Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

ELECTRONIC SUPPORTING INFORMATION

Spectroscopic signatures of the carbon buckyonions $C_{60}@C_{180}$ and $C_{60}@C_{240}$: a dispersion-corrected DFT study.

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Table 1 **Interaction energies for the encapsulations of C_{60} into C_{180} and C_{240} calculated with and without dispersion term and different basis set. For each geometry the level of theory for the single point energy is indicated in square brackets.**

	DZ kcal mol^{-1}	DZP kcal mol^{-1}	TZP kcal mol^{-1}	TZ2P kcal mol^{-1}
C60				
Geometry BLYP				
♦Electronic Internal Energy [E] (kcal mol^{-1}) [no_disp]	-10734.76	-11227.70	-11350.62	-11399.60
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp]	-10821.04	-11313.99	-11436.90	-11485.89
Geometry BLYP-D3				
♦Electronic Internal Energy [E] (kcal mol^{-1}) [no_disp]	**-10734.56**	**-11227.69**	**-11350.56**	**-11399.57**
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp]	-10820.85	-11313.98	-11436.85	-11485.86
C180				
Geometry BLYP-D3				
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp]				-35308.07
C240				
Geometry BLYP				
♦Electronic Internal Energy [E] (kcal mol^{-1}) [no_disp]	-44359.68	-46214.68	-46716.31	-46930.94
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp]	-44710.44	-46565.44	-47067.07	-47281.71
Geometry BLYP-D3				
♦Electronic Internal Energy [E] (kcal mol^{-1}) [no_disp]	**-44357.94**	**-46214.10**	**-46715.28**	**-46930.14**
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp]	-44708.99	-46565.15	-47066.33	-47281.19
C60@C180				
Geometry BLYP-D3				
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp]				-46526.67
ΔE				**267.26**
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp] ***[C_{3i} Symmetry ; No freqs calculated]***				-46530.12
ΔE				**263.81**
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp] ***[I_h Symmetry; Immaginary freqs]***				**-46478.56**
ΔE				**315.37**
C60@C240				
Geometry BLYP				
♦Electronic Internal Energy [E] (kcal mol^{-1}) [no_disp]	-55154.02	-57460.02	-57994.74	-58256.63
ΔE	**-59.58**	**-17.64**	**72.19**	**73.91**
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp]	-55813.91	-58119.91	-58654.63	-58916.52
ΔE	**-282.43**	**-240.48**	**-150.66**	**-148.92**
Geometry BLYP-D3				
♦Electronic Internal Energy [E] (kcal mol^{-1}) [no_disp]	**-55143.83**	**-57451.72**	**-57982.55**	**-58245.11**
ΔE	**-51.33**	**-9.93**	**83.29**	**84.60**
♦Electronic Internal Energy [E] (kcal mol^{-1}) [disp]	-55811.96	-58119.86	-58650.68	-58913.24
ΔE	**-282.12**	**-240.73**	**-147.50**	**-146.19**

Table 2 **BSSE corrections for $C_{60}@C_{240}$ at BLYP/*TBS*//BLYP-D3/DZP. (*TBS*= TZ2P, TZP, DZP, DZ)**

TZ2P

	C60@C240	C60	C240	
BSSE	**-58245.11**	-11402.20	-46928.31	Kcal mol^{-1}
Regular – disp	**-58245.11**	**-11399.57**	**-46930.14**	Kcal mol^{-1}
E BSSE	**85.40**			Kcal mol^{-1}
E Regular	**84.60**			Kcal mol^{-1}
BSSE correction	0.80			Kcal mol^{-1}

TZP

	C60@C240	C60	C240	
BSSE	**-57982.55**	-11354.60	-46712.33	Kcal mol^{-1}
Regular – disp	**-57982.55**	**-11350.56**	**-46715.28**	Kcal mol^{-1}
E BSSE	**84.38**			Kcal mol^{-1}
E Regular	**83.29**			Kcal mol^{-1}
BSSE correction	1.09			Kcal mol^{-1}

DZP

	C60@C240	C60	C240	
BSSE	**-57451.72**	-11258.23	-46267.40	Kcal mol^{-1}
Regular – disp	**-57451.72**	**-11227.69**	**-46214.10**	Kcal mol^{-1}
E BSSE	**73.91**			Kcal mol^{-1}
E Regular	**-9.93**			Kcal mol^{-1}
BSSE correction	83.84			Kcal mol^{-1}

DZ

	C60@C240	C60	C240	
BSSE	**-55143.83**	-10793.32	-44406.30	Kcal mol^{-1}
Regular – disp	**-55143.83**	**-10734.56**	**-44357.94**	Kcal mol^{-1}
E BSSE	**55.79**			Kcal mol^{-1}
E Regular	**-51.33**			Kcal mol^{-1}
BSSE correction	107.12			Kcal mol^{-1}

Table 3 **Interaction energies for the encapsulations of C_{60} into C_{180} and C_{240} calculated with and without dispersion term and TZ2P basis set. For each geometry the level of theory for the single point energy is indicated in square brackets.**

		TZ2P kcal mol^{-1}
C_{60}		
Geometry BLYP		
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [disp]	-11485.98
Geometry BLYP-D3		
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [nodisp]	-11399.72
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [disp]	-11485.98
C_{180}		
Geometry BLYP		
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [disp]	-35309.16
Geometry BLYP-D3		
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [nodisp]	-35047.37
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [disp]	-35309.18
C_{240}		
Geometry BLYP		
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [disp]	
Geometry BLYP-D3		
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [nodisp]	-46932.36
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [disp]	-47282.92
$C_{60}@C_{180}$		
Geometry BLYP		
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [disp]	-46526.76
	ΔE	**268.38**
Geometry BLYP-D3		
Electronic Internal Energy [E]	(kcal mol^{-1}) [disp]	-46527.56
	ΔE	**267.60**
Electronic Internal Energy [E] ***[C_{3i} Symmetry]***	(kcal mol^{-1}) [disp]	-46530.03
	ΔE	**265.13**
Electronic Internal Energy [E] ***[I_h Symmetry]***	(kcal mol^{-1}) [disp]	-46479.55
	ΔE	**315.61**
$C_{60}@C_{240}$		
Geometry BLYP-D3		
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [no_disp]	-58255.90
	ΔE	**76.18**
♦Electronic Internal Energy [E]	(kcal mol^{-1}) [disp]	-58917.65
	ΔE	**-148.75**

Fig. 1 Calculated IR spectra (BLYP-D3/DZP) for $C_{60}@C_{180}$. C_{3i} symmetry.

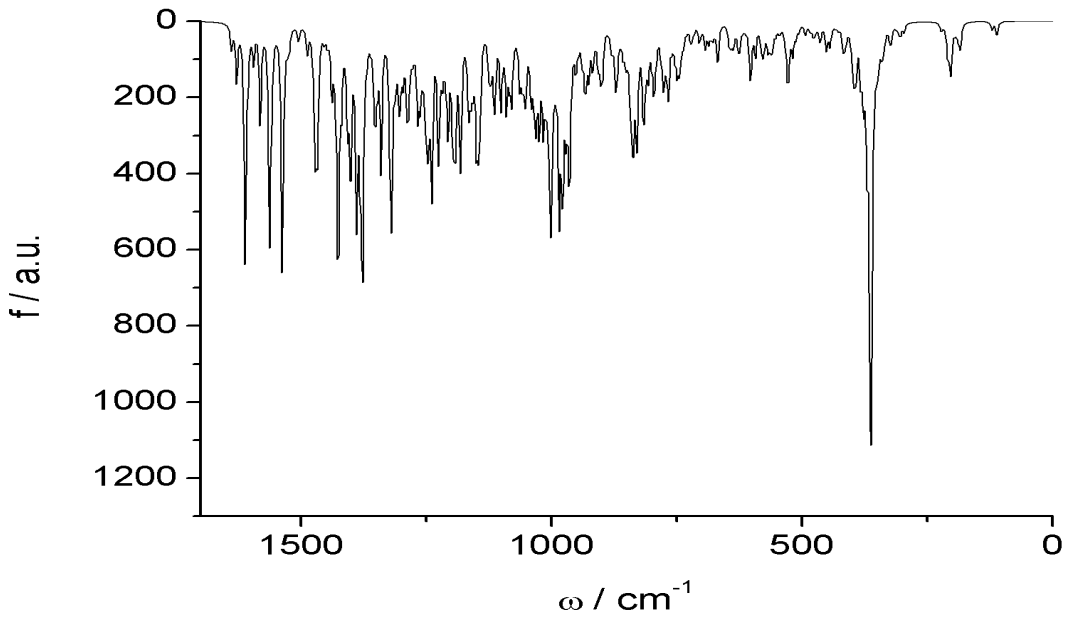

Fig. 2 Calculated IR spectra (BLYP-D3/DZP) for $C_{60}@C_{180}$. I_h symmetry. Top to bottom: C_{60}, C_{180}, $C_{60}@C_{180}$.

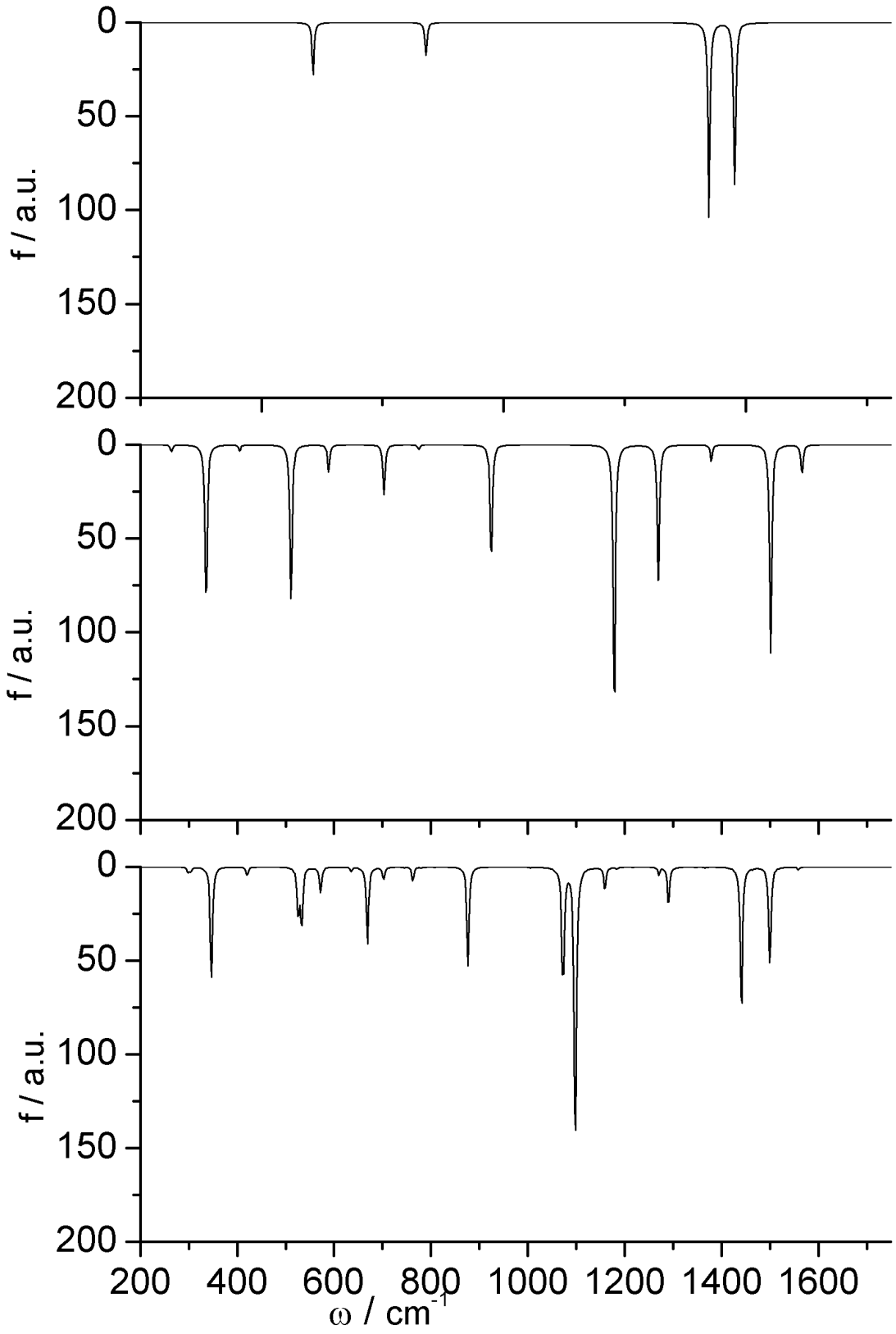

Fig. 3 C_{60} – HOMO level (Symmetry: I_h. Five degenerate orbitals. Isosurface 0.01)

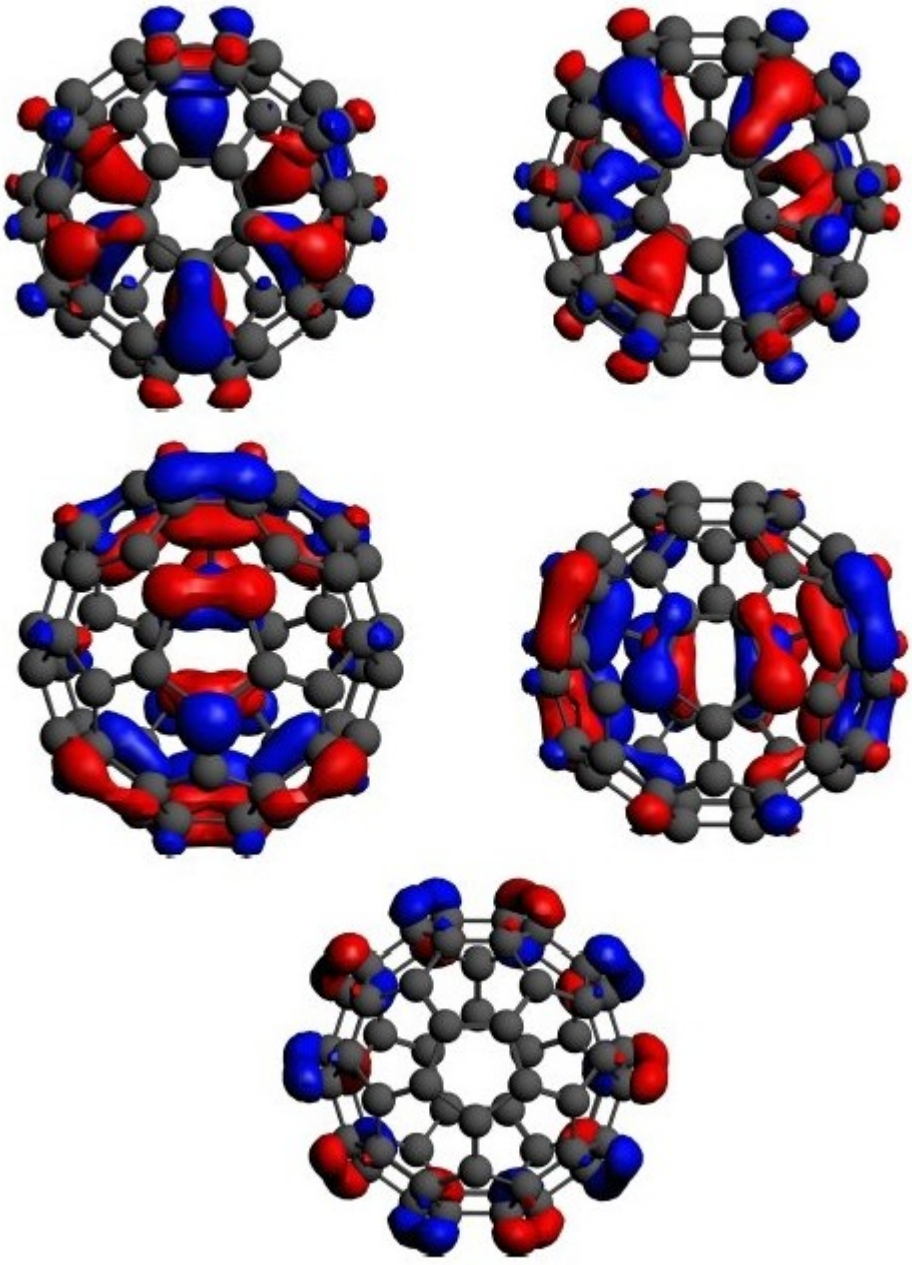

Fig. 4 C_{60} – LUMO level (Symmetry: I_h. Three degenerate orbitals. Isosurface 0.01)

