	-0.00760500	1.63979600	3.03160900
C	2.35364700	-1.33808400	2.59558100
C	-1.33568400	2.35761900	-2.58351700
C	1.26046900	-0.56744100	3.16533700
C	-0.56777700	1.27096000	-3.15189300
C	3.04791200	-2.73946100	0.78094200
C	-2.72125800	3.07293600	-0.76646200
C	2.68621000	-2.45541000	-1.72703500
C	-2.41987200	2.68005600	1.70603000
C	2.10369700	-2.62844700	1.91749300
C	-2.65759900	2.14391500	-1.93054700
C	0.87847600	-1.27554000	-3.13129600
C	-1.27755800	0.89199700	3.12471200
C	2.48715000	-3.24837500	-0.48761300
C	-3.26614500	2.53731200	0.49243500
C	1.40994100	-2.45759700	-2.46477100
C	-2.47166200	1.43123700	2.46666400
C	0.01653800	-1.23743100	3.34536100
C	-1.24784400	0.03134500	-3.29138700
C	-1.23912800	-0.51793200	3.34988100
C	-0.54220100	-1.22530600	-3.31128500
C	0.75183900	-3.18530200	1.90531800
C	-3.26576200	0.80800900	-1.91789500
C	1.10676300	-3.73546700	-0.51062700
C	-3.88017600	1.18215100	0.54220300
C	0.49601500	-3.35746600	-1.78099600
C	-3.42380800	0.54287100	1.80690600
C	-0.21867900	-2.56101600	2.75837500
C	-2.58972400	-0.19204900	-2.72697500
C	0.25687200	-3.84789200	0.67163200
C	-3.96627600	0.31385400	-0.66669900
C	-2.27971800	-1.40666400	2.81888200
C	-1.44952300	-2.25810200	-2.80712700
C	-0.93289300	-3.29499800	-1.95374100
C	-3.33419500	-0.89302200	1.97798400
C	-1.64303200	-2.67774300	2.50355100
C	-2.71842600	-1.61286200	-2.49531800
C	-1.15334900	-3.97757800	0.45924300
C	-4.02015900	-1.10096300	-0.44513000
C	-1.75775800	-3.78498100	-0.88273600
C	-3.82842800	-1.71761500	0.90957700
C	-2.11733300	-3.46518200	1.43265800
C	-3.50907400	-2.07873100	-1.41305700

C	-3.29828900	-3.02946500	0.72465600
C	-3.07942100	-3.24977500	-0.70452600
Pr	-1.42349000	0.93393400	-0.01627400
Pr	1.56011400	-0.88920500	-0.02994500

8. $\text{Pr}_2@C_{2v}(11188)-C_{72}$ (B3LYP/3-21G~MWB48)

singlet state :

C	-3.97237400	0.71699900	-1.13509400
C	-3.97237400	-0.71699900	-1.13509400
C	-3.85439000	1.16387000	0.27085400
C	-3.85439000	-1.16387000	0.27085400
C	-3.75893400	0.00000000	1.14226400
C	-3.22089000	-1.42415300	-2.13241800
C	-3.22089000	1.42415300	-2.13241800
C	-3.14947000	2.32515000	0.59693400
C	-3.14947000	-2.32515000	0.59693400
C	-2.97690500	0.00000000	2.36367100
C	-2.47387300	-0.70498300	-3.16567400
C	-2.47387300	0.70498300	-3.16567400
C	-2.43959900	-2.59064500	-1.77333600
C	-2.43959900	2.59064500	-1.77333600
C	-2.43298900	3.08318000	-0.43529800
C	-2.43298900	-3.08318000	-0.43529800
C	-2.38858700	-2.38965300	1.83418200
C	-2.38858700	2.38965300	1.83418200
C	-2.34240800	1.28981600	2.77383600
C	-2.34240800	-1.28981600	2.77383600
C	-1.23449200	-1.45510200	-3.50633000
C	-1.23449200	1.45510200	-3.50633000
C	-1.21697500	-2.59441900	-2.55791200
C	-1.21697500	2.59441900	-2.55791200
C	-1.23338200	-3.60783600	0.15134500
C	-1.23338200	3.60783600	0.15134500
C	-1.22538200	3.23449200	1.57547500
C	-1.22538200	-3.23449200	1.57547500
C	-1.21197300	1.27689400	3.71087000
C	-1.21197300	-1.27689400	3.71087000
C	-0.73968500	0.00000000	4.24518200
C	0.00000000	-0.77085300	-3.95939200
C	0.00000000	0.77085300	-3.95939200
C	0.00000000	3.12489600	-1.98510200
C	0.00000000	-3.12489600	-1.98510200
C	0.00000000	3.64018400	-0.60017800
C	0.00000000	-3.64018400	-0.60017800
C	0.00000000	-3.02539200	2.28854600

C	0.00000000	3.02539200	2.28854600
C	0.00000000	2.09130000	3.40735100
C	0.00000000	-2.09130000	3.40735100
C	0.73968500	0.00000000	4.24518200
C	1.21197300	1.27689400	3.71087000
C	1.21197300	-1.27689400	3.71087000
C	1.22538200	-3.23449200	1.57547500
C	1.22538200	3.23449200	1.57547500
C	1.23338200	-3.60783600	0.15134500
C	1.23338200	3.60783600	0.15134500
C	1.21697500	-2.59441900	-2.55791200
C	1.21697500	2.59441900	-2.55791200
C	1.23449200	-1.45510200	-3.50633000
C	1.23449200	1.45510200	-3.50633000
C	2.34240800	1.28981600	2.77383600
C	2.34240800	-1.28981600	2.77383600
C	2.38858700	-2.38965300	1.83418200
C	2.38858700	2.38965300	1.83418200
C	2.43298900	-3.08318000	-0.43529800
C	2.43298900	3.08318000	-0.43529800
C	2.43959900	2.59064500	-1.77333600
C	2.43959900	-2.59064500	-1.77333600
C	2.47387300	-0.70498300	-3.16567400
C	2.47387300	0.70498300	-3.16567400
C	2.97690500	0.00000000	2.36367100
C	3.14947000	-2.32515000	0.59693400
C	3.14947000	2.32515000	0.59693400
C	3.22089000	1.42415300	-2.13241800
C	3.22089000	-1.42415300	-2.13241800
C	3.75893400	0.00000000	1.14226400
C	3.85439000	-1.16387000	0.27085400
C	3.85439000	1.16387000	0.27085400
C	3.97237400	0.71699900	-1.13509400
C	3.97237400	-0.71699900	-1.13509400
Pr	0.00000000	0.00000000	1.79595000
Pr	0.00000000	0.00000000	-1.65707700

triplet state :

C	-3.95874200	0.72378900	-1.13993700
C	-3.95874200	-0.72378900	-1.13993700
C	-3.86169100	1.16806300	0.26024600
C	-3.86169100	-1.16806300	0.26024600
C	-3.75875900	0.00000000	1.12644200
C	-3.21230700	-1.42378500	-2.13731900
C	-3.21230700	1.42378500	-2.13731900

C	-3.15283900	2.33283900	0.59158400
C	-3.15283900	-2.33283900	0.59158400
C	-2.97717800	0.00000000	2.35046400
C	-2.47445100	-0.70968600	-3.17767500
C	-2.47445100	0.70968600	-3.17767500
C	-2.43254100	-2.59809400	-1.77498600
C	-2.43254100	2.59809400	-1.77498600
C	-2.43792900	3.08335200	-0.43521500
C	-2.43792900	-3.08335200	-0.43521500
C	-2.39456000	-2.39463300	1.83150200
C	-2.39456000	2.39463300	1.83150200
C	-2.34475300	1.29068600	2.76325900
C	-2.34475300	-1.29068600	2.76325900
C	-1.23121100	-1.43981900	-3.49575500
C	-1.23121100	1.43981900	-3.49575500
C	-1.22088100	-2.61667900	-2.56071200
C	-1.22088100	2.61667900	-2.56071200
C	-1.22757400	-3.59861300	0.15511800
C	-1.22757400	3.59861300	0.15511800
C	-1.22619500	3.24128100	1.58039000
C	-1.22619500	-3.24128100	1.58039000
C	-1.21001100	1.27458300	3.70143800
C	-1.21001100	-1.27458300	3.70143800
C	-0.74070500	0.00000000	4.24522100
C	0.00000000	-0.78167500	-3.96228400
C	0.00000000	0.78167500	-3.96228400
C	0.00000000	3.11796400	-1.98876200
C	0.00000000	-3.11796400	-1.98876200
C	0.00000000	3.64296100	-0.59116400
C	0.00000000	-3.64296100	-0.59116400
C	0.00000000	-3.02850900	2.28899100
C	0.00000000	3.02850900	2.28899100
C	0.00000000	2.09000300	3.40357500
C	0.00000000	-2.09000300	3.40357500
C	0.74070500	0.00000000	4.24522100
C	1.21001100	1.27458300	3.70143800
C	1.21001100	-1.27458300	3.70143800
C	1.22619500	-3.24128100	1.58039000
C	1.22619500	3.24128100	1.58039000
C	1.22757400	-3.59861300	0.15511800
C	1.22757400	3.59861300	0.15511800
C	1.22088100	-2.61667900	-2.56071200
C	1.22088100	2.61667900	-2.56071200
C	1.23121100	-1.43981900	-3.49575500

C	1.23121100	1.43981900	-3.49575500
C	2.34475300	1.29068600	2.76325900
C	2.34475300	-1.29068600	2.76325900
C	2.39456000	-2.39463300	1.83150200
C	2.39456000	2.39463300	1.83150200
C	2.43792900	-3.08335200	-0.43521500
C	2.43792900	3.08335200	-0.43521500
C	2.43254100	2.59809400	-1.77498600
C	2.43254100	-2.59809400	-1.77498600
C	2.47445100	-0.70968600	-3.17767500
C	2.47445100	0.70968600	-3.17767500
C	2.97717800	0.00000000	2.35046400
C	3.15283900	-2.33283900	0.59158400
C	3.15283900	2.33283900	0.59158400
C	3.21230700	1.42378500	-2.13731900
C	3.21230700	-1.42378500	-2.13731900
C	3.75875900	0.00000000	1.12644200
C	3.86169100	-1.16806300	0.26024600
C	3.86169100	1.16806300	0.26024600
C	3.95874200	0.72378900	-1.13993700
C	3.95874200	-0.72378900	-1.13993700
Pr	0.00000000	0.00000000	1.78975000
Pr	0.00000000	0.00000000	-1.62629700

9. Pr₂@D₂(10611)-C₇₂(Ad) (A)(B3LYP/6-31G(d)~MWB48)

singlet state (^SA):

C	-3.33006400	1.85058600	-0.47401000
C	-3.08920000	2.00513900	0.97229300
C	-2.37570800	2.68994700	-1.16391400
C	-3.08353200	0.75021800	1.75004400
C	-3.69036100	0.51322200	-0.95883600
C	-2.00070800	2.97947800	1.13188800
C	-1.56647300	3.39835800	-0.20151100
C	-3.47502900	-0.45252100	1.01953100
C	-1.76099700	2.18348300	-2.34437200
C	-2.05310700	0.62595600	2.72605500
C	-2.76791800	-0.10371600	-1.89503600
C	-1.00355300	2.82827400	2.16680900
C	-1.95533600	0.78643200	-2.70419800
C	-1.09881100	1.67032700	3.01456900
C	-0.18003900	3.72633400	-0.49313100
C	-2.52249800	-1.56030800	0.96903600
C	-0.42075300	2.55501500	-2.68820500
C	-1.42367300	-0.63790900	3.00294800
C	-2.17733600	-1.42043500	-1.63246400

C	0.30391800	3.35409600	1.93656200
C	-2.11223500	-2.10977300	-0.31540900
C	0.69662000	3.83621200	0.62311800
C	0.38901200	3.33870300	-1.79209800
C	-1.59899000	-1.73783900	2.09654100
C	-0.76043200	0.35570600	-3.36899400
C	0.06768000	1.05407900	3.57467700
C	0.16268300	1.45286200	-3.41707200
C	-0.13965400	-0.37138500	3.60235500
C	-1.02010800	-1.86123000	-2.38147500
C	1.46897900	2.77666400	2.54941700
C	-0.29832800	-0.98970600	-3.25584600
C	1.36901300	1.60452400	3.34932700
C	-0.98298800	-3.00607700	-0.37526100
C	2.11085400	3.63108800	0.49046500
C	1.80579600	3.17213200	-1.90056600
C	-0.52090400	-2.66565700	2.00293300
C	-0.31003100	-2.86332500	-1.62304500
C	2.60004900	2.96675000	1.65800000
C	2.66270600	3.33404500	-0.76619000
C	-0.23683700	-3.33249900	0.77475800
C	1.56834500	1.22427800	-3.44475300
C	0.95650400	-1.27033700	3.44426100
C	2.39594400	2.14566900	-2.73908200
C	0.73064200	-2.46254500	2.69578200
C	1.09314300	-1.22677000	-3.44047600
C	2.47767300	0.70507700	3.34551400
C	2.01975000	-0.12946100	-3.56802200
C	2.27979500	-0.71822100	3.42404000
C	1.10738000	-3.07220800	-1.74886500
C	3.67926400	2.03016900	1.58476400
C	3.76981300	2.42598000	-0.86941800
C	1.17707000	-3.56133400	0.68309300
C	3.62882400	1.71841000	-2.13990500
C	1.77796300	-3.06388900	1.91792100
C	1.77184700	-2.30549500	-2.76608700
C	3.65123800	0.95320200	2.54615600
C	1.87122000	-3.49136700	-0.56493700
C	4.33288100	1.79650400	0.28403600
C	3.29320300	-0.54260300	-3.04446900
C	3.36122100	-1.37030200	2.73241000
C	4.12753600	0.38892000	-2.30451700
C	3.12181800	-2.57372600	1.94906300
C	3.15037900	-1.93037500	-2.62819300

C	4.25626300	-0.31767500	2.26091500
C	3.30274800	-3.20674000	-0.49926600
C	5.04290500	0.53662800	0.05817700
C	4.97660300	-0.14029200	-1.25588000
C	3.94027500	-2.79758400	0.77394900
C	3.93955100	-2.45189100	-1.57091200
C	5.04057000	-0.50104500	1.08704400
C	4.93592100	-1.57252700	-0.99062200
C	4.95104000	-1.79588100	0.43390500
Pr	2.76899700	-0.69248100	-0.05582400
Pr	-1.17669900	0.71638800	0.02620500
C	-4.58346000	-0.29711200	-0.02663700
C	-5.81164000	0.52132600	0.51102200
H	-5.47159200	1.46501800	0.94225300
C	-5.16668400	-1.62015200	-0.61813300
H	-4.37527500	-2.24990700	-1.01960900
C	-6.79030600	0.83147100	-0.64123700
H	-7.60925600	1.45069600	-0.25157000
H	-6.29098200	1.42173300	-1.42117900
C	-6.15118000	-1.29928600	-1.76468400
H	-6.50217400	-2.24445400	-2.19969700
H	-5.64151400	-0.75337500	-2.56941300
C	-5.90617500	-2.41336100	0.48100500
H	-6.25659300	-3.36225700	0.05377000
H	-5.21923400	-2.67018500	1.29771500
C	-7.33943500	-0.47914400	-1.23250300
H	-8.03357400	-0.25462900	-2.05257800
C	-6.54697700	-0.28155800	1.60513700
H	-7.36628600	0.33281800	2.00182500
H	-5.87297900	-0.49008200	2.44621700
C	-7.09387000	-1.59520400	1.01899200
H	-7.61343400	-2.16336300	1.80125100
C	-8.07026100	-1.27946900	-0.13383500
H	-8.47250800	-2.21217400	-0.55267900
H	-8.92647300	-0.70431000	0.24454800
triplet state (¹ A)			
C	-3.31453000	1.86860200	-0.48011100
C	-3.07076400	2.02926600	0.95277800
C	-2.33810100	2.67372400	-1.17144700
C	-3.06129100	0.78697900	1.73208800
C	-3.67980300	0.53615600	-0.95270000
C	-1.96052500	2.98696500	1.10370900
C	-1.52723800	3.40296500	-0.21943400
C	-3.47520900	-0.42521200	1.01776800

C	-1.74222200	2.17600300	-2.35109400
C	-2.04174500	0.66041500	2.72019200
C	-2.76547200	-0.09348100	-1.88992700
C	-0.97474300	2.84359500	2.14513800
C	-1.95070700	0.78375300	-2.71184500
C	-1.08081000	1.69844000	3.00926000
C	-0.14916900	3.73360000	-0.51504100
C	-2.53637300	-1.53909300	0.97257000
C	-0.39742700	2.54385600	-2.70139500
C	-1.42016100	-0.60723200	2.99954300
C	-2.18584500	-1.41315400	-1.62593200
C	0.33731900	3.35765700	1.90518200
C	-2.13252900	-2.10477300	-0.30830500
C	0.72923900	3.84950100	0.60179900
C	0.41438800	3.33926700	-1.81388500
C	-1.60879900	-1.71606300	2.10178500
C	-0.76314900	0.34611500	-3.37773200
C	0.07968200	1.07790400	3.57515000
C	0.17273500	1.44258300	-3.42659500
C	-0.13643300	-0.34665200	3.59419900
C	-1.03402000	-1.86546900	-2.38012300
C	1.50184500	2.77826500	2.53595400
C	-0.30855700	-0.99741800	-3.25581500
C	1.38514000	1.61342200	3.34463800
C	-1.00833100	-3.00481500	-0.36464700
C	2.14155400	3.62538600	0.47039000
C	1.82429800	3.15094400	-1.91646700
C	-0.54182300	-2.64850300	2.01221000
C	-0.33095000	-2.86930500	-1.61826900
C	2.62694700	2.95194100	1.64770300
C	2.68967300	3.31564400	-0.77511100
C	-0.26397400	-3.32878400	0.78320200
C	1.57697200	1.20569600	-3.45538400
C	0.95189600	-1.26098200	3.44866100
C	2.40572200	2.12602300	-2.74991200
C	0.71007900	-2.45500000	2.70689100
C	1.08548700	-1.23911200	-3.43455200
C	2.48602000	0.70278800	3.34594000
C	2.02118700	-0.14882600	-3.57815700
C	2.27766900	-0.72407700	3.43694000
C	1.07932900	-3.08435900	-1.74220200
C	3.69859000	2.01107700	1.57955900
C	3.79115700	2.40030100	-0.87552700
C	1.14615300	-3.56986400	0.69313500

C	3.63211100	1.68432500	-2.13169700
C	1.74885500	-3.05961400	1.92038600
C	1.75286900	-2.31653200	-2.75685800
C	3.65397300	0.93453800	2.54191900
C	1.84201400	-3.49827700	-0.55339200
C	4.34853500	1.76465100	0.28007500
C	3.28892200	-0.56821700	-3.04884000
C	3.34812000	-1.38511900	2.74177800
C	4.12824100	0.35171500	-2.30112700
C	3.09745300	-2.57914100	1.95137100
C	3.13513800	-1.94923600	-2.61947400
C	4.24838000	-0.34620100	2.25868900
C	3.26684200	-3.21193500	-0.48587000
C	5.03662300	0.49990200	0.05589300
C	4.96282500	-0.18048500	-1.24508200
C	3.90504900	-2.80102400	0.77290900
C	3.91609200	-2.46013400	-1.55566900
C	5.01716100	-0.54452600	1.08410800
C	4.93835500	-1.61625000	-0.98209900
C	4.94995100	-1.83572500	0.43492800
Pr	2.66240900	-0.63990800	-0.06256800
Pr	-1.07838600	0.63421800	0.05067300
C	-4.58451800	-0.26388400	-0.02532900
C	-5.80566100	0.56352900	0.51439200
H	-5.45729100	1.50370900	0.94582100
C	-5.17800000	-1.58185100	-0.61737200
H	-4.39221800	-2.21794500	-1.02026600
C	-6.78268200	0.88248900	-0.63665500
H	-7.59693400	1.50716300	-0.24571200
H	-6.27873500	1.47025700	-1.41532200
C	-6.16052600	-1.25170600	-1.76317100
H	-6.51905300	-2.19346700	-2.19956500
H	-5.64675300	-0.70844900	-2.56712200
C	-5.92324600	-2.37154500	0.48033200
H	-6.28184000	-3.31665300	0.05135100
H	-5.23830500	-2.63540900	1.29640500
C	-7.34207900	-0.42298300	-1.22950600
H	-8.03483800	-0.19228600	-2.04909800
C	-6.54610100	-0.23595100	1.60764200
H	-7.36046600	0.38372400	2.00634200
H	-5.87290800	-0.45139900	2.44767600
C	-7.10390900	-1.54440600	1.02010200
H	-7.62762400	-2.10965600	1.80176500
C	-8.07850400	-1.21933500	-0.13166300

H	-8.48842800	-2.14826000	-0.55160100
H	-8.92990600	-0.63796800	0.24811400
10. Pr ₂ @D ₂ (10611)-C ₇₂ (Ad) (B)(B3LYP/6-31G(d)~MWB48)			
singlet state (^S B):			
C	2.15612500	3.40325800	0.02226700
C	3.08515000	2.34069700	0.26691400
C	1.64355700	3.31999300	-1.30860500
C	2.80572000	1.84144900	1.63157100
C	1.26246900	3.56710600	1.12593300
C	3.18541100	1.55674700	-1.02211300
C	2.21739700	2.16108900	-1.94270800
C	1.64690000	2.58993100	2.13042900
C	0.32002300	3.70195800	-1.56461700
C	2.88808900	0.42718000	1.96604800
C	-0.10833000	3.93096300	0.89243800
C	3.47494100	0.14477200	-1.08329400
C	-0.54812000	4.07713000	-0.47265200
C	3.31506900	-0.59852100	1.01171700
C	1.40904000	1.37439300	-2.84560400
C	0.61541400	2.01495300	2.98008800
C	-0.45431600	3.00985400	-2.55466600
C	1.80989300	-0.14275600	2.74606400
C	-1.06898800	3.51057400	1.85683700
C	2.52005900	-0.64999600	-1.82023600
C	-0.69204600	2.58719700	2.91070600
C	1.65061900	-0.03305900	-2.81740800
C	0.06134700	1.84080500	-3.20748100
C	0.72307300	0.60486800	3.33653200
C	-1.88426500	3.72860800	-0.85758100
C	2.36604700	-1.68935600	1.07963200
C	-1.83639100	3.10131700	-2.16159000
C	1.56378300	-1.47133200	2.25420700
C	-2.42206500	3.22838400	1.48269100
C	1.85655600	-1.90834200	-1.40987100
C	-2.82897300	3.29433200	0.11962800
C	1.74858700	-2.39707800	-0.04880500
C	-1.85837400	1.80734800	3.22794700
C	0.63592400	-0.96494900	-3.17398600
C	-0.90205600	0.87860200	-3.65740100
C	-0.44676000	-0.12830700	3.69409900
C	-2.92744800	2.17477600	2.34780100
C	0.72579600	-2.09861400	-2.31058000
C	-0.60491400	-0.52258200	-3.66685400
C	-1.74160400	0.48066700	3.65947400

C	-2.76941600	2.09355500	-2.53018300
C	0.35048900	-2.16886000	2.51991900
C	-2.30365900	1.01613700	-3.34146700
C	-0.62265100	-1.51397100	3.31669600
C	-3.84755500	2.38159600	-0.30035200
C	0.58751200	-3.17908900	0.26110800
C	-3.84876800	1.81625300	-1.62300000
C	-0.06515500	-3.12047600	1.55146400
C	-3.90585000	1.22572500	1.92334800
C	-0.44903900	-2.85678800	-1.98582000
C	-1.78785500	-1.26474700	-3.35808000
C	-2.72375100	-0.49511900	3.26582500
C	-2.87419100	-0.30214600	-3.20857700
C	-2.02065000	-1.76052400	3.09703500
C	-4.45361000	1.43547200	0.59791800
C	-0.43438600	-3.49540600	-0.70972000
C	-3.84620800	-0.14947700	2.44931300
C	-1.73986100	-2.45511600	-2.57067500
C	-4.51087600	0.53998400	-1.57759700
C	-1.45485700	-3.44752700	1.39703300
C	-4.00913100	-0.57103200	-2.38293400
C	-2.46841000	-2.74851300	2.16823100
C	-4.96417600	0.34690100	-0.19628500
C	-1.65604300	-3.75789700	-0.00234100
C	-4.44628400	-1.23618700	1.66662500
C	-2.96905100	-2.81952600	-1.88512200
C	-4.13396600	-1.91058000	-1.84377900
C	-3.77078100	-2.54613300	1.56695800
C	-5.05519700	-0.96527400	0.35922200
C	-2.90618200	-3.50875500	-0.61227800
C	-4.75413500	-2.08291100	-0.53031700
C	-3.99260900	-3.04230900	0.22233800
Pr	-2.60182300	-0.86257900	-0.05843900
Pr	1.13526400	0.67935800	0.10453200
C	4.40326400	-0.48117300	-0.04318900
C	5.60791200	0.42557600	0.37212900
H	5.25251300	1.40261800	0.70274800
C	5.00506500	-1.85525300	-0.48742100
H	4.20615300	-2.53498900	-0.78825400
C	6.38772400	-0.22956800	1.53297800
H	7.19523900	0.44825700	1.84017400
H	5.73755800	-0.36096800	2.40742000
C	5.79089600	-2.49527300	0.67791400
H	6.16127600	-3.47721200	0.35487200

H	5.12920900	-2.67345400	1.53510600
C	5.95436000	-1.64590600	-1.68745800
H	6.32650500	-2.62429800	-2.01905200
H	5.41036900	-1.21196200	-2.53677600
C	6.96298400	-1.58592500	1.08711300
H	7.51506200	-2.04473700	1.91731200
C	6.55769400	0.62315700	-0.83026900
H	7.36992300	1.29885600	-0.53165300
H	6.03270800	1.11155600	-1.66160400
C	7.12722700	-0.73460300	-1.28231000
H	7.79569900	-0.58815500	-2.14034900
C	7.90598000	-1.38062400	-0.11704300
H	8.32791000	-2.34430900	-0.43388600
H	8.75206100	-0.74157200	0.17098100
triplet state (^T B):			
C	2.15323800	3.42405200	-0.01731800
C	3.09006000	2.36771100	0.23215500
C	1.62466600	3.32354700	-1.33843600
C	2.79844900	1.86238100	1.58594000
C	1.25216200	3.58350400	1.08494200
C	3.16754300	1.56528900	-1.03612100
C	2.19370300	2.14803900	-1.95580800
C	1.63890200	2.61963300	2.09610900
C	0.30113100	3.70311200	-1.60260000
C	2.89009400	0.45672200	1.94799000
C	-0.12074200	3.94422600	0.84686500
C	3.45419200	0.15623100	-1.07709300
C	-0.56826300	4.08920400	-0.51553100
C	3.31776800	-0.58364700	1.01535700
C	1.39820500	1.35405700	-2.85383700
C	0.61578100	2.05184300	2.95655200
C	-0.46979900	2.99240900	-2.58228000
C	1.81417600	-0.10761800	2.74350300
C	-1.07517700	3.50955100	1.80939500
C	2.50473000	-0.65198000	-1.80483600
C	-0.69607900	2.61687400	2.88532000
C	1.64473200	-0.05399400	-2.81295200
C	0.04858200	1.81723300	-3.22292900
C	0.72915700	0.64630100	3.33056700
C	-1.90328100	3.72181000	-0.88963000
C	2.37146600	-1.66940700	1.09417200
C	-1.84887200	3.06952900	-2.17920200
C	1.56594300	-1.43879800	2.26985500
C	-2.44179700	3.23522500	1.44893200

C	1.85629100	-1.91516800	-1.38727500
C	-2.85387500	3.29772300	0.08641100
C	1.75508100	-2.39032300	-0.02250200
C	-1.86246600	1.84546700	3.21583800
C	0.64041600	-0.99971300	-3.16883600
C	-0.90871000	0.84608500	-3.64805800
C	-0.44004200	-0.08561400	3.67924000
C	-2.94092000	2.20396400	2.32892200
C	0.73476800	-2.12959200	-2.29791900
C	-0.60417400	-0.55859600	-3.64178100
C	-1.74199600	0.52344800	3.64442200
C	-2.78627400	2.05972200	-2.54173400
C	0.35892000	-2.14148200	2.54623600
C	-2.31434400	0.97879300	-3.34677800
C	-0.61298200	-1.47862600	3.33811900
C	-3.87579600	2.38375400	-0.32630500
C	0.59755800	-3.17848700	0.30265500
C	-3.87441300	1.80177300	-1.64610400
C	-0.04912000	-3.11776300	1.59682100
C	-3.90938400	1.24314200	1.90858700
C	-0.43773800	-2.87465500	-1.95620000
C	-1.78695700	-1.30235600	-3.33972200
C	-2.71948400	-0.46146600	3.26974500
C	-2.87601200	-0.34049200	-3.20369800
C	-2.01287900	-1.72347500	3.11893700
C	-4.45459300	1.43465200	0.58233900
C	-0.42505200	-3.49131100	-0.66353400
C	-3.83609800	-0.12898700	2.43953800
C	-1.73596900	-2.48604800	-2.54228300
C	-4.51228200	0.51399000	-1.58043300
C	-1.44018200	-3.43639800	1.44362100
C	-4.00858300	-0.60372700	-2.36754000
C	-2.45766500	-2.72673100	2.20044300
C	-4.94767200	0.32614800	-0.19904700
C	-1.64676100	-3.75407200	0.04591700
C	-4.42403700	-1.22163500	1.67263000
C	-2.96530000	-2.84713300	-1.85468100
C	-4.12348000	-1.93634400	-1.81058100
C	-3.75102400	-2.52427100	1.58965600
C	-5.03661000	-0.97571400	0.36280900
C	-2.90180100	-3.51859600	-0.56485200
C	-4.76002000	-2.10813900	-0.50200800
C	-3.99384900	-3.05423300	0.25530000
Pr	-2.48039300	-0.89764700	-0.08741000

Pr	1.03852000	0.68081000	0.15275900
C	4.39491400	-0.46611500	-0.04679900
C	5.60203000	0.44148300	0.35995900
H	5.24844100	1.41970300	0.68852400
C	4.99599200	-1.84083900	-0.49195000
H	4.19724900	-2.52259300	-0.78765800
C	6.38740300	-0.21118500	1.51880400
H	7.19659700	0.46707600	1.82060800
H	5.74147200	-0.34061100	2.39668400
C	5.78697400	-2.47868900	0.67131800
H	6.15606600	-3.46125300	0.34856500
H	5.12895600	-2.65545100	1.53154400
C	5.94004800	-1.63435400	-1.69642800
H	6.31025100	-2.61363600	-2.02771200
H	5.39259300	-1.20174200	-2.54423700
C	6.96059800	-1.56873300	1.07385100
H	7.51603900	-2.02585700	1.90281700
C	6.54699800	0.63587600	-0.84668600
H	7.36062400	1.31201000	-0.55281300
H	6.01839500	1.12236200	-1.67668600
C	7.11479100	-0.72276200	-1.29810700
H	7.77987200	-0.57841400	-2.15915400
C	7.89836000	-1.36672400	-0.13482200
H	8.31809700	-2.33155000	-0.45125100
H	8.74623900	-0.72772900	0.14796300

11. Pr₂@D₂(10611)-C₇₂ (Ad) (C)(B3LYP/6-31G(d)~MWB48)

singlet state (^SC):

C	-3.85987200	0.94325100	-0.41871300
C	-3.27167800	1.82805300	0.56550900
C	-3.09885200	1.06827600	-1.64696600
C	-2.83897100	1.19809900	1.82599700
C	-3.53118600	-0.86782600	0.60966600
C	-2.40451300	2.75803400	-0.14726400
C	-2.28944800	2.27769700	-1.53160700
C	-2.87868900	-0.28347400	1.81424800
C	-2.49676300	-0.09220300	-2.27816400
C	-1.72547300	1.82696900	2.47218700
C	-2.72144300	-1.74545800	-0.22897000
C	-1.27287500	3.34635500	0.50873100
C	-2.37882700	-1.43116000	-1.63590100
C	-1.01305800	2.94397100	1.86760600
C	-1.05048000	2.45101300	-2.26518100
C	-1.79040600	-1.03118500	2.45562600
C	-1.31106700	0.10574200	-3.08298700

C	-0.77129000	1.08536800	3.25203200
C	-1.79500400	-2.56305000	0.47956300
C	-0.16513000	3.74020100	-0.29834300
C	-1.42329600	-2.27723500	1.85823400
C	-0.07872500	3.32170600	-1.68936800
C	-0.59312300	1.36286000	-3.13103400
C	-0.77799800	-0.34644900	3.26086000
C	-1.19195500	-2.04666100	-2.20341800
C	0.33327400	2.93283600	2.36734500
C	-0.57423200	-1.13142600	-3.11599000
C	0.47468700	1.81457500	3.25869600
C	-0.70095500	-3.24686800	-0.13462300
C	1.16706600	3.79352600	0.22460600
C	-0.37558100	-2.99287300	-1.49211800
C	1.43384200	3.36574700	1.55695000
C	-0.14010000	-2.88002000	2.07870400
C	1.31205900	3.21758800	-2.01825800
C	0.79611800	1.30418900	-3.46740700
C	0.47492400	-0.99700200	3.51621300
C	0.31723300	-3.48145500	0.86396400
C	2.09455000	3.49714500	-0.85311100
C	1.73864000	2.24285000	-2.93376300
C	0.78598400	-2.26611600	2.93700600
C	0.82916000	-1.18301400	-3.39672300
C	1.72839200	1.15416000	3.41508100
C	1.49643400	0.04960100	-3.63998100
C	1.71285300	-0.25622100	3.61620200
C	0.99245400	-3.13326300	-1.86322500
C	2.71282800	2.78705800	1.81062500
C	1.58681100	-2.25805500	-2.83587800
C	2.87251600	1.71906600	2.75945800
C	1.70551000	-3.52376700	0.51981300
C	3.33934300	2.83495100	-0.62165100
C	3.00757000	1.59597900	-2.75573800
C	2.19032100	-2.32700100	2.64612600
C	2.87140900	0.23384700	-3.26220100
C	2.78492700	-1.08641300	3.13463500
C	2.00604500	-3.47149100	-0.88817800
C	3.68719600	2.60658200	0.76101300
C	2.68783900	-2.98827800	1.47866100
C	3.85221900	1.90337100	-1.64185400
C	2.98458900	-2.10630400	-2.52542500
C	3.99056800	0.90712700	2.35281800
C	3.65398200	-0.83469600	-2.72668800

