

Supporting Information

Conformational Control in [22]- and [24]Pentaphyrins(1.1.1.1) by *meso*-Substituents and their N-Fusion Reaction

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I. Nomenclature and conformational descriptor

The nomenclature for the different conformations of pentaphyrins is taken from the following review (Stępień, M.; Sprutta, N.; Latos-Grażyński, L. *Angew. Chem. Int. Ed.* 2011, 50, 4288). In the convex conformers **1a** and **2a**, all subunits (pyrrole rings and/or *meso*-bridges) have a *cis-cis* alignment, so all nitrogen atoms point inward. On the other hand, concave conformers contain inverted subunits with a *trans-trans* alignment.

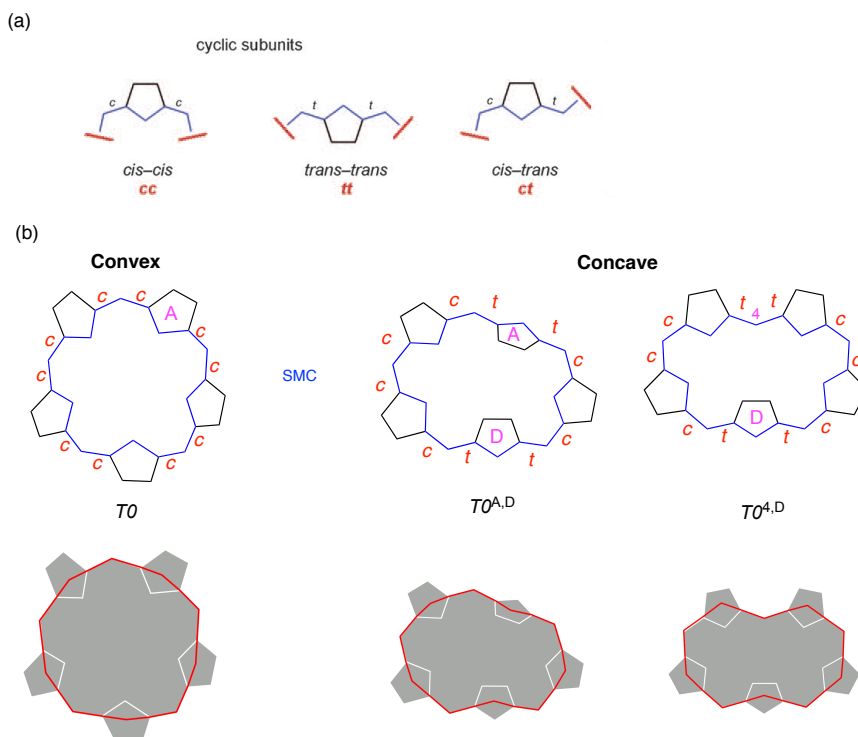


Figure S1. (a) Alignment types for cyclic subunits. The same alignment types are applicable to meso bridges. (b) Convex and concave conformations for non-fused pentaphyrins.

Figure S1 shows the three different alignment types for the individual subunits: *cis-cis* (*cc*), *trans-trans* (*tt*) and *cis-trans* (*ct*). The same definition are applicable to meso bridges. The inverted subunit has a *trans-trans* alignment. The *cis/trans* configuration is referred to the smallest macrocyclic circuit (SMC) displayed in blue in Figure S1. In a convex conformation, all subunits have a *cc* alignment, so the polygon formed by meso positions and centroids of pyrrolic subunits is convex. In concave conformations, one or more subunits are inverted and the polygon is concave. The topological descriptor Tn^x indicates the number of half-twists (n) and the subunits (pyrrole rings and/or *meso* carbon atoms) located between two transoid linkages (x).

II. Interrelation between the torsional parameters used to quantify the ring strain

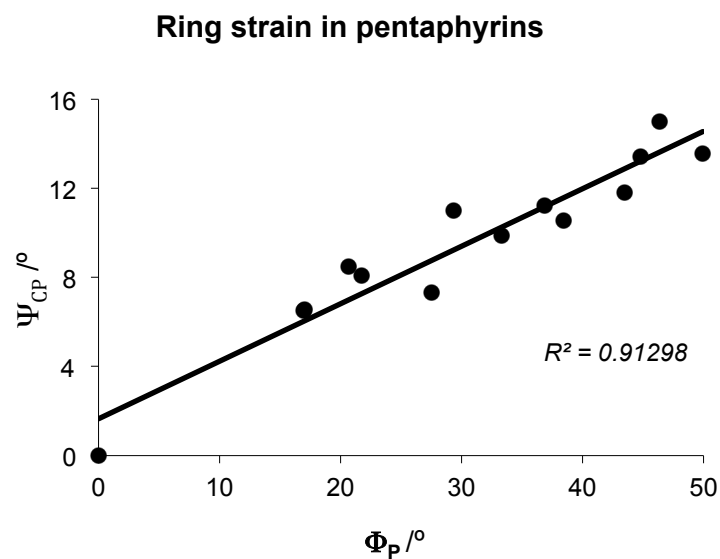


Figure S2. Dependence between the torsional parameters used for evaluating the ring strain in pentaphyrins. Ψ is the average absolute deviation from either 0° and 180° of the dihedral angles along the classical conjugation pathway (CP) and Φ_P is the average dihedral angle between the neighboring pyrrole rings.

III. Conformational interconversion pathways in non-fused [22]- and [24]pentaphyrins

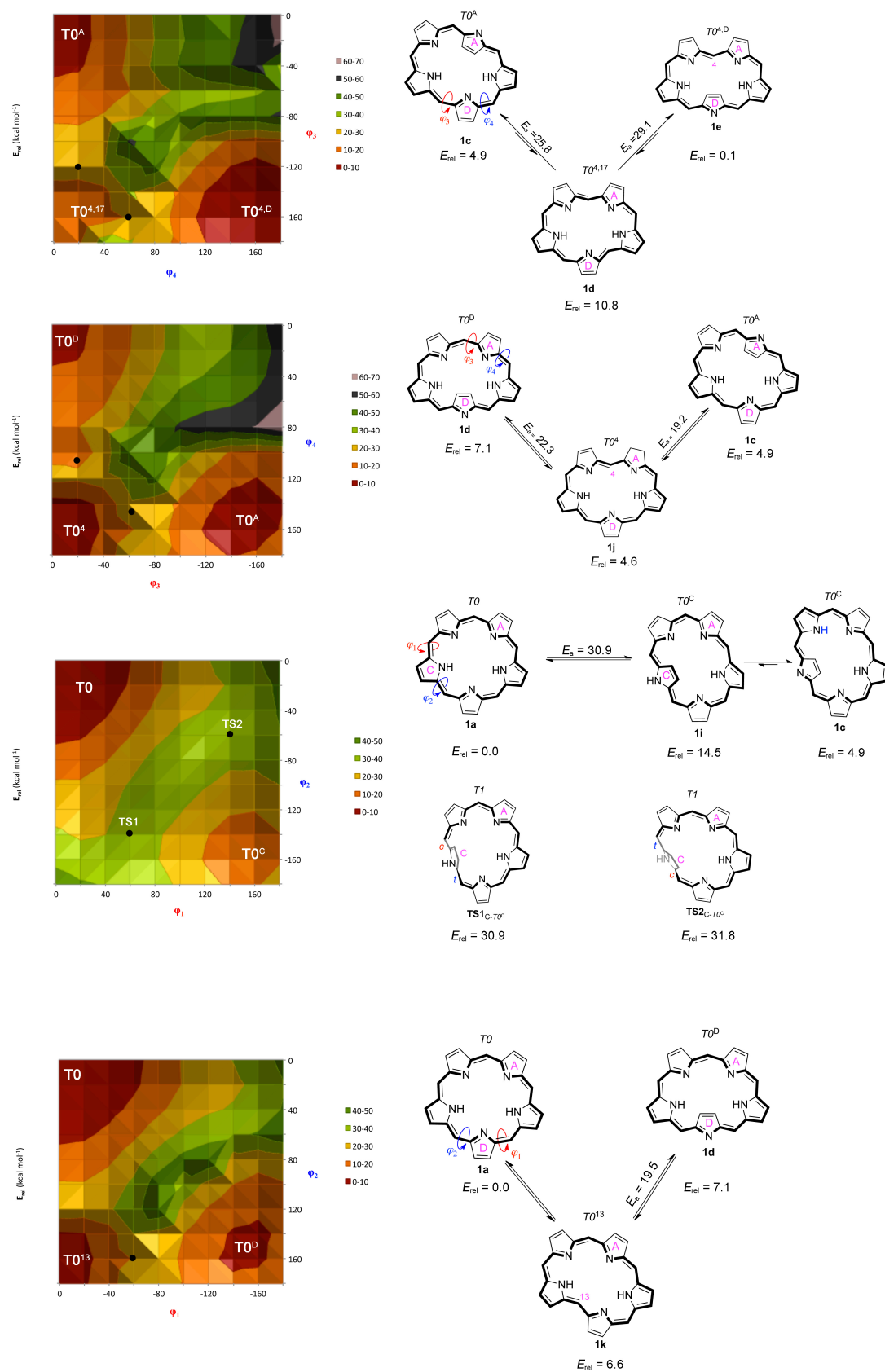


Figure S3. B3LYP/6-31G(d,p) relaxed energy potential surfaces for the [22]pentaphyrin obtained by rotating the dihedral angles φ_3 and φ_4 from the pyrrole-inverted conformers **1c** ($T0^A$) and **1d** ($T0^D$). The fully optimized geometries for the minima and the activation energy barriers are also shown. The isomerization pathways for the rotation of the imine-type pyrrole ring C ($T0 \rightarrow T0^C$) and the amine-type pyrrole ring D ($T0 \rightarrow T0^D$) from the convex conformation are also shown.

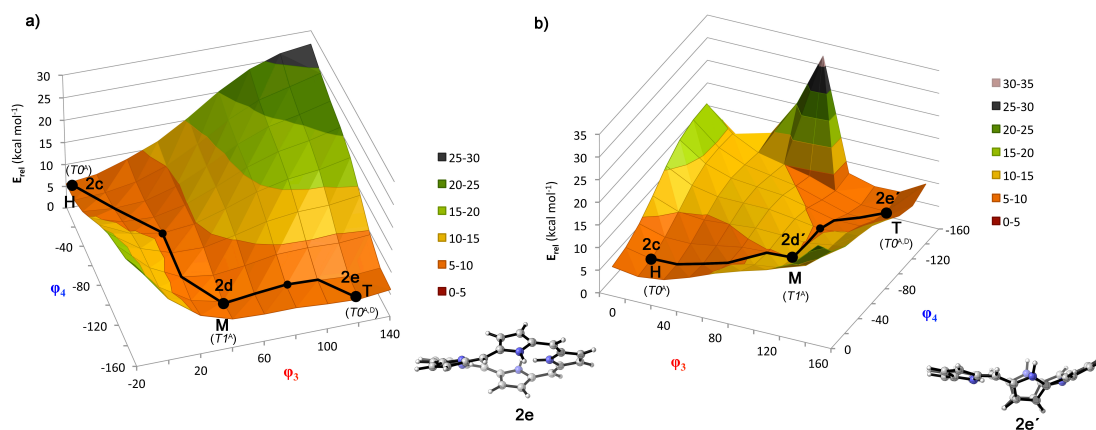


Figure S4. B3LYP/6-31G(d,p) relaxed energy potential surfaces for the $T0^A \rightarrow T0^{A,D}$ conformational interconversion in [24]pentaphyrin. Two non-equivalent isomerization pathways differing in the relative orientation of the inverted pyrrole rings A and D. Whereas A and D face toward the same direction in **2e**, they are stacked in **2e'**.

IV. Performance of the dispersion correction DFT-D in the conformational stability of unsubstituted [22]- and [24]pentaphyrin

Table S1. Relative energies (in kcal mol⁻¹) of the main conformers of [22]- and [24]pentaphyrins calculated with B3LYP and B3LYP-D.^a

[24]PP	Tn^X	E_{rel}	E_{rel} (DFT-D)	[22]PP		E_{rel}	E_{rel} (DFT-D)
2a (C)	$T0$	0.00	0.22	1a (C)	$T0$	0.00	4.87
2b (M)	$T1$	2.80	2.33	1b (H)	$T0^{22}$	16.17	20.77
2c (H)	$T0^A$	5.39	5.24	1c (H)	$T0^A$	4.86	6.65
2d (M)	$T1^A$	9.58	8.57	1d (H)	$T0^D$	7.09	8.36
2e (T)	$T0^{A,D}$	4.69	1.95	1e (H)	$T0^{4,D}$	0.09	0.00
2d' (M)	$T1^A$	5.06	2.16	1f (T)	$T0^{A,D}$	15.15	13.72
2e' (T)	$T0^{A,D}$	4.76	1.90	1f' (T)	$T0^{A,D}$	17.22	15.46
2f (T)	$T0^{4,D}$	3.27	0.00				
MAE			1.63	MAE			2.26

^a MAE is the mean absolute error between the B3LYP/6-31G** relative energies and the B3LYP-D/6-31G** energies.

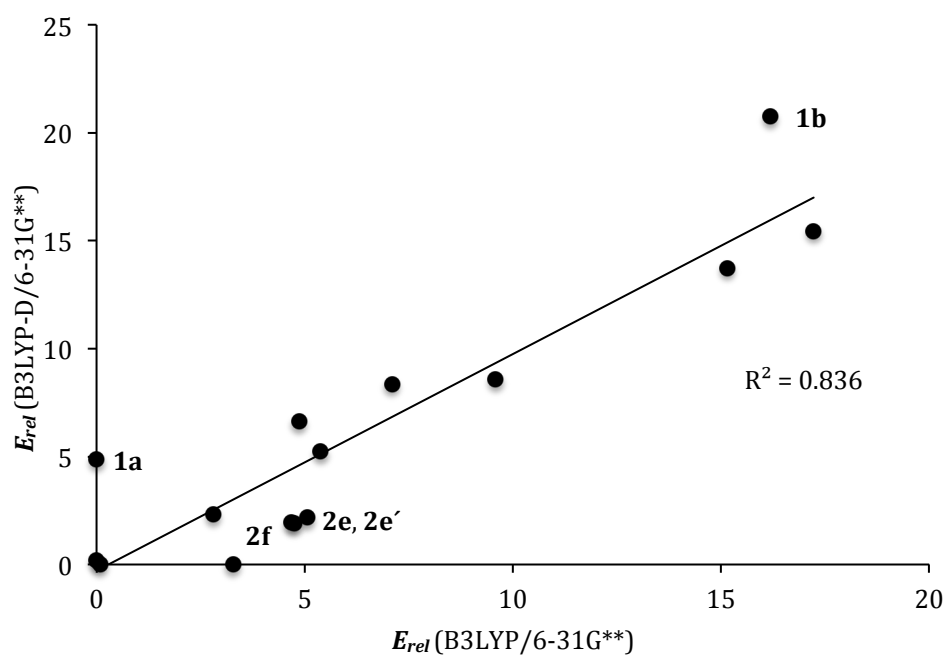


Figure S5. Deviations of the relative energies of the conformers of unsubstituted [22]- and [24]pentaphyrin calculated with B3LYP and B3LYP-D.

V. Solvation effects on the relative energies of [24]- and [22]pentaphyrins.

The effect of the solvent on the conformational stabilities of unsubstituted [24]- and [22]pentaphyrins has been assessed using the recently introduced solvation model SMD (A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378-6396) at the B3LYP/6-31G(d,p) level of theory. The free solvation energies in THF and DMSO are collected in Table S2. In the pentapyrrolic macrocycles, solvent plays a minor role in the stability of the different conformers of [22]PP and [24]PP. The convex conformations (**1a** and **2e**) are predominant in both THF and DMSO. In the case of the [24]PP, as the dielectric constant increases the Hückel conformers with one inverted pyrrole ring (**2c** and **2f**) become more stable. Interestingly, the opposite solvent-polarity-dependent behavior is found for the [22]pentaphyrin, so singly-inverted conformers **1c** and **1e** are destabilized in polar solvents. Previously, we have shown that the Hückel-Möbius conformational switch in [28]hexaphyrin and [32]heptaphyrin is strongly affected by solvent.

Table S2. Gibbs free energies (ΔG in kcal mol⁻¹) for the different Hückel and Möbius conformers of unsubstituted [24]- and [22]pentaphyrins calculated at 298 K in different solvents.

Compound	Tn^X	ΔG (298 K)	THF	DMSO
		ϵ	7.43	46.82
[22]pentaphyrin				
1a (H)	$T0$	0.00	0.00	0.00
1c (H)	$T0^A$	6.63	7.17	8.10
1d (H)	$T0^D$	8.87	8.70	9.27
1e (H)	$T0^{4,D}$	2.33	4.51	5.86
1f (H)	$T0^{A,D}$	17.41	17.29	18.14
[24]pentaphyrin				
2a (H)	$T0$	0.00	0.00	0.00
2b (M)	$T1$	2.96	4.51	4.83
2c (H)	$T0^A$	5.79	4.27	3.66
2d (M)	$T1^A$	6.21	5.66	5.46
2e (H)	$T0^{A,D}$	5.55	5.40	5.13
2f (H)	$T0^{4,D}$	4.67	3.35	2.88

VI. Dependence between relative energies and hydrogen bonding, ring strain and aromaticity in [22]- and [24]pentaphyrins.

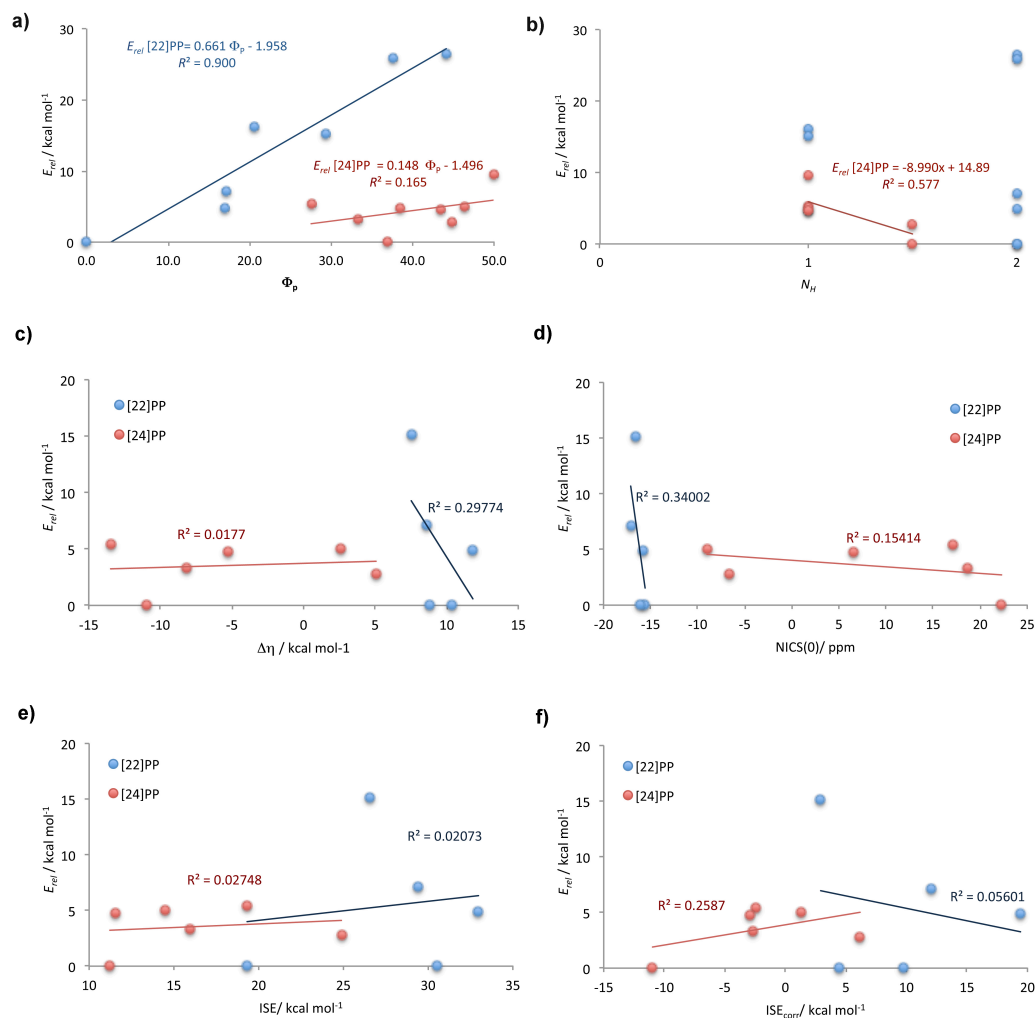


Figure S6. Dependence between relative energies of [22] and [24]pentaphyrin conformers and ring strain (Φ_p) [a]; hydrogen bonding (N_H) [b]; relative hardness [c]; nucleus-independent chemical shifts NICS(0) [d]; uncorrected aromatic stabilization energies (ISE) [e] and corrected aromatic stabilization energies (ISE_{corr}) [f].

VII. *Syn-anti* corrections for the isomerization stabilization energies (ISE)

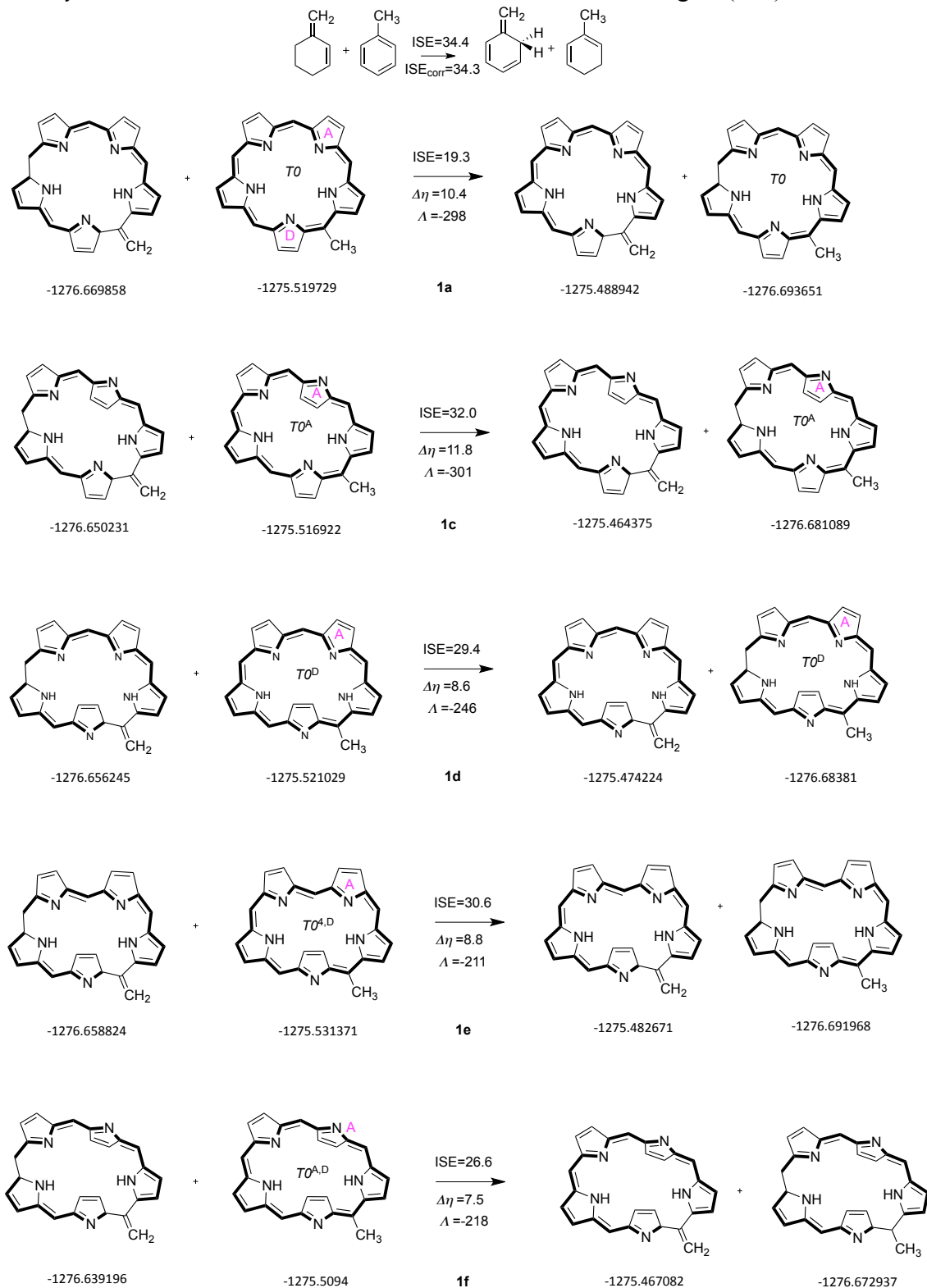


Figure S7. *Syn-anti* corrections applied for the ISE values computed for benzene and the different conformers of [22]pentaphyrin. Zero-point corrected energies in hartrees evaluated at B3LYP/6-31G(d,p) level of theory.