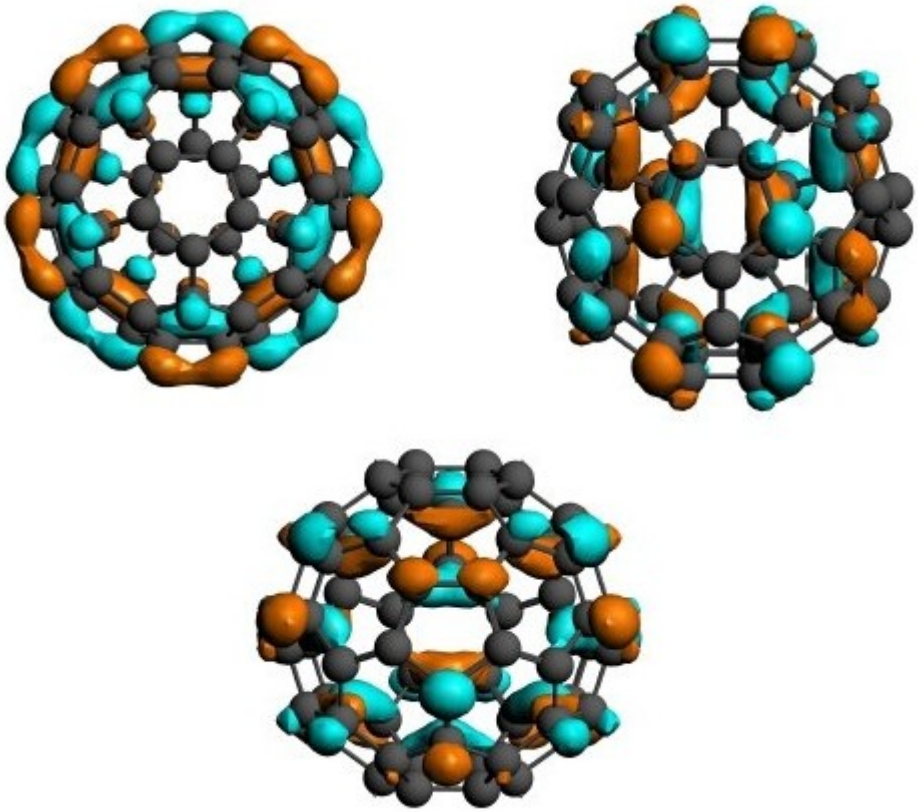

Fig. 5 C_{180} – HOMO level (Symmetry: I_h. Five degenerate orbitals. Isosurface 0.01)

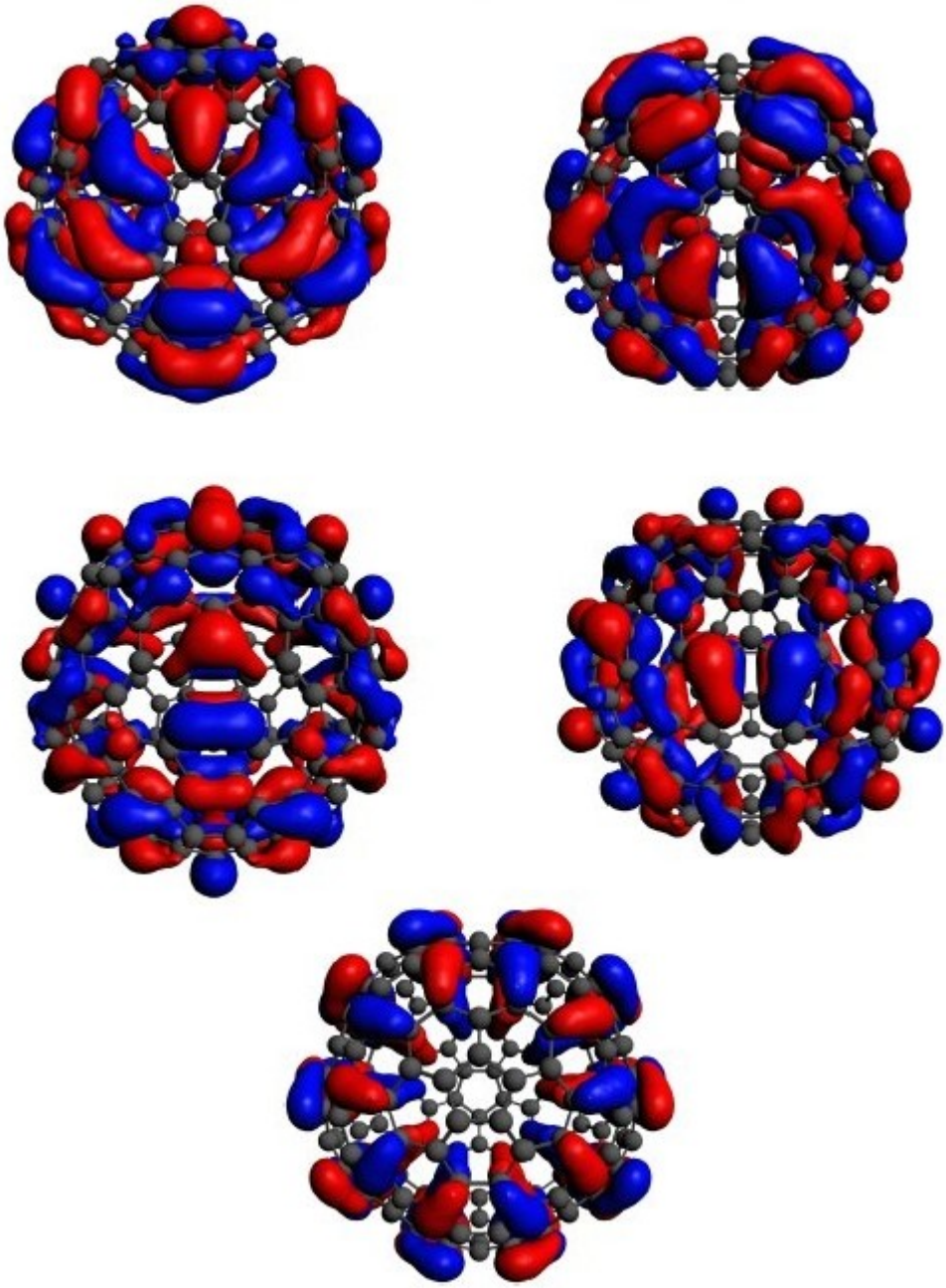

Fig.6 C_{180} – LUMO level (Symmetry: I_h. Three degenerate orbitals. Isosurface 0.01)

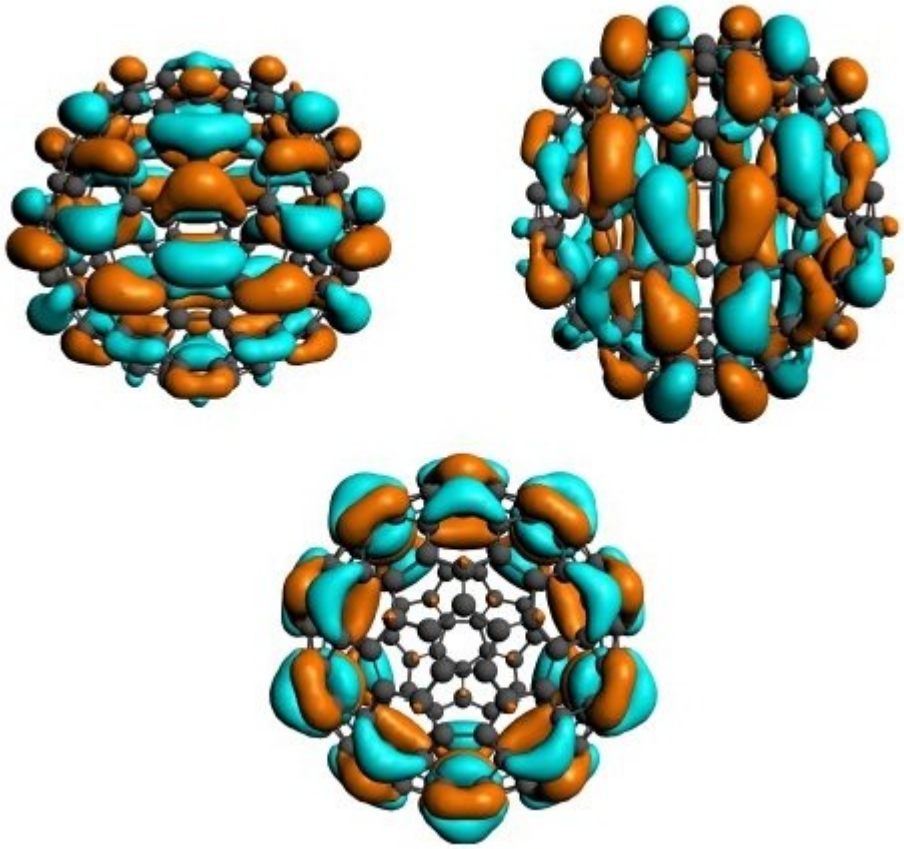

Fig. 7 C_{240} – HOMO level (Symmetry: I_h. Five degenerate orbitals. Isosurface 0.01)

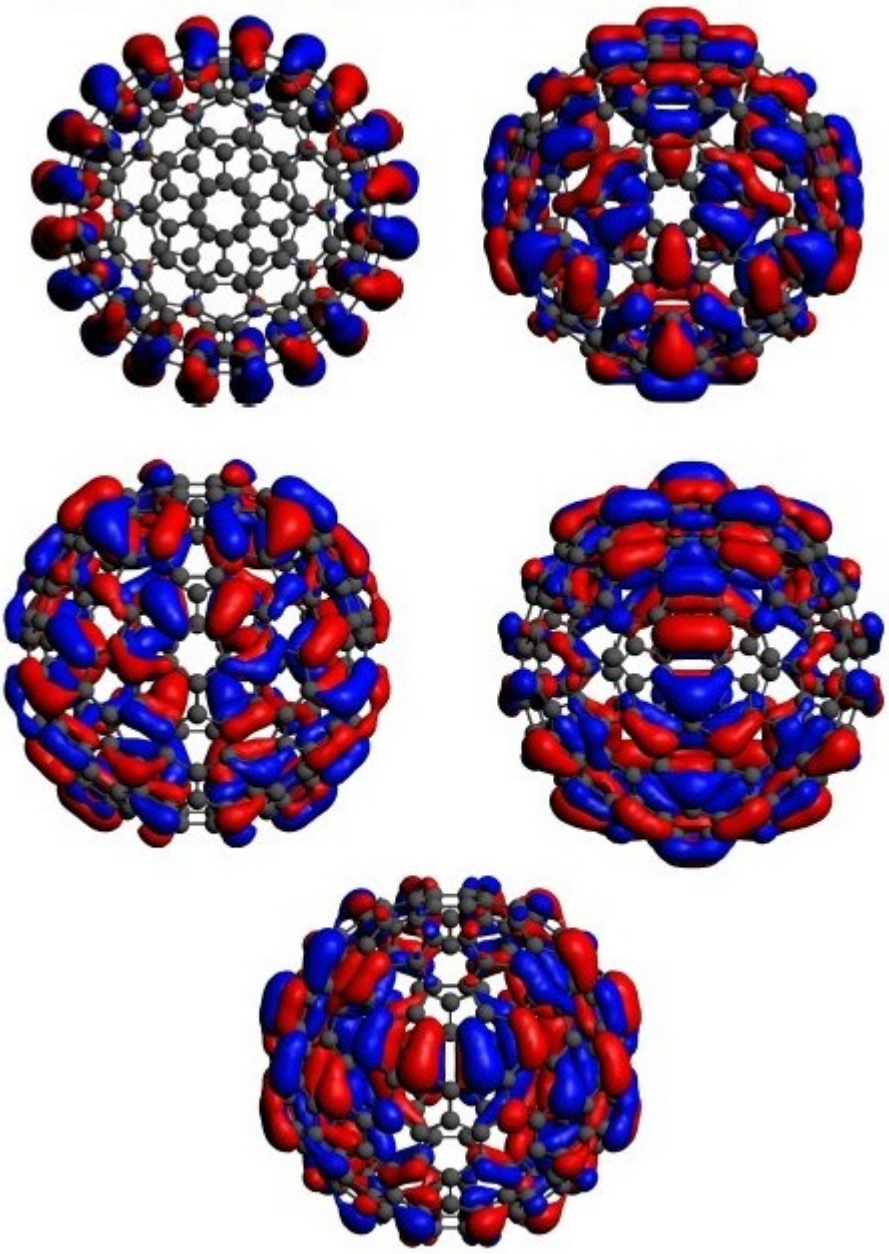

Fig. 8 C_{240} – LUMO level (Symmetry: I_h. Three degenerate orbitals. Isosurface 0.01)

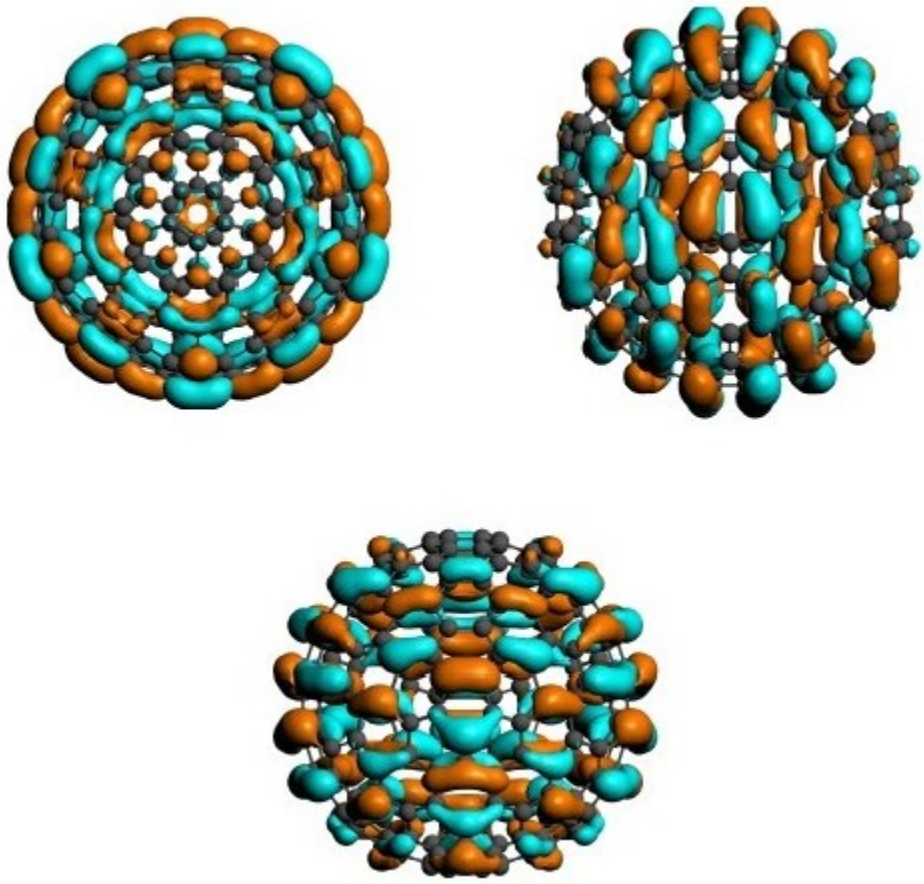

Fig. 9 $C_{60}@C_{180}$ – From top to bottom: HOMO level (two degenerate orbitals); HOMO-1 level (two degenerate orbitals); HOMO -2 level (one orbital) (Symmetry: C_{3i}. Isosurface 0.01)

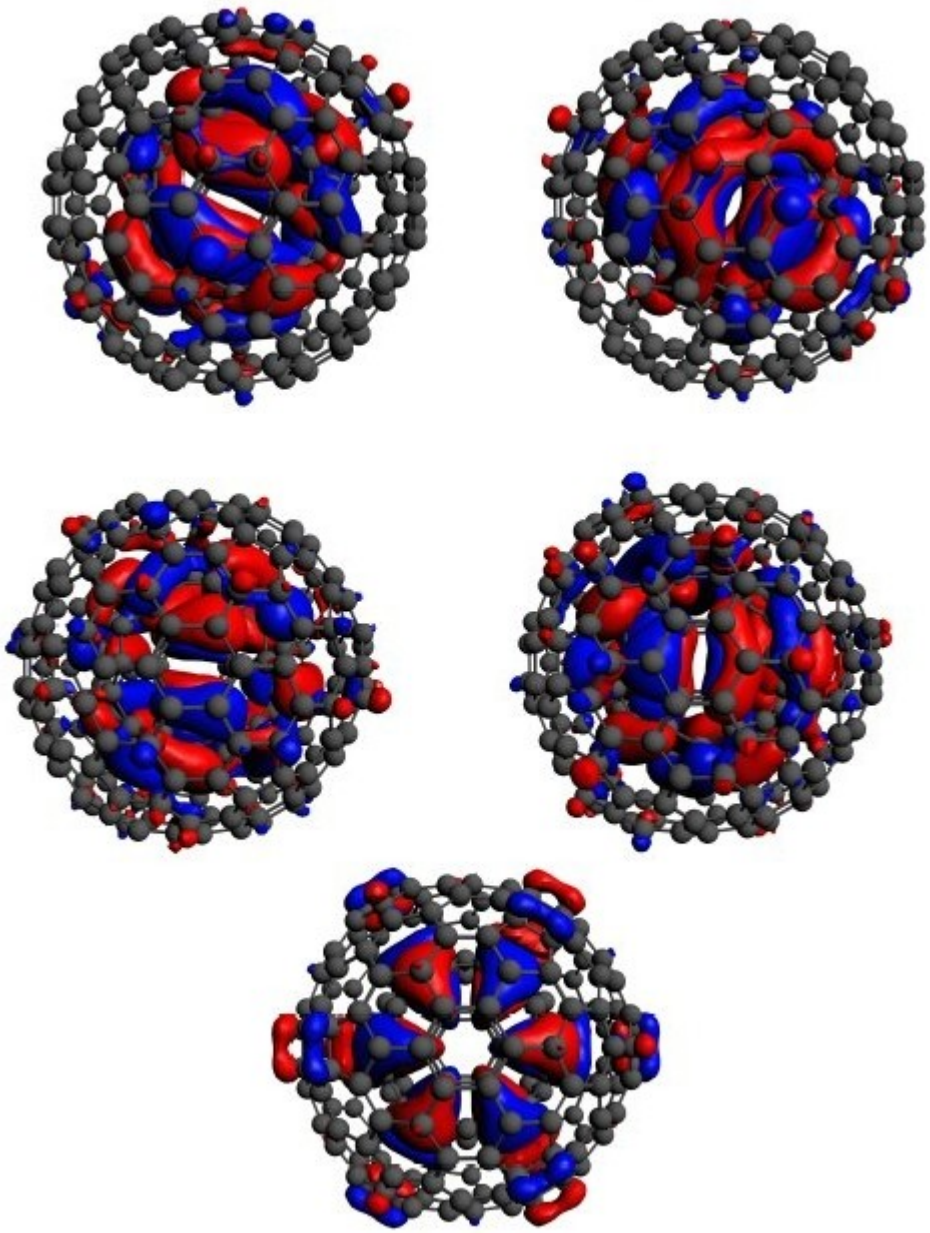

Fig. 10 $C_{60}@C_{180}$ – From bottom to top LUMO level (one orbital); LUMO+1 level (two degenerate orbitals) (Symmetry: C_{3i}. Isosurface 0.01)

