

A Benchmark Study of DFT Methods on the Electronic Properties of Lanthanofullerene: A Case Study of Ce@C_{2v}(9)-C₈₂ Anion

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Table S1: Comparison between the experimental results and calculated ^{13}C NMR chemical shifts (δ/ppm) of $[\text{Ce}@C_{2v}(9)\text{-C}_{82}]^-$ anion, 6-311G(d) basis set are used on C atoms, signed deviations (Δ), and root mean square deviations (RMSDs).

Num.	$\delta_{\text{Exp.}}^a$	Int. ^b	PW91PW91		BP86		TPSSTPSS		B3LYP		B3PW91		PBE1PBE		BHandHLYP		CAM-B3LYP		M06	
			δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ
1	111.60	4	140.46	28.86	140.43	28.83	140.83	29.23	136.81	25.21	137.01	25.41	136.21	24.61	119.06	7.46	134.8	23.2	143.60	32.00
2	112.80	2	146.78	33.98	146.58	33.78	146.66	33.86	144.49	31.69	144.94	32.14	144.63	31.83	129.31	16.51	143.91	31.11	144.66	31.86
3	146.60	2	137.58	-9.02	137.63	-8.97	136.47	-10.13	133.30	-13.30	132.93	-13.67	131.90	-14.70	136.87	-9.73	129.03	-17.57	133.87	-12.73
4	134.00	4	145.4	11.4	145.45	11.45	144.22	10.22	139.58	5.58	139.31	5.31	138.15	4.15	135.04	1.04	135.18	1.18	140.94	6.94
5	149.70	2	152.23	2.53	152.36	2.66	151.62	1.92	149.66	-0.04	149.29	-0.41	148.74	-0.96	149.98	0.28	148.15	-1.55	153.32	3.62
6	155.60	4	139.31	-16.29	139.24	-16.36	139.67	-15.93	138.74	-16.86	138.84	-16.76	138.79	-16.81	145.16	-10.44	137.91	-17.69	138.82	-16.78
7	143.60	4	136.72	-6.88	136.97	-6.63	137.39	-6.21	137.79	-5.81	137.4	-6.20	137.50	-6.10	144.21	0.61	138.50	-5.10	137.62	-5.98
8	132.10	2	131.13	-0.97	131.30	-0.80	130.88	-1.22	130.53	-1.57	129.74	-2.36	129.42	-2.68	132.50	0.40	129.57	-2.53	129.99	-2.11
9	164.20	4	144.84	-19.36	144.90	-19.3	145.15	-19.05	146.05	-18.15	146.18	-18.02	146.16	-18.04	151.49	-12.71	145.23	-18.97	145.87	-18.33
10	152.10	4	149.01	-3.09	148.90	-3.20	148.38	-3.72	147.41	-4.69	147.28	-4.82	146.92	-5.18	147.32	-4.78	144.32	-7.78	144.95	-7.15
11	157.10	4	156.97	-0.13	156.95	-0.15	156.65	-0.45	158.36	1.26	158.21	1.11	158.31	1.21	161.03	3.93	159.05	1.95	158.97	1.87
12	143.00	4	136.16	-6.84	136.26	-6.74	136.70	-6.30	137.31	-5.69	136.96	-6.04	137.06	-5.94	139.77	-3.23	137.63	-5.37	134.63	-8.37
13	153.70	4	149.79	-3.91	149.77	-3.93	149.50	-4.20	150.04	-3.66	149.86	-3.84	149.79	-3.91	151.17	-2.53	149.67	-4.03	148.41	-5.29
14	147.20	4	149.47	2.27	149.39	2.19	148.87	1.67	148.86	1.66	148.79	1.59	148.55	1.35	147.29	0.09	146.32	-0.88	147.79	0.59
15	142.70	4	142.01	-0.69	142.09	-0.61	142.37	-0.33	142.58	-0.12	142.20	-0.5	142.08	-0.62	142.45	-0.25	141.96	-0.74	140.76	-1.94
16	150.90	4	152.11	1.21	152.03	1.13	152.13	1.23	153.6	2.70	153.72	2.82	154.10	3.20	155.01	4.11	154.77	3.87	153.98	3.08
17	145.90	2	149.98	4.08	150.12	4.22	150.43	4.53	151.47	5.57	151.14	5.24	151.17	5.27	152.02	6.12	151.7	5.8	150.51	4.61
18	146.10	4	149.54	3.44	149.53	3.43	149.27	3.17	149.75	3.65	149.65	3.55	149.59	3.49	148.55	2.45	149.17	3.07	148.57	2.47
19	145.90	4	147.23	1.33	147.21	1.31	147.31	1.41	148.77	2.87	148.89	2.99	149.11	3.21	148.4	2.50	148.9	3.00	148.52	2.62
20	134.50	2	140.68	6.18	140.84	6.34	140.71	6.21	140.46	5.96	140.15	5.65	139.92	5.42	137.73	3.23	138.92	4.42	137.97	3.47
21	138.90	4	144.72	5.82	144.68	5.78	144.44	5.54	144.61	5.71	144.56	5.66	144.54	5.64	143.30	4.40	144.36	5.46	143.72	4.82
22	139.80	4	145.46	5.66	145.38	5.58	145.3	5.50	145.42	5.62	145.56	5.76	145.59	5.79	143.35	3.55	144.27	4.47	144.74	4.94
23	133.00	4	138.86	5.86	138.86	5.86	138.59	5.59	136.84	3.84	136.84	3.84	136.51	3.51	133.02	0.02	134.44	1.44	135.23	2.23
24	133.60	2	141.66	8.06	141.75	8.15	142.10	8.50	141.3	7.70	141.10	7.50	140.98	7.38	138.52	4.92	139.72	6.12	139.60	6.00
RMSD	--	--	11.56		11.52		11.51		10.81		10.89		10.82		6.07		10.82		11.59	

^a ^{13}C NMR lines of $[\text{Ce}@C_{2v}(9)\text{-C}_{82}]^-$ anion provided in ref 19, ^b Intensity of the NMR peaks.

Table S2: Comparison between the experimental results and calculated ¹³C NMR chemical shifts (δ /ppm) of [Ce@C_{2v}(9)-C₈₂]⁻ anion, 6-31G(d) basis set are used on C atoms, CEP-4G basis set are used on Ce, signed deviations (Δ), and root mean square deviations (RMSDs).

