Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Polyradical Character Assessment using Multireference Calculations and Comparison with Density-Functional Derived Fractional Occupation Number Weighted Density Analysis

Reed Nieman,[1,a] Jhonatas R. Carvalho,[1,a] Bhumika Jayee,[1,a,b] Andreas Hansen,[2] Adelia J. A. Aquino,[3] Miklos Kertesz,[4] Hans Lischka[1]*

[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX 79409-1061, USA

[2] Mulliken Center for Theoretical Chemistry, Universität Bonn, D- 53115 (Germany)

[3]Department of Mechanical Engineering, Texas Tech University, Lubbock, TX 79409-1061, USA

[4]Chemistry Department and Institute of Soft Matter, Georgetown University, Washington, District of Columbia 20057-1227, USA

[a] These authors contributed equally to this publication.

[b] Current address: Department of Chemistry and Chemical Biology, Northeastern University, Boston MA, 02115, USA

* email: Hans.Lischka@ttu.edu

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Table S1: RMSD values for the difference in Cartesian geometries and a comparison of N_{FOD} and N_U values for structures optimized without and with D3 contribution, respectively.

Str	RMSD (Å) no D3 vs. with D3	N_{FOD} (e) geom.: no D3/with D3			N_U (e) Geom.: no D3/with D3
		TPSS	B3LYP	M05-2X	MR-AQCC
3	0.008	2.00/2.13	2.65/2.75	4.14/4.23	1.97/2.30
12	0.006	1.72/1.72	2.36/2.35	3.59/3.58	2.14/2.29
15	0.001	1.48/1.48	2.30/2.30	3.94/3.94	1.64/1.64
28	0.000	0.81/0.81	1.26/1.26	2.04/2.04	0.99/0.99

Table S2: HOMO-LUMO f_i and NFOD values (M05-2X/def2-TZVP, TPSS/def2-TZVP, and B3LYP /def2-TZVP method with FT-UDFT approaches) for n-acenes (**1-4**) at TPSS optimized geometry. FT-DFT calculations performed with literature-recommended temperature (M05-2X: 16200 K, TPSS: 5000 K, B3LYP: 9000 K) and improved present temperature (M05-2X: 12200 K, TPSS: 6200 K, B3LYP: 8200 K, values italics). All values are given in units of e.

Str	FT-UDFT/M05-2X/FOD				FT-UDFT/TPSS/FOD				FT-UDFT/B3LYP/FOD			
	f_i Values		N_{FOD}		f_i Values		N_{FOD}		f_i Values		N_{FOD}	
1	-	-	-	-	-	-	-	-	-	-	-	-
	-	-			-	-			-	-		
2	1.32	*1.51*	2.96	*1.55*	-	-	-	-	1.41	*1.45*	1.78	*1.53*
	0.65	*0.50*			-	-			0.62	*0.57*		
3	1.18	*1.32*	4.14	*2.36*	1.24	*1.20*	2.00	*2.42*	1.23	*1.26*	2.65	*2.33*
	0.80	*0.70*			0.80	*0.85*			0.81	*0.78*		
4	1.02	*1.13*	5.49	*3.34*	1.07	*1.07*	2.82	*3.31*	1.04	*1.05*	3.68	*3.34*
	0.97	*0.90*			0.98	*0.99*			1.02	*1.01*		

Table S3: HOMO-LUMO f_i and N_{FOD} values (TPSS/def2-TZVP and B3LYP/def2-TZVP methods with FT-RDFT approach) for the *n*-acenes (**1-4**). FT-DFT calculations performed with literature-recommended temperature (TPSS: 5000 K, B3LYP: 9000 K) and improved present temperature (TPSS: 6200 K, B3LYP: 8200 K, values italics). All values are given in units of *e*.

Str		FT-RDFT/TPSS/FOD				FT-RDFT/B3LYP/FOD			
		f_i Values		N_{FOD}		f_i Values		N_{FOD}	
1	H	1.76	*1.67*	0.52	*0.80*	1.66	*1.71*	0.95	*0.76*
	L	0.25	*0.34*			0.35	*0.30*		
2	H	1.47	*1.40*	1.25	*1.60*	1.41	*1.45*	1.78	*1.53*
	L	0.56	*0.64*			0.62	*0.57*		
3	H	1.24	*1.20*	2.00	*2.42*	1.23	*1.26*	2.65	*2.33*
	L	0.80	*0.85*			0.81	*0.78*		
4	H	1.07	*1.07*	2.82	*3.31*	1.03	*1.04*	3.68	*3.34*
	L	0.98	*0.99*			1.02	*1.01*		

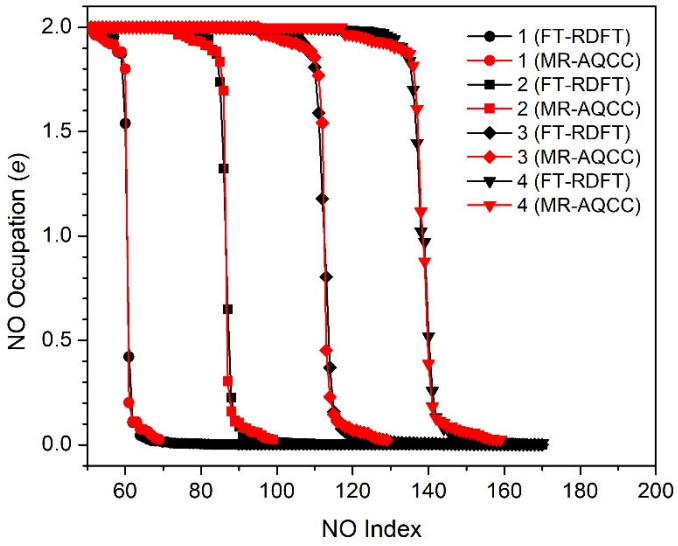

Figure S1: Comparison between FT-RDFT/M05-2X f_i occupation and MR-AQCC NO occupation for the *n*-acenes (**1-4**). FT-RDFT calculations performed at the literature-recommended FT of 16200 K.

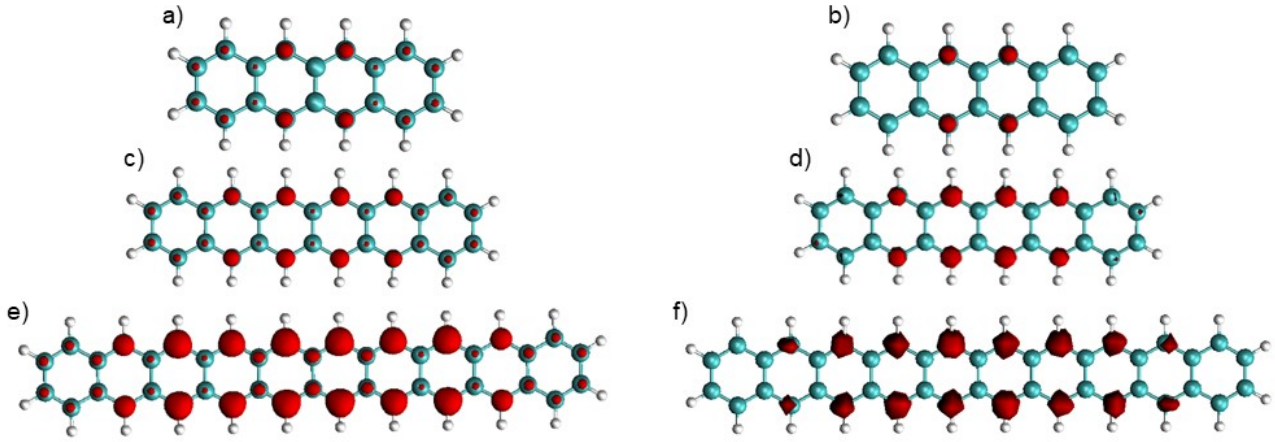

Figure S2: Total MR-AQCC unpaired density plots for a) **1**, c) **2,** and e) **4** and the corresponding FT-DFT FOD (TPSS density functional, literature-recommended temperature, 5000 K) for b) **1**, d) **2**, and f) **4**. The isovalue = 0.004 *e*/bohr^3

Table S4: HOMO-LUMO f_i and N_{FOD} values (M05-2X/def2-TZVP, TPSS/def2-TZVP, and B3LYP/def2-TZVP method with FT-UDFT approaches) for trans-diindenoacenes (**5-9**) and cis-diindenoacenes (**10-14**) at TPSS optimized geometry. FT-UDFT calculations performed with literature-recommended temperatures (M05-2X: 16200 K, TPSS: 5000 K, B3LYP: 9000 K) and improved present temperatures (M05-2X: 12200 K, TPSS: 6200 K, B3LYP: 8200 K, values in italics). All values are given in units of *e*.

Str		FT-UDFT/M05-2X/FOD				FT-UDFT/TPSS/FOD		FT-UDFT/B3LYP/FOD			
		f_i Values		N_{FOD}		f_i Values	N_{FOD}	f_i Values		N_{FOD}	
5	H	-	-	-	-	-	-	-	-	-	-
	L	-	-			-		-	-		
6	H	1.44	*1.58*	2.80	*1.51*	-	-	1.53	*1.56*	1.70	*1.46*
	L	0.73	*0.56*			-		0.65	*0.59*		
7	H	1.33	*1.45*	3.36	*1.91*	-	-	1.41	*1.43*	2.08	*1.81*
	L	0.78	*0.66*			-		0.72	*0.67*		
8	H	1.24	*1.33*	3.93	*2.32*	1.35 *1.31*	1.72 *2.16*	1.30	*1.32*	2.49	*2.19*
	L	0.82	*0.73*			0.65 *0.73*		0.77	*0.73*		
9	H	1.18	*1.25*	4.50	*2.71*	1.27 *1.24*	2.04 *2.54*	1.39	*1.43*	2.52	*2.14*
	L	0.84	*0.77*			0.68 *0.75*		0.65	*0.59*		
10	H	1.65	*1.47*	1.87	*1.66*	1.44 *1.41*	1.39 *1.65*	1.41	*1.43*	1.83	*1.65*
	L	0.46	*0.71*			0.68 *0.78*		0.80	*0.75*		
11	H	1.63	*1.38*	2.17	*1.94*	1.38 *1.35*	1.51 *1.82*	1.46	*1.50*	1.76	*1.52*
	L	0.45	*0.77*			0.71 *0.80*		0.67	*0.62*		
12	H	1.22	*1.28*	3.59	*2.25*	1.30 *1.27*	1.72 *2.08*	1.35	*1.36*	2.16	*1.92*
	L	0.89	*0.82*			0.76 *0.82*		0.77	*0.74*		
13	H	1.15	*1.20*	4.11	*2.58*	1.21 *1.19*	1.98 *2.39*	1.51	*1.54*	1.97	*1.66*
	L	0.90	*0.85*			0.78 *0.84*		0.54	*0.49*		
14	H	1.10	*1.14*	4.65	*2.93*	1.14 *1.13*	2.28 *2.74*	1.47	*1.50*	2.26	*1.92*
	L	0.91	*0.87*			0.81 *0.85*		0.54	*0.49*		

Table S5: HOMO-LUMO f_i and N_{FOD} values (TPSS/def2-TZVP and B3LYP/def2-TZVP methods with FT-RDFT approach) for trans-diindenoacenes (**5-9**) and cis-diindenoacenes (**10-14**) at TPSS optimized geometry. FT-RDFT calculations performed with literature-recommended temperature (TPSS: 5000 K, B3LYP: 9000 K) and improved present temperature (TPSS: 6200 K, B3LYP: 8200 K, values italics). All values are given in units of *e*.

Str		FT-RDFT/TPSS/FOD		FT-RDFT/B3LYP/FOD			
		f_i Values	N_{FOD}	f_i Values		N_{FOD}	
5	H	1.77 *1.70*	0.78 *1.12*	1.69	*1.73*	1.30	*1.08*
	L	0.37 *0.50*		0.52	*0.46*		
6	H	1.60 *1.54*	1.10 *1.47*	1.53	*1.56*	1.70	*1.46*
	L	0.50 *0.62*		0.65	*0.59*		
7	H	1.47 *1.42*	1.39 *1.80*	1.41	*1.43*	2.08	*1.81*
	L	0.59 *0.68*		0.72	*0.67*		
8	H	1.36 *1.31*	1.72 *2.18*	1.30	*1.32*	2.49	*2.19*
	L	0.65 *0.73*		0.77	*0.73*		
9	H	1.27 *1.24*	2.04 *2.54*	1.23	*1.25*	2.89	*2.56*
	L	0.68 *0.75*		0.79	*0.76*		
10	H	1.44 *1.41*	1.39 *1.65*	1.41	*1.43*	1.83	*1.65*
	L	0.68 *0.78*		0.80	*0.75*		
11	H	1.38 *1.35*	1.51 *1.82*	1.35	*1.36*	2.05	*1.84*
	L	0.71 *0.80*		0.83	*0.79*		
12	H	1.30 *1.27*	1.72 *2.08*	1.26	*1.28*	2.36	*2.11*
	L	0.76 *0.82*		0.85	*0.82*		
13	H	1.21 *1.19*	1.98 *2.39*	1.19	*1.20*	2.70	*2.42*
	L	0.79 *0.84*		0.87	*0.85*		
14	H	1.14 *1.13*	2.28 *2.74*	1.13	*1.14*	3.08	*2.76*
	L	0.81 *0.85*		0.88	*0.86*		

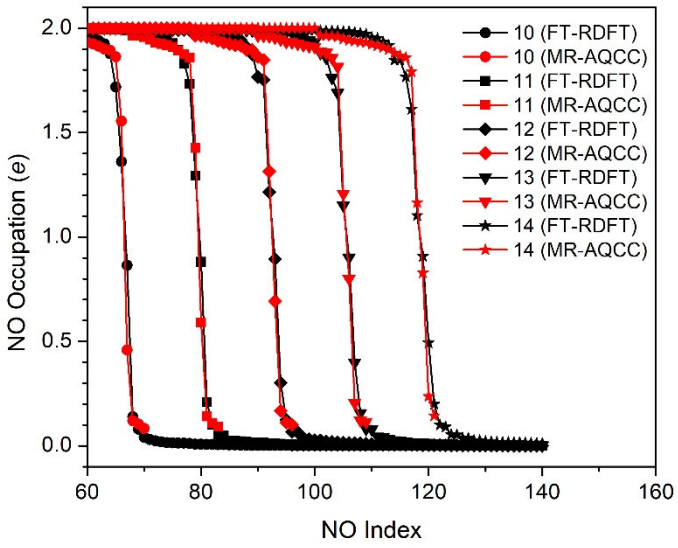

Figure S3: Comparison between FT-RDFT/M05-2X f_i occupation and MR-AQCC NO occupation for all cis-diindenoacenes (**10-14**). FT-RDFT calculations performed with the literature-recommended FT of 16200 K.