C	3.96033400	-0.53644800	2.53129800
C	3.24926900	-2.92962700	-1.35503500
C	4.53991000	1.51966600	1.14596400
C	3.99262600	-2.55166400	0.99177400
C	4.80664100	0.87075500	-1.24355400
C	4.73735200	-0.48482400	-1.82938400
C	4.65838600	-1.35768700	1.55999300
C	4.27656600	-2.57596800	-0.43917300
C	5.19241200	0.72596200	0.15872900
C	5.08544200	-1.42080400	-0.76846900
C	5.33818600	-0.68876200	0.44877600
Pr	2.90606700	-0.40661300	-0.01567100
Pr	-1.22724700	0.44647900	-0.02623600
C	-4.75585500	-0.17217500	0.03284200
C	-5.51194400	-0.94705200	-1.08630000
H	-4.81733600	-1.27575600	-1.86090900
C	-5.81218800	0.26299500	1.09868600
H	-5.32088500	0.80856500	1.90791800
C	-6.21552200	-2.18427600	-0.48612500
H	-6.70780300	-2.73893500	-1.29578200
H	-5.48020100	-2.86567700	-0.03877400
C	-6.50854500	-0.98221000	1.68479400
H	-7.21397100	-0.66212300	2.46312300
H	-5.77447600	-1.63728000	2.17240900
C	-6.86366400	1.18114700	0.43874500
H	-7.57341100	1.51836800	1.20560600
H	-6.38345000	2.08235100	0.03440600
C	-7.24761000	-1.74552400	0.57024000
H	-7.74252200	-2.62954100	0.99227100
C	-6.56779200	-0.02314200	-1.73230700
H	-7.06290500	-0.56783000	-2.54715400
H	-6.08584400	0.85308300	-2.18530300
C	-7.60021800	0.41976000	-0.67870700
H	-8.34572700	1.07670500	-1.14478500
C	-8.29741300	-0.82174500	-0.08367000
H	-9.04372200	-0.51333400	0.66139700
H	-8.83849000	-1.36393700	-0.87126700
triplet state (^T C):			
C	-3.87821300	0.98923400	-0.43428800
C	-3.27375500	1.86108200	0.54003500
C	-3.08815400	1.06635000	-1.63431000
C	-2.82117200	1.23710700	1.78738800
C	-3.53170700	-0.84043400	0.61343700
C	-2.37123700	2.75891100	-0.17453400

C	-2.26134700	2.27510400	-1.54389300
C	-2.87370200	-0.24826900	1.79976600
C	-2.49254200	-0.09561000	-2.25961900
C	-1.71248000	1.86254500	2.44139300
C	-2.72504900	-1.72414000	-0.21368300
C	-1.24824000	3.35939100	0.47845900
C	-2.38475000	-1.43072500	-1.62083800
C	-0.99280800	2.97720200	1.84309700
C	-1.03391100	2.43994700	-2.28493500
C	-1.79906100	-0.99448500	2.45364000
C	-1.30752900	0.08768100	-3.07409900
C	-0.76374500	1.12022100	3.23021300
C	-1.80657700	-2.54562200	0.50275600
C	-0.13598400	3.73075300	-0.33387600
C	-1.44309000	-2.25497300	1.87804500
C	-0.05696700	3.31596700	-1.72317800
C	-0.58411800	1.34355700	-3.14611300
C	-0.78425800	-0.31293000	3.25969500
C	-1.21220100	-2.06568600	-2.19218600
C	0.34924900	2.96443000	2.34786100
C	-0.58503300	-1.15338300	-3.10750100
C	0.48119000	1.84146000	3.24086000
C	-0.72475200	-3.25424100	-0.11179400
C	1.19742400	3.79268000	0.19558400
C	-0.40177600	-3.00656100	-1.47182000
C	1.45299800	3.37486100	1.53320200
C	-0.16273800	-2.85900400	2.10233500
C	1.33188000	3.19489000	-2.04775400
C	0.79893700	1.27305300	-3.48208600
C	0.45812900	-0.96774500	3.52535900
C	0.29384500	-3.47642500	0.88571000
C	2.11886000	3.47483900	-0.87488100
C	1.75318900	2.21594600	-2.95199100
C	0.76322200	-2.25041000	2.95381900
C	0.81819000	-1.21429600	-3.39322200
C	1.73091800	1.17252000	3.41132600
C	1.48869500	0.01522600	-3.64597100
C	1.69869700	-0.23623200	3.62327200
C	0.96995200	-3.14825900	-1.83968700
C	2.72689200	2.78395800	1.79316700
C	1.56985500	-2.28906500	-2.82822000
C	2.88068800	1.72464500	2.75963700
C	1.67629800	-3.53322700	0.54545700
C	3.35692200	2.81278000	-0.63917800

C	3.01629700	1.56261400	-2.76675000
C	2.16644900	-2.32522800	2.66729300
C	2.86176700	0.19718500	-3.24800200
C	2.76084100	-1.08042200	3.13344700
C	1.97717600	-3.48394200	-0.86515400
C	3.69484800	2.58584400	0.74828900
C	2.66035900	-2.99060900	1.49984000
C	3.86136800	1.86694000	-1.65035700
C	2.96615000	-2.14283000	-2.51648900
C	3.98750400	0.90009600	2.35699800
C	3.64222700	-0.87540000	-2.71127200
C	3.94424400	-0.54235900	2.53206000
C	3.22498000	-2.95137700	-1.33649100
C	4.53897800	1.49155800	1.14301000
C	3.95658700	-2.55586100	1.00890100
C	4.79534800	0.82856500	-1.24120900
C	4.71711900	-0.52354400	-1.80850900
C	4.62833500	-1.36999600	1.56017600
C	4.24301200	-2.58244600	-0.42394500
C	5.17309400	0.67982000	0.16706600
C	5.08438900	-1.45721800	-0.75057500
C	5.34333400	-0.72681900	0.45731100
Pr	2.78562900	-0.38102800	-0.01056600
Pr	-1.08957600	0.42814100	-0.03573700
C	-4.74918900	-0.14577900	0.03356800
C	-5.50828900	-0.92781500	-1.07989200
H	-4.81673200	-1.25627100	-1.85756200
C	-5.80619000	0.28629500	1.10194000
H	-5.31422100	0.83745200	1.90744200
C	-6.20389800	-2.16705200	-0.47426700
H	-6.69646500	-2.72656300	-1.28051000
H	-5.46380100	-2.84403100	-0.02785400
C	-6.49488400	-0.96036900	1.69445800
H	-7.19966100	-0.64155000	2.47395300
H	-5.75650400	-1.61099300	2.18179300
C	-6.86593400	1.19674600	0.44485700
H	-7.57519800	1.52973000	1.21418300
H	-6.39244900	2.09955800	0.03759400
C	-7.23413600	-1.73099400	0.58490000
H	-7.72289700	-2.61642400	1.01134500
C	-6.57158500	-0.01153100	-1.72455700
H	-7.06700000	-0.56115700	-2.53602800
H	-6.09612100	0.86601000	-2.18112600
C	-7.60241600	0.42872100	-0.66822900

H	-8.35303900	1.08073500	-1.13321400
C	-8.29113400	-0.81485500	-0.06814100
H	-9.03737700	-0.50904800	0.67809900
H	-8.83098100	-1.36240300	-0.85299300
12. Pr ₂ @D ₂ (10611)-C ₇₂ (Ad) (D)(B3LYP/6-31G(d)~MWB48)			
singlet state (^SD):			
C	3.08699500	2.00648100	0.92282500
C	3.32018300	1.84085300	-0.51681800
C	2.03956600	3.00483600	1.06038500
C	3.73048100	0.50753600	-0.94248300
C	3.03405400	0.75668400	1.70986600
C	2.34106500	2.64907500	-1.23859000
C	1.56673600	3.39698000	-0.25146100
C	3.46050700	-0.43890300	0.94628500
C	1.09890600	2.89968100	2.11142800
C	2.83674300	-0.11778500	-1.88081000
C	1.97372800	0.62911200	2.69696600
C	1.67691100	2.09577500	-2.39918100
C	1.10377100	1.74107800	2.97061700
C	1.96778200	0.70385300	-2.71403500
C	0.17057300	3.72856100	-0.47275800
C	2.53363700	-1.58087800	0.86761600
C	-0.25569500	3.34007600	1.94936900
C	2.17904200	-1.41669600	-1.69701300
C	1.44595300	-0.67797800	2.95634100
C	0.36091200	2.56148400	-2.69125100
C	1.71198200	-1.76041000	2.02025000
C	-0.35869900	3.42474900	-1.76351600
C	-0.74904000	3.75888200	0.67007600
C	2.03048400	-2.14027900	-0.42245100
C	-0.24292600	1.54359600	3.43639500
C	0.93615300	-0.14147800	-3.23382800
C	-1.07752300	2.55137400	2.83792800
C	1.07849300	-1.44186600	-2.64894000
C	0.12074500	-0.87447500	3.47274300
C	-0.61867800	1.73821900	-3.35447500
C	-0.74791300	0.23340400	3.69457000
C	-0.34994700	0.36726400	-3.61786500
C	0.58296700	-2.63222200	2.04252000
C	-1.76061300	3.19755400	-1.96263500
C	-2.15021800	3.57637900	0.43179900
C	0.89512400	-3.02967900	-0.35139000
C	-0.40595100	-2.11555600	2.93168300
C	-1.93903000	2.15530500	-2.92596000

C	-2.65177700	3.30916100	-0.88064600
C	0.21347200	-3.31191000	0.87719500
C	-2.44718000	2.29058100	2.54878600
C	-0.05066400	-2.30767100	-2.53629000
C	-2.99697100	2.87172400	1.36876800
C	-0.09489300	-3.16054600	-1.40348200
C	-2.14864400	0.01523700	3.52475100
C	-1.44253700	-0.54198200	-3.61743100
C	-3.00181000	1.04291100	2.99434500
C	-1.28717200	-1.88420700	-3.12171000
C	-1.79778300	-2.32015200	2.67792600
C	-3.03204600	1.23303400	-2.83219500
C	-3.78497200	2.43522300	-0.78727500
C	-1.17325700	-3.58070300	0.62094000
C	-4.04343100	2.20954200	0.63442700
C	-1.35174800	-3.54712400	-0.82282000
C	-2.67948400	-1.26409100	3.11611500
C	-2.78161300	-0.10131600	-3.31380400
C	-2.19704700	-3.14235700	1.52160600
C	-4.03011600	1.42033100	-1.76321500
C	-4.11027900	0.41931800	2.31850200
C	-2.54865000	-2.31699800	-2.58198200
C	-4.65549700	1.00390100	1.09975200
C	-2.60000000	-3.15852000	-1.40292300
C	-3.93825400	-1.02532100	2.47080300
C	-3.49074000	-1.22626500	-2.77898200
C	-3.53025600	-2.95639700	0.94958600
C	-4.83352300	0.28205300	-1.32574900
C	-5.19823400	0.10228600	0.09801300
C	-3.73403100	-3.01746600	-0.51379700
C	-4.42378700	-1.92662500	1.47659300
C	-4.57391400	-1.03981800	-1.88285300
C	-5.15077400	-1.33842500	0.36337200
C	-4.74938100	-2.02522700	-0.83940100
Pr	-2.78925600	-0.65982000	0.00384300
Pr	1.17944900	0.68264000	-0.06492500
C	4.63364200	-0.27533100	-0.01547400
C	5.21886000	-1.59520500	-0.60124800
H	4.42704800	-2.21220000	-1.02576100
C	5.83308100	0.54241400	0.56472300
H	5.47647400	1.48191000	0.99221700
C	6.23304300	-1.26688200	-1.71900100
H	6.59813500	-2.20776000	-2.15161000
H	5.74363200	-0.71525300	-2.53250900

C	6.84070800	0.85929400	-0.56081600
H	7.65041800	1.47608700	-0.14875600
H	6.36003300	1.45406700	-1.34926800
C	6.53674100	-0.27069900	1.67198900
H	7.34606700	0.33768700	2.09707300
H	5.83844900	-0.48526400	2.49148300
C	7.40450100	-0.44839500	-1.14655900
H	8.12093000	-0.21791400	-1.94549600
C	5.92635600	-2.39685500	0.51235200
H	6.28974700	-3.34298200	0.08997000
H	5.21628300	-2.65747700	1.30772700
C	7.09797400	-1.58072400	1.08926400
H	7.59589900	-2.15530400	1.88076300
C	8.10561600	-1.25601400	-0.03396800
H	8.95048300	-0.68287500	0.37192100
H	8.52028300	-2.18533000	-0.44820100

triplet state (**¹D**):

C	3.07791300	2.04018000	0.86394100
C	3.31031300	1.85445200	-0.56742400
C	2.01423000	3.01851800	0.98870900
C	3.72208800	0.53105000	-0.97182000
C	3.02235300	0.80540200	1.67498700
C	2.29724100	2.61767300	-1.28939600
C	1.53054800	3.38967600	-0.33113200
C	3.46190900	-0.40344700	0.95952300
C	1.08453600	2.94691900	2.04500600
C	2.82614800	-0.13230100	-1.87891000
C	1.97113900	0.70166300	2.67770800
C	1.64624100	2.04594800	-2.44080400
C	1.09926500	1.81499900	2.93947600
C	1.94749900	0.65433200	-2.73021700
C	0.14224000	3.72195000	-0.55852900
C	2.55293300	-1.55114400	0.90735100
C	-0.27470700	3.37793900	1.87440800
C	2.18555800	-1.43863100	-1.66599800
C	1.44651100	-0.60007800	2.95893800
C	0.32681300	2.50128800	-2.74131000
C	1.72889100	-1.70948800	2.06439800
C	-0.38789000	3.39153100	-1.84446700
C	-0.77497600	3.77664700	0.58672300
C	2.05105400	-2.14488000	-0.37305500
C	-0.24268400	1.62327600	3.41268200
C	0.93092200	-0.21198200	-3.23875900
C	-1.08499500	2.61111800	2.78211900

C	1.08489600	-1.49542400	-2.61449600
C	0.12590000	-0.79349300	3.50100300
C	-0.64487100	1.65341700	-3.39322100
C	-0.74298900	0.31849000	3.69885900
C	-0.36001700	0.27945100	-3.62255000
C	0.60607100	-2.58401000	2.10979800
C	-1.78897800	3.14240300	-2.02935900
C	-2.16898700	3.57762800	0.35785600
C	0.92171900	-3.03241100	-0.27740700
C	-0.39055500	-2.04535200	2.99204500
C	-1.96349600	2.06704500	-2.96842200
C	-2.67418400	3.27226900	-0.95484600
C	0.24037300	-3.29412600	0.96721900
C	-2.45809100	2.33929400	2.50530500
C	-0.03684000	-2.36984600	-2.47767100
C	-3.00817700	2.89237900	1.31147600
C	-0.06829700	-3.19164100	-1.32172300
C	-2.14435100	0.09256000	3.53858800
C	-1.44646400	-0.63906500	-3.58996700
C	-3.00840500	1.10851500	2.98954700
C	-1.27834000	-1.97431200	-3.07094100
C	-1.77703200	-2.26114500	2.74760300
C	-3.04832700	1.14532400	-2.85253400
C	-3.80376800	2.39574000	-0.83846600
C	-1.14396000	-3.57288900	0.72075800
C	-4.04255300	2.19611200	0.58538400
C	-1.32499800	-3.55648200	-0.71925900
C	-2.66144000	-1.19424300	3.15527900
C	-2.78350100	-0.20266900	-3.29481700
C	-2.17063300	-3.10546600	1.60561500
C	-4.04580600	1.35169300	-1.78657000
C	-4.10439300	0.46057300	2.32106900
C	-2.53431700	-2.40166600	-2.51868200
C	-4.64859000	0.99749500	1.08433700
C	-2.57912900	-3.20144900	-1.31119800
C	-3.91893100	-0.97512800	2.49671300
C	-3.48583800	-1.32236500	-2.73302100
C	-3.49232000	-2.93209400	1.02692500
C	-4.83142500	0.21950400	-1.31608200
C	-5.17958500	0.06717000	0.10630800
C	-3.70461900	-3.03169700	-0.42078800
C	-4.38992400	-1.88605600	1.51828400
C	-4.56088900	-1.12150900	-1.83331300
C	-5.15304400	-1.36425800	0.40690400

C	-4.75174100	-2.07807900	-0.77115600
Pr	-2.67402100	-0.60779700	-0.03215700
Pr	1.07820300	0.60338000	-0.05745600
C	4.61854700	-0.23756500	-0.02472300
C	5.21636400	-1.56273000	-0.59001300
H	4.43157600	-2.19140100	-1.00993500
C	5.81615100	0.59322100	0.54810200
H	5.45457500	1.53694100	0.96088500
C	6.23316400	-1.24425000	-1.70851800
H	6.60382800	-2.18925900	-2.12732100
H	5.74401400	-0.70552000	-2.53080800
C	6.82699300	0.89945200	-0.57737900
H	7.63240200	1.52468600	-0.16939900
H	6.34700500	1.48228500	-1.37478900
C	6.52053500	-0.20138600	1.66815300
H	7.32547300	0.41714700	2.08705200
H	5.82143900	-0.40837500	2.48885500
C	7.39925500	-0.41298300	-1.14361200
H	8.11708900	-0.18996700	-1.94345800
C	5.92579000	-2.34627100	0.53533700
H	6.29649700	-3.29490400	0.12490500
H	5.21599400	-2.60252400	1.33224800
C	7.09081500	-1.51630300	1.10574200
H	7.58861100	-2.07758100	1.90690200
C	8.10076900	-1.20190700	-0.01809200
H	8.94117000	-0.61879300	0.38291100
H	8.52180600	-2.13465100	-0.41804100

13. Pr₂@D₂(10611)-C₇₂ (Ad) (E)(B3LYP/6-31G(d)~MWB48)
singlet state (^SE):

C	3.25789900	1.78602500	0.52130700
C	3.82889100	0.86306500	-0.44986100
C	2.44602600	2.71469700	-0.22691300
C	3.57592300	-0.82902600	0.63686800
C	2.80123500	1.22640100	1.80603100
C	3.05160000	0.95840600	-1.69380500
C	2.28763200	2.22281300	-1.58401500
C	2.88707700	-0.26682500	1.81288900
C	1.37654300	3.36193300	0.41609900
C	2.78535100	-1.71920800	-0.18318200
C	1.64512400	1.86934900	2.43068700
C	2.40455300	-0.20784900	-2.30548000
C	1.01973300	2.99932800	1.76878100
C	2.36900300	-1.50895000	-1.59196200
C	1.03149400	2.43539700	-2.26823000

C	1.81168800	-1.04996100	2.43248800
C	0.19456900	3.72474500	-0.30220200
C	1.80902500	-2.54401400	0.45184800
C	0.78249200	1.07867800	3.25737700
C	1.25243600	0.08094000	-3.12831700
C	0.89594800	-0.36994200	3.27954400
C	0.63192100	1.40705400	-3.16917900
C	-0.00635900	3.27333600	-1.65012100
C	1.34659200	-2.28904700	1.79162000
C	-0.38606300	3.27913200	1.90791100
C	1.22851600	-2.39223200	-1.78718400
C	-0.88847300	3.76671000	0.64574100
C	0.92883400	-3.05826800	-0.55543200
C	-0.60530000	1.39831300	3.44754500
C	0.19896300	-0.86617200	-3.38372900
C	-1.21296600	2.48181600	2.75319900
C	0.16226300	-2.11244800	-2.70389100
C	-0.40360300	-0.90772700	3.57155300
C	-0.74406200	1.24341400	-3.53376300
C	-1.36194700	3.11986500	-2.07637000
C	0.06369200	-2.82058800	2.12326200
C	-1.34087400	0.16485900	3.66392100
C	-1.02964000	-0.14865100	-3.66048900
C	-1.72636300	2.11983900	-3.03179300
C	-0.80290800	-2.14343000	3.03714600
C	-2.22854900	3.51411400	0.23594800
C	-0.37733800	-3.53300800	-0.23205300
C	-2.46386400	3.25947300	-1.14870400
C	-0.77683700	-3.46751100	1.13304100
C	-2.59451400	2.35561000	2.41245100
C	-1.11613100	-2.69624800	-2.45391600
C	-3.11000100	2.89487400	1.18270100
C	-1.37854900	-3.43188300	-1.24342400
C	-2.70520600	-0.00069100	3.26191500
C	-2.32050500	-0.68044700	-3.33380900
C	-3.03410600	1.62242600	-2.71817800
C	-2.16825600	-2.34835900	2.64270500
C	-3.52315300	2.38164800	-1.56803700
C	-2.15155000	-3.23000000	1.47809700
C	-3.35647600	1.17703300	2.74057500
C	-2.33798000	-2.02991900	-2.83668900
C	-3.15350700	-1.32213600	2.79082900
C	-3.38123600	0.24781100	-2.90481600
C	-4.23549000	2.10133100	0.76724800

C	-2.76758000	-3.28718100	-0.90240800
C	-4.45992600	1.82107400	-0.64439900
C	-3.17866600	-3.16993600	0.48588600
C	-4.43175700	1.07995000	1.79302300
C	-3.37254900	-2.47646200	-1.94678100
C	-4.31787400	-1.40458500	1.90722300
C	-4.48587100	-0.25708800	-2.09341200
C	-5.06975200	0.55377800	-1.00004100
C	-4.34846600	-2.36874700	0.78564700
C	-4.98667100	-0.18735300	1.45625200
C	-4.48559800	-1.64612700	-1.65666700
C	-5.40819600	-0.37684900	0.07634400
C	-5.03631500	-1.71308200	-0.31684800
Pr	-2.91291700	-0.37211000	-0.00792600
Pr	1.21199500	0.38628200	-0.03522900
C	4.79892600	-0.16701900	0.03493900
C	5.55420400	-0.98854600	-1.04621100
H	4.85633100	-1.36965800	-1.79459200
C	5.84289500	0.35546700	1.06589800
H	5.34089000	0.93822900	1.84248100
C	6.59198000	-0.08386000	-1.74707900
H	7.09293200	-0.66345200	-2.53367300
H	6.09257100	0.75831600	-2.24402100
C	6.87659800	1.24986700	0.34881200
H	7.58370500	1.64454200	1.09031700
H	6.38006800	2.11690200	-0.10745400
C	6.56044500	-0.84337600	1.72078600
H	7.26555200	-0.46935700	2.47488300
H	5.83770300	-1.47778300	2.25084900
C	7.62094500	0.43381100	-0.72456800
H	8.35513500	1.07295100	-1.23143500
C	6.27894400	-2.17793400	-0.37872000
H	6.78040400	-2.77098200	-1.15475000
H	5.55352600	-2.84283000	0.10795200
C	7.30464900	-1.66126600	0.64829700
H	7.81433100	-2.51131400	1.11959800
C	8.33861300	-0.76092400	-0.06129300
H	9.08266100	-0.39936300	0.66173900
H	8.88536200	-1.33940900	-0.81852900
triplet state (^T E):			
C	3.26303300	1.82517800	0.41175300
C	3.82988300	0.84886300	-0.49989200
C	2.42566400	2.68994700	-0.37508300
C	3.57504900	-0.75930700	0.64225300

C	2.78912500	1.33132300	1.71139200
C	3.02610300	0.86283600	-1.73018200
C	2.26454200	2.12344900	-1.70417000
C	2.88414900	-0.14514200	1.80553800
C	1.36814500	3.38713100	0.22504800
C	2.77849500	-1.70136700	-0.10878700
C	1.64175500	2.01276400	2.30978500
C	2.38495000	-0.32654300	-2.28493400
C	1.01476500	3.10944000	1.59861100
C	2.35930900	-1.58885900	-1.51630500
C	1.01940900	2.30379000	-2.40516100
C	1.82802000	-0.89928100	2.47909300
C	0.18347900	3.70406900	-0.51330800
C	1.81651900	-2.50089200	0.58286300
C	0.78026500	1.26169700	3.17172300
C	1.23134500	-0.08729600	-3.12324100
C	0.90960800	-0.17791700	3.29397500
C	0.61949300	1.22892900	-3.25387900
C	-0.01709200	3.17887000	-1.83657100
C	1.36435600	-2.17724900	1.91358800
C	-0.38952400	3.38986600	1.72465100
C	1.23132100	-2.49376100	-1.66142500
C	-0.89438500	3.79276200	0.43061800
C	0.93811800	-3.08178300	-0.38672000
C	-0.60722100	1.59838200	3.36732100
C	0.18531100	-1.06125900	-3.33284300
C	-1.21489700	2.64314700	2.61531100
C	0.16109900	-2.26820900	-2.58428400
C	-0.38685500	-0.69869400	3.62468100
C	-0.75692200	1.03817500	-3.60583100
C	-1.36854100	2.98839200	-2.24144100
C	0.08437600	-2.68394800	2.27335600
C	-1.33216300	0.38039200	3.66002000
C	-1.04195400	-0.36636100	-3.65195000
C	-1.73565200	1.93006400	-3.14431100
C	-0.78492800	-1.95527000	3.15539800
C	-2.23752900	3.51721600	0.03955600
C	-0.36470500	-3.54611700	-0.02935300
C	-2.47021800	3.18431400	-1.32871700
C	-0.75572300	-3.39872100	1.33251000
C	-2.59724500	2.49599000	2.28235600
C	-1.11547000	-2.84111100	-2.29210800
C	-3.11964800	2.96661100	1.02277700
C	-1.36995600	-3.51449600	-1.04063500

C	-2.69191600	0.18871200	3.26590900
C	-2.32647100	-0.87997300	-3.28846300
C	-3.04364700	1.45249900	-2.80368900
C	-2.14915400	-2.19094000	2.78152800
C	-3.52260900	2.27073700	-1.69518500
C	-2.12929500	-3.13121600	1.66732800
C	-3.34478900	1.33110400	2.67033000
C	-2.33558800	-2.19715900	-2.70311500
C	-3.13480200	-1.15760300	2.86393100
C	-3.38840100	0.06733800	-2.90608400
C	-4.23445000	2.13834700	0.65215600
C	-2.75616800	-3.34780000	-0.70149400
C	-4.45802800	1.76487500	-0.73626800
C	-3.16225400	-3.13715000	0.67614800
C	-4.42104400	1.17331900	1.72804100
C	-3.36775500	-2.59433800	-1.78329700
C	-4.29128300	-1.29369900	1.98732500
C	-4.48322600	-0.38953100	-2.06041700
C	-5.05344500	0.47381900	-1.01226100
C	-4.32275100	-2.31220600	0.92851300
C	-4.96424500	-0.10897000	1.45752500
C	-4.47855200	-1.75158300	-1.53341200
C	-5.41596900	-0.39020700	0.11064800
C	-5.04207400	-1.73884100	-0.20305800
Pr	-2.79983100	-0.36426400	-0.01092600
Pr	1.07961900	0.35410600	-0.02984100
C	4.81187600	-0.15411200	0.03371400
C	5.56811100	-1.01734600	-1.01088600
H	4.87090200	-1.43020100	-1.74366700
C	5.84720100	0.41523100	1.04480400
H	5.33892900	1.02792600	1.79404400
C	6.60633400	-0.13950100	-1.74504500
H	7.11204100	-0.74929700	-2.50529000
H	6.10626800	0.68017000	-2.27742900
C	6.88022400	1.28189900	0.29556600
H	7.58459300	1.70899300	1.02174700
H	6.38152900	2.12656300	-0.19781000
C	6.56397900	-0.75522200	1.75100800
H	7.26565800	-0.35059200	2.49236300
H	5.83894700	-1.36807400	2.30336200
C	7.63004500	0.42297500	-0.74057700
H	8.36482600	1.04197200	-1.27116600
C	6.29337400	-2.17681300	-0.29340700
H	6.80010000	-2.79973300	-1.04220700

H	5.56748800	-2.82299200	0.21735100
C	7.31346400	-1.61549300	0.71542900
H	7.82382400	-2.44373500	1.22350700
C	8.34792000	-0.74173300	-0.02594000
H	9.08793900	-0.34899400	0.68487300
H	8.89944200	-1.34932200	-0.75652900
14. Pr ₂ @D ₂ (10611)-C ₇₂ (Ad) (F)(B3LYP/6-31G(d)~MWB48)			
singlet state (^S F):			
C	3.37112100	1.85172700	0.50932000
C	2.68296000	2.86269200	-0.22772900
C	2.73572600	1.75474500	1.83544000
C	2.43304600	2.39247600	-1.56436700
C	3.72835500	0.78494300	-0.44884900
C	1.65307400	3.45375800	0.57204400
C	1.67151800	2.77070000	1.86109400
C	2.95680800	1.03571500	-1.70027800
C	2.43763900	0.46241400	2.42752500
C	1.23938900	2.80354200	-2.17118200
C	3.28407400	-1.03800800	0.40706100
C	0.43409900	3.88264000	-0.05096100
C	2.67139200	-0.83111500	1.73092100
C	0.28105500	3.62642000	-1.46273700
C	0.42155600	2.60413900	2.58307300
C	2.11975400	0.04386500	-2.40962600
C	1.20351100	0.31643700	3.18115200
C	0.53682900	1.91949500	-3.04702900
C	2.44166200	-1.74265400	-0.54115200
C	-0.73505100	3.90454000	0.75651400
C	2.03212500	-1.31612100	-1.89928400
C	-0.72060400	3.30246000	2.07956600
C	0.20717600	1.35756900	3.31595600
C	0.93714100	0.54209600	-3.17113200
C	1.60774500	-1.71451900	2.13990200
C	-1.00539400	3.34582300	-2.02075200
C	0.76838800	-1.05271800	3.08318800
C	-0.84885400	2.32388800	-3.03306100
C	1.47274700	-2.68992600	-0.08059500
C	-2.03240700	3.69852300	0.18486500
C	1.05893000	-2.72430400	1.28011900
C	-2.17570100	3.38311100	-1.19801500
C	0.90548800	-2.15769900	-2.24608800
C	-2.05093900	2.82591100	2.33474900
C	-1.13191400	0.94420500	3.60536900
C	-0.11817600	-0.36023600	-3.54036900

C	0.56084800	-2.99738200	-1.14534600
C	-2.86798000	3.04736000	1.17933500
C	-2.25795500	1.68913500	3.12597700
C	-0.11896900	-1.71595300	-3.10072300
C	-0.58777900	-1.46352300	3.29207400
C	-1.88565100	1.39212200	-3.29636700
C	-1.52619300	-0.44925200	3.61831600
C	-1.50095300	0.06109500	-3.62587300
C	-0.24201400	-3.21514000	1.55414000
C	-3.26458500	2.53322500	-1.56126500
C	-1.05286200	-2.61619300	2.58485900
C	-3.14457800	1.57765700	-2.63041500
C	-0.77964500	-3.44016900	-0.88938400
C	-3.92335600	2.15186200	0.82940100
C	-3.34003600	0.79170800	2.82499300
C	-1.47164400	-2.15702200	-2.89513400
C	-2.89478300	-0.54858800	3.18754600
C	-2.34466000	-1.05302600	-3.27762800
C	-1.11923500	-3.65221300	0.49098000
C	-4.18633700	2.00904600	-0.58679800
C	-1.82933600	-3.04857100	-1.83561400
C	-4.22049300	1.01772800	1.71978000
C	-2.43517000	-2.75564400	2.21424600
C	-4.03950000	0.48323400	-2.37078700
C	-3.38948300	-1.70333400	2.50656900
C	-3.64307600	-0.88241900	-2.69614300
C	-2.46539500	-3.47185400	0.94886100
C	-4.74934000	0.80392000	-1.12971200
C	-3.21115200	-2.99648800	-1.37539700
C	-4.89203600	-0.16086000	1.16502300
C	-4.50516300	-1.51919400	1.59929300
C	-4.14288000	-1.95120100	-1.85161500
C	-3.51384200	-3.25034000	0.02424200
C	-5.20460100	-0.23168700	-0.26257600
C	-4.59756200	-2.38043300	0.43141000
C	-4.99616800	-1.60231900	-0.71209200
Pr	-2.73865100	-0.71078600	-0.12586700
Pr	1.18041900	0.69572000	0.15060700
C	4.57075800	-0.39688700	-0.06653600
C	5.29139700	-1.11958000	-1.23764700
H	4.58462800	-1.31234400	-2.04868500
C	5.60998100	-0.12556200	1.05783400
H	5.12608600	0.38581600	1.89509500
C	6.43535500	-0.22588800	-1.76558000

H	6.91264200	-0.72714400	-2.61781500
H	6.03453500	0.72457400	-2.14193100
C	6.75421300	0.75522800	0.51217800
H	7.46224700	0.96323700	1.32517700
H	6.36456100	1.72517100	0.17605400
C	6.18520900	-1.47252100	1.54852400
H	6.89025800	-1.28216900	2.36822500
H	5.38573500	-2.10247500	1.95997300
C	7.46385200	0.03267400	-0.64824300
H	8.27557800	0.66299400	-1.03314900
C	5.87261100	-2.45850100	-0.73528200
H	6.35184900	-2.97874300	-1.57482300
H	5.06779300	-3.11290200	-0.37589900
C	6.89451400	-2.19752300	0.38831400
H	7.30158500	-3.15206700	0.74537600
C	8.03771900	-1.31110500	-0.15014700
H	8.78125800	-1.13335300	0.63888900
H	8.55906300	-1.82466800	-0.96963400
triplet state (^T F):			
C	3.38764600	1.86626200	0.54528000
C	2.68952900	2.88627900	-0.16933900
C	2.71873300	1.71370200	1.83993700
C	2.42297400	2.43234000	-1.50414500
C	3.73161700	0.81673900	-0.42658800
C	1.64222400	3.44829400	0.63872400
C	1.65659300	2.74032300	1.90807700
C	2.94926700	1.07210200	-1.66119000
C	2.41983800	0.41964600	2.40904300
C	1.23394100	2.85358800	-2.11520600
C	3.26777600	-1.03075100	0.38275400
C	0.42311500	3.88651800	0.01898400
C	2.65395700	-0.85550500	1.70262400
C	0.27005500	3.66412800	-1.39943000
C	0.41302500	2.55434400	2.62848400
C	2.12802400	0.09234700	-2.39659500
C	1.19479500	0.25462400	3.18057400
C	0.53667500	1.97656100	-3.00365100
C	2.43921600	-1.72757500	-0.57397600
C	-0.74891500	3.86710100	0.82271500
C	2.04266900	-1.28240800	-1.92152600
C	-0.73438900	3.25931600	2.14046700
C	0.20176600	1.29400400	3.33993900
C	0.94594700	0.60162300	-3.15538100
C	1.61205400	-1.75813500	2.11013600

C	-1.01487500	3.38267500	-1.96005500
C	0.77014000	-1.11233900	3.06960600
C	-0.84860500	2.36712000	-2.97710000
C	1.48300300	-2.69790500	-0.12753900
C	-2.05486000	3.68590500	0.24420800
C	1.07140800	-2.75099200	1.23313700
C	-2.19240200	3.40103800	-1.14646500
C	0.92354800	-2.12665500	-2.28888300
C	-2.06326800	2.78000100	2.38397800
C	-1.13452800	0.87039700	3.60782600
C	-0.10450900	-0.29282200	-3.53259500
C	0.57986800	-2.99709900	-1.20211800
C	-2.88470700	3.02081700	1.22300500
C	-2.26763400	1.62709900	3.14280500
C	-0.10160100	-1.66493000	-3.12117400
C	-0.58503000	-1.52870700	3.26721500
C	-1.88614200	1.44201400	-3.27290000
C	-1.52456000	-0.51959400	3.60791800
C	-1.48849900	0.12077900	-3.62736000
C	-0.23470000	-3.24580000	1.49799000
C	-3.27891200	2.55956000	-1.53542800
C	-1.04675600	-2.67340100	2.54464100
C	-3.15067800	1.62085600	-2.62551000
C	-0.75761900	-3.43425000	-0.95415200
C	-3.92974900	2.12527300	0.85111300
C	-3.34563700	0.73206700	2.82721300
C	-1.45321300	-2.11648400	-2.93845000
C	-2.89221100	-0.60918900	3.16071300
C	-2.32273000	-1.00574800	-3.29772700
C	-1.10463900	-3.66115400	0.42735300
C	-4.18391800	2.00416400	-0.56778100
C	-1.81158000	-3.02428300	-1.89249500
C	-4.21879300	0.96860800	1.71660300
C	-2.42752200	-2.80601700	2.16707000
C	-4.02634100	0.51085300	-2.37500000
C	-3.38684000	-1.75985200	2.46660000
C	-3.62167300	-0.84540300	-2.70971900
C	-2.45483900	-3.49442400	0.88605600
C	-4.73114100	0.79764200	-1.12967700
C	-3.18970900	-2.97885300	-1.43342100
C	-4.87622000	-0.19943900	1.14446200
C	-4.49126400	-1.55710400	1.55304900
C	-4.11215700	-1.92524100	-1.87975700
C	-3.50307500	-3.25562800	-0.03399600