Num.	$\delta_{\text{Exp.}}^a$	Int. ^b	PW91PW91		BP86		TPSSTPSS		B3LYP		B3PW91		PBE1PBE		BHandHLYP		CAM-B3LYP		M06	
			δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ	δ	Δ
1	111.60	4	138.61	27.01	138.29	26.69	138.05	26.45	133.56	21.96	132.68	21.08	124.68	13.08	131.83	20.23	131.30	19.7	137.72	26.12
2	112.80	2	140.02	27.22	139.30	26.50	141.09	28.29	137.14	24.34	135.78	22.98	133.39	20.59	139.78	26.98	138.38	25.58	140.25	27.45
3	146.60	2	134.69	-11.91	135.91	-10.69	134.91	-11.69	130.69	-15.91	129.58	-17.02	128.29	-18.31	128.05	-18.55	127.34	-19.26	133.87	-12.73
4	134.00	4	142.30	8.30	141.80	7.80	142.05	8.05	137.56	3.56	137.60	3.60	130.79	-3.21	132.77	-1.23	133.44	-0.56	140.36	6.36
5	149.70	2	148.58	-1.12	148.27	-1.43	147.83	-1.87	149.07	-0.63	149.41	-0.29	140.73	-8.97	146.28	-3.42	147.03	-2.67	144.59	-5.11
6	155.60	4	138.58	-17.02	139.43	-16.17	139.22	-16.38	136.15	-19.45	135.90	-19.70	133.56	-22.04	135.83	-19.77	135.99	-19.61	138.98	-16.62
7	143.60	4	135.70	-7.90	136.55	-7.05	136.62	-6.98	136.95	-6.65	136.62	-6.98	133.56	-10.04	137.64	-5.96	137.17	-6.43	135.31	-8.29
8	132.10	2	134.76	2.66	135.48	3.38	134.90	2.80	130.81	-1.29	130.43	-1.67	123.81	-8.29	129.21	-2.89	129.15	-2.95	137.30	5.20
9	164.20	4	138.02	-26.18	137.97	-26.23	138.78	-25.42	144.09	-20.11	143.73	-20.47	139.92	-24.28	143.2	-21.00	142.96	-21.24	136.52	-27.68
10	152.10	4	143.36	-8.74	142.98	-9.12	143.37	-8.73	145.14	-6.96	144.96	-7.14	138.94	-13.16	141.91	-10.19	141.69	-10.41	142.17	-9.93
11	157.10	4	150.60	-6.50	149.96	-7.14	150.59	-6.51	156.28	-0.82	156.10	-1.00	149.80	-7.30	156.56	-0.54	156.15	-0.95	148.40	-8.70
12	143.00	4	134.30	-8.70	134.70	-8.30	135.35	-7.65	135.39	-7.61	134.91	-8.09	130.74	-12.26	136.36	-6.64	136.04	-6.96	135.26	-7.74
13	153.70	4	143.75	-9.95	143.55	-10.15	144.05	-9.65	147.67	-6.03	147.38	-6.32	142.22	-11.48	147.07	-6.63	147.09	-6.61	142.05	-11.65
14	147.20	4	145.08	-2.12	144.56	-2.64	144.9	-2.30	147.40	0.20	147.14	-0.06	140.86	-6.34	144.87	-2.33	144.62	-2.58	141.96	-5.24
15	142.70	4	138.07	-4.63	137.99	-4.71	138.93	-3.77	141.17	-1.53	140.56	-2.14	135.88	-6.82	141.22	-1.48	140.77	-1.93	136.80	-5.90
16	150.90	4	143.26	-7.64	142.52	-8.38	143.68	-7.22	151.62	0.72	151.55	0.65	145.96	-4.94	152.49	1.59	152.21	1.31	141.57	-9.33
17	145.90	2	146.93	1.03	146.72	0.82	147.60	1.70	150.10	4.20	149.76	3.86	143.7	-2.20	150.77	4.87	149.97	4.07	147.13	1.23
18	146.10	4	142.00	-4.10	141.29	-4.81	142.39	-3.71	147.93	1.83	147.57	1.47	142.23	-3.87	147.72	1.62	147.32	1.22	140.93	-5.17
19	145.90	4	141.35	-4.55	140.61	-5.29	141.76	-4.14	147.36	1.46	147.23	1.33	141.81	-4.09	147.34	1.44	147.08	1.18	140.31	-5.59
20	134.50	2	139.63	5.13	139.79	5.29	140.08	5.58	138.41	3.91	138.13	3.63	132.60	-1.90	137.56	3.06	137.24	2.74	140.39	5.89
21	138.90	4	144.78	5.88	144.90	6.00	144.65	5.75	142.41	3.51	142.22	3.32	137.04	-1.86	142.92	4.02	142.31	3.41	144.85	5.95
22	139.80	4	138.92	-0.88	138.20	-1.60	139.32	-0.48	143.58	3.78	143.45	3.65	138.27	-1.53	143.07	3.27	142.38	2.58	137.54	-2.26
23	133.00	4	141.76	8.76	142.16	9.16	141.51	8.51	134.99	1.99	134.80	1.80	129.57	-3.43	133.25	0.25	132.75	-0.25	140.35	7.35
24	133.60	2	140.70	7.10	140.65	7.05	141.33	7.73	140.24	6.64	139.93	6.33	134.52	0.92	139.67	6.07	138.62	5.02	140.48	6.88
RMSD	--	--	11.78		11.65		11.63		10.06		9.99		11.08		10.56		10.39		12.18	

^a ¹³C NMR lines of [Ce@C_{2v}(9)-C₈₂]⁻ anion provided in ref 19, ^b Intensity of the NMR peaks.

Cartesian coordinates of $[\text{Ce}@\text{C}_{82}(\text{C}_{2v}: 9)]^-$ anion calculated by all the considered DFT methods at 6-31G(d)//RCEP level.