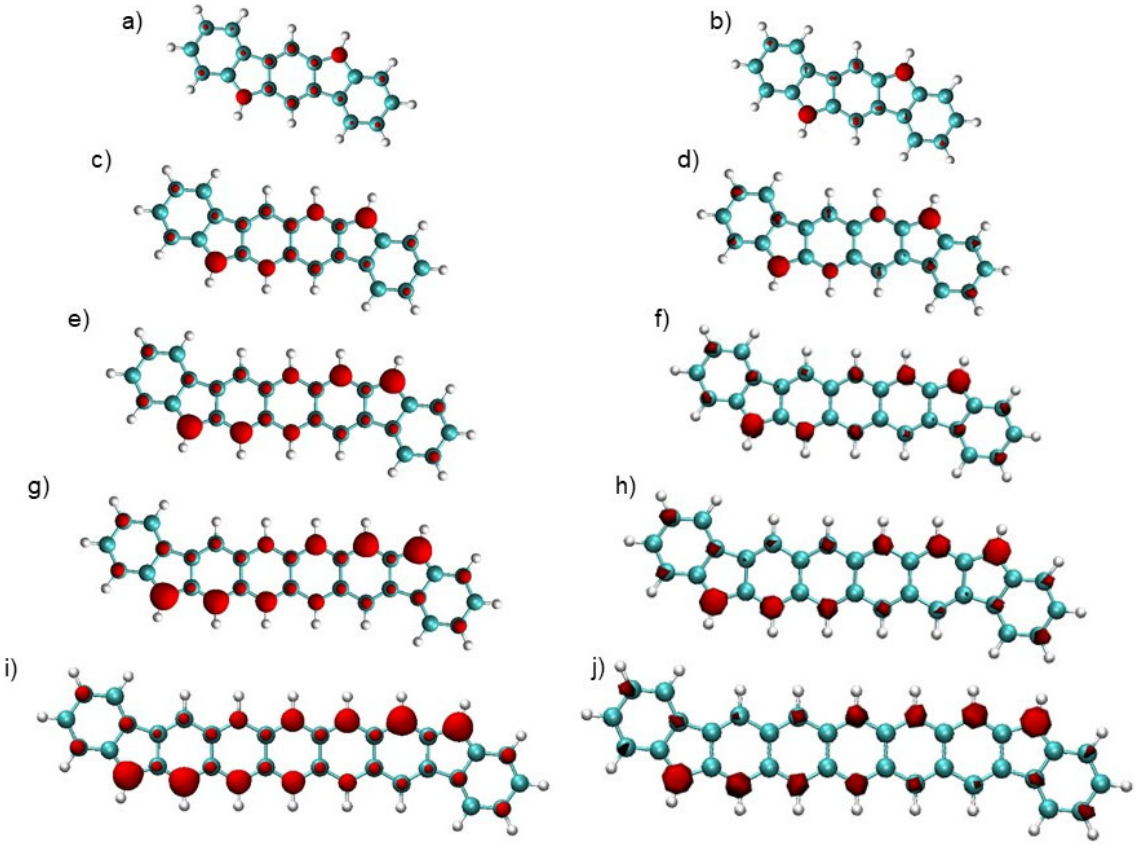

Figure S4: Total MR-AQCC unpaired density plots for a) **5**, c) **6**, e) **7**, g) **8**, and i) **9** and the corresponding FT-DFT FOD (TPSS density functional, literature-recommended temperature, 5000 K) for b) **5**, d) **6**, f) **7**, h) **8**, and j) **9**. The isovalue = 0.004 *e*/bohr^3

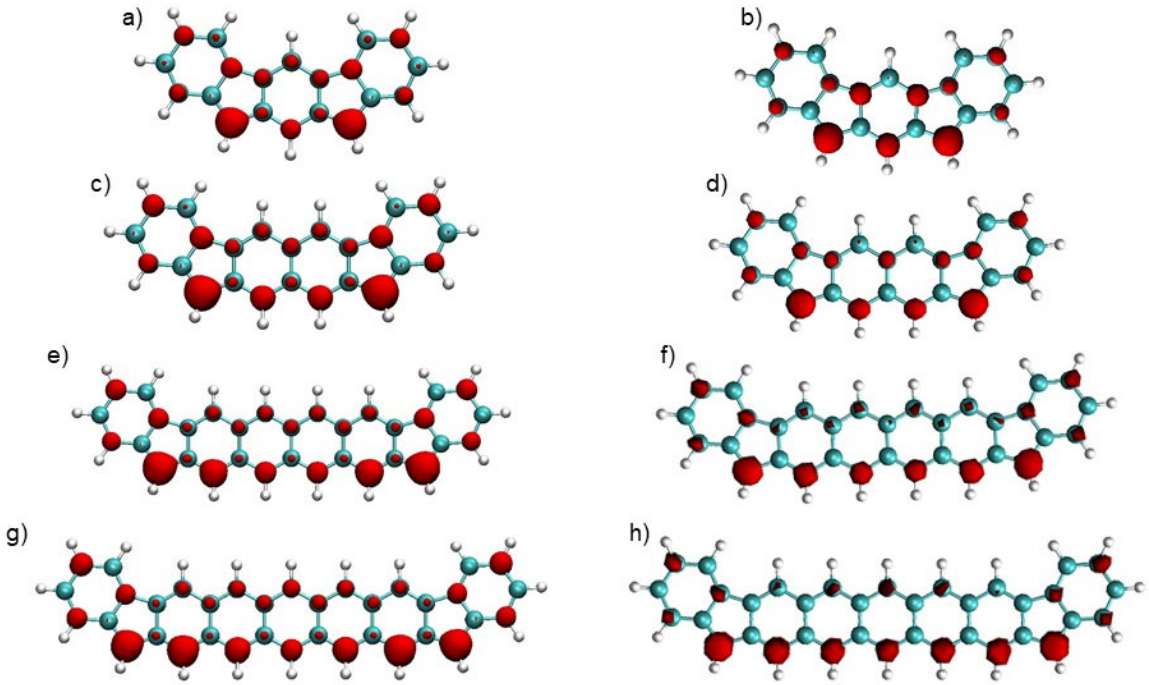

Figure S5: Total MR-AQCC unpaired density plots for a) **10**, c) **11**, e) **13**, and g) **14**and the corresponding FT-DFT FOD (TPSS density functional, literature-recommended temperature, 5000 K) for b) **10**, d) 11, f) **13**, and h) **14**. The isovalue = 0.004 *e*/bohr^3

Table S6: HOMO-LUMO f_i and N_{FOD} values (M05-2X/def2-TZVP, TPSS/def2-TZVP, and B3LYP/def2-TZVP method with FT-UDFT approaches) for the zethrenes (**15-19**) at TPSS optimized geometry. FT-DFT calculations performed with the literature-recommended temperature (M05-2X: 16200 K, TPSS: 5000 K, B3LYP: 9000 K) and improved present temperature (M05-2X: 12200 K, TPSS: 6200 K, B3LYP: 8200 K, values italics). The $N_{U,red.}$ and $N_{FOD,red.}$ values are provided in parentheses for structures with triplet ground states (**17** and **19**). All values are given in units of *e*.

Str		FT-UDFT/M05-2X/FOD			FT-UDFT/TPSS/FOD			FT-UDFT/B3LYP/FOD		
		f_i Values		N_{FOD} ($N_{FOD,red.}$)	f_i Values		N_{FOD} ($N_{FOD,red.}$)	f_i Values		N_{FOD} ($N_{FOD,red.}$)
15	H	1.21	*1.36*	3.94 *2.12*	-	-	-	1.31	*1.35*	2.30 *1.97*
	L	0.67	*0.56*		-	-		0.63	*0.60*	
16	H	1.19	*1.34*	3.18 *1.82*	1.35	*1.29*	1.39 *1.70*	1.38	*1.43*	1.75 *1.49*
	L	0.72	*0.62*		0.64	*0.71*		0.60	*0.56*	
17	H	1.73	*1.86*		1.89	*1.91*		1.81	*1.84*	
	S1	0.99	*1.01*	4.92 *3.23*	1.01	*1.00*	2.69 *2.33*	1.02	*1.02*	3.52 *3.19*
	S2	0.94	*0.96*	(2.92) *(1.23)*	0.98	*0.99*	(0.69) *(0.33)*	0.97	*0.97*	(1.52) *(1.19)*
	L	0.26	*0.14*		0.12	*0.10*		0.20	*0.17*	
18	H	-	-	-	-	-	-	-	-	-
	L	-	-		-	-		-	-	
19	H	1.79	*1.89*		1.93	*1.88*		1.87	*1.89*	
	S1	0.97	*0.99*	4.88 *3.31*	1.00	*1.00*	2.66 3.*19*	1.00	*1.00*	3.47 *3.13*
	S2	0.96	*0.98*	(2.88) *(1.31)*	0.99	*0.99*	(0.66) (1.*19)*	0.99	*0.99*	(1.47) *(1.13)*
	L	0.20	*0.11*		0.08	*0.13*		0.14	*0.11*	

Table S7: HOMO-LUMO f_i and N_{FOD} values (TPSS/def2-TZVP and B3LYP/def2-TZVP methods with FT-RDFT approach) for the zethrenes (**15, 16, 19**) at TPSS optimized geometry. FT-DFT calculations performed with literature-recommended temperature (TPSS: 5000 K, B3LYP: 9000 K) and improved present temperature (TPSS: 6200 K, B3LYP: 8200 K, values italics). All values are given in units of *e*.

Str[a]		FT-RDFT/TPSS/FOD			FT-RDFT/B3LYP/FOD		
		f_i Values		N_{FOD}	f_i Values		N_{FOD}
15	H	1.40	*1.33*	1.48 *1.95*	1.31	*1.35*	2.30 *1.97*
	L	0.55	*0.62*		0.63	*0.60*	
16	H	1.35	*1.29*	1.39 *1.70*	1.28	*1.31*	1.96 *1.72*
	L	0.64	*0.71*		0.70	*0.67*	
18	H	1.84	*1.76*	0.55 *0.97*	1.75	*1.79*	1.23 *0.95*
	L	0.14	*0.22*		0.23	*0.19*	

[a]Structures **17** and **19** have triplet ground states so the f_i and N_{FOD} values were not computed with FT-RDFT.