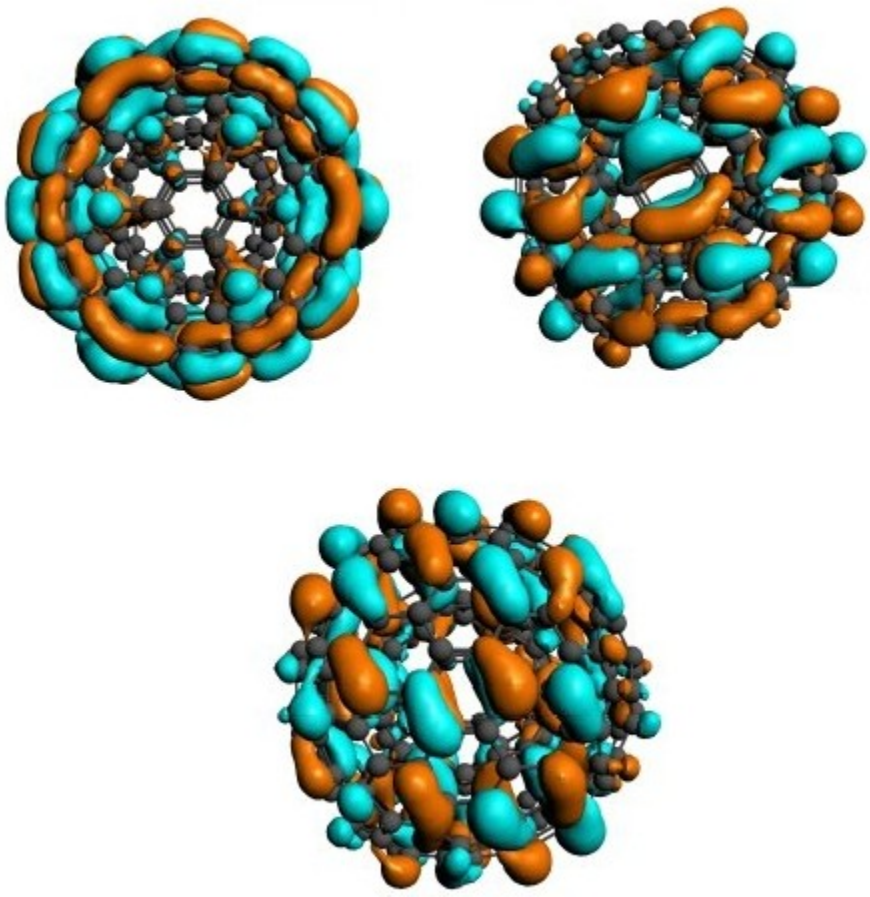

Fig. 11 $C_{60}@C_{240}$ – HOMO level (Symmetry: I_h. Five degenerate orbitals. Isosurface 0.01)

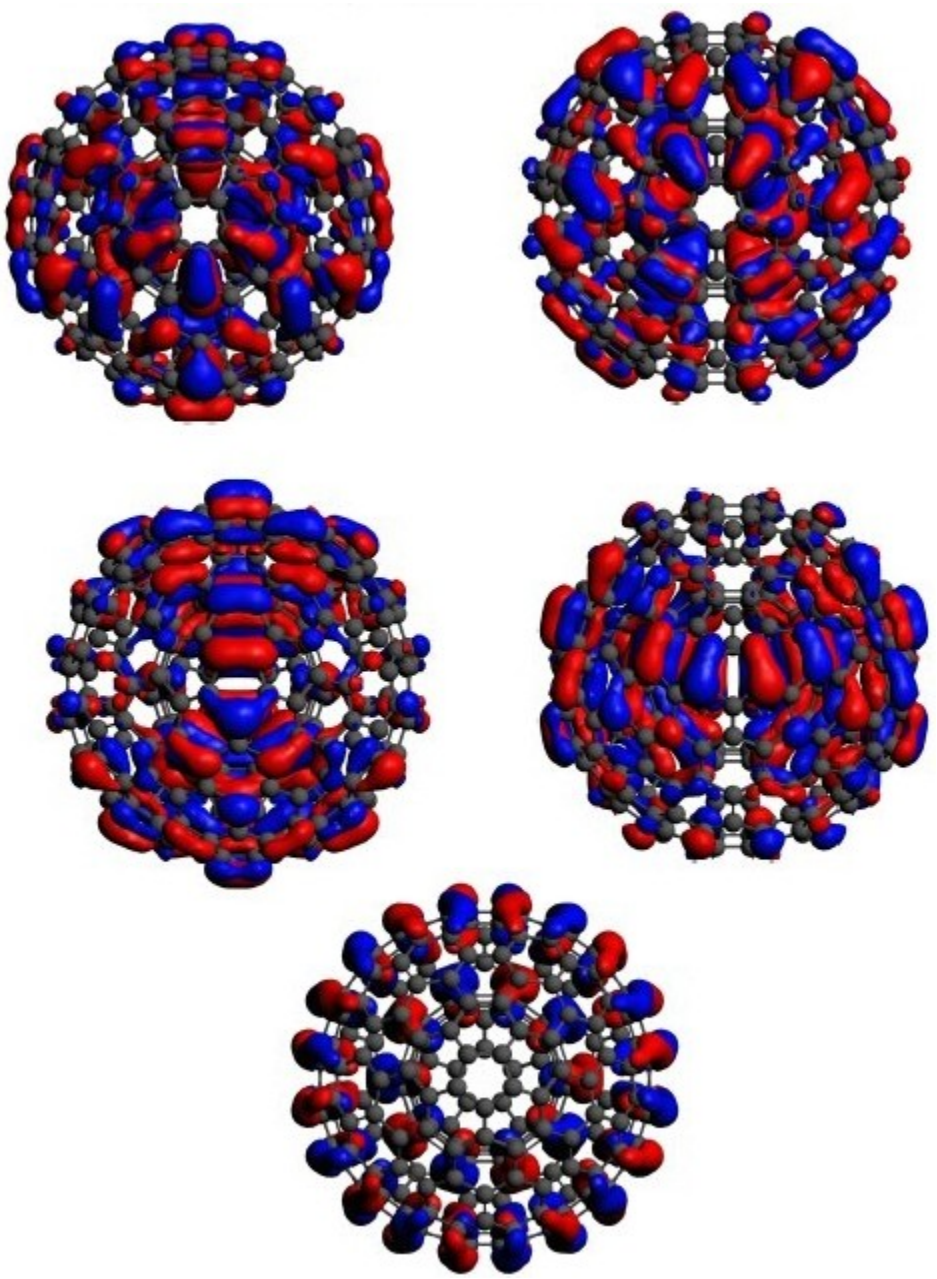

Fig. 12 $C_{60}@C_{240}$ – LUMO level (Symmetry: I_h. Three degenerate orbitals. Isosurface 0.01)

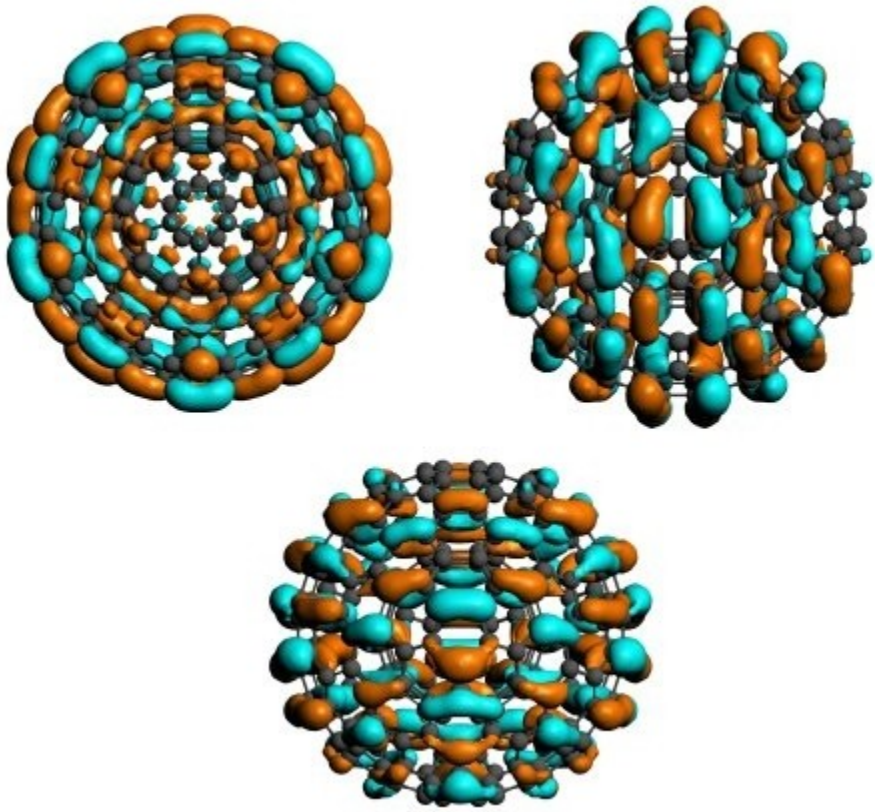

Table 4 **Calculated excitation energies B-P86 with DZP,TZP and TZ2P compared with calculated 6-31G+z/TZVP[a] and experimental data.**

C_{60} (B-P86)									
This work						REF.[a]		EXP[b]	
DZP		TZP		TZ2P		6-31G+s , TZVP aux[a]			
E_{calc}	f	E_{calc}	f	E_{calc}	f	E_{calc}	f	E_{exp}	f_{obs}
2.78	0.003	**2.77**	0.003	**2.78**	0.003	**2.82**	0.002	**3.04**	0.015
								3.30	
3.42	0.318	**3.39**	0.304	**3.39**	0.307	**3.51**	0.139	**3.78**	0.370
								4.06	
4.35	0.887	**4.28**	0.890	**4.29**	0.906	**4.48**	0.369	**4.35**	0.100
4.93	0.006	**4.84**	0.006	**4.86**	0.006				
5.06	0.015	**4.94**	0.011	**4.90**	0.006	**5.02**	0.000	**4.84**	2.270
						5.10	0.003		
5.37	0.781	**5.27**	0.814	**5.29**	0.822				
		5.70	0.014						
						5.47	0.765	**5.46**	0.220
5.83	0.046	**5.84**	0.876	**5.84**	0.871	**5.98**	0.812	**5.88**	3.09
5.92	0.705								
6.21	0.019	**6.25**	0.019	**6.26**	0.019				
6.43	0.020	**6.37**	0.024	**6.38**	0.023			**6.36**	
6.51	0.076	**6.44**	0.098	**6.45**	0.097				
6.64	0.172	**6.59**	0.156	**6.60**	0.154				

[a] **Rudiger Bauernschmitt et al. JACS 1998, 120, 5052-5029**
[b] **Koudoumas, E.; Ruth, A.; Couris, S.; Leach, S. Mol. Phys. 1996,88, 125.**

Table 5 **Calculated excitation energies BLYP with DZP, TZP and TZ2P *vs.* B-P86 with DZP, TZP and TZ2P.**

C_{60} (BLYP *vs* B-P86)											
BLYP						B-P86					
DZP		TZP		TZ2P		DZP		TZP		TZ2P	
Ecalc	f	Ecalc	f	Ecalc	f	Ecalc	f	Ecalc	f	Ecalc	f
2.78	0.003	**2.77**	0.003	**2.78**	0.003	**2.78**	0.003	**2.77**	0.003	**2.78**	0.003
3.42	0.323	**3.39**	0.304	**3.39**	0.307	**3.42**	0.318	**3.39**	0.304	**3.39**	0.307
4.35	0.880	**4.28**	0.890	**4.29**	0.906	**4.35**	0.887	**4.28**	0.890	**4.29**	0.906
4.93	0.000	**4.84**	0.006	**4.86**	0.006	**4.93**	0.006	**4.84**	0.006	**4.86**	0.006
5.06	0.016	**4.94**	0.011	**4.90**	0.006	**5.06**	0.015	**4.94**	0.011	**4.90**	0.006
5.37	0.781	**5.27**	0.814	**5.29**	0.822	**5.37**	0.781	**5.27**	0.814	**5.29**	0.822
		5.70	0.014					**5.70**	0.014		
5.83	0.046	**5.84**	0.876	**5.84**	0.871	**5.83**	0.046	**5.84**	0.876	**5.84**	0.871
5.92	0.705					**5.92**	0.705				
6.21	0.019	**6.25**	0.019	**6.26**	0.019	**6.21**	0.019	**6.25**	0.019	**6.26**	0.019
6.43	0.020	**6.37**	0.024	**6.38**	0.023	**6.43**	0.020	**6.37**	0.024	**6.38**	0.023
6.51	0.076	**6.44**	0.098	**6.45**	0.097	**6.51**	0.076	**6.44**	0.098	**6.45**	0.097
6.64	0.172	**6.59**	0.156	**6.60**	0.154	**6.64**	0.172	**6.59**	0.156	**6.60**	0.154

Table 6 **Calculated excitation energies (eV) and oscillators strength for C_{60}, C_{180},C_{240}, $C_{60}@C_{180}$, $C_{60}@C_{240}$. (BLYP/TZP).**

C60		C180		C240		C60@C180		C60@C240	
E_{calcd}	f	E_{calcd}	f	E_{calcd}	f	E_{calcd}	f	E_{calcd}	f
2.77	0.003	1.76	0.001	1.57	0.004	0.69	0.005	1.47	0.015
3.39	0.304	2.14	0.957	1.95	0.337	0.72	0.002	1.63	0.045
4.28	0.890	2.67	0.012	2.33	0.405	0.77	0.010	1.83	0.540
4.84	0.006	2.92	0.784	2.37	0.825	1.40	0.010	2.05	0.159
4.94	0.011	3.07	0.179	2.83	0.149	1.47	0.074	2.20	0.450
5.27	0.814	3.12	0.119	2.86	0.320	1.48	0.004	2.40	0.370
5.70	0.014	3.29	0.004	3.02	0.012	1.49	0.006	2.48	0.103
5.84	0.876	3.32	0.018	3.14	0.015	1.56	0.001	2.59	0.093
6.25	0.019	3.36	0.304	3.16	0.007	1.59	0.004	2.72	0.270
6.37	0.024	3.57	0.033	3.27	0.003	1.64	0.003	2.73	0.015
6.44	0.098	3.60	0.018	3.31	0.056	1.71	0.001	2.86	0.037
6.59	0.156	3.65	0.014	3.37	0.164	1.73	0.002	2.92	0.135
		3.78	0.391	3.41	0.019	1.76	0.002	3.02	0.081
		3.87	0.051	3.53	0.028	1.80	0.005	3.04	0.047
		3.92	0.044	3.55	0.424	1.81	0.001	3.11	0.025
		3.94	0.014	3.60	0.001	1.93	0.011	3.13	0.004
		4.04	0.092	3.63	0.068	1.95	0.013	3.26	0.048
		4.31	0.037	3.71	0.001	1.97	0.017	3.28	0.150
		4.37	0.559	3.85	0.111	2.00	0.296	3.31	0.028
		4.40	0.018	3.86	0.100	2.01	0.024	3.34	0.220
		4.41	0.001	3.89	0.020	2.03	0.008	3.39	0.200
		4.43	0.004	3.96	0.004	2.04	0.043	3.47	0.002
		4.47	0.032	4.02	0.082	2.06	0.158	3.53	0.003
		4.49	0.055	4.19	0.274	2.09	0.002	3.55	0.007
		4.50	0.001	4.26	0.017	2.11	0.001	3.57	0.210
		4.52	0.033	4.32	0.231	2.12	0.010	3.62	0.034
		4.55	0.044	4.34	0.010	2.13	0.007	3.65	0.008
		4.62	0.130	4.43	0.003	2.14	0.007	3.66	0.064
		4.67	0.611	4.55	1.348	2.18	0.003	3.72	0.003
		4.72	0.091	4.68	0.248	2.22	0.003	3.78	0.017
		4.80	0.260	4.71	0.120	2.51	0.001	3.81	0.001
		4.93	0.150	4.81	0.002	2.52	0.002	3.84	0.039
		5.00	0.111	4.82	0.021	2.55	0.003	3.86	0.012
		5.07	0.137	4.85	0.007	2.56	0.002	3.88	0.037
		5.09	0.151			2.57	0.003	3.89	0.022
		5.11	0.387			2.58	0.007	3.91	0.003
		5.22	0.037			2.60	0.001	3.94	0.001
		5.27	0.007			2.67	0.001	3.97	0.003
		5.32	0.003			2.68	0.005	4.03	0.027

5.36	0.020	2.69	0.004	4.05	0.029
5.37	0.059	2.70	0.014	4.11	0.002
5.40	0.066	2.71	0.010	4.14	0.136
5.43	0.032	2.72	0.002	4.22	0.052
5.47	0.449	2.73	0.003	4.26	0.002
5.53	0.003	2.74	0.001	4.27	0.012
		2.75	0.018	4.33	0.095
		2.77	0.020	4.35	0.114
		2.79	0.115	4.44	0.279
		2.80	0.036	4.45	0.007
		2.81	0.038	4.53	0.236
		2.82	0.052	4.54	0.800
		2.83	0.002	4.63	0.004
		2.84	0.002	4.68	0.125
		2.85	0.016	4.72	0.028
		2.86	0.001	4.72	0.003
		2.87	0.031	4.78	0.016
		2.90	0.020	4.79	0.024
		2.91	0.009	4.80	0.011
		2.92	0.018	4.83	0.011
		2.93	0.004	4.87	0.001
		2.94	0.024	4.88	0.053
		2.95	0.020	4.89	0.017
		2.96	0.033	4.90	0.002
		2.97	0.012		
		2.98	0.005		
		2.99	0.025		
		3.00	0.007		
		3.01	0.004		
		3.04	0.006		
		3.05	0.050		
		3.06	0.022		
		3.08	0.003		
		3.09	0.004		
		3.11	0.016		
		3.12	0.006		
		3.13	0.006		
		3.14	0.006		
		3.15	0.001		
		3.16	0.001		
		3.17	0.001		

Table 7 Calculated shielding constants in ppm (BLYP/TZP//BLYP-D3/TZP).