B3LYP:

C	1.21526000	4.00813800	-0.76252700
C	-1.21526000	4.00813800	-0.76252700
C	0.00000000	3.95185600	-1.50774100
C	1.21749100	3.92897400	0.67118100
C	-1.21749100	3.92897400	0.67118100
C	0.00000000	3.85226100	1.40016500
C	2.39346600	3.31556900	-1.21894200
C	-2.39346600	3.31556900	-1.21894200
C	2.38486700	3.18145600	1.09289900
C	-2.38486700	3.18145600	1.09289900
C	0.00000000	3.24930700	-2.80054000
C	0.00000000	3.06743100	2.60830000
C	3.08281300	2.74600400	-0.09499800
C	-3.08281300	2.74600400	-0.09499800
C	2.40821500	2.65460700	-2.43558600
C	-2.40821500	2.65460700	-2.43558600
C	1.20642600	2.64028600	-3.25708900
C	-1.20642600	2.64028600	-3.25708900
C	1.15883300	2.36402000	3.06033400
C	-1.15883300	2.36402000	3.06033400
C	2.35039700	2.36518200	2.24734500
C	-2.35039700	2.36518200	2.24734500
C	3.69141300	1.46054600	-0.18427600
C	-3.69141300	1.46054600	-0.18427600
C	3.09568400	1.40809800	-2.57742500
C	-3.09568400	1.40809800	-2.57742500
C	1.20481200	1.42227700	-4.00245400
C	-1.20481200	1.42227700	-4.00245400
C	0.73715200	1.23246700	3.86320600
C	-0.73715200	1.23246700	3.86320600
C	3.10361900	1.15961000	2.22773800
C	-3.10361900	1.15961000	2.22773800
C	3.66949000	0.73175700	-1.45223700
C	-3.66949000	0.73175700	-1.45223700
C	2.39727400	0.68593100	-3.60944000
C	-2.39727400	0.68593100	-3.60944000
C	0.00000000	0.73710300	-4.31773300
C	3.76670700	0.71372200	1.03567300
C	-3.76670700	0.71372200	1.03567300
C	1.49934500	0.00000000	3.81930600
C	-1.49934500	0.00000000	3.81930600

C	2.66759900	0.00000000	2.97552000
C	-2.66759900	0.00000000	2.97552000
C	3.76670700	-0.71372200	1.03567300
C	-3.76670700	-0.71372200	1.03567300
C	0.00000000	-0.73710300	-4.31773300
C	2.39727400	-0.68593100	-3.60944000
C	-2.39727400	-0.68593100	-3.60944000
C	3.66949000	-0.73175700	-1.45223700
C	-3.66949000	-0.73175700	-1.45223700
C	3.10361900	-1.15961000	2.22773800
C	-3.10361900	-1.15961000	2.22773800
C	0.73715200	-1.23246700	3.86320600
C	-0.73715200	-1.23246700	3.86320600
C	1.20481200	-1.42227700	-4.00245400
C	-1.20481200	-1.42227700	-4.00245400
C	3.09568400	-1.40809800	-2.57742500
C	-3.09568400	-1.40809800	-2.57742500
C	3.69141300	-1.46054600	-0.18427600
C	-3.69141300	-1.46054600	-0.18427600
C	2.35039700	-2.36518200	2.24734500
C	-2.35039700	-2.36518200	2.24734500
C	1.15883300	-2.36402000	3.06033400
C	-1.15883300	-2.36402000	3.06033400
C	1.20642600	-2.64028600	-3.25708900
C	-1.20642600	-2.64028600	-3.25708900
C	2.40821500	-2.65460700	-2.43558600
C	-2.40821500	-2.65460700	-2.43558600
C	3.08281300	-2.74600400	-0.09499800
C	-3.08281300	-2.74600400	-0.09499800
C	0.00000000	-3.06743100	2.60830000
C	0.00000000	-3.24930700	-2.80054000
C	2.38486700	-3.18145600	1.09289900
C	-2.38486700	-3.18145600	1.09289900
C	2.39346600	-3.31556900	-1.21894200
C	-2.39346600	-3.31556900	-1.21894200
C	0.00000000	-3.85226100	1.40016500
C	1.21749100	-3.92897400	0.67118100
C	-1.21749100	-3.92897400	0.67118100
C	0.00000000	-3.95185600	-1.50774100
C	1.21526000	-4.00813800	-0.76252700
C	-1.21526000	-4.00813800	-0.76252700
Ce	0.00000000	0.00000000	1.78260300

B3PW91

C	1.21261800	3.99942400	-0.76372400
C	-1.21261800	3.99942400	-0.76372400
C	0.00000000	3.94262200	-1.50730600
C	1.21469700	3.91852300	0.66690800
C	-1.21469700	3.91852300	0.66690800
C	0.00000000	3.84052000	1.39375400
C	2.38728800	3.30826500	-1.21815600
C	-2.38728800	3.30826500	-1.21815600
C	2.37803800	3.17295000	1.08714100
C	-2.37803800	3.17295000	1.08714100
C	0.00000000	3.24205400	-2.79566200
C	0.00000000	3.05425700	2.59642200
C	3.07467600	2.73893000	-0.09743000
C	-3.07467600	2.73893000	-0.09743000
C	2.40269000	2.64820200	-2.43329300
C	-2.40269000	2.64820200	-2.43329300
C	1.20372900	2.63397500	-3.25152900
C	-1.20372900	2.63397500	-3.25152900
C	1.15505000	2.35321900	3.04939600
C	-1.15505000	2.35321900	3.04939600
C	2.34336900	2.35770900	2.23901300
C	-2.34336900	2.35770900	2.23901300
C	3.68233200	1.45658200	-0.18734300
C	-3.68233200	1.45658200	-0.18734300
C	3.08889600	1.40502400	-2.57439800
C	-3.08889600	1.40502400	-2.57439800
C	1.20217800	1.41869600	-3.99561200
C	-1.20217800	1.41869600	-3.99561200
C	0.73511900	1.22862800	3.85732100
C	-0.73511900	1.22862800	3.85732100
C	3.09455700	1.15586500	2.21898900
C	-3.09455700	1.15586500	2.21898900
C	3.66114500	0.72959500	-1.45138800
C	-3.66114500	0.72959500	-1.45138800
C	2.39130100	0.68515800	-3.60340700
C	-2.39130100	0.68515800	-3.60340700
C	0.00000000	0.73464300	-4.31014600
C	3.75686800	0.71182600	1.03014400
C	-3.75686800	0.71182600	1.03014400
C	1.49679600	0.00000000	3.81401400
C	-1.49679600	0.00000000	3.81401400
C	2.65730500	0.00000000	2.96455300
C	-2.65730500	0.00000000	2.96455300