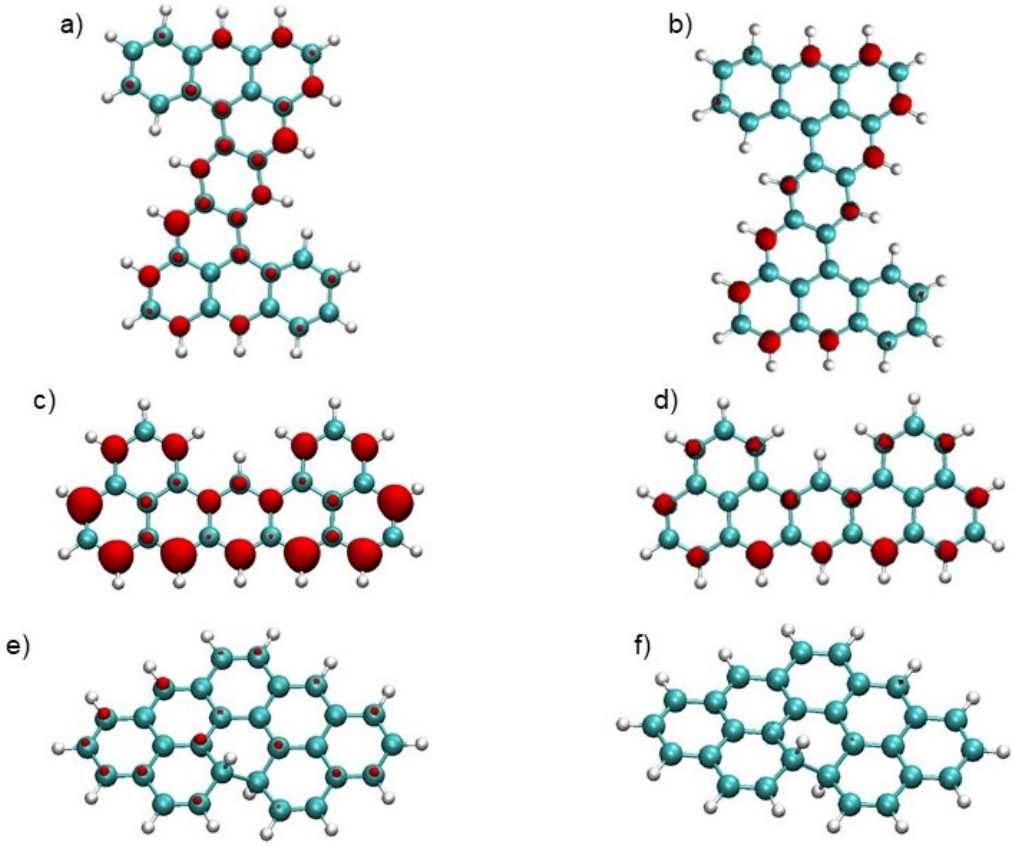

Figure S6: Total MR-AQCC unpaired density plots for a) **15**, c) **17**, and e) **18** and the corresponding FT-DFT FOD (TPSS density functional, literature-recommended temperature, 5000 K) for b) **15**, d) **17**, and f) **18**. The isovalue = 0.004 *e*/bohr^3

Table S8: HOMO-LUMO f_i and N_{FOD} values (TPSS/def2-TZVP and B3LYP/def2-TZVP methods with FT-RDFT approach) for **25-29** at TPSS optimized geometry. FT-DFT calculations performed with literature-recommended temperature (TPSS: 5000 K, B3LYP: 9000 K) and improved present temperature (TPSS: 6200 K, B3LYP: 8200 K, values italics). All values are given in units of *e*.

Str[a]		FT-RDFT/TPSS/FOD				FT-RDFT/B3LYP/FOD			
		f_i Values		N_{FOD}		f_i Values		N_{FOD}	
25	H	1.95	*1.90*	0.22	*0.43*	1.88	*1.90*	0.60	*0.44*
	L	0.10	*0.18*			0.21	*0.16*		
26	H	1.90	*1.84*	0.46	*0.84*	1.82	*1.86*	1.10	*0.84*
	L	0.18	*0.28*			0.30	*0.25*		
27	H	1.65	*1.56*	0.72	*0.97*	1.54	*1.58*	1.10	*0.94*
	L	0.35	*0.45*			0.47	*0.42*		
28	H	1.65	*1.56*	0.81	*1.11*	1.54	*1.59*	1.26	*1.07*
	L	0.36	*0.46*			0.48	*0.43*		
29	H	1.43	*1.38*	1.23	*1.46*	1.39	*1.42*	1.56	*1.41*
	L	0.57	*0.62*			0.62	*0.59*		

[a]Structures **20**-**24** have doublet or triplet ground states so the f_i and N_{FOD} values were not computed with FT-RDFT.

Table S9: HOMO-LUMO f_i and N_{FOD} values (M05-2X/def2-TZVP, TPSS/def2-TZVP, and B3LYP/def2-TZVP method with FT-UDFT approaches) for **20-29** at TPSS optimized geometry. FT-DFT calculations performed with literature-recommended temperature (M05-2X: 16200 K, TPSS: 5000 K, B3LYP: 9000 K) and improved present temperature (M05-2X: 12200 K, TPSS: 6200 K, B3LYP: 8200 K, values italics). The $N_{U,red.}$ and $N_{FOD,red.}$ values are provided in parentheses for structures with doublet or triplet ground states (**20**-**24**). All values are given in units of *e*.

Str		FT-UDFT/M05-2X/FOD				FT-UDFT/TPSS/FOD				FT-UDFT/B3LYP/FOD			
		f_i Values		N_{FOD} ($N_{FOD,red.}$)		f_i Values		N_{FOD} ($N_{FOD,red.}$)		f_i Values		N_{FOD} ($N_{FOD,red.}$)	
20	H	1.89	*1.95*	2.29 (1.29)	*1.62 (0.62)*	1.98	*1.96*	1.23 (0.23)	*1.47 (0.47)*	1.95	*1.96*	1.61 (0.61)	*1.46 (0.46)*
	S1	0.96	*0.98*			1.00	*1.00*			1.00	*1.00*		
	L	0.11	*0.06*			0.02	*0.05*			0.06	*0.04*		
21	H	1.85	*1.93*	4.21 (2.21)	*2.96 (0.96)*	1.96	*1.93*	2.43 (0.43)	*2.85 (0.85)*	1.91	*1.93*	3.08 (1.08)	*2.82 (0.82)*
	S1	0.99	*1.00*			1.01	*1.01*			1.01	*1.01*		
	S2	0.99	*1.00*			1.01	*1.01*			1.01	*1.01*		
	L	0.14	*0.07*			0.04	*0.07*			0.08	*0.06*		
22	H	1.87	*1.94*	3.56 (2.56)	*2.12 (1.12)*	1.85	*1.84*	2.11 (1.11)	*2.53 (1.53)*	1.91	*1.91*	2.31 (1.31)	*2.28 (1.28)*
	S1	1.21	*1.12*			1.23	*1.24*			1.15	*1.18*		
	L	0.25	*0.11*			0.10	*0.15*			0.15	*0.13*		
23	H	1.79	*1.89*	3.50 (2.50)	*2.17 (1.17)*	1.94	*1.90*	1.64 (0.64)	*2.02 (1.02)*	1.88	*1.90*	2.29 (1.29)	*2.01 (1.01)*
	S1	0.95	*0.96*			0.98	*0.98*			0.98	*0.98*		
	L	0.21	*0.11*			0.08	*0.12*			0.13	*0.11*		
24	H	1.76	*1.86*	2.36 (1.36)	*1.61 (0.61)*	1.89	*1.83*	1.35 (0.35)	*1.62 (0.62)*	1.85	*1.86*	1.66 (0.66)	*1.56 (0.56)*
	S1	1.11	*1.09*			1.10	*1.13*			1.10	*1.11*		
	L	0.15	*0.07*			0.03	*0.08*			0.09	*0.07*		
25	H	-	-	-	-	-	-	-	-	-	-	-	-
	L	-	-			-	-			-	-		
26	H	-	-	-	-	-	-	-	-	-	-	-	-
	L	-	-			-	-			-	-		
27	H	1.42	*1.61*	1.78	*0.94*	-	-	-	-	1.54	*1.58*	1.10	*0.94*
	L	0.53	*0.38*			-	-			0.47	*0.42*		
28	H	1.67	*1.80*	1.45	*0.66*	-	-	-	-	1.54	*1.59*	1.26	*1.07*
	L	0.30	*0.19*			-	-			0.48	*0.43*		
29	H	-	-	-	-	-	-	-	-	-	-	-	-
	L	-	-			-	-			-	-		

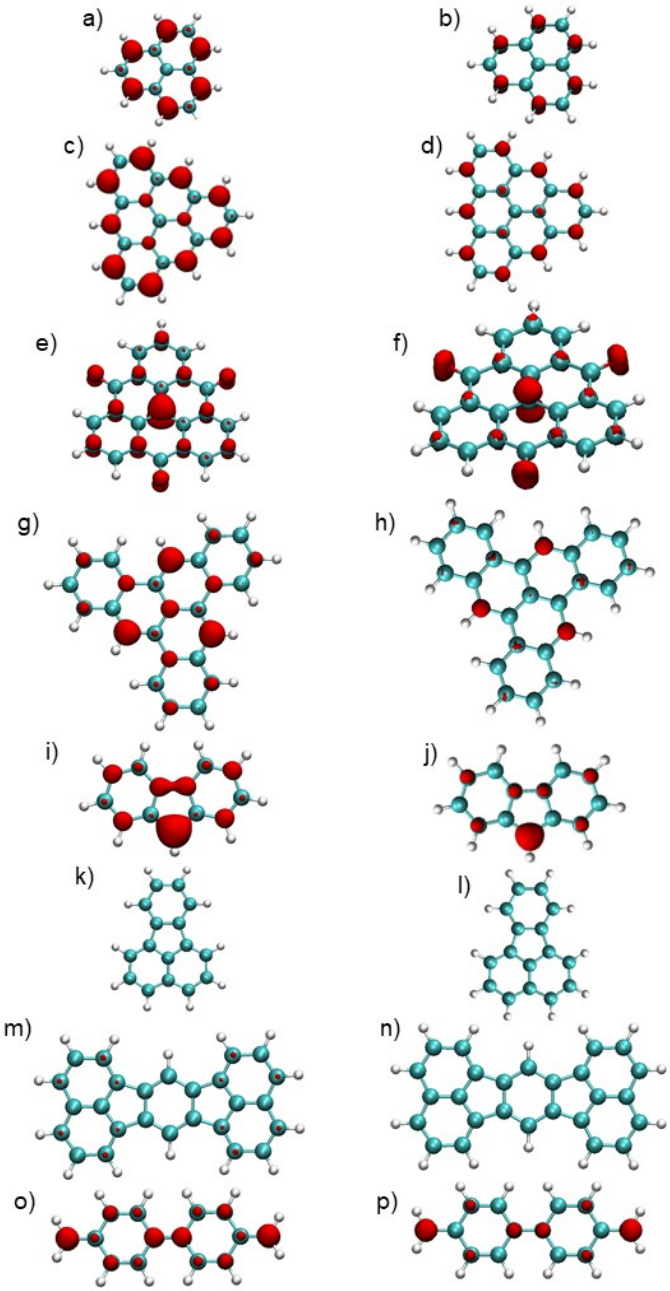

Figure S7: Total MR-AQCC unpaired density plots for a) **20**, c) 2**1**, e) **22** , g) **23**, i) **24**, k) **25**, m) **26**, and o) **27** and the corresponding FT-DFT FOD (TPSS density functional, literature-recommended temperature, 5000 K) for b) **20**, d) 2**1**, f) **22** , h) **23**, j) **24**, l) **25**, n) **26**, and p) **27**. The isovalue = 0.004 *e*/bohr^3

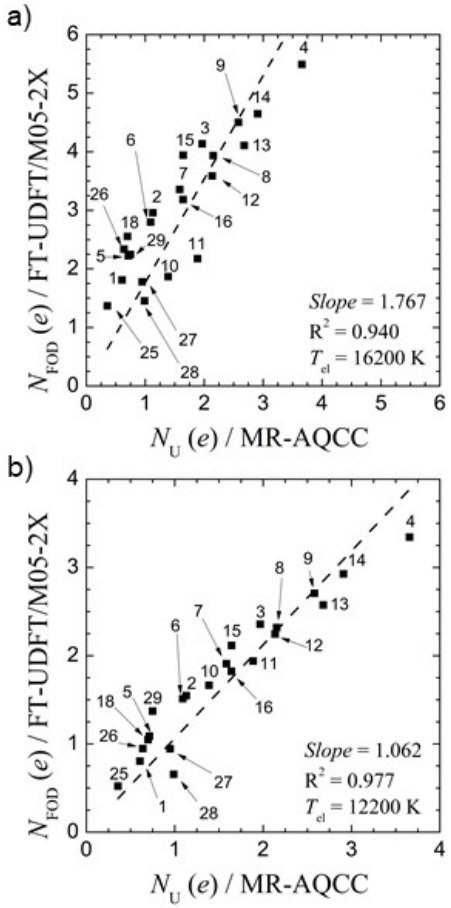

Figure S8: Comparison between MR-AQCC N_U values and FT-UDFT N_{FOD} numbers using the M05-2X density functional for structures with singlet ground electronic state (**1-16, 18, 25-29**) using a) the literature-recommended FT of 16200 K and b) the improved present FT of 12200 K. Included are the FT-RDFT structures for which there is no triplet instability: **1, 5, 18, 25, 26, 29.**

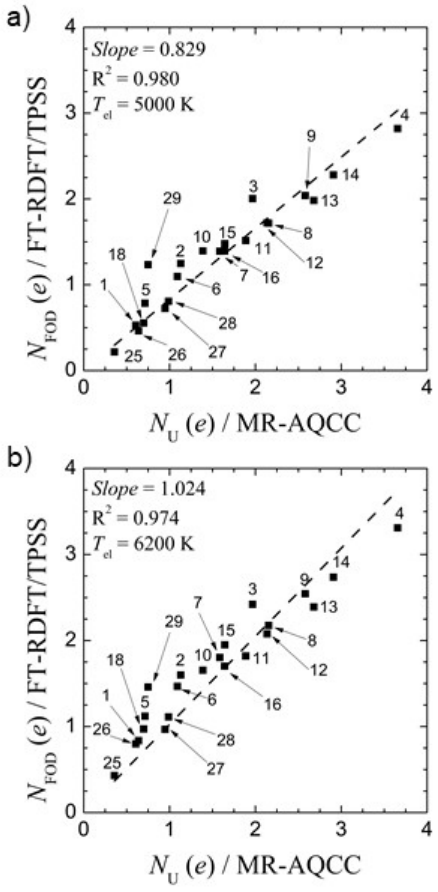

Figure S9: Comparison between MR-AQCC N_U values and FT-RDFT N_{FOD} numbers with the TPSS density functional for structures with singlet ground electronic state (**1-16, 18, 25-29**) using the a) literature-recommended FT of 5000 K and b) improved present FT of 6200 K.