C60	C180	C240	C60@C180				C60@C240
29.47	36.30	43.62	**49.90**	28.79	33.37	32.83	**40.48**
29.47	36.30	43.07	**48.67**	32.30	33.20	33.37	**40.48**
29.46	36.30	43.66	**45.09**	31.90	27.59	31.54	**40.48**
29.47	37.21	43.16	**49.91**	27.06	28.74	30.79	**40.48**
	43.61	43.59	**52.28**	28.46	35.96	36.04	43.55
	37.21	36.10	**58.48**	29.64	32.27	30.77	43.23
	43.61	36.12	**44.92**	27.75	28.80	28.80	43.55
	37.21	43.05	**59.03**	33.01	33.46	35.50	43.24
	37.21	36.11	**46.82**	33.41	32.99	31.90	43.56
	43.61	43.58	**51.65**	28.76	28.69	27.05	36.16
	36.30	43.06	**52.27**	35.48	29.72	35.47	36.17
	43.61	43.62	**58.47**	28.66	31.53	29.43	43.23
		36.11	**51.64**	32.78	33.38	33.24	36.17
		43.58	**48.67**	27.60	33.36	30.31	43.55
			45.06	32.01	27.29	31.26	43.23
			44.95	27.27	33.36	27.69	43.56
			45.00	29.41	29.74	29.49	36.18
			46.76	33.83	27.61	33.02	43.56
			51.72	27.78	33.40	33.93	
			50.15	29.45	28.82	28.71	
			48.66	27.07	30.27	28.81	
			46.79	28.51	31.25	35.34	
			59.08	32.02	31.89	27.67	
			52.26	33.87	32.30	28.80	
			50.07	31.52	35.32	33.16	
			50.10	30.72	31.28	29.48	
			50.18	33.36	27.65	27.31	
			58.53	32.87	35.34	36.00	
			59.04	30.23	32.25	28.73	
			44.91	29.72	28.61	27.42	

Table 8 NMR test. Calculated $\delta^{13}C$ (wrt benzene) for C_{60}, C_{180}, C_{240}, $C_{60}@C_{180}$, $C_{60}@C_{240}$ and relative $\Delta\delta^{13}C$ values (ppm) obtained with different basis set and different geometries. Averaged values.

		$\delta^{13}C$		
	GEOM	***DZ***	***DZP***	***TZP***
C_{60}	***BLYP/DZP***	21.4	19.4	16.8
	BLYP-D3/DZP	21.3	19.3	16.8
	BLYP/TZP	21.3	19.3	16.8
	BLYP-D3/TZP	21.3	19.3	16.8
C_{180}	***BLYP/DZP***	11.3	10.0	7.2
	BLYP-D3/DZP	11.1	9.9	7.0
	BLYP/TZP	11.4	10.1	7.3
	BLYP-D3/TZP	11.3	10.0	7.2
C_{240}	***BLYP/DZP***	9.0	7.7	4.9
	BLYP-D3/DZP	8.8	7.6	4.7
	BLYP/TZP	9.1	7.9	5.0
	BLYP-D3/TZP	9.0	7.7	4.9
$C_{60}@C_{180}$	***BLYP/DZP***	n.c [a]	n.c.	-4.0 (-20.7) @ 15.8 (+8.7)
	BLYP-D3/DZP	n.c.	n.c.	n.c.
	BLYP/TZP	n.c.	n.c.	n.c.
	BLYP-D3/TZP	0.8 (-20.5) @ 18.2 (+6.9)	-2.8 (-22.1) @ 18.2 (+8.2)	-4.1 (-20.9) @ 16.0 (+8.8)
$C_{60}@C_{240}$	***BLYP/DZP***	9.8 (-11.6) @ 8.7 (-0.3)	7.5 (-11.9) @ 8.0 (+0.3)	4.9 (-11.9) @ 5.1 (+0.2)
	BLYP-D3/DZP	11.4 (-9.9) @ 7.9 (-0.9)	9.1 (-10.2) @ 7.2 (-0.4)	6.7 (-10.1) @ 4.0 (-0.7)
	BLYP/TZP	8.8 (-12.5) @ 9.3 (+0.2)	6.6 (-12.7) @ 9.5 (+1.6)	4.0 (-12.8) @ 5.7 (+0.7)
	BLYP-D3/TZP	10.6 (-10.7) @ 8.5 (-0.3)	8.2 (-11.2) @ 7.7 (0.0)	4.8 (-11.1) @ 4.8 (-0.1)

[a] **n.c. = not calculated.**

Table 9 **Optimized structures cartesian coordinates, BLYP-D3/DZP, of C60, C180, C240, C60@C180 (Symmetry: *Ih*, D_{5d}, C_{3i}, C_i) and C60@C240.**

C60 (BLYP-D3/DZP; Symmetry: I_h)

C	-3.489600	-0.367958	0.595367
C	-1.428295	3.205102	0.595367
C	3.489600	-0.367958	0.595367
C	2.606865	2.348820	0.595367
C	0.728397	-3.432512	0.595367
C	3.039426	-1.753451	0.595367
C	-3.039426	-1.753451	0.595367
C	-0.728397	-3.432512	0.595367
C	-2.606865	2.348820	0.595367
C	1.428295	3.205102	0.595367
C	1.428295	-1.965880	-2.600469
C	-1.428295	-1.965880	-2.600469
C	-2.311030	0.750899	-2.600469
C	0.000000	2.429961	-2.600469
C	2.311030	0.750899	-2.600469
C	-2.606866	-1.582937	-1.834589
C	-2.311029	1.990122	-1.834589
C	1.178571	2.812900	-1.834589
C	3.039426	-0.251654	-1.834589
C	0.699897	-2.968431	-1.834589
C	-0.728397	1.002553	3.336387
C	0.728397	1.002553	3.336387
C	1.178572	-0.382941	3.336387
C	0.000000	-1.239224	3.336387
C	-1.178572	-0.382941	3.336387
C	-3.039426	0.251654	1.834589
C	-0.699897	2.968431	1.834589
C	2.606866	1.582937	1.834589
C	2.311029	-1.990122	1.834589
C	-1.178571	-2.812900	1.834589
C	3.039426	0.251654	1.834589
C	1.178571	-2.812900	1.834589
C	-2.311029	-1.990122	1.834589
C	-2.606866	1.582937	1.834589
C	0.699897	2.968431	1.834589
C	2.606866	-1.582937	-1.834589
C	-0.699897	-2.968431	-1.834589
C	-3.039426	-0.251654	-1.834589
C	-1.178571	2.812900	-1.834589
C	2.311029	1.990122	-1.834589
C	0.000000	1.239224	-3.336387
C	1.178572	0.382941	-3.336387
C	0.728397	-1.002553	-3.336387
C	-0.728397	-1.002553	-3.336387
C	-1.178572	0.382941	-3.336387
C	-3.039426	1.753451	-0.595367
C	0.728397	3.432512	-0.595367
C	3.489600	0.367958	-0.595367
C	1.428295	-3.205102	-0.595367
C	-2.606865	-2.348820	-0.595367
C	0.000000	-2.429961	2.600469
C	-2.311030	-0.750899	2.600469
C	-1.428295	1.965880	2.600469
C	1.428295	1.965880	2.600469
C	2.311030	-0.750899	2.600469
C	2.606865	-2.348820	-0.595367
C	-1.428295	-3.205102	-0.595367
C	-3.489600	0.367958	-0.595367
C	-0.728397	3.432512	-0.595367
C	3.039426	1.753451	-0.595367

C180 (BLYP-D3/DZP; Symmetry: I_h)

C	0.713863	-5.103556	3.650273
C	-0.713863	-5.103556	3.650273
C	-1.155051	-5.710827	2.435810
C	0.000000	-6.086148	1.685236
C	1.155051	-5.710827	2.435810
C	0.726469	-3.150066	5.096915
C	-0.726469	-3.150066	5.096915
C	-1.446700	-4.097095	4.274780
C	1.446700	-4.097095	4.274780
C	-3.220409	-4.432513	2.532138
C	-2.340832	-5.327766	1.813532
C	-2.771418	-3.814530	3.768063
C	3.220409	-4.432513	2.532138
C	2.771418	-3.814530	3.768063
C	2.340832	-5.327766	1.813532
C	-1.263838	-5.889525	-0.381928
C	-2.439310	-5.507591	0.381928
C	0.000000	-6.088409	0.292369
C	2.439310	-5.507591	0.381928
C	1.263838	-5.889525	-0.381928
C	0.713859	-0.982542	6.197240
C	-0.713859	-0.982542	6.197240
C	-1.446701	-1.991213	5.576300
C	1.446701	-1.991213	5.576300
C	-4.633175	-2.256010	3.650273
C	-5.074389	-2.863261	2.435810
C	-3.449514	-2.641965	4.274780
C	-2.771399	-1.664337	5.096915
C	-3.577348	-4.923797	-1.685236
C	-2.422284	-5.299078	-2.435810
C	-1.237810	-5.686160	-1.813532
C	-3.578677	-4.925626	-0.292369
C	0.000000	-5.478887	-2.532138
C	-4.484242	-4.021861	0.381928
C	-4.343650	-3.872634	1.813532
C	3.577348	-4.923797	-1.685236
C	2.422284	-5.299078	-2.435810
C	1.237810	-5.686160	-1.813532
C	3.578677	-4.925626	-0.292369
C	4.484242	-4.021861	0.381928
C	4.633175	-2.256010	3.650273
C	5.074389	-2.863261	2.435810
C	4.343650	-3.872634	1.813532
C	3.449514	-2.641965	4.274780
C	2.771399	-1.664337	5.096915
C	-4.343623	0.109821	4.274780
C	-5.074366	-0.898161	3.650273
C	-3.220382	-0.282511	5.096915
C	-2.340812	0.760576	5.576300
C	-1.155048	0.375298	6.197240
C	-5.788250	-0.666224	2.435810
C	-5.788271	-1.880723	1.685236
C	1.155048	0.375298	6.197240
C	0.000000	1.214489	6.197240
C	-5.025355	-2.934347	-1.813532
C	-4.291196	-3.941235	-2.435810
C	-5.210724	-3.021945	-0.381928
C	-5.790421	-1.881422	0.292369
C	1.237807	-4.164968	-4.274780
C	2.422268	-4.548462	-3.650273
C	0.000000	-4.715019	-3.768063
C	-1.237807	-4.164968	-4.274780
C	-2.422268	-4.548462	-3.650273
C	-3.577323	-3.709266	-3.650273
C	5.790421	-1.881422	0.292369
C	5.788271	-1.880723	1.685236
C	5.210724	-3.021945	-0.381928
C	5.025355	-2.934347	-1.813532
C	4.291196	-3.941235	-2.435810
C	3.577323	-3.709266	-3.650273
C	2.340812	0.760576	5.576300
C	3.220382	-0.282511	5.096915
C	4.343623	0.109821	4.274780
C	5.074366	-0.898161	3.650273
C	5.788250	-0.666224	2.435810
C	-1.263836	2.975465	5.096915
C	-2.439288	2.121449	5.096915
C	0.000000	2.461275	5.576300
C	-2.422268	4.548462	3.650273
C	-3.578616	2.464270	4.274780
C	-1.237807	4.164968	4.274780
C	0.000000	4.715019	3.768063
C	0.000000	5.478887	2.532138
C	3.577323	3.709266	3.650273
C	2.422268	4.548462	3.650273
C	1.237807	4.164968	4.274780
C	1.263836	2.975465	5.096915
C	2.439288	2.121449	5.096915
C	-5.790421	1.881422	-0.292369
C	-5.788271	1.880723	-1.685236
C	-5.790364	-0.579893	-1.813532
C	-5.991819	-0.617982	-0.381928
C	-5.991819	0.617982	0.381928
C	-5.790364	0.579893	1.813532
C	-5.210724	3.021945	0.381928
C	-4.484242	4.021861	-0.381928
C	-3.577323	3.709266	3.650273
C	-4.291196	3.941235	2.435810
C	-5.025355	2.934347	1.813532
C	-5.210731	1.693069	2.532138
C	-4.484249	1.457021	3.768063
C	-2.340812	-0.760576	-5.576300
C	-1.155048	-0.375298	-6.197240
C	0.000000	-2.461275	-5.576300
C	-1.263836	-2.975465	-5.096915
C	-2.439288	-2.121449	-5.096915
C	-3.578616	-2.464270	-4.274780
C	-3.220382	0.282511	-5.096915
C	-5.788250	0.666224	-2.435810
C	-5.074366	0.898161	-3.650273
C	-4.343623	-0.109821	-4.274780
C	-4.484249	-1.457021	-3.768063
C	-5.210731	-1.693069	-2.532138
C	4.343623	-0.109821	-4.274780
C	5.074366	0.898161	-3.650273
C	5.788250	0.666224	-2.435810
C	5.790364	-0.579893	-1.813532
C	5.210731	-1.693069	-2.532138
C	4.484249	-1.457021	-3.768063
C	3.578616	-2.464270	-4.274780
C	3.220382	0.282511	-5.096915
C	2.771399	1.664337	-5.096915
C	0.000000	-1.214489	-6.197240
C	1.155048	-0.375298	-6.197240
C	2.340812	-0.760576	-5.576300
C	2.439288	-2.121449	-5.096915
C	1.263836	-2.975465	-5.096915
C	5.025355	2.934347	1.813532
C	4.291196	3.941235	2.435810
C	3.578616	2.464270	4.274780
C	4.484249	1.457021	3.768063
C	5.210731	1.693069	2.532138
C	5.790364	0.579893	1.813532
C	5.788271	1.880723	-1.685236
C	5.790421	1.881422	-0.292369
C	5.991819	0.617982	0.381928
C	5.991819	-0.617982	-0.381928
C	5.210724	3.021945	0.381928
C	4.484242	4.021861	-0.381928
C	4.633175	2.256010	-3.650273
C	5.074389	2.863261	-2.435810
C	3.449514	2.641965	-4.274780
C	2.771418	3.814530	-3.768063
C	1.446700	4.097095	-4.274780
C	0.713863	5.103556	-3.650273
C	4.343650	3.872634	-1.813532
C	3.220409	4.432513	-2.532138
C	2.340832	5.327766	-1.813532
C	1.155051	5.710827	-2.435810
C	3.577348	4.923797	1.685236
C	2.422284	5.299078	2.435810
C	3.578677	4.925626	0.292369
C	2.439310	5.507591	-0.381928
C	1.237810	5.686160	1.813532
C	1.263838	5.889525	0.381928
C	0.000000	6.088409	-0.292369
C	0.000000	6.086148	-1.685236
C	-2.422284	5.299078	2.435810
C	-3.577348	4.923797	1.685236
C	-1.237810	5.686160	1.813532
C	-1.263838	5.889525	0.381928
C	-3.578677	4.925626	0.292369
C	-2.439310	5.507591	-0.381928
C	-2.340832	5.327766	-1.813532
C	-1.155051	5.710827	-2.435810
C	-5.074389	2.863261	-2.435810
C	-4.633175	2.256010	-3.650273
C	-4.343650	3.872634	-1.813532
C	-3.220409	4.432513	-2.532138
C	-0.713859	0.982542	-6.197240
C	0.713859	0.982542	-6.197240
C	1.446701	1.991213	-5.576300
C	0.726469	3.150066	-5.096915
C	-1.446701	1.991213	-5.576300
C	-0.726469	3.150066	-5.096915
C	-1.446700	4.097095	-4.274780
C	-0.713863	5.103556	-3.650273
C	-2.771399	1.664337	-5.096915
C	-3.449514	2.641965	-4.274780
C	-2.771418	3.814530	-3.768063