C	3.75686800	-0.71182600	1.03014400
C	-3.75686800	-0.71182600	1.03014400
C	0.00000000	-0.73464300	-4.31014600
C	2.39130100	-0.68515800	-3.60340700
C	-2.39130100	-0.68515800	-3.60340700
C	3.66114500	-0.72959500	-1.45138800
C	-3.66114500	-0.72959500	-1.45138800
C	3.09455700	-1.15586500	2.21898900
C	-3.09455700	-1.15586500	2.21898900
C	0.73511900	-1.22862800	3.85732100
C	-0.73511900	-1.22862800	3.85732100
C	1.20217800	-1.41869600	-3.99561200
C	-1.20217800	-1.41869600	-3.99561200
C	3.08889600	-1.40502400	-2.57439800
C	-3.08889600	-1.40502400	-2.57439800
C	3.68233200	-1.45658200	-0.18734300
C	-3.68233200	-1.45658200	-0.18734300
C	2.34336900	-2.35770900	2.23901300
C	-2.34336900	-2.35770900	2.23901300
C	1.15505000	-2.35321900	3.04939600
C	-1.15505000	-2.35321900	3.04939600
C	1.20372900	-2.63397500	-3.25152900
C	-1.20372900	-2.63397500	-3.25152900
C	2.40269000	-2.64820200	-2.43329300
C	-2.40269000	-2.64820200	-2.43329300
C	3.07467600	-2.73893000	-0.09743000
C	-3.07467600	-2.73893000	-0.09743000
C	0.00000000	-3.05425700	2.59642200
C	0.00000000	-3.24205400	-2.79566200
C	2.37803800	-3.17295000	1.08714100
C	-2.37803800	-3.17295000	1.08714100
C	2.38728800	-3.30826500	-1.21815600
C	-2.38728800	-3.30826500	-1.21815600
C	0.00000000	-3.84052000	1.39375400
C	1.21469700	-3.91852300	0.66690800
C	-1.21469700	-3.91852300	0.66690800
C	0.00000000	-3.94262200	-1.50730600
C	1.21261800	-3.99942400	-0.76372400
C	-1.21261800	-3.99942400	-0.76372400
Ce	0.00000000	0.00000000	1.79981500

PW91PW91

C	1.21889700	4.02261500	-0.76837200
C	-1.21889700	4.02261500	-0.76837200

C	0.00000000	3.96669900	-1.51790300
C	1.22085100	3.94200800	0.66985000
C	-1.22085100	3.94200800	0.66985000
C	0.00000000	3.86251200	1.40172700
C	2.40073800	3.32966100	-1.22528200
C	-2.40073800	3.32966100	-1.22528200
C	2.38918600	3.18938000	1.09135800
C	-2.38918600	3.18938000	1.09135800
C	0.00000000	3.26223000	-2.81039100
C	0.00000000	3.07349100	2.61029300
C	3.09122300	2.75634300	-0.09843900
C	-3.09122300	2.75634300	-0.09843900
C	2.41373100	2.66491500	-2.44733200
C	-2.41373100	2.66491500	-2.44733200
C	1.21091400	2.65127700	-3.26940800
C	-1.21091400	2.65127700	-3.26940800
C	1.16043900	2.36617400	3.06520800
C	-1.16043900	2.36617400	3.06520800
C	2.35391300	2.37050000	2.25094600
C	-2.35391300	2.37050000	2.25094600
C	3.69966800	1.46442400	-0.18935900
C	-3.69966800	1.46442400	-0.18935900
C	3.10365900	1.41286400	-2.58959100
C	-3.10365900	1.41286400	-2.58959100
C	1.20921400	1.42621200	-4.01607600
C	-1.20921400	1.42621200	-4.01607600
C	0.73834900	1.23740400	3.88123400
C	-0.73834900	1.23740400	3.88123400
C	3.10682500	1.16125600	2.22932500
C	-3.10682500	1.16125600	2.22932500
C	3.67713500	0.73335500	-1.45969400
C	-3.67713500	0.73335500	-1.45969400
C	2.40288500	0.69055400	-3.62372300
C	-2.40288500	0.69055400	-3.62372300
C	0.00000000	0.73710300	-4.33249100
C	3.77209900	0.71604200	1.03222500
C	-3.77209900	0.71604200	1.03222500
C	1.50177500	0.00000000	3.83482300
C	-1.50177500	0.00000000	3.83482300
C	2.66803800	0.00000000	2.97878200
C	-2.66803800	0.00000000	2.97878200
C	3.77209900	-0.71604200	1.03222500
C	-3.77209900	-0.71604200	1.03222500
C	0.00000000	-0.73710300	-4.33249100

C	2.40288500	-0.69055400	-3.62372300
C	-2.40288500	-0.69055400	-3.62372300
C	3.67713500	-0.73335500	-1.45969400
C	-3.67713500	-0.73335500	-1.45969400
C	3.10682500	-1.16125600	2.22932500
C	-3.10682500	-1.16125600	2.22932500
C	0.73834900	-1.23740400	3.88123400
C	-0.73834900	-1.23740400	3.88123400
C	1.20921400	-1.42621200	-4.01607600
C	-1.20921400	-1.42621200	-4.01607600
C	3.10365900	-1.41286400	-2.58959100
C	-3.10365900	-1.41286400	-2.58959100
C	3.69966800	-1.46442400	-0.18935900
C	-3.69966800	-1.46442400	-0.18935900
C	2.35391300	-2.37050000	2.25094600
C	-2.35391300	-2.37050000	2.25094600
C	1.16043900	-2.36617400	3.06520800
C	-1.16043900	-2.36617400	3.06520800
C	1.21091400	-2.65127700	-3.26940800
C	-1.21091400	-2.65127700	-3.26940800
C	2.41373100	-2.66491500	-2.44733200
C	-2.41373100	-2.66491500	-2.44733200
C	3.09122300	-2.75634300	-0.09843900
C	-3.09122300	-2.75634300	-0.09843900
C	0.00000000	-3.07349100	2.61029300
C	0.00000000	-3.26223000	-2.81039100
C	2.38918600	-3.18938000	1.09135800
C	-2.38918600	-3.18938000	1.09135800
C	2.40073800	-3.32966100	-1.22528200
C	-2.40073800	-3.32966100	-1.22528200
C	0.00000000	-3.86251200	1.40172700
C	1.22085100	-3.94200800	0.66985000
C	-1.22085100	-3.94200800	0.66985000
C	0.00000000	-3.96669900	-1.51790300
C	1.21889700	-4.02261500	-0.76837200
C	-1.21889700	-4.02261500	-0.76837200
Ce	0.00000000	0.00000000	1.81436300
PBE1PBE			
C	1.21074000	3.99349600	-0.76307000
C	-1.21074000	3.99349600	-0.76307000
C	0.00000000	3.93668800	-1.50563600
C	1.21284600	3.91231100	0.66509400
C	-1.21284600	3.91231100	0.66509400