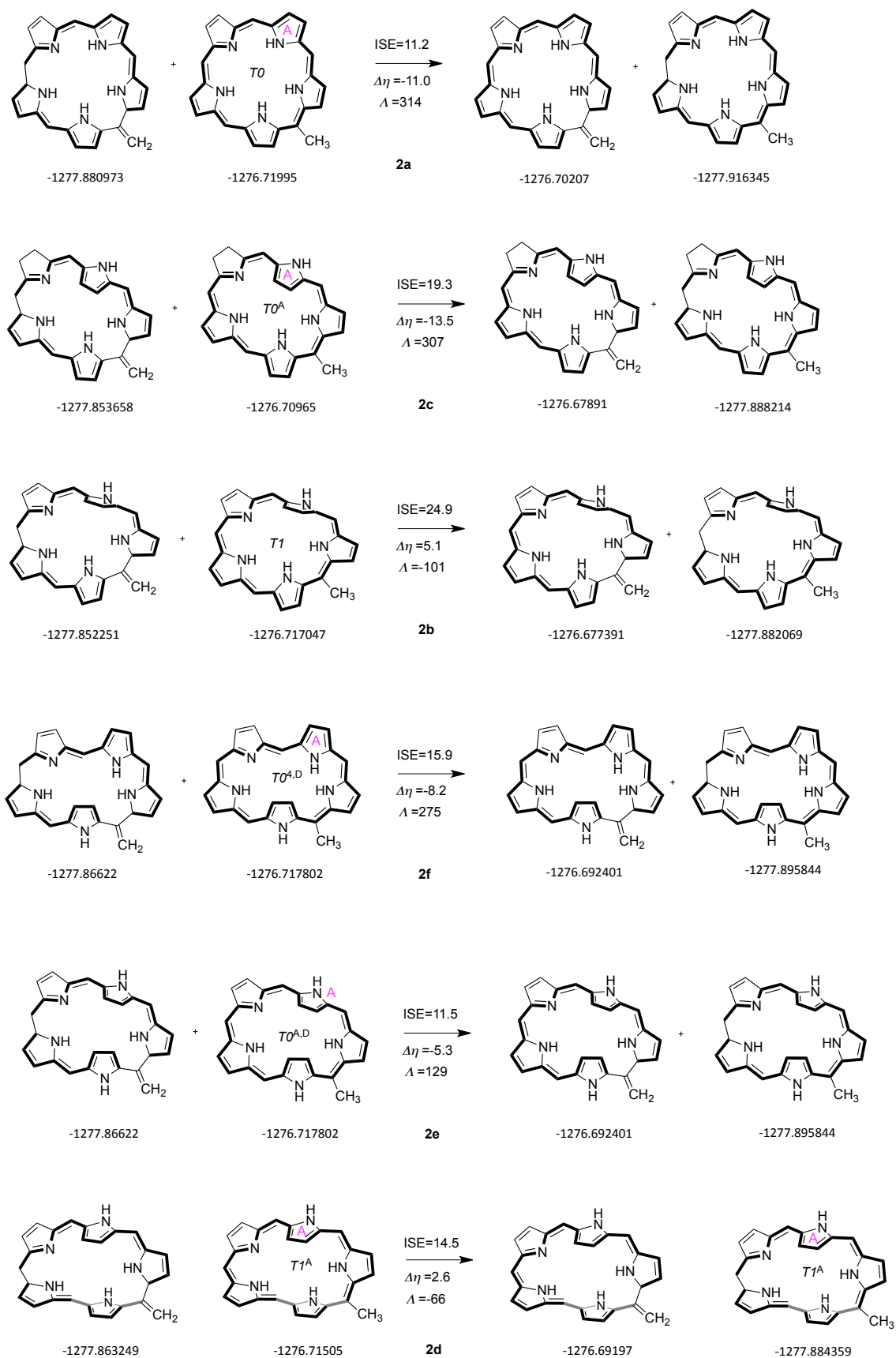


Figure S8. *Syn-anti* corrections applied for the ISE values computed for the Hückel and Möbius conformers of [24]pentaphyrin. Zero-point corrected energies in hartrees evaluated at B3LYP/6-31G(d,p) level of theory.

VIII. Mutual relationships between aromaticity indices of [24] and [22]pentaphyrins.

Table S3. Correlation coefficients (R) between energetic, magnetic, reactivity and structural descriptors of aromaticity for unsubstituted [24]- and [22]pentaphyrins ($n = 11$).

	ISE	ISE _{corr}	Λ	$\Delta\eta$	NICS	NICS(1)	NICS _{zz} (1)	HOMA
ISE	1							
ISE _{corr}	0.919	1						
Λ	-0.743	-0.885	1					
$\Delta\eta$	0.746	0.884	-0.992	1				
NICS(0)	-0.733	-0.883	0.985	-0.973	1			
NICS(1)	-0.734	-0.885	0.986	-0.973	1.000	1		
NICS _{zz} (1)	-0.719	-0.875	0.989	-0.973	0.998	0.998	1	
HOMA	0.772	0.834	-0.948	0.931	-0.908	-0.910	-0.913	1

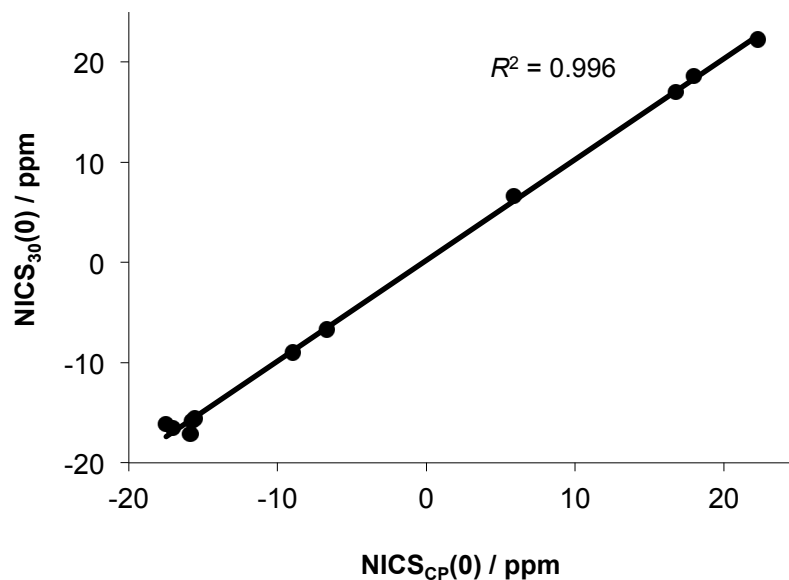


Figure S9. Interrelation between NICS values calculated at the geometrical center of 30 heavy atoms of the pentaphyrin framework [NICS₃₀] and those evaluate at the geometrical center of the heavy atoms belonging to the classical conjugation pathway [NICS_{CP}].

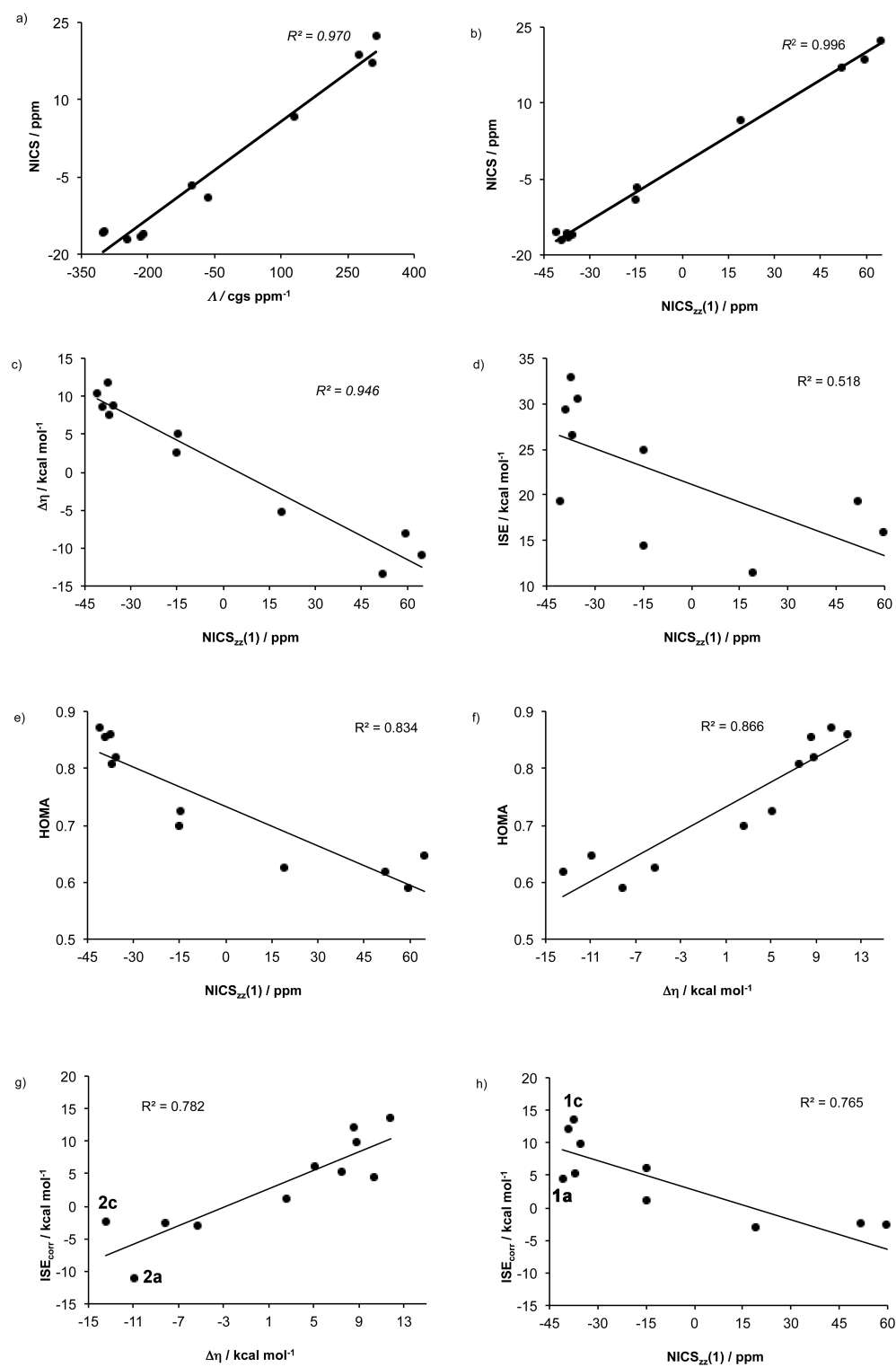


Figure S10. Dependence between the different aromaticity descriptors computed for quantifying the aromaticity of [24]- and [22]pentaphyrins ($n = 11$). The aromaticity descriptors of **1a-f** and **2a-f** are collected in Table 2.

IX. N-fusion reaction in [22]- and [24]pentaphyrins.

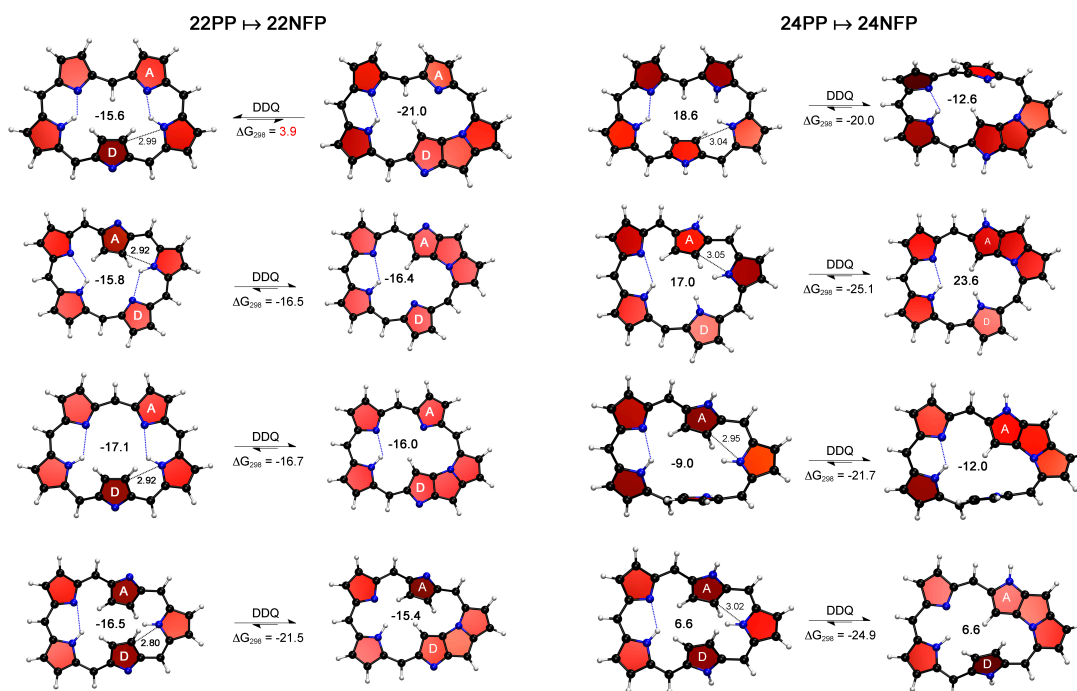


Figure S11. Computed Gibbs free energies (kcal mol⁻¹) for the N-fusion reactions of unsubstituted [22]- and [24]pentaphyrins(1.1.1.1.1). NICS values computed at the heavy atom center is also shown.

X. Dual descriptor in non-fused pentaphyrins.

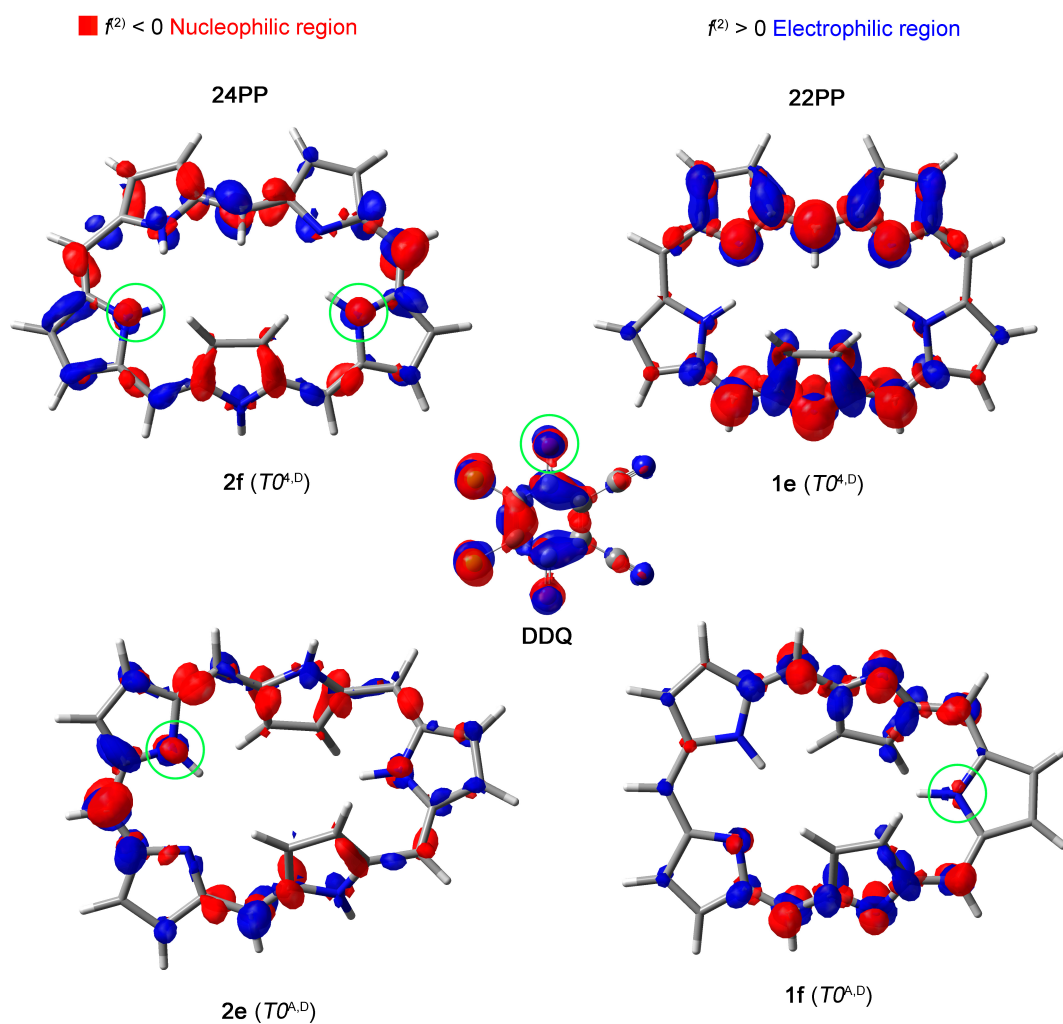


Figure S12. Dual descriptor isosurface (0.002 au) for the $T0^{4,D}$ and $T0^{A,D}$ conformers of non-fused [24]- and [22]pentaphyrins and DDQ.

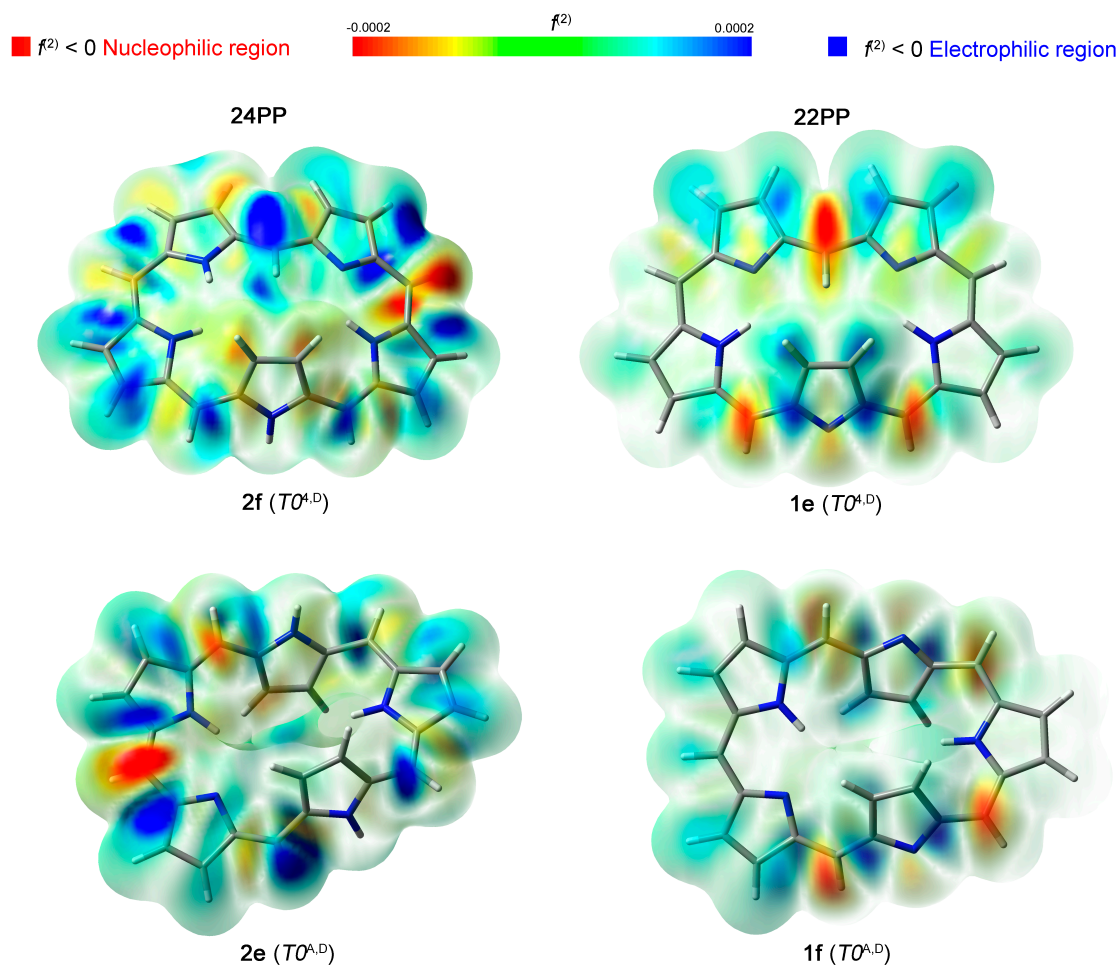


Figure S13. Dual descriptor mapped on a isodensity surface (0.002 au) of the most important conformers of non-fused [24]- and [22]pentaphyrins.

The dual descriptor has been also mapped on the isodensity surface (0.002 au), as shown in Figure S13. It allows a rapid visual comparison of the dual descriptor pattern of the different conformers. In each conformation, the blue and red colored regions for $f^{(2)}(r)$ invert after oxidation with DDQ. That is, nucleophilic regions in the [24]PP switch into electrophilic regions in the [22]PP counterpart and *vice versa*. In addition, the predicted electrophilic/nucleophilic centers are different for the $T0^{4,D}$ and $T0^{A,D}$ conformers with the same oxidation state, indicating that the reactivity is dependent on the conformation of the pentapyrrolic macrocycle.

XI. Conformations and relative energies of *meso*-substituted [22]pentaphyrins.

Table S4. Relative energies (E_{rel}), hydrogen bonding (N_H), ring strain (Φ_p), maximum deviation of dihedral angles from planarity (ψ_{MAX}), π -conjugation index (Π), and bond length alternation (Δr_{C-C}) of the $T0^{4,D}$ and $T0^{A,D}$ structures of *meso*-substituted[22]PP with 5 and 4 aryl groups.^a

Ar	N°	[22]PP	E_{rel}	N_H	Φ_p	ψ_{MAX}	Π	Δr_{C-C}	HOMA
C ₆ F ₅	5	$T0^{4,D}$	1.43	2	34.1	39.8	0.37	0.070	0.772
	5	$T0^{A,D}$	0.00	1	30.9	42.8	0.40	0.072	0.750
	4	$T0^{4,D}$	0.00	2	16.5	21.2	0.77	0.0650	0.775
	4	$T0^{A,D}$	13.03	1	30.7	43.46	0.41	0.0709	0.762
C ₆ H ₃ Cl ₂	5	$T0^{4,D}$	8.53	2	38.9	57.7	0.23	0.101	0.657
	5	$T0^{A,D}$	0.00	1	30.0	42.0	0.41	0.073	0.763
	4	$T0^{4,D}$	0.00	2	14.5	21.0	0.80	0.066	0.789
	4	$T0^{A,D}$	14.55	1	30.0	42.7	0.41	0.072	0.773

^a E_{rel} are given in kcal mol⁻¹, Φ_p and ψ_{MAX} in deg, and Δr_{C-C} in Å.

Table S5. Relative energies of the concave ($T0^{4,D}$) and triangular ($T0^{A,D}$) conformations of *meso*-aryl-substituted non-fused pentaphyrins computed with B3LYP and B3LYP-D.

Ar	N°	[22]PP	E_{rel}	E_{rel} (DFT-D)	Ar	N°	[24]PP	E_{rel}	E_{rel} (DFT-D)
C ₆ F ₅	5	$T0^{4,D}$	1.43	0.00	C ₆ F ₅	5	$T0^{4,D}$	7.97	0.65
	5	$T0^{A,D}$	0.00	1.18		5	$T0^{A,D}$	0.00	0.00
	4	$T0^{4,D}$	0.00	0.00		4	$T0^{4,D}$	1.29	0.00
	4	$T0^{A,D}$	13.03	13.10		4	$T0^{A,D}$	0.00	0.14
C ₆ H ₃ Cl ₂	5	$T0^{4,D}$	8.53	4.49	C ₆ H ₃ Cl ₂	5	$T0^{4,D}$	-(^a)	-(^a)
	5	$T0^{A,D}$	0.00	0.00		5	$T0^{A,D}$	0.00	0.00
	4	$T0^{4,D}$	0.00	0.00		4	$T0^{4,D}$	0.00	0.00
	4	$T0^{A,D}$	14.55	12.89		4	$T0^{A,D}$	1.19	2.36

^a The optimization of the $T0^{4,D}$ conformation for the *meso*-pentakis(2,6-dichlorophenyl)-substituted [24]pentaphyrin led to a $T0^{A,D}$ structure.

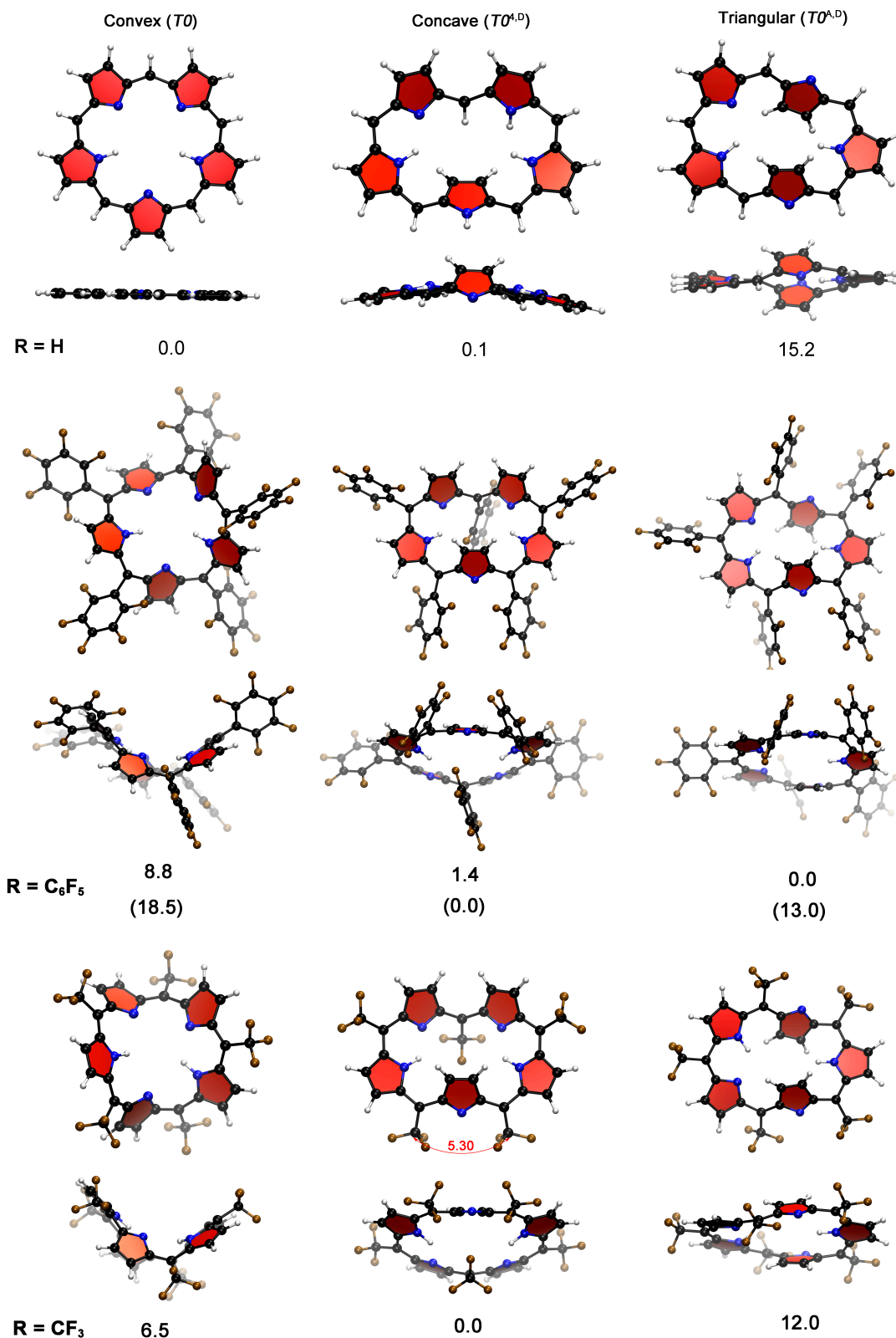
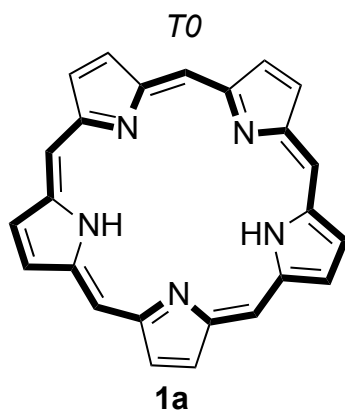


Figure S14. Convex ($T0$), concave ($T0^{4,D}$) and triangular ($T0^{A,D}$) conformations of *meso*-substituted non-fused [22]pentaphyrins, optimized at the B3LYP/6-31G(d,p) level of theory. The relative energies (in kcal mol⁻¹) are also shown. The conformational relative energies corresponding to the 5,10,15,20-tetrakis(pentafluorophenyl) [22]pentaphyrin with a free *meso* position are in parenthesis.