C240 (BLYP-D3/DZP; Symmetry: I_h)

C	3.215458	0.288172	6.158774
C	2.341975	-0.760954	6.641911
C	2.431977	-2.123135	6.158774
C	1.267699	-2.969032	6.158774
C	1.267669	-4.180518	5.410023
C	4.602345	-1.495392	5.173044
C	3.584177	-2.497476	5.410023
C	3.584044	-3.721525	4.653286
C	2.431850	-4.558643	4.653286
C	4.367640	-0.086226	5.410023
C	1.447420	1.992203	6.641911
C	0.714578	0.983533	7.257312
C	1.156212	-0.375676	7.257312
C	2.770743	1.656863	6.158774
C	4.646911	2.258614	4.653286
C	3.482813	2.636993	5.410023
C	5.087010	0.904129	4.653286
C	5.656047	-1.837761	4.333009
C	6.049407	0.496762	3.650894
C	6.370452	-0.854223	3.581546
C	-0.719563	3.147132	6.158774
C	-1.447420	1.992203	6.641911
C	-2.770743	1.656863	6.158774
C	-3.215458	0.288172	6.158774
C	-4.367640	-0.086226	5.410023
C	-0.714578	0.983533	7.257312
C	0.719563	3.147132	6.158774
C	6.799163	0.703948	1.272284
C	6.943719	-0.734396	1.188364
C	6.798966	-1.452581	-0.060746
C	6.354284	-2.821169	-0.060746
C	5.914409	-3.426942	-1.272284
C	6.811942	-1.462013	2.365775
C	6.354536	1.315992	2.496468
C	5.914448	2.670443	2.496468
C	3.495630	4.811321	4.333009
C	4.651705	4.435539	3.581546
C	5.186062	3.153863	3.650894
C	2.844405	3.914988	5.173044
C	1.431681	4.127227	5.410023
C	-1.431681	4.127227	5.410023
C	-2.844405	3.914988	5.173044
C	-3.482813	2.636993	5.410023
C	-4.646911	2.258614	4.653286
C	-5.087010	0.904129	4.653286
C	5.185920	4.675554	1.188364
C	4.651627	5.186753	2.365775
C	5.914409	3.426942	1.272284
C	6.354284	2.821169	0.060746
C	6.798966	1.452581	0.060746
C	6.943719	0.734396	-1.188364
C	6.799163	-0.703948	-1.272284
C	6.354536	-1.315992	-2.496468
C	5.914448	-2.670443	-2.496468
C	-0.712095	5.117425	4.653286
C	0.712095	5.117425	4.653286
C	1.396921	5.906836	3.650894
C	2.780992	5.794691	3.581546
C	3.495463	6.026755	2.365775
C	-3.495630	4.811321	4.333009
C	-1.431562	6.683920	1.272284
C	-2.844179	6.376929	1.188364
C	-3.482482	6.017328	-0.060746
C	-4.646673	5.171494	-0.060746
C	-5.086868	4.565954	-1.272284
C	-3.495463	6.026755	2.365775
C	-2.780992	5.794691	3.581546
C	-1.396921	5.906836	3.650894
C	5.655904	3.053377	-3.581546
C	4.602083	3.957641	-3.650894
C	3.584044	3.721525	-4.653286
C	3.584177	2.497476	-5.410023
C	2.431977	2.123135	-6.158774
C	4.367407	4.799762	-2.496468
C	5.086868	4.565954	-1.272284
C	6.049254	3.487277	-1.188364
C	6.370327	2.821166	-2.365775
C	6.811942	1.462013	-2.365775
C	0.719509	6.915073	0.060746
C	-0.719509	6.915073	0.060746
C	-0.712077	6.450187	2.496468
C	0.712077	6.450187	2.496468
C	1.431562	6.683920	1.272284
C	2.844179	6.376929	1.188364
C	3.215242	5.636859	-2.496468
C	2.770551	6.248857	-1.272284
C	3.482482	6.017328	-0.060746
C	4.646673	5.171494	-0.060746
C	1.447275	6.830810	-1.188364
C	0.714549	6.930329	-2.365775
C	2.341818	5.599820	-3.650894
C	2.431850	4.558643	-4.653286
C	1.267669	4.180518	-5.410023
C	1.267699	2.969032	-6.158774
C	1.156164	6.322630	-3.581546
C	-1.447275	6.830810	-1.188364
C	-2.770551	6.248857	-1.272284
C	-3.215242	5.636859	-2.496468
C	-4.367407	4.799762	-2.496468
C	-0.714549	6.930329	-2.365775
C	0.000000	-1.215714	7.257312
C	-1.156212	-0.375676	7.257312
C	0.000000	-2.462499	6.641911
C	-1.267699	-2.969032	6.158774
C	-2.341975	-0.760954	6.641911
C	-2.431977	-2.123135	6.158774
C	6.370327	-2.821166	2.365775
C	5.655904	-3.053377	3.581546
C	6.049254	-3.487277	1.188364
C	5.086868	-4.565954	1.272284
C	4.602083	-3.957641	3.650894
C	4.367407	-4.799762	2.496468
C	5.656047	1.837761	-4.333009
C	6.370452	0.854223	-3.581546
C	4.602345	1.495392	-5.173044
C	4.367640	0.086226	-5.410023
C	6.049407	-0.496762	-3.650894
C	5.087010	-0.904129	-4.653286
C	-1.156164	6.322630	-3.581546
C	0.000000	5.947120	-4.333009
C	-2.341818	5.599820	-3.650894
C	-2.431850	4.558643	-4.653286
C	0.000000	4.839192	-5.173044
C	-1.267669	4.180518	-5.410023
C	-4.651705	4.435539	3.581546
C	-4.651627	5.186753	2.365775
C	-5.186062	3.153863	3.650894
C	-5.914448	2.670443	2.496468
C	-5.185920	4.675554	1.188364
C	-5.914409	3.426942	1.272284
C	0.000000	-5.947120	4.333009
C	1.156164	-6.322630	3.581546
C	2.341818	-5.599820	3.650894
C	0.000000	-4.839192	5.173044
C	-1.156164	-6.322630	3.581546
C	0.714549	-6.930329	2.365775
C	-0.714549	-6.930329	2.365775
C	4.651627	-5.186753	-2.365775
C	4.651705	-4.435539	-3.581546
C	5.186062	-3.153863	-3.650894
C	5.185920	-4.675554	-1.188364
C	3.495463	-6.026755	-2.365775
C	3.495630	-4.811321	-4.333009
C	2.780992	-5.794691	-3.581546
C	3.482813	-2.636993	-5.410023
C	2.770743	-1.656863	-6.158774
C	3.215458	-0.288172	-6.158774
C	4.646911	-2.258614	-4.653286
C	2.844405	-3.914988	-5.173044
C	1.447420	-1.992203	-6.641911
C	0.719563	-3.147132	-6.158774
C	2.770551	-6.248857	1.272284
C	3.482482	-6.017328	0.060746
C	4.646673	-5.171494	0.060746
C	3.215242	-5.636859	2.496468
C	1.447275	-6.830810	1.188364
C	2.844179	-6.376929	-1.188364
C	1.431562	-6.683920	-1.272284
C	1.156212	0.375676	-7.257312
C	0.000000	1.215714	-7.257312
C	0.000000	2.462499	-6.641911
C	2.341975	0.760954	-6.641911
C	0.714578	-0.983533	-7.257312
C	-1.156212	0.375676	-7.257312
C	-0.714578	-0.983533	-7.257312
C	-2.431977	2.123135	-6.158774
C	-3.584177	2.497476	-5.410023
C	-3.584044	3.721525	-4.653286
C	-1.267699	2.969032	-6.158774
C	-2.341975	0.760954	-6.641911
C	-4.602345	1.495392	-5.173044
C	-4.367640	0.086226	-5.410023
C	-5.655904	3.053377	-3.581546
C	-6.370327	2.821166	-2.365775
C	-6.049254	3.487277	-1.188364
C	-4.602083	3.957641	-3.650894
C	-5.656047	1.837761	-4.333009
C	-6.811942	1.462013	-2.365775
C	-6.370452	0.854223	-3.581546
C	-6.798966	1.452581	0.060746
C	-6.799163	0.703948	1.272284
C	-6.354536	1.315992	2.496468
C	-6.354284	2.821169	0.060746
C	-6.943719	0.734396	-1.188364
C	-6.943719	-0.734396	1.188364
C	-6.798966	-1.452581	-0.060746
C	-6.370452	-0.854223	3.581546
C	-5.656047	-1.837761	4.333009
C	-4.602345	-1.495392	5.173044
C	-6.049407	0.496762	3.650894
C	-6.811942	-1.462013	2.365775
C	-5.655904	-3.053377	3.581546
C	-6.370327	-2.821166	2.365775
C	-3.584044	-3.721525	4.653286
C	-2.431850	-4.558643	4.653286
C	-1.267669	-4.180518	5.410023
C	-3.584177	-2.497476	5.410023
C	-4.602083	-3.957641	3.650894
C	-2.341818	-5.599820	3.650894
C	-3.215242	-5.636859	2.496468
C	-5.086868	-4.565954	1.272284
C	-4.367407	-4.799762	2.496468
C	-6.049254	-3.487277	1.188364
C	-6.354284	-2.821169	-0.060746
C	-6.354536	-1.315992	-2.496468
C	-6.799163	-0.703948	-1.272284
C	-6.049407	-0.496762	-3.650894
C	-5.087010	-0.904129	-4.653286
C	-2.770743	-1.656863	-6.158774
C	-3.215458	-0.288172	-6.158774
C	-1.447420	-1.992203	-6.641911
C	-0.719563	-3.147132	-6.158774
C	0.712095	-5.117425	-4.653286
C	1.431681	-4.127227	-5.410023
C	1.396921	-5.906836	-3.650894
C	0.712077	-6.450187	-2.496468
C	-0.719509	-6.915073	-0.060746
C	0.719509	-6.915073	-0.060746
C	-1.447275	-6.830810	1.188364
C	-2.770551	-6.248857	1.272284
C	-5.185920	-4.675554	-1.188364
C	-4.646673	-5.171494	0.060746
C	-5.914409	-3.426942	-1.272284
C	-4.651627	-5.186753	-2.365775
C	-5.186062	-3.153863	-3.650894
C	-5.914448	-2.670443	-2.496468
C	-4.646911	-2.258614	-4.653286
C	-4.651705	-4.435539	-3.581546
C	-2.844405	-3.914988	-5.173044
C	-3.482813	-2.636993	-5.410023
C	-1.431681	-4.127227	-5.410023
C	-3.495630	-4.811321	-4.333009
C	-1.396921	-5.906836	-3.650894
C	-0.712095	-5.117425	-4.653286
C	-0.712077	-6.450187	-2.496468
C	-2.780992	-5.794691	-3.581546
C	-2.844179	-6.376929	-1.188364
C	-1.431562	-6.683920	-1.272284
C	-3.482482	-6.017328	0.060746
C	-3.495463	-6.026755	-2.365775

C60@C180 (BLYP-D3/DZP; Symmetry: I_h)

C	-3.413857	-0.360402	0.583486
C	-1.397703	3.135400	0.583486
C	3.413857	-0.360402	0.583486
C	2.550029	2.298186	0.583486
C	0.712177	-3.358141	0.583486
C	2.973707	-1.715043	0.583486
C	-2.973707	-1.715043	0.583486
C	-0.712177	-3.358141	0.583486
C	-2.550029	2.298186	0.583486
C	1.397703	3.135400	0.583486
C	1.398290	-1.924581	-2.544775
C	-1.398290	-1.924581	-2.544775
C	-2.262480	0.735124	-2.544775
C	0.000000	2.378913	-2.544775
C	2.262480	0.735124	-2.544775
C	-2.550037	-1.549718	-1.795193
C	-2.261874	1.946340	-1.795193
C	1.152121	2.752622	-1.795193
C	2.973925	-0.245125	-1.795193
C	0.685865	-2.904118	-1.795193
C	-0.712305	0.980403	3.265916
C	0.712305	0.980403	3.265916
C	1.152533	-0.374481	3.265916
C	0.000000	-1.211845	3.265916
C	-1.152533	-0.374481	3.265916
C	-2.973925	0.245125	1.795193
C	-0.685865	2.904118	1.795193
C	2.550037	1.549718	1.795193
C	2.261874	-1.946340	1.795193
C	-1.152121	-2.752622	1.795193
C	2.973925	0.245125	1.795193
C	1.152121	-2.752622	1.795193
C	-2.261874	-1.946340	1.795193
C	-2.550037	1.549718	1.795193
C	0.685865	2.904118	1.795193
C	2.550037	-1.549718	-1.795193
C	-0.685865	-2.904118	-1.795193
C	-2.973925	-0.245125	-1.795193
C	-1.152121	2.752622	-1.795193
C	2.261874	1.946340	-1.795193
C	0.000000	1.211845	-3.265916
C	1.152533	0.374481	-3.265916
C	0.712305	-0.980403	-3.265916
C	-0.712305	-0.980403	-3.265916
C	-1.152533	0.374481	-3.265916
C	-2.973707	1.715043	-0.583486
C	0.712177	3.358141	-0.583486
C	3.413857	0.360402	-0.583486
C	1.397703	-3.135400	-0.583486
C	-2.550029	-2.298186	-0.583486
C	0.000000	-2.378913	2.544775
C	-2.262480	-0.735124	2.544775
C	-1.398290	1.924581	2.544775
C	1.398290	1.924581	2.544775
C	2.262480	-0.735124	2.544775
C	2.550029	-2.298186	-0.583486
C	-1.397703	-3.135400	-0.583486
C	-3.413857	0.360402	-0.583486
C	-0.712177	3.358141	-0.583486
C	2.973707	1.715043	-0.583486
C	0.720454	-5.135589	3.676397
C	-1.165594	-5.748569	2.451055
C	0.000000	-6.126712	1.693236
C	1.165594	-5.748569	2.451055
C	0.746019	-3.225340	5.218361
C	-0.746019	-3.225340	5.218361
C	-1.480709	-4.172307	4.364135
C	1.480709	-4.172307	4.364135
C	-3.297071	-4.538029	2.591360
C	-2.394489	-5.429998	1.845565
C	-2.837447	-3.905410	3.860515
C	3.297071	-4.538029	2.591360
C	2.837447	-3.905410	3.860515
C	2.394489	-5.429998	1.845565
C	-1.292145	-6.028497	-0.391956
C	-2.498094	-5.636661	0.391956
C	0.000000	-6.208228	0.288863
C	2.498094	-5.636661	0.391956
C	1.292145	-6.028497	-0.391956
C	0.720181	-0.991244	6.233269
C	-0.720181	-0.991244	6.233269
C	-1.481230	-2.038738	5.682897
C	1.481230	-2.038738	5.682897
C	-4.661603	-2.272177	3.676397
C	-5.107026	-2.884952	2.451055
C	-3.510535	-2.697552	4.364135
C	-2.836948	-1.706191	5.218361
C	-3.601191	-4.956614	-1.693236
C	-2.435938	-5.335809	-2.451055
C	-1.254490	-5.800406	-1.845565
C	-3.649105	-5.022562	-0.288863
C	0.000000	-5.609312	-2.591360
C	-4.588829	-4.117653	0.391956
C	-4.424297	-3.955256	1.845565
C	3.601191	-4.956614	-1.693236
C	2.435938	-5.335809	-2.451055
C	1.254490	-5.800406	-1.845565
C	3.649105	-5.022562	-0.288863
C	4.588829	-4.117653	0.391956
C	4.661603	-2.272177	3.676397
C	5.107026	-2.884952	2.451055
C	4.424297	-3.955256	1.845565
C	3.510535	-2.697552	4.364135
C	2.836948	-1.706191	5.218361
C	-4.425664	0.118924	4.364135
C	-5.106868	-0.901792	3.676397
C	-3.298014	-0.287178	5.218361
C	-2.396680	0.778728	5.682897
C	-1.165278	0.378622	6.233269
C	-5.827403	-0.667859	2.451055
C	-5.826849	-1.893258	1.693236
C	1.165278	0.378622	6.233269
C	0.000000	1.225245	6.233269
C	-5.128855	-2.985515	-1.845565
C	-4.321910	-3.965571	-2.451055
C	-5.334147	-3.091811	-0.391956
C	-5.904376	-1.918448	0.288863
C	1.254501	-4.245806	-4.364135
C	2.435764	-4.578251	-3.676397
C	0.000000	-4.827353	-3.860515
C	-1.254501	-4.245806	-4.364135
C	-2.435764	-4.578251	-3.676397
C	-3.601483	-3.731306	-3.676397
C	5.904376	-1.918448	0.288863
C	5.826849	-1.893258	1.693236
C	5.334147	-3.091811	-0.391956
C	5.128855	-2.985515	-1.845565
C	4.321910	-3.965571	-2.451055
C	3.601483	-3.731306	-3.676397
C	2.396680	0.778728	5.682897
C	3.298014	-0.287178	5.218361
C	4.425664	0.118924	4.364135
C	5.106868	-0.901792	3.676397
C	5.827403	-0.667859	2.451055
C	-1.292265	3.047854	5.218361
C	-2.499350	2.170856	5.218361
C	0.000000	2.520018	5.682897
C	-2.435764	4.578251	3.676397
C	-3.650339	2.505128	4.364135
C	-1.254501	4.245806	4.364135
C	0.000000	4.827353	3.860515
C	0.000000	5.609312	2.591360
C	3.601483	3.731306	3.676397
C	2.435764	4.578251	3.676397
C	1.254501	4.245806	4.364135
C	1.292265	3.047854	5.218361
C	2.499350	2.170856	5.218361
C	-5.904376	1.918448	-0.288863
C	-5.826849	1.893258	-1.693236
C	-5.904173	-0.599333	-1.845565
C	-6.132737	-0.634005	-0.391956
C	-6.132737	0.634005	0.391956
C	-5.904173	0.599333	1.845565
C	-5.334147	3.091811	0.391956
C	-4.588829	4.117653	-0.391956
C	-3.601483	3.731306	3.676397
C	-4.321910	3.965571	2.451055
C	-5.128855	2.985515	1.845565
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C	-2.396680	-0.778728	-5.682897
C	-1.165278	-0.378622	-6.233269
C	0.000000	-2.520018	-5.682897
C	-1.292265	-3.047854	-5.218361
C	-2.499350	-2.170856	-5.218361
C	-3.650339	-2.505128	-4.364135
C	-3.298014	0.287178	-5.218361
C	-5.827403	0.667859	-2.451055
C	-5.106868	0.901792	-3.676397
C	-4.425664	-0.118924	-4.364135
C	-4.591085	-1.491734	-3.860515
C	-5.334773	-1.733373	-2.591360
C	4.425664	-0.118924	-4.364135
C	5.106868	0.901792	-3.676397
C	5.827403	0.667859	-2.451055
C	5.904173	-0.599333	-1.845565
C	5.334773	-1.733373	-2.591360
C	4.591085	-1.491734	-3.860515
C	3.650339	-2.505128	-4.364135
C	3.298014	0.287178	-5.218361
C	2.836948	1.706191	-5.218361
C	0.000000	-1.225245	-6.233269
C	1.165278	-0.378622	-6.233269
C	2.396680	-0.778728	-5.682897
C	2.499350	-2.170856	-5.218361
C	1.292265	-3.047854	-5.218361
C	5.128855	2.985515	1.845565
C	4.321910	3.965571	2.451055
C	3.650339	2.505128	4.364135
C	4.591085	1.491734	3.860515
C	5.334773	1.733373	2.591360
C	5.904173	0.599333	1.845565
C	5.826849	1.893258	-1.693236
C	5.904376	1.918448	-0.288863
C	6.132737	0.634005	0.391956
C	6.132737	-0.634005	-0.391956
C	5.334147	3.091811	0.391956
C	4.588829	4.117653	-0.391956
C	4.661603	2.272177	-3.676397
C	5.107026	2.884952	-2.451055
C	3.510535	2.697552	-4.364135
C	2.837447	3.905410	-3.860515
C	1.480709	4.172307	-4.364135
C	0.720454	5.135589	-3.676397
C	4.424297	3.955256	-1.845565
C	3.297071	4.538029	-2.591360
C	2.394489	5.429998	-1.845565
C	1.165594	5.748569	-2.451055
C	3.601191	4.956614	1.693236
C	2.435938	5.335809	2.451055
C	3.649105	5.022562	0.288863
C	2.498094	5.636661	-0.391956
C	1.254490	5.800406	1.845565
C	1.292145	6.028497	0.391956
C	0.000000	6.208228	-0.288863
C	0.000000	6.126712	-1.693236
C	-2.435938	5.335809	2.451055
C	-3.601191	4.956614	1.693236
C	-1.254490	5.800406	1.845565
C	-1.292145	6.028497	0.391956
C	-3.649105	5.022562	0.288863
C	-2.498094	5.636661	-0.391956
C	-2.394489	5.429998	-1.845565
C	-1.165594	5.748569	-2.451055
C	-5.107026	2.884952	-2.451055
C	-4.661603	2.272177	-3.676397
C	-4.424297	3.955256	-1.845565
C	-3.297071	4.538029	-2.591360
C	-0.720181	0.991244	-6.233269
C	0.720181	0.991244	-6.233269
C	1.481230	2.038738	-5.682897
C	0.746019	3.225340	-5.218361
C	-1.481230	2.038738	-5.682897
C	-0.746019	3.225340	-5.218361
C	-1.480709	4.172307	-4.364135
C	-0.720454	5.135589	-3.676397
C	-2.836948	1.706191	-5.218361
C	-3.510535	2.697552	-4.364135
C	-2.837447	3.905410	-3.860515