C	-5.17514000	-0.25525700	-0.28991800
C	-4.59842600	-2.41016600	0.37419600
C	-4.99265600	-1.61438900	-0.75224700
Pr	-2.61167000	-0.72920800	-0.09599900
Pr	1.05318900	0.74435300	0.12272100
C	4.55833500	-0.38043000	-0.06918100
C	5.28772100	-1.07655100	-1.25173800
H	4.58958600	-1.24266300	-2.07618500
C	5.58834300	-0.14927300	1.07341300
H	5.09889000	0.34084600	1.91983800
C	6.44220500	-0.17464800	-1.74193300
H	6.92559400	-0.65401200	-2.60331300
H	6.05027200	0.78845300	-2.09457000
C	6.74383200	0.73944100	0.56605900
H	7.44466000	0.91801600	1.39229200
H	6.36380300	1.72126600	0.25546600
C	6.15119200	-1.51269900	1.53188600
H	6.84855100	-1.34934000	2.36403300
H	5.34430800	-2.14960300	1.91737400
C	7.46100000	0.04630300	-0.60754600
H	8.27981100	0.68260300	-0.96690900
C	5.85798700	-2.43198800	-0.78185000
H	6.34410000	-2.92975600	-1.63107400
H	5.04757500	-3.09384700	-0.44967500
C	6.86933900	-2.20861000	0.35931800
H	7.26741100	-3.17528700	0.69326200
C	8.02281700	-1.31402900	-0.14208000
H	8.75917300	-1.16301200	0.65918200
H	8.54951600	-1.80761000	-0.97039800

15. Pr₂@D₂(10611)-C₇₂ (Ad) (G)(B3LYP/6-31G(d)~MWB48)

singlet state (^SG):

C	-2.24212300	3.31425700	0.01710300
C	-3.14246200	2.21610700	0.24215000
C	-1.41119100	3.51119000	1.16180000
C	-3.24761000	1.49953700	-1.05936700
C	-1.68045400	3.25100500	-1.30276800
C	-2.84323500	1.66644000	1.61353100
C	-1.73411000	2.50421600	2.14425600
C	-2.27194600	2.09032200	-1.95686100
C	-0.08441300	3.93991300	0.95988300
C	-3.51054600	0.08509100	-1.11390100
C	-0.30884600	3.61870500	-1.51730100
C	-2.82383000	0.22708900	1.90006500
C	0.45326500	4.05829800	-0.37883900

C	-3.27439800	-0.73639800	0.88439400
C	-0.65696100	1.98211600	2.96770400
C	-1.46623200	1.27715700	-2.85837100
C	0.96179900	3.51284600	1.83552000
C	-2.50385200	-0.74220900	-1.74763800
C	0.38609900	2.96595200	-2.58082200
C	-1.78402100	-0.23503200	2.77198800
C	-0.20549800	1.81924300	-3.25755200
C	-0.78569000	0.62603800	3.37722800
C	0.70447800	2.53595100	2.84939700
C	-1.59078500	-0.18038300	-2.74351800
C	1.86309000	3.80502400	-0.29698200
C	-2.32825800	-1.76869800	0.48421300
C	2.19133500	3.50991000	1.07789000
C	-2.02890600	-1.87789300	-0.93629300
C	1.80130500	2.75871800	-2.51858900
C	-1.17821000	-1.54032700	2.63782000
C	2.54632600	3.14868500	-1.36555200
C	-1.38995300	-2.28865300	1.45041200
C	0.87650800	0.96491200	-3.65905300
C	0.34905800	-0.17930900	3.71622100
C	1.81914000	1.72082800	3.24258200
C	-0.50887700	-0.99282300	-3.17812000
C	2.11698800	1.52269000	-3.21498400
C	0.13192500	-1.51250500	3.25013400
C	1.64053300	0.37422600	3.68905200
C	0.70919000	-0.42634600	-3.67219800
C	3.24938900	2.62040000	1.40372800
C	-0.87579500	-2.64968300	-1.35871200
C	3.08071400	1.77466200	2.53948900
C	-0.17821600	-2.24189800	-2.53100000
C	3.69056600	2.35860400	-1.03485700
C	-0.36421200	-3.16070200	1.02054300
C	4.07131300	2.12939000	0.33170800
C	-0.12758600	-3.37363500	-0.37866900
C	3.21700300	0.68863400	-2.84590000
C	1.21669800	-2.31840900	2.76808300
C	2.75215200	-0.42383300	3.25950600
C	1.80318500	-1.29325600	-3.34062700
C	3.69253200	0.47039800	2.58706400
C	1.23614000	-2.46220700	-2.67927800
C	4.08540700	1.21017500	-1.81257900
C	0.89481900	-3.24422100	1.71801600
C	3.08685700	-0.77193400	-2.98156700

C	2.58428700	-1.77839200	2.83544100
C	4.77056600	0.87376600	0.41307100
C	1.27152600	-3.67256300	-0.55470700
C	4.58228900	0.00146100	1.56933900
C	1.98919000	-3.20019300	-1.71813200
C	4.84407700	0.34473500	-0.95310500
C	1.87891100	-3.65973700	0.76446200
C	3.93725400	-1.63670200	-2.16155300
C	3.60377300	-2.30627000	1.93593700
C	4.64823400	-1.43399900	1.35275400
C	3.39398700	-2.87883000	-1.57565800
C	4.86739500	-1.06314600	-1.18841200
C	3.23534000	-3.28652800	0.92588100
C	4.88450000	-1.92164000	-0.01057900
C	4.00933200	-3.03609700	-0.26899800
Pr	2.62486900	-0.88840100	-0.06681200
Pr	-1.10854700	0.82886600	0.02969400
C	-4.43966100	-0.53813700	-0.07941700
C	-5.60834900	0.36635300	0.42753200
H	-5.23396800	1.32552000	0.78347000
C	-5.09387100	-1.88250600	-0.55338700
H	-4.32475600	-2.56147200	-0.92533800
C	-6.61392100	0.62900700	-0.71587600
H	-7.39710600	1.30433200	-0.34653300
H	-6.12216300	1.14356700	-1.55159500
C	-6.09364700	-1.60534800	-1.69533700
H	-6.49589300	-2.56220100	-2.05426600
H	-5.58157500	-1.13870600	-2.54745100
C	-5.82737500	-2.56194000	0.62137000
H	-6.22840400	-3.52570700	0.28031900
H	-5.12378000	-2.78262500	1.43500800
C	-7.23107200	-0.69816500	-1.19364200
H	-7.94018000	-0.50461200	-2.00879700
C	-6.34310200	-0.32599300	1.59735500
H	-7.12448800	0.35074100	1.96816800
H	-5.65605200	-0.50221200	2.43505800
C	-6.96257200	-1.65427300	1.12725600
H	-7.48124000	-2.13813100	1.96486200
C	-7.96010200	-1.38368100	-0.01894100
H	-8.41240800	-2.32691800	-0.35504400
H	-8.78049900	-0.74637700	0.33871400
triplet state (^T G):			
C	-2.22393200	3.33922200	0.07287400
C	-3.12915600	2.24592100	0.28149200

C	-1.37725300	3.50679100	1.20826600
C	-3.22517400	1.53947000	-1.00937700
C	-1.65582800	3.28308900	-1.24291900
C	-2.80104900	1.65820500	1.62195300
C	-1.69940700	2.47467500	2.17424100
C	-2.25203800	2.13854300	-1.91165700
C	-0.05532600	3.94329000	1.02138100
C	-3.51177700	0.13234700	-1.09855800
C	-0.28497100	3.65679900	-1.45344700
C	-2.80138000	0.21897900	1.88757700
C	0.48407300	4.08700400	-0.31517900
C	-3.27582300	-0.73480000	0.87267800
C	-0.63878200	1.94083800	2.99636900
C	-1.46261400	1.33908700	-2.83116700
C	0.98862400	3.48569400	1.88969500
C	-2.51609400	-0.69759400	-1.75839200
C	0.40401300	3.00183000	-2.51725000
C	-1.76609300	-0.26451100	2.75858000
C	-0.19850800	1.88019700	-3.22730300
C	-0.77683500	0.57773800	3.38795800
C	0.72619600	2.49261900	2.88984000
C	-1.60132400	-0.12178400	-2.75077000
C	1.88775900	3.81304100	-0.23923700
C	-2.34415500	-1.77121300	0.45374700
C	2.21180100	3.48097600	1.13184300
C	-2.04532100	-1.85203100	-0.97269200
C	1.82505500	2.79925700	-2.47304500
C	-1.17556100	-1.57873000	2.60573300
C	2.57035500	3.17027400	-1.31363900
C	-1.39848800	-2.30213500	1.40551900
C	0.87686300	1.03224000	-3.64549100
C	0.35619800	-0.24174100	3.70980600
C	1.83065200	1.66388900	3.25851800
C	-0.51951100	-0.92661100	-3.19099800
C	2.12862300	1.57972800	-3.18998900
C	0.13296100	-1.57046600	3.21767500
C	1.64305200	0.30223300	3.68183000
C	0.70587000	-0.35377600	-3.67953700
C	3.27346500	2.58536500	1.44447100
C	-0.89192100	-2.62029200	-1.41089900
C	3.09511800	1.72382700	2.56701600
C	-0.19658200	-2.19191200	-2.57715200
C	3.71558600	2.37299500	-0.99594800
C	-0.37488400	-3.17046500	0.95544100

C	4.10196700	2.12131200	0.37028300
C	-0.14685800	-3.37117500	-0.44865300
C	3.22107400	0.73626100	-2.83396100
C	1.20992100	-2.37023700	2.72277900
C	2.75484300	-0.49301200	3.24620600
C	1.79461800	-1.23098400	-3.36553800
C	3.69152000	0.40843600	2.58819500
C	1.22239900	-2.40231900	-2.72127200
C	4.08855200	1.23296700	-1.78753600
C	0.88191800	-3.26951800	1.64743500
C	3.07870200	-0.72202500	-2.98669800
C	2.58248000	-1.84043900	2.79757600
C	4.77695300	0.85240500	0.42885500
C	1.25039300	-3.67025200	-0.63082300
C	4.58054100	-0.04661000	1.55871900
C	1.97344300	-3.16863700	-1.77786400
C	4.83592100	0.34104100	-0.93966400
C	1.86403700	-3.67648400	0.68564200
C	3.91535500	-1.60167400	-2.18310900
C	3.59637800	-2.35228700	1.88717300
C	4.63336800	-1.47655800	1.31254200
C	3.37347800	-2.84322000	-1.62317200
C	4.84734100	-1.05641000	-1.18986800
C	3.22196100	-3.30890600	0.84912100
C	4.89401700	-1.95215800	-0.05026900
C	4.00973200	-3.04714500	-0.32823600
Pr	2.51680600	-0.87064900	-0.04017700
Pr	-1.02434500	0.73038000	-0.00507000
C	-4.44462800	-0.50569200	-0.07714900
C	-5.59800800	0.39620200	0.46625600
H	-5.20862500	1.34081400	0.84391800
C	-5.11560800	-1.82934800	-0.58232100
H	-4.35673300	-2.50448000	-0.98149900
C	-6.61256700	0.70124600	-0.65790300
H	-7.38509600	1.37352100	-0.26139100
H	-6.12433500	1.23433000	-1.48399200
C	-6.12492900	-1.50956000	-1.70531900
H	-6.54053700	-2.45184600	-2.08690200
H	-5.61757100	-1.02374600	-2.54956300
C	-5.84365700	-2.53533000	0.57968400
H	-6.25794500	-3.48502500	0.21563200
H	-5.13385500	-2.78558100	1.37920000
C	-7.24788300	-0.60597700	-1.16551300
H	-7.96373200	-0.38308100	-1.96723600

C	-6.32723000	-0.32250600	1.62374000
H	-7.09837100	0.35063600	2.02148200
H	-5.63301600	-0.52858000	2.44860000
C	-6.96436200	-1.63134800	1.12371500
H	-7.47892200	-2.13379900	1.95293500
C	-7.97133700	-1.31789900	-0.00318100
H	-8.43733100	-2.24622500	-0.36152200
H	-8.78106400	-0.68266500	0.38157000

16. Pr₂@D₂(10611)-C₇₂ (Ad) (**H**)(B3LYP/6-31G(d)~MWB48)

singlet state (**^SH**):

C	-2.81284800	2.79916400	-0.73046200
C	-2.82664900	2.77943200	0.71886100
C	-1.63046200	3.49914800	-1.13994500
C	-3.28434200	1.47213500	1.15429900
C	-3.21723300	1.49223500	-1.24439300
C	-1.63536700	3.44107400	1.20383000
C	-0.89483300	3.91607200	0.03414900
C	-3.72688600	0.78007200	-0.05214200
C	-0.93214800	3.00976700	-2.26205600
C	-2.51778200	0.83478800	2.22041700
C	-2.36614900	0.87728700	-2.29064100
C	-0.92866700	2.86922800	2.31781100
C	-1.31357600	1.73216200	-2.85288300
C	-1.42640700	1.60371900	2.84858300
C	0.54697900	3.98630500	0.01958700
C	-3.05914200	-1.31584900	-0.00596500
C	0.48831100	3.17242000	-2.34411400
C	-2.12186700	-0.58157200	2.26878300
C	-2.06387300	-0.55576400	-2.30733600
C	0.47488500	3.12261000	2.38075200
C	-2.35446900	-1.53054700	-1.23378200
C	1.19384600	3.73203600	1.26565300
C	1.25197400	3.66748500	-1.22826600
C	-2.30705100	-1.58944300	1.22319800
C	-0.10141600	1.20031800	-3.42906600
C	-0.48193500	0.67239700	3.39409800
C	0.99112800	2.09728600	-3.15803200
C	-0.91395100	-0.65574200	3.07829400
C	-0.86149300	-1.05598200	-2.96070800
C	1.38251500	2.22504400	3.03471300
C	0.12911200	-0.20019100	-3.51634600
C	0.91735400	0.98093800	3.53636000
C	-1.35269100	-2.54703600	-1.28451200
C	2.54559800	3.26066600	1.31731400

C	2.61099000	3.23011200	-1.14167000
C	-1.32538300	-2.62516600	1.14984300
C	-0.45361800	-2.30316700	-2.35245700
C	2.68182200	2.33206900	2.39667900
C	3.25847000	3.05006900	0.12258300
C	-0.91241800	-3.17055100	-0.10733500
C	2.32691800	1.61930700	-3.02419000
C	0.03884700	-1.72387600	2.99769300
C	3.15998000	2.24822700	-2.05173100
C	-0.21036600	-2.74896100	2.05131400
C	1.48270500	-0.66299600	-3.54596800
C	1.84154000	-0.10195700	3.55934300
C	2.57790100	0.24242900	-3.32866700
C	1.40448000	-1.45110600	3.33366800
C	0.90855000	-2.74395700	-2.28634200
C	3.57571300	1.21974300	2.31349200
C	4.19552600	1.96871900	0.02394700
C	0.44246800	-3.62774800	-0.00723700
C	4.18132200	1.50599200	-1.36286400
C	0.86010200	-3.42744300	1.37527100
C	1.86006600	-1.94830100	-3.01300300
C	3.17746700	0.03482700	3.02949100
C	1.35968100	-3.48517100	-1.09657600
C	4.41784200	1.06970600	1.11247800
C	3.66396800	-0.48019300	-2.71625700
C	2.48682100	-2.18573700	2.72586900
C	4.48986800	0.15136700	-1.69588400
C	2.22743600	-3.18896100	1.70958400
C	3.23405200	-1.86838200	-2.60101200
C	3.61097800	-1.26670500	2.61279800
C	2.78014100	-3.47252100	-0.75048100
C	4.94108900	-0.24948600	0.76897800
C	5.03055400	-0.68771700	-0.64234900
C	3.21075400	-3.37712900	0.66258900
C	3.72446200	-2.69909600	-1.55162100
C	4.56564700	-1.41187600	1.56886400
C	4.71102400	-2.11522600	-0.65990500
C	4.40936300	-2.54713700	0.68287600
Pr	2.57855400	-0.98282400	-0.04116800
Pr	-1.06165300	1.14341800	0.05367600
C	-4.37884500	-0.57110400	-0.02196600
C	-5.27760700	-0.81742300	1.23200000
H	-4.70823700	-0.62307100	2.14421900
C	-5.25302900	-0.86913100	-1.28293700

H	-4.66068700	-0.70521800	-2.18717500
C	-6.50334900	0.12086000	1.19546300
H	-7.09843800	-0.04051100	2.10409500
H	-6.18650000	1.17159600	1.20980700
C	-6.47621500	0.07237500	-1.30535700
H	-7.05326000	-0.12086300	-2.21942900
H	-6.15566600	1.12111200	-1.35169800
C	-5.74035300	-2.33391100	-1.25416600
H	-6.31759000	-2.53386600	-2.16662800
H	-4.88666700	-3.02340700	-1.26333400
C	-7.35089800	-0.16408600	-0.05908600
H	-8.21647700	0.51037800	-0.08163300
C	-5.76278000	-2.28413900	1.24708400
H	-6.35525800	-2.45098400	2.15646700
H	-4.90890600	-2.97211200	1.29685300
C	-6.61124700	-2.57440300	-0.00588000
H	-6.94984800	-3.61827100	0.01206700
C	-7.83081800	-1.63011400	-0.03561900
H	-8.44744200	-1.83965100	-0.92044500
H	-8.46469000	-1.80568300	0.84441800
triplet state (^T H):			
C	2.79384900	2.81977700	0.68582900
C	2.80383000	2.77890300	-0.75455300
C	1.60385700	3.50638100	1.08691400
C	3.24116100	1.47228100	-1.17051100
C	3.18782700	1.51837000	1.21407600
C	1.59558300	3.41474100	-1.24236300
C	0.86119300	3.91730100	-0.09310900
C	3.69939400	0.78970200	0.03953300
C	0.91470000	3.04250900	2.21628400
C	2.48712600	0.81931100	-2.22755300
C	2.35925000	0.92518500	2.28324700
C	0.89791800	2.83155100	-2.35085300
C	1.30435300	1.78231600	2.83905300
C	1.39865200	1.56730200	-2.87321200
C	-0.57468500	3.98745900	-0.07898000
C	3.06573800	-1.28007800	0.02566400
C	-0.51038600	3.19926200	2.29595600
C	2.10945300	-0.60005600	-2.26451200
C	2.06422300	-0.50782400	2.32156900
C	-0.50832000	3.08155600	-2.41729600
C	2.36591200	-1.49183200	1.26259700
C	-1.22306200	3.71481000	-1.32278500
C	-1.27857000	3.68570700	1.17498300

C	2.30822600	-1.58564800	-1.20074400
C	0.09923800	1.25590300	3.42306500
C	0.47037400	0.62347600	-3.42432100
C	-1.00302700	2.14265600	3.12620900
C	0.91238300	-0.69805600	-3.08359100
C	0.87047200	-1.00757700	2.99564600
C	-1.40898400	2.16612100	-3.06962700
C	-0.12393900	-0.14332700	3.53200400
C	-0.93029800	0.91994900	-3.55563100
C	1.37177600	-2.51256300	1.32692300
C	-2.57017600	3.22556400	-1.36042900
C	-2.62700800	3.23640300	1.09872800
C	1.34492700	-2.62997800	-1.10802900
C	0.46867100	-2.26001000	2.39860200
C	-2.69901600	2.26692100	-2.42691600
C	-3.27904500	3.02961700	-0.17143200
C	0.93701900	-3.16084300	0.16458400
C	-2.33963700	1.65845000	3.00789100
C	-0.02996900	-1.77293500	-2.97628600
C	-3.17028300	2.27094900	2.02313800
C	0.23206500	-2.77547400	-2.00717500
C	-1.47752400	-0.60960500	3.56332400
C	-1.84686100	-0.17231900	-3.55240900
C	-2.58278900	0.28883200	3.33888000
C	-1.39782900	-1.51977600	-3.31268300
C	-0.88567400	-2.70847700	2.34154100
C	-3.58978700	1.15820100	-2.33048700
C	-4.21136100	1.94464200	-0.05445300
C	-0.41188600	-3.62860700	0.07480900
C	-4.17618200	1.50040400	1.33084100
C	-0.83504200	-3.43793200	-1.30699200
C	-1.84369600	-1.90087900	3.04946600
C	-3.17791300	-0.03822300	-3.02351900
C	-1.33341600	-3.46540300	1.15810300
C	-4.42750600	1.02099600	-1.12602600
C	-3.65730400	-0.44973300	2.73143200
C	-2.47190800	-2.25139400	-2.69146200
C	-4.47897400	0.14845500	1.69192500
C	-2.20601800	-3.22680200	-1.64967900
C	-3.21770400	-1.83328000	2.63046200
C	-3.60207200	-1.33983600	-2.58447500
C	-2.74637300	-3.45920400	0.80866000
C	-4.92793500	-0.29431500	-0.75643500
C	-5.00515300	-0.71143200	0.65190300

C	-3.18311800	-3.39325400	-0.59469800
C	-3.69742100	-2.66803800	1.58844400
C	-4.54211100	-1.47467800	-1.53146700
C	-4.70694900	-2.14117300	0.69720900
C	-4.40508900	-2.59671600	-0.62992800
Pr	-2.47397600	-0.93460800	0.01838900
Pr	0.96186400	1.05112100	-0.03877300
C	4.38701800	-0.54348700	0.02309800
C	5.27834600	-0.79084600	-1.23333600
H	4.69842900	-0.61949800	-2.14355200
C	5.26989200	-0.80961200	1.28263500
H	4.67834600	-0.64498700	2.18745500
C	6.48453200	0.17276000	-1.21707700
H	7.07807800	0.01170400	-2.12675800
H	6.14543300	1.21624800	-1.24327500
C	6.47416000	0.15642500	1.28591600
H	7.06133700	-0.01412000	2.19803500
H	6.13227700	1.19869200	1.32165600
C	5.78426200	-2.26502300	1.26942900
H	6.36944900	-2.44353500	2.18127700
H	4.94292900	-2.96965600	1.29068600
C	7.34485200	-0.07833300	0.03635200
H	8.19705800	0.61326200	0.04453900
C	5.79086700	-2.24793400	-1.23176500
H	6.37984500	-2.41683300	-2.14300200
H	4.94907300	-2.95187400	-1.26544500
C	6.65300000	-2.50429100	0.01934600
H	7.01304900	-3.54105900	0.01301600
C	7.85335300	-1.53482800	0.02873900
H	8.47977500	-1.72043500	0.91201200
H	8.48482100	-1.70927300	-0.85323900

17. Pr₂@D₂(10611)-C₇₂ (Ad) (I)(B3LYP/6-31G(d)~MWB48)

singlet state (^SI):

C	-2.70145700	2.81271900	-0.29624000
C	-3.34786500	1.81561700	0.50021200
C	-1.70470900	3.46867600	0.49297600
C	-3.72813100	0.72183900	-0.42458500
C	-2.41991400	2.30026600	-1.61811100
C	-2.68327100	1.75879600	1.81808300
C	-1.65893700	2.83591100	1.79030000
C	-2.95444700	0.92507400	-1.68746400
C	-0.53346200	3.92135000	-0.14512500
C	-3.31413800	-0.89505300	0.41093500
C	-1.17407900	2.67416700	-2.22941600

C	-2.33265600	0.47824200	2.44085700
C	-0.29472000	3.58200100	-1.53065600
C	-2.65661600	-0.77289100	1.74417700
C	-0.37832200	2.73335300	2.46382500
C	-2.16586300	-0.11920600	-2.36902600
C	0.71198400	3.93048900	0.55142500
C	-2.45525800	-1.74746400	-0.41639000
C	-0.58278300	1.72635500	-3.11569800
C	-1.11865300	0.45869500	3.22300200
C	-1.08611900	0.35867500	-3.19766700
C	-0.20347600	1.58981900	3.29686600
C	0.81492900	3.34757900	1.85873100
C	-1.98034600	-1.47003000	-1.75680600
C	1.12910300	3.50588900	-1.70544800
C	-1.71447500	-1.86277200	1.79483700
C	1.75716300	3.76595500	-0.43257400
C	-1.63186200	-2.48338600	0.50465700
C	0.82961600	1.70552000	-3.34702500
C	-0.31354000	-0.72717400	3.41432800
C	1.70268100	2.57284900	-2.62180800
C	-0.58596400	-1.90353800	2.67489000
C	0.03889900	-0.45986700	-3.56175800
C	1.10202300	1.08540000	3.61645400
C	2.10446400	2.83468300	2.21645900
C	-0.83674800	-2.25715300	-2.15656500
C	1.21846700	0.34357800	-3.65536300
C	1.05539400	-0.33920700	3.68648200
C	2.24612100	1.72439100	3.10459400
C	0.14016900	-1.77049100	-3.07578900
C	2.99717900	3.16111700	-0.09235600
C	-0.48940500	-3.23278100	0.10658400
C	3.19156500	2.76792600	1.26448700
C	-0.14338100	-3.17302300	-1.26709600
C	3.01521900	2.08782500	-2.33998900
C	0.49487400	-2.76751700	2.34106700
C	3.68043100	2.40900000	-1.10740700
C	0.52742000	-3.46167000	1.08040900
C	2.50722600	-0.17388100	-3.30897400
C	2.16704300	-1.14308100	3.25930700
C	3.39287600	0.95244900	2.71903100
C	1.42466100	-2.34372900	-2.77352800
C	4.02708100	1.64335700	1.59713700
C	1.23039000	-3.27441700	-1.67210200
C	3.44722800	0.77480200	-2.75571700

C	1.84984000	-2.42726900	2.69477800
C	2.63023400	-1.58811900	-2.92153800
C	3.40634800	-0.47186800	2.82398100
C	4.59108700	1.34210800	-0.78102200
C	1.89701800	-3.62228500	0.67711200
C	4.78290200	0.93524000	0.60873300
C	2.27243400	-3.51693900	-0.72030800
C	4.49838500	0.36412400	-1.86702200
C	2.71431700	-3.04858300	1.73111500
C	3.76720400	-2.00236700	-2.09914300
C	4.33636800	-1.17575300	1.94409100
C	5.06783800	-0.46449000	0.86973200
C	3.58693200	-3.00263900	-1.02739500
C	4.74127000	-1.02153900	-1.62604600
C	3.98266700	-2.49341200	1.43313100
C	5.13370500	-1.38518900	-0.27328400
C	4.45306100	-2.60595400	0.07216200
Pr	2.75162100	-0.70361200	-0.08508500
Pr	-1.13610400	0.75170400	0.08986700
C	-4.65242400	-0.38032900	-0.04621800
C	-5.67874900	-0.06910900	1.06948600
H	-5.19158000	0.48158200	1.88033900
C	-5.34663300	-1.15638000	-1.18832700
H	-4.63108900	-1.37370100	-1.98615300
C	-6.82694300	0.78073300	0.48365300
H	-7.54117700	1.01810200	1.28296400
H	-6.43932200	1.73737100	0.10856400
C	-6.49519300	-0.29288000	-1.75547300
H	-6.96956100	-0.83041100	-2.58692100
H	-6.09768500	0.64389500	-2.16841600
C	-5.91537300	-2.47818500	-0.62966400
H	-6.38864900	-3.03973800	-1.44566500
H	-5.10342800	-3.10631700	-0.24057200
C	-7.52636300	0.00447700	-0.64917800
H	-8.34267700	0.61149100	-1.06077000
C	-6.24172300	-1.39985500	1.61376500
H	-6.95120200	-1.18443800	2.42333400
H	-5.43553000	-2.00395000	2.05009100
C	-6.94151200	-2.17720200	0.48098600
H	-7.34270100	-3.11910900	0.87605800
C	-8.09006900	-1.32251000	-0.09667100
H	-8.60573300	-1.87361000	-0.89501700
H	-8.83661800	-1.11775100	0.68284900

triplet state (**T**):

C	-2.75038900	2.79864900	-0.33735500
C	-3.34378500	1.79947400	0.49032200
C	-1.74201500	3.48554300	0.42719100
C	-3.65594000	0.61325000	-0.36603500
C	-2.44289000	2.23237200	-1.65459200
C	-2.66798200	1.78152000	1.76420800
C	-1.67379700	2.87915600	1.74529700
C	-2.91066600	0.84979200	-1.66825500
C	-0.54657000	3.89468300	-0.22806200
C	-3.28410200	-0.79507400	0.37197900
C	-1.19726400	2.60632400	-2.28895700
C	-2.31111200	0.51283700	2.40250900
C	-0.30503300	3.52809500	-1.60742000
C	-2.63834400	-0.71795000	1.72584200
C	-0.38843200	2.77466800	2.42951500
C	-2.14735500	-0.17525700	-2.33932200
C	0.70447700	3.89740800	0.46898500
C	-2.45689900	-1.75292700	-0.40288000
C	-0.59049500	1.63387700	-3.14018500
C	-1.12919000	0.50706200	3.21701000
C	-1.08772000	0.27678900	-3.20030600
C	-0.21600700	1.64538400	3.28381800
C	0.81431600	3.35554500	1.80299400
C	-1.98201400	-1.52524800	-1.72974800
C	1.12327500	3.43854500	-1.77634900
C	-1.76895700	-1.84239200	1.82240300
C	1.74858900	3.71207100	-0.50846500
C	-1.69947400	-2.51033700	0.53403000
C	0.83401000	1.61119000	-3.38539700
C	-0.34362700	-0.68007500	3.41580700
C	1.70437500	2.48949400	-2.67513200
C	-0.63754100	-1.86739700	2.69625200
C	0.03226200	-0.55472400	-3.55451400
C	1.08822000	1.13305900	3.59459300
C	2.09941000	2.85186000	2.16865300
C	-0.86179700	-2.33028700	-2.12983800
C	1.21805800	0.25133700	-3.66284200
C	1.03259500	-0.29563100	3.68046300
C	2.23472300	1.75389400	3.07817400
C	0.12608700	-1.85639500	-3.06251300
C	2.99644900	3.11865300	-0.15326300
C	-0.54912800	-3.26019200	0.15334800
C	3.18700200	2.75778400	1.21282800
C	-0.18449900	-3.21373400	-1.21912900

C	3.01780600	2.01208900	-2.38392600
C	0.44855400	-2.73354400	2.36807600
C	3.68360400	2.35760000	-1.15185900
C	0.47652000	-3.46538200	1.12773600
C	2.50569400	-0.26496600	-3.31103700
C	2.13262500	-1.11128800	3.27637100
C	3.37537400	0.96601600	2.70548300
C	1.40677700	-2.42180600	-2.74190700
C	4.00120100	1.62768300	1.56554900
C	1.20394400	-3.30969500	-1.61286200
C	3.44075200	0.69012700	-2.76765600
C	1.80273900	-2.40124200	2.72391100
C	2.61827900	-1.67074200	-2.89126000
C	3.38019600	-0.45669300	2.83116200
C	4.57590100	1.28587100	-0.79983100
C	1.84710500	-3.64508800	0.73582700
C	4.75053800	0.89119000	0.58856800
C	2.24130000	-3.56187200	-0.66050200
C	4.47984900	0.28690600	-1.85739200
C	2.66768600	-3.05038200	1.77732900
C	3.73914600	-2.07574800	-2.05344700
C	4.29708300	-1.18245800	1.96128500
C	5.02292200	-0.50177700	0.87394000
C	3.56035100	-3.05718300	-0.97094300
C	4.70458400	-1.08580200	-1.57693600
C	3.94179300	-2.51019000	1.46951600
C	5.12263300	-1.44769900	-0.23818300
C	4.44120200	-2.65885700	0.12166800
Pr	2.60574200	-0.77879400	-0.03878300
Pr	-0.84048000	1.06935800	0.05149600
C	-4.69881100	-0.40766900	-0.03993600
C	-5.70404900	-0.08981500	1.07955300
H	-5.21250300	0.47515600	1.87799800
C	-5.37495300	-1.19714700	-1.17097600
H	-4.65841800	-1.41276800	-1.96909100
C	-6.86373100	0.74432200	0.49173700
H	-7.57684800	0.98403500	1.29156800
H	-6.48323100	1.69883200	0.10470500
C	-6.53549600	-0.34966600	-1.74039200
H	-7.01134100	-0.89881700	-2.56360800
H	-6.14700000	0.58662700	-2.16291900
C	-5.92855900	-2.51985200	-0.59683800
H	-6.40432400	-3.09409500	-1.40276200
H	-5.10711100	-3.13539900	-0.20763500

C	-7.56171700	-0.05066800	-0.62943000
H	-8.38702100	0.54356600	-1.04199600
C	-6.25086700	-1.42060600	1.64153700
H	-6.95892300	-1.20689700	2.45301800
H	-5.43381400	-2.01045300	2.07722300
C	-6.94880600	-2.21599500	0.51918100
H	-7.33935400	-3.15758900	0.92581000
C	-8.10894200	-1.37764100	-0.05976100
H	-8.62457300	-1.94182600	-0.84900800
H	-8.85228900	-1.17181300	0.72256300

18. Pr₂@D₂(10611)-C₇₂ (Ad) (J)(B3LYP/6-31G(d)~MWB48)

singlet state (^SJ):

C	-1.35197100	4.10250400	0.01006700
C	-2.49454100	3.21554800	0.03759300
C	-0.66232300	3.98099900	1.27583700
C	-2.55676700	2.51579000	-1.23917400
C	-0.66285500	3.96884900	-1.26160000
C	-2.51168300	2.48905300	1.30517200
C	-1.35142900	2.98530800	2.08381400
C	-1.42569600	2.97324600	-2.05608700
C	0.75709400	4.01171100	1.26554000
C	-2.93749400	1.15377900	-1.22211800
C	0.78801800	3.93378700	-1.25881700
C	-2.86541800	1.09133200	1.31262600
C	1.48263000	4.06635300	0.00833600
C	-3.42839500	0.47327600	0.04832700
C	-0.59197600	2.09361900	2.93675800
C	-0.72713200	2.02711000	-2.91608700
C	1.51136800	3.22168100	2.19578300
C	-2.27024500	0.22539400	-2.08761800
C	1.43208700	3.15520200	-2.27275800
C	-2.18227700	0.27018300	2.24348500
C	0.67077200	2.25560500	-3.13499800
C	-1.13083800	0.78037600	3.11326100
C	0.86694600	2.26570100	3.05418200
C	-1.21344800	0.64410000	-2.99052000
C	2.74700600	3.40922100	0.22428900
C	-3.01269300	-1.10346500	-0.21669400
C	2.78441400	2.92685600	1.58040000
C	-2.33079400	-1.09942400	-1.55907500
C	2.73175900	2.57836400	-2.07925300
C	-1.93068400	-1.15260400	2.05544500
C	3.39550600	2.67708900	-0.81897100
C	-2.21809000	-1.79563300	0.83665800