C	0.00000000	3.83413200	1.39096200
C	2.38388800	3.30317700	-1.21689600
C	-2.38388800	3.30317700	-1.21689600
C	2.37492700	3.16857700	1.08532100
C	-2.37492700	3.16857700	1.08532100
C	0.00000000	3.23721100	-2.79233700
C	0.00000000	3.04790100	2.59161500
C	3.07040200	2.73500300	-0.09765400
C	-3.07040200	2.73500300	-0.09765400
C	2.39931200	2.64406000	-2.43025300
C	-2.39931200	2.64406000	-2.43025300
C	1.20176800	2.62957600	-3.24735300
C	-1.20176800	2.62957600	-3.24735300
C	1.15340200	2.34899600	3.04495400
C	-1.15340200	2.34899600	3.04495400
C	2.33989200	2.35453900	2.23516100
C	-2.33989200	2.35453900	2.23516100
C	3.67684000	1.45463300	-0.18745900
C	-3.67684000	1.45463300	-0.18745900
C	3.08445400	1.40267900	-2.57071300
C	-3.08445400	1.40267900	-2.57071300
C	1.20025200	1.41669700	-3.99075600
C	-1.20025200	1.41669700	-3.99075600
C	0.73397200	1.22674800	3.85244200
C	-0.73397200	1.22674800	3.85244200
C	3.08932100	1.15383200	2.21500200
C	-3.08932100	1.15383200	2.21500200
C	3.65560500	0.72863900	-1.44952400
C	-3.65560500	0.72863900	-1.44952400
C	2.38786800	0.68405400	-3.59865600
C	-2.38786800	0.68405400	-3.59865600
C	0.00000000	0.73367700	-4.30526900
C	3.75114200	0.71081100	1.02862800
C	-3.75114200	0.71081100	1.02862800
C	1.49429700	0.00000000	3.80944800
C	-1.49429700	0.00000000	3.80944800
C	2.65210600	0.00000000	2.95975900
C	-2.65210600	0.00000000	2.95975900
C	3.75114200	-0.71081100	1.02862800
C	-3.75114200	-0.71081100	1.02862800
C	0.00000000	-0.73367700	-4.30526900
C	2.38786800	-0.68405400	-3.59865600
C	-2.38786800	-0.68405400	-3.59865600
C	3.65560500	-0.72863900	-1.44952400

C	-3.65560500	-0.72863900	-1.44952400
C	3.08932100	-1.15383200	2.21500200
C	-3.08932100	-1.15383200	2.21500200
C	0.73397200	-1.22674800	3.85244200
C	-0.73397200	-1.22674800	3.85244200
C	1.20025200	-1.41669700	-3.99075600
C	-1.20025200	-1.41669700	-3.99075600
C	3.08445400	-1.40267900	-2.57071300
C	-3.08445400	-1.40267900	-2.57071300
C	3.67684000	-1.45463300	-0.18745900
C	-3.67684000	-1.45463300	-0.18745900
C	2.33989200	-2.35453900	2.23516100
C	-2.33989200	-2.35453900	2.23516100
C	1.15340200	-2.34899600	3.04495400
C	-1.15340200	-2.34899600	3.04495400
C	1.20176800	-2.62957600	-3.24735300
C	-1.20176800	-2.62957600	-3.24735300
C	2.39931200	-2.64406000	-2.43025300
C	-2.39931200	-2.64406000	-2.43025300
C	3.07040200	-2.73500300	-0.09765400
C	-3.07040200	-2.73500300	-0.09765400
C	0.00000000	-3.04790100	2.59161500
C	0.00000000	-3.23721100	-2.79233700
C	2.37492700	-3.16857700	1.08532100
C	-2.37492700	-3.16857700	1.08532100
C	2.38388800	-3.30317700	-1.21689600
C	-2.38388800	-3.30317700	-1.21689600
C	0.00000000	-3.83413200	1.39096200
C	1.21284600	-3.91231100	0.66509400
C	-1.21284600	-3.91231100	0.66509400
C	0.00000000	-3.93668800	-1.50563600
C	1.21074000	-3.99349600	-0.76307000
C	-1.21074000	-3.99349600	-0.76307000
Ce	0.00000000	0.00000000	1.80060500

BHandHLYP

C	1.20575500	3.97783300	-0.75518200
C	-1.20575500	3.97783300	-0.75518200
C	0.00000000	3.92052100	-1.49281600
C	1.20813700	3.89838800	0.66735600
C	-1.20813700	3.89838800	0.66735600
C	0.00000000	3.82410900	1.39116700
C	2.37479400	3.28723800	-1.20855900
C	-2.37479400	3.28723800	-1.20855900

C	2.36777700	3.15918600	1.08754200
C	-2.36777700	3.15918600	1.08754200
C	0.00000000	3.22282300	-2.77979600
C	0.00000000	3.04543600	2.59240500
C	3.05933200	2.72329300	-0.09300600
C	-3.05933200	2.72329300	-0.09300600
C	2.39213100	2.63270300	-2.41508600
C	-2.39213100	2.63270300	-2.41508600
C	1.19598300	2.61714900	-3.23132800
C	-1.19598300	2.61714900	-3.23132800
C	1.15028300	2.34899300	3.04175100
C	-1.15028300	2.34899300	3.04175100
C	2.33205800	2.34872000	2.23163600
C	-2.33205800	2.34872000	2.23163600
C	3.66475300	1.45047700	-0.18150200
C	-3.66475300	1.45047700	-0.18150200
C	3.07378600	1.39682700	-2.55481100
C	-3.07378600	1.39682700	-2.55481100
C	1.19457000	1.41209400	-3.97239100
C	-1.19457000	1.41209400	-3.97239100
C	0.73045600	1.22275100	3.83319500
C	-0.73045600	1.22275100	3.83319500
C	3.07970700	1.15095100	2.21257500
C	-3.07970700	1.15095100	2.21257500
C	3.64469200	0.72716300	-1.44018200
C	-3.64469200	0.72716300	-1.44018200
C	2.38077400	0.67849800	-3.58094900
C	-2.38077400	0.67849800	-3.58094900
C	0.00000000	0.73373100	-4.28584300
C	3.73846900	0.70782700	1.03168300
C	-3.73846900	0.70782700	1.03168300
C	1.48691700	0.00000000	3.79231200
C	-1.48691700	0.00000000	3.79231200
C	2.64622200	0.00000000	2.95527800
C	-2.64622200	0.00000000	2.95527800
C	3.73846900	-0.70782700	1.03168300
C	-3.73846900	-0.70782700	1.03168300
C	0.00000000	-0.73373100	-4.28584300
C	2.38077400	-0.67849800	-3.58094900
C	-2.38077400	-0.67849800	-3.58094900
C	3.64469200	-0.72716300	-1.44018200
C	-3.64469200	-0.72716300	-1.44018200
C	3.07970700	-1.15095100	2.21257500
C	-3.07970700	-1.15095100	2.21257500