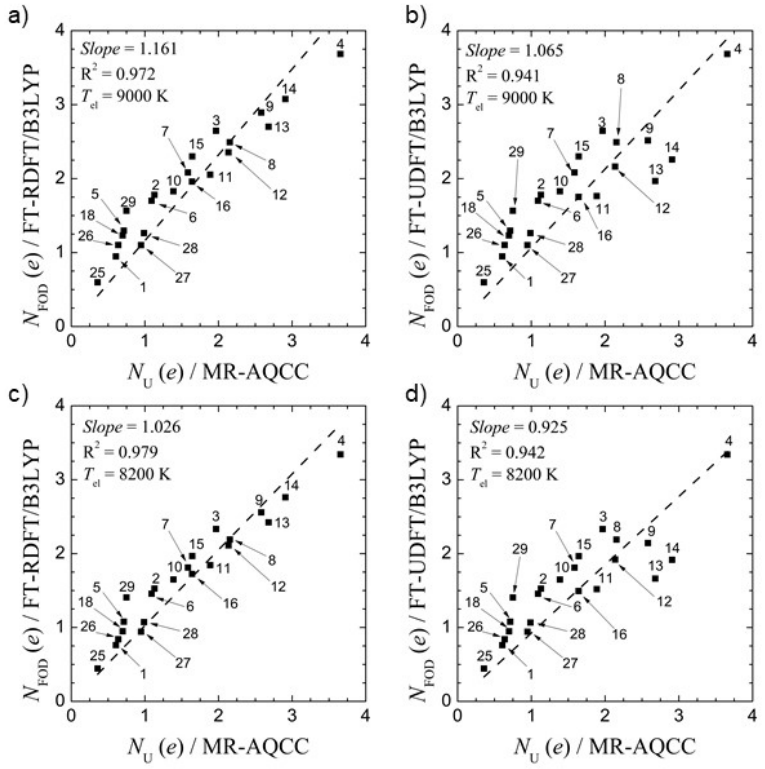

Figure S10: Comparison between MR-AQCC N_U values and a,c) FT-RDFT and b,d) FT-UDFT N_{FOD} numbers with the B3LYP density functional for structures with singlet ground electronic state (**1-16, 18, 25-29**) using the a,b) literature-recommended FT of 9000 K and c,d) improved present FT of 8200 K. Included in the FT-UDFT plots b,d) are the FT-RDFT structures for which there is no triplet instability: **1, 5, 18, 25, 26, 29**.

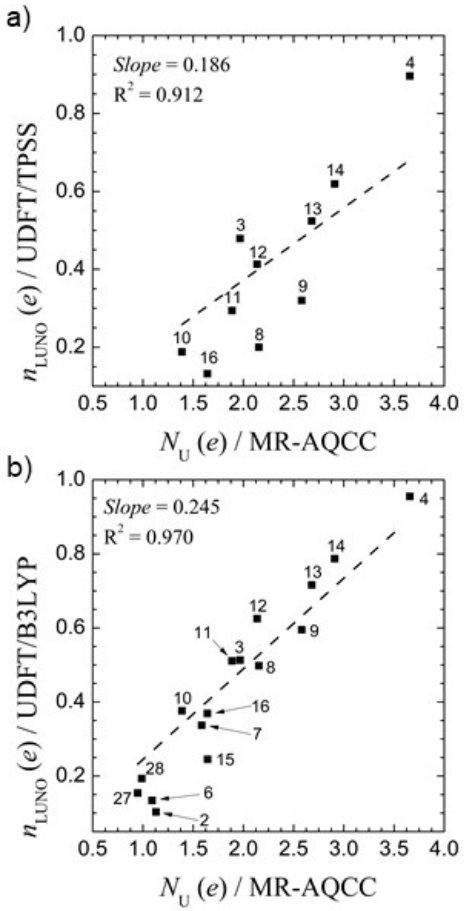

Figure S11. Comparison between the MR-AQCC and a) UDFT/TPSS and b) UDFT/B3LYP LUNO occupation for all UDFT structures with singlet ground state.

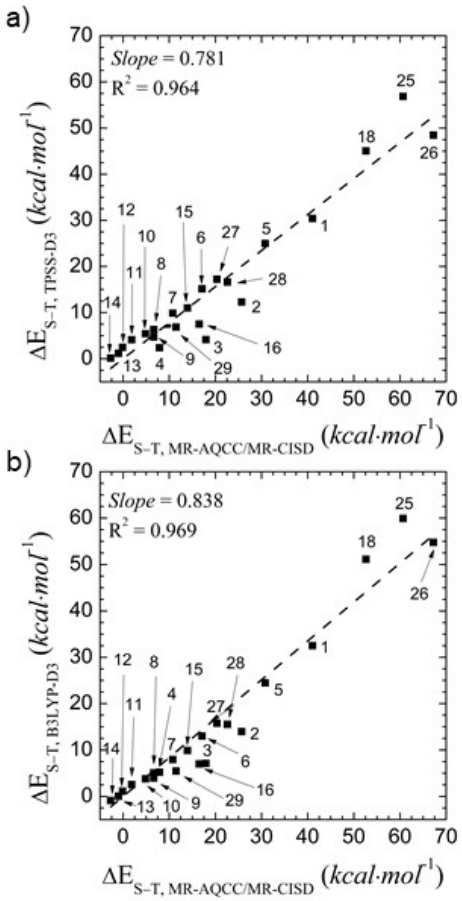

Figure S12. Comparison between the MR-AQCC/MR-CISD+Q and a) TPSS and b) B3LYP singlet/triplet energy (ΔE_{S-T}) for structures with singlet ground electronic state (MR-AQCC: **1-15, 18, 25, 27-29**; MR-CISD+Q: **16**, **26**)..

Optimized Geometries:

Cartesian coordinates are in Å

```
Structure 1,         TPSS
C    0.0000000    0.0000000    0.7268362
C    0.0000000    0.0000000   -0.7268362
C    0.0000000    2.4503076    0.7260090
C    0.0000000   -2.4503076    0.7260090
C    0.0000000    2.4503076   -0.7260090
C    0.0000000   -2.4503076   -0.7260090
C   -0.0000000    1.2341554    1.4069158
C   -0.0000000   -1.2341554    1.4069158
C   -0.0000000    1.2341554   -1.4069158
C   -0.0000000   -1.2341554   -1.4069158
C    0.0000000    4.8870981    0.7138033
C    0.0000000   -4.8870981    0.7138033
C    0.0000000    4.8870981   -0.7138033
C   -0.0000000   -4.8870981   -0.7138033
C   -0.0000000    3.7078954    1.4084613
C    0.0000000   -3.7078954    1.4084613
C   -0.0000000    3.7078954   -1.4084613
C   -0.0000000   -3.7078954   -1.4084613
H   -0.0000000    1.2344783    2.4954285
H    0.0000000   -1.2344783    2.4954285
H   -0.0000000    1.2344783   -2.4954285
H   -0.0000000   -1.2344783   -2.4954285
H    0.0000000    5.8344541    1.2459907
H    0.0000000   -5.8344541    1.2459907
H   -0.0000000    5.8344541   -1.2459907
H    0.0000000   -5.8344541   -1.2459907
H    0.0000000    3.7065523    2.4960405
H   -0.0000000   -3.7065523    2.4960405
H    0.0000000    3.7065523   -2.4960405
H   -0.0000000   -3.7065523   -2.4960405

Structure 2,         TPSS
C    0.0000000    4.9063312    0.7283517
C    0.0000000   -4.9063312    0.7283517
C    0.0000000    4.9063312   -0.7283517
C    0.0000000   -4.9063312   -0.7283517
C   -0.0000000    6.1670107    1.4100209
C    0.0000000   -6.1670107    1.4100209
C    0.0000000    6.1670107   -1.4100209
C    0.0000000   -6.1670107   -1.4100209
C   -0.0000000    7.3441562    0.7153330
C    0.0000000   -7.3441562    0.7153330
```

```
C    0.0000000    7.3441562   -0.7153330
C    0.0000000   -7.3441562   -0.7153330
C   -0.0000000    3.6952175    1.4091281
C    0.0000000   -3.6952175    1.4091281
C   -0.0000000    3.6952175   -1.4091281
C   -0.0000000   -3.6952175   -1.4091281
C    0.0000000    2.4540163    0.7302636
C    0.0000000   -2.4540163    0.7302636
C    0.0000000    2.4540163   -0.7302636
C    0.0000000   -2.4540163   -0.7302636
C    0.0000000    0.0000000    0.7309610
C    0.0000000    0.0000000   -0.7309610
C    0.0000000    1.2311673    1.4104143
C    0.0000000   -1.2311673    1.4104143
C    0.0000000    1.2311673   -1.4104143
C   -0.0000000   -1.2311673   -1.4104143
H    0.0000000    6.1661433    2.4975913
H   -0.0000000   -6.1661433    2.4975913
H    0.0000000    6.1661433   -2.4975913
H   -0.0000000   -6.1661433   -2.4975913
H    0.0000000    8.2922097    1.2463237
H    0.0000000   -8.2922097    1.2463237
H    0.0000000    8.2922097   -1.2463237
H    0.0000000   -8.2922097   -1.2463237
H   -0.0000000    3.6956874    2.4976009
H    0.0000000   -3.6956874    2.4976009
H    0.0000000    3.6956874   -2.4976009
H   -0.0000000   -3.6956874   -2.4976009
H    0.0000000    1.2312031    2.4987034
H   -0.0000000   -1.2312031    2.4987034
H    0.0000000    1.2312031   -2.4987034
H    0.0000000   -1.2312031   -2.4987034

Structure 3,         TPSS
C    0.0000000    7.3639973    0.7289102
C    0.0000000   -7.3639973    0.7289102
C   -0.0000000    7.3639965   -0.7289096
C    0.0000000   -7.3639965   -0.7289096
C    0.0000000    8.6254804    1.4102088
C    0.0000000   -8.6254804    1.4102088
C    0.0000000    8.6254801   -1.4102093
C    0.0000000   -8.6254801   -1.4102093
C   -0.0000000    9.8021391    0.7158015
C    0.0000000   -9.8021391    0.7158015
C    0.0000000    9.8021382   -0.7158017
C    0.0000000   -9.8021382   -0.7158017
C    0.0000000    6.1543409    1.4097198
```

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C    0.0000000   -6.1543409    1.4097198
C    0.0000000    6.1543410   -1.4097213
C    0.0000000   -6.1543410   -1.4097213
C   -0.0000000    4.9112630    0.7312335
C   -0.0000000   -4.9112630    0.7312335
C    0.0000000    4.9112603   -0.7312352
C    0.0000000   -4.9112603   -0.7312352
C    0.0000000    2.4561176    0.7325508
C    0.0000000   -2.4561176    0.7325508
C    0.0000000    2.4561139   -0.7325582
C    0.0000000   -2.4561139   -0.7325582
C   -0.0000000    3.6911053    1.4113196
C    0.0000000   -3.6911053    1.4113196
C    0.0000000    3.6911033   -1.4113239
C    0.0000000   -3.6911033   -1.4113239
C   -0.0000000    0.0000000    0.7329462
C   -0.0000000    0.0000000   -0.7329571
C    0.0000000    1.2301795    1.4119673
C    0.0000000   -1.2301795    1.4119673
C    0.0000000    1.2301779   -1.4119750
C   -0.0000000   -1.2301779   -1.4119750
H   -0.0000000    8.6248349    2.4977217
H   -0.0000000   -8.6248349    2.4977217
H    0.0000000    8.6248354   -2.4977205
H   -0.0000000   -8.6248354   -2.4977205
H    0.0000000   10.7496634    1.2476598
H    0.0000000  -10.7496634    1.2476598
H    0.0000000   10.7496620   -1.2476601
H   -0.0000000  -10.7496620   -1.2476601
H    0.0000000    6.1551988    2.4982078
H    0.0000000   -6.1551988    2.4982078
H    0.0000000    6.1551988   -2.4982052
H    0.0000000   -6.1551988   -2.4982052
H    0.0000000    3.6915703    2.4996434
H    0.0000000   -3.6915703    2.4996434
H    0.0000000    3.6915695   -2.4996347
H    0.0000000   -3.6915695   -2.4996347
H   -0.0000000    1.2303717    2.5002760
H    0.0000000   -1.2303717    2.5002760
H   -0.0000000    1.2303711   -2.5002601
H    0.0000000   -1.2303711   -2.5002601