C	1.55182900	1.19002900	-3.51106900
C	-0.31146300	-0.32926300	3.50334200
C	1.65537600	1.14103400	3.45464400
C	-0.32249900	-0.38267400	-3.41976200
C	2.82279200	1.36962800	-2.87367200
C	-0.77905900	-1.51554900	2.86054200
C	1.06699800	-0.14056800	3.70323300
C	1.05467200	-0.10749600	-3.70652700
C	3.52727800	1.76331000	1.92929400
C	-1.35766800	-2.06676800	-1.90819400
C	2.98566700	0.90849200	2.93533300
C	-0.40473700	-1.73343800	-2.91830200
C	4.24817000	1.59637200	-0.44672300
C	-1.35555000	-2.84716900	0.44212100
C	4.35287000	1.16519800	0.92137400
C	-0.98118400	-3.05946500	-0.93753600
C	3.61359300	0.24830500	-2.46907600
C	0.12666600	-2.54161000	2.45101800
C	1.99915200	-1.16889100	3.34050900
C	1.84070700	-1.25267200	-3.35794800
C	3.23112400	-0.50834000	2.91346100
C	0.91253900	-2.29565800	-2.92224700
C	4.43004800	0.44065200	-1.29435700
C	-0.25077600	-3.26832600	1.27199600
C	3.14311300	-1.11415200	-2.78279000
C	1.56299200	-2.39742200	2.75646500
C	4.67442900	-0.23908600	0.94086700
C	0.32208300	-3.65226200	-0.96269800
C	4.10569600	-1.11427900	1.95558800
C	1.30877900	-3.28122600	-1.96764700
C	4.80371000	-0.66086300	-0.45317900
C	0.72509500	-3.87432900	0.42067000
C	3.62280000	-2.23550700	-1.97966200
C	2.54085600	-3.11393600	1.94541800
C	3.83627400	-2.49331300	1.58910600
C	2.70833900	-3.34134700	-1.61403800
C	4.51068700	-2.00237700	-0.84180900
C	2.09457200	-3.89336500	0.79275200
C	4.14124600	-2.92208800	0.21926700
C	3.07109400	-3.75832700	-0.26238000
Pr	2.19177500	-1.39349400	0.01249800
Pr	-0.50290100	1.70479900	-0.04991900
C	-4.45432000	-0.63371700	-0.03893500
C	-5.21092400	-1.05460000	1.23150400

H	-4.55316700	-1.01813300	2.10431200
C	-5.39227200	-0.68026600	-1.25752000
H	-4.85548900	-0.37749900	-2.16127600
C	-6.40082700	-0.09269700	1.45171500
H	-6.93063700	-0.37841600	2.37031300
H	-6.03652100	0.93284600	1.59902000
C	-6.57979400	0.27815200	-1.01965600
H	-7.24005600	0.26250300	-1.89722800
H	-6.21697200	1.30910100	-0.91113200
C	-5.91234300	-2.12403100	-1.42923900
H	-6.56525600	-2.17296000	-2.31092100
H	-5.07211600	-2.80571700	-1.61463000
C	-7.35337900	-0.15235500	0.24176800
H	-8.19934600	0.52776000	0.40525700
C	-5.73613300	-2.49596400	1.04717400
H	-6.26234300	-2.80970300	1.95870900
H	-4.89593800	-3.18885700	0.90889500
C	-6.68495200	-2.55495100	-0.16645000
H	-7.05632700	-3.58001000	-0.29374000
C	-7.87310700	-1.59535000	0.06291600
H	-8.56576700	-1.64279200	-0.78874900
H	-8.44026300	-1.90340400	0.95219200
triplet state (TJ):			
C	1.34573600	4.10504300	0.06516000
C	2.48671200	3.23603200	0.02374800
C	0.65049600	4.00989400	-1.19740000
C	2.51906900	2.48570800	1.27029300
C	0.63641600	3.92284900	1.33554400
C	2.48748600	2.52037200	-1.24253600
C	1.34183000	3.02715600	-2.02499000
C	1.38540200	2.91794400	2.09990200
C	-0.77571600	4.01880200	-1.18479200
C	2.91454100	1.14516300	1.24941600
C	-0.81294100	3.89506500	1.33622900
C	2.85384000	1.12778700	-1.28184400
C	-1.50956200	4.04762200	0.06954200
C	3.40884200	0.48649400	-0.02485700
C	0.59610500	2.14539600	-2.90127100
C	0.70856100	1.96569100	2.95037500
C	-1.52231300	3.23251000	-2.12808900
C	2.26833500	0.19680300	2.11226400
C	-1.45262500	3.08388600	2.33072300
C	2.19972100	0.32326900	-2.23745400
C	-0.69329100	2.18225000	3.17453600

C	1.14704200	0.84167600	-3.10368800
C	-0.86932400	2.29886300	-3.01185900
C	1.21138900	0.59069400	3.02103800
C	-2.76710400	3.37845300	-0.16206100
C	3.02997500	-1.07690500	0.21192000
C	-2.79398500	2.91615200	-1.52286000
C	2.35208400	-1.11332100	1.56256600
C	-2.76024900	2.50336000	2.12675800
C	1.96036900	-1.10742300	-2.06874400
C	-3.41513400	2.61999000	0.86590300
C	2.24393400	-1.75846600	-0.85587800
C	-1.56685900	1.10255700	3.53489300
C	0.32961100	-0.26597300	-3.49954200
C	-1.64760400	1.18342400	-3.44000600
C	0.32917600	-0.44712100	3.43550800
C	-2.84095200	1.28399900	2.89318000
C	0.80601600	-1.45980700	-2.86651300
C	-1.04500200	-0.09112800	-3.70895400
C	-1.06026000	-0.18764500	3.71698900
C	-3.53394000	1.75486400	-1.90192300
C	1.38335900	-2.09568500	1.89484600
C	-2.97693400	0.92745600	-2.92255600
C	0.42215000	-1.77542600	2.89885600
C	-4.26016300	1.54192100	0.46835700
C	1.38365100	-2.81842600	-0.47884400
C	-4.35990400	1.13705800	-0.91136200
C	1.00909500	-3.06207800	0.90031400
C	-3.62526700	0.16449100	2.47059700
C	-0.08718000	-2.50521500	-2.48644300
C	-1.96755100	-1.13650000	-3.36421900
C	-1.83886800	-1.33301600	3.34221300
C	-3.19497200	-0.49332300	-2.91560000
C	-0.90467300	-2.34579700	2.87548800
C	-4.43005400	0.37104800	1.29274200
C	0.29396100	-3.24513100	-1.31658800
C	-3.14069400	-1.19733400	2.75917000
C	-1.52267100	-2.36874600	-2.79313800
C	-4.65869700	-0.27147200	-0.95361300
C	-0.28210200	-3.67688900	0.91220100
C	-4.06814500	-1.12585200	-1.96752800
C	-1.28183200	-3.33075800	1.91553200
C	-4.78374400	-0.72178000	0.42629000
C	-0.68046800	-3.87955600	-0.47549300
C	-3.59666800	-2.30478100	1.93028400

C	-2.49025900	-3.10091700	-1.98961600
C	-3.78454900	-2.50267200	-1.62084800
C	-2.68069400	-3.39545000	1.54865300
C	-4.47022700	-2.05985700	0.78283100
C	-2.04550600	-3.89529000	-0.84655700
C	-4.11220700	-2.97823400	-0.27681200
C	-3.04270500	-3.80861000	0.19903500
Pr	-2.07311500	-1.36917600	-0.00895000
Pr	0.30554800	1.71156800	-0.00904600
C	4.47145000	-0.59549800	0.04802300
C	5.23340400	-0.98463200	-1.22799400
H	4.57544100	-0.94393000	-2.10027300
C	5.40871800	-0.64559800	1.26595500
H	4.86815400	-0.36289600	2.17385500
C	6.41109400	-0.00454300	-1.43297600
H	6.94447900	-0.26996600	-2.35553700
H	6.03328200	1.01811800	-1.56503000
C	6.58419300	0.33150400	1.04312200
H	7.24359800	0.31081500	1.92120100
H	6.20806200	1.35909400	0.94988200
C	5.94819900	-2.08497700	1.41695300
H	6.60168800	-2.13740000	2.29795800
H	5.11730300	-2.78068000	1.59260700
C	7.36387500	-0.07042200	-0.22373700
H	8.20116600	0.62271000	-0.37643600
C	5.77676900	-2.42227300	-1.06470300
H	6.30666200	-2.71547100	-1.98082600
H	4.94517200	-3.12747000	-0.93720700
C	6.72617300	-2.48729800	0.14819000
H	7.11040600	-3.50937600	0.26022300
C	7.90196200	-1.50928500	-0.06621400
H	8.59502700	-1.56070400	0.78486100
H	8.47318200	-1.79679300	-0.95972000

19. Pr₂@D₂(10611)-C₇₂ (Ad) (**K**)(B3LYP/6-31G(d)~MWB48)

singlet state (**^SK**):

C	1.98549300	3.58262800	0.55660200
C	2.78013700	2.81328800	-0.36612300
C	0.84048000	4.11353100	-0.14970900
C	3.23981400	1.62779100	0.31773500
C	1.87834100	2.85320500	1.80607600
C	2.12317500	2.82134000	-1.67749700
C	0.88721800	3.64036300	-1.52795000
C	2.65889200	1.61236800	1.64252700
C	-0.39283900	4.12858800	0.55284200

C	3.50836700	0.41257000	-0.47552600
C	0.60886000	2.85554300	2.50042200
C	2.06614000	1.53858200	-2.36939000
C	-0.49056100	3.58086100	1.90017400
C	2.71272000	0.39174100	-1.77901000
C	-0.35952200	3.26754800	-2.18748000
C	2.19965000	0.36786900	2.28223900
C	-1.63510200	3.90853900	-0.12322300
C	3.08158700	-0.99162500	0.27098100
C	0.29425300	1.71114700	3.28887900
C	0.89165600	1.30780600	-3.17058100
C	1.10417100	0.50590800	3.20647800
C	-0.27062300	2.18301300	-3.12220700
C	-1.64632200	3.46766600	-1.49423900
C	2.38374200	-0.90364300	1.59941900
C	-1.84545600	3.14042000	2.07525700
C	2.10378200	-0.90642100	-1.92887500
C	-2.56287700	3.37061400	0.84611200
C	2.28319300	-1.71455700	-0.77570400
C	-1.07044100	1.31505800	3.51921600
C	0.41298600	-0.01381800	-3.45487300
C	-2.14837400	2.00527200	2.89468000
C	1.00397500	-1.14420100	-2.83618300
C	0.23368600	-0.59529800	3.48526800
C	-1.41962500	1.39431700	-3.47214300
C	-2.77951200	2.68362000	-1.89168700
C	1.49311000	-1.97081100	1.89923400
C	-1.10921800	-0.12182100	3.67686600
C	-1.02021100	0.03996700	-3.68126500
C	-2.67102800	1.66997300	-2.89326900
C	0.44297500	-1.82866600	2.86349000
C	-3.63350900	2.52033700	0.45371100
C	1.35814900	-2.73892000	-0.45788000
C	-3.77572800	2.23858000	-0.93739500
C	1.03982300	-2.94996300	0.92044400
C	-3.30940900	1.24294100	2.56963000
C	0.18374900	-2.27659300	-2.60042300
C	-4.07457300	1.51873900	1.38268200
C	0.37084300	-3.09079500	-1.43355600
C	-2.23603800	-0.90732000	3.28471400
C	-1.87586900	-1.05739600	-3.34916000
C	-3.56953900	0.59373500	-2.58193600
C	-0.66305600	-2.66459300	2.50371100
C	-4.31093600	0.98118200	-1.38135500

C	-0.26498600	-3.39521800	1.30039700
C	-3.39770500	-0.17020300	2.84531700
C	-1.22632900	-2.26823200	-2.92864400
C	-2.01286000	-2.26060300	2.74221300
C	-3.23165300	-0.76866000	-2.83828500
C	-4.70072200	0.29836900	0.94747500
C	-0.89980200	-3.64197900	-1.05669900
C	-4.82718500	0.00312000	-0.47390200
C	-1.25250000	-3.79623400	0.34092800
C	-4.33784800	-0.73403300	1.91793200
C	-1.87200400	-3.18763600	-2.04150100
C	-3.03751800	-2.86220400	1.88976300
C	-3.91958500	-1.77398000	-2.03533700
C	-4.76831500	-1.38724500	-0.88594000
C	-2.64581600	-3.67083100	0.71262400
C	-4.23194300	-2.10090000	1.52393400
C	-3.23060400	-3.00782600	-1.67733600
C	-4.56883600	-2.41026900	0.14381200
C	-3.61784300	-3.38400300	-0.33516900
Pr	-2.40563700	-1.19449500	0.02799800
Pr	0.69873200	1.51395400	-0.08324400
C	4.52535300	-0.62972800	-0.07219500
C	5.47894700	-0.29972500	1.08898300
H	4.96360400	0.28423200	1.85707600
C	5.25973900	-1.44875000	-1.14687200
H	4.58902800	-1.67473700	-1.98014100
C	5.98055300	-1.62344300	1.70880000
H	6.64616300	-1.39891900	2.55305000
H	5.13489400	-2.19589000	2.11160800
C	5.76367000	-2.76526600	-0.51683100
H	6.27219100	-3.36538500	-1.28333500
H	4.91355700	-3.35935300	-0.15666300
C	6.45999000	-0.62827700	-1.67024600
H	6.97315300	-1.20020200	-2.45509800
H	6.10694300	0.30311200	-2.13289500
C	6.72838800	-2.45086700	0.64407800
H	7.08514300	-3.38790500	1.09084300
C	6.68006600	0.50895600	0.55082600
H	7.35083600	0.75870700	1.38385100
H	6.33495900	1.45925600	0.12195800
C	7.42906900	-0.31716300	-0.51327900
H	8.28311700	0.25890000	-0.89235800
C	7.92836500	-1.63777100	0.11237500
H	8.47924300	-2.22363300	-0.63632100

H	8.63047700	-1.42394400	0.93011000
triplet state (^T K):			
C	1.99228500	3.62029600	0.45893200
C	2.76968500	2.82784300	-0.44582400
C	0.82582000	4.10341000	-0.24625200
C	3.20582700	1.64928700	0.24845300
C	1.87873900	2.91045800	1.72089900
C	2.07714100	2.77086500	-1.73768700
C	0.85832900	3.58103200	-1.61722500
C	2.65122100	1.66524500	1.58453700
C	-0.39921400	4.13901900	0.45014400
C	3.48100900	0.41762400	-0.50898700
C	0.61484000	2.92965700	2.42386100
C	2.02323200	1.47568500	-2.39878300
C	-0.49517100	3.63500700	1.81684900
C	2.69301200	0.34923800	-1.80733700
C	-0.38661900	3.20672900	-2.27192400
C	2.20522500	0.43593100	2.25456200
C	-1.65041000	3.89037700	-0.21921900
C	3.08257200	-0.97429300	0.27143300
C	0.29942900	1.79332800	3.22721600
C	0.85290800	1.22832900	-3.19905500
C	1.11944400	0.58779900	3.18411800
C	-0.29891900	2.10025900	-3.17987000
C	-1.66973200	3.42432800	-1.58438500
C	2.39109200	-0.85432000	1.60186800
C	-1.84363600	3.19176400	2.00449800
C	2.09861500	-0.95560300	-1.92831100
C	-2.56422900	3.37901000	0.76090900
C	2.29067700	-1.73578200	-0.75653600
C	-1.06044600	1.40641100	3.48830000
C	0.38316600	-0.10964600	-3.46000300
C	-2.14469500	2.08027100	2.85236100
C	0.98949500	-1.21616400	-2.81818200
C	0.25553700	-0.50413500	3.49975100
C	-1.44948000	1.29503800	-3.50523200
C	-2.79689800	2.62471000	-1.94901300
C	1.50608800	-1.90952900	1.93243400
C	-1.09121400	-0.02671100	3.68386400
C	-1.04406400	-0.06949800	-3.68711100
C	-2.68952400	1.57827900	-2.92969400
C	0.46258800	-1.75048700	2.90671100
C	-3.64295200	2.51851800	0.39867300
C	1.36890000	-2.74876100	-0.40531100

C	-3.78488600	2.20391300	-0.98419400
C	1.05281400	-2.91793900	0.98180700
C	-3.30761900	1.30907600	2.55156600
C	0.17240800	-2.34578500	-2.54516300
C	-4.08370400	1.55293200	1.35959300
C	0.37546700	-3.13422200	-1.36249000
C	-2.21472900	-0.81979800	3.31277100
C	-1.89380400	-1.15791200	-3.32281600
C	-3.58799100	0.50767900	-2.58720800
C	-0.63994300	-2.59699200	2.57445200
C	-4.30903700	0.92338800	-1.39500100
C	-0.24809200	-3.34766800	1.37973400
C	-3.37761600	-0.09611800	2.85378800
C	-1.23642300	-2.35282200	-2.86589700
C	-1.98918400	-2.18687400	2.79757800
C	-3.24649400	-0.86160500	-2.80869300
C	-4.68962000	0.31437000	0.95342600
C	-0.89044800	-3.68211900	-0.96342300
C	-4.81116900	-0.02922100	-0.45323700
C	-1.24154600	-3.79425400	0.43898600
C	-4.31177600	-0.68994900	1.93724100
C	-1.87441200	-3.25643200	-1.95094000
C	-3.00748500	-2.81001600	1.96341200
C	-3.91760800	-1.84170400	-1.96911000
C	-4.73947000	-1.42728100	-0.82357200
C	-2.62982400	-3.65334800	0.81376500
C	-4.19629300	-2.05667100	1.56878900
C	-3.22897300	-3.07224600	-1.57747000
C	-4.56379100	-2.43275600	0.22195400
C	-3.62439000	-3.41998500	-0.23281100
Pr	-2.26338900	-1.19120400	0.01711000
Pr	0.57337600	1.46967500	-0.04805300
C	4.51700800	-0.60335300	-0.07624200
C	5.46910600	-0.23472300	1.07443300
H	4.94958000	0.35991400	1.83134700
C	5.26179800	-1.43297100	-1.13571300
H	4.59329700	-1.68441900	-1.96316200
C	5.98588600	-1.53924300	1.72293700
H	6.64990700	-1.28829200	2.56094100
H	5.14700800	-2.11186900	2.13940400
C	5.77928800	-2.73048400	-0.47747400
H	6.29314900	-3.34196200	-1.23136500
H	4.93496800	-3.32470500	-0.10423500
C	6.45294000	-0.61117300	-1.67677100

H	6.97144100	-1.19396100	-2.45006400
H	6.08980000	0.30656700	-2.15838800
C	6.74144300	-2.38169000	0.67564500
H	7.10810800	-3.30524800	1.14208000
C	6.66143500	0.57474000	0.51886700
H	7.32900000	0.84940900	1.34663800
H	6.30634500	1.51184300	0.06963900
C	7.41939800	-0.26590700	-0.52732500
H	8.26741500	0.31088500	-0.91859000
C	7.93244900	-1.56775700	0.12594500
H	8.48907100	-2.16372100	-0.61041800
H	8.63294200	-1.32960500	0.93839200
20. #10611 C ₇₂ (B3LYP/6-31G(d))			
C	-4.41994900	0.71306900	-0.13718500
C	-4.41994800	-0.71306900	0.13718400
C	-3.86426200	-0.93214500	1.42113000
C	-3.56371000	0.37723900	1.99733400
C	-3.91980800	1.38343100	0.99636400
C	-3.86426200	0.93214500	-1.42113000
C	-3.56371100	-0.37723900	-1.99733500
C	-3.91980800	-1.38343100	-0.99636400
C	-3.09524700	-2.50062300	-0.81164900
C	-2.67882600	-2.88125000	0.49919800
C	-2.98549000	-2.04717300	1.62637400
C	-1.97581000	-1.88114000	2.61279600
C	-1.74834200	-0.62702400	3.23951800
C	-2.44564600	0.56122200	2.83086100
C	-1.66816500	1.82492300	2.73699000
C	-2.00889400	2.76115300	1.73278900
C	-3.09524700	2.50062300	0.81164900
C	-2.67882600	2.88125000	-0.49919800
C	-2.98549100	2.04717300	-1.62637400
C	-1.97581000	1.88114000	-2.61279600
C	-1.74834100	0.62702400	-3.23951800
C	-2.44564600	-0.56122300	-2.83086100
C	-1.66816500	-1.82492300	-2.73699000
C	-2.00889300	-2.76115300	-1.73279000
C	-0.98580800	-3.47180700	-1.01037300
C	-1.37397100	-3.50556300	0.37082900
C	-0.38761000	-3.39616400	1.38416800
C	-0.69702000	-2.58794300	2.52594200
C	0.30316900	-1.81880600	3.16224000
C	-0.34756100	-0.59006700	3.59760200
C	0.34754600	0.59021200	3.59757300

C	-0.30317000	1.81893200	3.16216800
C	0.69702300	2.58804200	2.52584300
C	0.38761700	3.39622000	1.38403500
C	-0.98580900	3.47180700	1.01037300
C	-1.37397200	3.50556400	-0.37082900
C	-0.38761000	3.39616400	-1.38416800
C	-0.69702000	2.58794300	-2.52594200
C	0.30316900	1.81880600	-3.16223900
C	-0.34756100	0.59006700	-3.59760100
C	0.34754700	-0.59021200	-3.59757200
C	-0.30316900	-1.81893300	-3.16216800
C	0.69702300	-2.58804300	-2.52584200
C	0.38761800	-3.39622000	-1.38403500
C	1.37398100	-3.50556100	-0.37070000
C	0.98581300	-3.47176000	1.01052100
C	2.00888400	-2.76107500	1.73289800
C	1.66816000	-1.82481000	2.73707100
C	2.44564300	-0.56110300	2.83089500
C	1.74834000	0.62714900	3.23949800
C	1.97581300	1.88124500	2.61273200
C	2.98549600	2.04723100	1.62630700
C	2.67882900	2.88126900	0.49909100
C	1.37398100	3.50556100	0.37070000
C	0.98581300	3.47176000	-1.01052100
C	2.00888300	2.76107500	-1.73289800
C	1.66816000	1.82481000	-2.73707100
C	2.44564300	0.56110300	-2.83089500
C	1.74834000	-0.62715000	-3.23949800
C	1.97581300	-1.88124500	-2.61273200
C	2.98549600	-2.04723000	-1.62630600
C	2.67883000	-2.88126800	-0.49909100
C	3.09523900	-2.50056800	0.81173700
C	3.91981300	-1.38338800	0.99641600
C	3.56371100	-0.37714900	1.99735800
C	3.86426000	0.93219600	1.42111200
C	4.41994800	0.71306300	0.13715400
C	3.91981200	1.38338800	-0.99641600
C	3.09523800	2.50056900	-0.81173700
C	3.56371200	0.37714900	-1.99735800
C	3.86426000	-0.93219600	-1.42111100
C	4.41994900	-0.71306300	-0.13715400
21. #10610C ₇₂ (B3LYP/6-31G(d))			
C	4.29017300	-0.29819000	-1.11457400
C	4.39207000	-0.57922200	0.32178700

C	3.73474800	-1.77811600	0.59292400
C	3.26157500	-2.33643000	-0.68814700
C	3.59750100	-1.37777000	-1.73230600
C	3.86991500	1.01795200	-1.27568900
C	3.77068800	1.62921700	0.07924500
C	4.08794100	0.60676800	1.04023300
C	3.35729000	0.50894900	2.24037000
C	2.81869800	-0.76294500	2.64132100
C	2.93575300	-1.90099900	1.79568100
C	1.84589500	-2.81223500	1.73864600
C	1.46521900	-3.43735500	0.51760700
C	2.07495600	-3.07733500	-0.74604500
C	1.18974500	-2.91485900	-1.91825700
C	1.49188600	-1.89480400	-2.86447700
C	2.68439000	-1.10569300	-2.75199300
C	2.34997900	0.26300400	-3.06360500
C	2.89864500	1.33372700	-2.29125300
C	2.07037700	2.45214800	-2.05611500
C	2.07655800	3.14538100	-0.76455600
C	2.79484700	2.60305600	0.36013700
C	2.11713900	2.58578500	1.68082700
C	2.40519400	1.51591000	2.57414100
C	1.34240200	0.88677100	3.35019200
C	1.58189500	-0.50805800	3.36968500
C	0.49576900	-1.44168200	3.32797300
C	0.65013200	-2.62456100	2.55106000
C	-0.45525700	-3.20354200	1.86495400
C	0.06166000	-3.72036500	0.60617900
C	-0.73367700	-3.68100100	-0.52253800
C	-0.17716100	-3.25241300	-1.79170800
C	-1.20756700	-2.52294500	-2.46735000
C	-0.92174300	-1.30983200	-3.15308200
C	0.44999700	-1.04648800	-3.38496600
C	0.96808300	0.29117300	-3.47621900
C	0.13278800	1.41156500	-3.22818700
C	0.75804500	2.54372600	-2.61158500
C	0.00287800	3.42282600	-1.75366300
C	0.81793600	3.75694100	-0.59464100
C	0.20673600	3.80713400	0.67717800
C	0.83179200	3.19309000	1.79365300
C	-0.22180800	2.61621700	2.63016800
C	0.01560800	1.42038500	3.35398100
C	-1.06795700	0.51050900	3.48011900
C	-0.82575500	-0.93272200	3.45579400

C	-1.93770500	-1.56400800	2.83918100
C	-1.77065800	-2.66969100	1.95379600
C	-2.66603200	-2.77148300	0.78695200
C	-2.11892200	-3.27435800	-0.43509400
C	-2.42302400	-2.65254500	-1.69313900
C	-3.39980000	-1.67226600	-1.78559900
C	-3.11811800	-0.41212200	-2.47769900
C	-1.85773500	-0.17504700	-3.06495500
C	-1.30965000	1.19812900	-3.04952800
C	-2.02952900	2.19176100	-2.33933700
C	-1.35151400	3.25085800	-1.62683200
C	-1.99697500	3.39457500	-0.32092300
C	-1.22521800	3.62619500	0.80267400
C	-1.48510700	2.86260500	2.01143800
C	-2.55396500	1.92120100	2.07139600
C	-2.33389000	0.77241400	2.89348400
C	-2.91497800	-0.51739800	2.55835000
C	-3.80725800	-0.64563900	1.53345100
C	-3.73770700	-1.83129800	0.66312400
C	-4.13902500	-1.38494000	-0.60970700
C	-4.38940600	0.04505000	-0.56933400
C	-3.80036300	0.62473400	-1.72254100
C	-3.20623700	1.86970300	-1.57601000
C	-3.12520600	2.50195000	-0.27472400
C	-3.44790100	1.77820100	0.91277100
C	-4.14005200	0.53074500	0.72590600

22. #10616C₇₂ (B3LYP/6-31G(d))

C	4.20710500	-1.46091300	0.02007500
C	4.28034100	-0.59578400	-1.06798400
C	4.10147100	0.77834400	-0.61204600
C	3.98168400	0.76062300	0.80628800
C	4.02063200	-0.65548500	1.20095100
C	3.28755900	-2.54414900	-0.28506500
C	2.81757700	-2.35312400	-1.62887300
C	3.44369000	-1.12623300	-2.10717400
C	2.69953000	-0.25281500	-2.86550700
C	2.68729900	1.18548000	-2.58198100
C	3.32893400	1.68787600	-1.39760200
C	2.66480000	2.73265500	-0.70913300
C	2.63710400	2.77458900	0.72644900
C	3.15245600	1.69800400	1.49824600
C	2.36130200	1.23111900	2.65226200
C	2.37993400	-0.17385900	2.95954500
C	3.17459900	-1.10706300	2.18072700

C	2.41600700	-2.35124600	2.01076900
C	2.40808500	-3.01915500	0.72489400
C	1.17167300	-3.56076000	0.29104300
C	0.72614400	-3.42224000	-1.06677500
C	1.47924700	-2.68735000	-2.00804600
C	0.73524000	-1.81354500	-2.93549900
C	1.39552200	-0.63806100	-3.36383700
C	0.68259100	0.58662700	-3.58391300
C	1.43254300	1.68955400	-2.99985800
C	0.73671300	2.73767700	-2.31113700
C	1.42146900	3.30432600	-1.20242100
C	0.69836000	3.83287800	-0.08331400
C	1.42424000	3.47440700	1.11310600
C	0.72562800	3.07612100	2.23906500
C	1.17840900	1.92800000	2.99659800
C	0.00000000	1.23764100	3.45617800
C	0.00000000	-0.18176800	3.60942900
C	1.22165300	-0.86095100	3.37030700
C	1.23079900	-2.20328500	2.74745000
C	0.00000000	-2.82230200	2.35259300
C	0.00000000	-3.53810200	1.12657600
C	-1.17167300	-3.56075900	0.29104300
C	-0.72614500	-3.42224000	-1.06677500
C	-1.47924700	-2.68735000	-2.00804600
C	-0.73524000	-1.81354400	-2.93549800
C	-1.39552300	-0.63806000	-3.36383700
C	-0.68259200	0.58662700	-3.58391300
C	-1.43254300	1.68955400	-2.99985800
C	-0.73671300	2.73767700	-2.31113700
C	-1.42146900	3.30432600	-1.20242100
C	-0.69836000	3.83287800	-0.08331400
C	-1.42423900	3.47440700	1.11310600
C	-0.72562800	3.07612100	2.23906500
C	-1.17840900	1.92800000	2.99659800
C	-2.36130100	1.23111900	2.65226200
C	-2.37993400	-0.17385900	2.95954500
C	-1.22165200	-0.86095100	3.37030700
C	-1.23079900	-2.20328500	2.74744900
C	-2.41600800	-2.35124600	2.01076900
C	-2.40808600	-3.01915500	0.72489400
C	-3.28755900	-2.54415000	-0.28506500
C	-2.81757700	-2.35312400	-1.62887300
C	-3.44369000	-1.12623200	-2.10717300
C	-2.69953000	-0.25281500	-2.86550800

C	-2.68729900	1.18548000	-2.58198000
C	-3.32893400	1.68787600	-1.39760200
C	-2.66480000	2.73265500	-0.70913200
C	-2.63710400	2.77458900	0.72644900
C	-3.15245600	1.69800400	1.49824600
C	-3.98168400	0.76062300	0.80628800
C	-4.02063200	-0.65548400	1.20095200
C	-3.17459900	-1.10706400	2.18072700
C	-4.20710400	-1.46091300	0.02007500
C	-4.28034200	-0.59578400	-1.06798400
C	-4.10147100	0.77834500	-0.61204600
23. #10528 C ₇₂ (B3LYP/6-31G(d))			
C	-4.01889700	-0.53750400	1.18008700
C	-4.08178600	-1.44969200	0.05539700
C	-3.22993800	-2.51898100	0.32064800
C	-2.71940500	-2.35565500	1.69469800
C	-3.18170700	-1.07103500	2.17844300
C	-3.86100500	0.78039900	0.70540900
C	-3.84789900	0.73302100	-0.74944000
C	-3.94413700	-0.66787500	-1.13620200
C	-3.16612100	-1.14899600	-2.17627000
C	-2.41122500	-2.37907300	-2.00511000
C	-2.37411500	-3.03799300	-0.72719500
C	-1.15776500	-3.63361400	-0.32784600
C	-0.70360500	-3.58511200	1.05873400
C	-1.45104700	-2.84261200	2.04500700
C	-0.70936200	-2.10022000	3.02400100
C	-1.16771400	-0.79309600	3.46756800
C	-2.33282900	-0.19766000	2.93625200
C	-2.32136500	1.24167600	2.61735500
C	-3.06541700	1.71384400	1.43762000
C	-2.56600800	2.79647900	0.67714500
C	-2.57119900	2.77264200	-0.77857900
C	-3.08134200	1.64998100	-1.50209900
C	-2.34181700	1.16509100	-2.68228000
C	-2.38271200	-0.23676100	-2.97212900
C	-1.21961300	-0.93830300	-3.40643000
C	-1.22350700	-2.25278700	-2.78658800
C	0.00000100	-2.87387000	-2.39337400
C	0.00000100	-3.61724000	-1.16945600
C	1.15776700	-3.63361400	-0.32784500
C	0.70360600	-3.58511200	1.05873500
C	1.45104800	-2.84261100	2.04500700
C	0.70936200	-2.10022000	3.02400100

C	1.16771400	-0.79309500	3.46756800
C	0.00000000	-0.01792100	3.75761100
C	-0.00000100	1.34875200	3.53371400
C	-1.17822000	1.98800200	2.99624300
C	-0.72645800	3.13350300	2.23778400
C	-1.41434200	3.54053100	1.10385300
C	-0.69161100	3.97570500	-0.07769700
C	-1.42049800	3.48369900	-1.23556000
C	-0.71925200	3.03634700	-2.36170700
C	-1.16843400	1.86140100	-3.07066900
C	0.00000000	1.16228300	-3.54415000
C	0.00000100	-0.25274600	-3.66524000
C	1.21961400	-0.93830200	-3.40643000
C	1.22350900	-2.25278600	-2.78658800
C	2.41122700	-2.37907100	-2.00510900
C	2.37411700	-3.03799200	-0.72719400
C	3.22993900	-2.51898000	0.32064900
C	2.71940600	-2.35565400	1.69469800
C	3.18170700	-1.07103300	2.17844400
C	2.33282900	-0.19765800	2.93625200
C	2.32136400	1.24167700	2.61735500
C	1.17821800	1.98800200	2.99624300
C	0.72645600	3.13350400	2.23778400
C	1.41434000	3.54053100	1.10385300
C	0.69160800	3.97570600	-0.07769700
C	1.42049600	3.48369900	-1.23556000
C	0.71925100	3.03634800	-2.36170700
C	1.16843400	1.86140100	-3.07066900
C	2.34181700	1.16509200	-2.68227900
C	2.38271300	-0.23676000	-2.97212800
C	3.16612200	-1.14899400	-2.17626900
C	3.94413800	-0.66787400	-1.13620100
C	4.08178700	-1.44969000	0.05539700
C	4.01889700	-0.53750200	1.18008700
C	3.86100500	0.78040200	0.70540900
C	3.06541600	1.71384500	1.43762100
C	2.56600600	2.79648000	0.67714500
C	2.57119800	2.77264400	-0.77857800
C	3.08134100	1.64998300	-1.50209900
C	3.84789900	0.73302400	-0.74943900
24. #11188C ₇₂ (B3LYP/6-31G(d))			
C	-0.71213600	4.12982000	-0.00004900
C	0.71213500	4.12982000	0.00005000
C	1.15866300	3.56115800	-1.22358500