XII. Cartesian coordinates of B3LYP/6-31G(d,p) optimized geometries

Unsubstituted [22]pentaphyrin **1**

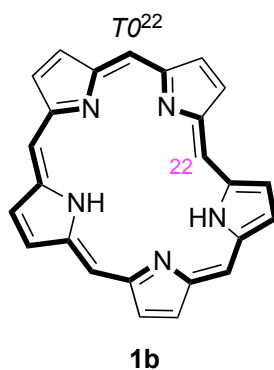
1a



Sum of electronic and zero-point Energies= -1236.238326

C	1.30990500	-3.49040400	-0.00004700
N	1.78700100	-2.21611200	-0.00002800
C	3.13980700	-2.35796200	-0.00006800
C	4.09711200	-1.34107800	-0.00005200
C	3.98133200	0.04440500	-0.00001300
C	5.10832900	0.92643100	-0.00006500
C	4.63979100	2.20856100	0.00001600
C	3.20624500	2.16447200	0.00004700
C	2.44147600	3.32875800	0.00010300
C	1.07600700	3.62904300	0.00010200
N	-0.00018900	2.79401400	0.00002700
C	-1.07647100	3.62892000	0.00000700
C	-2.44191600	3.32848700	-0.00008500
C	-3.20653200	2.16410500	-0.00012800
C	-4.64008500	2.20800100	-0.00023600
C	-5.10845200	0.92580000	-0.00015700
C	-3.98133000	0.04392500	-0.00005700
C	-4.09693400	-1.34157000	0.00004500
C	-3.13948900	-2.35833800	0.00009000
N	-1.78670800	-2.21633000	0.00001600
C	-1.30946000	-3.49057600	0.00007000
C	0.00024700	-3.98960600	-0.00000400
C	-0.67454900	5.03865300	0.00008000
C	0.67393100	5.03872700	0.00015300
N	-2.84779400	0.83231600	-0.00004000
C	-2.40511800	-4.47276000	0.00021100
C	-3.55164100	-3.76239300	0.00021000
N	2.84768500	0.83263600	0.00004500
C	2.40568200	-4.47246300	-0.00011400
C	3.55212300	-3.76196200	-0.00014200
H	-1.35378900	5.88145700	0.00008000
H	1.35308400	5.88160400	0.00022200
H	-3.07098900	4.21454900	-0.00013100
H	3.07044500	4.21489600	0.00015300
H	-1.90283500	0.46397500	0.00002800
H	-6.13615400	0.59030800	-0.00019800
H	-5.21154000	3.12571500	-0.00034200
H	-5.12799000	-1.68391100	0.00009800
H	-2.27574000	-5.54755400	0.00028000
H	-4.57404900	-4.11783900	0.00028000
H	0.00031500	-5.07769000	-0.00000100
H	1.90277800	0.46416200	0.00016100
H	6.13608200	0.59109300	-0.00015900
H	5.21113500	3.12634300	-0.00000100
H	5.12821300	-1.68328800	-0.00007000
H	2.27643600	-5.54727200	-0.00013800
H	4.57457600	-4.11728100	-0.00018900

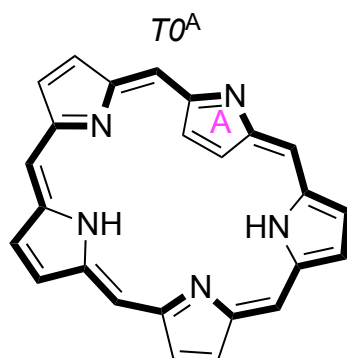
1b



Sum of electronic and zero-point Energies= -1236.212550

C	2.99226000	-2.64918400	-0.01541800
N	1.96738800	-2.15787400	0.69030600
C	0.96035900	-3.07085600	0.58206900
C	-0.27566700	-2.55314800	0.94947600
C	-1.59317700	-2.82628600	0.56690200
C	-2.35126900	-3.93023700	0.06743400
C	-3.60943400	-3.46177800	-0.26537400
C	-3.62809600	-2.05004300	-0.02583400
C	-4.52707700	-1.02784700	-0.37525800
C	-4.19723000	0.32936800	-0.33063300
N	-2.94677600	0.83032300	-0.02624800
C	-3.06055900	2.17546500	-0.08927400
C	-2.09554600	3.18932700	0.08527700
C	-0.70954700	3.34374700	0.19579500
C	-0.16595900	4.66810600	0.35134400
C	1.19190200	4.59133200	0.34809200
C	1.56992600	3.21620900	0.18805000
C	2.90720000	2.84677100	0.07467300
C	3.59898200	1.63108400	-0.09582200
N	3.07351300	0.39288900	-0.09825900
C	4.13480900	-0.44958300	-0.31444500
C	4.09426000	-1.84563700	-0.36763600
C	-4.43654500	2.56136900	-0.42248200
C	-5.13163900	1.41214600	-0.60034900
N	0.38414700	2.48941300	0.12375000
C	5.37757900	0.30878100	-0.49480400
C	5.05193700	1.61025200	-0.32040000
N	-2.43063700	-1.73814600	0.53993100
C	2.69608100	-4.01183500	-0.49142200
C	1.40527000	-4.26118200	-0.14387500
H	-4.78700300	3.57974200	-0.53294200
H	-6.17275300	1.28982800	-0.86966700
H	-2.56643800	4.16888900	0.09925700
H	-5.51300500	-1.30529000	-0.73277600
H	0.35833600	1.48707100	-0.00828700
H	1.90325800	5.40061000	0.43662700
H	-0.77898300	5.55381800	0.44311300
H	3.56201300	3.71368900	0.11490300
H	6.35258300	-0.12165200	-0.68570100
H	5.69845800	2.47816700	-0.35849200
H	4.98035000	-2.34219100	-0.75768900
H	-2.15708300	-0.74736300	0.59178000
H	-1.99854800	-4.94976000	0.00181700
H	-4.43281600	-4.03612000	-0.66737100
H	-0.15431100	-1.57421100	1.40802700
H	3.36261900	-4.64723700	-1.06181000
H	0.81694600	-5.14228000	-0.36365200

1c

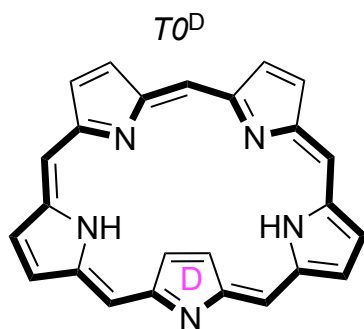


1c

Sum of electronic and zero-point Energies= -1236.230576

C	-1.12928700	-3.02069700	0.39535700
N	-0.06328800	-3.77655900	0.03240200
C	1.01789000	-3.05036500	0.42256800
C	2.31102400	-3.34326500	-0.02464600
C	3.31004100	-2.37613000	-0.15581400
C	4.70699600	-2.54646500	-0.42114300
C	5.29116800	-1.30280300	-0.46641600
C	4.26185400	-0.32668000	-0.27060900
C	4.35371800	1.06458000	-0.28006100
C	3.32275200	2.00001000	-0.13421400
N	1.97525900	1.75397500	-0.02678100
C	1.40310500	2.98435800	0.09505800
C	0.06980400	3.44023800	0.18141800
C	-1.27211900	3.03592800	0.12424100
C	-2.29350700	4.05211200	0.14978700
C	-3.51424300	3.45995800	0.01727700
C	-3.31080400	2.04768100	-0.07386900
C	-4.34043100	1.12043700	-0.22553500
C	-4.24815600	-0.27632400	-0.25848100
N	-3.08685200	-0.93698200	-0.07274800
C	-3.38561800	-2.26250900	-0.20266200
C	-2.42543600	-3.27148300	-0.07794900
C	3.61786100	3.42640000	-0.07571200
C	2.42742600	4.04062200	0.08577700
N	3.09520600	-1.01406400	-0.07809600
C	-0.72613000	-1.86702600	1.20712500
C	0.62466000	-1.88267900	1.22255600
N	-1.94043300	1.83053700	0.00110800
C	-4.80227700	-2.44386700	-0.51720000
C	-5.35094600	-1.20156500	-0.52364000
H	2.51999800	-4.34482300	-0.38772100
H	5.19274500	-3.50679700	-0.52509300
H	6.33480200	-1.06989100	-0.62642800
H	5.35260500	1.46955200	-0.40934000
H	0.07655400	4.52168100	0.28689000
H	-2.07900800	5.10762900	0.24306700
H	-4.48524700	3.93436500	-0.01171400
H	-5.33001000	1.55593500	-0.32790000
H	-2.65229600	-4.26715700	-0.44908500
H	4.60515800	3.86497900	-0.14036600
H	2.22476800	5.10038300	0.17398600
H	2.20312900	-0.52932000	-0.02871900
H	-1.40122500	-1.18879600	1.70336100
H	1.28613900	-1.22590000	1.76980300
H	-1.54667200	0.89627300	-0.04257000
H	-5.29454500	-3.39464500	-0.67634700
H	-6.38222300	-0.92462500	-0.70231000

1d

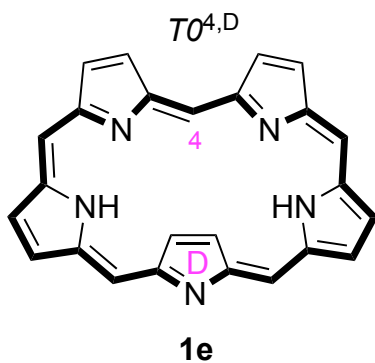


1d

Sum of electronic and zero-point Energies= -1236.227029

C	1.34605500	2.95135100	0.12003300
N	1.96649300	1.74429700	-0.01866000
C	3.30167500	2.03963900	-0.11572100
C	4.35869700	1.13218700	-0.27147300
C	4.28754200	-0.25845100	-0.27705800
C	5.32968700	-1.22290700	-0.47295700
C	4.75919800	-2.47174600	-0.43878500
C	3.35688200	-2.31790400	-0.18060600
C	2.37340600	-3.29837100	-0.05005300
C	1.07454900	-3.02252100	0.39873500
N	-0.00003500	-3.75729300	0.01453300
C	-1.07461500	-3.02250600	0.39876500
C	-2.37347000	-3.29835400	-0.05002000
C	-3.35693700	-2.31787600	-0.18060700
C	-4.75924200	-2.47167900	-0.43882700
C	-5.32970800	-1.22282500	-0.47295800
C	-4.28754100	-0.25839800	-0.27708000
C	-4.35866300	1.13224200	-0.27149700
C	-3.30163400	2.03966900	-0.11572000
N	-1.96646700	1.74433400	-0.01863400
C	-1.34598200	2.95135600	0.12003100
C	0.00003700	3.37163800	0.20171200
C	3.55004800	3.47374100	-0.03318700
C	2.33803400	4.04174000	0.13365600
N	3.12606100	-0.95917100	-0.09813800
C	-0.67575000	-1.86530100	1.20809900
C	0.67571000	-1.86531300	1.20811300
C	-3.54998300	3.47378800	-0.03314400
C	-2.33797400	4.04176300	0.13372600
N	-3.12607900	-0.95914400	-0.09814900
H	4.52198400	3.94679800	-0.08655800
H	2.09885300	5.09230300	0.23827400
H	5.34921900	1.55940600	-0.39264000
H	0.00003100	4.45184900	0.32529400
H	2.23111300	-0.47495600	-0.05696000
H	5.25589800	-3.42641600	-0.54337400
H	6.37191700	-0.97778900	-0.62370000
H	2.59749900	-4.29799600	-0.40911100
H	-1.33161800	-1.19786700	1.74852200
H	1.33156900	-1.19788600	1.74855100
H	-2.59756400	-4.29797300	-0.40909700
H	-4.52192800	3.94682700	-0.08652600
H	-2.09873900	5.09230400	0.23844100
H	-5.34916800	1.55948800	-0.39269900
H	-5.25596100	-3.42633800	-0.54343700
H	-6.37193200	-0.97769000	-0.62371400
H	-2.23111100	-0.47497400	-0.05699400

1e

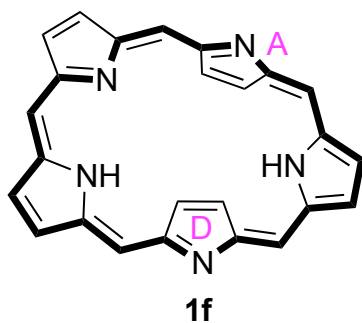


Sum of electronic and zero-point Energies= -1236.238189

C	-1.31527600	2.52919100	0.17747100
N	-2.24550800	1.53431400	0.22900300
C	-3.45645900	2.07717700	-0.02480200
C	-4.59443600	1.25603100	-0.17682800
C	-4.51899300	-0.14591000	-0.15707600
C	-5.49660000	-1.15908800	-0.45184700
C	-4.85311200	-2.37469800	-0.46849600
C	-3.46400300	-2.15686600	-0.15424600
C	-2.39564100	-3.06510800	-0.13658800
C	-1.08332600	-2.76429800	0.27255600
N	-0.00007800	-3.46459200	-0.16184100
C	1.08313600	-2.76430800	0.27248700
C	2.39547700	-3.06512400	-0.13664700
C	3.46379400	-2.15690000	-0.15431100
C	4.85290800	-2.37486200	-0.46865500
C	5.49649000	-1.15934800	-0.45203700
C	4.51896400	-0.14606600	-0.15713100
C	4.59457000	1.25584200	-0.17673500
C	3.45663600	2.07706000	-0.02443800
N	2.24572900	1.53422400	0.22948500
C	1.31545900	2.52912700	0.17769000
C	0.00009700	2.07349800	0.31603600
C	0.67650100	-1.65101000	1.14037200
C	-0.67659900	-1.65102600	1.14042400
N	3.33480300	-0.80737700	0.05042200
C	1.97963000	3.80076300	-0.08650600
C	3.31155900	3.52315900	-0.20223900
N	-3.33489500	-0.80736000	0.05051600
C	-1.97943900	3.80088800	-0.08647300
C	-3.31137300	3.52329700	-0.20236800
H	1.33060500	-1.01048100	1.71498000
H	-1.33064700	-1.01047300	1.71505900
H	2.57058400	-4.04660700	-0.56705400
H	-2.57073000	-4.04653600	-0.56712400
H	2.48862400	-0.22617800	0.15195500
H	6.54405000	-0.97197700	-0.64470800
H	5.29017900	-3.34356400	-0.66833200
H	5.55644100	1.71055500	-0.38897800
H	1.50040800	4.76685900	-0.17398000
H	4.11339500	4.22258800	-0.40394000
H	0.00003700	1.00369100	0.49832700
H	-2.48856800	-0.22644800	0.15173300
H	-6.54416600	-0.97166800	-0.64444900
H	-5.29059400	-3.34336900	-0.66785600
H	-5.55631300	1.71081500	-0.38891100
H	-1.50023000	4.76701100	-0.17369000
H	-4.11321600	4.22279600	-0.40380700

1f (A and D are stacked)

TO^{A,D}

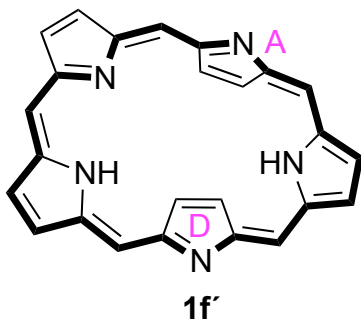


Sum of electronic and zero-point Energies= -1236.214177

C	-0.10070100	-2.83693300	-0.24678100
N	-1.35342700	-3.31588900	0.05353400
C	-2.20641700	-2.44124900	-0.51413600
C	-3.60404100	-2.38246400	-0.24186100
C	-4.22785000	-1.13971200	-0.11630100
C	-5.59696200	-0.68513000	-0.03430900
C	-5.59649900	0.68805700	0.04854600
C	-4.22580600	1.14288000	0.09908800
C	-3.59897800	2.38359800	0.23199300
C	-2.20071400	2.43564800	0.50210300
N	-1.34119600	3.31845100	-0.04409000
C	-0.09125500	2.84479300	0.26833600
C	1.07275000	3.39004600	-0.27362700
C	2.33661000	2.77671700	-0.32114900
C	3.59112300	3.41074800	-0.58881800
C	4.58640700	2.46669000	-0.48029400
C	3.97110500	1.20946500	-0.19314900
C	4.57477200	-0.04369200	-0.03290400
C	3.91803400	-1.26588800	0.14755400
N	2.56367300	-1.42323800	0.06648600
C	2.32585400	-2.73400600	0.33859900
C	1.05967900	-3.35976400	0.31922900
C	-0.16894700	-1.70370900	-1.16793800
C	-1.48627200	-1.45577400	-1.34678400
N	-3.47522800	0.00237400	-0.02066600
C	-1.48866800	1.44164300	1.32719500
C	-0.16877800	1.69617400	1.17027400
N	2.61785900	1.44407900	-0.09743400
C	3.57258700	-3.43392800	0.64298800
C	4.57101600	-2.52646500	0.48454900
H	0.68327400	-1.22385900	-1.62374300
H	-1.94048000	-0.74339700	-2.02283400
H	-4.15210300	-3.28693500	0.00072600
H	-6.46272200	-1.33199800	-0.07325000
H	-6.46135500	1.33411300	0.11245000
H	-4.14708400	3.29259900	0.00749900
H	-1.94630800	0.71715700	1.98735100
H	0.65833500	1.21378200	1.67215100
H	0.99317100	4.37038600	-0.73452300
H	3.70466600	4.46668800	-0.79151700
H	5.65098400	2.61595800	-0.59651200
H	5.66048500	-0.05396100	-0.04147800
H	0.97334400	-4.32565500	0.81076500
H	1.96997700	0.66337000	-0.01075700
H	3.65472300	-4.48229400	0.89965700
H	5.63690500	-2.67359600	0.60344700
H	-2.46588200	0.00074100	-0.03865200

1f' (A and D facing toward the same direction)

TO^{A,D}



Sum of electronic and zero-point Energies= -1236.210877

C	0.13549200	2.96874000	0.13213400
N	1.35299200	3.37836600	-0.34936200
C	2.25051800	2.56535600	0.24552100
C	3.58298800	2.39721500	-0.22036200
C	4.17989500	1.13770800	-0.23742700
C	5.47439500	0.67398900	-0.66721300
C	5.46290200	-0.70059500	-0.68784200
C	4.16050300	-1.15520500	-0.27190600
C	3.54604700	-2.40652400	-0.28663400
C	2.21535300	-2.57256900	0.18378400
N	1.30450000	-3.37228800	-0.41138900
C	0.09773400	-2.98255200	0.10582600
C	-1.12311500	-3.46533400	-0.36314000
C	-2.37079000	-2.83025500	-0.23228200
C	-3.65810100	-3.42608900	-0.39756400
C	-4.61293500	-2.45397500	-0.20684200
C	-3.94161100	-1.21419900	0.02054400
C	-4.51988800	0.06133100	0.04368200
C	-3.87668900	1.30180800	0.00025300
N	-2.52354400	1.48751300	0.04635600
C	-2.32882500	2.80325400	-0.24347700
C	-1.07406700	3.44211900	-0.36590500
C	0.28578600	1.96486300	1.18561200
C	1.61519500	1.73456200	1.28145600
N	3.45832900	-0.00750100	0.03464500
C	1.59957700	-1.76487400	1.24611200
C	0.26763200	-1.99684200	1.17364200
N	-2.59217800	-1.49137700	0.04253200
C	-3.60084600	3.48205400	-0.48077100
C	-4.57166700	2.55443300	-0.28395500
H	-0.52351200	1.55806000	1.77305300
H	2.13525400	1.12282000	2.00449000
H	4.06989000	3.21213000	-0.74611900
H	6.30412600	1.32075600	-0.91771800
H	6.28187800	-1.35345800	-0.95720200
H	4.02102700	-3.21424700	-0.83380200
H	2.13033700	-1.16995800	1.97505500
H	-0.51172300	-1.61941200	1.82162500
H	-1.11216600	-4.39641500	-0.92293000
H	-3.81742800	-4.47569300	-0.60225400
H	-5.68733100	-2.56819400	-0.24941500
H	-5.60410400	0.07385500	-0.01948900
H	-1.04257300	4.36554200	-0.93936400
H	-1.90967200	-0.73747400	0.03943200
H	-3.71303200	4.52845700	-0.73392000
H	-5.64462500	2.67707700	-0.35970700
H	2.45008700	0.00265900	0.08932600

TS1_{1a-1b} conformational interconversion $T0 \rightarrow T0^A$

Sum of electronic and zero-point Energies= -1236.196013

C	-1.46748500	-2.74330900	1.22805100
N	-0.96407800	-2.66176100	-0.09095200
C	0.29479200	-2.99461600	0.00179100
C	1.21867200	-3.13356100	-1.13653400
C	2.31930200	-2.34903100	-1.23753400
C	3.55841100	-2.55912600	-1.97717600
C	4.45768300	-1.62401200	-1.57696000
C	3.79183600	-0.70934300	-0.66032000
C	4.25525400	0.45457900	-0.09139600
C	3.41332900	1.42781900	0.52390800
N	2.07282000	1.45365200	0.42705200
C	1.69215300	2.67978800	0.95421900
C	0.51657400	3.37209100	0.78728800
C	-0.70302300	3.16759300	0.05287700
C	-1.39535900	4.23815200	-0.56160200
C	-2.51078200	3.71922000	-1.20447100
C	-2.55001300	2.33585100	-0.93759900
C	-3.64457800	1.47098700	-1.19324200
C	-3.85251700	0.22156200	-0.65869300
N	-2.90768000	-0.37385500	0.17017100
C	-3.47429100	-1.48299600	0.61873600
C	-2.71690300	-2.32526300	1.54219600
C	2.86206100	3.37207400	1.51711500
C	3.93526500	2.60770500	1.22321300
N	-1.41745700	2.02704400	-0.20309500
C	-4.82456900	-1.65813100	0.10421400
C	-5.04782800	-0.59818800	-0.72749900
N	2.52586100	-1.20102700	-0.47625600
C	-0.42132500	-3.20608300	2.14132000
C	0.70276200	-3.29730200	1.39305500
H	2.83582500	4.33657000	2.00801900
H	4.97964700	2.79987100	1.43395500
H	0.56540800	4.38946300	1.16876100
H	5.31016700	0.68696400	-0.18804300
H	-1.28378000	1.09197800	0.17658100
H	-3.25383200	4.25789400	-1.77595300
H	-1.06142800	5.26602200	-0.54718200
H	-4.42927000	1.89586600	-1.81390700
H	-5.48679400	-2.48547700	0.32363900
H	-5.93335200	-0.38581100	-1.31300400
H	-3.12456000	-2.53429100	2.53078200
H	1.80497900	-0.61153900	-0.06638300
H	3.72082900	-3.38215300	-2.66019000
H	5.48849200	-1.52531900	-1.88998300
H	1.06792200	-3.94270300	-1.84546900
H	-0.52969300	-3.33817400	3.21007200
H	1.70664000	-3.54628700	1.71012200

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-43.0736	36.9512	41.9437
Red. masses --	4.5447	5.6113	5.9941
Frc consts --	0.0050	0.0045	0.0062
IR Inten --	3.2081	0.1901	0.1079

TS2_{1b-1c} conformational interconversion $T0 \rightarrow T0^A$

C	-1.83959300	-3.07899300	0.49599200
N	-1.25463400	-2.97779100	-0.66840900
C	0.12314200	-3.09030800	-0.39359200
C	1.04089600	-2.81114900	-1.34337900
C	2.42573200	-2.47413900	-0.98409700

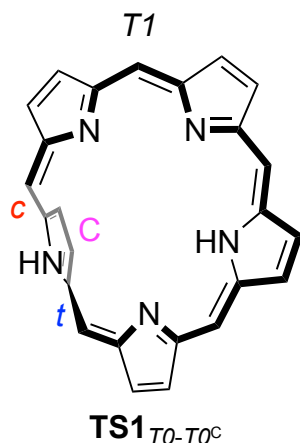
C	3.64083000	-3.16947900	-0.95897800
C	4.61464200	-2.29223300	-0.45126000
C	3.98247000	-1.06569300	-0.17841600
C	4.46469400	0.15862500	0.33777300
C	3.73231500	1.31724600	0.51057000
N	2.37925000	1.47569200	0.19827400
C	2.12586900	2.77715800	0.38248200
C	0.93837200	3.53695200	0.11954900
C	-0.39306900	3.33444900	-0.16750800
C	-1.24434800	4.47374700	-0.47042400
C	-2.50856900	4.04201600	-0.67219800
C	-2.53829900	2.60696500	-0.47460400
C	-3.70866200	1.88335300	-0.48213700
C	-3.96589500	0.51520500	-0.17664300
N	-3.06064400	-0.43147800	0.02419200
C	-3.79603600	-1.57274800	0.37401200
C	-3.26075800	-2.78732900	0.66733700
C	3.31435900	3.49395000	0.84931900
C	4.30813800	2.57655900	0.94298500
N	-1.23012600	2.22062000	-0.21091500
C	-5.23394500	-1.26607400	0.40010000
C	-5.34700100	0.02165400	0.01988800
N	2.65685600	-1.21828900	-0.51616500
C	-0.89252800	-3.38541500	1.59184700
C	0.33827000	-3.35600100	1.03730100
H	3.35616900	4.55313900	1.06927600
H	5.33610300	2.72438200	1.24808000
H	1.15556000	4.60183500	0.14483300
H	5.51833600	0.19397700	0.59974900
H	-0.97767200	1.26364500	-0.00313700
H	-3.38422800	4.62849400	-0.91358400
H	-0.87332900	5.48828300	-0.52075900
H	-4.59069000	2.48266700	-0.68691500
H	-6.01828500	-1.97196600	0.64120800
H	-6.24734000	0.61105000	-0.10255400
H	-3.91048300	-3.56043400	1.07263500
H	2.00244600	-0.43991400	-0.41552900
H	3.77924000	-4.19551100	-1.26758500
H	5.66297600	-2.50465900	-0.29297000
H	0.68960700	-2.64632700	-2.36032100
H	-1.15818600	-3.54424900	2.62925100
H	1.29872000	-3.49560100	1.51396100