Structure 4,         TPSS
C    0.0000000    7.4002310    0.7256661
C    0.0000000   -7.4002310    0.7256661
C    0.0000000    7.4002320   -0.7256696
C    0.0000000   -7.4002320   -0.7256696
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C	0.0000000	8.6220252	1.4036195
C	0.0000000	-8.6220252	1.4036195
C	0.0000000	8.6220258	-1.4036218
C	0.0000000	-8.6220258	-1.4036218
C	0.0000000	9.8540946	0.7215452
C	0.0000000	-9.8540946	0.7215452
C	0.0000000	9.8540948	-0.7215474
C	0.0000000	-9.8540948	-0.7215474
C	0.0000000	6.1529885	1.4047807
C	-0.0000000	-6.1529885	1.4047807
C	0.0000000	6.1529889	-1.4047841
C	0.0000000	-6.1529889	-1.4047841
C	0.0000000	4.9383045	0.7287547
C	0.0000000	-4.9383045	0.7287547
C	0.0000000	4.9383054	-0.7287591
C	0.0000000	-4.9383054	-0.7287591
C	0.0000000	2.4706251	0.7303879
C	0.0000000	-2.4706251	0.7303879
C	-0.0000000	2.4706255	-0.7303930
C	0.0000000	-2.4706255	-0.7303930
C	-0.0000000	3.6893500	1.4042480
C	0.0000000	-3.6893500	1.4042480
C	0.0000000	3.6893499	-1.4042517
C	0.0000000	-3.6893499	-1.4042517
C	0.0000000	0.0000000	0.7308852
C	-0.0000000	0.0000000	-0.7308905
C	-0.0000000	1.2293334	1.4033379
C	0.0000000	-1.2293334	1.4033379
C	0.0000000	1.2293332	-1.4033415
C	0.0000000	-1.2293332	-1.4033415
C	0.0000000	11.1007845	1.4038719
C	0.0000000	-11.1007845	1.4038719
C	0.0000000	11.1007853	-1.4038728
C	0.0000000	-11.1007853	-1.4038728
C	-0.0000000	12.2896929	0.7084268
C	0.0000000	-12.2896929	0.7084268
C	-0.0000000	12.2896935	-0.7084279
C	0.0000000	-12.2896935	-0.7084279
H	0.0000000	8.6233993	2.4922327
H	-0.0000000	-8.6233993	2.4922327
H	0.0000000	8.6233996	-2.4922285
H	0.0000000	-8.6233996	-2.4922285
H	-0.0000000	6.1538867	2.4934098
H	0.0000000	-6.1538867	2.4934098
H	0.0000000	6.1538870	-2.4934031
H	0.0000000	-6.1538870	-2.4934031
H	-0.0000000	3.6898774	2.4929979

```
H    0.0000000   -3.6898774    2.4929979
H    0.0000000    3.6898775   -2.4929888
H    0.0000000   -3.6898775   -2.4929888
H   -0.0000000    1.2295513    2.4921804
H    0.0000000   -1.2295513    2.4921804
H    0.0000000    1.2295512   -2.4921693
H   -0.0000000   -1.2295512   -2.4921693
H    0.0000000   11.0998258    2.4914425
H    0.0000000  -11.0998258    2.4914425
H    0.0000000   11.0998257   -2.4914410
H    0.0000000  -11.0998257   -2.4914410
H    0.0000000   13.2342565    1.2453906
H    0.0000000  -13.2342565    1.2453906
H   -0.0000000   13.2342581   -1.2453905
H    0.0000000  -13.2342581   -1.2453905

Structure 5,         TPSS
C    1.4479132   -0.0024265    0.0000000
C   -1.4479132    0.0024265    0.0000000
C    0.6973477    1.2145285    0.0000000
C   -0.6973477   -1.2145285    0.0000000
C   -0.7660864    1.1874432    0.0000000
C    0.7660864   -1.1874432    0.0000000
C    1.1163174    2.5338031    0.0000000
C   -1.1163174   -2.5338031    0.0000000
C   -0.0422358    3.4002312    0.0000000
C    0.0422358   -3.4002312    0.0000000
C   -1.2129844    2.5817331    0.0000000
C    1.2129844   -2.5817331    0.0000000
C   -0.1538955    4.7934407    0.0000000
C    0.1538955   -4.7934407    0.0000000
C   -1.4281327    5.3672910    0.0000000
C    1.4281327   -5.3672910    0.0000000
C   -2.4741889    3.1658292    0.0000000
C    2.4741889   -3.1658292    0.0000000
C   -2.5738748    4.5637387    0.0000000
C    2.5738748   -4.5637387    0.0000000
H    2.5354794    0.0322910    0.0000000
H   -2.5354794   -0.0322910    0.0000000
H    2.1471910    2.8727558    0.0000000
H   -2.1471910   -2.8727558    0.0000000
H    0.7329717    5.4220368    0.0000000
H   -0.7329717   -5.4220368    0.0000000
H   -1.5325966    6.4487992    0.0000000
H    1.5325966   -6.4487992    0.0000000
H   -3.3751991    2.5576298    0.0000000
H    3.3751991   -2.5576298    0.0000000
```

```
H   -3.5551235    5.0303776    0.0000000
H    3.5551235   -5.0303776    0.0000000

Structure 6,         TPSS
C   -0.7300315    0.0097830    0.0000000
C    0.7300315   -0.0097830    0.0000000
C    1.4025772   -1.2256528    0.0000000
C   -1.4025772    1.2256528    0.0000000
C   -1.4455248   -1.2354174   -0.0000000
C    1.4455248    1.2354174   -0.0000000
C    0.6878183   -2.4433022    0.0000000
C   -0.6878183    2.4433022    0.0000000
C   -0.7727303   -2.4231535   -0.0000000
C    0.7727303    2.4231535    0.0000000
C    1.1168213   -3.7691240   -0.0000000
C   -1.1168213    3.7691240   -0.0000000
C   -0.0358393   -4.6294256   -0.0000000
C    0.0358393    4.6294256   -0.0000000
C   -1.2138689   -3.8143253   -0.0000000
C    1.2138689    3.8143253    0.0000000
C   -0.1480812   -6.0271840    0.0000000
C    0.1480812    6.0271840    0.0000000
C   -1.4185817   -6.6003775    0.0000000
C    1.4185817    6.6003775    0.0000000
C   -2.4746575   -4.4033549    0.0000000
C    2.4746575    4.4033549    0.0000000
C   -2.5701039   -5.7990006    0.0000000
C    2.5701039    5.7990006    0.0000000
H    2.4911595   -1.2319440    0.0000000
H   -2.4911595    1.2319440    0.0000000
H   -2.5335953   -1.1996173    0.0000000
H    2.5335953    1.1996173    0.0000000
H    2.1482482   -4.1048307    0.0000000
H   -2.1482482    4.1048307    0.0000000
H    0.7396240   -6.6546690   -0.0000000
H   -0.7396240    6.6546690   -0.0000000
H   -1.5218009   -7.6819985   -0.0000000
H    1.5218009    7.6819985   -0.0000000
H   -3.3767678   -3.7967754    0.0000000
H    3.3767678    3.7967754    0.0000000
H   -3.5492344   -6.2700341    0.0000000
H    3.5492344    6.2700341    0.0000000

Structure 7,         TPSS
C    0.7177773   -1.2379623    0.0000000
C   -0.7177773    1.2379623    0.0000000
C   -0.7401565   -1.2236191    0.0000000
```

```
C    0.7401565    1.2236191    0.0000000
C    1.4019066   -2.4556171    0.0000000
C   -1.4019066    2.4556171    0.0000000
C   -1.4533413   -2.4692070    0.0000000
C    1.4533413    2.4692070    0.0000000
C    0.6921784   -3.6697803    0.0000000
C   -0.6921784    3.6697803    0.0000000
C   -0.7729983   -3.6526444    0.0000000
C    0.7729983    3.6526444    0.0000000
C    1.1214639   -4.9991920    0.0000000
C   -1.1214639    4.9991920    0.0000000
C   -0.0294472   -5.8566191    0.0000000
C    0.0294472    5.8566191    0.0000000
C   -1.2100678   -5.0429611    0.0000000
C    1.2100678    5.0429611   -0.0000000
C   -0.1435688   -7.2560022    0.0000000
C    0.1435688    7.2560022    0.0000000
C   -1.4133688   -7.8276186    0.0000000
C    1.4133688    7.8276186    0.0000000
C   -2.4715190   -5.6324705    0.0000000
C    2.4715190    5.6324705    0.0000000
C   -2.5670755   -7.0270214    0.0000000
C    2.5670755    7.0270214    0.0000000
C   -1.4008055   -0.0066407    0.0000000
C    1.4008055    0.0066407    0.0000000
H    2.4903427   -2.4550050    0.0000000
H   -2.4903427    2.4550050    0.0000000
H   -2.5413625   -2.4391253    0.0000000
H    2.5413625    2.4391253    0.0000000
H    2.1526607   -5.3347050    0.0000000
H   -2.1526607    5.3347050    0.0000000
H    0.7435066   -7.8843534    0.0000000
H   -0.7435066    7.8843534    0.0000000
H   -1.5164126   -8.9092602    0.0000000
H    1.5164126    8.9092602    0.0000000
H   -3.3735840   -5.0257625    0.0000000
H    3.3735840    5.0257625    0.0000000
H   -3.5455128   -7.4992575    0.0000000
H    3.5455128    7.4992575    0.0000000
H   -2.4898456    0.0032365   -0.0000000
H    2.4898456   -0.0032365    0.0000000

Structure 8,         TPSS
C    0.7179962   -2.4632592    0.0000000
C   -0.7179984    2.4632576    0.0000000
C   -0.7422733   -2.4523332    0.0000000
C    0.7422632    2.4523335    0.0000000
```

C	1.4047886	-3.6890221	0.0000000
C	-1.4047893	3.6890223	0.0000000
C	-1.4520349	-3.7000175	0.0000000
C	1.4520204	3.7000319	0.0000000
C	0.6971654	-4.8970767	0.0000000
C	-0.6971984	4.8970749	0.0000000
C	-0.7688948	-4.8815712	0.0000000
C	0.7688453	4.8815830	0.0000000
C	1.3981292	-1.2272119	0.0000000
C	-1.3981223	1.2272108	0.0000000
C	-1.4100704	-1.2383287	0.0000000
C	1.4100662	1.2383285	0.0000000
C	-0.7267255	0.0046425	0.0000000
C	0.7267202	-0.0046477	0.0000000
C	1.1268163	-6.2319226	0.0000000
C	-1.1268158	6.2319070	0.0000000
C	-0.0249405	-7.0866654	0.0000000
C	0.0249112	7.0866735	0.0000000
C	-1.2054590	-6.2725538	0.0000000
C	1.2054183	6.2725672	0.0000000
C	-0.1413769	-8.4860282	0.0000000
C	0.1413783	8.4860222	0.0000000
C	-1.4118294	-9.0565066	0.0000000
C	1.4118333	9.0565093	0.0000000
C	-2.4672458	-6.8604012	0.0000000
C	2.4672259	6.8604028	0.0000000
C	-2.5650190	-8.2552899	0.0000000
C	2.5650365	8.2553034	0.0000000
H	2.4929585	-3.6865715	0.0000000
H	-2.4929315	3.6865730	0.0000000
H	-2.5400416	-3.6722190	0.0000000
H	2.5400401	3.6722035	0.0000000
H	2.4869655	-1.2320491	0.0000000
H	-2.4869318	1.2320441	0.0000000
H	-2.4989453	-1.2319608	0.0000000
H	2.4989724	1.2319362	0.0000000
H	2.1582362	-6.5663734	0.0000000
H	-2.1581969	6.5663520	0.0000000
H	0.7448806	-9.1152854	0.0000000
H	-0.7448729	9.1152611	0.0000000
H	-1.5157056	-10.1382999	0.0000000
H	1.5157121	10.1383061	0.0000000
H	-3.3682499	-6.2520102	0.0000000
H	3.3682600	6.2520269	0.0000000
H	-3.5439508	-8.7263924	0.0000000
H	3.5439799	8.7264245	0.0000000

Structure 9, TPSS

C	1.2212303	0.7345787	0.0000000
C	-1.2212305	-0.7345688	0.0000000
C	1.2332272	-0.7216366	0.0000000
C	-1.2332283	0.7216461	0.0000000
C	-0.0009525	-1.4075024	0.0000000
C	0.0009519	1.4075123	0.0000000
C	2.4645934	1.4199958	0.0000000
C	-2.4645924	-1.4199858	0.0000000
C	3.6785981	0.7547436	0.0000000
C	-3.6785953	-0.7547330	0.0000000
C	2.4635157	-1.3898268	0.0000000
C	-2.4635165	1.3898368	0.0000000
C	3.6937127	-0.7070640	0.0000000
C	-3.6937136	0.7070747	0.0000000
C	4.9249353	1.4688262	0.0000000
C	-4.9249308	-1.4688196	0.0000000
C	6.1078526	0.7897791	0.0000000
C	-6.1078508	-0.7897797	0.0000000
C	4.9251612	-1.3893369	0.0000000
C	-4.9251659	1.3893423	0.0000000
C	6.1288842	-0.6771445	0.0000000
C	-6.1288876	0.6771455	0.0000000
C	7.4978775	1.2325937	0.0000000
C	-7.4978764	-1.2325991	0.0000000
C	8.3166222	0.0559537	0.0000000
C	-8.3166257	-0.0559616	0.0000000
C	7.4665219	-1.1003020	0.0000000
C	-7.4665282	1.1002987	0.0000000
C	8.0794107	2.4967911	0.0000000
C	-8.0794065	-2.4967989	0.0000000
C	9.4744317	2.6015118	0.0000000
C	-9.4744266	-2.6015212	0.0000000
C	9.7149428	0.1786558	0.0000000
C	-9.7149474	-0.1786670	0.0000000
C	10.2801359	1.4521752	0.0000000
C	-10.2801359	-1.4521896	0.0000000
H	0.0047241	-2.4961513	0.0000000
H	-0.0047176	2.4961612	0.0000000
H	2.4558657	2.5088247	0.0000000
H	-2.4558625	-2.5088144	0.0000000
H	2.4706965	-2.4784926	0.0000000
H	-2.4706915	2.4785013	0.0000000
H	4.8935114	2.5567438	0.0000000
H	-4.8935090	-2.5567372	0.0000000
H	4.9266622	-2.4773825	0.0000000
H	-4.9266669	2.4773878	0.0000000