C	0.73045600	-1.22275100	3.83319500
C	-0.73045600	-1.22275100	3.83319500
C	1.19457000	-1.41209400	-3.97239100
C	-1.19457000	-1.41209400	-3.97239100
C	3.07378600	-1.39682700	-2.55481100
C	-3.07378600	-1.39682700	-2.55481100
C	3.66475300	-1.45047700	-0.18150200
C	-3.66475300	-1.45047700	-0.18150200
C	2.33205800	-2.34872000	2.23163600
C	-2.33205800	-2.34872000	2.23163600
C	1.15028300	-2.34899300	3.04175100
C	-1.15028300	-2.34899300	3.04175100
C	1.19598300	-2.61714900	-3.23132800
C	-1.19598300	-2.61714900	-3.23132800
C	2.39213100	-2.63270300	-2.41508600
C	-2.39213100	-2.63270300	-2.41508600
C	3.05933200	-2.72329300	-0.09300600
C	-3.05933200	-2.72329300	-0.09300600
C	0.00000000	-3.04543600	2.59240500
C	0.00000000	-3.22282300	-2.77979600
C	2.36777700	-3.15918600	1.08754200
C	-2.36777700	-3.15918600	1.08754200
C	2.37479400	-3.28723800	-1.20855900
C	-2.37479400	-3.28723800	-1.20855900
C	0.00000000	-3.82410900	1.39116700
C	1.20813700	-3.89838800	0.66735600
C	-1.20813700	-3.89838800	0.66735600
C	0.00000000	-3.92052100	-1.49281600
C	1.20575500	-3.97783300	-0.75518200
C	-1.20575500	-3.97783300	-0.75518200
Ce	0.00000000	0.00000000	1.75485700

CAM-B3LYP

C	1.20945200	3.99040500	-0.75985800
C	-1.20945200	3.99040500	-0.75985800
C	0.00000000	3.93277800	-1.49972100
C	1.21181700	3.90927500	0.66674800
C	-1.21181700	3.90927500	0.66674800
C	0.00000000	3.83275200	1.39229000
C	2.38395400	3.29801900	-1.21518600
C	-2.38395400	3.29801900	-1.21518600
C	2.37633500	3.16826300	1.08900100
C	-2.37633500	3.16826300	1.08900100
C	0.00000000	3.23266200	-2.79129800

C	0.00000000	3.04861500	2.59531600
C	3.07128100	2.73223200	-0.09607600
C	-3.07128100	2.73223200	-0.09607600
C	2.40105500	2.64201700	-2.42566000
C	-2.40105500	2.64201700	-2.42566000
C	1.19964600	2.62598000	-3.24476900
C	-1.19964600	2.62598000	-3.24476900
C	1.15365200	2.35190200	3.04806900
C	-1.15365200	2.35190200	3.04806900
C	2.33925800	2.35471500	2.23494800
C	-2.33925800	2.35471500	2.23494800
C	3.67747800	1.45532200	-0.18513900
C	-3.67747800	1.45532200	-0.18513900
C	3.08468800	1.40132500	-2.56531400
C	-3.08468800	1.40132500	-2.56531400
C	1.19815300	1.41704800	-3.98796100
C	-1.19815300	1.41704800	-3.98796100
C	0.73390800	1.22617300	3.84875700
C	-0.73390800	1.22617300	3.84875700
C	3.08922300	1.15307400	2.21628400
C	-3.08922300	1.15307400	2.21628400
C	3.65674100	0.72980000	-1.44754300
C	-3.65674100	0.72980000	-1.44754300
C	2.38945900	0.68055700	-3.59579800
C	-2.38945900	0.68055700	-3.59579800
C	0.00000000	0.73630400	-4.30242900
C	3.75172600	0.71001000	1.03213400
C	-3.75172600	0.71001000	1.03213400
C	1.49273100	0.00000000	3.80649400
C	-1.49273100	0.00000000	3.80649400
C	2.65486100	0.00000000	2.96269900
C	-2.65486100	0.00000000	2.96269900
C	3.75172600	-0.71001000	1.03213400
C	-3.75172600	-0.71001000	1.03213400
C	0.00000000	-0.73630400	-4.30242900
C	2.38945900	-0.68055700	-3.59579800
C	-2.38945900	-0.68055700	-3.59579800
C	3.65674100	-0.72980000	-1.44754300
C	-3.65674100	-0.72980000	-1.44754300
C	3.08922300	-1.15307400	2.21628400
C	-3.08922300	-1.15307400	2.21628400
C	0.73390800	-1.22617300	3.84875700
C	-0.73390800	-1.22617300	3.84875700
C	1.19815300	-1.41704800	-3.98796100

C	-1.19815300	-1.41704800	-3.98796100
C	3.08468800	-1.40132500	-2.56531400
C	-3.08468800	-1.40132500	-2.56531400
C	3.67747800	-1.45532200	-0.18513900
C	-3.67747800	-1.45532200	-0.18513900
C	2.33925800	-2.35471500	2.23494800
C	-2.33925800	-2.35471500	2.23494800
C	1.15365200	-2.35190200	3.04806900
C	-1.15365200	-2.35190200	3.04806900
C	1.19964600	-2.62598000	-3.24476900
C	-1.19964600	-2.62598000	-3.24476900
C	2.40105500	-2.64201700	-2.42566000
C	-2.40105500	-2.64201700	-2.42566000
C	3.07128100	-2.73223200	-0.09607600
C	-3.07128100	-2.73223200	-0.09607600
C	0.00000000	-3.04861500	2.59531600
C	0.00000000	-3.23266200	-2.79129800
C	2.37633500	-3.16826300	1.08900100
C	-2.37633500	-3.16826300	1.08900100
C	2.38395400	-3.29801900	-1.21518600
C	-2.38395400	-3.29801900	-1.21518600
C	0.00000000	-3.83275200	1.39229000
C	1.21181700	-3.90927500	0.66674800
C	-1.21181700	-3.90927500	0.66674800
C	0.00000000	-3.93277800	-1.49972100
C	1.20945200	-3.99040500	-0.75985800
C	-1.20945200	-3.99040500	-0.75985800
Ce	0.00000000	0.00000000	1.78166300
M06			
C	1.21018300	3.99190500	-0.75942100
C	-1.21018300	3.99190500	-0.75942100
C	0.00000000	3.93301300	-1.50100600
C	1.21198600	3.90963000	0.66769900
C	-1.21198600	3.90963000	0.66769900
C	0.00000000	3.83624100	1.39504100
C	2.38257100	3.30107900	-1.21373000
C	-2.38257100	3.30107900	-1.21373000
C	2.37430100	3.16771100	1.08869500
C	-2.37430100	3.16771100	1.08869500
C	0.00000000	3.23484900	-2.78757300
C	0.00000000	3.05512000	2.59879000
C	3.06780800	2.73302300	-0.09485800
C	-3.06780800	2.73302300	-0.09485800