Sum of electronic and zero-point Energies= -1236.197188

***** 1 imaginary frequencies (negative Signs) *****
Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering
activities (A⁴/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-87.6166	29.7607	42.4033
Red. masses --	4.1462	5.7527	5.7880
Frc consts --	0.0188	0.0030	0.0061
IR Inten --	0.2693	0.0134	0.0416

TS1_{1a-li} conformational interconversion $T0 \rightarrow T0^C$



Sum of electronic and zero-point Energies= -1236.189164

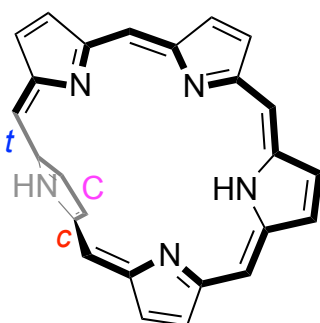
***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering
 activities (A⁴/AMU), depolarization ratios for plane and unpolarized
 incident light, reduced masses (AMU), force constants (mDyne/A),
 and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-93.1922	37.2322	40.9085
Red. masses --	3.7310	5.6600	5.7069
Frc consts --	0.0191	0.0046	0.0056
IR Inten --	2.3766	0.5797	0.0507
C	3.75283100	0.72071400	-0.49188300
N	3.03509400	-0.31657500	-0.11693200
C	3.96523300	-1.27295000	0.32654100
C	3.57207300	-2.44563200	0.88609100
C	2.15120900	-2.79795800	0.93472800
C	1.23759000	-2.80937200	1.98603900
C	-0.04739900	-2.92248300	1.42511800
C	0.09538900	-3.03606900	0.03805400
C	-0.88708000	-3.28081300	-0.97021200
C	-2.13141500	-2.70315400	-0.96270000
N	-2.43513000	-1.59818700	-0.17348200
C	-3.72789400	-1.36544300	-0.37011200
C	-4.39055200	-0.21328500	0.16707700
C	-3.78408300	0.96034300	0.52943300
C	-4.47259000	2.15577600	0.97401200
C	-3.56876700	3.15946500	1.05661400
C	-2.26371700	2.64879600	0.65826100
C	-1.18668900	3.49285300	0.47157900
C	0.13566800	3.34116400	-0.03840500
N	0.87316300	2.23819000	-0.18069900
C	2.08285500	2.68027300	-0.70735400
C	3.27788000	2.02269100	-0.88293400
C	-4.33006700	-2.34157400	-1.28067200
C	-3.31191300	-3.14223300	-1.69504400
N	-2.43811900	1.30527700	0.41176000
C	2.03939200	4.13709200	-0.95219600
C	0.84834600	4.55783000	-0.49449800
N	1.45244400	-2.99974100	-0.22573400
C	5.21107800	0.46002400	-0.36983600
C	5.33617900	-0.77493200	0.15825000
H	-5.36779800	-2.36701100	-1.58903500
H	-3.35581600	-3.98028200	-2.37911500
H	-5.47513000	-0.22758600	0.21637500
H	-0.64518500	-3.98289000	-1.76739100
H	-1.72359500	0.63935200	0.13588700
H	-3.74376900	4.19147000	1.32826700
H	-5.53560600	2.19825300	1.16860900
H	-1.44307800	4.52890800	0.67538200

H	2.84907800	4.72019800	-1.37226900
H	0.44860300	5.56380100	-0.46864800
H	4.06747600	2.65717100	-1.28045700
H	1.84588800	-2.80660800	-1.13465100
H	1.48718700	-2.69744800	3.03119400
H	-0.99259600	-2.96350200	1.94462500
H	4.31445400	-3.11172400	1.32069800
H	5.99684900	1.15997400	-0.62725200
H	6.23955100	-1.31155100	0.41768600

TS2_{1a-li} conformational interconversion $T0 \rightarrow T0^C$

T1



TS2_{T0-T0^C}

Sum of electronic and zero-point Energies= -1236.187579

C	3.74659100	-1.19893900	-0.36297600
N	2.54004700	-1.64795600	-0.07705300
C	2.32381900	-2.71157400	-0.94986600
C	1.11306200	-3.35348500	-0.97736200
C	0.12801800	-3.18212700	0.04464800
C	0.26286700	-3.10630700	1.43413700
C	-1.02283000	-2.97462300	1.98803700
C	-1.92941000	-2.91276100	0.93155800
C	-3.35226500	-2.58203900	0.87963400
C	-3.80277900	-1.41801500	0.34249700
N	-2.97282800	-0.36593600	-0.08004300
C	-3.80049600	0.58920900	-0.47664600
C	-3.46101300	1.92622100	-0.84395700
C	-2.30303000	2.65298000	-0.68113300
C	-2.27707800	4.09571600	-0.85230300
C	-1.06960700	4.55235600	-0.45584100
C	-0.24076800	3.42006100	-0.07665800
C	1.05045800	3.60114500	0.35357400
C	2.17219600	2.74385600	0.60731400
N	2.29410700	1.46058600	0.29668800
C	3.63495900	1.15201900	0.55635800
C	4.29689400	0.00197500	0.21890700
C	-5.21920300	0.17343700	-0.38374100
C	-5.21589500	-1.06288800	0.15238600
N	-1.03634400	2.28965500	-0.24930100
C	4.33371100	2.32337200	1.09979600
C	3.42452200	3.31873900	1.13835000
N	-1.22538200	-3.10170200	-0.22816100
C	4.40658000	-2.00146800	-1.40299500
C	3.48822900	-2.92125000	-1.80136600
H	-6.06986600	0.78244400	-0.66406800
H	-6.05838800	-1.69759600	0.39526300
H	-4.29915400	2.52556000	-1.18682200
H	-4.07792600	-3.28622600	1.28172000
H	-0.75649700	1.34008400	-0.03709700
H	-0.72123100	5.57574800	-0.42737700
H	-3.12548100	4.66776600	-1.20178300
H	1.29457200	4.65431000	0.46778700
H	5.37587500	2.34745100	1.39197000
H	3.55822700	4.34277500	1.46456900
H	5.37993700	0.02751800	0.33053700
H	-1.61484300	-2.91388800	-1.13972900
H	1.20436900	-3.16678100	1.95774100

H	-1.27809600	-2.88624600	3.03411300
H	0.87838300	-3.99649100	-1.82518400
H	5.39946800	-1.83426200	-1.80195100
H	3.58826400	-3.67835800	-2.56871700

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1 A	2 A	3 A
Frequencies --	-83.3147	37.0794	40.3638
Red. masses --	3.7903	5.5719	5.6788
Frc consts --	0.0155	0.0045	0.0055
IR Inten --	5.5384	0.4160	0.0857

TS1_{1a-1k} conformational interconversion *T0*→*T0*^D

C	-0.61406000	2.99733100	0.02200000
N	-1.37654600	1.92525300	-0.13802300
C	-2.39658400	2.32269000	-1.01884000
C	-3.53737600	1.59357900	-1.26717600
C	-3.87948500	0.34177500	-0.68722300
C	-5.12184800	-0.32264200	-0.58546000
C	-4.95004700	-1.40691100	0.28114700
C	-3.59313400	-1.43497800	0.65695300
C	-2.81521100	-2.28847700	1.52468900
C	-1.53939200	-2.65123200	1.20843700
N	-1.04434700	-2.54321400	-0.10833600
C	0.22523600	-2.85704600	-0.02977700
C	1.12414900	-3.02869500	-1.18178600
C	2.26954900	-2.30773900	-1.28572600
C	3.49183100	-2.55548100	-2.04438600
C	4.42970800	-1.65716000	-1.64600700
C	3.81034400	-0.73386900	-0.70254500
C	4.30624700	0.39768600	-0.09644500
C	3.45968800	1.33243600	0.58063300
N	2.13070700	1.36101100	0.43460400
C	1.70267800	2.51335200	1.08505700
C	0.52564900	3.18593900	0.91603700
C	0.64477200	-3.15018900	1.35659100
C	-0.47971200	-3.08944500	2.11246500
N	2.52875000	-1.18328700	-0.51248600
C	2.84209100	3.14118000	1.78094500
C	3.93784400	2.43224700	1.43513300
N	-2.98369800	-0.37515100	0.05255800
C	-1.09012600	4.13130800	-0.77570300
C	-2.18209100	3.69188000	-1.45246100
H	1.65428200	-3.38415600	1.66929300
H	-0.57649200	-3.22718800	3.18329200
H	0.90154900	-3.80396400	-1.90915300
H	-3.23106000	-2.56830300	2.49015800
H	1.83422300	-0.55016500	-0.11478000
H	5.45867500	-1.59324200	-1.97463300
H	3.61943600	-3.37696100	-2.73706800
H	5.36290500	0.62277000	-0.18638900
H	2.78273600	4.03559900	2.38971800
H	4.96859300	2.60652900	1.71815100
H	0.49929400	4.15597900	1.41218400
H	-2.03199000	-0.04116800	0.20419600
H	-6.03665500	-0.01516700	-1.07221300
H	-5.69470100	-2.13149400	0.57866700
H	-4.28985600	2.04863100	-1.90553400
H	-0.62463200	5.10767400	-0.81279100
H	-2.80467100	4.23710900	-2.15062600

Sum of electronic and zero-point Energies= -1236.195660

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A),

and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-21.6451	39.0644	47.2114
Red. masses --	4.7016	5.4436	5.7567
Frc consts --	0.0013	0.0049	0.0076
IR Inten --	5.1150	0.1590	0.1197

TS2_{1k-1d} conformational interconversion $T0 \rightarrow T0^D$

C	-0.51176400	3.23196500	-0.18406600
N	-1.30060300	2.08492500	-0.25017700
C	-2.52948600	2.53006200	-0.55421200
C	-3.75411300	1.79984800	-0.59156600
C	-4.01066900	0.48534100	-0.28148600
C	-5.33125900	-0.08465600	-0.04963400
C	-5.17951200	-1.35431000	0.39472200
C	-3.75847500	-1.67463600	0.39903500
C	-3.16558500	-2.83340800	0.79292100
C	-1.73298500	-3.04699500	0.61807000
N	-1.17202300	-2.90025300	-0.56030300
C	0.21293000	-2.94824600	-0.32050800
C	1.11256600	-2.78360400	-1.31990100
C	2.49382500	-2.39895700	-1.03215200
C	3.75343300	-2.98289600	-1.23016400
C	4.70928300	-2.10540500	-0.69415000
C	4.02444600	-0.97620100	-0.20550800
C	4.47823600	0.24939700	0.33903200
C	3.69873300	1.36570300	0.56946000
N	2.34097400	1.45985500	0.25509800
C	2.01588400	2.73780000	0.46229700
C	0.80465500	3.45732600	0.16219300
C	0.46971500	-3.16713400	1.10999000
C	-0.74664500	-3.28538300	1.69007000
N	2.68450800	-1.20338800	-0.40886800
C	3.16293900	3.50379800	0.96336600
C	4.20644800	2.64176500	1.03867600
N	-3.11082100	-0.51880500	-0.03742000
C	-1.32306800	4.42421600	-0.49751900
C	-2.56986600	3.98815800	-0.74865100
H	1.44505700	-3.25567800	1.56826000
H	-0.97758600	-3.46839900	2.73165500
H	0.75375300	-2.79326800	-2.34705300
H	-3.77676100	-3.59356800	1.26983500
H	2.00171100	-0.45731500	-0.24249400
H	5.78075800	-2.24825800	-0.66644400
H	3.93107500	-3.94942800	-1.67917000
H	5.54063000	0.32665200	0.55260400
H	3.14775200	4.55872200	1.20626600
H	5.22328500	2.83785300	1.35352300
H	1.00534300	4.52593700	0.21256000
H	-2.11035000	-0.39041600	-0.11393100
H	-6.25271700	0.46590500	-0.18224300
H	-5.95170500	-2.05437000	0.68311800
H	-4.63760300	2.39979800	-0.78594600
H	-0.94474900	5.43836900	-0.51728100
H	-3.45014400	4.55985700	-1.01344600

Sum of electronic and zero-point Energies= -1236.196793

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering
 activities (A⁴/AMU), depolarization ratios for plane and unpolarized
 incident light, reduced masses (AMU), force constants (mDyne/A),
 and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-73.1650	32.4444	39.1447
Red. masses --	4.0757	5.7903	5.6845
Frc consts --	0.0129	0.0036	0.0051
IR Inten --	1.9560	0.2107	0.0959

TS1_{1c-1g} conformational interconversion $T0^A \rightarrow T0^{4,D}$

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-65.3039	43.5306	52.8737
Red. masses --	4.5368	5.9430	6.0810
Frc consts --	0.0114	0.0066	0.0100
IR Inten --	3.7869	0.4691	0.4720

Sum of electronic and zero-point Energies= -1236.189345

C	1.20098400	2.67906600	0.52684200
N	2.19903800	1.78425800	0.47605100
C	3.17370300	2.29604500	-0.34772900
C	4.16180500	1.46553800	-0.88325200
C	4.22743100	0.07140300	-0.64784800
C	4.88106900	-0.99218000	-1.31759900
C	4.35333700	-2.19572900	-0.82907600
C	3.40317200	-1.86755800	0.15791100
C	2.53686300	-2.58066200	1.11316700
C	1.23345700	-2.91348600	0.92153600
N	0.54140100	-2.87488800	-0.29516700
C	-0.73705400	-2.84133100	0.03569400
C	-1.83249100	-2.86118000	-0.91252500
C	-2.95229500	-2.07539300	-0.83020300
C	-4.17648700	-2.16203100	-1.61378600
C	-4.97091600	-1.10633500	-1.29355800
C	-4.24336700	-0.26089300	-0.36230100
C	-4.45980200	1.07496200	-0.07802900
C	-3.41393700	1.92774900	0.39570700
N	-2.26926900	1.45266200	0.89144700
C	-1.34781600	2.49277900	0.82209700
C	-0.02963800	2.15323300	1.02679400
C	0.28466900	-3.03690100	2.04417200
C	-0.94303700	-2.89947300	1.50106400
N	3.37802700	-0.52092000	0.26520600
C	1.56672100	3.88353000	-0.20495200
C	2.80329100	3.64674200	-0.74011300
N	-3.09857500	-0.95341100	-0.02315000
C	-2.00769800	3.70418500	0.35058700
C	-3.30511100	3.36727300	0.12263200
H	4.84903500	1.88233500	-1.61408500
H	5.63361300	-0.88209100	-2.08654000
H	4.62527700	-3.19730300	-1.12831300
H	2.88416100	-2.57149800	2.14627600
H	-1.74600900	-3.52763200	-1.76510800
H	-4.38871400	-2.95862600	-2.31408200
H	-5.94721500	-0.87079500	-1.69550800
H	-5.36985700	1.52868400	-0.45531000
H	0.09401000	1.15058400	1.42692500
H	0.55519500	-3.11617800	3.08937900
H	-1.90327700	-2.87888400	1.99938600
H	2.67312600	0.07449600	0.72588100
H	0.96048800	4.77118700	-0.32394000
H	3.38394700	4.30729500	-1.37181700
H	-2.35146800	-0.42054900	0.43588100
H	-1.54606600	4.67481700	0.22855800
H	-4.10171400	4.00412800	-0.24168400

TS2_{1g-1e} conformational interconversion $T0^A \rightarrow T0^{4,D}$

Sum of electronic and zero-point Energies= -1236.191860

C	1.02961800	2.71661500	-0.27877500
N	2.02137400	1.76365000	-0.49695700
C	3.18404700	2.33406000	-0.20103200
C	4.39607000	1.57847000	-0.15356700
C	4.40947400	0.19745900	-0.16236500
C	5.54181000	-0.69015100	0.06367500

C	5.07579400	-1.95725000	0.17138000
C	3.62074600	-1.93857700	0.01276400
C	2.78388500	-2.98891400	0.23865500
C	1.31289300	-2.97520500	0.26135900
N	0.54095000	-2.85196100	-0.78936500
C	-0.78272700	-2.79905600	-0.27829600
C	-1.85426400	-2.62480500	-1.08573000
C	-3.16380700	-2.12790600	-0.60017300
C	-4.43917800	-2.63933600	-0.28214600
C	-5.24294800	-1.55074400	0.09881500
C	-4.45589500	-0.37676200	0.00804800
C	-4.66754000	0.99648400	0.31878100
C	-3.66937600	1.96525500	0.19691300
N	-2.43964800	1.60520200	-0.29715200
C	-1.59440700	2.62669200	-0.13938000
C	-0.24904700	2.26011900	-0.46422500
C	0.53743500	-3.07757900	1.52282400
C	-0.76017600	-2.91907700	1.18606700
N	3.29902600	-0.61478500	-0.25787400
C	1.64467000	3.96976800	0.14927400
C	2.98565000	3.74563100	0.17226300
N	-3.21527900	-0.79414700	-0.42408200
C	-2.30193900	3.76057800	0.44109700
C	-3.59564500	3.35055300	0.63898000
H	5.33842900	2.09270100	-0.00109500
H	6.56521100	-0.35245400	0.15708600
H	5.64349700	-2.85619100	0.37077400
H	3.25768300	-3.90773100	0.57767800
H	-1.67668300	-2.62662400	-2.16026400
H	-4.73075000	-3.67890600	-0.32355800
H	-6.27724200	-1.59430000	0.41211000
H	-5.63742500	1.27997600	0.71751900
H	-0.23662200	1.24742900	-0.85700600
H	0.96365500	-3.20923100	2.50929400
H	-1.62932400	-2.90801700	1.82956500
H	2.38212300	-0.18865500	-0.39350800
H	1.12444800	4.89051700	0.37832700
H	3.76775200	4.44684600	0.43688500
H	-2.48408200	-0.06744000	-0.54723500
H	-1.88108800	4.72958500	0.67408600
H	-4.40540700	3.92885200	1.06612600

***** 1 imaginary frequencies (negative Signs) *****
Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-105.4120	17.0852	45.2765
Red. masses --	4.1726	4.8569	5.2217
Frc consts --	0.0273	0.0008	0.0063
IR Inten --	1.6017	1.1092	1.9813

TS1_{1d-1j} conformational interconversion $T0^D \rightarrow T0^A$

Sum of electronic and zero-point Energies= -1236.195504

C	-3.10661900	-1.53836400	-1.14786100
N	-2.73667500	-0.43239100	-0.37668400
C	-3.60092600	0.52444300	-0.68837900
C	-3.57159000	1.84325700	-0.14676000
C	-2.49900100	2.52339300	0.38724000
C	-2.57757600	3.86192400	0.93823700
C	-1.32196900	4.28524700	1.21639100
C	-0.37941200	3.25300600	0.82099100
C	0.97119500	3.50335600	0.74657200
C	2.08396700	2.81393900	0.16130900
N	2.23900900	1.49940600	-0.03672500
C	3.42387300	1.37326500	-0.76213200
C	4.00062100	0.16793000	-1.12635700
C	3.59678200	-1.10481200	-0.67253700
C	3.91503000	-2.40863100	-1.10226800
C	3.14732800	-3.30453100	-0.34744500
C	2.39820400	-2.54787700	0.56555800

C	1.43606400	-2.88960600	1.61258100
C	0.14842000	-3.20350000	1.34117100
N	-0.33980700	-3.25302100	0.02094900
C	-1.61460400	-2.98395500	0.13384000
C	-2.51110200	-2.75225700	-1.00035300
C	-4.58804900	0.06885900	-1.68907800
C	-4.23860200	-1.19503000	-2.01735600
N	-1.15486700	2.17717400	0.40088400
C	4.00079500	2.67649300	-1.02420400
C	3.19365600	3.57755500	-0.40344700
C	-0.96022200	-3.07267800	2.29704700
C	-2.05707100	-2.86026000	1.53985500
N	2.69558600	-1.23808200	0.36445400
H	-5.40076500	0.66324700	-2.08806800
H	-4.71473200	-1.86276900	-2.72366700
H	-4.49430500	2.41305300	-0.20316700
H	-2.70871000	-3.55540100	-1.70514800
H	-0.80594600	1.29694300	0.04469100
H	-1.01830200	5.24322800	1.61609800
H	-3.50637400	4.39935700	1.07311900
H	1.21752400	4.51395300	1.06265700
H	4.91326200	2.86131600	-1.57670100
H	3.29352900	4.65493200	-0.37034100
H	4.84748300	0.20145900	-1.80634700
H	-0.86168600	-3.03011500	3.37368100
H	-3.06472300	-2.62157900	1.85190600
H	1.70795900	-2.66276600	2.64253600
H	4.61147500	-2.65280300	-1.89235200
H	3.12866100	-4.38167300	-0.42047300
H	2.19779700	-0.41898000	0.71573700

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1 A	2 A	3 A
Frequencies --	-24.1793	36.0162	41.3983
Red. masses --	4.8942	5.2946	6.0797
Frc consts --	0.0017	0.0040	0.0061
IR Inten --	6.5524	2.6713	1.0093

TS2_{ij-1c} conformational interconversion $T0^D \rightarrow T0^A$

Sum of electronic and zero-point Energies= -1236.200467

C	-2.38545400	-2.46121500	-0.94427200
N	-2.56611500	-1.26964100	-0.39775100
C	-3.94152800	-1.14191700	-0.21788700
C	-4.48031200	0.03073900	0.25962700
C	-3.78139000	1.23694300	0.50164900
C	-4.34621000	2.46737400	0.90271600
C	-3.34256000	3.41886700	0.86410200
C	-2.14134400	2.78416300	0.44725300
C	-0.95075400	3.53297900	0.20568700
C	0.37393900	3.32778600	-0.12454000
N	1.14989700	2.17767800	-0.23019100
C	2.38502800	2.62398000	-0.51897500
C	3.61653400	1.90937700	-0.58771000
C	3.93660600	0.60071300	-0.30474000
C	5.29460300	0.10634100	-0.11628900
C	5.23314800	-1.17855900	0.30468400
C	3.83583700	-1.58463400	0.34239400
C	3.32209200	-2.78151000	0.72881200
C	1.89153700	-3.05729100	0.60224000
N	1.29709800	-2.95244600	-0.56328100
C	-0.08125500	-3.01900800	-0.28210000
C	-1.00263400	-2.84464700	-1.25565200
C	-4.61559900	-2.34177500	-0.66533000
C	-3.63689600	-3.16811600	-1.14900800
N	-2.43623300	1.46076800	0.25820000
C	2.43099300	4.08781800	-0.65935600
C	1.18746200	4.52476800	-0.38942000

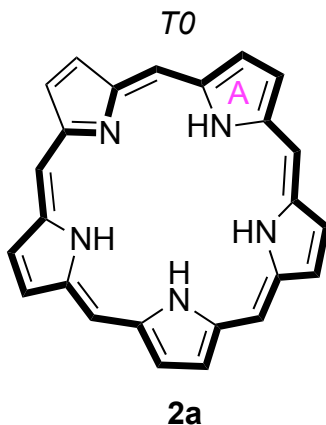
C	0.94270800	-3.29048700	1.70586200
C	-0.29218800	-3.21584300	1.15565200
N	3.10663400	-0.45942300	-0.05376400
H	-5.68255300	-2.52236400	-0.63472800
H	-3.74784400	-4.15510500	-1.57790400
H	-5.55345300	0.07558400	0.42613600
H	-0.66088900	-2.83328400	-2.28928600
H	-1.82894800	0.70717100	-0.05988000
H	-3.42430600	4.47251100	1.09142200
H	-5.38532400	2.61203000	1.16425000
H	-1.17714900	4.59262200	0.29634600
H	3.31464900	4.66366900	-0.90288800
H	0.81602800	5.54149600	-0.37100000
H	4.48064400	2.53653000	-0.78457600
H	1.20620000	-3.43655800	2.74560700
H	-1.25298300	-3.30212600	1.64355700
H	3.99184400	-3.52155700	1.15633000
H	6.17656900	0.71586700	-0.25945500
H	6.05417700	-1.83409200	0.56104200
H	2.10018200	-0.41202500	-0.12987000

***** 1 imaginary frequencies (negative Signs) *****
Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-73.5483	32.4077	39.7162
Red. masses --	4.1295	5.8442	5.7171
Frc consts --	0.0132	0.0036	0.0053
IR Inten --	1.6681	0.0243	0.0320

Unsubstituted [24]pentaphyrin 2

2a

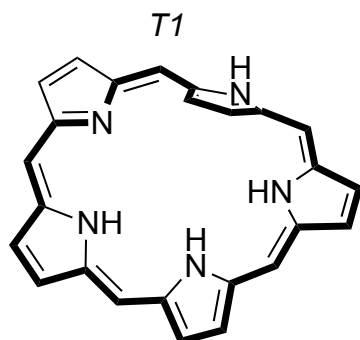


Sum of electronic and zero-point Energies= -1237.431873

C	-1.17611800	3.41014900	0.86090500
C	-0.66379300	4.67758500	1.17455900
C	0.59447500	4.79066900	0.58045200
C	0.87374600	3.58328500	-0.07948200
C	2.07677800	3.31257700	-0.82355500
C	2.81367600	2.17424100	-0.95448300
C	4.12879600	2.11378000	-1.56913600
C	4.69611000	0.92145300	-1.27258200
C	3.75675300	0.13212200	-0.50123400
C	4.00716300	-1.08701400	0.04993700
C	3.11254900	-2.02327400	0.67428100
C	3.43646200	-3.06250000	1.54597000
C	2.29703800	-3.86977200	1.70314200
C	1.27135000	-3.33136800	0.92300000
C	0.04397000	-3.97537800	0.56258200
C	-1.07969000	-3.52970400	-0.07371400

C	-2.06958600	-4.40661000	-0.66742600
C	-3.03451300	-3.65363500	-1.24703300
C	-2.75910200	-2.25757700	-0.96381700
C	-3.66950900	-1.24474200	-1.10159900
C	-3.66748200	0.05490300	-0.49658400
N	-2.61230700	0.75717800	-0.05782900
C	-3.16969300	1.86695400	0.58619700
C	-2.50989600	2.97841300	1.05422300
N	2.56996300	0.89401500	-0.43017700
N	1.76656200	-2.16312500	0.35669000
N	-1.50747000	-2.21962500	-0.35318100
N	-0.20193500	2.74628000	0.12769700
C	-4.93527800	0.70166700	-0.16839000
C	-4.62078300	1.80339600	0.55683200
H	-1.18722200	5.42576200	1.75380800
H	1.27092000	5.63247800	0.62479300
H	2.54692200	4.20302800	-1.22941400
H	4.56082700	2.93056100	-2.13146300
H	5.67817500	0.56781900	-1.55716300
H	5.03840100	-1.42078800	-0.01324300
H	4.40626300	-3.20355200	2.00241100
H	2.20874500	-4.76735200	2.29935800
H	0.04750400	-5.04374600	0.75744300
H	-1.98643500	-5.48534600	-0.65976800
H	-3.91065400	-3.99422400	-1.78175200
H	-4.61312900	-1.54293800	-1.54834300
H	-3.13100800	3.71142000	1.56287700
H	1.95437400	0.78530400	0.36573300
H	1.34649600	-1.72245800	-0.44964000
H	-1.24182100	-1.39910000	0.17885400
H	-0.41022700	1.87905400	-0.35400500
H	-5.91536700	0.32333100	-0.42923700
H	-5.28699400	2.53998200	0.98806800