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H     7.8057491   -2.1301316    0.0000000
H    -7.8057636    2.1301269    0.0000000
H     7.4667635    3.3949187    0.0000000
H    -7.4667529   -3.3949223    0.0000000
H     9.9409009    3.5826420    0.0000000
H    -9.9408870   -3.5826557    0.0000000
H    10.3482491   -0.7047095    0.0000000
H   -10.3482666    0.7046903    0.0000000
H    11.3615469    1.5604361    0.0000000
H   -11.3615462   -1.5604594    0.0000000

Structure 10,         TPSS
C     1.2006915    0.7050972    0.0000000
C     1.2012468   -0.7391711    0.0000000
C     0.0000009    1.4250576    0.0000000
C    -0.0000002   -1.4511690    0.0000000
C    -1.2006567    0.7051124    0.0000000
C    -1.2012003   -0.7391785    0.0000000
C    -2.5492748    1.1655349    0.0000000
C    -3.4028744    0.0391592    0.0000000
C    -2.5832698   -1.1545322    0.0000000
C    -4.8105540   -0.0623216    0.0000000
C    -5.3925330   -1.3185441    0.0000000
C    -3.2000555   -2.4108043    0.0000000
C    -4.5906487   -2.4825610    0.0000000
C     2.5492693    1.1655038    0.0000000
C     3.4028884    0.0391489    0.0000000
C     2.5832654   -1.1545169    0.0000000
C     4.8105347   -0.0623297    0.0000000
C     5.3925173   -1.3185351    0.0000000
C     3.2000609   -2.4107829    0.0000000
C     4.5906431   -2.4825438    0.0000000
H     0.0000026    2.5135069    0.0000000
H     0.0000047   -2.5394341    0.0000000
H    -2.8622766    2.2042428    0.0000000
H    -5.4246518    0.8348279    0.0000000
H    -6.4743070   -1.4177185    0.0000000
H    -2.6091766   -3.3230223    0.0000000
H    -5.0751630   -3.4557664    0.0000000
H     2.8622613    2.2041820    0.0000000
H     5.4246363    0.8348030    0.0000000
H     6.4742809   -1.4177158    0.0000000
H     2.6091902   -3.3229890    0.0000000
H     5.0751481   -3.4557395    0.0000000

Structure 11,         TPSS
C     0.0000143    1.3776484    0.0000000
```

C	-0.0000042	-0.0712536	0.0000000
C	-1.2289171	2.0788150	0.0000000
C	-1.2390082	-0.7613088	0.0000000
C	-2.4328165	1.3846666	0.0000000
C	-2.4320763	-0.0677726	0.0000000
C	-3.7808425	1.8402716	0.0000000
C	-4.6323406	0.7062782	0.0000000
C	-3.8182233	-0.4862988	0.0000000
C	-6.0395424	0.5992046	0.0000000
C	-6.6170445	-0.6605249	0.0000000
C	-4.4264522	-1.7441106	0.0000000
C	-5.8176451	-1.8238407	0.0000000
C	1.2289284	2.0788026	0.0000000
C	2.4328280	1.3846780	0.0000000
C	1.2390578	-0.7612911	0.0000000
C	2.4320447	-0.0677875	0.0000000
C	3.7808419	1.8402608	0.0000000
C	4.6323243	0.7062815	0.0000000
C	3.8182369	-0.4862918	0.0000000
C	6.0395394	0.5991964	0.0000000
C	6.6170288	-0.6605179	0.0000000
C	4.4264422	-1.7441057	0.0000000
C	5.8176403	-1.8238413	0.0000000
H	-1.2134674	3.1673152	0.0000000
H	-1.2252595	-1.8498676	0.0000000
H	-4.0995686	2.8765777	0.0000000
H	-6.6595528	1.4921227	0.0000000
H	-7.6989540	-0.7602929	0.0000000
H	-3.8302032	-2.6529121	0.0000000
H	-6.2995751	-2.7978300	0.0000000
H	1.2134978	3.1673225	0.0000000
H	1.2252541	-1.8498636	0.0000000
H	4.0995633	2.8765635	0.0000000
H	6.6595267	1.4921309	0.0000000
H	7.6989397	-0.7602873	0.0000000
H	3.8302073	-2.6529050	0.0000000
H	6.2995775	-2.7978318	0.0000000

Structure 12, TPSS

C	-1.2292512	2.0476390	0.0000000
C	-1.2297028	0.5962667	0.0000000
C	-2.4595286	2.7543279	0.0000000
C	-2.4756245	-0.0972782	0.0000000
C	-3.6612081	2.0601760	0.0000000
C	-3.6594066	0.5990450	0.0000000
C	-5.0080461	2.5093064	0.0000000
C	-5.8601411	1.3707112	0.0000000

C	-5.0488707	0.1798415	0.0000000
C	-7.2657686	1.2616935	0.0000000
C	-7.8421506	-0.0005224	0.0000000
C	-5.6523463	-1.0785025	0.0000000
C	-7.0446059	-1.1626911	0.0000000
C	-0.0000000	2.7224876	0.0000000
C	1.2292512	2.0476390	0.0000000
C	-0.0000000	-0.0756015	0.0000000
C	1.2297028	0.5962667	0.0000000
C	2.4595286	2.7543279	0.0000000
C	3.6612081	2.0601760	0.0000000
C	2.4756245	-0.0972782	0.0000000
C	3.6594066	0.5990450	0.0000000
C	5.0080461	2.5093064	0.0000000
C	5.8601411	1.3707112	0.0000000
C	5.0488707	0.1798415	0.0000000
C	7.2657686	1.2616935	0.0000000
C	7.8421506	-0.0005224	0.0000000
C	5.6523463	-1.0785025	0.0000000
C	7.0446059	-1.1626911	0.0000000
H	-2.4419874	3.8424249	0.0000000
H	-2.4631739	-1.1856189	0.0000000
H	-5.3301720	3.5444483	0.0000000
H	-7.8881144	2.1529969	0.0000000
H	-8.9242264	-0.0998776	0.0000000
H	-5.0529950	-1.9853095	0.0000000
H	-7.5248251	-2.1374378	0.0000000
H	-0.0000000	3.8113590	0.0000000
H	0.0000000	-1.1647216	0.0000000
H	2.4419874	3.8424249	0.0000000
H	2.4631739	-1.1856189	0.0000000
H	5.3301720	3.5444483	0.0000000
H	7.8881144	2.1529969	0.0000000
H	8.9242264	-0.0998776	0.0000000
H	5.0529950	-1.9853095	0.0000000
H	7.5248251	-2.1374378	0.0000000

Structure 13, TPSS

C	-2.4560820	1.3912188	0.0000000
C	-2.4569061	-0.0666813	0.0000000
C	-3.6893337	2.0959596	0.0000000
C	-3.7083734	-0.7599755	0.0000000
C	-4.8909525	1.4015049	0.0000000
C	-4.8878073	-0.0640102	0.0000000
C	-1.2305819	2.0634386	0.0000000
C	-0.0000033	1.3807708	0.0000000
C	-1.2381961	-0.7434810	0.0000000

C	-0.0000046	-0.0693707	0.0000000
C	1.2305770	2.0634388	0.0000000
C	2.4560781	1.3912181	0.0000000
C	1.2381888	-0.7434824	0.0000000
C	2.4569009	-0.0666830	0.0000000
C	3.6893348	2.0959607	0.0000000
C	4.8909521	1.4015054	0.0000000
C	3.7083710	-0.7599786	0.0000000
C	4.8878094	-0.0640098	0.0000000
C	-6.2356771	1.8461620	0.0000000
C	-7.0891028	0.7041945	0.0000000
C	-6.2792030	-0.4851139	0.0000000
C	-8.4932758	0.5940789	0.0000000
C	-9.0691470	-0.6700983	0.0000000
C	-6.8793485	-1.7436787	0.0000000
C	-8.2725977	-1.8309632	0.0000000
C	6.2356802	1.8461631	0.0000000
C	7.0891067	0.7041959	0.0000000
C	6.2792040	-0.4851132	0.0000000
C	8.4932799	0.5940817	0.0000000
C	9.0691513	-0.6700981	0.0000000
C	6.8793504	-1.7436806	0.0000000
C	8.2726001	-1.8309637	0.0000000
H	-3.6725588	3.1839334	0.0000000
H	-3.6957605	-1.8482891	0.0000000
H	-1.2260529	3.1520218	0.0000000
H	-1.2412830	-1.8323823	0.0000000
H	1.2260469	3.1520234	0.0000000
H	1.2412769	-1.8323835	0.0000000
H	3.6725588	3.1839358	0.0000000
H	3.6957569	-1.8482909	0.0000000
H	-6.5602692	2.8805419	0.0000000
H	-9.1174270	1.4840778	0.0000000
H	-10.1513108	-0.7692123	0.0000000
H	-6.2780384	-2.6492396	0.0000000
H	-8.7512793	-2.8063025	0.0000000
H	6.5602721	2.8805426	0.0000000
H	9.1174353	1.4840798	0.0000000
H	10.1513173	-0.7692119	0.0000000
H	6.2780402	-2.6492438	0.0000000
H	8.7512834	-2.8063064	0.0000000

Structure 14, TPSS

C	1.2264167	2.0940155	0.0000000
C	-1.2264152	2.0940184	0.0000000
C	1.2270883	0.6393980	0.0000000
C	-1.2270979	0.6393999	0.0000000

C	-0.0000032	2.7744383	0.0000000
C	0.0000017	-0.0397064	0.0000000
C	2.4614718	2.7757850	0.0000000
C	-2.4614736	2.7757887	0.0000000
C	3.6853732	2.1043112	0.0000000
C	-3.6853761	2.1043131	0.0000000
C	2.4720654	-0.0337720	0.0000000
C	-2.4720643	-0.0337679	0.0000000
C	3.6853940	0.6427996	0.0000000
C	-3.6853938	0.6427968	0.0000000
C	4.9200112	2.8057544	0.0000000
C	-4.9200030	2.8057571	0.0000000
C	6.1222604	2.1092578	0.0000000
C	-6.1222663	2.1092522	0.0000000
C	4.9390187	-0.0526735	0.0000000
C	-4.9390314	-0.0526655	0.0000000
C	6.1168539	0.6411622	0.0000000
C	-6.1168362	0.6411519	0.0000000
C	7.4649872	2.5490273	0.0000000
C	-7.4649932	2.5490242	0.0000000
C	8.3187672	1.4038094	0.0000000
C	-8.3187650	1.4038111	0.0000000
C	7.5090097	0.2165585	0.0000000
C	-7.5090041	0.2165527	0.0000000
C	9.7212386	1.2929280	0.0000000
C	-9.7212455	1.2929261	0.0000000
C	10.2966861	0.0269959	0.0000000
C	-10.2966851	0.0269950	0.0000000
C	8.1060679	-1.0424619	0.0000000
C	-8.1060624	-1.0424651	0.0000000
C	9.5002879	-1.1324262	0.0000000
C	-9.5002861	-1.1324289	0.0000000
H	-0.0000058	3.8628194	0.0000000
H	0.0000002	-1.1283982	0.0000000
H	2.4569719	3.8642854	0.0000000
H	-2.4569817	3.8642896	0.0000000
H	2.4747503	-1.1226089	0.0000000
H	-2.4747496	-1.1226093	0.0000000
H	4.9052045	3.8936316	0.0000000
H	-4.9052140	3.8936320	0.0000000
H	4.9238956	-1.1409120	0.0000000
H	-4.9238884	-1.1409211	0.0000000
H	7.7942548	3.5819800	0.0000000
H	-7.7942536	3.5819838	0.0000000
H	10.3451273	2.1831361	0.0000000
H	-10.3451163	2.1831470	0.0000000
H	11.3789641	-0.0718629	0.0000000

```
H  -11.3789648   -0.0718544    0.0000000
H    7.5023469   -1.9465047    0.0000000
H   -7.5023385   -1.9465015    0.0000000
H    9.9773592   -2.1085535    0.0000000
H   -9.9773599   -2.1085487    0.0000000