C	0.00016500	3.31395500	-2.05090600
C	-1.15847500	3.56115800	-1.22367200
C	-1.15866400	3.56115800	1.22358700
C	-0.00016600	3.31395400	2.05090700
C	1.15847400	3.56115800	1.22367300
C	2.30589600	2.70550800	1.26893100
C	2.95477200	2.31854300	0.00017200
C	2.30608500	2.70552900	-1.26868400
C	2.36813900	1.81287100	-2.36966900
C	1.21443200	1.56097700	-3.21476300
C	0.00021400	2.26527100	-3.00122400
C	-1.21398100	1.56097100	-3.21490300
C	-2.36781500	1.81287600	-2.36992600
C	-2.30589600	2.70550800	-1.26893000
C	-2.95477300	2.31854200	-0.00017100
C	-2.30608500	2.70552800	1.26868500
C	-2.36814000	1.81287000	2.36967000
C	-1.21443300	1.56097500	3.21476400
C	-0.00021400	2.26527000	3.00122500
C	1.21398000	1.56097000	3.21490400
C	2.36781500	1.81287600	2.36992600
C	3.14453200	0.60594900	2.31864200
C	3.83960600	0.28731500	1.16210000
C	3.75107500	1.14847500	0.00022700
C	3.83976900	0.28729800	-1.16164500
C	3.14484900	0.60592500	-2.31826800
C	2.42741600	-0.41875500	-3.04853900
C	1.21077700	0.17081200	-3.55805800
C	0.00025100	-0.58072200	-3.63731100
C	-1.21029600	0.17084400	-3.55819300
C	-2.42700700	-0.41872900	-3.04882700
C	-3.14453200	0.60594900	-2.31864200
C	-3.83960600	0.28731400	-1.16210000
C	-3.75107600	1.14847400	-0.00022600
C	-3.83976900	0.28729700	1.16164500
C	-3.14485000	0.60592300	2.31826900
C	-2.42741600	-0.41875700	3.04853900
C	-1.21077700	0.17081100	3.55805800
C	-0.00025100	-0.58072400	3.63731100
C	1.21029600	0.17084300	3.55819400
C	2.42700800	-0.41872900	3.04882600
C	2.43279100	-1.72707600	2.59244400
C	3.20513900	-2.08192000	1.41861500
C	3.90855800	-1.09708300	0.72135400

C	3.90865700	-1.09709300	-0.72087200
C	3.20532900	-2.08193900	-1.41821500
C	2.43314100	-1.72710900	-2.59214900
C	1.20628000	-2.49532900	-2.59465300
C	0.00021000	-1.95755200	-3.12825300
C	-1.20593100	-2.49531300	-2.59479900
C	-2.43279000	-1.72707500	-2.59244500
C	-3.20513800	-2.08192000	-1.41861600
C	-3.90855700	-1.09708400	-0.72135400
C	-3.90865600	-1.09709400	0.72087200
C	-3.20532800	-2.08194000	1.41821400
C	-2.43314000	-1.72711100	2.59214800
C	-1.20627900	-2.49533100	2.59465300
C	-0.00021000	-1.95755400	3.12825300
C	1.20593200	-2.49531400	2.59479700
C	1.20500400	-3.31499600	1.41864600
C	2.44015400	-3.07202500	0.69418100
C	2.44024800	-3.07203600	-0.69386800
C	1.20519000	-3.31500800	-1.41848800
C	0.00005000	-3.63255500	-0.73525100
C	-1.20500300	-3.31499500	-1.41864800
C	-2.44015400	-3.07202500	-0.69418200
C	-2.44024700	-3.07203700	0.69386600
C	-1.20518900	-3.31500900	1.41848600
C	-0.00005000	-3.63255500	0.73525000
25. #10557C ₇₂ (B3LYP/6-31G(d))			
C	2.97448600	-2.09900800	-2.12848500
C	3.88406300	-1.89667200	-1.01067100
C	3.33085800	-2.53179200	0.10427600
C	2.16619000	-3.30095900	-0.35636200
C	1.92205900	-2.95099400	-1.72929000
C	2.71221600	-0.87324600	-2.74031500
C	3.61549000	0.11669400	-2.12518600
C	4.26567600	-0.52428700	-0.98419600
C	4.32001600	0.14772700	0.23996600
C	3.80481000	-0.50610900	1.43177800
C	3.27774400	-1.83616500	1.37006500
C	2.19169800	-2.13277600	2.23813300
C	1.11765400	-3.05823500	1.83529300
C	1.08224300	-3.57173000	0.49901200
C	-0.20043200	-3.72953200	-0.09536100
C	-0.43481400	-3.30710600	-1.45662600
C	0.59794800	-2.71618700	-2.21467800
C	0.30256700	-1.48775600	-2.96473800

C	1.37576100	-0.52371800	-3.14663600
C	1.06824600	0.89969600	-3.17677400
C	1.96424300	1.85061600	-2.59920200
C	3.22932200	1.43313100	-2.03451600
C	3.46471900	2.20259800	-0.82207200
C	3.94942600	1.54540100	0.31169300
C	3.30996500	1.77366400	1.59010400
C	3.18380200	0.49872400	2.26710900
C	2.04546600	0.21104400	3.06407100
C	1.63575800	-1.16203000	3.10597400
C	0.24878500	-1.52281300	3.30506800
C	-0.07151900	-2.69596600	2.49510700
C	-1.37088300	-2.85206700	1.90540100
C	-1.40624000	-3.48270000	0.63527200
C	-2.43760600	-3.14288300	-0.32167300
C	-1.81125500	-2.91801100	-1.59033600
C	-2.17854700	-1.82301100	-2.42214300
C	-1.09589000	-1.05312700	-3.05438600
C	-1.34233800	0.32446300	-3.27667200
C	-0.28464700	1.28853400	-3.22720400
C	-0.76366100	2.47618000	-2.56493500
C	0.08089500	3.21682200	-1.70259100
C	1.47233400	2.94696300	-1.82169700
C	2.37813100	3.14290200	-0.70438300
C	1.84526800	3.44636800	0.54494400
C	2.30694000	2.72604900	1.70937300
C	1.16351600	2.47918000	2.55941500
C	1.01478900	1.24622500	3.24323300
C	-0.33302700	0.83882000	3.51549200
C	-0.70124900	-0.56847500	3.53731700
C	-2.05428800	-0.72734000	3.04165500
C	-2.42352600	-1.86356400	2.23884500
C	-3.50478500	-1.67968600	1.35454800
C	-3.52684100	-2.37381700	0.06835000
C	-4.09124600	-1.51151900	-0.89000400
C	-3.41479700	-1.17142100	-2.08298200
C	-3.56670600	0.27509500	-2.22554200
C	-2.54994700	0.98496300	-2.80776000
C	-2.16061600	2.29274500	-2.28844700
C	-2.71127100	2.76935600	-1.10881600
C	-1.83493900	3.37141000	-0.12076400
C	-0.46114200	3.64513900	-0.40377500
C	0.42686300	3.67963900	0.69959300
C	0.02638500	3.14473800	1.97561100

C	-1.30083200	2.68027800	2.18741400
C	-1.45755100	1.53338100	3.02028100
C	-2.53644000	0.57165300	2.76031500
C	-3.51876900	0.80401600	1.75199100
C	-4.09362300	-0.36149500	1.13952400
C	-4.52339400	-0.29086100	-0.21155400
C	-4.22674700	0.81075800	-1.02475400
C	-3.72019300	1.98631100	-0.42551500
C	-3.39437400	1.99332900	0.96294500
C	-2.25219500	2.89244400	1.15187400
26. #10626C ₇₂ (B3LYP/6-31G(d))			
C	-4.26271400	1.39512200	-0.12568400
C	-4.55102300	-0.00424800	0.19657200
C	-3.99675300	-0.29274200	1.46558400
C	-3.45845100	0.95364200	2.01250400
C	-3.63420300	1.98222100	0.98722600
C	-3.70375900	1.46677900	-1.41845900
C	-3.79283800	0.11138800	-1.97162700
C	-4.27374400	-0.79797900	-0.92749100
C	-3.63325400	-2.04527400	-0.74545500
C	-3.17882400	-2.42910900	0.54920400
C	-3.30710000	-1.53832100	1.66552700
C	-2.26036600	-1.53035900	2.63249200
C	-1.82843500	-0.33373200	3.25246200
C	-2.32024100	0.95552700	2.83452500
C	-1.34519500	2.06677000	2.72170300
C	-1.51332300	3.01168000	1.67845100
C	-2.61608700	2.90313600	0.75177600
C	-2.11094400	3.10130300	-0.57472400
C	-2.54801000	2.29194200	-1.66343700
C	-1.53966700	1.85100900	-2.63135900
C	-1.74648200	0.58300800	-3.24190900
C	-2.81260400	-0.30943600	-2.83389800
C	-2.24898900	-1.65943700	-2.73150600
C	-2.63500700	-2.48993200	-1.69811100
C	-1.60961600	-3.23461000	-1.00006700
C	-1.95960400	-3.22496200	0.37961700
C	-0.95019400	-3.25861400	1.37495800
C	-1.11408900	-2.44199500	2.53507800
C	0.00138200	-1.84435800	3.15792900
C	-0.43905100	-0.52493000	3.60309500
C	0.43905200	0.52502100	3.60308300
C	-0.00138200	1.84443800	3.15788300
C	1.11408900	2.44205900	2.53501700

C	0.95019400	3.25864900	1.37487600
C	-0.38026600	3.51213900	0.95204100
C	-0.72764100	3.50813300	-0.44579200
C	0.23873300	3.21630200	-1.42703800
C	-0.16059000	2.35501400	-2.55124700
C	0.87270400	1.60613200	-3.16470100
C	0.63965600	0.25289800	-3.59835000
C	-0.63965600	-0.25298800	-3.59834400
C	-0.87270400	-1.60621100	-3.16466200
C	0.16058900	-2.35507800	-2.55118800
C	-0.23873400	-3.21633800	-1.42695800
C	0.72764200	-3.50814400	-0.44570500
C	0.38026600	-3.51211500	0.95212900
C	1.51332200	-3.01163800	1.67852600
C	1.34519500	-2.06670100	2.72175400
C	2.32024200	-0.95545600	2.83454900
C	1.82843600	0.33381400	3.25245400
C	2.26036600	1.53042500	2.63245500
C	3.30710000	1.53836200	1.66548800
C	3.17882500	2.42912200	0.54914300
C	1.95960300	3.22497000	0.37953600
C	1.60961500	3.23458500	-1.00014800
C	2.63500700	2.48988900	-1.69817400
C	2.24898900	1.65936800	-2.73154700
C	2.81260400	0.30936500	-2.83390600
C	1.74648200	-0.58308900	-3.24189400
C	1.53966700	-1.85107500	-2.63131300
C	2.54800900	-2.29198200	-1.66338000
C	2.11094400	-3.10131800	-0.57464700
C	2.61608600	-2.90311500	0.75184700
C	3.63420500	-1.98219800	0.98727600
C	3.45845100	-0.95359200	2.01252900
C	3.99675400	0.29277900	1.46557800
C	4.55101900	0.00425200	0.19657100
C	4.27374600	0.79795600	-0.92751200
C	3.63325300	2.04525400	-0.74550600
C	3.79283800	-0.11143800	-1.97162600
C	3.70376000	-1.46681600	-1.41842500
C	4.26271100	-1.39512400	-0.12564900
27. #10612C ₇₂ (B3LYP/6-31G(d))			
C	-4.40131400	0.17568600	0.67487100
C	-4.40132300	-0.17569500	-0.67487500
C	-3.84314500	-1.50990700	-0.82723500
C	-3.56081900	-2.01853600	0.47513800

C	-3.86718200	-0.93316000	1.41595700
C	-3.84314900	1.50990000	0.82723700
C	-3.56082100	2.01852600	-0.47513600
C	-3.86718700	0.93315100	-1.41595800
C	-2.99280100	0.67773700	-2.45030200
C	-2.55947200	-0.68355600	-2.76106900
C	-2.95175400	-1.77633800	-1.91127500
C	-1.99610500	-2.79894800	-1.71862900
C	-1.82308600	-3.43268300	-0.43631600
C	-2.47456700	-2.91427300	0.71114700
C	-1.66294000	-2.73818900	1.93131400
C	-1.90766400	-1.59191600	2.74222800
C	-2.99279900	-0.67774000	2.45030300
C	-2.55947600	0.68355100	2.76107300
C	-2.95175700	1.77633100	1.91127600
C	-1.99611200	2.79894400	1.71863100
C	-1.82309200	3.43267500	0.43631700
C	-2.47457400	2.91426900	-0.71114800
C	-1.66294600	2.73818700	-1.93131300
C	-1.90767000	1.59191400	-2.74222900
C	-0.84449400	0.82393300	-3.28229300
C	-1.23845300	-0.58703400	-3.25227600
C	-0.25721000	-1.60258300	-3.06054500
C	-0.70671500	-2.76660200	-2.37556000
C	0.20409300	-3.56762400	-1.61015200
C	-0.46323900	-3.93277400	-0.37729400
C	0.24796200	-3.90863800	0.80902000
C	-0.33674200	-3.22986200	1.96024600
C	0.71964300	-2.51177400	2.60928600
C	0.50572200	-1.21403800	3.17155200
C	-0.84449100	-0.82393500	3.28229600
C	-1.23845300	0.58703100	3.25227500
C	-0.25721200	1.60258200	3.06054500
C	-0.70672100	2.76660000	2.37555900
C	0.20408600	3.56762600	1.61015200
C	-0.46324700	3.93277600	0.37729500
C	0.24795200	3.90863500	-0.80901900
C	-0.33675100	3.22986300	-1.96024700
C	0.71963600	2.51177600	-2.60928500
C	0.50571800	1.21403900	-3.17155300
C	1.54988700	0.18675700	-3.07549100
C	1.16376600	-1.23166200	-3.00829000
C	2.05144800	-2.13938400	-2.37353300
C	1.55865100	-3.28124500	-1.62588000

C	2.33683600	-3.40474300	-0.41113600
C	1.67074500	-3.65453400	0.79459500
C	1.96472600	-2.83096000	1.94624000
C	2.97382600	-1.88677100	1.90316800
C	2.79032600	-0.57810300	2.51482200
C	1.54988900	-0.18675400	3.07549100
C	1.16376400	1.23166400	3.00829000
C	2.05144500	2.13938800	2.37353300
C	1.55864400	3.28124700	1.62588000
C	2.33682700	3.40474600	0.41113500
C	1.67073700	3.65453600	-0.79459500
C	1.96471900	2.83096500	-1.94624200
C	2.97382000	1.88677700	-1.90317000
C	2.79032400	0.57810800	-2.51482400
C	3.60941800	-0.34948400	-1.77964500
C	3.24546200	-1.68463500	-1.70635900
C	3.38932300	-2.41726000	-0.45986300
C	3.75774600	-1.71976500	0.69400300
C	4.14820200	-0.33056500	0.61381800
C	3.60941800	0.34949200	1.77964300
C	3.24545900	1.68464200	1.70635800
C	3.38931800	2.41726700	0.45986200
C	3.75774100	1.71977300	-0.69400400
C	4.14820100	0.33057400	-0.61382000
28. #10693 C ₇₂ (B3LYP/6-31G(d))			
C	3.53285300	-2.30391900	0.84296100
C	3.73344300	-2.07266000	-0.56342200
C	4.01031400	-0.70217700	-0.78530800
C	4.02828400	-0.04875800	0.51306500
C	3.74874300	-1.06940800	1.51835100
C	2.34378000	-3.03998500	1.01197300
C	1.82394600	-3.36518500	-0.33450400
C	2.73312000	-2.76373500	-1.29365200
C	2.22078700	-2.17181000	-2.44250700
C	2.60628900	-0.81139300	-2.80270600
C	3.43885500	-0.04923400	-1.92929900
C	3.14092400	1.33159700	-1.79985100
C	3.25776700	2.00094800	-0.52277900
C	3.56044600	1.27925100	0.67502200
C	2.81863600	1.63684400	1.90414600
C	2.50238200	0.60310100	2.83304200
C	2.92781700	-0.77137100	2.59116900
C	1.86268600	-1.66300700	2.96033800
C	1.46214100	-2.73566100	2.08409500

C	0.05205300	-3.02747600	1.91065900
C	-0.45358200	-3.45622800	0.58618900
C	0.45360100	-3.45622800	-0.58617400
C	-0.05203600	-3.02748400	-1.91064500
C	0.85820000	-2.37884700	-2.79051300
C	0.44826300	-1.21191300	-3.54792600
C	1.49101600	-0.21118900	-3.46446200
C	1.16130400	1.17139700	-3.30548400
C	2.06599400	1.94465000	-2.53098900
C	1.61585800	3.09317500	-1.77162400
C	2.34909300	3.11398700	-0.52291900
C	1.70805100	3.50857700	0.64928000
C	1.91255700	2.72772900	1.87025400
C	0.67150700	2.70522900	2.57919900
C	0.25912600	1.56587000	3.32045600
C	1.24843300	0.56015400	3.49924200
C	0.87275300	-0.84719300	3.59375500
C	-0.44825700	-1.21190100	3.54793200
C	-0.85818800	-2.37883800	2.79052400
C	-2.22077500	-2.17180900	2.44251400
C	-2.73310300	-2.76374200	1.29366300
C	-1.82392800	-3.36519300	0.33451900
C	-2.34376300	-3.04000200	-1.01195900
C	-1.46212800	-2.73567800	-2.08408200
C	-1.86267800	-1.66302900	-2.96033100
C	-0.87275200	-0.84721600	-3.59375100
C	-1.24843700	0.56013200	-3.49924200
C	-0.25913400	1.56585300	-3.32046300
C	-0.67152100	2.70521400	-2.57920900
C	0.28958700	3.48536100	-1.80435300
C	-0.35531500	3.97344900	-0.61164500
C	0.35529600	3.97345200	0.61162700
C	-0.28960400	3.48536800	1.80433800
C	-1.61587300	3.09317700	1.77161000
C	-2.06600400	1.94465200	2.53097900
C	-1.16131000	1.17140800	3.30547900
C	-1.49101800	-0.21118000	3.46446100
C	-2.60628600	-0.81139100	2.80271100
C	-3.43885500	-0.04924100	1.92929800
C	-4.01031000	-0.70219000	0.78530900
C	-3.73343000	-2.07267500	0.56342700
C	-3.53284300	-2.30394200	-0.84295000
C	-3.74873900	-1.06943400	-1.51834700
C	-2.92781300	-0.77139500	-2.59116200

C	-2.50238700	0.60307800	-2.83304400
C	-2.81864400	1.63682400	-1.90415200
C	-1.91257200	2.72771300	-1.87026600
C	-1.70806700	3.50856700	-0.64929500
C	-2.34910800	3.11398100	0.52290500
C	-3.25777600	2.00093600	0.52276900
C	-3.14093100	1.33159100	1.79984500
C	-3.56045300	1.27923300	-0.67502700
C	-4.02828400	-0.04877900	-0.51306200
29. #10615 C ₇₂ (B3LYP/6-31G(d))			
C	-4.08318900	-1.55055600	-0.82265200
C	-4.30724400	-1.01846600	0.44810800
C	-4.18494500	0.42662500	0.40434500
C	-3.92812500	0.79978900	-0.95011800
C	-3.82874000	-0.45143100	-1.71433100
C	-3.13288400	-2.64143700	-0.71501900
C	-2.80933700	-2.82166600	0.67001000
C	-3.53903600	-1.78639000	1.39084700
C	-2.90893700	-1.12977800	2.42147700
C	-2.96045400	0.32867500	2.53631800
C	-3.53849000	1.11003900	1.47793500
C	-2.89069200	2.33333400	1.16602300
C	-2.75454400	2.77756600	-0.19356200
C	-3.11855300	1.92899600	-1.27362300
C	-2.18414400	1.82884700	-2.41019900
C	-2.03066300	0.55972200	-3.04702400
C	-2.83304300	-0.57788000	-2.65864100
C	-2.00427300	-1.78435700	-2.72741500
C	-2.12443700	-2.79346300	-1.70905300
C	-0.92925600	-3.43159600	-1.31231500
C	-0.63900700	-3.69447000	0.07386100
C	-1.49995600	-3.22764700	1.08635800
C	-0.87711500	-2.60455300	2.27321100
C	-1.62516600	-1.59369300	2.92192600
C	-0.99576000	-0.45095100	3.50704500
C	-1.76626600	0.74111900	3.17584900
C	-1.09152400	1.96598900	2.86228300
C	-1.73297200	2.79366400	1.90542900
C	-0.97076700	3.66775200	1.05348000
C	-1.58148300	3.63124200	-0.25978100
C	-0.77808800	3.62839800	-1.38456500
C	-1.04973700	2.66978100	-2.45011400
C	0.21754500	2.20495000	-2.93496200
C	0.41996000	0.84028700	-3.32053000

C	-0.75416200	0.06644300	-3.42361700
C	-0.73566800	-1.38431200	-3.19848000
C	0.47309800	-2.04290500	-2.83555700
C	0.32388800	-3.15784300	-1.96465700
C	1.37927900	-3.52889400	-1.06650900
C	0.80380500	-3.71974500	0.23533700
C	1.44215300	-3.20780300	1.39304700
C	0.58668800	-2.56677900	2.40351800
C	1.16027000	-1.49516800	3.13061100
C	0.37143500	-0.39610100	3.59772000
C	1.08452300	0.85040700	3.36809900
C	0.37684900	2.02170500	2.97195100
C	1.10163700	2.92252900	2.14470800
C	0.41167700	3.75433900	1.18344700
C	1.24320600	3.87205600	0.00867000
C	0.65514300	3.78071900	-1.25500400
C	1.26256600	2.93867300	-2.25930900
C	2.47503300	2.32186800	-2.02025300
C	2.72839900	0.97361800	-2.48836000
C	1.70397100	0.17972500	-3.05555800
C	1.73864200	-1.28186700	-2.83057500
C	2.82845100	-1.82913800	-2.12234800
C	2.63986900	-2.96689000	-1.21613700
C	3.40225600	-2.75232900	-0.04926900
C	2.80151900	-2.76186100	1.22796400
C	3.27533800	-1.54813600	1.89091100
C	2.45661600	-0.93037600	2.79148800
C	2.36969400	0.52316500	2.85978300
C	3.02974000	1.34401300	1.89331600
C	2.39409200	2.57992300	1.60213000
C	2.48148000	3.17079000	0.28024300
C	3.12471400	2.47101600	-0.73077300
C	3.84496800	1.25145600	-0.44312300
C	3.71583300	0.40340000	-1.60853200
C	3.82219000	-0.97433900	-1.49504600
C	4.14480700	-1.51050000	-0.21954100
C	4.04727200	-0.73741200	0.94555900
C	3.85005000	0.68811400	0.86354600
30. #10538 C ₇₂ (B3LYP/6-31G(d))			
C	2.30726000	3.45540100	-0.88561500
C	1.10073000	4.16525400	-0.61572400
C	0.77867700	3.95244000	0.74186600
C	1.88397100	3.23187600	1.37261500
C	2.79497800	2.86565100	0.33272000

C	2.12665500	2.64090900	-2.01770200
C	0.77593200	2.86118100	-2.53179900
C	0.15116600	3.79256400	-1.62983100
C	-1.17816100	3.59625400	-1.28929400
C	-1.58382000	3.61659900	0.12937400
C	-0.58168900	3.70272100	1.15181200
C	-0.79360200	2.90946600	2.30927900
C	0.32450300	2.24710800	2.98425400
C	1.64624100	2.35427000	2.46309800
C	2.48596500	1.21114500	2.58128200
C	3.41639100	0.86668700	1.52735500
C	3.45344500	1.60229000	0.31236900
C	3.53793600	0.86086900	-0.96190700
C	2.76865000	1.36713700	-2.11125800
C	2.15620900	0.45046800	-2.99175000
C	0.78175200	0.63451400	-3.44923900
C	0.03934700	1.79966700	-3.11585300
C	-1.38724300	1.65488500	-2.84912900
C	-1.96248100	2.61405400	-1.96068000
C	-3.02611500	2.24968200	-1.04966500
C	-2.72319600	2.78520100	0.27577400
C	-2.92989200	1.96890200	1.43006500
C	-1.95771200	2.10188600	2.46487500
C	-1.56948400	0.95822600	3.26302700
C	-0.14810300	1.02835200	3.53371400
C	0.65635700	-0.15713400	3.56790100
C	2.01116800	-0.00854600	3.17239000
C	2.74352200	-1.10509800	2.57310900
C	3.60903700	-0.55567300	1.55227700
C	3.82293000	-1.24564800	0.36566600
C	3.77614400	-0.53125100	-0.90068800
C	3.21799000	-1.44092300	-1.87710400
C	2.40025700	-0.95490600	-2.89218300
C	1.17805100	-1.64422100	-3.24514500
C	0.16654000	-0.64219400	-3.53059600
C	-1.21110600	-0.84425300	-3.20842700
C	-2.01893000	0.33857100	-2.93806400
C	-3.25523200	0.14605100	-2.23796600
C	-3.69602100	1.07966100	-1.20928700
C	-4.12902000	0.32425000	-0.02293100
C	-3.63889600	0.68757400	1.27944000
C	-3.26907900	-0.39855300	2.13162500
C	-2.18709000	-0.25634300	3.08324800
C	-1.40412800	-1.47930200	3.11969300

C	0.00048700	-1.45139300	3.34154700
C	0.74311700	-2.50987800	2.74342300
C	2.13615800	-2.33408300	2.37867800
C	2.40322600	-3.08990900	1.17445500
C	3.23868400	-2.55649400	0.18412700
C	2.87194800	-2.68539800	-1.20869300
C	1.70340000	-3.35708800	-1.56065300
C	0.84117000	-2.81526100	-2.59523700
C	-0.53373700	-3.04592400	-2.23217700
C	-1.56231400	-2.13175800	-2.60086300
C	-2.74863900	-2.22826200	-1.82176600
C	-3.61910900	-1.12628400	-1.76589000
C	-4.17471200	-1.01709600	-0.41975700
C	-3.61608100	-2.06137000	0.35849400
C	-3.19786000	-1.75281800	1.64839400
C	-2.00535700	-2.38347100	2.19458700
C	-1.21826600	-3.27040500	1.40880900
C	0.14815500	-3.38376200	1.77827800
C	1.16966000	-3.74463600	0.80407500
C	0.83237400	-3.89014000	-0.53573000
C	-0.54210400	-3.69960400	-0.95774500
C	-1.58448400	-3.47011400	-0.00638700
C	-2.74651700	-2.85256800	-0.50696100

31. #10849 C₇₂ (B3LYP/6-31G(d))

C	-2.52789800	0.01999000	-3.25681700
C	-3.55317600	0.64499900	-2.44969700
C	-3.03774600	1.88119800	-1.98617200
C	-1.76121300	2.10620800	-2.63481500
C	-1.42251100	0.88678600	-3.35439500
C	-2.36392000	-1.32674000	-2.87002400
C	-3.38290700	-1.58873800	-1.85133800
C	-4.05404900	-0.31891400	-1.55045400
C	-4.27858800	0.03606700	-0.20254100
C	-3.84185200	1.31655600	0.27408300
C	-3.21218200	2.25053700	-0.60617300
C	-2.23115300	3.10637500	-0.04087700
C	-1.09415600	3.52798600	-0.79060700
C	-0.75978800	2.88034600	-2.02897300
C	0.64016000	2.56088300	-2.31841900
C	0.96576600	1.30862500	-3.04279900
C	-0.10782600	0.36625000	-3.37267100
C	0.07931800	-1.06613500	-3.18848700
C	-1.06389100	-1.88553800	-2.79074700
C	-0.85939100	-2.94151400	-1.79747100

C	-1.85934900	-3.18359800	-0.80389200
C	-3.11599800	-2.47672700	-0.83072300
C	-3.48492000	-2.16724400	0.54372900
C	-4.01689100	-0.92640100	0.85076900
C	-3.51079800	-0.20133900	2.01311500
C	-3.38208700	1.16972700	1.66089200
C	-2.32171700	1.96287600	2.19186000
C	-1.85935000	3.03738500	1.37468300
C	-0.53978000	3.53587100	1.49890800
C	-0.06195100	3.85831800	0.15872500
C	1.25583000	3.67449800	-0.17112300
C	1.62004700	3.09338700	-1.45123500
C	2.89185400	2.45416900	-1.26949400
C	3.26382400	1.41992500	-2.11730400
C	2.26803500	0.80884900	-2.97293700
C	2.51597500	-0.63347200	-2.95939300
C	1.42121400	-1.55501900	-2.90827300
C	1.59391000	-2.70178700	-2.07731200
C	0.45246400	-3.29829700	-1.43546700
C	0.80772400	-3.65318000	-0.08273100
C	-0.13504700	-3.53692700	0.97036900
C	-1.49403300	-3.42129900	0.56586000
C	-2.46909800	-2.76264000	1.40111400
C	-2.06595400	-2.12522300	2.56531500
C	-2.58351500	-0.80650200	2.87263900
C	-1.51918900	-0.04031300	3.43100700
C	-1.36949900	1.34563300	3.12993000
C	-0.04684900	1.87938100	3.21996000
C	0.35656900	2.99289400	2.43131800
C	1.75297300	2.81696400	2.08095500
C	2.20690200	3.17701100	0.82186400
C	3.20858900	2.39889900	0.14454000
C	3.75234900	1.21266800	0.72727300
C	4.25989500	0.22610500	-0.18977200
C	4.07716800	0.39361600	-1.58613300
C	3.67477600	-0.85999500	-2.18135400
C	3.71790400	-1.85989100	-1.17705900
C	2.70983200	-2.81360400	-1.16637500
C	2.18830300	-3.30986600	0.09711500
C	2.59970600	-2.72589600	1.29074600
C	1.64172100	-2.47878200	2.33225400
C	0.29164100	-2.90795100	2.22677100
C	-0.67973600	-2.17272300	2.97559400
C	-0.36036000	-0.91188100	3.55918500

C	0.96069600	-0.38799900	3.50193200
C	1.11629100	1.01706400	3.38789000
C	2.21677900	1.57745100	2.66795000
C	3.18955400	0.75949100	2.01020100
C	3.10414600	-0.64339500	2.25286700
C	3.53798700	-1.60793400	1.26481800
C	4.11242400	-1.19836200	0.07843200
C	1.97604100	-1.20916900	2.93939100
32. #11029 C ₇₂ (B3LYP/6-31G(d))			
C	4.41667900	-0.40420400	0.16535100
C	4.02889500	-1.80642600	0.24323300
C	3.44992600	-2.20269600	-0.97370900
C	3.52116600	-1.02256200	-1.84913100
C	4.07704500	0.10834700	-1.09528500
C	3.99584900	0.23340400	1.36014700
C	3.26821200	-0.72211900	2.17418800
C	3.36980400	-2.01135100	1.48140500
C	2.30755800	-2.90104200	1.50014100
C	1.84048000	-3.51609200	0.29094500
C	2.29810200	-3.05842400	-0.98126700
C	1.28893200	-2.86260300	-2.02950800
C	1.41451900	-1.73500900	-2.89417200
C	2.51441100	-0.79481700	-2.74676000
C	2.02231100	0.54931600	-3.00050400
C	2.50568300	1.66811000	-2.25479100
C	3.51913600	1.42958800	-1.21697000
C	3.42352100	2.19050900	-0.01589300
C	3.54664900	1.54385500	1.26901200
C	2.47915300	1.99510900	2.12161300
C	1.69289100	1.07628500	2.85776300
C	2.08478300	-0.34989500	2.84518800
C	1.04383000	-1.38117600	3.01628000
C	1.16882800	-2.63971800	2.35583600
C	0.03385000	-3.31794300	1.81274000
C	0.44787600	-3.84727800	0.51998200
C	-0.44787600	-3.84727800	-0.51998300
C	-0.03385000	-3.31794300	-1.81274100
C	-1.16882800	-2.63971700	-2.35583600
C	-1.04383000	-1.38117600	-3.01628100
C	0.28219700	-0.98421900	-3.30610100
C	0.65692000	0.42779200	-3.36307400
C	-0.29371200	1.44616700	-3.10647500
C	0.23788600	2.65579200	-2.56520900
C	1.59711100	2.74483500	-2.10915900

C	1.60150100	3.57774700	-0.91281400
C	2.43843200	3.23814900	0.13784400
C	1.89113900	3.15402700	1.48109900
C	0.57701000	3.50201900	1.71963600
C	-0.23788700	2.65579100	2.56521000
C	0.29371200	1.44616700	3.10647500
C	-0.65692000	0.42779200	3.36307400
C	-0.28219700	-0.98422000	3.30610100
C	-1.41452000	-1.73500900	2.89417200
C	-1.28893200	-2.86260400	2.02950800
C	-2.29810100	-3.05842300	0.98126700
C	-1.84048000	-3.51609200	-0.29094500
C	-2.30755700	-2.90104100	-1.50014000
C	-3.36980500	-2.01135200	-1.48140600
C	-3.26821200	-0.72211900	-2.17418800
C	-2.08478300	-0.34989400	-2.84518900
C	-1.69289100	1.07628500	-2.85776400
C	-2.47915300	1.99510900	-2.12161300
C	-1.89113900	3.15402700	-1.48109900
C	-0.57700900	3.50201800	-1.71963600
C	0.24986000	4.01652500	-0.65347300
C	-0.24986100	4.01652500	0.65347300
C	-1.60150100	3.57774700	0.91281500
C	-1.59711100	2.74483500	2.10915900
C	-2.50568300	1.66811000	2.25479200
C	-2.02231100	0.54931600	3.00050400
C	-2.51441200	-0.79481800	2.74676200
C	-3.52116500	-1.02256200	1.84913000
C	-3.44992600	-2.20269700	0.97370900
C	-4.02889300	-1.80642500	-0.24323300
C	-4.41667800	-0.40420400	-0.16535200
C	-3.99584800	0.23340400	-1.36014800
C	-3.54664900	1.54385500	-1.26901200
C	-3.42352100	2.19050900	0.01589300
C	-2.43843100	3.23814900	-0.13784400
C	-3.51913500	1.42958800	1.21697000
C	-4.07704400	0.10834700	1.09528500

33. #10554 C₇₂ (B3LYP/6-31G(d))

C	3.27833700	-2.18749300	-1.58932200
C	4.14604400	-1.49548400	-0.65093700
C	3.72790700	-1.83947600	0.63826800
C	2.71955800	-2.90872800	0.51132300
C	2.43119500	-3.07460600	-0.88221300
C	2.77255000	-1.26579400	-2.51553000