2b

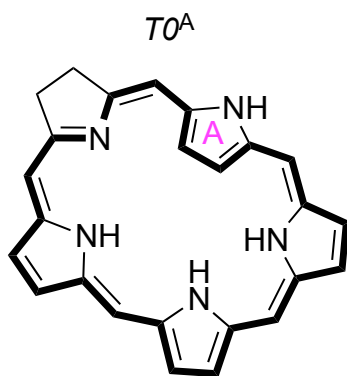


Sum of electronic and zero-point Energies= -1237.427414

C	1.49623400	-2.98369600	1.00456200
C	0.55639100	-3.66262500	1.79832500
C	-0.65827200	-3.67358400	1.10044400
C	-0.44523300	-3.07114500	-0.15446500
C	-1.36323300	-3.03020300	-1.28565400
C	-2.49804600	-2.27208700	-1.22937100
C	-3.72889700	-2.31859400	-1.99124100
C	-4.60306500	-1.40985800	-1.46639100
C	-3.93238500	-0.66572500	-0.42737000
C	-4.33089700	0.48368500	0.21937500
C	-3.47549000	1.47219900	0.77550100
C	-3.84120400	2.60828200	1.52233300
C	-2.73905900	3.45107800	1.59974600
C	-1.66398000	2.85516800	0.90308500
C	-0.47389600	3.53682300	0.55009900
C	0.72233900	3.25152000	-0.08889300
C	1.55065200	4.30109200	-0.62869300
C	2.65133500	3.74789300	-1.20813400
C	2.61249400	2.32766600	-0.98240800
C	3.69416800	1.47924100	-1.13771900

C	3.86484000	0.18782000	-0.57786500
N	2.87704200	-0.60418800	-0.12331800
C	3.51243500	-1.60361100	0.60627100
C	2.84763900	-2.63012600	1.24823100
N	-2.66606500	-1.22410900	-0.32463600
N	-2.11731900	1.61146100	0.48118100
N	1.38536500	2.05528100	-0.38295600
N	0.85782200	-2.65793500	-0.17772200
C	5.18031300	-0.33233800	-0.21055100
C	4.95307700	-1.41349500	0.58094200
H	0.75390000	-4.08019500	2.77607900
H	-1.58372600	-4.14391400	1.40237300
H	-1.18857600	-3.66906300	-2.14691500
H	-3.90678100	-3.00121600	-2.81094700
H	-5.60688300	-1.19584500	-1.80920800
H	-5.38783100	0.72757500	0.20060400
H	-4.82575400	2.77683900	1.93614500
H	-2.68614000	4.41538800	2.08630000
H	-0.56071700	4.59827500	0.76604800
H	1.28201200	5.34825700	-0.58822300
H	3.46509100	4.25719000	-1.70580200
H	4.58217500	1.94593200	-1.55313600
H	3.38986300	-3.21684800	1.98450000
H	-2.06974600	-1.11630600	0.48339300
H	-1.67547300	1.08385800	-0.25857500
H	1.23887300	1.15196700	0.05540900
H	1.28359600	-2.02669800	-0.84718300
H	6.12956400	0.11953300	-0.47001900
H	5.67907100	-2.05057400	1.07035000

2c



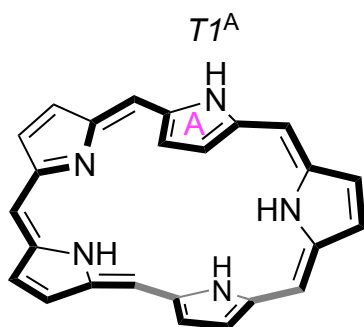
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Sum of electronic and zero-point Energies= -1237.423285

C	0.60078300	-3.05856600	0.46632000
C	0.33685300	-2.10052200	1.44363500
C	-1.05992700	-2.05893800	1.63878400
C	-1.64870200	-2.97320800	0.76169600
C	-3.03852200	-3.10038000	0.33595500
C	-3.71748600	-1.98895700	-0.06455300
C	-5.06862800	-1.85371000	-0.59098000
C	-5.30065200	-0.54517200	-0.86432400
C	-4.11873200	0.23050700	-0.52248000
C	-3.97757000	1.58562800	-0.60318900
C	-2.87892700	2.44924200	-0.27209700
C	-3.00589300	3.81507300	-0.00054400
C	-1.73785300	4.32319000	0.28115100
C	-0.79885900	3.28557400	0.16845400
C	0.60256700	3.54495800	0.30082300
C	1.84035200	2.94810800	0.21852300
C	3.03356400	3.77748700	0.26534700
C	4.12915100	3.00452400	0.07698500
C	3.69457600	1.63293200	-0.06312900
C	4.51757000	0.54760000	-0.26411500
C	4.11206800	-0.81326800	-0.35250200
N	2.87665000	-1.24355100	-0.09008000
C	2.89762600	-2.61534100	-0.33739700
C	1.83244800	-3.45441500	-0.14879200

N	2.30827800	1.64433500	0.02823300
C	4.22255600	-3.02455000	-0.79842000
C	4.99202300	-1.90965500	-0.77852800
N	-0.62009300	-3.61450500	0.11163800
N	-1.52561300	2.13594000	-0.13885400
N	-3.18656700	-0.69781100	-0.08047600
H	1.09663000	-1.52906700	1.95338400
H	-1.59866300	-1.46015300	2.36121800
H	-3.51668500	-4.07138100	0.25390200
H	-5.74381900	-2.68617700	-0.73530600
H	-6.19996300	-0.11105600	-1.28101600
H	-4.87032800	2.12456800	-0.90423300
H	-3.94534700	4.34960700	0.01162100
H	-1.48591000	5.34173800	0.54184500
H	0.72694200	4.60832800	0.48633800
H	2.99817200	4.85056500	0.39843900
H	5.16420300	3.31449300	0.03678700
H	5.57472300	0.76427100	-0.37578000
H	1.92487800	-4.48158200	-0.49731000
H	1.80280400	0.76463700	0.03589200
H	4.51022000	-4.03485200	-1.06130300
H	6.03601500	-1.81006900	-1.04845900
H	-0.75723600	-4.20192400	-0.69698900
H	-1.11182400	1.28234900	-0.48216800
H	-2.33570300	-0.47398700	0.41016500

2d



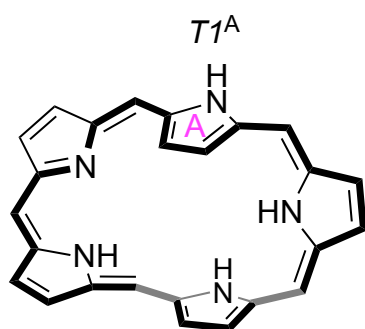
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Sum of electronic and zero-point Energies= -1237.423810

C	-0.34095600	2.75654200	-0.27760200
C	-0.25728600	1.65790000	-1.15359500
C	1.08030300	1.47521700	-1.49525800
C	1.84938600	2.45668200	-0.83747600
C	3.27564200	2.53211800	-0.69148000
C	4.01334100	1.38660700	-0.48590600
C	5.40995900	1.21463100	-0.14454400
C	5.59685800	-0.06143000	0.30618600
C	4.32578300	-0.75506500	0.27057800
C	3.91887000	-1.91138800	0.88679400
C	2.53644100	-2.33856500	0.89835000
C	1.68186800	-2.57800400	1.98156700
C	0.37096800	-2.69355700	1.49181000
C	0.41221800	-2.59956000	0.09164900
C	-0.60656400	-2.93847900	-0.86782300
C	-1.93480900	-2.58208100	-0.78599700
C	-3.07715000	-3.25762100	-1.36536200
C	-4.21191400	-2.61113000	-0.96643600
C	-3.82478800	-1.43893100	-0.21644400
C	-4.60200900	-0.36053700	0.17912600
C	-4.06547100	0.91272300	0.50886300
N	-2.76046700	1.20889700	0.35390600
C	-2.62514400	2.54690000	0.64490800
C	-1.46127900	3.26995600	0.42156900
N	1.73691500	-2.36389900	-0.23488100
N	-2.45313100	-1.50561900	-0.07946700
C	-3.90559100	3.09256500	1.08269100
C	-4.81197500	2.08331300	0.96569500
N	3.44603500	0.12150600	-0.36342800

N	0.95127600	3.26864800	-0.17184400
H	-1.11383400	1.09822500	-1.49180000
H	1.48095900	0.75023100	-2.18939500
H	3.76939300	3.49274700	-0.58267000
H	6.15107000	2.00066800	-0.20265100
H	6.51511000	-0.49247400	0.68225500
H	4.62187400	-2.41677200	1.54081200
H	1.99210900	-2.59910800	3.01719800
H	-0.52474900	-2.88788100	2.06413200
H	-0.33645800	-3.63027400	-1.66356500
H	-3.00908200	-4.16360000	-1.95288700
H	-5.23458800	-2.87378400	-1.20188700
H	-5.68008100	-0.46873800	0.12256100
H	-1.41482800	4.29069000	0.79592900
H	2.09122900	-2.29218000	-1.17634100
H	-1.94797600	-0.66560000	0.20181900
H	-4.08653700	4.11895200	1.37710000
H	-5.87378000	2.11414900	1.17652200
H	2.44669300	0.03143700	-0.23241800
H	1.22885800	3.93375300	0.53410200

2d'



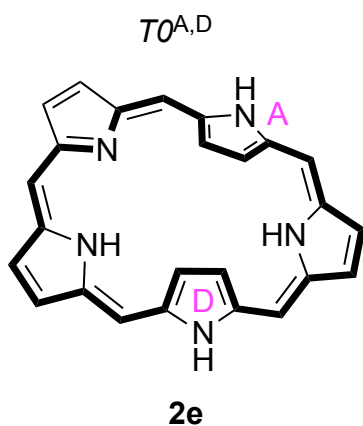
2d'

Sum of electronic and zero-point Energies= -1237.416610

C	0.14259600	2.92372800	0.74668400
C	0.25819300	1.80362800	1.57551200
C	1.62251900	1.49913400	1.70318400
C	2.35377000	2.41139400	0.92163600
C	3.68172800	2.32282600	0.35923200
C	4.13751100	1.12357900	-0.12898200
C	5.17031700	0.86324900	-1.12298700
C	4.96475800	-0.37519200	-1.64755300
C	3.82991400	-0.98465200	-0.96557900
C	3.10234200	-2.10644800	-1.22280700
C	2.06570200	-2.54722700	-0.28510700
C	2.23019900	-3.02478400	1.01426800
C	0.97259900	-3.44468600	1.49117900
C	0.02360200	-3.17299700	0.50659000
C	-1.39068900	-3.47596000	0.51317600
C	-2.47710900	-2.72804900	0.14778100
C	-3.82431300	-3.26047100	0.03247100
C	-4.66384800	-2.25976400	-0.33195500
C	-3.90470700	-1.02923600	-0.40204300
C	-4.42243500	0.23278600	-0.58568600
C	-3.73095900	1.47033700	-0.46501900
N	-2.45881900	1.60360900	-0.06274400
C	-2.19424700	2.96607200	-0.12064700
C	-0.99649200	3.57094700	0.19345100
N	-2.58094300	-1.37050600	-0.17052900
C	-3.36879300	3.69216500	-0.59464700
C	-4.33774600	2.76370300	-0.78767200
N	1.43913900	3.32662600	0.43985200
N	0.71308200	-2.62552500	-0.56378300
N	3.48147400	-0.08428200	0.03875300
H	-0.57869200	1.30171200	2.03628600
H	2.05553600	0.72583000	2.32297400
H	4.20387700	3.22877300	0.06716400
H	5.91582500	1.58644300	-1.42657300

H	5.51745500	-0.84578200	-2.44968500
H	3.32559600	-2.69383800	-2.10957000
H	3.18086600	-3.09370100	1.52390600
H	0.75175400	-3.87857900	2.45659500
H	-1.64097900	-4.46120600	0.89948600
H	-4.06537000	-4.30322500	0.19040800
H	-5.72904000	-2.31979800	-0.50992200
H	-5.48345800	0.28266000	-0.80887800
H	-0.89898200	4.62604900	-0.05793500
H	-1.89756100	-0.64154900	0.01049500
H	-3.42871300	4.76487100	-0.73051800
H	-5.35202200	2.91352000	-1.13618500
H	1.64799600	3.94842000	-0.32707300
H	0.29098800	-2.37355600	-1.44440800
H	2.56090600	-0.12099800	0.45571500

2e

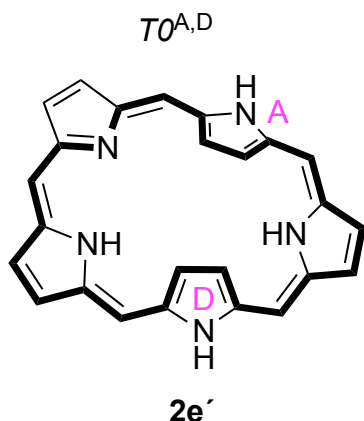


Sum of electronic and zero-point Energies= -1237.424287

C	-0.06164500	-2.77349500	-0.23819400
C	-0.12112000	-1.83015300	-1.26869200
C	-1.47185100	-1.61959300	-1.58244800
C	-2.25350500	-2.41569300	-0.73795700
C	-3.70409100	-2.33538700	-0.53603300
C	-4.23611600	-1.10906900	-0.25367200
C	-5.61502000	-0.62608300	-0.16422200
C	-5.59845900	0.70811900	0.09219300
C	-4.20980200	1.14926300	0.22204800
C	-3.64868900	2.36306400	0.49771000
C	-2.20307300	2.41827500	0.73366900
C	-1.44758900	1.61678900	1.58850300
C	-0.08335000	1.84442700	1.32417700
C	0.00440300	2.79766300	0.30851600
C	1.16411200	3.36553300	-0.32636400
C	2.37544000	2.73611000	-0.44807500
C	3.64093900	3.33762600	-0.83036500
C	4.62068400	2.40127400	-0.72339700
C	4.01448800	1.14559100	-0.31842300
C	4.62118800	-0.07375200	-0.10782200
C	3.92388300	-1.28211600	0.20300700
N	2.59653900	-1.42130700	0.09756800
C	2.31178300	-2.71902300	0.50887000
C	1.07348600	-3.31705600	0.43674500
N	-1.29870400	3.16127900	-0.00396900
N	2.66826400	1.40517700	-0.16217300
C	3.53940100	-3.38606700	0.93225700
C	4.55056700	-2.50912900	0.70218400
N	-3.46118100	0.00600700	0.00466500
N	-1.37573600	-3.14812800	0.03142600
H	0.74811700	-1.38169100	-1.72276800
H	-1.87083600	-0.96105700	-2.34107800
H	-4.35081100	-3.19955500	-0.64933000
H	-6.48603800	-1.25073700	-0.31184900
H	-6.45432800	1.35997500	0.20770200
H	-4.27554500	3.24604700	0.57622400
H	-1.86313100	0.94879900	2.32966300
H	0.75910500	1.40577200	1.83825700
H	1.10267900	4.38422800	-0.70052900

H	3.75253200	4.37903100	-1.10184400
H	5.67789700	2.52886400	-0.91308400
H	5.70327500	-0.11090800	-0.17384200
H	0.96525800	-4.29511400	0.90297900
H	-1.55302500	3.72664700	-0.79939300
H	2.01724600	0.63976300	-0.00671800
H	3.60685700	-4.40204700	1.30127400
H	5.61010100	-2.65049500	0.87575900
H	-2.45306400	-0.00400200	0.00833300
H	-1.65694300	-3.70742100	0.82232400

2e'

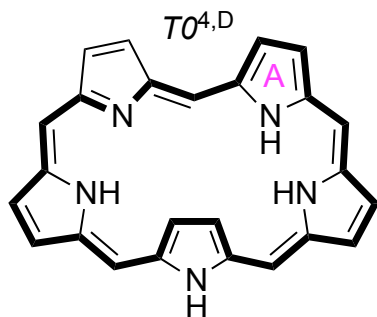


Sum of electronic and zero-point Energies= -1237.424406

C	0.08351100	2.91748600	0.28486300
C	0.31356300	2.02712200	1.33264500
C	1.69758400	1.79357400	1.40297900
C	2.32259100	2.51066100	0.37145400
C	3.66569300	2.37659500	-0.16979800
C	4.22393300	1.13080600	-0.28943600
C	5.44870300	0.66614700	-0.93352400
C	5.42594300	-0.69432400	-0.98667700
C	4.18849700	-1.16674000	-0.37532100
C	3.59215200	-2.39784600	-0.33499200
C	2.26355400	-2.53940400	0.24293200
C	1.69743500	-1.90130600	1.34989400
C	0.30775100	-2.14471900	1.34268100
C	0.02079500	-2.95041100	0.24501500
C	-1.24061400	-3.48510000	-0.20455200
C	-2.43698300	-2.82364200	-0.17721300
C	-3.74214500	-3.40860700	-0.43447900
C	-4.68419800	-2.43876200	-0.32991300
C	-4.01751600	-1.17687300	-0.05802600
C	-4.59842200	0.07004200	-0.06945800
C	-3.91967600	1.32744000	-0.08478600
N	-2.60635800	1.50124700	0.09589200
C	-2.36513900	2.84297200	-0.20539100
C	-1.13921000	3.46430200	-0.21118000
N	-2.67600300	-1.47231800	0.08787700
C	-3.61235300	3.51014000	-0.56964700
C	-4.58939300	2.57810900	-0.46150500
N	1.32999200	3.24785500	-0.24141100
N	1.23082900	-3.22111500	-0.37881400
N	3.57956200	-0.02381200	0.11974700
H	-0.46003900	1.63313800	1.97349900
H	2.21666200	1.20160300	2.14232100
H	4.17522700	3.23211000	-0.60139300
H	6.21432300	1.32035200	-1.32923000
H	6.17127700	-1.34061600	-1.43121900
H	4.07203500	-3.23833900	-0.82660000
H	2.25377500	-1.36241700	2.10265100
H	-0.41502500	-1.82491000	2.07945600
H	-1.26483400	-4.50969800	-0.56831400
H	-3.89407100	-4.45786300	-0.65007500
H	-5.75314300	-2.53727600	-0.46270400
H	-5.67328400	0.09344100	-0.21684300
H	-1.10027500	4.46375100	-0.64250000

H	-1.98543700	-0.73001700	0.15043600
H	-3.70591100	4.55356500	-0.84409400
H	-5.64904000	2.69046400	-0.65450000
H	1.45322400	3.71306200	-1.12809100
H	1.30484500	-3.62984500	-1.29792300
H	2.59721400	-0.01947400	0.36270400

2f



2f

Sum of electronic and zero-point Energies= -1237.426655

C	3.48351000	2.04960600	0.07009100
N	2.33848400	1.56640900	0.54928100
C	1.38002900	2.57256300	0.41499000
C	0.08561500	2.19256600	0.67405500
C	-1.20711400	2.68933100	0.34544400
N	-2.24159500	1.77094900	0.48985200
C	-3.40275800	2.20840900	-0.09544700
C	-4.54102200	1.33953500	-0.26627400
C	-4.47227800	-0.03079700	-0.23349000
C	-5.51527100	-1.01751100	-0.46064200
C	-4.96659900	-2.26360800	-0.43719300
C	-3.54369100	-2.14747800	-0.17306700
C	-2.55609700	-3.09014500	-0.10865400
C	-1.20093300	-2.76410500	0.29832900
N	-0.06387900	-3.34145500	-0.24407200
C	1.08437100	-2.76764300	0.28468700
C	2.41399200	-3.08807600	-0.18408700
C	3.44580700	-2.18754400	-0.21552500
C	4.81598700	-2.38099400	-0.67653800
C	5.45717600	-1.18214200	-0.65291500
C	4.51708800	-0.16815000	-0.19250900
C	4.62236500	1.20727200	-0.17919300
C	3.32307600	3.45876300	-0.30734700
C	2.01002800	3.77080500	-0.11355500
C	-3.12209100	3.49844400	-0.58449300
C	-1.76978300	3.78737900	-0.32350400
N	-3.31243400	-0.77659800	0.01004800
C	-0.75240300	-1.84741700	1.25249100
C	0.65773500	-1.85212100	1.24759600
N	3.36175500	-0.84825900	0.12845300
H	1.52406600	4.71930100	-0.30159600
H	4.10228600	4.10207300	-0.69779900
H	6.47520200	-0.97691800	-0.95601900
H	5.21812400	-3.33382200	-0.99466100
H	1.30580700	-1.28799800	1.90188900
H	-1.39503500	-1.30805400	1.93385900
H	-5.48379400	-3.20425700	-0.57258700
H	-6.55531000	-0.76782700	-0.62433600
H	-3.81829000	4.11801600	-1.13241800
H	-1.23343700	4.67358000	-0.63165900
H	0.05373500	1.18046100	1.07437200
H	-2.39901500	-0.41632700	-0.23250400
H	2.52981900	-0.29697700	0.35641100
H	-0.06871000	-3.93343700	-1.06069400
H	-2.17984100	0.95930800	1.08460500
H	-2.80335300	-4.11495600	-0.37120600
H	2.60441600	-4.08458800	-0.57285400
H	5.55382400	1.65865900	-0.50196100
H	-5.48725500	1.79478700	-0.53527200

TS1_{2a-2b} conformational interconversion *T0*→*T1*

Sum of electronic and zero-point Energies= -1237.427340

C	1.48017400	-3.00834900	1.00228600
C	0.57779000	-3.74783000	1.78226700
C	-0.64500900	-3.78330100	1.09603300
C	-0.47211700	-3.12627400	-0.13400000
C	-1.40997500	-3.07968800	-1.25723100
C	-2.50667700	-2.27305200	-1.22192900
C	-3.74263200	-2.31001500	-1.98189400
C	-4.59723800	-1.37876300	-1.47167500
C	-3.91038600	-0.62609000	-0.44671900
C	-4.30598000	0.52258200	0.19498700
C	-3.45184000	1.50587700	0.77045500
C	-3.81771500	2.62703900	1.53523000
C	-2.71363300	3.46977300	1.62631600
C	-1.64199100	2.88560100	0.91901400
C	-0.45040300	3.57034600	0.56669600
C	0.73837300	3.27797000	-0.07647700
C	1.57649500	4.31996600	-0.61970100
C	2.66424800	3.75540800	-1.20961500
C	2.61100200	2.33345100	-0.98570800
C	3.68046100	1.47440100	-1.14928400
C	3.84290500	0.18164500	-0.58451200
N	2.85370300	-0.60375400	-0.12543200
C	3.48951400	-1.60970500	0.59849500
C	2.83241400	-2.64344200	1.23185000
N	-2.64438200	-1.19441100	-0.34597100
N	-2.09598700	1.65065700	0.47488600
N	1.38429900	2.07363900	-0.38017900
N	0.81240700	-2.65816400	-0.15667800
C	5.15841600	-0.34492200	-0.22515800
C	4.93089000	-1.42597000	0.56549200
H	0.80363800	-4.19105500	2.74245100
H	-1.54976300	-4.29453400	1.39379600
H	-1.29290700	-3.77880800	-2.08087300
H	-3.93504700	-3.00636400	-2.78668000
H	-5.60029400	-1.15609800	-1.81142800
H	-5.36140900	0.77210300	0.16467900
H	-4.80195100	2.78888900	1.95239500
H	-2.66044200	4.42588600	2.12867700
H	-0.53388900	4.63142800	0.78553600
H	1.32060800	5.37015600	-0.57434200
H	3.48002000	4.25578100	-1.71301800
H	4.57067800	1.93012100	-1.57193400
H	3.38874600	-3.24395800	1.94632200
H	-2.06401900	-1.10617200	0.47646100
H	-1.65177500	1.12946800	-0.26802400
H	1.23361700	1.17384400	0.06396200
H	1.21705500	-2.01110000	-0.82408200
H	6.10792700	0.10283700	-0.49055700
H	5.65639700	-2.06812700	1.04895300

***** 1 imaginary frequencies (negative Signs) *****
Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-22.8316	34.6362	39.8022
Red. masses --	5.0101	5.5844	5.9054
Frc consts --	0.0015	0.0039	0.0055
IR Inten --	0.1538	0.0271	0.1353

TS2_{2b-2c} conformational interconversion *T1*→*T0*^A

Sum of electronic and zero-point Energies= -1237.416907

***** 1 imaginary frequencies (negative Signs) *****
Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-65.4123	36.4130	42.0797
Red. masses --	4.2171	5.6994	5.5301
Frc consts --	0.0106	0.0045	0.0058
IR Inten --	1.3740	0.0567	0.5512

C	1.19538400	-3.04625500	0.92760900
C	0.45718100	-2.57456400	1.99815300
C	-0.91257000	-2.62367300	1.63047100
C	-0.99415200	-3.14742800	0.34182600
C	-2.14784600	-3.36393500	-0.51553900
C	-3.06425700	-2.37953400	-0.72394400
C	-4.35226000	-2.42497900	-1.39084100
C	-4.95080600	-1.21095100	-1.26793700
C	-4.05618300	-0.31386700	-0.56032500
C	-4.26306000	1.00499300	-0.25472700
C	-3.32950000	1.96478900	0.24471200
C	-3.64026700	3.20117700	0.83090900
C	-2.45034100	3.89364100	1.03699400
C	-1.38042500	3.10259800	0.57752600
C	-0.05863000	3.60883600	0.45595200
C	1.20183200	3.21214700	0.05673100
C	2.21206900	4.20477400	-0.23171500
C	3.33194100	3.58593200	-0.68689700
C	3.11037300	2.16272000	-0.63084900
C	4.08412600	1.20431600	-0.84599000
C	4.01566900	-0.17703100	-0.54787300
N	2.94083500	-0.83044500	-0.10298600
C	3.38927100	-2.12429800	0.18434200
C	2.64188800	-3.13871000	0.69130800
N	-2.91763400	-1.05751600	-0.28868800
N	-1.94174500	1.90103900	0.14884300
N	1.79745800	1.97538200	-0.22894900
N	0.29903000	-3.42038400	-0.05016000
C	5.21022100	-1.04701000	-0.60418200
C	4.82445800	-2.24631700	-0.13024800
H	0.87073800	-2.22453700	2.93300600
H	-1.76090900	-2.36946500	2.25198900
H	-2.30466500	-4.32852100	-0.99098000
H	-4.74582300	-3.30532600	-1.88084100
H	-5.91381700	-0.91048900	-1.65899600
H	-5.26448400	1.38680100	-0.42262500
H	-4.64186800	3.52866100	1.07150700
H	-2.33350400	4.87955500	1.46574800
H	-0.06114100	4.67136000	0.68464000
H	2.04074200	5.26820100	-0.13016000
H	4.26069000	4.03878600	-1.00477800
H	5.04692400	1.58668000	-1.16852900
H	3.14924500	-4.07586200	0.91671400
H	-2.23030500	-0.80983700	0.40755800
H	-1.46540800	1.24193500	-0.44964800
H	1.48776900	1.04785300	0.04527400
H	0.56906100	-3.68238000	-0.98561300
H	6.19192200	-0.73947000	-0.94318900
H	5.41453600	-3.14469700	-0.00029000