Structure 15,         TPSS
C   -1.0569598    5.2951420    0.0000000
C    1.0569598   -5.2951420    0.0000000
C   -1.2452426    3.8572285    0.0000000
C    1.2452426   -3.8572285    0.0000000
C   -2.1702126    6.1869133    0.0000000
C    2.1702126   -6.1869133    0.0000000
C   -2.6123332    3.4487188    0.0000000
C    2.6123332   -3.4487188    0.0000000
C   -3.4598178    5.7285754    0.0000000
C    3.4598178   -5.7285754    0.0000000
C   -3.6696263    4.3338101    0.0000000
C    3.6696263   -4.3338101    0.0000000
C    1.3587880    5.0470620    0.0000000
C   -1.3587880   -5.0470620    0.0000000
C    1.2071083    3.6108796    0.0000000
C   -1.2071083   -3.6108796    0.0000000
C    0.2240623    5.8485996    0.0000000
C   -0.2240623   -5.8485996    0.0000000
C   -0.0787146    2.9858279    0.0000000
C    0.0787146   -2.9858279    0.0000000
C    3.7934647    4.8814991    0.0000000
C   -3.7934647   -4.8814991    0.0000000
C    3.6806492    3.4852115    0.0000000
C   -3.6806492   -3.4852115    0.0000000
C    2.6515797    5.6485877    0.0000000
C   -2.6515797   -5.6485877    0.0000000
C    2.4339530    2.8462456    0.0000000
C   -2.4339530   -2.8462456    0.0000000
C    2.3653905    1.4380211    0.0000000
C   -2.3653905   -1.4380211    0.0000000
C    1.1601870    0.7690571    0.0000000
C   -1.1601870   -0.7690571    0.0000000
C   -0.1027592    1.4984900    0.0000000
C    0.1027592   -1.4984900    0.0000000
C    1.2000106   -0.6615186    0.0000000
C   -1.2000106    0.6615186    0.0000000
H   -1.9569876    7.2533464    0.0000000
H    1.9569876   -7.2533464    0.0000000
H   -2.8823319    2.4100165    0.0000000
H    2.8823319   -2.4100165    0.0000000
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H   -4.3005453    6.4160753    0.0000000
H    4.3005453   -6.4160753    0.0000000
H   -4.6821117    3.9391942    0.0000000
H    4.6821117   -3.9391942    0.0000000
H    0.3330729    6.9312830    0.0000000
H   -0.3330729   -6.9312830    0.0000000
H    4.7739855    5.3493352    0.0000000
H   -4.7739855   -5.3493352    0.0000000
H    4.5749591    2.8667805    0.0000000
H   -4.5749591   -2.8667805    0.0000000
H    2.7077905    6.7341780    0.0000000
H   -2.7077905   -6.7341780    0.0000000
H    3.2941875    0.8707659    0.0000000
H   -3.2941875   -0.8707659    0.0000000
H    2.2073532   -1.0365163    0.0000000
H   -2.2073532    1.0365163    0.0000000

Structure 16,         TPSS
C   -2.9133717    1.0939524    0.0000000
C    2.9133717    1.0939524    0.0000000
C   -3.6178654   -0.1463396    0.0000000
C    3.6178654   -0.1463396    0.0000000
C   -3.6705113    2.2761689    0.0000000
C    3.6705113    2.2761689    0.0000000
C   -5.0489656   -0.1735814    0.0000000
C    5.0489656   -0.1735814    0.0000000
C   -5.0690987    2.2509413    0.0000000
C    5.0690987    2.2509413    0.0000000
C   -5.7570778    1.0501047    0.0000000
C    5.7570778    1.0501047    0.0000000
C   -2.8944330   -1.3794573    0.0000000
C    2.8944330   -1.3794573    0.0000000
C   -3.6010003   -2.5927188    0.0000000
C    3.6010003   -2.5927188    0.0000000
C   -5.7172114   -1.4282568    0.0000000
C    5.7172114   -1.4282568    0.0000000
C   -5.0013316   -2.6114448    0.0000000
C    5.0013316   -2.6114448    0.0000000
C   -1.4489450    1.0877922    0.0000000
C    1.4489450    1.0877922    0.0000000
C   -0.7392160   -0.1778626    0.0000000
C    0.7392160   -0.1778626    0.0000000
C   -1.4719994   -1.3483039    0.0000000
C    1.4719994   -1.3483039    0.0000000
C   -0.7007737    2.2567829    0.0000000
C    0.7007737    2.2567829    0.0000000
H   -3.1742523    3.2409526    0.0000000
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H     3.1742523    3.2409526    0.0000000
H    -5.6167627    3.1897196    0.0000000
H     5.6167627    3.1897196    0.0000000
H    -6.8439868    1.0329409    0.0000000
H     6.8439868    1.0329409    0.0000000
H    -3.0438404   -3.5266122    0.0000000
H     3.0438404   -3.5266122    0.0000000
H    -6.8041874   -1.4405281    0.0000000
H     6.8041874   -1.4405281    0.0000000
H    -5.5257673   -3.5632850    0.0000000
H     5.5257673   -3.5632850    0.0000000
H    -0.9678964   -2.3103353    0.0000000
H     0.9678964   -2.3103353    0.0000000
H    -1.2018383    3.2193707    0.0000000
H     1.2018383    3.2193707    0.0000000

Structure 17,          TPSS
C     1.2218281   -0.0000000    0.6384254
C    -1.2218281    0.0000000    0.6384254
C     2.4920189   -0.0000000   -0.1118454
C    -2.4920189   -0.0000000   -0.1118454
C     1.2294240    0.0000000    2.0645524
C    -1.2294240    0.0000000    2.0645524
C     3.6997905    0.0000000    0.6615515
C    -3.6997905    0.0000000    0.6615515
C     2.4471425    0.0000000    2.7851746
C    -2.4471425    0.0000000    2.7851746
C     3.6725941    0.0000000    2.0870656
C    -3.6725941    0.0000000    2.0870656
C     4.9624911    0.0000000   -0.0433098
C    -4.9624911    0.0000000   -0.0433098
C     6.1565289    0.0000000    0.7316290
C    -6.1565289    0.0000000    0.7316290
C     4.9026337    0.0000000    2.8086656
C    -4.9026337    0.0000000    2.8086656
C     6.1076307    0.0000000    2.1124209
C    -6.1076307   -0.0000000    2.1124209
C     2.5615210    0.0000000   -1.5088711
C    -2.5615210    0.0000000   -1.5088711
C     3.7905160    0.0000000   -2.1745232
C    -3.7905160   -0.0000000   -2.1745232
C     4.9705735    0.0000000   -1.4525382
C    -4.9705735    0.0000000   -1.4525382
C     0.0000000    0.0000000   -0.0471643
C     0.0000000    0.0000000    2.7632098
H     7.1049184    0.0000000    0.1979448
H    -7.1049184    0.0000000    0.1979448
```

```
H     4.8800806    0.0000000    3.8930587
H    -4.8800806    0.0000000    3.8930587
H     7.0323905    0.0000000    2.6898672
H    -7.0323905    0.0000000    2.6898672
H     1.6570922    0.0000000   -2.1071353
H    -1.6570922   -0.0000000   -2.1071353
H     3.8104688    0.0000000   -3.2603122
H    -3.8104688    0.0000000   -3.2603122
H     0.0000000    0.0000000   -1.1271620
H     0.0000000    0.0000000    3.8478796
H     2.4427439    0.0000000    3.8694232
H    -2.4427439    0.0000000    3.8694232
H     5.9269743    0.0000000   -1.9710568
H    -5.9269743    0.0000000   -1.9710568

Structure 18,         TPSS
C    -0.6779230    0.0410569    2.5223601
C     0.6779273   -0.0410564    2.5223745
C    -1.4339932    0.0520731    1.2949367
C     1.4339996   -0.0520716    1.2949371
C    -0.7255333   -0.0093417    0.0488079
C     0.7255316    0.0093440    0.0488151
C    -2.8261526    0.0703460    1.2903243
C     2.8261463   -0.0703461    1.2903222
C    -3.5558321    0.0224311    0.0886320
C     3.5558416   -0.0224320    0.0886443
C    -1.4308062   -0.1436135   -1.1520019
C     1.4307984    0.1436142   -1.1519981
C    -2.8422800   -0.1003274   -1.1525650
C     2.8422740    0.1003292   -1.1525640
C    -0.6511008   -0.4238246   -2.4274414
C     0.6510973    0.4238223   -2.4274365
C    -1.4932813   -0.2955727   -3.6666502
C     1.4932751    0.2955742   -3.6666552
C    -3.5779843   -0.1419676   -2.3834241
C     3.5779947    0.1419662   -2.3834343
C    -2.8321588   -0.1980504   -3.6304755
C     2.8321619    0.1980505   -3.6304713
C    -4.9795093    0.0692012    0.0613578
C     4.9794981   -0.0692007    0.0613403
C    -5.6621191    0.0124648   -1.1311787
C     5.6621158   -0.0124640   -1.1311728
C    -4.9612835   -0.0851445   -2.3554433
C     4.9612737    0.0851444   -2.3554402
H    -1.2270273    0.0751640    3.4607115
H     1.2270242   -0.0751639    3.4607129
H    -3.3631527    0.1137948    2.2359889
```

```
H     3.3631549   -0.1137967    2.2359934
H    -0.9878689   -0.3560823   -4.6265427
H     0.9878724    0.3560843   -4.6265401
H    -3.4007731   -0.1561113   -4.5576885
H     3.4007774    0.1561100   -4.5576962
H    -5.5167151    0.1522936    1.0029061
H     5.5167233   -0.1522950    1.0029123
H    -6.7479737    0.0509482   -1.1394512
H     6.7479694   -0.0509505   -1.1394516
H    -5.5137004   -0.1088068   -3.2918715
H     5.5137100    0.1088056   -3.2918779
H    -0.3170032   -1.4803428   -2.3746524
H     0.3170049    1.4803438   -2.3746527

Structure 19,         TPSS
C    -1.8459963   -1.9328018   -0.3967365
C    -3.0574462   -1.2311617   -0.0957939
C    -1.9101301   -3.3073793   -0.7272218
C    -4.3015076   -1.9379334   -0.0996005
C    -3.1281058   -3.9858520   -0.7335078
C    -4.3075536   -3.3226423   -0.4183119
C    -3.0174459    0.1688902    0.1709916
C    -4.2339200    0.8198723    0.4669076
C    -5.4905867   -1.2318360    0.2005527
C    -5.4445424    0.1248624    0.4853980
C    -0.6166644   -1.2432372   -0.3365918
C    -0.5230319    0.1241152   -0.0128937
C    -1.7466868    0.8691570    0.1259543
C     0.7470550    0.8176943    0.0747819
C     0.7473183    2.2402401   -0.0666659
C    -1.6825039    2.2855663    0.1368509
C    -0.4929406    2.9455353   -0.0208790
C     2.0239927    0.1605188    0.2900565
C     3.2352746    0.8850093    0.0446543
C     1.9516770    2.9377726   -0.2585525
C     3.1963461    2.2817979   -0.2797687
C     2.1474115   -1.1458720    0.8173152
C     3.3904807   -1.7643887    0.9636754
C     4.5063599    0.2373020    0.1667159
C     4.5565215   -1.1075554    0.6043597
C     5.6892753    0.9682505   -0.1245210
C     4.4060908    2.9692725   -0.5433803
C     5.6314422    2.3101079   -0.4805084
H    -0.9886103   -3.8328800   -0.9652003
H    -3.1534379   -5.0431136   -0.9835640
H    -5.2554665   -3.8549736   -0.4209138
H    -4.2387220    1.8770889    0.7086514
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```
H   -6.4373758   -1.7662220    0.2043774
H   -6.3601647    0.6588414    0.7255583
H   -2.5989378    2.8624226    0.1973327
H   -0.4731734    4.0298771   -0.0956683
H    3.4367514   -2.7707282    1.3712777
H    5.5220612   -1.5983240    0.6973327
H    4.3635312    4.0275008   -0.7884020
H    6.5482259    2.8533411   -0.6935121
H    1.9164067    4.0148095   -0.4087105
H    6.6475460    0.4602571   -0.0489093
H    1.2618918   -1.6661748    1.1617322
H    0.2792350   -1.7870140   -0.6146626

Structure 20,         TPSS
C   -0.0000000    0.0000000   -1.4303654
C   -0.0000000    0.0000000   -0.0001356
C   -0.0000000    2.4433986   -1.4109789
C   -0.0000000   -2.4433986   -1.4109789
C    0.0000000    2.4522796   -0.0189532
C    0.0000000   -2.4522796   -0.0189532
C    0.0000000    1.2422587   -2.1144949
C    0.0000000   -1.2422587   -2.1144949
C    0.0000000    1.2387629    0.7150937
C    0.0000000   -1.2387629    0.7150937
C   -0.0000000    1.2099746    2.1329936
C    0.0000000   -1.2099746    2.1329936
C    0.0000000    0.0000000    2.8212496
H   -0.0000000    3.3846332   -1.9544794
H   -0.0000000   -3.3846332   -1.9544794
H    0.0000000    3.3948459    0.5230617
H    0.0000000   -3.3948459    0.5230617
H   -0.0000000    1.2439102   -3.2016684
H   -0.0000000   -1.2439102   -3.2016684
H    0.0000000    2.1506005    2.6780150
H    0.0000000   -2.1506005    2.6780150
H   -0.0000000    0.0000000    3.9080750

Structure 21,         TPSS
C    4.1699974   -0.5533327    0.0000000
C    1.4310877   -0.1882345    0.0000000
C    3.7031544    0.7427337    0.0000000
C    3.3804350   -1.6820328    0.0000000
C    2.2773497    0.9660653    0.0000000
C    1.9460852   -1.5227262    0.0000000
C    0.0005778    0.0009712    0.0000000
C   -0.5504860    1.3345148    0.0000000
C   -0.8785619   -1.1433253    0.0000000
```

```
C    1.7356949    2.2588857    0.0000000
C    1.0875166   -2.6304585    0.0000000
C    0.3470335    2.4493632    0.0000000
C   -0.3028595   -2.4531665    0.0000000
C   -1.9726224    1.4885285    0.0000000
C   -2.2926312   -0.9242502    0.0000000
C   -2.4956687    2.8335962    0.0000000
C   -3.1461626   -2.0875412    0.0000000
C   -0.2357036    3.7696193    0.0000000
C   -1.2068136   -3.5775854    0.0000000
C   -1.6080834    3.8868905    0.0000000
C   -2.5628688   -3.3353787    0.0000000
C   -2.8218311    0.3735589    0.0000000
H    5.2590822   -0.7000459    0.0000000
H    4.3480741    1.6154413    0.0000000
H    3.7728617   -2.6937708    0.0000000
H    2.3974378    3.1199431    0.0000000
H    1.5025837   -3.6340582    0.0000000
H   -3.5743199    2.9524522    0.0000000
H   -4.2188622   -1.9233977    0.0000000
H    0.4415682    4.6174001    0.0000000
H   -0.7721396   -4.5717561    0.0000000
H   -2.0301050    4.9015680    0.0000000
H   -3.2322980   -4.2066531    0.0000000
H   -3.8985225    0.5161818    0.0000000