C	2.39871100	2.64276500	-2.42676700
C	-2.39871100	2.64276500	-2.42676700
C	1.20142200	2.62873600	-3.24342700
C	-1.20142200	2.62873600	-3.24342700
C	1.15348400	2.35391400	3.04848300
C	-1.15348400	2.35391400	3.04848300
C	2.33945600	2.35530700	2.23914200
C	-2.33945600	2.35530700	2.23914200
C	3.67118900	1.45283700	-0.18481800
C	-3.67118900	1.45283700	-0.18481800
C	3.08318700	1.40173100	-2.56782900
C	-3.08318700	1.40173100	-2.56782900
C	1.19977500	1.41670200	-3.98716700
C	-1.19977500	1.41670200	-3.98716700
C	0.73292000	1.22597400	3.84548700
C	-0.73292000	1.22597400	3.84548700
C	3.08992000	1.15463300	2.22020100
C	-3.08992000	1.15463300	2.22020100
C	3.65100400	0.72772000	-1.44605000
C	-3.65100400	0.72772000	-1.44605000
C	2.38691900	0.68365600	-3.59620000
C	-2.38691900	0.68365600	-3.59620000
C	0.00000000	0.73310800	-4.29870300
C	3.74652600	0.71049900	1.03206000
C	-3.74652600	0.71049900	1.03206000
C	1.49292000	0.00000000	3.80469300
C	-1.49292000	0.00000000	3.80469300
C	2.65495900	0.00000000	2.96386700
C	-2.65495900	0.00000000	2.96386700
C	3.74652600	-0.71049900	1.03206000
C	-3.74652600	-0.71049900	1.03206000
C	0.00000000	-0.73310800	-4.29870300
C	2.38691900	-0.68365600	-3.59620000
C	-2.38691900	-0.68365600	-3.59620000
C	3.65100400	-0.72772000	-1.44605000
C	-3.65100400	-0.72772000	-1.44605000
C	3.08992000	-1.15463300	2.22020100
C	-3.08992000	-1.15463300	2.22020100
C	0.73292000	-1.22597400	3.84548700
C	-0.73292000	-1.22597400	3.84548700
C	1.19977500	-1.41670200	-3.98716700
C	-1.19977500	-1.41670200	-3.98716700
C	3.08318700	-1.40173100	-2.56782900
C	-3.08318700	-1.40173100	-2.56782900

C	3.67118900	-1.45283700	-0.18481800
C	-3.67118900	-1.45283700	-0.18481800
C	2.33945600	-2.35530700	2.23914200
C	-2.33945600	-2.35530700	2.23914200
C	1.15348400	-2.35391400	3.04848300
C	-1.15348400	-2.35391400	3.04848300
C	1.20142200	-2.62873600	-3.24342700
C	-1.20142200	-2.62873600	-3.24342700
C	2.39871100	-2.64276500	-2.42676700
C	-2.39871100	-2.64276500	-2.42676700
C	3.06780800	-2.73302300	-0.09485800
C	-3.06780800	-2.73302300	-0.09485800
C	0.00000000	-3.05512000	2.59879000
C	0.00000000	-3.23484900	-2.78757300
C	2.37430100	-3.16771100	1.08869500
C	-2.37430100	-3.16771100	1.08869500
C	2.38257100	-3.30107900	-1.21373000
C	-2.38257100	-3.30107900	-1.21373000
C	0.00000000	-3.83624100	1.39504100
C	1.21198600	-3.90963000	0.66769900
C	-1.21198600	-3.90963000	0.66769900
C	0.00000000	-3.93301300	-1.50100600
C	1.21018300	-3.99190500	-0.75942100
C	-1.21018300	-3.99190500	-0.75942100
Ce	0.00000000	0.00000000	1.77556300

TPSSTPSS

C	1.21919300	4.02332300	-0.76966700
C	-1.21919300	4.02332300	-0.76966700
C	0.00000000	3.96818100	-1.51951500
C	1.22082400	3.94161400	0.66845300
C	-1.22082400	3.94161400	0.66845300
C	0.00000000	3.86106700	1.40020000
C	2.40067600	3.32960000	-1.22642000
C	-2.40067600	3.32960000	-1.22642000
C	2.38935700	3.18956100	1.09046700
C	-2.38935700	3.18956100	1.09046700
C	0.00000000	3.26339900	-2.81267100
C	0.00000000	3.06795700	2.60718600
C	3.09120900	2.75636400	-0.09960500
C	-3.09120900	2.75636400	-0.09960500
C	2.41417800	2.66479400	-2.44851800
C	-2.41417800	2.66479400	-2.44851800
C	1.21100400	2.65110200	-3.27105100

C	-1.21100400	2.65110200	-3.27105100
C	1.15976500	2.36250200	3.06380800
C	-1.15976500	2.36250200	3.06380800
C	2.35443500	2.37042500	2.24984300
C	-2.35443500	2.37042500	2.24984300
C	3.70154100	1.46518200	-0.19036200
C	-3.70154100	1.46518200	-0.19036200
C	3.10421400	1.41307800	-2.59096600
C	-3.10421400	1.41307800	-2.59096600
C	1.20933100	1.42651300	-4.01771700
C	-1.20933100	1.42651300	-4.01771700
C	0.73893200	1.23764600	3.88647000
C	-0.73893200	1.23764600	3.88647000
C	3.10625900	1.16098100	2.22757100
C	-3.10625900	1.16098100	2.22757100
C	3.67974400	0.73377600	-1.46125100
C	-3.67974400	0.73377600	-1.46125100
C	2.40316700	0.69039700	-3.62470600
C	-2.40316700	0.69039700	-3.62470600
C	0.00000000	0.73753800	-4.33520500
C	3.77280100	0.71589300	1.03173200
C	-3.77280100	0.71589300	1.03173200
C	1.50312000	0.00000000	3.84041500
C	-1.50312000	0.00000000	3.84041500
C	2.66464200	0.00000000	2.97652800
C	-2.66464200	0.00000000	2.97652800
C	3.77280100	-0.71589300	1.03173200
C	-3.77280100	-0.71589300	1.03173200
C	0.00000000	-0.73753800	-4.33520500
C	2.40316700	-0.69039700	-3.62470600
C	-2.40316700	-0.69039700	-3.62470600
C	3.67974400	-0.73377600	-1.46125100
C	-3.67974400	-0.73377600	-1.46125100
C	3.10625900	-1.16098100	2.22757100
C	-3.10625900	-1.16098100	2.22757100
C	0.73893200	-1.23764600	3.88647000
C	-0.73893200	-1.23764600	3.88647000
C	1.20933100	-1.42651300	-4.01771700
C	-1.20933100	-1.42651300	-4.01771700
C	3.10421400	-1.41307800	-2.59096600
C	-3.10421400	-1.41307800	-2.59096600
C	3.70154100	-1.46518200	-0.19036200
C	-3.70154100	-1.46518200	-0.19036200
C	2.35443500	-2.37042500	2.24984300