C	3.47018700	0.00026800	-2.28534200
C	4.26573300	-0.13630000	-1.06454500
C	4.22111100	0.87490800	-0.10573600
C	3.86028500	0.54234500	1.26708800
C	3.56457500	-0.81063800	1.63500700
C	2.55130900	-1.00082100	2.61611600
C	1.64041000	-2.16139800	2.56794700
C	1.69239000	-3.07035100	1.46586600
C	0.45276100	-3.61928600	1.02091500
C	0.18500700	-3.77660400	-0.38888300
C	1.10542300	-3.29159200	-1.35003600
C	0.59945200	-2.43395900	-2.43561000
C	1.38881400	-1.30852500	-2.90139200
C	0.72364100	-0.04940200	-3.22573400
C	1.45110400	1.16317800	-3.04958200
C	2.81431400	1.17826900	-2.54479200
C	2.95817400	2.31767700	-1.65730700
C	3.60741600	2.14325800	-0.42763300
C	2.98887400	2.65276900	0.77710800
C	3.09723300	1.63769400	1.80846700
C	2.03315300	1.43025400	2.73034000
C	1.85459400	0.08553900	3.19185700
C	0.54404000	-0.41041300	3.56590900
C	0.40843300	-1.79877000	3.14255400
C	-0.85498400	-2.30867000	2.68030500
C	-0.79041300	-3.30605400	1.67267100
C	-1.85143200	-3.43848600	0.69589200
C	-1.23399100	-3.68491300	-0.58628700
C	-1.72992000	-3.05982400	-1.72383300
C	-0.80517200	-2.35446700	-2.60292900
C	-1.45110300	-1.16317500	-3.04958300
C	-0.72364000	0.04940500	-3.22573500
C	-1.38881300	1.30852800	-2.90139000
C	-0.59945200	2.43396200	-2.43560700
C	0.80517300	2.35447000	-2.60292600
C	1.72992000	3.05982500	-1.72382900
C	1.23399100	3.68491500	-0.58628400
C	1.85143100	3.43848300	0.69589500
C	0.79041200	3.30605300	1.67267400
C	0.85498300	2.30866600	2.68030700
C	-0.40843300	1.79876600	3.14255500
C	-0.54404000	0.41041000	3.56590800
C	-1.85459500	-0.08554200	3.19185700
C	-2.03315300	-1.43025700	2.73033800

C	-3.09723300	-1.63769700	1.80846500
C	-2.98887300	-2.65276800	0.77710400
C	-3.60741700	-2.14325900	-0.42763600
C	-2.95817200	-2.31767400	-1.65730800
C	-2.81431400	-1.17826600	-2.54479500
C	-3.47018500	-0.00026600	-2.28534200
C	-2.77254900	1.26579700	-2.51553000
C	-3.27833500	2.18749400	-1.58932000
C	-2.43119600	3.07460800	-0.88221000
C	-1.10542200	3.29159300	-1.35003300
C	-0.18500700	3.77660600	-0.38887900
C	-0.45276100	3.61928400	1.02091800
C	-1.69239100	3.07035000	1.46586800
C	-1.64041100	2.16139400	2.56794700
C	-2.55130900	1.00081900	2.61611600
C	-3.56457600	0.81063600	1.63500700
C	-3.86028600	-0.54234500	1.26708600
C	-4.22110900	-0.87490700	-0.10573700
C	-4.26573500	0.13630100	-1.06454700
C	-4.14604200	1.49548300	-0.65093600
C	-3.72790900	1.83947700	0.63827000
C	-2.71955800	2.90872800	0.51132600
34. #10689C ₇₂ (B3LYP/6-31G(d))			
C	4.21337500	-0.80116200	0.63472800
C	4.19373600	-0.76897100	-0.82519300
C	3.92225300	0.53945800	-1.25300800
C	3.83143200	1.38312000	-0.05345200
C	4.02448600	0.52075000	1.10620800
C	3.42045900	-1.86945100	1.07035100
C	2.96966000	-2.60321700	-0.13554000
C	3.46639200	-1.88185900	-1.29967000
C	2.63868000	-1.70522700	-2.41899300
C	2.41666200	-0.39558800	-2.95520900
C	3.01650500	0.74183600	-2.35411500
C	2.26165700	1.94322900	-2.35418300
C	2.28692200	2.83003100	-1.23705600
C	2.94317800	2.46979600	-0.00075700
C	2.23406500	2.76078400	1.26634400
C	2.38039400	1.85564200	2.35422800
C	3.24699500	0.69936700	2.24571000
C	2.58487000	-0.42666900	2.84191600
C	2.55264200	-1.70503300	2.19422100
C	1.33220800	-2.49923100	2.24200300
C	0.97173500	-3.35634400	1.10625300

C	1.74286900	-3.25869400	-0.16044300
C	1.01341800	-3.28935600	-1.45674200
C	1.42158600	-2.43873900	-2.50221100
C	0.44135900	-1.61072300	-3.20317100
C	1.03415400	-0.35100800	-3.42978800
C	0.26388700	0.85348700	-3.40019200
C	0.94787400	2.02259400	-2.97379600
C	0.24552100	3.09832800	-2.34207900
C	1.05815800	3.57694500	-1.23826900
C	0.44617800	3.93198800	-0.04405300
C	1.00686600	3.47601000	1.21921200
C	-0.08660100	3.17406300	2.09183200
C	-0.02075500	2.08667100	3.00357500
C	1.26171300	1.49973900	3.17483200
C	1.40562100	0.09526800	3.49094500
C	0.29527800	-0.70137700	3.62598900
C	0.28120000	-2.03848600	3.08425000
C	-1.09237300	-2.33394200	2.80450600
C	-1.41967600	-3.23970400	1.82647400
C	-0.36213100	-3.79612000	1.00699600
C	-0.96665200	-4.05178400	-0.27528400
C	-0.36258000	-3.64518500	-1.46691200
C	-1.35275700	-2.90736900	-2.25774700
C	-0.96104600	-1.76371300	-2.98830300
C	-1.80687300	-0.56183600	-3.00532400
C	-1.18979500	0.75610900	-3.21538200
C	-1.86200300	1.90268000	-2.71113200
C	-1.13398600	3.05710300	-2.23173800
C	-1.78108900	3.55213400	-1.02703100
C	-0.99353900	3.95227800	0.06285700
C	-1.32251800	3.48686000	1.38923400
C	-2.45501300	2.71378900	1.59747600
C	-2.40356400	1.56994600	2.49655000
C	-1.21463700	1.24872100	3.20162800
C	-1.03817200	-0.12921300	3.52080000
C	-1.90301100	-1.14009000	3.01708500
C	-2.99428800	-0.83590100	2.15325100
C	-3.33549700	-1.78111300	1.07956000
C	-2.59711400	-3.01035700	0.98931100
C	-2.33296400	-3.60513700	-0.26026300
C	-2.56726900	-2.90245500	-1.47884300
C	-3.33936100	-1.75359300	-1.43023200
C	-3.02537200	-0.62453500	-2.27905000
C	-3.59286200	0.54276700	-1.65800600

C	-3.04042200	1.78473700	-1.88601300
C	-2.96015500	2.76327800	-0.80935700
C	-3.31445800	2.37588700	0.48735900
C	-3.82925400	1.04513300	0.73364400
C	-3.26894100	0.55056900	1.97610200
C	-4.03294600	0.16722400	-0.32115000
C	-3.81431200	-1.24513800	-0.15574700
35. #10629C ₇₂ (B3LYP/6-31G(d))			
C	4.33973100	-0.54437000	0.93683100
C	4.48668500	-0.17851300	-0.41830900
C	4.03794700	1.18866300	-0.59928500
C	3.70676700	1.71902900	0.68645900
C	3.85910800	0.60197100	1.63453000
C	3.67668800	-1.82426300	1.02829300
C	3.57170500	-2.31070800	-0.32965300
C	4.00512200	-1.23661800	-1.23552600
C	3.21942400	-0.92392900	-2.34682400
C	2.84018300	0.44812800	-2.62618100
C	3.23853200	1.50963700	-1.74131800
C	2.33818600	2.59251800	-1.59977700
C	2.13054400	3.23688900	-0.33863300
C	2.67322800	2.68258900	0.85440900
C	1.78572800	2.58751200	2.03316700
C	1.91530800	1.43730600	2.87796400
C	2.90884900	0.41070000	2.60785600
C	2.31393900	-0.89840000	2.82908500
C	2.60055300	-2.00618200	1.94355300
C	1.48622400	-2.88385100	1.58949900
C	1.52019400	-3.48724700	0.29848300
C	2.50140800	-3.10643600	-0.68191900
C	1.79188700	-2.87825100	-1.93901600
C	2.11088700	-1.77464700	-2.72024800
C	1.05304900	-0.95009000	-3.23078100
C	1.52768600	0.42700200	-3.18819400
C	0.61668500	1.50947500	-3.05520400
C	1.09482400	2.65349200	-2.35306000
C	0.19494700	3.50504500	-1.65084400
C	0.79976600	3.81907600	-0.37080400
C	0.01221300	3.83127000	0.75977800
C	0.49206800	3.16747900	1.96572500
C	-0.64591200	2.55522100	2.57774700
C	-0.51356200	1.32679100	3.27967700
C	0.78730200	0.78768300	3.41542400
C	1.01721200	-0.66805500	3.32433700

C	-0.06531000	-1.56190100	3.10118100
C	0.16832100	-2.71206100	2.22453500
C	-0.97282700	-3.27215700	1.59510100
C	-0.90442000	-3.73589000	0.22930200
C	0.29846500	-3.76648600	-0.41580800
C	0.42356600	-3.24505500	-1.76701500
C	-0.64075000	-2.51323500	-2.34450300
C	-0.30622200	-1.27151700	-3.06462700
C	-1.28220600	-0.17485400	-3.13469100
C	-0.81646200	1.22987100	-3.09691300
C	-1.68349300	2.21229500	-2.55317500
C	-1.17488000	3.30433400	-1.75406900
C	-2.01658800	3.42203200	-0.58812100
C	-1.41990300	3.62102500	0.65739200
C	-1.83083500	2.82237400	1.77848600
C	-2.88767100	1.88059900	1.67763300
C	-2.79063500	0.71813400	2.52270400
C	-1.60679700	0.42317000	3.24659000
C	-1.37877500	-1.02107700	3.22275100
C	-2.49500500	-1.61664000	2.57540500
C	-2.30000000	-2.73595200	1.76731000
C	-3.02120200	-2.83732700	0.51135700
C	-2.09221500	-3.31361700	-0.47614100
C	-1.96526400	-2.67128000	-1.74981500
C	-2.96431600	-1.71378800	-2.08699000
C	-2.60365900	-0.45738000	-2.76033200
C	-3.46453000	0.57846000	-2.22229400
C	-2.96306600	1.85121000	-2.00718800
C	-3.11371100	2.49054300	-0.71670400
C	-3.60468900	1.75260500	0.40013500
C	-4.26269800	0.50198900	0.10275900
C	-4.12473400	-0.66522300	0.98771500
C	-3.39379500	-0.54838700	2.14674400
C	-3.96844600	-1.86682000	0.16173500
C	-4.00687000	-1.43466700	-1.18119700
C	-4.26348200	0.00075900	-1.20649300
36. #10530 C ₇₂ (B3LYP/6-31G(d))			
C	-3.89209300	-1.62143800	0.42653400
C	-3.61932400	-2.18367400	-0.89483600
C	-2.59248700	-3.09928300	-0.76712600
C	-2.26888200	-3.21655700	0.68227600
C	-3.04501800	-2.24040000	1.39026400
C	-3.99251500	-0.24348700	0.32188400
C	-3.82733000	0.11686600	-1.10188900

C	-3.55421700	-1.09997100	-1.83319000
C	-2.55037800	-1.10921100	-2.79853000
C	-1.54932400	-2.15553900	-2.79342600
C	-1.53261500	-3.13151300	-1.75236900
C	-0.27395600	-3.60264700	-1.32646500
C	0.00718500	-3.87888600	0.08918900
C	-0.96946900	-3.56004000	1.10549900
C	-0.49996600	-2.98339400	2.32265000
C	-1.24580100	-1.93589500	2.96544700
C	-2.47592100	-1.45652700	2.44564100
C	-2.75314500	-0.01474400	2.48284700
C	-3.48383800	0.59722300	1.37426400
C	-3.20410800	1.92809000	0.98786100
C	-3.08418600	2.30326400	-0.41422100
C	-3.23846700	1.33966800	-1.46689000
C	-2.28768600	1.36315500	-2.59083500
C	-1.92205800	0.12343100	-3.19004700
C	-0.55573600	-0.16661600	-3.51630900
C	-0.31787400	-1.56679800	-3.25227200
C	0.94790800	-2.02096300	-2.81318100
C	0.93388300	-3.14894900	-1.92654400
C	1.98115300	-3.33577100	-0.95831100
C	1.38692200	-3.70978700	0.32015400
C	1.86565600	-3.08521500	1.53780000
C	0.90116100	-2.70711900	2.50572800
C	1.03752800	-1.47113000	3.23698400
C	-0.28308500	-1.03744600	3.55177400
C	-0.57065700	0.31007300	3.65424200
C	-1.82601700	0.82009100	3.17997500
C	-1.60231400	2.19046500	2.79747100
C	-2.29845700	2.75171300	1.73591700
C	-1.63038300	3.65494800	0.81673600
C	-2.13280800	3.36045400	-0.51585200
C	-1.26193000	3.41929800	-1.61649900
C	-1.31106100	2.38636200	-2.63187700
C	0.03644200	2.12308700	-3.06521100
C	0.47019100	0.80286300	-3.38671400
C	1.82000600	0.35922100	-3.02639500
C	2.06964100	-1.06725200	-2.75165000
C	3.17386200	-1.41304500	-1.93546900
C	3.10560400	-2.54645100	-1.01230700
C	3.72875300	-2.15844000	0.22401600
C	3.04641000	-2.28829600	1.47110100
C	3.11978800	-0.99390500	2.11266800

C	2.06938000	-0.52443600	2.92483500
C	1.75126100	0.91578700	2.93556900
C	0.47266700	1.29360300	3.41229000
C	-0.18708800	2.48798200	2.96526100
C	0.45352800	3.34403500	2.08634600
C	-0.29304500	3.97003400	1.00113000
C	0.59461800	4.06934100	-0.13913400
C	0.10469100	3.81987700	-1.43292000
C	0.90042700	3.03435600	-2.35460500
C	2.16819800	2.61974000	-2.00441300
C	2.65909300	1.31719600	-2.40004600
C	3.63509100	0.93009100	-1.42242300
C	3.94135600	-0.39979900	-1.24387200
C	4.24960000	-0.85075900	0.08457000
C	3.82269500	-0.09122000	1.20890500
C	3.41888600	1.26594400	1.05902200
C	2.42819200	1.81737700	1.98906500
C	1.77071700	3.01813900	1.61057200
C	1.87606800	3.55054100	0.25938700
C	2.68144300	2.90068700	-0.67228800
C	3.50323400	1.81159800	-0.26775900
37. #11037 C ₇₂ (B3LYP/6-31G(d))			
C	3.85130800	-1.90867100	-0.72958000
C	3.85131300	-1.90867400	0.72955300
C	2.82317100	-2.74274100	1.19535200
C	2.26788900	-3.36967800	-0.00001100
C	2.82316300	-2.74273600	-1.19537600
C	3.99721700	-0.57079400	-1.17051200
C	4.09574800	0.30696000	-0.00001100
C	3.99722500	-0.57079900	1.17048900
C	3.24977500	-0.17788600	2.27282200
C	2.24977800	-1.04940700	2.83797400
C	1.93832900	-2.30049300	2.25076800
C	0.53984300	-2.74235500	2.25212300
C	0.13206400	-3.58802600	1.18389300
C	0.96661000	-3.75382700	-0.00000800
C	0.13205700	-3.58802200	-1.18390300
C	0.53982800	-2.74234800	-2.25213300
C	1.93831400	-2.30048400	-2.25078500
C	2.24975900	-1.04939700	-2.83798800
C	3.24975900	-0.17787700	-2.27284000
C	2.77038000	1.17385400	-2.35134100
C	2.94330200	2.08458000	-1.27678400
C	3.51795200	1.58264600	-0.00000700

C	2.94331300	2.08457800	1.27677500
C	2.77039600	1.17384600	2.35133100
C	1.57058400	1.16805600	3.15472800
C	1.21503200	-0.20088400	3.38663300
C	-0.13789400	-0.62366600	3.46029100
C	-0.49504100	-1.93541300	2.91044900
C	-1.85342200	-2.13660700	2.53275700
C	-2.21359100	-2.97473000	1.42050100
C	-1.21680800	-3.64605200	0.73096400
C	-1.21681300	-3.64605100	-0.73096600
C	-2.21360000	-2.97472700	-1.42049400
C	-1.85344000	-2.13660100	-2.53275200
C	-0.49506000	-1.93540500	-2.91045200
C	-0.13791900	-0.62365600	-3.46029100
C	1.21501000	-0.20087200	-3.38663900
C	1.57056000	1.16806400	-3.15473300
C	0.57603700	2.16464900	-2.97326400
C	0.83875400	3.20822800	-2.05101300
C	2.02464300	3.17670900	-1.22857000
C	1.72834300	3.83735900	-0.00000100
C	2.02465400	3.17670500	1.22857200
C	0.83877300	3.20822100	2.05101500
C	0.57606000	2.16464100	2.97326600
C	-0.77027400	1.78341200	3.17999400
C	-1.11570900	0.42094900	3.47909600
C	-2.45544900	0.19366500	3.01427300
C	-2.82524600	-1.06061600	2.56603800
C	-3.71393500	-1.18612700	1.42094000
C	-3.32461600	-2.37274400	0.69873100
C	-3.32462100	-2.37274300	-0.69871600
C	-3.71394500	-1.18612500	-1.42092200
C	-2.82526500	-1.06061200	-2.56602500
C	-2.45547000	0.19367100	-3.01425900
C	-1.11573300	0.42095500	-3.47909000
C	-0.77029700	1.78342100	-3.17998500
C	-1.82767300	2.34404200	-2.36347200
C	-1.54535300	3.20787400	-1.27059400
C	-0.22239300	3.74285200	-1.22733400
C	0.35355700	4.18257900	0.00000500
C	-0.22238200	3.74284900	1.22733900
C	-1.54534400	3.20786900	1.27060800
C	-1.82765700	2.34403600	2.36348500
C	-2.89255100	1.38351800	2.30995700
C	-3.65721300	1.27057900	1.16118700

C	-4.10883300	-0.04076800	0.72149000
C	-4.10883800	-0.04076700	-0.72146700
C	-3.65722100	1.27058000	-1.16116500
C	-2.89256800	1.38352200	-2.30993800
C	-3.34545900	2.08210900	0.00001200
C	-2.27286900	3.00180600	0.00000900
38. #11078 C ₇₂ (B3LYP/6-31G(d))			
C	3.53957000	-2.30925900	0.57763500
C	2.62446800	-3.43542300	0.39475900
C	2.15203700	-3.44240700	-0.92508500
C	2.87006500	-2.35573700	-1.60529200
C	3.69694000	-1.62824100	-0.62701100
C	3.19544300	-1.63496900	1.77734200
C	2.05324100	-2.32407500	2.35402600
C	1.74720100	-3.46208000	1.49964400
C	0.42415900	-3.81196100	1.27593100
C	-0.04554400	-4.04373300	-0.06630900
C	0.76329400	-3.70034600	-1.19159000
C	0.11571300	-2.96614400	-2.29134200
C	0.86232900	-1.95752600	-2.96478000
C	2.23438300	-1.65376400	-2.58903500
C	2.46460600	-0.23283700	-2.73941700
C	3.29842400	0.48953800	-1.83078200
C	3.80263500	-0.19567100	-0.64082300
C	3.77520200	0.49593900	0.64004500
C	3.32699400	-0.22701000	1.83009400
C	2.43919400	0.42705700	2.73926700
C	1.28724700	-0.23010000	3.24132600
C	1.00696500	-1.60051600	2.97693100
C	-0.39749300	-2.02429800	2.82012000
C	-0.64112700	-3.17883300	2.03394100
C	-1.84322700	-3.31999500	1.26287200
C	-1.47354400	-3.79269800	-0.05781800
C	-2.09989000	-3.24710300	-1.16628400
C	-1.28912900	-2.77436700	-2.27784800
C	-1.89437500	-1.56710200	-2.76700300
C	-1.11070900	-0.46365500	-3.21446300
C	0.27182100	-0.73002300	-3.36882900
C	1.26421700	0.33103100	-3.24100800
C	0.87655700	1.67478200	-2.97620800
C	1.86243700	2.47921300	-2.35430600
C	3.05567000	1.88270400	-1.77790100
C	3.34556100	2.58211500	-0.57830900
C	3.55644400	1.91560300	0.62617600

C	2.67504800	2.57543000	1.60475200
C	2.09716900	1.82529600	2.58871900
C	0.70530200	2.01939700	2.96454800
C	0.21393200	0.74912900	3.36898400
C	-1.14333500	0.37441300	3.21484200
C	-1.47575700	-1.03348600	2.95140700
C	-2.71708000	-1.29797100	2.31736400
C	-2.87795900	-2.41166700	1.42126100
C	-3.65286700	-1.98057500	0.27408200
C	-3.22628300	-2.35410300	-1.00333500
C	-3.12613700	-1.34861400	-2.03786100
C	-3.56644100	-0.05840300	-1.81178000
C	-2.81179300	1.07905000	-2.31705800
C	-1.55327900	0.91339900	-2.95069000
C	-0.55681900	1.98625300	-2.81927000
C	-0.89082400	3.11793600	-2.03333100
C	0.12104700	3.83373200	-1.27579700
C	1.46765300	3.58979500	-1.50004100
C	2.34444700	3.63253100	-0.39518900
C	1.87305300	3.60176300	0.92477700
C	0.46835200	3.74866400	1.19132500
C	-0.11901900	2.96561900	2.29107000
C	-1.50433600	2.66358500	2.27785900
C	-2.01209200	1.41238000	2.76712300
C	-3.22260300	1.09712700	2.03799700
C	-3.55913400	-0.22376700	1.81183000
C	-4.09271900	-0.62824400	0.52158100
C	-4.12994900	0.30255700	-0.52133700
C	-3.79801700	1.68534600	-0.27378600
C	-3.05991100	2.17655100	-1.42093100
C	-2.10041800	3.16401300	-1.26252300
C	-1.76919100	3.66465700	0.05812300
C	-0.36529700	4.02756400	0.06642900
C	-2.35020200	3.07094900	1.16660700
C	-3.40232100	2.09158500	1.00358400
39. #11097C ₇₂ (B3LYP/6-31G(d))			
C	-3.87109200	-1.31448400	1.14732400
C	-3.91392600	-1.92334300	-0.18815900
C	-2.89145000	-2.88115800	-0.27159500
C	-2.36886800	-3.02185600	1.08395400
C	-2.88465400	-1.95214000	1.92047100
C	-3.97329300	0.08059700	1.03774400
C	-4.18483200	0.36920500	-0.38837300
C	-4.06264200	-0.89231200	-1.13325600

C	-3.26972700	-0.94155600	-2.28601100
C	-2.24227400	-1.94518100	-2.41687300
C	-1.97767800	-2.89138600	-1.39024400
C	-0.59044400	-3.33386200	-1.17798800
C	-0.23274500	-3.75337600	0.13027000
C	-1.09118900	-3.44605600	1.26380400
C	-0.28452600	-2.90196300	2.33480000
C	-0.67872500	-1.73110500	3.02971000
C	-2.02034900	-1.18341700	2.75146000
C	-2.26419400	0.25075400	2.81926200
C	-3.16665600	0.90886100	1.86333700
C	-2.80210400	2.23322800	1.32586500
C	-2.99277400	2.47523500	-0.06557100
C	-3.65634600	1.51601300	-0.92139700
C	-2.96043000	1.49591800	-2.20137100
C	-2.74809400	0.28680000	-2.85204200
C	-1.46260200	0.01820700	-3.43947800
C	-1.15208500	-1.35847100	-3.17461200
C	0.18179000	-1.80526300	-3.03628100
C	0.48561300	-2.85012100	-2.04990200
C	1.82667800	-2.93863300	-1.59109400
C	2.14162500	-3.33473600	-0.24423900
C	1.10692700	-3.68025400	0.61770600
C	1.08610500	-3.16722200	1.98063800
C	2.09405100	-2.31436100	2.40267400
C	1.75107000	-1.13600500	3.15660000
C	0.39214000	-0.84001200	3.47380700
C	0.08795600	0.51895800	3.68800000
C	-1.23734100	1.05249400	3.40572300
C	-1.10655000	2.42255300	3.10603100
C	-1.74128600	2.95163700	1.94129400
C	-0.74073900	3.63479100	1.17646600
C	-0.81887600	3.67204400	-0.23507900
C	-1.98637300	3.13373600	-0.84894400
C	-1.91566600	2.48254800	-2.14042100
C	-0.67703300	2.29288900	-2.80483300
C	-0.44495800	1.01180300	-3.48248000
C	0.88246100	0.52389300	-3.60067600
C	1.18923100	-0.86559800	-3.40879100
C	2.53072800	-0.96310100	-2.88293300
C	2.84242200	-1.97737800	-1.99450000
C	3.69689900	-1.70010000	-0.85331800
C	3.24914000	-2.53336600	0.23704300
C	3.21419300	-2.01851000	1.53507500

C	3.57392900	-0.63980600	1.77595400
C	2.65878600	-0.09236400	2.75355200
C	2.25908000	1.26910000	2.71487300
C	1.03132200	1.55548100	3.36963700
C	0.28706800	2.73670800	3.04940700
C	0.54119100	3.40550400	1.84324100
C	1.73821800	3.14585700	1.08967600
C	1.66829200	3.41143900	-0.29992900
C	0.39249800	3.62137600	-0.97562700
C	0.45324300	2.97904000	-2.24793400
C	1.79342800	2.47997000	-2.43634000
C	2.00943800	1.29245000	-3.11971100
C	3.04109900	0.37558600	-2.67670800
C	3.78846600	0.66258800	-1.53596700
C	4.11834100	-0.38897300	-0.60590700
C	4.01280100	0.16377500	0.73532200
C	3.57365200	1.54762600	0.63957400
C	2.67116100	2.11082900	1.57329900
C	3.49605500	1.86484600	-0.76609700
C	2.54542100	2.76313100	-1.22891400
40. #10784 C ₇₂ (B3LYP/6-31G(d))			
C	-4.04508500	-0.61427800	1.33294300
C	-4.22631800	-0.89590800	-0.07320200
C	-3.51769100	-2.05240500	-0.41118000
C	-2.85447600	-2.51119000	0.81591500
C	-3.16802500	-1.59001500	1.88340100
C	-3.79093900	0.76143000	1.46800400
C	-3.76176300	1.38175500	0.12643100
C	-4.08165700	0.32045200	-0.81191500
C	-3.43300800	0.27655800	-2.03680100
C	-2.85200400	-0.96637600	-2.51664700
C	-2.83568300	-2.11711600	-1.67362700
C	-1.69233300	-2.94617200	-1.73749800
C	-1.14776600	-3.55867600	-0.53545700
C	-1.62306400	-3.19601500	0.76744200
C	-0.65179900	-3.00442400	1.85932400
C	-0.90922600	-1.96174000	2.86549100
C	-2.16252100	-1.20217700	2.82182500
C	-2.15526500	0.17493100	3.21027500
C	-2.89067600	1.16118600	2.44962900
C	-2.06071500	2.30062900	2.22202300
C	-2.03554100	2.94599500	0.93726500
C	-2.82795100	2.38340500	-0.18441600
C	-2.25669600	2.42328500	-1.55057200

C	-2.59030300	1.36626200	-2.43398100
C	-1.60457300	0.81085000	-3.33846500
C	-1.70936400	-0.63033100	-3.31594900
C	-0.54101800	-1.44767800	-3.35593600
C	-0.60592900	-2.66985500	-2.62557100
C	0.58373100	-3.27254400	-2.06364400
C	0.23110300	-3.82861400	-0.77049000
C	1.13843100	-3.78216000	0.28398900
C	0.68866700	-3.38901100	1.61126100
C	1.80040400	-2.72506800	2.24284700
C	1.56022500	-1.69732100	3.13778300
C	0.21180700	-1.33957800	3.47429600
C	0.21654100	0.08145000	3.76904700
C	-0.93662400	0.81896300	3.59564400
C	-0.85802200	2.12534100	2.99522100
C	0.37893800	2.67058200	2.57896500
C	0.28835600	3.61319900	1.51166800
C	-0.88004000	3.67582100	0.65216200
C	-0.41122100	3.86759000	-0.72962900
C	-1.00444300	3.13715400	-1.80122600
C	-0.10036800	2.64539000	-2.80481800
C	-0.38246000	1.42322600	-3.49424800
C	0.82581700	0.62217300	-3.60031800
C	0.77011600	-0.79524300	-3.50515900
C	1.92290900	-1.42087900	-2.95453300
C	1.82152900	-2.68804800	-2.24468300
C	2.80245600	-2.71178500	-1.18155900
C	2.46953100	-3.27357000	0.06637000
C	2.88785700	-2.61533600	1.27832700
C	3.63093800	-1.43848000	1.21363600
C	3.34730100	-0.34984300	2.12785400
C	2.35709500	-0.48017000	3.08777800
C	1.49715300	0.63286000	3.40541400
C	1.61147400	1.88976900	2.74555900
C	2.67993000	2.02625300	1.75007500
C	2.53812300	2.99022700	0.70540200
C	1.40483400	3.83354800	0.68413100
C	0.98007300	4.05956400	-0.67780900
C	1.86803900	3.33821400	-1.51984300
C	1.33092000	2.66465500	-2.60203200
C	1.87677000	1.37978000	-3.00672600
C	2.91501600	0.75263800	-2.25860500
C	2.96430900	-0.66279600	-2.33558200
C	3.51052600	-1.46395400	-1.24056500

C	3.93004300	-0.84038500	-0.06918000
C	3.82910600	0.59601700	0.06002500
C	3.48470200	0.90091700	1.42514800
C	3.38903000	1.41296500	-1.02655500
C	2.86077000	2.67410700	-0.67414800
41. #11032C ₇₂ (B3LYP/6-31G(d))			
C	-4.24989800	0.72903100	-0.93953100
C	-4.24989800	-0.72903200	-0.93953100
C	-4.04707400	-1.20280300	0.36237300
C	-3.96773400	-0.00000100	1.20487100
C	-4.04707400	1.20280200	0.36237300
C	-3.44209400	1.16146900	-2.02359700
C	-2.83822900	0.00000000	-2.66112000
C	-3.44209400	-1.16146900	-2.02359700
C	-2.69439200	-2.30732400	-1.84364700
C	-2.66233400	-2.97587700	-0.56104100
C	-3.18779800	-2.33495900	0.59779700
C	-2.36784500	-2.35385600	1.81893700
C	-2.38356400	-1.18745200	2.66136400
C	-3.14556900	0.00000000	2.29458800
C	-2.38356400	1.18745100	2.66136400
C	-2.36784500	2.35385500	1.81893700
C	-3.18779800	2.33495900	0.59779700
C	-2.66233400	2.97587700	-0.56104100
C	-2.69439300	2.30732400	-1.84364800
C	-1.39673600	2.41496900	-2.46178800
C	-0.73169600	1.27261700	-2.99386700
C	-1.47399200	0.00000000	-3.04412400
C	-0.73169500	-1.27261700	-2.99386800
C	-1.39673600	-2.41496900	-2.46178800
C	-0.68758000	-3.43397300	-1.73672800
C	-1.42504500	-3.71807300	-0.51979400
C	-0.72510600	-3.84577600	0.66995700
C	-1.17928600	-3.12534600	1.84060600
C	0.00000100	-2.68623600	2.54864700
C	0.00000100	-1.46164500	3.26897000
C	-1.22506900	-0.73648400	3.32304700
C	-1.22506900	0.73648300	3.32304800
C	0.00000000	1.46164400	3.26896900
C	0.00000000	2.68623600	2.54864800
C	-1.17928600	3.12534600	1.84060600
C	-0.72510700	3.84577700	0.66995800
C	-1.42504600	3.71807100	-0.51979300
C	-0.68758100	3.43397400	-1.73672800

C	0.68758000	3.43397400	-1.73672900
C	1.39673500	2.41496900	-2.46178800
C	0.73169500	1.27261700	-2.99386800
C	1.47399200	0.00000100	-3.04412500
C	0.73169500	-1.27261700	-2.99386800
C	1.39673500	-2.41496900	-2.46178800
C	0.68758100	-3.43397500	-1.73673000
C	1.42504500	-3.71807000	-0.51979400
C	0.72510800	-3.84577800	0.66995700
C	1.17928700	-3.12534600	1.84060600
C	2.36784600	-2.35385500	1.81893700
C	2.38356500	-1.18745100	2.66136400
C	1.22507000	-0.73648300	3.32304800
C	1.22507000	0.73648300	3.32304800
C	2.38356400	1.18745100	2.66136300
C	2.36784500	2.35385600	1.81893800
C	1.17928600	3.12534600	1.84060600
C	0.72510600	3.84577800	0.66995800
C	1.42504400	3.71807000	-0.51979300
C	2.66233400	2.97587700	-0.56104200
C	2.69439200	2.30732500	-1.84364900
C	3.44209300	1.16146900	-2.02359800
C	2.83822900	0.00000100	-2.66112200
C	3.44209500	-1.16146900	-2.02359900
C	2.69439200	-2.30732300	-1.84364700
C	2.66233400	-2.97587700	-0.56104200
C	3.18779800	-2.33495800	0.59779600
C	4.04707500	-1.20280300	0.36237300
C	3.96773400	0.00000000	1.20487000
C	3.14556900	0.00000000	2.29458800
C	4.04707300	1.20280300	0.36237300
C	3.18779800	2.33495900	0.59779600
C	4.24989700	0.72903200	-0.93953200
C	4.24989600	-0.72903000	-0.93953100
42. #10534 C ₇₂ (B3LYP/6-31G(d))			
C	1.82456600	-3.79208000	-0.52318000
C	3.06074900	-3.13238800	-0.31838600
C	3.04206600	-2.61466800	1.00653300
C	1.84889400	-3.11588400	1.67694900
C	1.06976200	-3.82357300	0.69483800
C	1.21508000	-3.35220300	-1.73489400
C	2.08204600	-2.35262300	-2.31531700
C	3.22731500	-2.23009300	-1.42283100
C	3.74897700	-0.97927100	-1.20951900

C	4.00517000	-0.50847300	0.17236900
C	3.53082700	-1.29161900	1.29026700
C	2.93170700	-0.56921100	2.36155500
C	1.76661100	-1.07934800	3.04258900
C	1.20105400	-2.32922900	2.66477300
C	-0.21327400	-2.45395000	2.77330700
C	-0.97205200	-3.22230800	1.82053800
C	-0.34325400	-3.74993900	0.65241800
C	-1.02410000	-3.57475500	-0.65256200
C	-0.19647100	-3.27251600	-1.83689400
C	-0.67695400	-2.33798300	-2.79051100
C	0.16824700	-1.28201500	-3.29710200
C	1.54388800	-1.21368600	-2.97693700
C	2.14858900	0.10341600	-2.80047900
C	3.30315900	0.15218100	-1.97337400
C	3.61245400	1.31601600	-1.19628300
C	3.95690400	0.89945100	0.17326400
C	3.38201200	1.62209200	1.27922800
C	2.84552600	0.86040700	2.34695600
C	1.59556200	1.23641900	2.96961800
C	0.93391200	0.03567400	3.38365100
C	-0.48913500	-0.06195400	3.41859400
C	-1.03640200	-1.36275600	3.24190900
C	-2.34559100	-1.54927100	2.68479100
C	-2.29806900	-2.68618900	1.78362400
C	-3.00121000	-2.65260300	0.58771000
C	-2.34258100	-3.07834600	-0.64034400
C	-2.85586300	-2.23067300	-1.70174200
C	-2.01608300	-1.83909100	-2.73400300
C	-1.99891900	-0.45972700	-3.18042700
C	-0.63210000	-0.09348500	-3.44519900
C	-0.12518200	1.19625200	-3.14398500
C	1.31400600	1.31464700	-2.90256700
C	1.78451000	2.50235600	-2.29282500
C	2.95615500	2.49443800	-1.44216800
C	2.70659000	3.37564700	-0.32965700
C	2.76454000	2.88645700	1.01464900
C	1.54118900	3.27976200	1.67637000
C	0.87260700	2.39392500	2.57251900
C	-0.60137500	2.33655100	2.59977900
C	-1.28507200	1.11344800	3.04406900
C	-2.61628600	0.88189700	2.59943500
C	-3.13663700	-0.45594400	2.38740700
C	-3.95852700	-0.46059400	1.19022700