Structure 22,         TPSS
C    0.0000000    0.0000000    4.2577137
C    0.0000000    0.0000000    1.4357858
C   -1.2063267    0.0000000    3.5587177
C    1.2063267    0.0000000    3.5587177
C   -1.2222341    0.0000000    2.1620941
C    1.2222341   -0.0000000    2.1620941
C    0.0000000    0.0000000    0.0001377
C   -1.2433559    0.0000000   -0.7178025
C    1.2433559    0.0000000   -0.7178025
C   -2.5259711   -0.0000000    1.4583835
C    2.5259711    0.0000000    1.4583835
C   -2.4835593    0.0000000   -0.0225584
C    2.4835593    0.0000000   -0.0225584
C   -1.2612928    0.0000000   -2.1393649
C    1.2612928    0.0000000   -2.1393649
C   -2.4787021    0.0000000   -2.8241005
C    2.4787021    0.0000000   -2.8241005
C   -3.6851024    0.0000000   -0.7347732
C    3.6851024    0.0000000   -0.7347732
C   -3.6872306   -0.0000000   -2.1289738
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```
C     3.6872306   -0.0000000   -2.1289738
C     0.0000000    0.0000000   -2.9168202
O    -3.5956836    0.0000000    2.0764672
O     3.5956836    0.0000000    2.0764672
O     0.0000000    0.0000000   -4.1521470
H     0.0000000    0.0000000    5.3437565
H    -2.1612203   -0.0000000    4.0760802
H     2.1612203    0.0000000    4.0760802
H    -2.4492765    0.0000000   -3.9097122
H     2.4492765   -0.0000000   -3.9097122
H    -4.6107034   -0.0000000   -0.1665211
H     4.6107034    0.0000000   -0.1665211
H    -4.6278125    0.0000000   -2.6721496
H     4.6278125   -0.0000000   -2.6721496

Structure 23,         TPSS
C    -0.0000049    0.0000737    0.0000000
C    -0.7419124   -1.2314001    0.0000000
C    -0.6957601    1.2582548    0.0000000
C    -2.1367272   -1.1763090    0.0000000
C    -2.1517956    1.2816556    0.0000000
C    -2.8569897    0.0399525    0.0000000
C    -2.9092591    2.4727747    0.0000000
C    -4.2932620    2.4497426    0.0000000
C    -4.2770319    0.0416614    0.0000000
C    -4.9860417    1.2232438    0.0000000
C     2.1858795    1.2224928    0.0000000
C     1.4373990   -0.0266030    0.0000000
C     1.4630837    2.4539235    0.0000000
C     0.0496391    2.4384604    0.0000000
C     4.2682832    2.4925199    0.0000000
C     3.5961068    1.2824989    0.0000000
C     3.5525388    3.7058783    0.0000000
C     2.1747619    3.6827040    0.0000000
C     2.0870586   -1.2620542    0.0000000
C     1.3937482   -2.4938390    0.0000000
C    -0.0340089   -2.5038874    0.0000000
C     2.1022996   -3.7244984    0.0000000
C     1.4336139   -4.9293589    0.0000000
C     0.0248273   -4.9423851    0.0000000
C    -0.6871201   -3.7552631    0.0000000
H    -2.7158213   -2.0942347    0.0000000
H    -2.4077725    3.4348911    0.0000000
H    -4.8470479    3.3845008    0.0000000
H    -4.7964614   -0.9139134    0.0000000
H    -6.0723993    1.2123289    0.0000000
H    -0.4549553    3.3992687    0.0000000
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```
H    5.3546438    2.5049404    0.0000000
H    4.1782296    0.3671475    0.0000000
H    4.0864029    4.6521745    0.0000000
H    1.6071431    4.6106254    0.0000000
H    3.1715053   -1.3053608    0.0000000
H    3.1895445   -3.6962848    0.0000000
H    1.9866390   -5.8647100    0.0000000
H   -0.5077805   -5.8894017    0.0000000
H   -1.7711958   -3.8022103    0.0000000

Structure 24,         TPSS
C   -1.6676780   -0.0000000   -1.4528376
C    1.6676780    0.0000000   -1.4528376
C   -3.0332804    0.0000000   -1.1290404
C    3.0332804    0.0000000   -1.1290404
C   -0.7324978    0.0000000   -0.4274181
C    0.7324978    0.0000000   -0.4274181
C   -3.4573813    0.0000000    0.2065743
C    3.4573813   -0.0000000    0.2065743
C   -1.1605167    0.0000000    0.9413354
C    1.1605167    0.0000000    0.9413354
C   -2.5301213   -0.0000000    1.2490689
C    2.5301213    0.0000000    1.2490689
C    0.0000000    0.0000000    1.7777509
H    0.0000000    0.0000000    2.8624783
H   -1.3571340    0.0000000   -2.4946723
H    1.3571340    0.0000000   -2.4946723
H   -3.7723600    0.0000000   -1.9256292
H    3.7723600   -0.0000000   -1.9256292
H   -4.5208747    0.0000000    0.4293286
H    4.5208747   -0.0000000    0.4293286
H   -2.8654670    0.0000000    2.2831758
H    2.8654670   -0.0000000    2.2831758

Structure 25,         TPSS
C    0.0000000    0.0000000    0.9219464
C    0.0000000    0.0000000    2.3267675
C   -1.1708351    0.0000000    0.1230582
C    1.1708351    0.0000000    0.1230582
C   -2.3975069    0.0000000    0.7603753
C    2.3975069    0.0000000    0.7603753
C   -2.4285977    0.0000000    2.1808911
C    2.4285977    0.0000000    2.1808911
C   -1.2780937    0.0000000    2.9529410
C    1.2780937    0.0000000    2.9529410
C   -0.7141768    0.0000000   -1.2776219
C    0.7141768    0.0000000   -1.2776219
```

```
C   -1.4144301    0.0000000   -2.4809075
C    1.4144301    0.0000000   -2.4809075
C   -0.6988796    0.0000000   -3.6832604
C    0.6988796    0.0000000   -3.6832604
H   -3.3333920    0.0000000    0.2072295
H    3.3333920    0.0000000    0.2072295
H   -3.3956593    0.0000000    2.6770552
H    3.3956593    0.0000000    2.6770552
H   -1.3531037    0.0000000    4.0376201
H    1.3531037    0.0000000    4.0376201
H   -2.5014714    0.0000000   -2.4937177
H    2.5014714    0.0000000   -2.4937177
H   -1.2355843    0.0000000   -4.6280198
H    1.2355843    0.0000000   -4.6280198

Structure 26,         TPSS
C   -3.3962308    0.0000000    0.0000000
C    3.3962308    0.0000000    0.0000000
C   -4.8005105    0.0000000    0.0000000
C    4.8005105    0.0000000    0.0000000
C   -3.2349503   -2.3976138    0.0000000
C   -3.2349503    2.3976138    0.0000000
C    3.2349503   -2.3976138    0.0000000
C    3.2349503    2.3976138    0.0000000
C   -2.5965159   -1.1704349    0.0000000
C   -2.5965159    1.1704349    0.0000000
C    2.5965159   -1.1704349    0.0000000
C    2.5965159    1.1704349    0.0000000
C   -4.6551065   -2.4285523    0.0000000
C   -4.6551065    2.4285523    0.0000000
C    4.6551065   -2.4285523    0.0000000
C    4.6551065    2.4285523    0.0000000
C   -5.4271659   -1.2778501    0.0000000
C   -5.4271659    1.2778501    0.0000000
C    5.4271659   -1.2778501    0.0000000
C    5.4271659    1.2778501    0.0000000
C    0.0000000   -1.4323483    0.0000000
C    0.0000000    1.4323483    0.0000000
C   -1.1973245   -0.7161534    0.0000000
C   -1.1973245    0.7161534    0.0000000
C    1.1973245   -0.7161534    0.0000000
C    1.1973245    0.7161534    0.0000000
H   -2.6821683   -3.3336753    0.0000000
H   -2.6821683    3.3336753    0.0000000
H    2.6821683   -3.3336753    0.0000000
H    2.6821683    3.3336753    0.0000000
H   -5.1516473   -3.3955451    0.0000000
```

```
H   -5.1516473    3.3955451    0.0000000
H    5.1516473   -3.3955451    0.0000000
H    5.1516473    3.3955451    0.0000000
H   -6.5118809   -1.3519831    0.0000000
H   -6.5118809    1.3519831    0.0000000
H    6.5118809   -1.3519831    0.0000000
H    6.5118809    1.3519831    0.0000000
H    0.0000000   -2.5199524    0.0000000
H    0.0000000    2.5199524    0.0000000

Structure 27,         TPSS
C    0.7078299    0.0000000    0.0000000
C   -0.7078299    0.0000000    0.0000000
C    3.6122715    0.0000000    0.0000000
C   -3.6122715    0.0000000    0.0000000
C    1.4797607    1.2187636    0.0000000
C    1.4797607   -1.2187636    0.0000000
C   -1.4797607    1.2187636    0.0000000
C   -1.4797607   -1.2187636    0.0000000
C    2.8400318    1.2239970    0.0000000
C    2.8400318   -1.2239970    0.0000000
C   -2.8400318    1.2239970    0.0000000
C   -2.8400318   -1.2239970    0.0000000
C    4.9781234    0.0000000    0.0000000
C   -4.9781234    0.0000000    0.0000000
H    0.9646771    2.1731519    0.0000000
H    0.9646771   -2.1731519    0.0000000
H   -0.9646771    2.1731519    0.0000000
H   -0.9646771   -2.1731519    0.0000000
H    3.3779243    2.1695568    0.0000000
H    3.3779243   -2.1695568    0.0000000
H   -3.3779243    2.1695568    0.0000000
H   -3.3779243   -2.1695568    0.0000000
H    5.5432655    0.9268544    0.0000000
H    5.5432655   -0.9268544    0.0000000
H   -5.5432655    0.9268544    0.0000000
H   -5.5432655   -0.9268544    0.0000000

Structure 28,         TPSS
C    1.2468875    0.7049965    0.0000000
C   -1.2468875   -0.7049965    0.0000000
C    2.4597686    1.3585677    0.0000000
C   -2.4597686   -1.3585677    0.0000000
C    3.7178035    0.6566229    0.0000000
C   -3.7178035   -0.6566229    0.0000000
C   -1.2116506    0.7544125    0.0000000
C    1.2116506   -0.7544125    0.0000000
```

```
C   -0.0032897    1.4065053    0.0000000
C    0.0032897   -1.4065053    0.0000000
C   -3.6559966    0.7975852    0.0000000
C    3.6559966   -0.7975852    0.0000000
C   -2.4732882    1.4571781    0.0000000
C    2.4732882   -1.4571781    0.0000000
C    4.9139823    1.3179404    0.0000000
C   -4.9139823   -1.3179404    0.0000000
H    2.4794239    2.4468817    0.0000000
H   -2.4794239   -2.4468817    0.0000000
H    0.0179348    2.4950849    0.0000000
H   -0.0179348   -2.4950849    0.0000000
H   -4.5944161    1.3467834    0.0000000
H    4.5944161   -1.3467834    0.0000000
H   -2.4500577    2.5448392    0.0000000
H    2.4500577   -2.5448392    0.0000000
H    5.8562706    0.7786664    0.0000000
H   -5.8562706   -0.7786664    0.0000000
H    4.9594363    2.4027585    0.0000000
H   -4.9594363   -2.4027585    0.0000000

Structure 29,         TPSS
C    0.0000000    0.0000000   -2.4337403
C   -1.1342336    0.0000000   -1.5989911
C    1.1342336    0.0000000   -1.5989911
C   -2.5128484    0.0000000   -1.8523705
C    2.5128484    0.0000000   -1.8523705
C   -3.4303856   -0.0000000   -0.7925785
C    3.4303856    0.0000000   -0.7925785
C   -3.0248218    0.0000000    0.5432671
C    3.0248218    0.0000000    0.5432671
C   -1.6532034    0.0000000    0.8819559
C    1.6532034    0.0000000    0.8819559
C   -1.2720066    0.0000000    2.2361226
C    1.2720066    0.0000000    2.2361226
C    0.0000000    0.0000000    2.8188984
C   -0.6923089    0.0000000   -0.1952137
C    0.6923089    0.0000000   -0.1952137
H    0.0000000    0.0000000   -3.5160833
H   -2.8808975    0.0000000   -2.8758527
H    2.8808975    0.0000000   -2.8758527
H   -4.4934742    0.0000000   -1.0191401
H    4.4934742    0.0000000   -1.0191401
H   -3.7637515   -0.0000000    1.3398344
H    3.7637515    0.0000000    1.3398344
H   -2.1007373    0.0000000    2.9447888
H    2.1007373    0.0000000    2.9447888
```

H	0.0000000	0.0000000	3.9072810