C60@C180 (BLYP-D3/DZP; Symmetry: D_{5d})

C	-2.977125	1.718225	0.584755
C	0.714147	3.362374	0.584755
C	2.554111	-2.300453	0.584755
C	3.418491	0.359837	0.584755
C	-1.398597	-3.139983	0.584755
C	1.398597	-3.139983	0.584755
C	-3.418491	0.359837	0.584755
C	-2.554111	-2.300453	0.584755
C	-0.714147	3.362374	0.584755
C	2.977125	1.718225	0.584755
C	0.000000	-2.378981	-2.544418
C	-2.262545	-0.735145	-2.544418
C	-1.398330	1.924636	-2.544418
C	1.398330	1.924636	-2.544418
C	2.262545	-0.735145	-2.544418
C	-2.983922	0.246627	-1.800292
C	-0.687526	2.914090	-1.800292
C	2.559007	1.554380	-1.800292
C	2.269080	-1.953430	-1.800292
C	-1.156639	-2.761666	-1.800292
C	0.000000	1.220078	3.281895
C	1.160363	0.377025	3.281895
C	0.717144	-0.987063	3.281895
C	-0.717144	-0.987063	3.281895
C	-1.160363	0.377025	3.281895
C	-2.269080	1.953430	1.800292
C	1.156639	2.761666	1.800292
C	2.983922	-0.246627	1.800292
C	0.687526	-2.914090	1.800292
C	-2.559007	-1.554380	1.800292
C	2.559007	-1.554380	1.800292
C	-0.687526	-2.914090	1.800292
C	-2.983922	-0.246627	1.800292
C	-1.156639	2.761666	1.800292
C	2.269080	1.953430	1.800292
C	1.156639	-2.761666	-1.800292
C	-2.269080	-1.953430	-1.800292
C	-2.559007	1.554380	-1.800292
C	0.687526	2.914090	-1.800292
C	2.983922	0.246627	-1.800292
C	0.717144	0.987063	-3.281895
C	1.160363	-0.377025	-3.281895
C	0.000000	-1.220078	-3.281895
C	-1.160363	-0.377025	-3.281895
C	-0.717144	0.987063	-3.281895
C	-1.398597	3.139983	-0.584755
C	2.554111	2.300453	-0.584755
C	2.977125	-1.718225	-0.584755
C	-0.714147	-3.362374	-0.584755
C	-3.418491	-0.359837	-0.584755
C	-1.398330	-1.924636	2.544418
C	-2.262545	0.735145	2.544418
C	0.000000	2.378981	2.544418
C	2.262545	0.735145	2.544418
C	1.398330	-1.924636	2.544418
C	0.714147	-3.362374	-0.584755
C	-2.977125	-1.718225	-0.584755
C	-2.554111	2.300453	-0.584755
C	1.398597	3.139983	-0.584755
C	3.418491	-0.359837	-0.584755
C	-4.678164	-2.278130	3.684714
C	-5.123766	-0.906710	3.684714
C	-5.834076	-0.670176	2.455798
C	-5.820595	-1.891226	1.693997
C	-5.113786	-2.887000	2.455798
C	-2.826665	-1.695930	5.188630
C	-3.283663	-0.289436	5.188630
C	-4.419376	0.113458	4.350222
C	-3.508661	-2.689433	4.350222
C	-5.318954	1.728233	2.580682
C	-5.894982	0.595412	1.842006
C	-4.573056	1.485876	3.839885
C	-3.287294	-4.524573	2.580682
C	-2.826304	-3.890074	3.839885
C	-4.419166	-3.946682	1.842006
C	-6.125255	-0.631960	-0.390603
C	-6.125255	0.631960	0.390603
C	-5.889797	-1.913711	0.290995
C	-4.583979	-4.111601	0.390603
C	-5.326892	-3.089068	-0.390603
C	-0.720527	-0.991720	6.250050
C	-1.165837	0.378803	6.250050
C	-2.379083	0.773011	5.657214
C	-1.470354	-2.023769	5.657214
C	-3.612263	3.745217	3.684714
C	-4.325947	3.971368	2.455798
C	-3.642039	2.505854	4.350222
C	-2.486413	2.164247	5.188630
C	-5.820595	1.891226	-1.693997
C	-5.834076	0.670176	-2.455798
C	-5.894982	-0.595412	-1.842006
C	-5.889797	1.913711	-0.290995
C	-5.318954	-1.728233	-2.580682
C	-5.326892	3.089068	0.390603
C	-5.119115	2.983285	1.842006
C	-3.597326	-4.951294	-1.693997
C	-4.325947	-3.971368	-2.455798
C	-5.119115	-2.983285	-1.842006
C	-3.640095	-5.010160	-0.290995
C	-2.493838	-5.630178	0.390603
C	-0.720999	-5.153179	3.684714
C	-1.165453	-5.755632	2.455798
C	-2.387920	-5.422469	1.842006
C	-1.473567	-4.168015	4.350222
C	-0.739438	-3.212390	5.188630
C	-1.257757	4.238136	4.350222
C	-2.445663	4.592802	3.684714
C	-1.289978	3.033508	5.188630
C	0.000000	2.501516	5.657214
C	0.000000	1.225833	6.250050
C	-2.440204	5.341440	2.455798
C	-3.597326	4.951294	1.693997
C	0.720527	-0.991720	6.250050
C	1.165837	0.378803	6.250050
C	-4.419166	3.946682	-1.842006
C	-5.113786	2.887000	-2.455798
C	-4.583979	4.111601	-0.390603
C	-3.640095	5.010160	0.290995
C	-3.642039	-2.505854	-4.350222
C	-3.612263	-3.745217	-3.684714
C	-4.573056	-1.485876	-3.839885
C	-4.419376	-0.113458	-4.350222
C	-5.123766	0.906710	-3.684714
C	-4.678164	2.278130	-3.684714
C	0.000000	-6.192899	0.290995
C	0.000000	-6.120136	1.693997
C	-1.291778	-6.020750	-0.390603
C	-1.255379	-5.790453	-1.842006
C	-2.440204	-5.341440	-2.455798
C	-2.445663	-4.592802	-3.684714
C	1.470354	-2.023769	5.657214
C	0.739438	-3.212390	5.188630
C	1.473567	-4.168015	4.350222
C	0.720999	-5.153179	3.684714
C	1.165453	-5.755632	2.455798
C	2.486413	2.164247	5.188630
C	1.289978	3.033508	5.188630
C	2.379083	0.773011	5.657214
C	3.612263	3.745217	3.684714
C	1.257757	4.238136	4.350222
C	3.642039	2.505854	4.350222
C	4.573056	1.485876	3.839885
C	5.318954	1.728233	2.580682
C	4.678164	-2.278130	3.684714
C	5.123766	-0.906710	3.684714
C	4.419376	0.113458	4.350222
C	3.283663	-0.289436	5.188630
C	2.826665	-1.695930	5.188630
C	0.000000	6.192899	-0.290995
C	0.000000	6.120136	-1.693997
C	-2.387920	5.422469	-1.842006
C	-2.493838	5.630178	-0.390603
C	-1.291778	6.020750	0.390603
C	-1.255379	5.790453	1.842006
C	1.291778	6.020750	0.390603
C	2.493838	5.630178	-0.390603
C	2.445663	4.592802	3.684714
C	2.440204	5.341440	2.455798
C	1.255379	5.790453	1.842006
C	0.000000	5.592679	2.580682
C	0.000000	4.808396	3.839885
C	-1.470354	2.023769	-5.657214
C	-0.720527	0.991720	-6.250050
C	-2.379083	-0.773011	-5.657214
C	-3.283663	0.289436	-5.188630
C	-2.826665	1.695930	-5.188630
C	-3.508661	2.689433	-4.350222
C	-0.739438	3.212390	-5.188630
C	-1.165453	5.755632	-2.455798
C	-0.720999	5.153179	-3.684714
C	-1.473567	4.168015	-4.350222
C	-2.826304	3.890074	-3.839885
C	-3.287294	4.524573	-2.580682
C	1.257757	-4.238136	-4.350222
C	2.445663	-4.592802	-3.684714
C	2.440204	-5.341440	-2.455798
C	1.255379	-5.790453	-1.842006
C	0.000000	-5.592679	-2.580682
C	0.000000	-4.808396	-3.839885
C	-1.257757	-4.238136	-4.350222
C	1.289978	-3.033508	-5.188630
C	2.486413	-2.164247	-5.188630
C	-1.165837	-0.378803	-6.250050
C	0.000000	-1.225833	-6.250050
C	0.000000	-2.501516	-5.657214
C	-1.289978	-3.033508	-5.188630
C	-2.486413	-2.164247	-5.188630
C	4.419166	-3.946682	1.842006
C	5.113786	-2.887000	2.455798
C	3.508661	-2.689433	4.350222
C	2.826304	-3.890074	3.839885
C	3.287294	-4.524573	2.580682
C	2.387920	-5.422469	1.842006
C	3.597326	-4.951294	-1.693997
C	3.640095	-5.010160	-0.290995
C	2.493838	-5.630178	0.390603
C	1.291778	-6.020750	-0.390603
C	4.583979	-4.111601	0.390603
C	5.326892	-3.089068	-0.390603
C	3.612263	-3.745217	-3.684714
C	4.325947	-3.971368	-2.455798
C	3.642039	-2.505854	-4.350222
C	4.573056	-1.485876	-3.839885
C	4.419376	-0.113458	-4.350222
C	5.123766	0.906710	-3.684714
C	5.119115	-2.983285	-1.842006
C	5.318954	-1.728233	-2.580682
C	5.894982	-0.595412	-1.842006
C	5.834076	0.670176	-2.455798
C	5.820595	-1.891226	1.693997
C	5.834076	-0.670176	2.455798
C	5.889797	-1.913711	0.290995
C	6.125255	-0.631960	-0.390603
C	5.894982	0.595412	1.842006
C	6.125255	0.631960	0.390603
C	5.889797	1.913711	-0.290995
C	5.820595	1.891226	-1.693997
C	4.325947	3.971368	2.455798
C	3.597326	4.951294	1.693997
C	5.119115	2.983285	1.842006
C	5.326892	3.089068	0.390603
C	3.640095	5.010160	0.290995
C	4.583979	4.111601	-0.390603
C	4.419166	3.946682	-1.842006
C	5.113786	2.887000	-2.455798
C	1.165453	5.755632	-2.455798
C	0.720999	5.153179	-3.684714
C	2.387920	5.422469	-1.842006
C	3.287294	4.524573	-2.580682
C	0.720527	0.991720	-6.250050
C	1.165837	-0.378803	-6.250050
C	2.379083	-0.773011	-5.657214
C	3.283663	0.289436	-5.188630
C	1.470354	2.023769	-5.657214
C	2.826665	1.695930	-5.188630
C	3.508661	2.689433	-4.350222
C	4.678164	2.278130	-3.684714
C	0.739438	3.212390	-5.188630
C	1.473567	4.168015	-4.350222
C	2.826304	3.890074	-3.839885

C60@C180 (BLYP-D3/DZP; Symmetry: C_{3i})