C	-3.87072600	-1.53548700	0.29176700
C	-3.78772700	-1.27437800	-1.12865900
C	-3.81730100	0.03889700	-1.60203600
C	-2.87211300	0.45555700	-2.62866100
C	-2.40820300	1.78934800	-2.34245100
C	-1.05942700	2.18238100	-2.57498100
C	-0.53647700	3.27494100	-1.76211100
C	0.87015800	3.47046700	-1.71263500
C	1.48520200	4.03954900	-0.55063500
C	0.77636800	4.03890600	0.69860700
C	-0.58437000	3.91723100	0.66605100
C	-1.29371200	3.18380400	1.69796200
C	-2.56540700	2.82890100	1.14620600
C	-3.24233800	1.72288400	1.61072900
C	-4.01462400	0.89137500	0.69418600
C	-3.95429700	1.13995300	-0.67995400
C	-3.13628000	2.23675500	-1.17929700
C	-2.53314600	3.11658700	-0.29009100
C	-1.27512000	3.68974200	-0.60274800
43. #10981C ₇₂ (B3LYP/6-31G(d))			
C	3.95305000	-1.81272500	-0.80432600
C	4.32982100	-0.41428100	-0.84877800
C	4.25033000	0.13948900	0.44387400
C	3.92138800	-0.96354800	1.35124300
C	3.74526500	-2.17964900	0.54954600
C	2.96734200	-2.04037400	-1.78746800
C	2.76713800	-0.78396800	-2.52589600
C	3.66869500	0.18952600	-1.94659500
C	3.26807000	1.51012300	-1.81674600
C	3.38321900	2.19142800	-0.54506000
C	3.69724500	1.45613200	0.63459600
C	2.87179900	1.70223900	1.82677700
C	2.54108500	0.59352500	2.66676300
C	3.06793200	-0.73166000	2.41141200
C	2.03669100	-1.69656400	2.76693100
C	1.86639200	-2.84700300	2.00707200
C	2.70352700	-3.05937000	0.83415700
C	1.83752800	-3.51469600	-0.22105400
C	1.87004200	-2.90570700	-1.51655200
C	0.61348900	-2.66246700	-2.22520300
C	0.43256200	-1.41300300	-2.97838400
C	1.50307000	-0.40476000	-3.00322800
C	1.16146700	1.03576900	-3.03863500
C	2.07577500	1.95962400	-2.47601300

C	1.61860000	3.14020300	-1.77163800
C	2.38866800	3.23771000	-0.54274000
C	1.73650600	3.58543000	0.63260300
C	1.93240600	2.76389600	1.81303500
C	0.66302300	2.66154100	2.48441300
C	0.24137000	1.44082900	3.08808900
C	1.23247000	0.44118800	3.21259300
C	0.88590800	-0.97412700	3.21894100
C	-0.43256200	-1.41300200	2.97838500
C	-0.61348700	-2.66246500	2.22520300
C	0.54262300	-3.31636700	1.73599700
C	0.56745400	-3.84172300	0.38139300
C	-0.56745200	-3.84172200	-0.38139300
C	-0.54262200	-3.31636800	-1.73599700
C	-1.86639100	-2.84700700	-2.00707400
C	-2.03669000	-1.69656500	-2.76692700
C	-0.88590800	-0.97412900	-3.21894000
C	-1.23247000	0.44118700	-3.21259300
C	-0.24137000	1.44082800	-3.08808900
C	-0.66302400	2.66154000	-2.48441400
C	0.28503500	3.49680400	-1.78969100
C	-0.35432300	4.01654900	-0.59982900
C	0.35432100	4.01654800	0.59982800
C	-0.28503600	3.49680500	1.78969000
C	-1.61860100	3.14020200	1.77163600
C	-2.07577600	1.95962500	2.47601400
C	-1.16146800	1.03577000	3.03863500
C	-1.50307000	-0.40476000	3.00322900
C	-2.76713800	-0.78396700	2.52589700
C	-2.96734200	-2.04037600	1.78747000
C	-1.87004100	-2.90570600	1.51655300
C	-1.83752700	-3.51469600	0.22105400
C	-2.70352400	-3.05937000	-0.83415400
C	-3.74526700	-2.17965300	-0.54954500
C	-3.92138700	-0.96355000	-1.35124300
C	-3.06793400	-0.73166200	-2.41141300
C	-2.54108500	0.59352300	-2.66676300
C	-2.87180000	1.70223800	-1.82677800
C	-1.93240700	2.76389500	-1.81303600
C	-1.73650700	3.58542900	-0.63260400
C	-2.38866900	3.23771000	0.54273800
C	-3.38322000	2.19142700	0.54506000
C	-3.26807000	1.51012200	1.81674400
C	-3.66869700	0.18952500	1.94659600

C	-4.32981900	-0.41428200	0.84877800
C	-3.95304600	-1.81272500	0.80432500
C	-4.25033100	0.13948800	-0.44387400
C	-3.69724600	1.45613000	-0.63459700
44. #11158C ₇₂ (B3LYP/6-31G(d))			
C	2.04153900	3.56844900	-0.56471800
C	2.34562900	2.99268600	-1.85554700
C	1.12459100	2.80363700	-2.55581000
C	0.08017000	3.38561300	-1.73115100
C	0.67671800	3.83971800	-0.47620100
C	2.74688300	2.87048600	0.45811300
C	3.54774300	1.85759400	-0.19197900
C	3.25198700	1.94225300	-1.63843300
C	3.09622500	0.78005900	-2.38373100
C	1.96586700	0.63865900	-3.26435100
C	0.88555500	1.58997900	-3.25766000
C	-0.49281700	1.09865200	-3.36783100
C	-1.58102200	1.80156200	-2.67046700
C	-1.24370400	2.92163100	-1.77654700
C	-2.02252400	3.15022200	-0.59614400
C	-1.40132700	3.49852100	0.67016600
C	-0.00267400	3.67377600	0.77257500
C	0.72469700	3.09387800	1.90538100
C	2.10331600	2.62999300	1.70560000
C	2.56343500	1.47970200	2.40723200
C	3.40784900	0.50594300	1.79338700
C	3.79791100	0.61545000	0.41916600
C	3.79796000	-0.61526600	-0.41904000
C	3.40798000	-0.50578700	-1.79327000
C	2.56362000	-1.47956900	-2.40713000
C	1.69741400	-0.76722300	-3.32192100
C	0.41953400	-1.22350900	-3.54209700
C	-0.67791300	-0.27889700	-3.65406700
C	-1.86363500	-0.98560300	-3.27047000
C	-2.91543100	-0.30478300	-2.68011000
C	-2.77938500	1.09919000	-2.39696400
C	-3.57088200	1.36645800	-1.20238000
C	-3.19218600	2.37431900	-0.31932900
C	-3.27993000	2.16367900	1.11232100
C	-2.15665600	2.85831400	1.70839000
C	-1.48173700	2.30806200	2.79228500
C	-0.05506100	2.42554000	2.89395400
C	0.41932400	1.22353900	3.54211300
C	1.69723600	0.76731200	3.32198500

C	1.96576800	-0.63855800	3.26443600
C	3.09615800	-0.77989800	2.38384700
C	3.25198900	-1.94209100	1.63853300
C	3.54782500	-1.85743100	0.19210600
C	2.74705200	-2.87034800	-0.45801200
C	2.10353400	-2.62989600	-1.70552000
C	0.72493800	-3.09383600	-1.90535700
C	-0.05481700	-2.42555100	-2.89397100
C	-1.48148800	-2.30813600	-2.79234300
C	-2.15642600	-2.85842400	-1.70846700
C	-3.27975700	-2.16384500	-1.11244500
C	-3.67508300	-0.92471500	-1.60353700
C	-4.08609100	0.11895800	-0.69345200
C	-4.08611500	-0.11916800	0.69329500
C	-3.67520800	0.92452800	1.60339900
C	-2.91556900	0.30463700	2.68000600
C	-1.86383000	0.98551200	3.27040300
C	-0.67808100	0.27887000	3.65404000
C	-0.49290000	-1.09866900	3.36781400
C	0.88550600	-1.58992500	3.25769700
C	1.12461900	-2.80357400	2.55585000
C	2.34572100	-2.99259000	1.85563800
C	2.04171900	-3.56840600	0.56480900
C	0.67692200	-3.83966500	0.47622600
C	-0.00244400	-3.67376500	-0.77257900
C	-1.40110600	-3.49858400	-0.67022000
C	-2.02238600	-3.15032700	0.59608200
C	-3.19206100	-2.37447800	0.31921100
C	-3.57086700	-1.36664200	1.20225100
C	-2.77943700	-1.09933000	2.39686300
C	-1.58104100	-1.80163600	2.67040800
C	-1.24362900	-2.92168100	1.77650100
C	0.08028600	-3.38557900	1.73117300
45. #11184 C ₇₂ (B3LYP/6-31G(d))			
C	-2.39219000	3.21814000	1.22220300
C	-3.26366800	2.88745200	0.10334000
C	-4.00935400	1.73644100	0.43488800
C	-3.57089300	1.31851000	1.77009900
C	-2.46564100	2.20066000	2.17906300
C	-1.15525700	3.66449500	0.73615100
C	-1.21367300	3.55960800	-0.70593100
C	-2.48328600	2.95782000	-1.06539600
C	-2.51807400	1.91040200	-2.03889800
C	-3.50166400	0.89174100	-1.81819200

C	-4.21254400	0.77968000	-0.56003800
C	-4.26541200	-0.63302600	-0.20627000
C	-3.94940000	-1.02485200	1.09696700
C	-3.52320500	-0.02188500	2.06506500
C	-2.40935800	-0.55503400	2.82070800
C	-1.31041900	0.27894500	3.19878700
C	-1.26442700	1.67704300	2.78510000
C	0.01488300	2.29111300	2.47326900
C	0.04153900	3.33192400	1.43855600
C	1.21367400	3.55960700	0.70593100
C	1.15525800	3.66449500	-0.73615000
C	-0.04153800	3.33192400	-1.43855500
C	-0.01488200	2.29111300	-2.47326900
C	-1.26889600	1.57609700	-2.75239000
C	-1.17167400	0.27965100	-3.30540400
C	-2.17279000	-0.73838400	-3.06385200
C	-3.29655800	-0.45313700	-2.31011100
C	-3.76514400	-1.40328200	-1.31881900
C	-3.03984600	-2.57817300	-1.09274600
C	-2.71772300	-2.98046300	0.25646400
C	-3.13299000	-2.19376600	1.32318100
C	-2.20045200	-1.90262400	2.40243200
C	-0.91653400	-2.51247900	2.45558900
C	0.08390400	-1.78204600	3.14003800
C	-0.09451800	-0.38607100	3.44279200
C	1.17167400	0.27965000	3.30540400
C	1.26889700	1.57609600	2.75239000
C	2.51807500	1.91040000	2.03889800
C	2.48328600	2.95781800	1.06539600
C	3.26367000	2.88745200	-0.10334000
C	2.39219100	3.21813900	-1.22220200
C	2.46564200	2.20066000	-2.17906300
C	1.26442700	1.67704300	-2.78509900
C	1.31041800	0.27894600	-3.19878700
C	0.09451800	-0.38607000	-3.44279200
C	-0.08390400	-1.78204600	-3.14003800
C	-1.48569400	-2.00169200	-2.89919000
C	-1.89020900	-2.89233900	-1.91187800
C	-0.88635300	-3.53679800	-1.08548300
C	-1.38283500	-3.56181700	0.25683500
C	-0.50335800	-3.40184200	1.35989900
C	0.88635200	-3.53679800	1.08548200
C	1.89020800	-2.89234000	1.91187700
C	1.48569300	-2.00169300	2.89918900

C	2.17279000	-0.73838500	3.06385100
C	3.29655800	-0.45313800	2.31011100
C	3.50166400	0.89173900	1.81819200
C	4.21254600	0.77967900	0.56003800
C	4.00935300	1.73643900	-0.43488800
C	3.57089400	1.31850900	-1.77009800
C	3.52320500	-0.02188600	-2.06506500
C	2.40935800	-0.55503500	-2.82070800
C	2.20045100	-1.90262400	-2.40243200
C	0.91653200	-2.51247900	-2.45559000
C	0.50335700	-3.40184200	-1.35990000
C	1.38283300	-3.56181700	-0.25683500
C	2.71772200	-2.98046300	-0.25646400
C	3.03984600	-2.57817400	1.09274600
C	3.76514300	-1.40328300	1.31881800
C	4.26541200	-0.63302700	0.20627000
C	3.94940000	-1.02485300	-1.09696800
C	3.13298900	-2.19376700	-1.32318100

46. #10780 C₇₂ (B3LYP/6-31G(d))

C	-3.84770200	-1.90049700	0.62313200
C	-3.82542300	-1.88591200	-0.83129700
C	-2.79057300	-2.71183600	-1.28658000
C	-2.14343800	-3.27225700	-0.09710600
C	-2.78790800	-2.70435400	1.08269600
C	-4.04013300	-0.57636400	1.07817700
C	-4.09437500	0.31060100	-0.09791000
C	-3.97316400	-0.54720900	-1.27885400
C	-3.21169900	-0.12487800	-2.37244900
C	-2.23555300	-0.99810700	-2.95909800
C	-1.99338900	-2.28438900	-2.40404100
C	-0.66651900	-2.76780600	-2.46121000
C	-0.10459400	-3.50754200	-1.37180300
C	-0.78298600	-3.58870900	-0.09676700
C	0.00568400	-3.40670800	1.14233900
C	-0.60465600	-2.70476100	2.27781800
C	-2.00573200	-2.29350800	2.20975100
C	-2.40373200	-1.07210200	2.83661900
C	-3.35412500	-0.18266100	2.21837500
C	-2.85319300	1.16623800	2.31464100
C	-2.98291300	2.07423200	1.23166700
C	-3.52259800	1.58790600	-0.06615700
C	-2.89830100	2.09215500	-1.31642000
C	-2.69621600	1.21061800	-2.39679000
C	-1.42476400	1.18229900	-3.10775200

C	-1.12953500	-0.16921100	-3.41424200
C	0.21546400	-0.65259000	-3.45299100
C	0.39862300	-2.01555100	-3.09540200
C	1.63323600	-2.47211300	-2.52988900
C	1.31727400	-3.38545100	-1.44597700
C	2.07317500	-3.37149300	-0.28449100
C	1.41608500	-3.39333700	1.01648300
C	2.25675600	-2.63993800	1.91033000
C	1.67217200	-1.90212200	2.92654400
C	0.25729300	-1.95943700	3.13294200
C	-0.14017200	-0.66916300	3.64983400
C	-1.42720600	-0.22521200	3.47152700
C	-1.66775100	1.14992600	3.12734600
C	-0.57962400	2.04738500	2.89836000
C	-0.85330900	3.11871800	2.02351300
C	-2.04898700	3.13542200	1.22707800
C	-1.71158600	3.79005900	-0.00468400
C	-1.98536700	3.18671700	-1.24591800
C	-0.76417300	3.23644500	-2.04305800
C	-0.39837700	2.14062300	-2.86053400
C	1.00267400	1.70518500	-2.94549600
C	1.31243100	0.30144200	-3.24901900
C	2.56220200	-0.22346500	-2.81801200
C	2.70651700	-1.60804000	-2.41958000
C	3.58018600	-1.68029100	-1.25859100
C	3.26103200	-2.54801800	-0.20145900
C	3.37719800	-2.08896400	1.16145700
C	3.81934700	-0.79145200	1.42776900
C	3.14305900	0.00972500	2.43778300
C	2.12065200	-0.54126000	3.18932300
C	0.97745900	0.25082700	3.53486300
C	0.80297700	1.57513400	3.05733100
C	1.86777600	2.15344400	2.22391600
C	1.53718500	3.20150000	1.25242500
C	0.21183700	3.73309000	1.23194100
C	-0.35653000	4.23423100	0.03704100
C	0.22697400	3.90564900	-1.22635300
C	1.53020100	3.46416800	-1.24946700
C	1.94883400	2.44766800	-2.19081000
C	3.13232500	1.83739700	-1.65127600
C	3.45442000	0.53838800	-1.98052000
C	4.04247600	-0.34753200	-0.98145700
C	4.16480800	0.09171400	0.34147600
C	3.72096800	1.42826300	0.70271000

C	3.02716200	1.36836400	1.97279800
C	3.28925400	2.30633200	-0.27878000
C	2.24058500	3.23237400	0.00223000
47. #10848 C ₇₂ (B3LYP/6-31G(d))			
C	-2.83275100	-0.63843100	-2.93422400
C	-3.73251700	0.24244700	-2.22504600
C	-3.13361700	1.52514200	-2.14414200
C	-1.90403700	1.47717000	-2.90596500
C	-1.69266700	0.08700000	-3.31555500
C	-2.71752100	-1.86125300	-2.23289100
C	-3.63846900	-1.78676500	-1.10177800
C	-4.19654500	-0.43109200	-1.07466200
C	-4.24595000	0.27008500	0.15049400
C	-3.73581000	1.60308100	0.24089800
C	-3.16581800	2.24575400	-0.90409400
C	-2.10850600	3.16154100	-0.67074300
C	-1.02727700	3.29616500	-1.58247900
C	-0.82159200	2.31559900	-2.61207400
C	0.53418700	1.82715700	-2.88697200
C	0.73325800	0.40575600	-3.22777500
C	-0.41040400	-0.50568900	-3.26867800
C	-0.29378800	-1.87685200	-2.76998700
C	-1.45443300	-2.49232600	-2.12623400
C	-1.24088000	-3.32455400	-0.93395700
C	-2.13228600	-3.21252600	0.18268700
C	-3.31362700	-2.41348000	0.08988600
C	-3.49576100	-1.72546200	1.36813600
C	-3.92664200	-0.41485700	1.39853400
C	-3.26157300	0.53622000	2.27555600
C	-3.12237600	1.76602800	1.56179000
C	-1.99905400	2.61523500	1.77822600
C	-1.59344800	3.42475100	0.67462000
C	-0.26305900	3.90609000	0.55784200
C	0.09780100	3.83226800	-0.84752700
C	1.37478100	3.49961500	-1.22408100
C	1.60729100	2.53038400	-2.29463800
C	2.86235500	1.89706700	-2.01739400
C	3.07659500	0.58472300	-2.41966200
C	2.00229600	-0.15944800	-3.01771300
C	2.16306200	-1.55991700	-2.65394600
C	1.02761400	-2.40053900	-2.46520700
C	1.16144100	-3.45026200	-1.49238600
C	0.04987700	-3.76077500	-0.63527100
C	0.53534900	-3.82813600	0.74986000

C	-0.21758400	-3.22750200	1.79782800
C	-1.60250900	-3.10166900	1.52989600
C	-2.41459900	-2.16430300	2.24184800
C	-1.80877900	-1.27852900	3.12032800
C	-2.24047000	0.10778000	3.13271000
C	-1.09551900	0.92488800	3.36162000
C	-0.96878700	2.19857500	2.74058500
C	0.35550600	2.69017700	2.59352200
C	0.69957300	3.57856800	1.52741000
C	2.06919600	3.33033800	1.13604700
C	2.41377900	3.31751300	-0.21620300
C	3.35263200	2.35090100	-0.72482800
C	3.94502500	1.42450200	0.13880700
C	4.21700300	0.08453900	-0.30782700
C	3.84021000	-0.32126400	-1.59136500
C	3.32148500	-1.65242100	-1.80636800
C	3.34712800	-2.58215100	-0.74907300
C	2.32268000	-3.52532400	-0.68070300
C	1.91428700	-3.69049600	0.71522300
C	2.57961800	-2.69976300	1.49048200
C	1.85512800	-1.90671700	2.43225800
C	0.45218100	-2.25758200	2.67294000
C	-0.37960700	-1.30727100	3.32251100
C	0.04891200	0.04558200	3.50835200
C	1.36221100	0.46449100	3.17816800
C	1.50930000	1.84093400	2.84710600
C	2.57832200	2.28181400	2.00080500
C	3.49092800	1.35032400	1.52172500
C	3.41168300	-0.03646900	1.90929500
C	3.97868100	-0.80913000	0.82858200
C	3.59064600	-2.10952700	0.62488200
C	2.30624200	-0.52772100	2.65998700
48. #10962C ₇₂ (B3LYP/6-31G(d))			
C	4.42689900	-0.61456100	-0.75416600
C	4.50374100	0.63508200	0.02282700
C	4.03570500	0.37375800	1.32879900
C	3.88861300	-1.07892200	1.43578100
C	4.09134800	-1.66730600	0.11202900
C	3.71712500	-0.36243700	-1.94678900
C	3.54405600	1.08808200	-2.02069700
C	3.99640000	1.68251900	-0.75612800
C	3.19588200	2.64922800	-0.12698100
C	2.75645300	2.44562100	1.22484300
C	3.07355500	1.25907600	1.94454200

C	2.05276700	0.69824100	2.84227000
C	2.05927600	-0.70838600	3.03159500
C	2.90904000	-1.58894600	2.25372300
C	2.10733600	-2.73810200	1.83940200
C	2.24282600	-3.23948900	0.55357600
C	3.19748400	-2.63931300	-0.35570000
C	2.52026300	-2.44504900	-1.60518000
C	2.66146600	-1.25231400	-2.36709200
C	1.46091300	-0.69590900	-3.02247400
C	1.41879100	0.70686300	-3.19971000
C	2.42959300	1.59054200	-2.63599800
C	1.74477700	2.75851600	-2.09828500
C	2.10087000	3.25510300	-0.84854800
C	1.05589000	3.59503100	0.09007400
C	1.45283900	3.07921600	1.36449900
C	0.49522700	2.62837300	2.29919700
C	0.78660000	1.41160300	3.06787600
C	-0.33076100	0.68240200	3.54201700
C	-0.32051300	-0.75662700	3.55041000
C	0.84289600	-1.43007800	3.26708400
C	0.79924700	-2.61660400	2.44788200
C	-0.39409100	-3.00161700	1.79612700
C	-0.23951800	-3.56551400	0.44529000
C	1.05115000	-3.57787500	-0.17215200
C	1.23005300	-3.08908800	-1.50710600
C	0.12300000	-2.68278600	-2.28229500
C	0.18205800	-1.41547500	-3.00906600
C	-1.06471500	-0.69774000	-3.23025800
C	-1.06195100	0.75934900	-3.22251100
C	0.17988000	1.42394600	-3.18764000
C	0.36206000	2.66027600	-2.46509600
C	-0.66909000	3.17695600	-1.64367800
C	-0.30976900	3.64087600	-0.29714100
C	-1.25875100	3.48454500	0.74247900
C	-0.86142900	2.98830200	2.02847800
C	-1.96765400	2.22692300	2.55895000
C	-1.69687100	1.07283500	3.27525700
C	-2.47791300	-0.12863700	3.02855000
C	-1.58443900	-1.26098000	3.08893400
C	-1.65343600	-2.32603300	2.15404600
C	-2.78974700	-2.33604100	1.22243900
C	-2.63685200	-3.03050400	-0.02394800
C	-1.32566800	-3.52961500	-0.43295100
C	-1.12875900	-3.17787000	-1.82132000

C	-2.32102900	-2.58080500	-2.26398000
C	-2.31167800	-1.33109300	-2.89049900
C	-3.43606000	-0.56928900	-2.32309400
C	-3.34840700	0.79770300	-2.20581900
C	-2.16957200	1.48456700	-2.68504100
C	-1.96516000	2.63664500	-1.86257600
C	-2.96703100	2.62738600	-0.81096300
C	-2.61038000	3.02395200	0.47442800
C	-3.05940700	2.25179300	1.60877000
C	-3.84467500	1.11211800	1.41271500
C	-3.52088700	-0.11112200	2.11796700
C	-3.71277100	-1.23870600	1.22671100
C	-4.28068900	-0.71873000	-0.00098000
C	-3.99282100	-1.34717700	-1.21298700
C	-3.29211700	-2.57556700	-1.18060900
C	-4.26395800	0.73522600	0.08163900
C	-3.82751100	1.48364700	-1.01175000
49. #11163C ₇₂ (B3LYP/6-31G(d))			
C	2.83716100	-2.56859200	-1.69018100
C	3.23823500	-2.83022200	-0.30946400
C	2.12911700	-3.37173300	0.37219700
C	1.09181600	-3.60870200	-0.62659700
C	1.54545500	-3.06134800	-1.89491300
C	3.20969100	-1.25861700	-2.05194600
C	4.01696800	-0.74753400	-0.94593100
C	3.94884800	-1.71375000	0.16236800
C	3.67973100	-1.26204500	1.46024900
C	2.63221900	-1.88125600	2.22438100
C	1.76921900	-2.88374200	1.66579200
C	0.35335300	-2.91447300	2.05712100
C	-0.67024100	-3.35554900	1.09863200
C	-0.26737900	-3.62120200	-0.29308200
C	-1.16889200	-3.32085500	-1.36700600
C	-0.71247300	-2.67072700	-2.56421100
C	0.65761300	-2.35168200	-2.74871200
C	1.04470700	-1.01926400	-3.21975800
C	2.29283800	-0.41790600	-2.76773600
C	2.36483300	1.02891500	-2.53596400
C	3.25093300	1.49991500	-1.52416300
C	3.98424800	0.59073900	-0.67068600
C	3.86519300	1.07687400	0.70618700
C	3.64987500	0.16884800	1.73361900
C	2.62662100	0.43696400	2.71270200
C	2.08089400	-0.84612900	3.07028500

C	0.78797700	-0.93953400	3.51547000
C	-0.05923300	-2.04056500	3.09475700
C	-1.40918400	-1.58720700	3.22343000
C	-2.39401800	-2.08315400	2.37756000
C	-2.01813500	-2.97961200	1.31456500
C	-2.93675100	-2.73122600	0.20814400
C	-2.51798800	-2.88918900	-1.10398500
C	-2.89690600	-1.92389800	-2.11576400
C	-1.75581100	-1.78216800	-3.00114800
C	-1.41113900	-0.54385100	-3.51215000
C	-0.02062400	-0.14218900	-3.59428900
C	0.04393500	1.25812800	-3.36730300
C	1.20775100	1.87554600	-2.83812300
C	1.00246900	3.09414500	-2.14135300
C	1.88995700	3.49071300	-1.08404100
C	2.92835000	2.64871500	-0.72891500
C	3.14488600	2.30566900	0.67910500
C	2.14477800	2.60995700	1.65779600
C	1.80661600	1.59813200	2.65834600
C	0.42862900	1.50022000	3.16617600
C	-0.01224600	0.24718100	3.66189500
C	-1.39166900	-0.17806900	3.58246200
C	-2.35690100	0.66811500	3.06746900
C	-3.42202500	0.14546300	2.23557800
C	-3.45096700	-1.21036500	1.90560500
C	-3.79301600	-1.61473400	0.56183000
C	-4.10857000	-0.64778200	-0.40274200
C	-3.64722500	-0.80731400	-1.76419700
C	-3.26592600	0.50390300	-2.26667700
C	-2.18920500	0.62058800	-3.14206400
C	-1.29894400	1.73052000	-3.02788400
C	-1.49937400	2.73321000	-2.05511400
C	-0.34199800	3.50969900	-1.72972400
C	-0.23657800	4.13971100	-0.48079400
C	1.12145500	4.10396300	-0.04416700
C	1.13638600	3.54751500	1.25608000
C	-0.24044100	3.40027900	1.70980200
C	-0.60437300	2.40227900	2.64016200
C	-1.96269200	1.96515600	2.57458000
C	-2.78118800	2.24929200	1.42653500
C	-3.68620500	1.14067300	1.22333600
C	-4.01349300	0.75927100	-0.07061200
C	-3.44456200	1.46986600	-1.21043600
C	-2.55454100	2.55500000	-1.04465600

C	-2.28162200	3.00776300	0.33388100
C	-1.09022100	3.72326100	0.59839500
50. #11030 C ₇₂ (B3LYP/6-31G(d))			
C	-4.32662000	0.72692900	-0.56393300
C	-4.32661900	-0.72692900	-0.56393200
C	-3.99243600	-1.19982600	0.71486000
C	-3.81995700	0.00000000	1.54618300
C	-3.99243500	1.19982500	0.71485900
C	-3.61946700	1.16006200	-1.71607100
C	-3.06845000	0.00000000	-2.40055800
C	-3.61946800	-1.16006400	-1.71607000
C	-2.86355000	-2.30985100	-1.60957800
C	-2.72528000	-2.98708200	-0.34204700
C	-3.12757900	-2.33861600	0.86165900
C	-2.17786000	-2.35729500	1.98472100
C	-2.05745000	-1.18307300	2.78656900
C	-2.86086400	0.00000000	2.52269300
C	-2.05745000	1.18307300	2.78656900
C	-2.17786000	2.35729500	1.98472000
C	-3.12757900	2.33861600	0.86165900
C	-2.72528000	2.98708200	-0.34204700
C	-2.86355100	2.30985100	-1.60958000
C	-1.62179200	2.41853200	-2.33423800
C	-0.99200000	1.27221100	-2.89488700
C	-1.73571500	0.00000000	-2.88530200
C	-0.99200000	-1.27221200	-2.89488600
C	-1.62179100	-2.41853300	-2.33423700
C	-0.86618300	-3.45880300	-1.69082000
C	-1.50410300	-3.75427900	-0.41746100
C	-0.70945300	-3.92897000	0.70299700
C	-1.01554000	-3.16410300	1.90467300
C	0.23546800	-2.75097000	2.47632200
C	0.39784900	-1.46123400	3.06316000
C	-0.79812600	-0.72997000	3.25720700
C	-0.79812700	0.72997100	3.25720600
C	0.39784900	1.46123500	3.06316000
C	0.23546800	2.75097100	2.47632200
C	-1.01554000	3.16410400	1.90467300
C	-0.70945400	3.92896900	0.70299600
C	-1.50410500	3.75427900	-0.41746200
C	-0.86618400	3.45880200	-1.69082000
C	0.50389600	3.48418000	-1.81193700
C	1.17160600	2.42916300	-2.53634700
C	0.47065600	1.27036700	-2.98366500

C	1.20268100	0.00000000	-3.04110100
C	0.47065600	-1.27036700	-2.98366500
C	1.17160700	-2.42916300	-2.53634700
C	0.50389700	-3.48418000	-1.81193600
C	1.33084900	-3.87528000	-0.68459000
C	0.72738300	-4.02321300	0.56801500
C	1.30723300	-3.34855400	1.70860400
C	2.51801600	-2.69154900	1.59882400
C	2.72563100	-1.40949400	2.25593600
C	1.66680200	-0.73545800	2.91392900
C	1.66680200	0.73545900	2.91392900
C	2.72563000	1.40949600	2.25593600
C	2.51801500	2.69155000	1.59882400
C	1.30723200	3.34855500	1.70860300
C	0.72738200	4.02321400	0.56801400
C	1.33084800	3.87527900	-0.68459100
C	2.58549500	3.17928800	-0.80575500
C	2.50828000	2.34793500	-1.99863200
C	3.19884100	1.15753000	-2.06590200
C	2.57534000	0.00000000	-2.66314300
C	3.19884200	-1.15753100	-2.06590100
C	2.50828100	-2.34793500	-1.99863100
C	2.58549600	-3.17928700	-0.80575500
C	3.22245800	-2.66980600	0.32919100
C	3.95470900	-1.42755700	0.25471900
C	3.70545700	-0.69341800	1.48314500
C	3.70545600	0.69341900	1.48314400
C	3.95470900	1.42755800	0.25471900
C	3.22245700	2.66980700	0.32919000
C	4.02029600	0.72079000	-0.94805200
C	4.02029700	-0.72079000	-0.94805200

51. #10958 C₇₂ (B3LYP/6-31G(d))

C	4.50685200	0.18436400	-0.71402400
C	4.50685100	-0.18436400	0.71402400
C	3.92473000	-1.46016500	0.84738800
C	3.76241700	-1.98577900	-0.51308600
C	4.07259000	-0.91860400	-1.46569300
C	3.92473000	1.46016500	-0.84738700
C	3.76241700	1.98577900	0.51308700
C	4.07259000	0.91860400	1.46569400
C	3.20386300	0.68520100	2.54435500
C	2.65098500	-0.62237300	2.74959500
C	2.91621300	-1.69839700	1.85420200
C	1.83139200	-2.64874700	1.56942100

C	1.82109700	-3.25609700	0.28555600
C	2.72131900	-2.83928700	-0.77304900
C	1.93944700	-2.71827100	-2.00385900
C	2.16251200	-1.64281300	-2.84780100
C	3.20386300	-0.68520200	-2.54435500
C	2.65098500	0.62237200	-2.74959500
C	2.91621400	1.69839700	-1.85420100
C	1.83139200	2.64874700	-1.56942100
C	1.82109800	3.25609700	-0.28555600
C	2.72131900	2.83928600	0.77304900
C	1.93944700	2.71827100	2.00386000
C	2.16251100	1.64281300	2.84780100
C	1.01992000	0.94434300	3.37882900
C	1.32810500	-0.45267000	3.33420500
C	0.31160100	-1.41504500	3.17940700
C	0.55357700	-2.55539800	2.28917800
C	-0.59476800	-3.16389700	1.72646200
C	-0.58922100	-3.60707800	0.35502600
C	0.58922100	-3.60707800	-0.35503200
C	0.59476800	-3.16389500	-1.72646700
C	-0.55357700	-2.55539500	-2.28918200
C	-0.31160100	-1.41504000	-3.17940900
C	1.01992000	-0.94434300	-3.37882800
C	1.32810600	0.45267000	-3.33420600
C	0.31160200	1.41504500	-3.17940600
C	0.55357800	2.55539800	-2.28917800
C	-0.59476800	3.16389700	-1.72646200
C	-0.58922100	3.60707800	-0.35502600
C	0.58922100	3.60707700	0.35503200
C	0.59476800	3.16389500	1.72646700
C	-0.55357800	2.55539500	2.28918200
C	-0.31160200	1.41504000	3.17940800
C	-1.32810600	0.45266500	3.33420600
C	-1.01992100	-0.94434900	3.37882700
C	-2.16251200	-1.64281800	2.84779900
C	-1.93944700	-2.71827400	2.00385500
C	-2.72131900	-2.83928800	0.77304400
C	-1.82109700	-3.25609700	-0.28556200
C	-1.83139200	-2.64874500	-1.56942500
C	-2.91621300	-1.69839400	-1.85420400
C	-2.65098500	-0.62236800	-2.74959600
C	-1.32810500	-0.45266500	-3.33420600
C	-1.01992000	0.94434900	-3.37882700
C	-2.16251100	1.64281700	-2.84779800