TS1_{2c-2d} conformational interconversion $T0^A \rightarrow T1^A$

Sum of electronic and zero-point Energies= -1237.417825

C	0.46487600	-2.96299800	-0.16059000
C	0.35052200	-1.98373600	-1.15793500
C	-0.99962400	-1.87503700	-1.50422500
C	-1.73149000	-2.77985100	-0.71908100
C	-3.16648300	-2.86138300	-0.54714200
C	-3.88408500	-1.70818300	-0.37269000
C	-5.30117300	-1.51284700	-0.11689600
C	-5.50795000	-0.21044700	0.21665600
C	-4.24072000	0.49326000	0.18321700
C	-3.96142900	1.76012300	0.60294400
C	-2.69476900	2.44359500	0.64670100
C	-2.34489700	3.49098300	1.49573600
C	-1.01939600	3.86996600	1.20430500
C	-0.55253700	3.07110600	0.16734700
C	0.66844100	3.33915800	-0.61274100

C	1.89609700	2.74649800	-0.66413200
C	3.07994800	3.44182000	-1.17478800
C	4.17443800	2.68800000	-0.92824200
C	3.74585800	1.43578200	-0.32954000
C	4.54740200	0.38194700	0.03076700
C	4.07657400	-0.90755600	0.43527400
N	2.79934600	-1.27239000	0.30692600
C	2.73174900	-2.59205100	0.73046700
C	1.60593600	-3.37427500	0.58021000
N	-1.57183900	2.17987600	-0.13929000
N	2.36501600	1.52052000	-0.20333100
C	4.03607100	-3.02912300	1.20867300
C	4.88831200	-1.99003500	0.99037100
N	-3.31154100	-0.43694500	-0.29113100
N	-0.81541500	-3.47677400	0.03494200
H	1.18913300	-1.44515700	-1.56775800
H	-1.43222100	-1.24299700	-2.26684400
H	-3.67044900	-3.81832800	-0.45958000
H	-6.03876400	-2.30227600	-0.16861900
H	-6.44795200	0.25489100	0.48313900
H	-4.78708600	2.31292300	1.03986900
H	-2.98811100	3.90209300	2.26177400
H	-0.44616800	4.65395600	1.67859900
H	0.66317300	4.32292800	-1.07935500
H	3.04092500	4.43124400	-1.61027100
H	5.20741300	2.92940200	-1.13997000
H	5.61921900	0.53233300	-0.04678900
H	1.59856000	-4.35986200	1.04240700
H	-1.59044700	1.63169900	-0.98623500
H	1.83158700	0.72138100	0.12079200
H	4.26858800	-4.01192700	1.59931500
H	5.94968800	-1.94280900	1.19977800
H	-2.32357700	-0.34819500	-0.09472800
H	-1.07250300	-4.06960700	0.80967000

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-63.1161	38.4239	46.0759
Red. masses --	4.3333	6.0454	5.5952
Frc consts --	0.0102	0.0053	0.0070
IR Inten --	1.4860	0.3570	0.0789

TS_{2d-2e} conformational interconversion $T1^A \rightarrow T0^{A,D}$

Sum of electronic and zero-point Energies= -1237.423144

C	-0.28509500	2.76679600	-0.28335000
C	-0.19403300	1.69995500	-1.18944100
C	1.15442800	1.50549400	-1.49659000
C	1.91300200	2.44840500	-0.78416600
C	3.34989900	2.50084000	-0.62189400
C	4.04765100	1.34029800	-0.41809500
C	5.46749300	1.10100500	-0.20013200
C	5.64478500	-0.19772000	0.16127700
C	4.33851800	-0.84829100	0.22053300
C	3.94404100	-2.04247500	0.74429200
C	2.50246400	-2.31969400	0.88614100
C	1.65145900	-2.02353000	1.94761900
C	0.32103900	-2.20494800	1.51390900
C	0.35344200	-2.64648100	0.18781600
C	-0.71363200	-3.14185700	-0.64571400
C	-2.01024900	-2.69279400	-0.64526800
C	-3.18053100	-3.39724800	-1.13463900
C	-4.28693500	-2.65698500	-0.84771500
C	-3.85893900	-1.41023600	-0.24721400
C	-4.61743900	-0.29853700	0.07166900
C	-4.06312400	0.97669400	0.37859000
N	-2.75624200	1.25085600	0.24602800
C	-2.60313000	2.58861000	0.56005600
C	-1.42613200	3.29153800	0.38650500
N	1.69208700	-2.70554700	-0.16649400

N	-2.48886300	-1.50109900	-0.11048000
C	-3.88522800	3.14998700	0.97578700
C	-4.80316800	2.15757700	0.82873000
N	3.44330200	0.09754700	-0.26244200
N	1.01130200	3.24569900	-0.10969300
H	-1.04732600	1.16142300	-1.56773900
H	1.56823000	0.78516100	-2.18752200
H	3.87602300	3.44966800	-0.58427800
H	6.23147700	1.86064900	-0.30121700
H	6.57659200	-0.68342000	0.41850700
H	4.68367800	-2.69371900	1.19979700
H	1.97646900	-1.67659800	2.91863500
H	-0.57866000	-2.08193200	2.09955300
H	-0.50813900	-4.01583000	-1.26007600
H	-3.14508600	-4.37783900	-1.59062300
H	-5.31853000	-2.90765800	-1.05528000
H	-5.69650900	-0.39301600	0.01385800
H	-1.37878500	4.30935300	0.76899700
H	2.03665100	-2.95480600	-1.08073400
H	-1.95362800	-0.66555400	0.11929400
H	-4.05497900	4.17529700	1.28040400
H	-5.86822900	2.20116800	1.02001100
H	2.44964200	0.01873300	-0.09465300
H	1.27647600	3.89830000	0.61238300

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering
 activities (A⁴/AMU), depolarization ratios for plane and unpolarized
 incident light, reduced masses (AMU), force constants (mDyne/A),
 and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-41.9284	43.8555	54.4424
Red. masses --	4.1941	5.7200	5.7898
Frc consts --	0.0043	0.0065	0.0101
IR Inten --	0.2267	0.3315	0.6850

TS1_{2c-2d} conformational interconversion $T0^A \rightarrow T1^A$

Sum of electronic and zero-point Energies= -1237.416587

C	-0.00075400	-2.95394500	0.75687700
C	-0.15072700	-1.83870600	1.58515700
C	-1.52514900	-1.57490200	1.71066500
C	-2.22558800	-2.51047700	0.93172200
C	-3.55911300	-2.46939800	0.37326300
C	-4.05912200	-1.29168200	-0.11599000
C	-5.12942200	-1.07419800	-1.08158900
C	-4.99510400	0.17201400	-1.60517600
C	-3.87127200	0.83389200	-0.94826200
C	-3.24149500	2.01009100	-1.20413000
C	-2.21280900	2.53512200	-0.29055000
C	-2.40308600	3.21452600	0.90863200
C	-1.14623700	3.65486600	1.36823400
C	-0.17385700	3.20157700	0.47605000
C	1.23741800	3.49264600	0.50370300
C	2.35265300	2.77661100	0.15717500
C	3.67496000	3.36755800	0.05663800
C	4.56049400	2.40955200	-0.31454300
C	3.85782300	1.14773400	-0.39777200
C	4.43381900	-0.08845100	-0.59041300
C	3.79797600	-1.35444700	-0.47257000
N	2.53413500	-1.54196800	-0.06802700
C	2.32831000	-2.91518100	-0.12133800
C	1.15961200	-3.56626000	0.20219400
N	2.51843800	1.42594800	-0.16928600
C	3.53274400	-3.59100400	-0.59727200
C	4.45951800	-2.62215700	-0.79484100
N	-1.28299700	-3.39487700	0.44737600
N	-0.84728600	2.51077500	-0.52057800
N	-3.44497400	-0.05747500	0.03245500
H	0.66992300	-1.31120600	2.04639500
H	-1.98317400	-0.81380800	2.32769600
H	-4.05876100	-3.39407100	0.10104000
H	-5.85371400	-1.82771300	-1.36199600

H	-5.59254600	0.62294600	-2.38619800
H	-3.56193800	2.60479000	-2.05580700
H	-3.36677900	3.39268700	1.36428200
H	-0.94090000	4.22587800	2.26326300
H	1.46469200	4.48387900	0.88832700
H	3.86813500	4.41894300	0.22336900
H	5.62234200	2.51929300	-0.48817100
H	5.49598800	-0.08858600	-0.81314800
H	1.10208900	-4.62680000	-0.03788800
H	1.87342700	0.66232000	0.01128400
H	3.63887000	-4.66042600	-0.73071500
H	5.47855700	-2.72856300	-1.14546900
H	-1.47299000	-4.02797300	-0.31515000
H	-0.41390200	2.14157100	-1.35329600
H	-2.52008500	0.01772400	0.43342300

***** 1 imaginary frequencies (negative Signs) *****
Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-22.7627	34.4889	43.9952
Red. masses --	4.7369	5.3444	6.0278
Frc consts --	0.0014	0.0037	0.0069
IR Inten --	0.6035	0.3987	0.3719

TS_{2d'-2e'} conformational interconversion $T1^A \rightarrow T0^{A,D}$

Sum of electronic and zero-point Energies= -1237.416538

C	0.13830200	2.93359900	0.68375400
C	0.26667800	1.82937900	1.53177800
C	1.63207900	1.52902200	1.64656300
C	2.35215500	2.42582200	0.83579900
C	3.67987700	2.33114000	0.27450500
C	4.15079800	1.11835500	-0.16527000
C	5.20987700	0.82225000	-1.12133100
C	5.03640000	-0.44638700	-1.58271800
C	3.89095700	-1.03474800	-0.90136700
C	3.18126200	-2.17742400	-1.11781400
C	2.09839900	-2.55364000	-0.20837300
C	2.16337500	-2.80725400	1.16067200
C	0.87947100	-3.20119800	1.59740900
C	0.01756900	-3.14329200	0.50820600
C	-1.39129200	-3.51226100	0.42153300
C	-2.47865200	-2.75711600	0.09019800
C	-3.82470000	-3.29498800	-0.06608800
C	-4.67105700	-2.28196700	-0.36567200
C	-3.91981600	-1.04125700	-0.37159200
C	-4.44642400	0.21838000	-0.52376700
C	-3.75950200	1.46260500	-0.41253200
N	-2.48109200	1.60274200	-0.03891600
C	-2.21924700	2.96549800	-0.12438100
C	-1.01139700	3.57212300	0.14495700
N	-2.59629600	-1.38523800	-0.14392300
C	-3.40498700	3.68288700	-0.58023800
C	-4.37685600	2.74984600	-0.73738900
N	1.43061300	3.33033300	0.34868400
N	0.78125600	-2.75272100	-0.57926100
N	3.50275200	-0.08605700	0.04160100
H	-0.56325700	1.33563200	2.01341400
H	2.07363600	0.76922700	2.27648500
H	4.19676600	3.23145900	-0.04271800
H	5.95263100	1.53948800	-1.44503200
H	5.61756200	-0.95018700	-2.34354600
H	3.43995600	-2.81321000	-1.96023500
H	3.06593600	-2.74765400	1.75262900
H	0.58905400	-3.48188400	2.60021200
H	-1.62762600	-4.53661300	0.70238700
H	-4.05665200	-4.34705100	0.03161300
H	-5.73587000	-2.33876900	-0.54747600
H	-5.50918700	0.26408400	-0.73971900

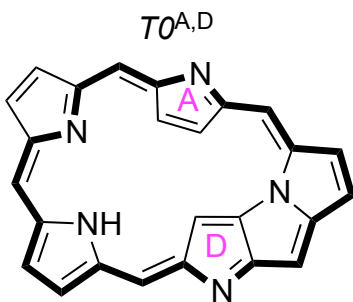
H	-0.91779800	4.62175400	-0.13016300
H	-1.90306200	-0.66583800	0.03234100
H	-3.47002700	4.75330600	-0.73084500
H	-5.39880100	2.89314900	-1.06560900
H	1.62865200	3.93895000	-0.43154100
H	0.42187500	-2.64441800	-1.51515900
H	2.57596900	-0.12108700	0.44462400

***** 1 imaginary frequencies (negative Signs) *****
Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-37.7193	38.6816	44.9314
Red. masses --	4.2759	5.6532	5.8833
Frc consts --	0.0036	0.0050	0.0070
IR Inten --	1.2353	0.9141	0.2559

Unsubstituted N-fused [22]pentaphyrin 3

3a



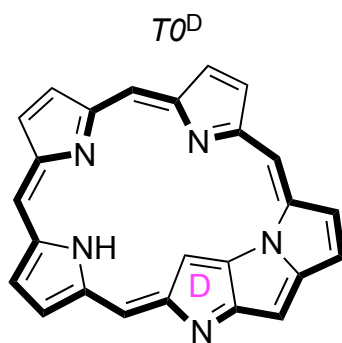
3a

Sum of electronic and zero-point Energies= -1235.018438

N	-2.24949000	1.66756400	-0.00934600
N	-2.94224500	-1.06949100	0.02635400
N	0.55405300	-3.31345600	-0.29241900
N	3.44852200	-0.08982400	-0.01053900
N	2.10763200	3.15830500	-0.00585500
C	-1.63928800	2.90065700	-0.03407700
C	-2.69051600	3.86947700	-0.02028900
C	-3.89671900	3.20681500	0.00233500
C	-3.62233600	1.80950700	0.00879500
C	-4.54188700	0.74943300	-0.01215900
C	-4.22687500	-0.60841300	-0.04335700
C	-5.15806900	-1.70593500	-0.27897500
C	-4.39403600	-2.82425200	-0.40574700
C	-3.01296800	-2.40561100	-0.18408700
C	-1.86354400	-3.22823500	-0.25545900
C	-0.62178700	-2.84594500	0.23637500
C	-0.37614800	-1.83211200	1.26798700
C	0.96156000	-1.63089700	1.27157900
C	1.50159500	-2.51167500	0.23162800
C	2.84010000	-2.51996600	-0.23139900
C	3.71893900	-1.45125000	-0.22083400
C	5.14484000	-1.52925800	-0.39332400
C	5.70666200	-0.28108200	-0.24086500
C	4.64893400	0.64393200	-0.03291700
C	4.41174300	2.02403400	0.02203000
C	3.01095700	2.17860700	0.01354200
C	2.39606100	0.84105000	-0.05601800
C	1.05966900	1.02441100	-0.17337000
C	0.89769800	2.49768700	-0.09672900
C	-0.27010200	3.24460600	-0.05841000
H	-2.52446800	4.93759900	-0.03489000
H	-4.88799700	3.63817000	0.01042000

H	-6.23352000	-1.61673700	-0.36468200
H	-4.71985700	-3.83799600	-0.59962300
H	-1.13205800	-1.38538200	1.89575100
H	1.53986900	-0.98113100	1.91255300
H	5.66895000	-2.46143400	-0.55644500
H	6.75700200	-0.02990400	-0.28756400
H	0.27787000	0.29347900	-0.28346300
H	-1.84661800	0.73181900	0.00585600
H	-1.92609200	-4.15702000	-0.81702400
H	3.20438800	-3.43856400	-0.68294500
H	5.16784200	2.79553600	0.01514200
H	-0.09164200	4.31543500	-0.01530000
H	-5.58987900	1.03095200	-0.05267300

3b



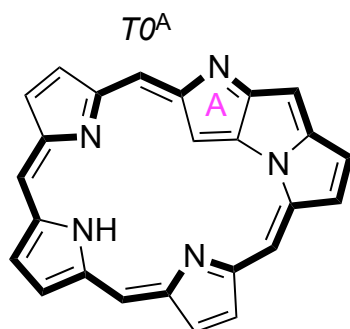
3b

Sum of electronic and zero-point Energies= -1235.022890

N	-2.47056200	-1.71771900	0.00001700
N	-2.79822200	1.04412700	-0.00013900
N	0.61140100	2.14721900	-0.00006300
N	3.34891200	-0.41422500	0.00002800
N	1.70091400	-3.50915400	-0.00003700
C	-1.98050000	-2.99602900	-0.00000600
C	-3.11237600	-3.87186200	-0.00001000
C	-4.25236200	-3.10228300	0.00001400
C	-3.84482100	-1.73601500	0.00002800
C	-4.62705400	-0.57885500	0.00007800
C	-4.13301600	0.72421400	0.00004300
C	-4.96832500	1.91586300	0.00006000
C	-4.10900000	2.96217000	0.00004400
C	-2.75555500	2.39456000	0.00003300
C	-1.65456200	3.27584900	0.00008200
C	-0.25988900	3.20870500	0.00002500
C	0.46282500	4.48741700	0.00002300
C	1.77312000	4.17842200	-0.00003100
C	1.84168000	2.71014100	-0.00007500
C	3.13999800	2.14738900	-0.00009500
C	3.77150100	0.91200200	-0.00005100
C	5.21334700	0.84569700	-0.00004700
C	5.63288700	-0.46244700	0.00002400
C	4.46989900	-1.26863600	0.00006100
C	4.09457700	-2.61639000	0.00005700
C	2.69120800	-2.62118600	0.00000900
C	2.20569900	-1.23211300	-0.00002200
C	0.85471500	-1.26867000	-0.00007200
C	0.55988400	-2.73892400	-0.00000600
C	-0.64472800	-3.42443500	-0.00000300
H	-3.04129400	-4.95055900	-0.00002300
H	-5.27960400	-3.43913400	0.00002500
H	-6.05048100	1.92701000	0.00011100
H	-4.33855200	4.02008800	0.00008700
H	-0.00317900	5.46432800	0.00007400
H	2.62714400	4.84359600	-0.00003300
H	5.83893700	1.72791800	-0.00008800
H	6.65021300	-0.82708500	0.00004400
H	0.17336900	-0.42810900	-0.00010100
H	-5.70389400	-0.71444200	0.00012900
H	-0.52044200	-4.50319900	0.00000100
H	4.76748400	-3.46144200	0.00007900

H	3.89299900	2.93099700	-0.00013500
H	-1.99232300	4.31005500	0.00016300
H	-1.98239600	-0.81926400	0.00004900

3c



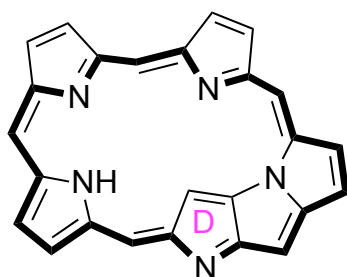
3c

Sum of electronic and zero-point Energies= -1235.025979

N	2.33946000	-1.74712800	-0.00004500
N	2.83488700	1.07721400	-0.00002700
N	-0.50950400	2.19734000	-0.00002700
N	-3.33379100	-0.38451400	-0.00002400
N	-1.77877900	-3.53089900	-0.00009900
C	1.91513100	-3.02924500	0.00003700
C	3.04296200	-3.96354100	0.00005600
C	4.16568000	-3.20408000	0.00004200
C	3.70555600	-1.82023700	0.00002100
C	4.54086800	-0.70832500	-0.00000100
C	4.13845600	0.63035900	-0.00003300
C	4.98146100	1.78000000	-0.00007100
C	4.17123300	2.88720100	-0.00006700
C	2.80693500	2.44915300	-0.00004800
C	1.73276000	3.34818200	-0.00002600
C	0.33892100	3.27670700	0.00000000
C	-0.39923900	4.54124000	0.00003000
C	-1.70405900	4.20761000	0.00008100
C	-1.75313500	2.73849100	0.00004100
C	-3.05168500	2.17475000	0.00007300
C	-3.71332200	0.95281000	0.00004600
C	-5.15755300	0.93083700	0.00007600
C	-5.61770300	-0.36338600	0.00004600
C	-4.47970800	-1.20444700	0.00000100
C	-4.14495800	-2.56364300	-0.00000800
C	-2.74274300	-2.61215800	-0.00003900
C	-2.21603700	-1.23750700	-0.00005200
C	-0.86943600	-1.31729400	-0.00010500
C	-0.61771200	-2.79294300	0.00002800
C	0.58125900	-3.48574200	0.00006700
H	2.95832500	-5.04251800	0.00008900
H	5.19941400	-3.52470500	0.00005700
H	6.06196600	1.74662200	-0.00008400
H	4.47019100	3.92621700	-0.00007700
H	0.05028000	5.52579600	0.00003900
H	-2.56848100	4.85909000	0.00013500
H	-5.75581100	1.83180200	0.00011400
H	-6.64579700	-0.69639100	0.00005700
H	-0.13359000	-0.53085900	-0.00012600
H	2.05499300	0.42424500	-0.00001800
H	5.61265200	-0.88119800	0.00000100
H	0.45415300	-4.56501000	0.00009700
H	-4.84400200	-3.38734300	-0.00000600
H	-3.79517000	2.96721100	0.00013100
H	2.09138400	4.37419900	-0.00002600

3d

T0^{4,D}



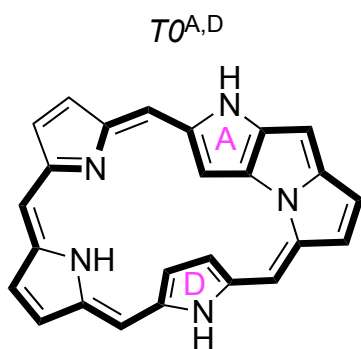
3d

Sum of electronic and zero-point Energies= -1235.001438

C	2.47518300	-2.53274400	0.33897700
N	1.44143000	-3.36210800	0.35487300
C	0.34260300	-2.54543900	0.15195500
C	-0.88046600	-3.19080600	0.02344200
C	-2.21134800	-2.74250000	-0.15867400
C	-3.31416800	-3.53506600	-0.61317800
C	-4.41843600	-2.71348600	-0.72608600
C	-4.03153900	-1.40613800	-0.30643400
C	-4.75281600	-0.19581700	-0.27208500
C	-4.18181600	1.00139900	0.17880600
N	-2.98734900	0.96656900	0.83409600
C	-2.45288000	2.20129200	0.75992600
C	-1.07294200	2.19463600	1.08991600
C	0.02569900	2.78403900	0.49741900
N	1.19181700	2.04877100	0.57201200
C	2.04056700	2.62900700	-0.27390100
C	3.31993800	2.10043600	-0.57055800
C	3.85393400	0.84815100	-0.32684000
C	5.27514500	0.61857600	-0.42659300
C	5.57709600	-0.67285100	-0.08285500
C	4.34907000	-1.33125900	0.18404900
C	3.87836600	-2.62434100	0.39609600
N	-2.69193000	-1.48190400	0.01941200
N	3.30195200	-0.38838700	0.05879300
C	-4.49027800	2.37655200	-0.19520700
C	-3.38603700	3.11921400	0.12695800
C	0.18895700	3.92269000	-0.40131600
C	1.46399500	3.84620600	-0.86391800
C	2.09091100	-1.12279100	0.12103600
C	0.73830800	-1.10520300	0.00772100
H	-3.24816500	-4.58440800	-0.86512300
H	-5.40650700	-2.98703100	-1.06984500
H	-5.39116900	2.71730600	-0.68967800
H	-3.23581000	4.17830700	-0.03436600
H	-0.56082600	4.66598600	-0.63695100
H	1.96054600	4.51243500	-1.55879600
H	5.97305300	1.40106600	-0.69333500
H	6.55424100	-1.13300200	-0.04325000
H	0.08532100	-0.26799600	-0.17881500
H	-5.74311900	-0.18999600	-0.71722300
H	-0.77789500	-4.27257700	0.03297900
H	4.48562100	-3.50934100	0.51658600
H	4.02189300	2.78691800	-1.03730000
H	-0.80208900	1.32141000	1.67672800
H	-2.26879600	-0.66220800	0.47216800

Unsubstituted N-fused [24]pentaphyrin **4**

4a

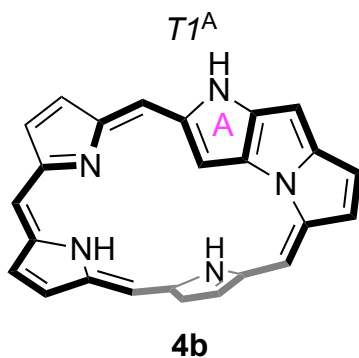


4a

Sum of electronic and zero-point Energies= -1236.234370

N	2.12303500	3.06471800	0.06016600
N	3.49694000	-0.08813800	-0.09156400
N	0.44224000	-3.14726200	-0.25273700
N	-3.06301500	-1.05692300	0.00236000
N	-2.22647200	1.65991100	0.02816200
C	0.86803800	2.43382400	0.07010000
C	1.07939100	1.03994500	0.01151100
C	2.46911600	0.85363100	-0.03086400
C	3.10104700	2.12037100	-0.01906700
C	4.51129800	1.97840800	-0.11878900
C	4.71544600	0.60810900	-0.18651200
H	2.25506300	4.06287500	0.06075000
C	5.74902600	-0.36824900	-0.42672200
H	0.49219800	-3.60702700	-1.14903300
C	5.16127100	-1.59122800	-0.50643300
H	-2.24187200	-0.46777900	0.11609800
C	3.72115400	-1.47007000	-0.26922400
H	0.28786100	0.31303800	-0.00916100
C	2.84298000	-2.50550500	-0.18624300
H	6.80113800	-0.14189500	-0.53262400
C	1.49196100	-2.44486900	0.31821100
H	5.65039900	-2.54370500	-0.66031500
C	0.96754900	-1.75287900	1.40551500
H	1.54421600	-1.15518500	2.09565500
C	-0.42152100	-1.99307400	1.44460300
H	-1.12695800	-1.61842700	2.17200300
C	-0.74399300	-2.83739500	0.38400800
H	-4.86185600	-3.74527200	-0.66650100
C	-2.04353300	-3.28699400	-0.07637700
H	-6.26258900	-1.46427800	-0.69047000
C	-3.10538600	-2.43438300	-0.17400600
H	-4.85523800	3.73464700	-0.10972300
C	-4.49426300	-2.74340200	-0.48926300
H	-2.48816000	5.01838900	0.09378800
C	-5.20595400	-1.58715300	-0.49362500
C	-4.29624400	-0.48680400	-0.21613400
C	-4.54569600	0.86364400	-0.20765900
C	-3.54983900	1.88107500	-0.06589300
C	-3.86221900	3.30777400	-0.04780600
C	-2.67264900	3.95179400	0.05684900
C	-1.64345300	2.91880600	0.08854000
C	-0.29985200	3.23706800	0.11405200
H	3.22985800	-3.47626600	-0.49153200
H	5.26978700	2.74502200	-0.16784600
H	-0.10149900	4.30811100	0.15008400
H	-5.57059900	1.18484700	-0.35912600
H	-2.19292500	-4.32790000	-0.34938800