C	0.679177	1.233442	3.218306
C	-1.185579	3.283164	0.245591
C	0.694921	-1.215851	-3.205084
C	-0.728231	1.204819	-3.217961
C	2.290474	-2.628873	0.244141
C	1.411485	-2.123631	-2.366038
C	1.399881	-0.006050	3.204924
C	2.279768	-2.112361	1.578892
C	-0.735057	3.019087	1.574025
C	-1.175741	2.274601	-2.378914
C	-1.131387	-3.297793	-0.243940
C	-1.133403	-2.283676	2.365777
C	-2.558107	0.119313	2.379086
C	-3.436204	0.615032	-0.245855
C	-2.532258	-1.492667	-1.857091
C	-0.705489	-1.209251	3.204732
C	-2.559260	1.446902	1.857104
C	-2.982027	0.873096	-1.574239
C	-1.381984	-2.155762	-2.379059
C	0.029243	-3.438968	0.579029
C	2.250564	2.668110	-0.245747
C	2.247258	2.145727	-1.574121
C	2.969475	0.917811	-1.578918
C	3.421814	0.668862	-0.244060
C	2.963581	1.744614	0.578872
C	1.381984	2.155762	2.379059
C	-0.029243	3.438968	-0.579029
C	0.705489	1.209251	-3.204732
C	2.559260	-1.446902	-1.857104
C	2.982027	-0.873096	1.574239
C	1.407858	0.028175	-3.218239
C	2.993084	-1.694326	-0.578817
C	2.544398	0.160416	2.366005
C	0.689417	3.030594	1.578792
C	-0.026471	2.939427	-1.857154
C	-0.689417	-3.030594	-1.578792
C	0.026471	-2.939427	1.857154
C	-1.407858	-0.028175	3.218239
C	-2.993084	1.694326	0.578817
C	-2.544398	-0.160416	-2.366005
C	-3.421814	-0.668862	0.244060
C	-2.963581	-1.744614	-0.578872
C	-2.250564	-2.668110	0.245747
C	-2.247258	-2.145727	1.574121
C	-2.969475	-0.917811	1.578918
C	-1.411485	2.123631	2.366038
C	-2.279768	2.112361	-1.578892
C	-0.679177	-1.233442	-3.218306
C	1.185579	-3.283164	-0.245591
C	0.728231	-1.204819	3.217961
C	3.436204	-0.615032	0.245855
C	2.532258	1.492667	1.857091
C	1.131387	3.297793	0.243940
C	1.133403	2.283676	-2.365777
C	2.558107	-0.119313	-2.379086
C	0.735057	-3.019087	-1.574025
C	1.175741	-2.274601	2.378914
C	-0.694921	1.215851	3.205084
C	-2.290474	2.628873	-0.244141
C	-1.399881	0.006050	-3.204924
C	6.320703	0.751681	0.198716
C	6.050782	1.193948	1.541449
C	5.899841	0.027929	2.374098
C	6.071500	-1.134310	1.544176
C	6.331177	-0.688022	0.199046
C	5.411623	2.854952	-0.694939
C	5.143605	3.310966	0.692825
C	5.415512	2.413914	1.826747
C	5.938542	1.503824	-0.928587
C	4.533520	1.310083	3.960148
C	5.102259	0.022780	3.531961
C	4.692072	2.511523	3.103410
C	5.698669	-0.710555	-2.175645
C	5.701089	0.771503	-2.182189
C	5.952692	-1.441825	-0.927384
C	4.720866	-2.469152	3.109623
C	4.551269	-1.269429	3.967673
C	5.434602	-2.358013	1.825772
C	5.439328	-2.799166	-0.693037
C	5.178298	-3.259220	0.694702
C	4.018092	4.691033	-1.544363
C	3.761343	5.138970	-0.199200
C	4.224851	4.434236	0.927204
C	4.759451	3.527622	-1.826007
C	2.891104	3.619196	4.359571
C	2.736521	2.448683	5.185118
C	3.780463	3.654366	3.270424
C	3.464525	4.579839	2.175482
C	2.765866	-2.425338	5.191374
C	2.934326	-3.593134	4.366794
C	3.829803	-3.624986	3.280845
C	3.487834	-1.238338	4.980787
C	3.518566	-4.551430	2.181879
C	2.874315	0.013118	5.452632
C	3.471609	1.270065	4.978437
C	4.059640	-4.643439	-1.541773
C	3.811486	-5.098220	-0.198991
C	4.271626	-4.391075	0.928337
C	4.798443	-3.483221	-1.827004
C	4.521188	-2.807870	-3.103626
C	4.579071	0.744671	-4.367066
C	4.579930	-0.694301	-4.359678
C	5.055117	-1.446946	-3.270586
C	5.054430	1.504310	-3.281166
C	4.498946	2.853964	-3.109925
C	1.224272	5.129286	3.281043
C	1.644518	4.337967	4.367031
C	2.182224	5.322894	2.182051
C	1.666811	5.894729	0.928492
C	2.509298	5.849763	-0.198851
C	0.717416	3.608230	5.191656
C	1.392217	2.442808	5.700853
C	2.925844	5.123619	-2.374330
C	1.991438	5.837355	-1.541641
C	0.729840	-1.249142	6.043815
C	1.419225	-2.427015	5.700641
C	1.488499	0.008023	5.995378
C	0.716862	1.256843	6.044029
C	1.727738	-5.876058	0.927108
C	2.569851	-5.827029	-0.199313
C	2.233910	-5.290383	2.175381
C	1.274417	-5.101241	3.270321
C	1.688595	-4.313339	4.359382
C	0.752207	-3.594188	5.184941
C	2.835781	-2.371626	-4.978620
C	3.488954	-1.145700	-5.185251
C	3.401498	-3.271354	-3.960455
C	2.571163	-4.407792	-3.532481
C	2.974403	-5.095847	-2.374517
C	2.053625	-5.825471	-1.544501
C	2.531655	4.430369	-3.532250
C	3.375251	3.307073	-3.967996
C	2.816473	2.401428	-4.980870
C	3.483481	1.182683	-5.191574
C	2.811648	0.015576	-5.700857
C	-0.295579	6.110094	-0.692795
C	0.233267	6.114088	0.694946
C	0.617261	5.897116	-1.826795
C	-2.569851	5.827029	0.199313
C	-0.675400	5.885765	1.826086
C	-1.727738	5.876058	-0.927108
C	-2.233910	5.290383	-2.175381
C	-3.518566	4.551430	-2.181879
C	-0.752207	3.594188	-5.184941
C	-1.688595	4.313339	-4.359382
C	-1.274417	5.101241	-3.270321
C	0.171110	5.319369	-3.103439
C	1.132327	4.581305	-3.960148
C	-2.835781	2.371626	4.978620
C	-3.488954	1.145700	5.185251
C	-1.446893	-0.007402	6.044000
C	-0.751232	1.285321	5.995862
C	-1.448586	2.482849	5.452881
C	-0.671577	3.639972	4.981068
C	-3.401498	3.271354	3.960455
C	-4.521188	2.807870	3.103626
C	-2.053625	5.825471	1.544501
C	-2.974403	5.095847	2.374517
C	-2.571163	4.407792	3.532481
C	-1.176518	4.576706	3.968179
C	-0.222282	5.323275	3.109974
C	-2.531655	-4.430369	3.532250
C	-2.925844	-5.123619	2.374330
C	-0.617261	-5.897116	1.826795
C	-0.171110	-5.319369	3.103439
C	-1.132327	-4.581305	3.960148
C	-0.636031	-3.641525	4.978333
C	-3.375251	-3.307073	3.967996
C	-2.811648	-0.015576	5.700857
C	-3.483481	-1.182683	5.191574
C	-2.816473	-2.401428	4.980870
C	-1.425893	-2.495769	5.452577
C	-0.737489	-1.292992	5.995328
C	-1.224272	-5.129286	-3.281043
C	-1.644518	-4.337967	-4.367031
C	-0.717416	-3.608230	-5.191656
C	0.671577	-3.639972	-4.981068
C	1.176518	-4.576706	-3.968179
C	0.222282	-5.323275	-3.109974
C	0.675400	-5.885765	-1.826086
C	-2.182224	-5.322894	-2.182051
C	-3.464525	-4.579839	-2.175482
C	-1.991438	-5.837355	1.541641
C	-2.509298	-5.849763	0.198851
C	-1.666811	-5.894729	-0.928492
C	-0.233267	-6.114088	-0.694946
C	0.295579	-6.110094	0.692795
C	-0.729840	1.249142	-6.043815
C	-1.419225	2.427015	-5.700641
C	0.636031	3.641525	-4.978333
C	1.425893	2.495769	-5.452577
C	0.737489	1.292992	-5.995328
C	1.446893	0.007402	-6.044000
C	-1.392217	-2.442808	-5.700853
C	-0.716862	-1.256843	-6.044029
C	0.751232	-1.285321	-5.995862
C	1.448586	-2.482849	-5.452881
C	-1.488499	-0.008023	-5.995378
C	-2.874315	-0.013118	-5.452632
C	-2.891104	-3.619196	-4.359571
C	-2.736521	-2.448683	-5.185118
C	-3.780463	-3.654366	-3.270424
C	-4.692072	-2.511523	-3.103410
C	-5.415512	-2.413914	-1.826747
C	-6.050782	-1.193948	-1.541449
C	-3.471609	-1.270065	-4.978437
C	-4.533520	-1.310083	-3.960148
C	-5.102259	-0.022780	-3.531961
C	-5.899841	-0.027929	-2.374098
C	-2.765866	2.425338	-5.191374
C	-2.934326	3.593134	-4.366794
C	-3.487834	1.238338	-4.980787
C	-4.551269	1.269429	-3.967673
C	-3.829803	3.624986	-3.280845
C	-4.720866	2.469152	-3.109623
C	-5.434602	2.358013	-1.825772
C	-6.071500	1.134310	-1.544176
C	-3.811486	5.098220	0.198991
C	-4.059640	4.643439	1.541773
C	-4.271626	4.391075	-0.928337
C	-5.178298	3.259220	-0.694702
C	-4.798443	3.483221	1.827004
C	-5.439328	2.799166	0.693037
C	-5.952692	1.441825	0.927384
C	-6.331177	0.688022	-0.199046
C	-4.579930	0.694301	4.359678
C	-4.579071	-0.744671	4.367066
C	-5.055117	1.446946	3.270586
C	-5.698669	0.710555	2.175645
C	-4.018092	-4.691033	1.544363
C	-3.761343	-5.138970	0.199200
C	-4.224851	-4.434236	-0.927204
C	-5.143605	-3.310966	-0.692825
C	-4.759451	-3.527622	1.826007
C	-5.411623	-2.854952	0.694939
C	-5.938542	-1.503824	0.928587
C	-6.320703	-0.751681	-0.198716
C	-4.498946	-2.853964	3.109925
C	-5.054430	-1.504310	3.281166
C	-5.701089	-0.771503	2.182189

C60@C180 (BLYP-D3/DZP; Symmetry: C_i)

C	-2.979671	1.635970	0.785284
C	0.713645	3.276672	0.982893
C	2.551338	-2.351813	0.307158
C	3.419527	0.289221	0.625065
C	-1.396024	-3.188516	0.205833
C	1.399374	-3.187120	0.207591
C	-3.420298	0.285584	0.620998
C	-2.549065	-2.354606	0.304110
C	-0.718402	3.275943	0.982144
C	2.977153	1.639250	0.788899
C	0.002871	-2.051211	-2.798278
C	-2.259918	-0.425950	-2.612028
C	-1.404089	2.224099	-2.305265
C	1.404277	2.225735	-2.303566
C	2.263745	-0.423414	-2.609550
C	-2.985729	0.459491	-1.758762
C	-0.689620	3.117944	-1.445996
C	2.561733	1.761809	-1.600953
C	2.269207	-1.721961	-2.017721
C	-1.153100	-2.528363	-2.115259
C	-0.002501	0.814023	3.386341
C	1.154825	-0.018747	3.290234
C	0.716588	-1.373888	3.140280
C	-0.718920	-1.374768	3.139586
C	-1.158843	-0.020080	3.289082
C	-2.269060	1.721471	2.017953
C	1.153275	2.527817	2.115529
C	2.985943	-0.459836	1.758999
C	0.689571	-3.117926	1.446254
C	-2.561760	-1.762006	1.601296
C	2.561678	-1.759191	1.604272
C	-0.688001	-3.118803	1.445402
C	-2.987628	-0.463075	1.755653
C	-1.158518	2.526682	2.114259
C	2.265014	1.723973	2.020751
C	1.158654	-2.527145	-2.113815
C	-2.264806	-1.724531	-2.020555
C	-2.561626	1.758985	-1.603858
C	0.688034	3.118717	-1.445058
C	2.987529	0.462788	-1.755334
C	0.718700	1.374488	-3.139220
C	1.158826	0.019880	-3.288816
C	0.002373	-0.814312	-3.386534
C	-1.154840	0.018497	-3.290157
C	-0.716644	1.373604	-3.140022
C	-1.399304	3.186993	-0.207110
C	2.549089	2.354411	-0.303851
C	2.979900	-1.636334	-0.785197
C	-0.713555	-3.277009	-0.982482
C	-3.419307	-0.289790	-0.625079
C	-1.404591	-2.226113	2.304090
C	-2.263900	0.423134	2.609843
C	-0.002760	2.050903	2.798591
C	2.260299	0.425552	2.612412
C	1.404121	-2.224318	2.305643
C	0.718390	-3.276350	-0.981576
C	-2.976772	-1.639585	-0.788809
C	-2.551369	2.351820	-0.306909
C	1.396074	3.188394	-0.205461
C	3.420556	-0.285986	-0.621064
C	-4.675831	-2.367339	3.629346
C	-5.122927	-0.997330	3.662391
C	-5.837369	-0.731898	2.440113
C	-5.824506	-1.933088	1.651129
C	-5.113955	-2.946945	2.388533
C	-2.827620	-1.824612	5.149248
C	-3.287020	-0.417344	5.186641
C	-4.421608	0.006459	4.354576
C	-3.507667	-2.795903	4.287082
C	-5.319750	1.661556	2.619595
C	-5.898374	0.548768	1.855914
C	-4.573556	1.388893	3.871133
C	-3.289283	-4.590212	2.476429
C	-2.826790	-3.986352	3.753611
C	-4.420275	-3.992350	1.751208
C	-6.128150	-0.621598	-0.404800
C	-6.128180	0.622393	0.405751
C	-5.890609	-1.919756	0.247209
C	-4.584905	-4.119497	0.296122
C	-5.327300	-3.076735	-0.460349
C	-0.719336	-1.142513	6.216875
C	-1.165296	0.226892	6.256147
C	-2.380570	0.633842	5.676426
C	-1.470699	-2.164724	5.608770
C	-3.610967	3.652396	3.768324
C	-4.324996	3.907673	2.545013
C	-3.636207	2.394242	4.397864
C	-2.481238	2.031000	5.229199
C	-5.824561	1.933760	-1.650224
C	-5.837693	0.732581	-2.439255
C	-5.898743	-0.548035	-1.855018
C	-5.890677	1.920494	-0.246300
C	-5.320199	-1.660868	-2.618794
C	-5.327146	3.077450	0.461209
C	-5.117471	2.935088	1.909133
C	-3.598336	-4.907458	-1.806900
C	-4.325481	-3.907089	-2.544312
C	-5.117721	-2.934356	-1.908307
C	-3.643909	-5.003914	-0.406771
C	-2.493892	-5.636027	0.260689
C	-0.721242	-5.240326	3.564217
C	-1.165405	-5.812286	2.322219
C	-2.389762	-5.466056	1.717070
C	-1.476409	-4.279626	4.260854
C	-0.741309	-3.347257	5.124044
C	-1.255732	4.126175	4.440225
C	-2.445744	4.499988	3.788389
C	-1.286653	2.902401	5.254670
C	0.000496	2.365937	5.721271
C	0.000508	1.074292	6.280096
C	-2.440949	5.279891	2.578045
C	-3.597810	4.907959	1.807450
C	0.720048	-1.142636	6.216804
C	1.166226	0.226732	6.256124
C	-4.420027	3.992757	-1.750474
C	-5.113989	2.947480	-2.387720
C	-4.584651	4.120075	-0.295399
C	-3.643496	5.004321	0.407296
C	-3.636923	-2.393646	-4.397208
C	-3.611669	-3.651880	-3.767751
C	-4.574179	-1.388249	-3.870398
C	-4.422077	-0.005820	-4.353809
C	-5.123346	0.997975	-3.661637
C	-4.676101	2.367903	-3.628640
C	-0.000170	-6.190026	0.148020
C	-0.000056	-6.161732	1.552534
C	-1.292178	-6.005400	-0.528958
C	-1.256819	-5.741702	-1.974883
C	-2.441530	-5.279459	-2.577663
C	-2.446478	-4.499578	-3.788014
C	1.471153	-2.164927	5.608571
C	0.741637	-3.347406	5.124062
C	1.476514	-4.279679	4.260621
C	0.721314	-5.240351	3.564161
C	1.165327	-5.812491	2.322030
C	2.482099	2.030724	5.228870
C	1.287622	2.902252	5.254460
C	2.381425	0.633606	5.676203
C	3.611699	3.652005	3.767682
C	1.256661	4.125961	4.439916
C	3.636885	2.393799	4.397139
C	4.574101	1.388408	3.870295
C	5.320129	1.660980	2.618722
C	4.676132	-2.367789	3.628606
C	5.123362	-0.997836	3.661584
C	4.422042	0.005975	4.353729
C	3.287556	-0.417697	5.186059
C	2.827989	-1.824839	5.148667
C	0.000182	6.189704	-0.148171
C	0.000083	6.161640	-1.552701
C	-2.389438	5.466220	-1.716787
C	-2.493443	5.636132	-0.260381
C	-1.291661	6.005320	0.529067
C	-1.256211	5.741701	1.974992
C	1.292104	6.004998	0.528840
C	2.493767	5.635812	-0.260812
C	2.446604	4.499773	3.787991
C	2.441575	5.279503	2.577575
C	1.256797	5.741510	1.974780
C	0.000336	5.526594	2.709648
C	0.000436	4.713097	3.946684
C	-1.471200	2.165159	-5.608746
C	-0.720017	1.142798	-6.216842
C	-2.381372	-0.633424	-5.676131
C	-3.287546	0.417858	-5.186069
C	-2.828066	1.825076	-5.148870
C	-3.507951	2.796352	-4.286526
C	-0.741700	3.347662	-5.124168
C	-1.165374	5.812632	-2.322222
C	-0.721480	5.240609	-3.564346
C	-1.476620	4.279918	-4.260773
C	-2.826855	3.986589	-3.753073
C	-3.289092	4.590427	-2.475912
C	1.255730	-4.126000	-4.440349
C	2.445725	-4.499851	-3.788458
C	2.440953	-5.279836	-2.578161
C	1.256239	-5.741797	-1.975127
C	-0.000348	-5.526506	-2.709690
C	-0.000473	-4.712758	-3.946618
C	-1.256666	-4.125802	-4.440097
C	1.286682	-2.902274	-5.254933
C	2.481250	-2.030826	-5.229292
C	-1.166154	-0.226536	-6.256350
C	-0.000445	-1.074084	-6.280290
C	-0.000484	-2.365743	-5.721495
C	-1.287614	-2.902061	-5.254671
C	-2.482101	-2.030585	-5.228955
C	4.419942	-3.992565	1.750384
C	5.114019	-2.947385	2.387687
C	3.507913	-2.796180	4.286431
C	2.826770	-3.986432	3.752977
C	3.289023	-4.590278	2.475817
C	2.389578	-5.466289	1.716677
C	3.597822	-4.907884	-1.807548
C	3.643541	-5.004283	-0.407403
C	2.493531	-5.636257	0.260270
C	1.291729	-6.005557	-0.529185
C	4.584592	-4.119945	0.295321
C	5.327214	-3.077371	-0.461278
C	3.610893	-3.652218	-3.768358
C	4.324961	-3.907536	-2.545066
C	3.636107	-2.394035	-4.397834
C	4.573474	-1.388707	-3.871093
C	4.421489	-0.006283	-4.354504
C	5.122929	0.997450	-3.662431
C	5.117528	-2.935004	-1.909214
C	5.319776	-1.661449	-2.619661
C	5.898416	-0.548665	-1.855999
C	5.837436	0.732012	-2.440222
C	5.824599	-1.933671	1.650167
C	5.837678	-0.732477	2.439178
C	5.890747	-1.920422	0.246236
C	6.128147	-0.622284	-0.405821
C	5.898560	0.548123	1.854910
C	6.128001	0.621670	0.404709
C	5.890505	1.919806	-0.247288
C	5.824592	1.933210	-1.651244
C	4.325576	3.907218	2.544253
C	3.598394	4.907559	1.806803
C	5.117719	2.934455	1.908220
C	5.327271	3.076805	0.460266
C	3.643881	5.003941	0.406670
C	4.584826	4.119521	-0.296230
C	4.420081	3.992265	-1.751224
C	5.114010	2.947026	-2.388615
C	1.165338	5.812375	-2.322417
C	0.721189	5.240493	-3.564544
C	2.389648	5.465988	-1.717201
C	3.289124	4.590127	-2.476438
C	0.719336	1.142675	-6.216816
C	1.165340	-0.226706	-6.256241
C	2.380589	-0.633669	-5.676494
C	3.286981	0.417532	-5.186623
C	1.470643	2.164937	-5.608897
C	2.827626	1.824793	-5.149392
C	3.507556	2.795994	-4.287083
C	4.675879	2.367481	-3.629417
C	0.741232	3.347404	-5.124068
C	1.476342	4.279775	-4.261024
C	2.826652	3.986367	-3.753632