C	-1.93944700	2.71827400	-2.00385500
C	-2.72131900	2.83928800	-0.77304400
C	-1.82109700	3.25609700	0.28556100
C	-1.83139200	2.64874400	1.56942500
C	-2.91621400	1.69839500	1.85420400
C	-2.65098600	0.62236800	2.74959600
C	-3.20386300	-0.68520500	2.54435300
C	-4.07259000	-0.91860700	1.46569200
C	-3.76241700	-1.98577900	0.51308300
C	-3.92472900	-1.46016400	-0.84739000
C	-4.50685100	-0.18436300	-0.71402500
C	-4.07259000	0.91860700	-1.46569200
C	-3.20386300	0.68520500	-2.54435400
C	-3.76241700	1.98578000	-0.51308300
C	-3.92473000	1.46016400	0.84738900
C	-4.50685200	0.18436300	0.71402400
52. #10627C ₇₂ (B3LYP/6-31G(d))			
C	4.26168200	-0.33807000	1.25364000
C	4.51747100	0.08213300	-0.08543300
C	4.01532000	1.41693200	-0.26633500
C	3.53116500	1.88000100	1.00751300
C	3.65206100	0.74695500	1.93647300
C	3.68206600	-1.64741900	1.24580500
C	3.73554800	-2.10123000	-0.12915700
C	4.17191400	-0.97184700	-0.96655500
C	3.44735400	-0.67016600	-2.12746100
C	3.01008000	0.67530800	-2.39309600
C	3.28768400	1.72933900	-1.45846100
C	2.32457700	2.76305700	-1.36480100
C	1.98981300	3.36496700	-0.11539700
C	2.45166100	2.79140500	1.10708900
C	1.46094600	2.60975000	2.18819300
C	1.53280800	1.42481700	2.97541500
C	2.60258400	0.46673600	2.79275700
C	2.06217200	-0.87271300	2.90155500
C	2.53196300	-1.92870700	2.05058500
C	1.54094200	-2.88544800	1.58616000
C	1.74371800	-3.45618800	0.29251500
C	2.75601400	-2.95275600	-0.58878700
C	2.11564800	-2.71801600	-1.89125900
C	2.41409400	-1.57164700	-2.60453900
C	1.33510600	-0.79175200	-3.14729600
C	1.72625200	0.59479300	-3.03988300
C	0.75229600	1.62201400	-2.94224800

C	1.13175500	2.77721000	-2.20038700
C	0.15197900	3.59192300	-1.56605700
C	0.65011600	3.91279900	-0.24084500
C	-0.22045300	3.89024200	0.82696600
C	0.16698900	3.16675800	2.04071500
C	-0.99999600	2.50076700	2.51879000
C	-0.93055300	1.17893100	3.06386900
C	0.36531000	0.69473800	3.31881100
C	0.68315200	-0.73299900	3.21879400
C	-0.30106200	-1.67423100	2.85994400
C	0.16313400	-2.83861900	2.09670300
C	-0.82366900	-3.59138800	1.40964000
C	-0.61799100	-3.98045500	0.02118700
C	0.61231800	-3.81415000	-0.53101700
C	0.77064800	-3.19236300	-1.83525500
C	-0.31432500	-2.48986100	-2.41970400
C	-0.01832000	-1.19391600	-3.05180200
C	-1.04430300	-0.15558900	-3.10783300
C	-0.66072300	1.26460000	-3.05572100
C	-1.60823400	2.20658600	-2.57332600
C	-1.19984300	3.34058400	-1.77460600
C	-2.13902700	3.49199000	-0.68521600
C	-1.64032100	3.70605700	0.60835900
C	-2.12695000	2.89443000	1.69548500
C	-3.17026100	2.00583000	1.50650600
C	-3.15287800	0.69523200	2.13450100
C	-2.00679000	0.22072700	2.82927300
C	-1.69971200	-1.21480100	2.78703300
C	-2.63652200	-2.06878800	2.14687600
C	-2.18495200	-3.25539100	1.51618700
C	-2.81219900	-3.35334900	0.21011500
C	-1.79806800	-3.60997500	-0.73760900
C	-1.65492600	-2.76703300	-1.89924100
C	-2.66435100	-1.79294800	-2.10661500
C	-2.35703600	-0.51506900	-2.72075500
C	-3.27935200	0.46233400	-2.19725400
C	-2.89981400	1.78855700	-2.08931700
C	-3.21253700	2.54778400	-0.88968800
C	-3.78166700	1.87703700	0.19549500
C	-4.23805500	0.51280400	0.05762500
C	-3.94312900	-0.17888200	1.30622000
C	-3.70998800	-1.53636600	1.31878300
C	-3.72546500	-2.28805300	0.06537100
C	-3.72460300	-1.57647200	-1.14253100

C	-4.05026600	-0.16947000	-1.14546000
53. #10797 C ₇₂ (B3LYP/6-31G(d))			
C	3.54160900	1.07040000	2.11161000
C	3.89115400	1.93420100	0.98808500
C	2.86460000	2.87637000	0.81937500
C	1.91425800	2.67961600	1.91156500
C	2.30128900	1.47685000	2.62639700
C	3.81171700	-0.26662200	1.78142700
C	4.45600500	-0.25510000	0.45843300
C	4.33853000	1.10863800	-0.06729900
C	3.80970500	1.31153300	-1.36067500
C	2.81280400	2.31106400	-1.56934000
C	2.35390400	3.13965400	-0.49590200
C	1.02971200	3.62804900	-0.58040400
C	0.20139200	3.74513000	0.58383900
C	0.57450200	3.06460500	1.79133200
C	-0.43638100	2.29608500	2.52242500
C	-0.05029000	0.99824700	3.10746800
C	1.31692400	0.51406300	3.00734600
C	1.60651600	-0.89832400	2.79650500
C	2.86739400	-1.28684100	2.15220700
C	2.90775200	-2.47212100	1.35130100
C	3.65825300	-2.50571700	0.14832100
C	4.25773900	-1.33223300	-0.37877300
C	3.68250800	-1.12164400	-1.72763500
C	3.42996400	0.15639000	-2.16497800
C	2.18289400	0.45051100	-2.84292400
C	1.84521800	1.79816600	-2.54002000
C	0.50804300	2.26564900	-2.59319200
C	0.16658200	3.32470700	-1.70162500
C	-1.18410400	3.51111300	-1.27828300
C	-1.16542300	3.75966100	0.15341200
C	-2.14935600	3.21611000	0.95587500
C	-1.78935000	2.50509900	2.17677100
C	-2.79404600	1.49570800	2.38381900
C	-2.43998400	0.28939500	2.96653900
C	-1.06191900	0.03957900	3.30590500
C	-0.79525300	-1.36450300	3.11809300
C	0.48196100	-1.82955800	2.75531600
C	0.52788500	-2.99920200	1.86496300
C	1.69683000	-3.24831900	1.13550300
C	1.62577500	-3.58857800	-0.26086700
C	2.78140800	-3.04320800	-0.86043500
C	2.69849100	-2.16265000	-1.96524000

C	1.42788100	-1.89184800	-2.57006200
C	1.17214900	-0.54007800	-3.04878500
C	-0.19015600	-0.07061700	-3.24240700
C	-0.53095000	1.34722500	-3.04881700
C	-1.87932200	1.68512000	-2.75861200
C	-2.19985300	2.74876900	-1.83307400
C	-3.32884500	2.33160000	-1.02048300
C	-3.29884100	2.55582200	0.36190600
C	-3.72818200	1.51612800	1.26754500
C	-4.24851500	0.31765000	0.77367900
C	-3.91382700	-0.94052600	1.42008100
C	-3.03118900	-0.94858900	2.50579400
C	-2.01939200	-1.97235000	2.61913800
C	-1.96565500	-2.99735200	1.68065200
C	-0.67890800	-3.47563400	1.26477000
C	-0.74515700	-3.74444100	-0.15040200
C	0.40022800	-3.56176500	-0.96023800
C	0.30227400	-2.73587500	-2.17460100
C	-0.98690600	-2.32955900	-2.55832000
C	-1.22858200	-1.02673800	-3.12848000
C	-2.58549500	-0.65149400	-2.81466300
C	-2.90242900	0.67947600	-2.61392400
C	-3.79553400	1.06237300	-1.52922200
C	-4.28596700	0.08765600	-0.65952300
C	-3.98368800	-1.31669800	-0.89404200
C	-3.79603800	-1.95958500	0.39326200
C	-2.85021800	-2.97399000	0.53106000
C	-2.05952400	-3.38971200	-0.60771000
C	-2.17996800	-2.71924800	-1.82170300
C	-3.16660400	-1.67769900	-1.96905800

54. #11026C₇₂ (B3LYP/6-31G(d))

C	3.33365900	-2.89100600	-0.42563200
C	4.10617700	-1.71431000	-0.67489600
C	4.08576500	-0.91296800	0.53328000
C	3.38153000	-1.68110200	1.53110800
C	2.82730800	-2.86208400	0.92722100
C	2.37824000	-3.03366600	-1.48461500
C	2.45417300	-1.89166600	-2.37505000
C	3.56075500	-1.10491400	-1.86232600
C	3.50493500	0.27335000	-1.96194400
C	3.85223300	1.12491600	-0.81339500
C	3.94021100	0.51452000	0.49341600
C	3.25362900	1.18597300	1.61637700
C	2.69281100	0.38864300	2.66767000

C	2.69038600	-1.03643600	2.56794400
C	1.41735500	-1.55432900	3.02042400
C	0.73547700	-2.61169700	2.31256000
C	1.47501800	-3.28479200	1.23810200
C	0.71520100	-3.85348200	0.16494800
C	1.14340400	-3.58604200	-1.20558500
C	-0.00001000	-3.19407700	-1.97655900
C	-0.00000400	-1.99724700	-2.77392500
C	1.27190100	-1.28456300	-2.92010800
C	1.27146800	0.16676300	-3.11480300
C	2.43308000	0.89445400	-2.68756300
C	2.34299600	2.24840000	-2.18955500
C	3.17171200	2.36106700	-0.99739700
C	2.65248600	3.07868900	0.10624700
C	2.66485700	2.47236600	1.40740900
C	1.43604300	2.88323900	2.09606700
C	0.74127600	1.96998100	2.95120400
C	1.42933100	0.77373100	3.30549700
C	0.70116300	-0.43207500	3.55417900
C	-0.70117600	-0.43207100	3.55418100
C	-1.41737400	-1.55432000	3.02042200
C	-0.73550200	-2.61169300	2.31256000
C	-1.47504500	-3.28478100	1.23809800
C	-0.71523100	-3.85348000	0.16494700
C	-1.14342800	-3.58603300	-1.20558700
C	-2.37825900	-3.03364800	-1.48462100
C	-2.45418100	-1.89164800	-2.37505600
C	-1.27190300	-1.28455400	-2.92011300
C	-1.27145800	0.16677200	-3.11480500
C	0.00000800	0.89693600	-3.20016100
C	0.00001300	2.29333600	-2.88474900
C	1.15356300	2.94373900	-2.30320200
C	0.71683400	3.85076900	-1.25061600
C	1.43310900	3.85031500	-0.02889700
C	0.70954500	3.75448700	1.21970300
C	-0.70952300	3.75449400	1.21970100
C	-1.43602900	2.88324600	2.09606200
C	-0.74127000	1.96998600	2.95120200
C	-1.42933500	0.77373900	3.30549300
C	-2.69281400	0.38866100	2.66766500
C	-2.69040200	-1.03642000	2.56794300
C	-3.38154500	-1.68108000	1.53110200
C	-2.82733300	-2.86206600	0.92721700
C	-3.33368200	-2.89098300	-0.42564100

C	-4.10618400	-1.71428100	-0.67490400
C	-3.56075800	-1.10488900	-1.86233600
C	-3.50492500	0.27337400	-1.96194800
C	-2.43306500	0.89447200	-2.68756800
C	-2.34297300	2.24841700	-2.18956200
C	-1.15353500	2.94374800	-2.30320300
C	-0.71680400	3.85077700	-1.25062000
C	-1.43308000	3.85032500	-0.02889900
C	-2.65246400	3.07870800	0.10624000
C	-2.66484300	2.47238300	1.40740600
C	-3.25362600	1.18599600	1.61637200
C	-3.94020700	0.51454600	0.49340800
C	-4.08577400	-0.91294100	0.53327300
C	-3.85222400	1.12494200	-0.81340300
C	-3.17168700	2.36108600	-0.99740100
55. #10730 C ₇₂ (B3LYP/6-31G(d))			
C	-3.98346900	0.89594400	-1.74551000
C	-4.12533700	1.80127100	-0.60465500
C	-3.09773500	2.75952100	-0.66310900
C	-2.31642000	2.46479400	-1.86176700
C	-2.82289700	1.24436000	-2.45827800
C	-4.24269000	-0.42937100	-1.32208100
C	-4.49500500	-0.38634600	0.12051200
C	-4.34442900	1.01620600	0.54743700
C	-3.60464800	1.30995800	1.71795100
C	-2.65330900	2.37204000	1.72020300
C	-2.39922400	3.12760100	0.53110500
C	-1.09597300	3.64366100	0.36644600
C	-0.44691100	3.63272500	-0.90964500
C	-0.96637800	2.80381500	-1.95960200
C	-0.04652000	1.89805100	-2.67895600
C	-0.48718200	0.53457400	-3.02141400
C	-1.90709100	0.22776600	-2.91442400
C	-2.31038000	-1.11663800	-2.70563400
C	-3.45252400	-1.44536700	-1.86309100
C	-3.09895500	-2.58328900	-1.05417300
C	-3.35914000	-2.56496700	0.32669600
C	-3.99247700	-1.40305100	0.91443300
C	-3.24516500	-1.08453300	2.13812300
C	-3.04682300	0.23001100	2.51209900
C	-1.75416500	0.63995400	3.00993100
C	-1.53766900	1.98564400	2.58290900
C	-0.23494800	2.50229900	2.41098400
C	-0.06579100	3.47825600	1.37311100

C	1.19769300	3.66839700	0.74962500
C	0.96275800	3.72639300	-0.68380800
C	1.83359800	3.08429700	-1.53627400
C	1.32343400	2.14366100	-2.53656400
C	2.31038300	1.11664000	-2.70563100
C	1.90709400	-0.22776300	-2.91442300
C	0.48718400	-0.53457200	-3.02141500
C	0.04652300	-1.89804800	-2.67895900
C	-1.32343200	-2.14365800	-2.53656700
C	-1.83359700	-3.08429600	-1.53627700
C	-0.96275800	-3.72639100	-0.68381100
C	-1.19769400	-3.66839900	0.74962200
C	-2.32250800	-3.00937700	1.23521100
C	-2.18638300	-2.04616700	2.30280400
C	-0.90381200	-1.67765800	2.80057800
C	-0.67281700	-0.27289100	3.15882100
C	0.67281400	0.27288800	3.15882100
C	0.90381000	1.67765600	2.80057900
C	2.18638000	2.04616500	2.30280500
C	2.32250700	3.00937700	1.23521500
C	3.35913900	2.56496600	0.32670000
C	3.09895600	2.58329100	-1.05417000
C	3.45252500	1.44536800	-1.86308900
C	4.24269200	0.42937200	-1.32207900
C	3.98347100	-0.89594200	-1.74551000
C	2.82290000	-1.24435700	-2.45827800
C	2.31642200	-2.46479300	-1.86176700
C	0.96638000	-2.80381300	-1.95960400
C	0.44691200	-3.63272200	-0.90964700
C	1.09597200	-3.64366200	0.36644400
C	0.06579000	-3.47825700	1.37310900
C	0.23494600	-2.50230100	2.41098300
C	1.53766700	-1.98564500	2.58290900
C	1.75416300	-0.63995700	3.00993200
C	3.04682100	-0.23001300	2.51210100
C	3.24516300	1.08453000	2.13812500
C	3.99247600	1.40305000	0.91443600
C	4.49500500	0.38634600	0.12051500
C	4.34442900	-1.01620600	0.54743900
C	4.12533600	-1.80126900	-0.60465300
C	3.09773500	-2.75952100	-0.66310900
C	2.39922400	-3.12760200	0.53110400
C	2.65330900	-2.37204200	1.72020300
C	3.60464600	-1.30995900	1.71795200

56. #11185C₇₂ (B3LYP/6-31G(d))

C	2.45594700	3.01776900	-1.51936400
C	3.46780600	2.57989500	-0.57593400
C	4.01957000	1.36374500	-1.04376000
C	3.30802000	1.02337800	-2.28103900
C	2.26750900	2.02394400	-2.49770900
C	1.37469900	3.58605800	-0.82007200
C	1.65006400	3.42386400	0.58724700
C	2.91638400	2.69837600	0.71410100
C	3.04944200	1.63515200	1.66247800
C	3.86303800	0.52142300	1.25899800
C	4.30416200	0.36658300	-0.11480500
C	4.13847800	-1.03124600	-0.48175300
C	3.53209100	-1.35641300	-1.69984700
C	3.03738100	-0.29361300	-2.56213700
C	1.73151100	-0.68115400	-3.06447900
C	0.67687500	0.26077300	-3.23321600
C	0.94001400	1.66016200	-2.90133400
C	-0.15319700	2.49818300	-2.43826800
C	0.06431500	3.44369100	-1.33673800
C	-0.97323600	3.66530100	-0.39982200
C	-0.70994900	3.58038000	1.01053400
C	0.59984900	3.25458100	1.49938000
C	0.75007400	2.26527400	2.57899100
C	1.95871300	1.42091900	2.62284500
C	1.83718500	0.12854500	3.19131300
C	2.62386800	-0.99158600	2.72965100
C	3.61660800	-0.80327100	1.77747600
C	3.78295200	-1.77022800	0.70863400
C	2.91847600	-2.86111300	0.62566000
C	2.31838700	-3.20629100	-0.64118500
C	2.57542200	-2.43164300	-1.76669100
C	1.47055200	-2.01268500	-2.62107600
C	0.15319800	-2.49818200	-2.43826900
C	-0.94001300	-1.66016200	-2.90133400
C	-0.67687400	-0.26077200	-3.23321600
C	-1.73151100	0.68115400	-3.06447900
C	-1.47055100	2.01268500	-2.62107700
C	-2.57542100	2.43164200	-1.76669100
C	-2.31838700	3.20629100	-0.64118500
C	-2.91847600	2.86111200	0.62565900
C	-1.89928300	3.06696500	1.63632400
C	-1.76186900	2.15691300	2.67545500
C	-0.44594800	1.77413100	3.14745000

C	-0.55604400	0.40165900	3.57270400
C	0.55604300	-0.40165900	3.57270200
C	0.44594700	-1.77413200	3.14745000
C	1.76186800	-2.15691300	2.67545500
C	1.89928200	-3.06696500	1.63632400
C	0.70994800	-3.58038000	1.01053400
C	0.97323600	-3.66530100	-0.39982300
C	-0.06431500	-3.44369100	-1.33673800
C	-1.37469800	-3.58605800	-0.82007300
C	-2.45594600	-3.01776800	-1.51936500
C	-2.26750900	-2.02394300	-2.49770900
C	-3.30802000	-1.02337700	-2.28104000
C	-3.03738100	0.29361300	-2.56213900
C	-3.53209000	1.35641300	-1.69984800
C	-4.13847800	1.03124600	-0.48175400
C	-3.78295300	1.77022900	0.70863300
C	-3.61660800	0.80327100	1.77747500
C	-2.62387000	0.99158600	2.72965100
C	-1.83718600	-0.12854500	3.19131200
C	-1.95871500	-1.42091900	2.62284500
C	-0.75007400	-2.26527500	2.57899000
C	-0.59984900	-3.25458200	1.49938000
C	-1.65006300	-3.42386300	0.58724600
C	-2.91638500	-2.69837600	0.71410100
C	-3.46780300	-2.57989300	-0.57593500
C	-4.01957200	-1.36374600	-1.04376100
C	-4.30416100	-0.36658300	-0.11480600
C	-3.86303900	-0.52142300	1.25899700
C	-3.04944200	-1.63515100	1.66247600

57. #10978C₇₂ (B3LYP/6-31G(d))

C	4.14039400	-1.16937600	-1.01547800
C	4.25320200	0.26277500	-1.14949200
C	4.19087800	0.86837000	0.12532700
C	4.12209100	-0.22348600	1.09858800
C	4.10974300	-1.49413600	0.36282400
C	3.12834200	-1.62155900	-1.89770600
C	2.61007600	-0.47252300	-2.63608200
C	3.38862600	0.67291200	-2.19660200
C	2.78530700	1.90699700	-2.08464500
C	2.91213000	2.68491600	-0.86872500
C	3.44143500	2.08146400	0.30957400
C	2.67167000	2.24926800	1.55174400
C	2.58330900	1.14152200	2.45022200
C	3.30884400	-0.08627100	2.20804200

C	2.47750800	-1.19111700	2.67152000
C	2.47068000	-2.39928100	1.98866100
C	3.26604300	-2.52935000	0.76525600
C	2.44825800	-3.20552000	-0.19411000
C	2.25614800	-2.66263400	-1.50854500
C	0.92367300	-2.69684800	-2.10748500
C	0.37029300	-1.51952100	-2.76804600
C	1.23936200	-0.34767200	-2.94878700
C	0.65289600	1.00659400	-3.00581300
C	1.47146300	2.10810600	-2.63080800
C	0.92752000	3.26590400	-1.96982600
C	1.77411200	3.56393300	-0.82299000
C	1.16790600	3.87427800	0.38676400
C	1.57306400	3.14366300	1.57306500
C	0.38064600	2.86549600	2.33105100
C	0.19779400	1.61129100	2.98117000
C	1.34663100	0.79694300	3.07568800
C	1.24275700	-0.65219600	3.15208300
C	0.00479800	-1.31484600	2.98932000
C	0.00786100	-2.62698800	2.33127700
C	1.24662000	-3.11592400	1.84051000
C	1.31103400	-3.74128700	0.52389900
C	0.18362300	-4.07309300	-0.15114900
C	0.02828700	-3.65095400	-1.54835500
C	-1.33831500	-3.54021700	-1.76295100
C	-1.91381300	-2.40796300	-2.36879600
C	-1.07700300	-1.33970800	-2.82784700
C	-1.66115300	0.00949900	-2.84791800
C	-0.79455400	1.18188100	-2.92694800
C	-1.30151300	2.43363800	-2.46442100
C	-0.43329700	3.43818400	-1.90153100
C	-1.04963800	3.96327400	-0.69264500
C	-0.26181900	4.10055400	0.44997900
C	-0.73133900	3.52724600	1.69470000
C	-1.99675200	2.97598500	1.78726400
C	-2.20848700	1.72843100	2.50595600
C	-1.11895200	0.97420000	3.00916800
C	-1.21275400	-0.49582600	3.00085500
C	-2.40060100	-1.08876400	2.52367000
C	-2.40404300	-2.38343300	1.84460300
C	-1.21472500	-3.13712500	1.69990000
C	-1.10736500	-3.94913700	0.50982000
C	-2.06272800	-3.83095700	-0.51329900
C	-3.15892100	-2.96592500	-0.42384000

C	-3.15532900	-2.14971200	-1.64182100
C	-3.65232700	-0.87747900	-1.60318700
C	-2.97028800	0.18647200	-2.31052800
C	-3.36462000	1.41346600	-1.67012500
C	-2.54925700	2.52393400	-1.74994800
C	-2.37218700	3.39566000	-0.60013300
C	-2.88207400	2.98625500	0.63703800
C	-3.73021700	1.82030200	0.72290100
C	-3.34896000	1.08557300	1.91733900
C	-3.45649100	-0.29694400	1.95455500
C	-4.00548900	-1.02215000	0.82548500
C	-3.40876700	-2.33430500	0.80954100
C	-4.21661600	-0.33215500	-0.37179600
C	-4.05462700	1.09740000	-0.42697800
58. #10777 C ₇₂ (B3LYP/6-31G(d))			
C	1.62973300	-3.96620900	-0.60140800
C	2.87825000	-3.25552600	-0.43152300
C	2.96670100	-2.76684900	0.89454900
C	1.73130400	-3.16323900	1.55688900
C	0.90286400	-3.89982900	0.59451000
C	1.04403100	-3.54120800	-1.83091200
C	1.84417700	-2.45478700	-2.37058400
C	3.03538700	-2.38210200	-1.52705100
C	3.64622200	-1.15228100	-1.31850800
C	4.00674200	-0.72998700	-0.00158800
C	3.55429000	-1.48028700	1.12800700
C	3.03835500	-0.73334600	2.22771600
C	1.89492300	-1.18363200	2.93289400
C	1.13260400	-2.33638300	2.51627500
C	-0.34394000	-2.30678000	2.62973400
C	-1.17800200	-3.03206200	1.66060000
C	-0.52352200	-3.75619000	0.56903500
C	-1.13000300	-3.74192500	-0.72075800
C	-0.32538500	-3.47540000	-1.89737100
C	-0.95671300	-2.41852900	-2.64822900
C	-0.22702600	-1.26977200	-3.06373900
C	1.23522900	-1.28015700	-2.87914100
C	1.96591200	0.00000100	-2.75286700
C	3.20326000	0.00000200	-2.06499500
C	3.64621900	1.15228500	-1.31850800
C	4.00674400	0.72999300	-0.00158700
C	3.55428800	1.48029000	1.12800500
C	3.03835500	0.73335000	2.22771700
C	1.89492200	1.18363500	2.93289300

C	1.22716300	0.00000000	3.41614500
C	-0.12476800	0.00000000	3.57139900
C	-0.91594300	-1.18934000	3.27938200
C	-2.24135000	-0.72921700	3.00589300
C	-3.04531900	-1.42522700	2.11599300
C	-2.51097600	-2.58154400	1.44704700
C	-3.12399200	-2.61352800	0.12898800
C	-2.39741600	-3.10363900	-0.93950900
C	-2.30895700	-2.32897500	-2.16716900
C	-3.00870600	-1.15247100	-2.29579500
C	-2.35135300	-0.00000200	-2.86227800
C	-0.95358600	-0.00000100	-3.15725200
C	-0.22702900	1.26977100	-3.06374000
C	1.23522800	1.28015800	-2.87914100
C	1.84417500	2.45479000	-2.37058700
C	3.03538700	2.38210700	-1.52705600
C	2.87824200	3.25552500	-0.43152300
C	2.96670000	2.76685500	0.89455000
C	1.73130000	3.16324300	1.55689100
C	1.13260000	2.33638600	2.51627600
C	-0.34394400	2.30678100	2.62973500
C	-0.91594600	1.18933900	3.27938100
C	-2.24135200	0.72921400	3.00589400
C	-3.04532100	1.42522300	2.11599200
C	-3.92344900	0.69861400	1.21086800
C	-3.92344600	-0.69861900	1.21086800
C	-3.94668600	-1.42510300	-0.03560600
C	-3.91669000	-0.72062300	-1.24455800
C	-3.91669100	0.72061600	-1.24455900
C	-3.00870800	1.15246500	-2.29579600
C	-2.30896200	2.32897100	-2.16717100
C	-0.95671800	2.41852600	-2.64823000
C	-0.32539100	3.47540100	-1.89737200
C	1.04402600	3.54120800	-1.83091100
C	1.62972600	3.96621500	-0.60141000
C	0.90285700	3.89983200	0.59451000
C	-0.52352900	3.75619200	0.56903700
C	-1.17800700	3.03206000	1.66060100
C	-2.51098100	2.58154100	1.44704800
C	-3.12399500	2.61352100	0.12898600
C	-3.94668800	1.42509600	-0.03560700
C	-2.39742200	3.10363600	-0.93951000
C	-1.13000800	3.74192200	-0.72075900

59. #11190C₇₂ (B3LYP/6-31G(d))

C	-1.64869500	-3.22571600	-1.68075300
C	-0.79802600	-4.04296900	-0.82992000
C	-1.31830900	-3.95828800	0.51035800
C	-2.48517100	-3.09088500	0.47197300
C	-2.59185000	-2.51800600	-0.84855500
C	-1.13213900	-2.61216400	-2.80052200
C	0.27108000	-2.77264200	-3.14758600
C	1.12151700	-3.38594900	-2.22406500
C	0.58140700	-4.02774400	-1.05321200
C	1.46266100	-3.71570600	0.06106800
C	0.96496100	-3.63514200	1.34289800
C	-0.44875100	-3.86073100	1.59976500
C	-0.81039500	-3.07358900	2.75039000
C	-2.03401400	-2.40005700	2.78772700
C	-2.83085100	-2.33792900	1.57242800
C	-3.29640300	-0.98346600	1.39419700
C	-3.24003700	-0.33299000	0.12790200
C	-2.87186600	-1.13481300	-1.04406200
C	-2.32208200	-0.48148300	-2.23685300
C	-1.53908000	-1.26743100	-3.13084200
C	-0.46605700	-0.69167700	-3.90553100
C	0.68577000	-1.57700100	-3.83518300
C	1.94243400	-1.01951500	-3.58525000
C	2.72713900	-1.54170600	-2.47755700
C	2.33031900	-2.68511800	-1.81984800
C	2.45014100	-2.76169600	-0.38358400
C	2.79776000	-1.62398900	0.40036800
C	2.26796600	-1.53825100	1.76563300
C	1.43556000	-2.59767900	2.22902400
C	0.38393900	-2.37026700	3.19099900
C	0.28294600	-1.14648600	3.81495400
C	-1.01966100	-0.54064700	4.04217900
C	-2.13974100	-1.12044800	3.44036600
C	-3.00049400	-0.28230200	2.62048200
C	-2.82997800	1.08438000	2.60078800
C	-2.94880600	1.80213500	1.35430500
C	-3.05872600	1.12257500	0.10685300
C	-2.50857000	1.77586300	-1.08579100
C	-2.14000800	0.97399000	-2.25759800
C	-1.19134300	1.51815500	-3.17067800
C	-0.29534700	0.67498200	-3.92514300
C	1.03908900	1.25158400	-3.87606300
C	2.12113500	0.40941400	-3.60615800
C	3.01316300	0.75377400	-2.51018400

	C	3.25880100	-0.43135800	-1.72401100
	C	3.22031900	-0.40625800	-0.30002200
	C	3.11283000	0.89715900	0.36436000
	C	2.58228800	0.98298500	1.72933000
	C	2.16011700	-0.23479000	2.42987400
	C	1.22964000	-0.10341200	3.50076600
	C	0.56962900	1.14891600	3.78258400
	C	-0.84126000	0.88831700	4.02114900
	C	-1.78664200	1.70816400	3.39940600
	C	-1.37203700	2.90381600	2.71177300
	C	-2.16364200	3.00483700	1.49588400
	C	-1.64741300	3.61842400	0.37598400
	C	-1.89659400	3.05277700	-0.92820100
	C	-0.81159400	3.48367800	-1.77700200
	C	-0.46552400	2.73066800	-2.87729700
	C	0.93308500	2.53122600	-3.22353000
	C	1.91134900	2.94241400	-2.31457400
	C	2.91184800	1.97759800	-1.88636400
	C	3.05232300	2.06297000	-0.45249000
	C	2.33107500	3.24243900	-0.03815700
	C	1.83318200	3.32302800	1.24359500
	C	2.03761100	2.22700800	2.16006700
	C	0.96605200	2.29237800	3.12472200
	C	-0.02058900	3.25477700	2.65986600
	C	0.51924700	3.89660700	1.48890600
	C	-0.30344800	4.17420600	0.39390000
	C	0.21713700	4.08949000	-0.94625800
	C	1.54962100	3.72956700	-1.16398300
60.	#11105C ₇₂ (B3LYP/6-31G(d))			
	C	-2.05571900	-3.20099600	1.78808400
	C	-2.75375100	-3.41831700	0.49779700
	C	-1.79246000	-3.77201000	-0.45087500
	C	-0.59631600	-4.12230500	0.30859600
	C	-0.72868700	-3.57327700	1.67157000
	C	-2.45168900	-1.95219000	2.30288000
	C	-3.58843700	-1.51826100	1.49262300
	C	-3.66564800	-2.37148200	0.30484800
	C	-3.70592500	-1.75712500	-0.96024200
	C	-2.64268100	-2.02570500	-1.90617000
	C	-1.64686700	-2.98826700	-1.66291000
	C	-0.30773900	-2.74637200	-2.20332500
	C	0.72869000	-3.57327600	-1.67157000
	C	0.59631900	-4.12230500	-0.30859600
	C	1.79246400	-3.77200900	0.45087500

C	1.64686900	-2.98826500	1.66290900
C	0.30774100	-2.74637200	2.20332400
C	-0.06124000	-1.44985900	2.76342500
C	-1.46080800	-1.02624900	2.75870300
C	-1.80883500	0.40110100	2.70973400
C	-3.04323200	0.77582500	2.09967900
C	-3.85379100	-0.18234100	1.37916300
C	-4.23431000	0.39969500	0.09597300
C	-4.04872600	-0.36551700	-1.06145100
C	-3.27249200	0.20112800	-2.14832900
C	-2.31522400	-0.78466800	-2.58584600
C	-0.98240000	-0.43019900	-2.91238800
C	0.06124200	-1.44985800	-2.76342500
C	1.46080800	-1.02624800	-2.75870300
C	2.45169000	-1.95218800	-2.30288000
C	2.05572100	-3.20099400	-1.78808400
C	2.75375300	-3.41831400	-0.49779700
C	3.66565000	-2.37147900	-0.30484900
C	3.70592700	-1.75712200	0.96024100
C	2.64268200	-2.02570300	1.90617000
C	2.31522500	-0.78466700	2.58584600
C	0.98240000	-0.43019800	2.91238800
C	0.63323300	0.99781300	2.94940100
C	-0.76270300	1.41315200	2.80981500
C	-1.03540100	2.72002300	2.30956700
C	-2.20848100	2.99022400	1.51651100
C	-3.18859300	2.02713700	1.40466100
C	-3.83728400	1.78099900	0.12311200
C	-3.30238500	2.38550800	-1.01786100
C	-2.93458200	1.53794000	-2.14306200
C	-1.64316200	1.94840000	-2.62687500
C	-0.63323300	0.99781300	-2.94940100
C	0.76270200	1.41315300	-2.80981500
C	1.80883500	0.40110300	-2.70973500
C	3.04323100	0.77582700	-2.09967900
C	3.85379200	-0.18233800	-1.37916400
C	3.58843800	-1.51825800	-1.49262300
C	4.23430900	0.39969900	-0.09597300
C	4.04872600	-0.36551400	1.06145100
C	3.27249200	0.20113000	2.14832900
C	2.93458000	1.53794200	2.14306300
C	1.64316100	1.94840100	2.62687500
C	1.32744300	3.19413200	1.96282200
C	0.01322900	3.56689600	1.79685500

C	-0.43764500	4.15469900	0.54305800
C	-1.81980500	3.78522500	0.36448200
C	-2.29344500	3.40521600	-0.89628100
C	-1.32744600	3.19413100	-1.96282100
C	-0.01323200	3.56689700	-1.79685500
C	1.03539900	2.72002400	-2.30956700
C	2.20847800	2.99022600	-1.51651000
C	3.18859200	2.02713900	-1.40466100
C	3.83728200	1.78100100	-0.12311200
C	3.30238300	2.38551000	1.01786100
C	2.29344200	3.40521700	0.89628100
C	1.81980200	3.78522600	-0.36448200
C	0.43764100	4.15469800	-0.54305800