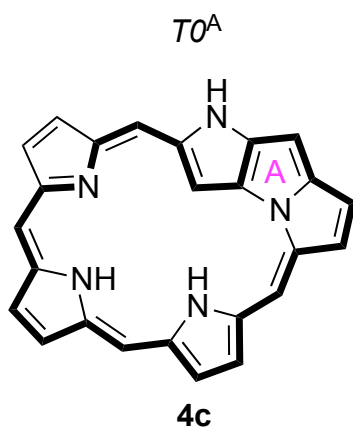
4b



Sum of electronic and zero-point Energies= -1236.228209

N	-2.42513600	1.39855500	0.39444100
N	-2.86303000	-1.18827700	-0.15091700
N	1.02402100	-2.34985200	-0.20857900
N	3.36539400	0.07329600	-0.30636300
N	1.64608700	3.06184500	-0.49416100
C	-1.94975900	2.68280900	0.49404300
C	-3.05907800	3.61633800	0.66559500
C	-4.19759100	2.87594700	0.62041300
C	-3.77596400	1.49420800	0.41381700
C	-4.64715800	0.42059900	0.08591000
C	-4.17764900	-0.82670300	-0.29550500
C	-4.80908400	-1.88653800	-1.05350500
C	-3.83840600	-2.76541800	-1.44497300
C	-2.57889400	-2.33705900	-0.86843900
C	-1.31700900	-2.87520500	-0.93442200
C	-0.31509900	-2.54586600	0.04953900
C	-0.44748100	-2.55753500	1.44943200
C	0.83028300	-2.43538700	2.01167700
C	1.74674300	-2.27053500	0.96781800
C	3.17075100	-2.05687200	0.99053000
C	3.86976300	-1.10085200	0.31101400
C	5.30340300	-1.05910400	0.09808900
C	5.63547900	0.07804100	-0.58704100
C	4.44242800	0.83837600	-0.79065700
C	4.04077600	2.15298500	-1.04583100
C	2.69347900	2.19982800	-0.64453600
C	2.26225900	0.92828400	-0.17928200
C	0.92498900	1.01550400	0.21682000
C	0.54043700	2.37127800	0.02450200
C	-0.64150700	3.09971200	0.29365500
H	-2.96303000	4.68945100	0.77618600
H	-5.22265000	3.21860900	0.68400700
H	-5.86253600	-1.92362000	-1.29710300
H	-3.96546700	-3.66215200	-2.03666400
H	-1.38132500	-2.70406500	1.97208800
H	1.08253200	-2.42224700	3.06286400
H	5.96676100	-1.85885600	0.39865100
H	6.62556100	0.38259700	-0.89843100
H	0.28934500	0.26183700	0.65260200
H	-2.19524400	-0.45457200	0.11372000
H	1.43151000	-2.27907600	-1.12822500
H	1.61175000	4.01851200	-0.80562300
H	-5.70689100	0.62856700	-0.01251400
H	-0.51577600	4.18178700	0.26786300
H	4.67225900	2.95388200	-1.40076200
H	3.76170400	-2.72281900	1.61499900
H	-1.09652600	-3.61782000	-1.69660200

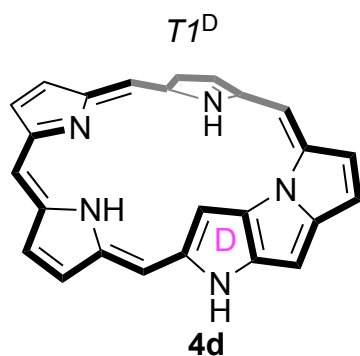
4c



Sum of electronic and zero-point Energies= -1236.228507

N	-2.40243800	-1.71300800	0.13354900
N	-2.89138900	1.04321800	-0.16702500
N	0.53922700	2.26524900	0.00499700
N	3.37477400	-0.37178900	-0.09380100
N	1.74959900	-3.40258200	-0.09651600
C	-1.94718400	-3.01670900	0.26666300
C	-3.07001300	-3.94180400	0.34016600
C	-4.19372100	-3.18865700	0.23183700
C	-3.74128200	-1.80715400	0.09550700
C	-4.61550900	-0.69733200	-0.09231400
C	-4.20523300	0.60514700	-0.22394300
C	-5.02720400	1.78230900	-0.41080300
C	-4.21174500	2.86387200	-0.43359600
C	-2.83349800	2.42650900	-0.25811500
C	-1.80064400	3.32196100	-0.16520300
C	-0.38820900	3.29756500	0.07113500
C	0.31961000	4.45719800	0.42103000
C	1.66498000	4.12588000	0.54335800
C	1.81520000	2.75925700	0.26598700
C	3.11710500	2.16704100	0.21689600
C	3.76427800	0.97455700	0.05035000
C	5.22579100	0.95460900	-0.07134500
C	5.67021800	-0.30546100	-0.30145300
C	4.52194300	-1.17155400	-0.30561600
C	4.19252500	-2.51130200	-0.39030600
C	2.78643200	-2.53392300	-0.19823400
C	2.27686400	-1.22672500	-0.00747900
C	0.88801800	-1.31816800	0.20370600
C	0.56522400	-2.69065400	0.13430800
C	-0.63727000	-3.43266600	0.25346700
H	-2.98870300	-5.01629700	0.44779700
H	-5.22575100	-3.51543300	0.22990500
H	-6.10443200	1.75942200	-0.50217600
H	-4.49185000	3.90243400	-0.54854400
H	-0.13686500	5.42463100	0.57491000
H	2.48087400	4.78416100	0.80768600
H	5.82076800	1.85616700	-0.01099400
H	6.69120300	-0.62834200	-0.44833100
H	0.16998500	-0.55802800	0.46382100
H	-2.15913700	0.35436000	-0.00967300
H	0.35489100	1.35450900	-0.38750000
H	1.79019700	-4.39891600	-0.23670300
H	-5.68145800	-0.89121500	-0.13905200
H	-0.49988100	-4.51212500	0.30501400
H	4.87299800	-3.33529400	-0.54055000
H	3.84970200	2.96128700	0.33427700
H	-2.15101000	4.34828000	-0.22432400

4d

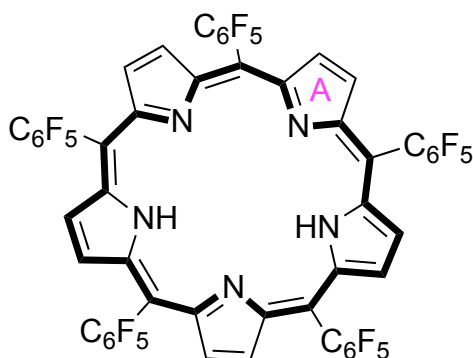


Sum of electronic and zero-point Energies= -1236.228197

N	-2.49807500	1.38348400	0.43106400
N	-2.79134200	-1.20168500	-0.12592400
N	1.08759700	-2.34152000	-0.17505300
N	3.35229000	0.09209600	-0.29538100
N	1.57596400	3.04240600	-0.56200200
C	-1.99243100	2.66530300	0.48889200
C	-3.13400100	3.53100000	0.68731900
C	-4.26722400	2.76852000	0.67623900
C	-3.87805400	1.39616200	0.45589500
C	-4.66456100	0.29683900	0.13247900
C	-4.09394200	-0.92860500	-0.29890300
C	-4.72256600	-1.93989800	-1.15532700
C	-3.72383500	-2.76591200	-1.56881200
C	-2.51106600	-2.31431600	-0.89076800
C	-1.23445600	-2.82924800	-0.95240600
C	-0.26074900	-2.51589500	0.05259800
C	-0.42759800	-2.50745100	1.45036800
C	0.83510400	-2.38919200	2.04107100
C	1.77908700	-2.24004200	1.01552900
C	3.19725700	-2.00184100	1.06183200
C	3.88305900	-1.05183100	0.35866300
C	5.31397300	-0.98760000	0.14161700
C	5.61977500	0.13076500	-0.58726400
C	4.41219100	0.85864400	-0.81550400
C	3.98253500	2.15645600	-1.11092900
C	2.63843600	2.19171000	-0.69923500
C	2.23639600	0.93260000	-0.18527800
C	0.90268700	1.01454400	0.23617900
C	0.49419200	2.35668900	0.00400600
C	-0.69298500	3.08535600	0.27720200
H	-3.06521800	4.60544100	0.79494800
H	-5.29024200	3.10707400	0.76776200
H	-5.76756800	-1.96920400	-1.43876100
H	-3.79895300	-3.62273700	-2.22664400
H	-1.37972600	-2.62466200	1.94466900
H	1.06272600	-2.36083900	3.09757300
H	5.99430700	-1.76406700	0.46430700
H	6.60255200	0.44225100	-0.91484800
H	0.30382900	0.25994400	0.72295000
H	1.51844600	-2.27415900	-1.08426800
H	1.51907900	3.98533600	-0.90948300
H	-5.73734200	0.44047300	0.06547000
H	-0.58059700	4.16737900	0.25042900
H	4.59560600	2.95703300	-1.49765600
H	3.79038600	-2.63664900	1.71554300
H	-0.96496700	-3.51000800	-1.75727200
H	-2.03469600	0.49738100	0.20356600

Meso-pentakis(pentafluorophenyl)-substituted pentaphyrins (7)

22PP



7

1a (T0)

Sum of electronic and zero-point Energies= -4871.917791

C	-1.01405600	-3.21404200	0.22783500
N	-1.46680800	-1.97487300	0.39999000
C	-2.43297200	-2.07867500	1.39068300
C	-3.34800900	-1.07285600	1.66812400
C	-3.43542300	0.15979600	0.96294100
C	-4.58887500	0.97361300	0.83746000
C	-4.32048100	1.93337100	-0.11893300
C	-2.97259200	1.76947500	-0.53380000
C	-2.26972700	2.67220600	-1.39029900
C	-0.92092900	2.99322900	-1.32931000
N	-0.01464700	2.46076800	-0.42123900
C	1.00444800	3.32611300	-0.40923600
C	2.17235300	3.26747800	0.43202400
C	2.85895600	2.12541800	0.80664800
C	4.11256600	2.09457800	1.53344400
C	4.65036000	0.85699600	1.40554400
C	3.74366200	0.04391000	0.62571300
C	4.00473500	-1.21563500	0.10695300
C	3.03406900	-2.04090300	-0.55288400
N	1.72712500	-2.00899800	-0.29183400
C	1.19318000	-3.07435900	-1.00274800
C	-0.02903400	-3.66106000	-0.73838500
C	0.81885300	4.41400400	-1.37434500
C	-0.35532300	4.16628900	-1.99599500
N	2.63805400	0.83186500	0.37041600
C	2.22517800	-3.69201500	-1.84994900
C	3.38347100	-3.07578500	-1.53729500
N	-2.47095500	0.68805500	0.13946300
C	-1.65496000	-4.16550300	1.14141900
C	-2.50036900	-3.43879100	1.91041600
H	1.51572200	5.21795700	-1.56551900
H	-0.81817800	4.73756000	-2.78712300
H	1.80943200	0.51055300	-0.11571700
H	5.58936600	0.50616500	1.80614900
H	4.53535200	2.93972600	2.05450200
H	2.07095800	-4.49699600	-2.55373700
H	4.37027000	-3.26623700	-1.93622200
H	-1.56781400	0.24511700	-0.00390900
H	-5.51677100	0.82220300	1.36779000
H	-4.98142000	2.71527900	-0.46037700
H	-1.44128000	-5.22342600	1.20446500
H	-3.12737400	-3.78615900	2.71860500
C	-0.35527900	-4.97684000	-1.37008000
C	0.37600500	-6.14656800	-1.12676300
C	-1.47337000	-5.09468800	-2.20704800
C	0.03086400	-7.36707800	-1.70269800
C	-1.83508000	-6.30271800	-2.79641900

C	-1.07835600	-7.44407600	-2.54122000
C	5.38927100	-1.75066800	0.21423700
C	5.64512100	-2.97603200	0.84811700
C	6.49569400	-1.09023400	-0.34026500
C	6.92627300	-3.51328400	0.93744000
C	7.78658000	-1.60542900	-0.25746500
C	8.00189100	-2.82334000	0.38288500
C	2.73966400	4.59057000	0.82763800
C	1.99745200	5.46320600	1.63621300
C	3.98684600	5.05216700	0.38575300
C	2.47184400	6.71913900	2.00464800
C	4.48377600	6.30295400	0.74418900
C	3.72163900	7.13972900	1.55593700
C	-4.41252100	-1.31199900	2.68940000
C	-4.41953100	-0.58792200	3.88736100
C	-5.44870300	-2.23182900	2.49518600
C	-5.39916100	-0.77702400	4.85862800
C	-6.43912800	-2.43763400	3.45308800
C	-6.41316800	-1.70649100	4.63830800
C	-3.15154000	3.44103700	-2.32560700
C	-3.71285600	2.80500700	-3.43888500
C	-3.48653600	4.78433900	-2.12510000
C	-4.55071400	3.47275100	-4.32798100
C	-4.32434000	5.47285900	-3.00010000
C	-4.85763100	4.81324400	-4.10492300
F	7.13250600	-4.67872100	1.55958900
F	9.23478900	-3.32705800	0.46550400
F	8.81589200	-0.94694400	-0.80176700
F	6.33202900	0.07180000	-0.98793400
F	4.64014300	-3.66272600	1.40413800
F	4.74201500	4.29018900	-0.41843700
F	5.67869500	6.71025500	0.30192600
F	4.18840900	8.34062800	1.90317800
F	1.74124900	7.51906000	2.78804100
F	0.79616300	5.08976900	2.09091100
F	-3.00806800	5.44670600	-1.06409900
F	-4.62629600	6.75700400	-2.78055300
F	-5.66074200	5.46449700	-4.94822800
F	-3.43593000	1.51761700	-3.67894400
F	-5.05925400	2.83903200	-5.38940800
F	-5.37122000	-0.07708700	5.99713400
F	-7.35804000	-1.89629200	5.56108400
F	-7.41771700	-3.32284800	3.23690500
F	-5.51737100	-2.94016800	1.36109500
F	-3.45674200	0.30976300	4.12944600
F	1.43094300	-6.12556200	-0.30136500
F	0.74931600	-8.46565800	-1.44509700
F	-1.41528200	-8.60863900	-3.09880600
F	-2.89783200	-6.37437500	-3.60446300
F	-2.21900800	-4.01685200	-2.47646000

1c ($T0^A$)

Sum of electronic and zero-point Energies= -4871.916000

C	-2.17554600	-1.94760800	-0.85291500
N	-3.25713800	-1.13652500	-0.79085500
C	-2.82681800	0.05076700	-1.28376000
C	-3.58146300	1.22832200	-1.10856600
C	-2.93557000	2.45587500	-0.87220900
C	-3.48997300	3.76897200	-0.80672800
C	-2.50369900	4.62964800	-0.39360200
C	-1.31173800	3.86708700	-0.18126000
C	-0.08287200	4.30689600	0.34776700
C	1.10569200	3.56582500	0.47341800
N	1.35948700	2.29556600	-0.01031000
C	2.69883800	2.12794700	0.13461800
C	3.59282200	1.09905400	-0.32805000
C	3.54649300	-0.29831500	-0.48269100
C	4.70256500	-1.04930600	-0.91508200
C	4.48548800	-2.37114000	-0.68509800
C	3.16274500	-2.52559400	-0.16422000
C	2.60257500	-3.76203600	0.20342500
C	1.22733800	-4.02049600	0.38816900
N	0.27914400	-3.10811000	0.09504500
C	-0.91395900	-3.75274800	0.23025600

C	-2.13986000	-3.16996600	-0.13993400
C	2.30654300	4.16329900	1.04179200
C	3.30406400	3.28982500	0.80295600
N	-1.60432200	2.57456400	-0.51673600
C	-1.06942700	-1.31508000	-1.57808100
C	-1.47143400	-0.04570200	-1.82622000
N	2.61037600	-1.25351800	-0.10073000
C	-0.71132600	-5.11819000	0.71367300
C	0.62971600	-5.29352200	0.79847600
H	-4.51089600	4.01483200	-1.05824000
H	-2.58787400	5.69608600	-0.25034800
H	5.59176700	-0.61391700	-1.33899700
H	5.16035800	-3.18766500	-0.89007800
H	2.36874100	5.11542100	1.54675600
H	4.33939300	3.38821300	1.09043100
H	-0.92767700	1.82453100	-0.41294800
H	-0.14724300	-1.79534400	-1.85835800
H	-0.94694300	0.71972100	-2.38183300
H	1.65338400	-1.09296500	0.19109200
H	-1.48768500	-5.84437200	0.90860300
H	1.16222400	-6.18345800	1.10224800
C	-3.42069500	-3.78435500	0.28092400
C	-3.68752600	-4.10027200	1.62013500
C	-4.44392800	-4.04083000	-0.64345100
C	-4.90146100	-4.64835800	2.02431200
C	-5.66336400	-4.58952000	-0.26081200
C	-5.89392300	-4.89314500	1.07917200
C	-5.05445800	1.13348300	-1.01210600
C	-5.77896700	1.61636600	0.08754500
C	-5.79172700	0.49718800	-2.02312700
C	-7.16243800	1.49148500	0.17310500
C	-7.17444700	0.36362800	-1.95707300
C	-7.86262900	0.86214000	-0.85299700
C	-0.06560100	5.73431600	0.80142000
C	0.61804400	6.72436600	0.08696100
C	-0.74699400	6.13943200	1.95438600
C	0.63363300	8.05462400	0.49943700
C	-0.74780900	7.46392200	2.38552700
C	-0.05340200	8.42445000	1.65360600
C	4.94423400	1.68114200	-0.66747300
C	5.10356700	2.46730500	-1.81390900
C	6.07337700	1.50452400	0.14030300
C	6.32658100	3.04154700	-2.15406200
C	7.30487700	2.07276200	-0.17429400
C	7.43061800	2.84363300	-1.32870200
C	3.55110200	-4.90671100	0.34041100
C	3.49595000	-6.01980100	-0.50828000
C	4.53211300	-4.92379200	1.34077700
C	4.36306300	-7.10055500	-0.36863800
C	5.41227400	-5.99135800	1.49708100
C	5.32515200	-7.08499500	0.63873100
F	6.33245200	-5.97624800	2.46664700
F	6.16215400	-8.11405200	0.77976900
F	4.28527700	-8.14441300	-1.20034100
F	2.59584700	-6.06483200	-1.49878900
F	4.64088400	-3.89354200	2.18924200
F	4.06364000	2.67809000	-2.62902700
F	6.44693300	3.77748500	-3.26343500
F	5.98388300	0.78148200	1.26534400
F	8.60689500	3.38997000	-1.64167800
F	8.36274800	1.88887900	0.62296000
F	-1.42207100	5.24076200	2.68242900
F	-1.40483700	7.81628200	3.49513500
F	1.28544000	6.40478700	-1.02868700
F	1.29626200	8.97635700	-0.20687800
F	-0.04658100	9.69616600	2.05706000
F	-5.14602100	2.19767400	1.11599600
F	-7.81960300	1.95865900	1.24035500
F	-9.18903200	0.74096600	-0.78071000
F	-7.84669300	-0.23001900	-2.94831900
F	-5.17201200	0.02301900	-3.10831600
F	-2.77179100	-3.85661800	2.56863900
F	-5.12237200	-4.92984100	3.31379300
F	-7.06070100	-5.42184900	1.45442700
F	-6.61211200	-4.83563600	-1.17138400
F	-4.25734800	-3.78613800	-1.94239700

1d ($T0^D$)

Sum of electronic and zero-point Energies= -4871.913232

C	-2.85952400	1.63078900	-0.10622600
N	-1.60367800	2.07484300	-0.03134100
C	-1.61844200	3.31491600	-0.67802900
C	-0.58323500	4.24524100	-0.64987800
C	0.70676300	4.02867200	-0.09708900
C	1.78131900	4.94409100	0.07222000
C	2.86840500	4.23462700	0.54467000
C	2.48139500	2.87448200	0.67841200
C	3.26621600	1.72957000	0.97788700
C	2.66226300	0.49417700	1.23570500
N	3.25509300	-0.67506300	0.83872800
C	2.29497500	-1.60474600	0.94023200
C	2.45334600	-2.89266100	0.33462900
C	1.36150200	-3.62499700	-0.11690900
C	1.32481300	-4.98981400	-0.58639400
C	0.03129000	-5.32247500	-0.85280100
C	-0.79671100	-4.17451300	-0.55988900
C	-2.18282100	-4.06435500	-0.53026700
C	-2.86501400	-2.88890800	-0.06817200
N	-2.37960100	-1.63625100	-0.05407800
C	-3.36623400	-0.86451900	0.55354800
C	-3.52797900	0.51036000	0.56661100
C	-2.92602800	3.57707900	-1.25752800
C	-3.71425500	2.54807000	-0.87466400
N	1.15758500	2.80362500	0.30502200
C	1.09003700	-1.07079100	1.58207400
C	1.31610000	0.25618700	1.74852000
C	-4.18340800	-2.97698100	0.56647200
C	-4.46009900	-1.74030400	1.02037500
N	0.05376400	-3.17533600	-0.15926300
H	-3.19504100	4.42862800	-1.86533000
H	-4.75034300	2.37496000	-1.12577300
H	0.56148700	1.97992800	0.25863500
H	3.84772500	4.62242100	0.78272200
H	1.73543200	6.00253300	-0.13563200
H	0.22573300	-1.62950500	1.91060700
H	0.66938600	0.97783300	2.22825600
H	-4.76878000	-3.87683500	0.69090900
H	-5.33205900	-1.42930000	1.57438000
H	2.18998000	-5.63208200	-0.65555900
H	-0.33714300	-6.27743400	-1.19459000
H	-0.28839100	-2.22660800	-0.02856100
C	4.73922300	1.80176800	0.85588700
C	5.38489100	2.30569000	-0.28285700
C	5.56156900	1.32364600	1.88825600
C	6.77202300	2.34982400	-0.38650300
C	6.94932200	1.36165700	1.80467200
C	7.55709200	1.87557900	0.66137100
C	3.82816500	-3.38915500	0.09274900
C	4.75619900	-3.47205400	1.14117100
C	4.28716100	-3.74452600	-1.18286000
C	6.06552800	-3.89425800	0.93818500
C	5.59248800	-4.17321000	-1.40770900
C	6.48575200	-4.24673100	-0.34259200
C	-3.00831100	-5.25258800	-0.87650800
C	-2.92651700	-6.46680800	-0.18103600
C	-3.94452600	-5.19063100	-1.91900200
C	-3.71195100	-7.56762700	-0.51299200
C	-4.74645300	-6.27514500	-2.26383500
C	-4.62781300	-7.47000600	-1.55778300
C	-4.73588200	1.03582000	1.30566400
C	-6.03729600	1.00980800	0.79723900
C	-4.56061500	1.63121400	2.55962900
C	-7.11900300	1.53721900	1.49714100
C	-5.62636500	2.15785700	3.28533300
C	-6.91128100	2.10982900	2.75035500
C	-0.82362400	5.60242800	-1.22794000
C	-0.16734500	6.02415100	-2.39008500
C	-1.69745400	6.51378600	-0.62418500
C	-0.37123400	7.28947100	-2.93484600
C	-1.91730900	7.78406500	-1.15150500
C	-1.25076400	8.17197700	-2.31151000

F	5.02035800	0.84074300	3.01068500
F	7.70187100	0.91557200	2.81564700
F	8.88731500	1.91645300	0.57173700
F	7.35344000	2.83017200	-1.49117500
F	4.67287200	2.73973400	-1.33153100
F	3.47049500	-3.66379000	-2.24424900
F	5.99492700	-4.50157600	-2.64091200
F	7.73878000	-4.65901500	-0.54616200
F	6.91949500	-3.97513400	1.96436000
F	4.38677600	-3.16165100	2.38832100
F	-2.07763300	-6.59795800	0.84975700
F	-4.08175300	-4.06149500	-2.62462000
F	-5.62108400	-6.18011200	-3.27037700
F	-5.38901600	-8.51727200	-1.88045900
F	-3.60490800	-8.70899600	0.17615900
F	-3.33774000	1.69367600	3.10123600
F	-6.26711300	0.49156200	-0.42034800
F	-8.35027300	1.49876900	0.97608300
F	-7.94086500	2.61305000	3.43428600
F	-5.42420900	2.70407300	4.48864800
F	-2.34662700	6.17956200	0.49773100
F	-2.75588000	8.63245500	-0.54817100
F	-1.45428500	9.38626300	-2.82465200
F	0.26543200	7.65860200	-4.05050600
F	0.67938300	5.19801400	-3.01682400

1d ($T0^{4,D}$)

Sum of electronic and zero-point Energies= -4871.929542

C	3.54438000	-2.73726600	0.02631500
N	2.43230000	-2.21840000	0.62004800
C	1.50490400	-3.20260600	0.64455900
C	0.21164600	-2.85005700	1.14229400
C	-1.00857200	-3.29216000	0.61062800
N	-2.12219400	-2.50318600	0.71069000
C	-3.10700300	-3.13776100	0.04304600
C	-4.32214400	-2.47429900	-0.30221900
C	-4.37712200	-1.07780900	-0.42439800
C	-5.46651200	-0.21292200	-0.80020800
C	-4.98360300	1.06627400	-0.89621300
C	-3.56747800	1.03339400	-0.63836000
C	-2.59621500	2.04492900	-0.76670100
C	-1.22787700	1.71446900	-0.99790900
N	-0.20721400	2.51932900	-0.64840200
C	0.92841500	1.82939700	-0.95682800
C	2.21792600	2.31946100	-0.67227600
C	3.34504400	1.45164200	-0.62540400
C	4.72891700	1.71691000	-0.87016900
C	5.40796900	0.51736300	-0.83338500
C	4.46788500	-0.51294100	-0.51807000
C	4.61570700	-1.91595800	-0.39380500
C	3.34018000	-4.15159200	-0.25885300
C	2.04510400	-4.42636000	0.07272600
C	-2.65008200	-4.44865400	-0.42312200
C	-1.32074300	-4.50541700	-0.14192400
N	-3.26881700	-0.26978600	-0.32623700
C	-0.74410200	0.49059500	-1.65222100
C	0.60580400	0.56210600	-1.62478500
N	3.24585100	0.10654100	-0.39910900
H	1.54453800	-5.38138500	0.00253700
H	4.06268200	-4.82823300	-0.69463500
H	6.46181400	0.36525300	-1.01433300
H	5.13585400	2.68788500	-1.11239900
H	1.31064500	-0.12682300	-2.06646700
H	-1.35564100	-0.27201100	-2.11224000
H	-5.52954600	1.94775600	-1.19993400
H	-6.47618500	-0.54266800	-0.99705800
H	-3.23630200	-5.18336600	-0.95579000
H	-0.64252400	-5.31277900	-0.37553000
C	5.90177900	-2.54315400	-0.78733400
C	6.60425600	-3.37072900	0.10200000
C	7.80802400	-3.97779500	-0.24567700
C	8.34323500	-3.77031700	-1.51477200
C	7.67082400	-2.95811700	-2.42510200
C	6.46785000	-2.36196100	-2.05803800