C60@C240 (BLYP-D3/DZP: Symmetry: I_h)

C	-3.210753	-0.288105	6.148974	C	-3.210735	-5.628584	-2.492184	C	1.266182	-2.964578	-6.148974	C	-2.838626	-6.366434	1.184989
C	-2.339048	0.760003	6.629252	C	-2.766919	-6.239520	-1.270355	C	2.339048	-0.760003	-6.629252	C	3.578343	-3.715807	-4.646344
C	-2.428209	2.120315	6.148974	C	-3.477790	-6.008592	-0.061003	C	4.593064	-1.492377	-5.164524	C	2.318453	-0.753311	-2.609668
C	-1.266182	2.964578	6.148974	C	-4.639814	-5.164332	-0.061003	C	4.360926	-0.085609	-5.401559	C	0.000000	-2.437765	-2.609668
C	-1.266181	4.173941	5.401559	C	-1.445599	-6.819056	-1.184989	C	5.644970	-3.048262	-3.574822	C	-2.318453	-0.753311	-2.609668
C	-4.593064	1.492377	5.164524	C	-0.713648	-6.917668	-2.360712	C	6.358563	-2.816397	-2.360712	C	2.615993	1.587820	-1.840870
C	-3.578383	2.494029	5.401559	C	-2.339032	-5.589370	-3.644421	C	6.038593	-3.482051	-1.184989	C	2.318493	-1.997294	-1.840870
C	-3.578343	3.715807	4.646344	C	-2.428173	-4.551454	-4.646344	C	4.593006	-3.951762	-3.644421	C	-1.183086	-2.822215	-1.840870
C	-2.428173	4.551454	4.646344	C	-1.266181	-4.173941	-5.401559	C	5.644952	-1.834156	-4.325167	C	-3.049680	0.253069	-1.840870
C	-4.360926	0.085609	5.401559	C	-1.266182	-2.964578	-6.148974	C	6.799622	-1.458957	-2.360712	C	-0.701720	2.978621	-1.840870
C	-1.445611	-1.989713	6.629252	C	-1.154678	-6.310650	-3.574822	C	6.358600	-0.851934	-3.574822	C	0.731208	-1.006422	3.347645
C	-0.713634	-0.982232	7.243266	C	1.445599	-6.819056	-1.184989	C	6.789207	-1.450818	0.061003	C	-0.731208	-1.006422	3.347645
C	-1.154683	0.375179	7.243266	C	2.766919	-6.239520	-1.270355	C	6.789161	-0.703379	1.270355	C	-1.183120	0.384419	3.347645
C	-2.766898	-1.654151	6.148974	C	3.210735	-5.628584	-2.492184	C	6.345274	-1.314262	2.492184	C	0.000000	1.244006	3.347645
C	-4.639711	-2.254959	4.646344	C	4.360930	-4.792919	-2.492184	C	6.345353	-2.816859	0.061003	C	1.183120	0.384419	3.347645
C	-3.477744	-2.632547	5.401559	C	0.713648	-6.917668	-2.360712	C	6.932023	-0.732358	-1.184989	C	3.049680	-0.253069	1.840870
C	-5.079037	-0.902853	4.646344	C	0.000000	1.214106	7.243266	C	6.932023	0.732358	1.184989	C	0.701720	-2.978621	1.840870
C	-5.644952	1.834156	4.325167	C	1.154683	0.375179	7.243266	C	6.789207	1.450818	-0.061003	C	-2.615993	-1.587820	1.840870
C	-6.038607	-0.497341	3.644421	C	0.000000	2.459421	6.629252	C	6.358600	0.851934	3.574822	C	-2.318493	1.997294	1.840870
C	-6.358600	0.851934	3.574822	C	1.266182	2.964578	6.148974	C	5.644952	1.834156	4.325167	C	1.183086	2.822215	1.840870
C	0.718173	-3.142637	6.148974	C	2.339048	0.760003	6.629252	C	4.593064	1.492377	5.164524	C	-3.049680	-0.253069	1.840870
C	1.445611	-1.989713	6.629252	C	2.428209	2.120315	6.148974	C	6.038607	-0.497341	3.644421	C	-1.183086	2.822215	1.840870
C	2.766898	-1.654151	6.148974	C	-6.358563	2.816397	2.360712	C	6.799622	1.458957	2.360712	C	2.318493	1.997294	1.840870
C	3.210753	-0.288105	6.148974	C	-5.644970	3.048262	3.574822	C	5.644970	3.048262	3.574822	C	2.615993	-1.587820	1.840870
C	4.360926	0.085609	5.401559	C	-6.038593	3.482051	1.184989	C	6.358563	2.816397	2.360712	C	-0.701720	-2.978621	1.840870
C	0.713634	-0.982232	7.243266	C	-5.079111	4.559614	1.270355	C	3.578343	3.715807	4.646344	C	-2.615993	1.587820	-1.840870
C	-0.718173	-3.142637	6.148974	C	-4.593006	3.951762	3.644421	C	2.428173	4.551454	4.646344	C	0.701720	2.978621	-1.840870
C	-6.789161	-0.703379	1.270355	C	-4.360930	4.792919	2.492184	C	1.266181	4.173941	5.401559	C	3.049680	0.253069	-1.840870
C	-6.932023	0.732358	1.184989	C	-5.644952	-1.834156	-4.325167	C	3.578383	2.494029	5.401559	C	1.183086	-2.822215	-1.840870
C	-6.789207	1.450818	-0.061003	C	-6.358600	-0.851934	-3.574822	C	4.593006	3.951762	3.644421	C	-2.318493	-1.997294	-1.840870
C	-6.345353	2.816859	-0.061003	C	-4.593064	-1.492377	-5.164524	C	2.339032	5.589370	3.644421	C	0.000000	-1.244006	-3.347645
C	-5.905982	3.421523	-1.270355	C	-4.360926	-0.085609	-5.401559	C	3.210735	5.628584	2.492184	C	-1.183120	-0.384419	-3.347645
C	-6.799622	1.458957	2.360712	C	-6.038607	0.497341	-3.644421	C	5.079111	4.559614	1.270355	C	-0.731208	1.006422	-3.347645
C	-6.345274	-1.314262	2.492184	C	-5.079037	0.902853	-4.646344	C	4.360930	4.792919	2.492184	C	0.731208	1.006422	-3.347645
C	-5.905938	-2.666398	2.492184	C	1.154678	-6.310650	-3.574822	C	6.038593	3.482051	1.184989	C	1.183120	-0.384419	-3.347645
C	-3.488772	-4.801883	4.325167	C	0.000000	-5.935454	-4.325167	C	6.345353	2.816859	-0.061003	C	3.049781	-1.759773	-0.596915
C	-4.643461	-4.426720	3.574822	C	2.339032	-5.589370	-3.644421	C	6.345274	1.314262	-2.492184	C	-0.731210	-3.444314	-0.596915
C	-5.177666	-3.147047	3.644421	C	2.428173	-4.551454	-4.646344	C	6.789161	0.703379	-1.270355	C	-3.501693	-0.368930	-0.596915
C	-2.838669	-3.907093	5.164524	C	0.000000	-4.829433	-5.164524	C	6.038607	0.497341	-3.644421	C	-1.432956	3.216303	-0.596915
C	-1.429019	-4.121032	5.401559	C	1.266181	-4.173941	-5.401559	C	5.079037	0.902853	-4.646344	C	2.616078	2.356714	-0.596915
C	1.429019	-4.121032	5.401559	C	4.643461	-4.426720	3.574822	C	2.766898	1.654151	-6.148974	C	0.000000	2.437765	2.609668
C	2.838669	-3.907093	5.164524	C	4.643456	-5.177039	2.360712	C	3.210753	0.288105	-6.148974	C	2.318453	0.753311	2.609668
C	3.477744	-2.632547	5.401559	C	5.177666	-3.147047	3.644421	C	1.445611	1.989713	-6.629252	C	1.432882	-1.972194	2.609668
C	4.639711	-2.254959	4.646344	C	5.905938	-2.666398	2.492184	C	0.718173	3.142637	-6.148974	C	-1.432882	-1.972194	2.609668
C	5.079037	-0.902853	4.646344	C	5.177655	-4.667031	1.184989	C	-0.710844	5.109448	-4.646344	C	-2.318453	0.753311	2.609668
C	-5.177655	-4.667031	1.184989	C	5.905982	-3.421523	1.270355	C	-1.429019	4.121032	-5.401559	C	-2.616078	2.356714	-0.596915
C	-4.643456	-5.177039	2.360712	C	0.000000	5.935454	4.325167	C	-1.393032	5.896744	-3.644421	C	1.432956	3.216303	-0.596915
C	-5.905982	-3.421523	1.270355	C	-1.154678	6.310650	3.574822	C	-0.710860	6.440843	-2.492184	C	3.501693	-0.368930	-0.596915
C	-6.345353	-2.816859	0.061003	C	-2.339032	5.589370	3.644421	C	0.718170	6.905247	-0.061003	C	0.731210	-3.444314	-0.596915
C	-6.789207	-1.450818	0.061003	C	0.000000	4.829433	5.164524	C	-0.718170	6.905247	-0.061003	C	-3.049781	-1.759773	-0.596915
C	-6.932023	-0.732358	-1.184989	C	1.154678	6.310650	3.574822	C	1.445599	6.819056	1.184989				
C	-6.789161	0.703379	-1.270355	C	-0.713648	6.917668	2.360712	C	2.766919	6.239520	1.270355				
C	-6.345274	1.314262	-2.492184	C	0.713648	6.917668	2.360712	C	5.177655	4.667031	-1.184989				
C	-5.905938	2.666398	-2.492184	C	-4.643456	5.177039	-2.360712	C	4.639814	5.164332	0.061003				
C	0.710844	-5.109448	4.646344	C	-4.643461	4.426720	-3.574822	C	5.905982	3.421523	-1.270355				
C	-0.710844	-5.109448	4.646344	C	-5.177666	3.147047	-3.644421	C	4.643456	5.177039	-2.360712				
C	-1.393032	-5.896744	3.644421	C	-5.177655	4.667031	-1.184989	C	5.177666	3.147047	-3.644421				
C	-2.775153	-5.784126	3.574822	C	-3.488750	6.015982	-2.360712	C	5.905938	2.666398	-2.492184				
C	-3.488750	-6.015982	2.360712	C	-3.488772	4.801883	-4.325167	C	4.639711	2.254959	-4.646344				
C	3.488772	-4.801883	4.325167	C	-2.775153	5.784126	-3.574822	C	4.643461	4.426720	-3.574822				
C	1.429013	-6.674232	1.270355	C	-3.477744	2.632547	-5.401559	C	2.838669	3.907093	-5.164524				
C	2.838626	-6.366434	1.184989	C	-2.766898	1.654151	-6.148974	C	3.477744	2.632547	-5.401559				
C	3.477790	-6.008592	-0.061003	C	-3.210753	0.288105	-6.148974	C	1.429019	4.121032	-5.401559				
C	4.639814	-5.164332	-0.061003	C	-4.639711	2.254959	-4.646344	C	3.488772	4.801883	-4.325167				
C	5.079111	-4.559614	-1.270355	C	-2.838669	3.907093	-5.164524	C	1.393032	5.896744	-3.644421				
C	3.488750	-6.015982	2.360712	C	-1.445611	1.989713	-6.629252	C	0.710844	5.109448	-4.646344				
C	2.775153	-5.784126	3.574822	C	-0.718173	3.142637	-6.148974	C	0.710860	6.440843	-2.492184				
C	1.393032	-5.896744	3.644421	C	-2.766919	6.239520	1.270355	C	2.775153	5.784126	-3.574822				
C	-5.644970	-3.048262	-3.574822	C	-3.477790	6.008592	0.061003	C	2.838626	6.366434	-1.184989				
C	-4.593006	-3.951762	-3.644421	C	-4.639814	5.164332	0.061003	C	1.429013	6.674232	-1.270355				
C	-3.578343	-3.715807	-4.646344	C	-3.210735	5.628584	2.492184	C	3.477790	6.008592	0.061003				
C	-3.578383	-2.494029	-5.401559	C	-1.445599	6.819056	1.184989	C	3.488750	6.015982	-2.360712				
C	-2.428209	-2.120315	-6.148974	C	-2.838626	6.366434	-1.184989	C	3.501693	0.368930	0.596915				
C	-4.360930	-4.792919	-2.492184	C	-1.429013	6.674232	-1.270355	C	1.432956	-3.216303	0.596915				
C	-5.079111	-4.559614	-1.270355	C	-1.154683	-0.375179	-7.243266	C	-3.501693	0.368930	0.596915				
C	-6.038593	-3.482051	-1.184989	C	0.000000	-1.214106	-7.243266	C	-2.616078	-2.356714	0.596915				
C	-6.358563	-2.816397	-2.360712	C	0.000000	-2.459421	-6.629252	C	-0.731210	3.444314	0.596915				
C	-6.799622	-1.458957	-2.360712	C	-2.339048	-0.760003	-6.629252	C	-3.049781	1.759773	0.596915				
C	-0.718170	-6.905247	0.061003	C	-0.713634	0.982232	-7.243266	C	3.049781	1.759773	0.596915				
C	0.718170	-6.905247	0.061003	C	1.154683	-0.375179	-7.243266	C	0.731210	3.444314	0.596915				
C	0.710860	-6.440843	2.492184	C	0.713634	0.982232	-7.243266	C	2.616078	-2.356714	0.596915				
C	-0.710860	-6.440843	2.492184	C	2.428209	-2.120315	-6.148974	C	-1.432956	-3.216303	0.596915				
C	-1.429013	-6.674232	1.270355	C	3.578383	-2.494029	-5.401559	C	-1.432882	1.972194	-2.60966				