C	-2.35443500	-2.37042500	2.24984300
C	1.15976500	-2.36250200	3.06380800
C	-1.15976500	-2.36250200	3.06380800
C	1.21100400	-2.65110200	-3.27105100
C	-1.21100400	-2.65110200	-3.27105100
C	2.41417800	-2.66479400	-2.44851800
C	-2.41417800	-2.66479400	-2.44851800
C	3.09120900	-2.75636400	-0.09960500
C	-3.09120900	-2.75636400	-0.09960500
C	0.00000000	-3.06795700	2.60718600
C	0.00000000	-3.26339900	-2.81267100
C	2.38935700	-3.18956100	1.09046700
C	-2.38935700	-3.18956100	1.09046700
C	2.40067600	-3.32960000	-1.22642000
C	-2.40067600	-3.32960000	-1.22642000
C	0.00000000	-3.86106700	1.40020000
C	1.22082400	-3.94161400	0.66845300
C	-1.22082400	-3.94161400	0.66845300
C	0.00000000	-3.96818100	-1.51951500
C	1.21919300	-4.02332300	-0.76966700
C	-1.21919300	-4.02332300	-0.76966700
Ce	0.00000000	0.00000000	1.82211600
BP86			
C	1.22156500	4.03121300	-0.76976400
C	-1.22156500	4.03121300	-0.76976400
C	0.00000000	3.97498000	-1.52073800
C	1.22349400	3.95053500	0.67160200
C	-1.22349400	3.95053500	0.67160200
C	0.00000000	3.87108000	1.40503600
C	2.40586100	3.33648400	-1.22777600
C	-2.40586100	3.33648400	-1.22777600
C	2.39458000	3.19639400	1.09410500
C	-2.39458000	3.19639400	1.09410500
C	0.00000000	3.26926500	-2.81652200
C	0.00000000	3.08067300	2.61646900
C	3.09793100	2.76211000	-0.09842300
C	-3.09793100	2.76211000	-0.09842300
C	2.41909100	2.67073600	-2.45240600
C	-2.41909100	2.67073600	-2.45240600
C	1.21362700	2.65720600	-3.27658700
C	-1.21362700	2.65720600	-3.27658700
C	1.16305900	2.37178800	3.07211000
C	-1.16305900	2.37178800	3.07211000

C	2.35927100	2.37569100	2.25610000
C	-2.35927100	2.37569100	2.25610000
C	3.70794900	1.46753300	-0.18934000
C	-3.70794900	1.46753300	-0.18934000
C	3.11048800	1.41595000	-2.59501500
C	-3.11048800	1.41595000	-2.59501500
C	1.21188900	1.42938300	-4.02469600
C	-1.21188900	1.42938300	-4.02469600
C	0.74002200	1.24013800	3.88931900
C	-0.74002200	1.24013800	3.88931900
C	3.11408400	1.16402800	2.23457400
C	-3.11408400	1.16402800	2.23457400
C	3.68545100	0.73499300	-1.46274900
C	-3.68545100	0.73499300	-1.46274900
C	2.40824700	0.69188900	-3.63138900
C	-2.40824700	0.69188900	-3.63138900
C	0.00000000	0.73882100	-4.34131900
C	3.78097600	0.71759400	1.03491400
C	-3.78097600	0.71759400	1.03491400
C	1.50488100	0.00000000	3.84239900
C	-1.50488100	0.00000000	3.84239900
C	2.67411300	0.00000000	2.98527400
C	-2.67411300	0.00000000	2.98527400
C	3.78097600	-0.71759400	1.03491400
C	-3.78097600	-0.71759400	1.03491400
C	0.00000000	-0.73882100	-4.34131900
C	2.40824700	-0.69188900	-3.63138900
C	-2.40824700	-0.69188900	-3.63138900
C	3.68545100	-0.73499300	-1.46274900
C	-3.68545100	-0.73499300	-1.46274900
C	3.11408400	-1.16402800	2.23457400
C	-3.11408400	-1.16402800	2.23457400
C	0.74002200	-1.24013800	3.88931900
C	-0.74002200	-1.24013800	3.88931900
C	1.21188900	-1.42938300	-4.02469600
C	-1.21188900	-1.42938300	-4.02469600
C	3.11048800	-1.41595000	-2.59501500
C	-3.11048800	-1.41595000	-2.59501500
C	3.70794900	-1.46753300	-0.18934000
C	-3.70794900	-1.46753300	-0.18934000
C	2.35927100	-2.37569100	2.25610000
C	-2.35927100	-2.37569100	2.25610000
C	1.16305900	-2.37178800	3.07211000
C	-1.16305900	-2.37178800	3.07211000

C	1.21362700	-2.65720600	-3.27658700
C	-1.21362700	-2.65720600	-3.27658700
C	2.41909100	-2.67073600	-2.45240600
C	-2.41909100	-2.67073600	-2.45240600
C	3.09793100	-2.76211000	-0.09842300
C	-3.09793100	-2.76211000	-0.09842300
C	0.00000000	-3.08067300	2.61646900
C	0.00000000	-3.26926500	-2.81652200
C	2.39458000	-3.19639400	1.09410500
C	-2.39458000	-3.19639400	1.09410500
C	2.40586100	-3.33648400	-1.22777600
C	-2.40586100	-3.33648400	-1.22777600
C	0.00000000	-3.87108000	1.40503600
C	1.22349400	-3.95053500	0.67160200
C	-1.22349400	-3.95053500	0.67160200
C	0.00000000	-3.97498000	-1.52073800
C	1.22156500	-4.03121300	-0.76976400
C	-1.22156500	-4.03121300	-0.76976400
Ce	0.00000000	0.00000000	1.81660300