C	2.40877500	3.75977300	-0.40090700
C	3.12607800	4.20890200	0.71932000
C	3.28867700	5.56062100	1.00501100
C	2.72423100	6.51348100	0.16130900
C	2.00693100	6.10556600	-0.96107400
C	1.85694500	4.74942700	-1.23244900
C	-2.98823100	3.46241700	-0.64425800
C	-2.52636300	4.43370100	-1.55023400
C	-2.85963300	5.77801400	-1.42438100
C	-3.67734200	6.19384900	-0.37582600
C	-4.15615700	5.26005000	0.53905200
C	-3.80963600	3.91985900	0.39919600
C	-5.54455200	-3.26173800	-0.63565500
C	-6.63622300	-3.29328100	0.24031300
C	-7.79120700	-4.01916100	-0.04128000
C	-7.87504700	-4.74495300	-1.22702100
C	-6.80694900	-4.73545900	-2.12081200
C	-5.66775100	-3.99256700	-1.82190900
F	6.13247800	-3.58532000	1.33545300
F	8.45540200	-4.75010400	0.63201800
F	9.49513000	-4.34791100	-1.85779200
F	8.17465400	-2.76846700	-3.64881900
F	5.84154400	-1.61236100	-2.97557800
F	3.66036800	3.32768700	1.57747100
F	3.97081700	5.94765500	2.08883600
F	2.87454600	7.81290700	0.42391800
F	1.47937700	7.02152300	-1.78039800
F	1.19437300	4.41484500	-2.34242900
F	-1.77234000	4.08201300	-2.59536900
F	-2.41655700	6.67151000	-2.31525300
F	-4.00650000	7.48108700	-0.25326000
F	-4.93528900	5.65652500	1.55184200
F	-4.27067600	3.06470200	1.32348800
F	-6.58955800	-2.60636200	1.38918100
F	-8.81432100	-4.02604200	0.81904800
F	-8.97496900	-5.44709700	-1.50614400
F	-6.88585600	-5.42535800	-3.26364500
F	-4.66355800	-3.99994900	-2.71279200
H	-2.41278700	-0.62289000	0.10091600
H	2.46373700	-0.41702300	0.00501000
C	0.21939300	-1.88989200	2.29069000
C	0.73343600	-2.37287600	3.50501800
C	-0.26524800	-0.58356700	2.31098800
C	0.74795300	-1.61259900	4.66915300
C	-0.26401000	0.20132200	3.46134100
C	0.24330000	-0.31543000	4.64885800
F	1.21549300	-3.62259000	3.57700100
F	-0.71276000	-0.00371700	1.18674800
F	-0.73255400	1.45303700	3.42269200
F	0.25154100	0.42760100	5.75775600
F	1.23583800	-2.12358600	5.80508900

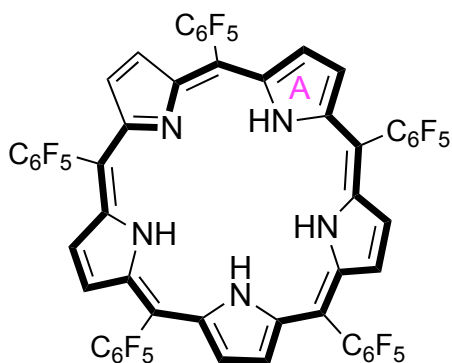
1f ($T0^{A,D}$)

Sum of electronic and zero-point Energies= -4871.931826

C	2.72112700	-0.05763200	-0.70527800
N	3.16963000	-1.33676400	-0.47665000
C	2.20495500	-2.14042400	-0.93914200
C	2.18072000	-3.55873800	-0.68269600
C	0.94969300	-4.13787900	-0.34328800
C	0.46480900	-5.49137900	-0.21113200
C	-0.86436600	-5.44586000	0.12448100
C	-1.25257600	-4.06253900	0.26663400
C	-2.43658200	-3.40091900	0.62164900
C	-2.35493500	-1.98861400	0.90033600
N	-3.26054300	-1.10513200	0.46246500
C	-2.72404100	0.13208600	0.72031000
C	-3.33722300	1.30349600	0.25666100
C	-2.68915700	2.56268400	0.15472600
C	-3.31966500	3.83669900	0.04454300
C	-2.34124400	4.80118200	-0.00744800
C	-1.07549700	4.14658300	0.03869800
C	0.21026900	4.72937400	-0.02713400
C	1.42017100	4.01672700	-0.07458400
N	1.50725300	2.65056900	-0.15279000

C	2.83189000	2.36556700	-0.12196400
C	3.40221700	1.05877700	-0.20936400
C	1.46925100	-0.06573500	-1.45668800
C	1.14058200	-1.37204600	-1.60966800
N	-0.12519000	-3.34418500	-0.03690800
C	-1.23605700	-1.31567300	1.57794400
C	-1.46944600	0.01591700	1.45725100
N	-1.32943600	2.79734200	0.14920400
C	3.62592300	3.58541100	-0.00085400
C	2.74717200	4.61707800	0.00287400
H	0.96378400	0.80866200	-1.83633900
H	0.31570400	-1.78452000	-2.17552700
H	1.05838400	-6.37794800	-0.37889800
H	-1.51874400	-6.28940800	0.28786100
H	-0.43849400	-1.79670500	2.12822800
H	-0.89441800	0.82395800	1.88744700
H	-4.38818900	3.99115000	0.04621000
H	-2.48504000	5.86829800	-0.08176700
H	-0.56558700	2.12544800	0.09409500
H	4.70483100	3.63425100	0.03490800
H	2.96764400	5.67231900	0.07349100
H	-0.08969600	-2.33502600	-0.03937200
C	4.79176700	0.86326300	0.27987500
C	5.16663200	1.21816300	1.58253100
C	5.78236400	0.28491300	-0.52655000
C	6.45653100	1.01632200	2.06453600
C	7.07806200	0.07604300	-0.06496500
C	7.41624700	0.44103500	1.23616300
C	0.26764800	6.22096500	-0.04196200
C	0.73683400	6.92345200	-1.15854600
C	-0.13901800	6.98215800	1.06057600
C	0.80308300	8.31436200	-1.18157300
C	-0.08560300	8.37354000	1.05877100
C	0.38904000	9.04155800	-0.06785500
C	-4.75035200	1.22133900	-0.19383600
C	-5.13519200	1.60237200	-1.48629300
C	-5.75655100	0.71875300	0.64353100
C	-6.45087100	1.49969100	-1.92823300
C	-7.07757800	0.60858400	0.22142500
C	-7.42598500	0.99886200	-1.06982000
C	3.44129300	-4.31617100	-0.64029100
C	3.76680200	-5.20468400	0.39808600
C	4.41352800	-4.14589600	-1.64240700
C	4.97568300	-5.89147900	0.43741700
C	5.62880900	-4.82107700	-1.61939500
C	5.91224000	-5.69860000	-0.57502400
C	-3.74873800	-4.06472800	0.58107900
C	-4.70037200	-3.83531900	1.59117100
C	-4.14313000	-4.91828200	-0.46293500
C	-5.96073500	-4.42212500	1.57053300
C	-5.39803500	-5.51715100	-0.49992700
C	-6.31220900	-5.26778600	0.52056400
F	6.77469900	1.36178700	3.31767200
F	8.65796700	0.24458400	1.68505100
F	8.00342300	-0.46569200	-0.86523700
F	5.51208800	-0.05749400	-1.78957300
F	4.26666500	1.75296000	2.42065400
F	2.91548600	-5.40078800	1.41736600
F	5.24859400	-6.72254200	1.44958900
F	7.07309700	-6.35468000	-0.54732400
F	6.51916000	-4.64588200	-2.60070900
F	4.17443200	-3.33794200	-2.67969800
F	1.13513700	6.25871500	-2.25019100
F	1.25282800	8.95335200	-2.26586100
F	0.44627100	10.37412000	-0.08027400
F	-0.47856400	9.06830700	2.13096300
F	-0.59243600	6.37305100	2.16435900
F	-4.22264700	2.06513500	-2.35321000
F	-6.77908800	1.86818900	-3.17169500
F	-8.69150200	0.89776300	-1.48056900
F	-8.01640700	0.13862300	1.04990000
F	-5.47235900	0.35430900	1.89692100
F	-4.39863300	-3.05497400	2.63354400
F	-3.31417300	-5.16490800	-1.48950300
F	-5.73596100	-6.31712400	-1.51742000
F	-7.51677600	-5.83980000	0.49515200
F	-6.83055400	-4.19247200	2.55913000

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2a (T0)

Sum of electronic and zero-point Energies= -4873.134287

C	2.06577800	3.16563100	-0.31492700
C	1.95469200	4.25119200	-1.27990300
C	0.64583700	4.48569200	-1.52437400
C	-0.15421500	3.60786000	-0.67864900
N	0.75573200	2.75257000	-0.06302100
C	3.17977500	2.62989100	0.26247000
C	-1.49624100	3.64567800	-0.42671200
C	3.14856900	1.36873100	1.01505900
N	2.68642000	0.21566600	0.40533200
C	3.02620800	-0.89549900	1.15739700
C	3.62675800	-0.41783500	2.32249600
C	3.70556700	0.98673200	2.23235600
C	3.00512700	-2.23136400	0.59181200
C	2.06723900	-2.70636400	-0.30173900
N	0.76811500	-2.23314200	-0.51282000
C	0.12231500	-3.01954500	-1.45520300
C	1.13602500	-3.89576900	-2.01076900
C	2.26655700	-3.75982000	-1.27408500
C	-1.24442800	-3.10753900	-1.64710200
C	-2.12762200	2.79289600	0.59379800
N	-2.21454800	1.42560500	0.55520400
C	-2.95363400	0.96774500	1.63374600
C	-3.28568600	2.09262600	2.40611500
C	-2.78103000	3.22220200	1.75497300
C	-3.44696500	-0.36809600	1.73941000
C	-3.11886300	-1.41402200	0.89046800
N	-2.04052900	-1.42613400	0.00220700
C	-2.21262300	-2.52766000	-0.74385700
C	-3.43526400	-3.23767700	-0.38645900
C	-3.96057800	-2.57725600	0.67682400
H	2.79957300	4.75173300	-1.72915400
H	0.23186500	5.21380700	-2.20547000
H	2.42248600	0.17129900	-0.56819600
H	3.97765200	-1.03458000	3.13759600
H	4.12282100	1.66432500	2.96139500
H	0.97650700	-4.56970300	-2.83837700
H	3.20037700	-4.28583700	-1.40961400
H	-1.91061800	0.79753300	-0.18291500
H	-3.84429500	2.07175100	3.32991200
H	-2.85990400	4.25181500	2.07274500
H	-3.79924100	-4.14420200	-0.84863600
H	-4.86393600	-2.81403500	1.22085800
H	0.22450700	-1.67405600	0.13847100
H	0.51666800	2.20770800	0.75331100
C	-4.47935200	-0.61443000	2.78904200
C	-4.21889100	-1.47872100	3.85973000
C	-5.74132200	-0.00767500	2.75604600
C	-5.16051900	-1.72475000	4.85630900
C	-6.69762000	-0.24022400	3.74097600

C	-6.40487200	-1.10304000	4.79497500
C	-2.37150600	4.66906900	-1.04944000
C	-3.53568900	4.28125100	-1.73172200
C	-2.14212600	6.04897400	-0.95040700
C	-4.41525600	5.20041600	-2.29260300
C	-3.00142200	6.98851900	-1.51537800
C	-4.14430400	6.56359100	-2.18683900
C	4.51326400	3.26207100	0.04110600
C	5.20887000	3.88589300	1.08237000
C	5.15221100	3.22617200	-1.20310000
C	6.47383300	4.43939200	0.90782000
C	6.41103100	3.78500800	-1.40990600
C	7.07604900	4.39156300	-0.34755800
C	4.15653200	-3.10668700	0.92636800
C	3.97162300	-4.39090600	1.46394200
C	5.48683400	-2.68762500	0.75639500
C	5.04126300	-5.21015000	1.81689900
C	6.56879200	-3.48741100	1.10815900
C	6.34520900	-4.75612500	1.64016000
C	-1.77302600	-4.03412000	-2.68906600
C	-1.62319500	-5.42571700	-2.63847900
C	-2.51128700	-3.52451400	-3.76598400
C	-2.14929900	-6.26632900	-3.61721200
C	-3.05522500	-4.34362100	-4.75136600
C	-2.87113400	-5.72227800	-4.67638500
F	4.82223600	-6.42358800	2.33530100
F	2.73623300	-4.86342200	1.67622900
F	7.37735300	-5.53351700	1.97417300
F	7.82121100	-3.05693900	0.91758500
F	5.75042000	-1.49113800	0.21476400
F	4.65426700	3.96011500	2.30440000
F	4.54455100	2.64545300	-2.25138600
F	6.98615300	3.73548400	-2.61669500
F	8.28485800	4.92727900	-0.53204700
F	7.10482400	5.02830000	1.92929300
F	-1.07316200	6.51240700	-0.28171300
F	-3.81736300	2.97783900	-1.86783700
F	-5.50605700	4.78665100	-2.94615000
F	-4.97566000	7.45687500	-2.72858100
F	-2.74373900	8.29655800	-1.39776800
F	-3.03034300	-2.08612400	3.96063300
F	-4.87551300	-2.54890300	5.87012100
F	-7.31560800	-1.33315900	5.74295700
F	-7.89681500	0.34828500	3.67509500
F	-6.06879400	0.81002100	1.74800900
F	-0.95966600	-5.99584900	-1.62121500
F	-1.98084300	-7.59151200	-3.53585200
F	-3.38354700	-6.51905900	-5.61753400
F	-3.74431000	-3.81745300	-5.77016800
F	-2.70372800	-2.20301400	-3.87363500

2b (TI)

Sum of electronic and zero-point Energies= -4873.137749

C	2.03657800	-2.30327500	1.59955900
C	1.18628100	-3.19061600	2.29212400
C	0.25419300	-3.68170600	1.38069500
C	0.57146400	-3.15715100	0.10614000
C	-0.04934800	-3.46600700	-1.17026200
C	-1.42585700	-3.26204800	-1.24362900
C	-2.47450500	-3.82861900	-2.04585700
C	-3.67791500	-3.34806100	-1.59446500
C	-3.42710900	-2.39210300	-0.54961200
C	-4.27404200	-1.53009300	0.14774500
C	-3.81867800	-0.31895100	0.74884300
C	-4.46099500	0.49881300	1.70299800
C	-3.77541600	1.70007400	1.78224000
C	-2.69271900	1.66775500	0.87071500
C	-1.94912800	2.78841700	0.40246000
C	-0.74354200	2.87002300	-0.31915500
C	-0.42407600	3.95399100	-1.20619900
C	0.83653900	3.77098000	-1.69500000
C	1.39636900	2.60919000	-1.06770700
C	2.75303000	2.27350200	-1.01718200
C	3.30808200	1.27865600	-0.16145500

N	2.59638900	0.27853100	0.39829300
C	3.43757400	-0.30725000	1.32595900
C	3.08446200	-1.45238200	2.05204300
N	-2.05826600	-2.37767600	-0.38495600
N	-2.68437200	0.38666200	0.33037000
N	0.36836500	2.03179400	-0.32690800
N	1.64964900	-2.33782000	0.27454500
C	4.66200500	1.32428400	0.37687300
C	4.71862000	0.37159700	1.34752400
H	1.25259100	-3.42332700	3.34514600
H	-0.52240300	-4.40992800	1.56790500
H	-2.31988000	-4.54477100	-2.83949400
H	-4.65457800	-3.58268800	-1.99075000
H	-5.32674800	0.21046900	2.27922800
H	-4.01195900	2.53630700	2.42322800
H	-1.11167000	4.74521500	-1.46470800
H	1.35523400	4.39699700	-2.40479300
H	-1.58727000	-1.94610500	0.39668600
H	-2.21496900	0.17299400	-0.53874200
H	0.57973500	1.27668700	0.31970200
H	1.96745000	-1.62842300	-0.37731800
H	5.43638800	2.02386000	0.09428700
H	5.56175700	0.11512900	1.97425200
C	-2.61169900	4.10641100	0.64238600
C	-1.99687100	5.09850300	1.42050100
C	-3.86990700	4.41909700	0.10638700
C	-2.59787300	6.33165200	1.66104300
C	-4.48963100	5.64436500	0.33408500
C	-3.84955900	6.60470000	1.11492400
C	3.71522500	3.11370600	-1.78825500
C	4.46154800	2.55384300	-2.83350700
C	3.96414500	4.45978400	-1.49187300
C	5.39499700	3.28944500	-3.55890500
C	4.88756100	5.21853800	-2.20753900
C	5.60789100	4.62919800	-3.24348400
C	3.80224900	-1.80513400	3.29618900
C	3.98355500	-0.87505900	4.33386800
C	4.33358900	-3.08874900	3.50868400
C	4.65362800	-1.19736300	5.51062500
C	5.00337300	-3.43091200	4.67937200
C	5.16538000	-2.48073000	5.68493800
C	0.74790300	-3.95554400	-2.30038600
C	0.49614600	-3.57463000	-3.63383400
C	1.84150800	-4.82636700	-2.11347200
C	1.25925600	-4.03317300	-4.70205600
C	2.62609300	-5.28140700	-3.16706700
C	2.33244800	-4.88984600	-4.47130000
C	-5.73423800	-1.83357700	0.19769500
C	-6.35686400	-2.24723300	1.38035500
C	-6.55235000	-1.71908200	-0.93173400
C	-7.71897100	-2.52768600	1.44692400
C	-7.91390200	-2.01061000	-0.89720200
C	-8.50036500	-2.41345000	0.29979300
F	-1.98662400	7.24891000	2.41818200
F	-4.43478100	7.78304800	1.33793500
F	-5.68546800	5.91172100	-0.20303700
F	-4.50826700	3.53465500	-0.67111000
F	-0.80051300	4.87136300	1.97584700
F	5.09775700	6.50267300	-1.89550700
F	3.31090100	5.06060600	-0.48752700
F	6.49858800	5.34672800	-3.93238600
F	6.08172200	2.72166400	-4.55679700
F	4.27979600	1.26948800	-3.16998400
F	3.48394500	0.36271400	4.22904100
F	4.79462300	-0.28703000	6.48056900
F	5.80836900	-2.79881100	6.81018800
F	5.50643000	-4.66022000	4.83722500
F	4.23144600	-4.02746600	2.55948200
F	-0.49504800	-2.71374400	-3.91882100
F	0.98068500	-3.63517300	-5.94894500
F	3.07280000	-5.33190500	-5.49025000
F	3.64698000	-6.11449500	-2.93723800
F	2.15282400	-5.26075000	-0.88472700
F	-6.02586300	-1.33258200	-2.10448800
F	-8.65993900	-1.89639200	-2.00130000
F	-9.80565100	-2.68843300	0.34837800
F	-8.27678400	-2.91496700	2.59918200

F	-5.63713400	-2.36261400	2.50838200
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2e (T0^{A,D})

Sum of electronic and zero-point Energies=	-4873.146197
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C	-0.82402600	-2.59284000	-0.53158100
C	-0.52335400	-1.62255000	-1.49013400
C	-1.69728200	-0.88479300	-1.73756400
C	-2.71224900	-1.39693600	-0.92888900
N	-2.16325700	-2.44178700	-0.22228200
C	-0.00189500	-3.62634000	0.06279800
C	-4.06716000	-0.84211900	-0.71708100
C	1.36985700	-3.51742800	0.18139100
N	2.14214900	-2.37800100	-0.02291400
C	3.48580100	-2.66976300	0.06947200
C	3.57276300	-4.08991500	0.34877700
C	2.31280000	-4.58695300	0.44050000
C	4.52342500	-1.76689000	-0.11579600
C	4.31699100	-0.36103800	-0.33932900
N	3.13977800	0.25350700	-0.17342400
C	3.36302000	1.59698300	-0.46806800
C	4.74922800	1.78394700	-0.89317400
C	5.35371000	0.57890900	-0.77692500
C	2.43371400	2.60701000	-0.29708800
C	-4.13676400	0.45512500	-0.27729900
N	-3.01673300	1.17835500	0.08448500
C	-3.32013400	2.45978000	0.49963800
C	-4.77520700	2.55414100	0.38849500
C	-5.25766200	1.36813600	-0.05850300
C	-2.35782600	3.35820200	0.88567300
C	-0.97368200	2.84303600	0.97596000
N	0.07339700	3.24741300	0.18637300
C	1.16879500	2.41602800	0.36933200
C	0.80808400	1.48895600	1.35313300
C	-0.51640000	1.76020800	1.73387300
H	0.42959500	-1.50136800	-1.98317600
H	-1.81599400	-0.06934000	-2.43694200
H	1.83301300	-1.41218200	-0.10882200
H	4.49761400	-4.63758000	0.45077800
H	2.03142600	-5.61585100	0.60967000
H	5.20107500	2.71464500	-1.20408600
H	6.38579000	0.34028900	-0.98869600
H	-2.07759200	0.81261800	0.03812800
H	-5.35111600	3.43220900	0.64111200
H	-6.29241300	1.11976000	-0.24340100
H	1.47156100	0.73751100	1.75002400
H	-1.09627400	1.24605900	2.48738800
H	-0.02529900	3.92063200	-0.55722300
H	-2.66621600	-2.97352500	0.47066200
C	-2.69250900	4.74915100	1.27633400
C	-2.11005200	5.85788100	0.64830400
C	-3.58325500	5.03740600	2.32109800
C	-2.37483600	7.16868800	1.02900400
C	-3.87912200	6.34025800	2.71418500
C	-3.26752200	7.41238500	2.07011000
C	2.78335600	3.99504500	-0.74056200
C	2.13770500	4.61689200	-1.81258000
C	3.75893000	4.75190300	-0.07958200
C	2.44033900	5.91007700	-2.22776300
C	4.09098100	6.04445300	-0.48020300
C	3.43010600	6.62596500	-1.55926800
C	5.91973700	-2.28876700	-0.06207800
C	6.71891900	-2.38322800	-1.20765600
C	6.49984500	-2.71113300	1.14042500
C	8.02668700	-2.85993800	-1.16727800
C	7.80072000	-3.20514500	1.20582000
C	8.56823900	-3.27658700	0.04632800
C	-0.67256900	-4.86551900	0.52982200
C	-0.52461600	-5.35036300	1.84009300
C	-1.52291200	-5.60249700	-0.31282800
C	-1.16769100	-6.50326600	2.28391600
C	-2.18292000	-6.75046500	0.11405600
C	-2.00244100	-7.20556800	1.41862800
C	-5.28240800	-1.62282800	-1.05569200

C	-6.20013400	-1.19226400	-2.02550200
C	-5.56541900	-2.85633900	-0.45500100
C	-7.32540300	-1.93572100	-2.37292700
C	-6.67276000	-3.62685400	-0.79092700
C	-7.56123300	-3.16222000	-1.75777000
F	-4.18560600	4.03877700	2.98607600
F	-4.73287300	6.56580200	3.71862200
F	-3.53895400	8.66497000	2.44260800
F	-1.79680500	8.19104200	0.38971200
F	-1.26953700	5.67774600	-0.39430300
F	1.15148100	3.96463100	-2.46342600
F	1.79411800	6.46128700	-3.25984500
F	3.73859900	7.86499500	-1.94649900
F	5.03424700	6.73248200	0.17085100
F	4.41361600	4.23881100	0.96945100
F	6.23016100	-1.99741200	-2.39595400
F	8.75902800	-2.93352200	-2.28522100
F	9.81863700	-3.74367700	0.09768100
F	8.31917700	-3.60220500	2.37396500
F	5.79541100	-2.65579000	2.27978200
F	0.24425000	-4.69525000	2.72085800
F	-1.00195900	-6.92825000	3.54112800
F	-2.62593500	-8.30890400	1.83568400
F	-2.97375000	-7.42845900	-0.72433000
F	-1.70826800	-5.21388000	-1.58098400
F	-4.75663500	-3.33424000	0.51855300
F	-6.89918400	-4.79349600	-0.17831600
F	-8.63398500	-3.88486600	-2.08646100
F	-8.17053900	-1.48601400	-3.30656900
F	-6.00984500	-0.02525300	-2.66081700

2e' (T0^{A,D})

Sum of electronic and zero-point Energies= -4873.143737

C	-2.07180500	-2.52933400	-1.04015500
C	-1.50485200	-1.73288100	-2.04199600
C	-1.94201100	-0.41039800	-1.85603100
C	-2.80147100	-0.39720000	-0.75655700
C	-3.55589400	0.67815400	-0.17208700
C	-3.15359100	2.00350800	-0.20499200
N	-1.87732300	2.46011700	-0.53350300
C	-1.94544300	3.79516900	-0.45729300
C	-0.82520600	4.69370500	-0.55103500
C	0.50605600	4.30332200	-0.53127900
C	1.66643300	5.16418500	-0.39874600
C	2.76277100	4.38450300	-0.23262200
C	2.36494300	2.99495000	-0.32515700
C	3.20081100	1.89692000	-0.27641500
C	2.81153100	0.59265300	-0.77459300
C	2.04290800	0.25492900	-1.88698900
C	2.05632600	-1.14841200	-2.00453700
C	2.81144500	-1.67048400	-0.95053200
C	2.96862000	-3.08257700	-0.56084300
C	1.82931400	-3.85230300	-0.50981700
C	1.59780500	-5.26420700	-0.22218900
C	0.25927200	-5.50057800	-0.23766800
C	-0.43529800	-4.25166100	-0.53342700
C	-1.76833800	-3.91245600	-0.64422700
N	-2.89076700	-1.70666600	-0.30461400
C	-4.03463400	3.13270900	0.07585300
C	-3.29821000	4.25018600	-0.11738700
N	0.98574500	3.00964600	-0.53547500
N	3.28434600	-0.59073300	-0.23760100
N	0.57007500	-3.32433100	-0.70369300
F	-0.26452200	6.49376800	1.62883400
F	-0.84795500	9.12422200	1.56843100
F	-2.04199200	10.21734500	-0.63040500
F	-2.64006700	8.64460300	-2.77977500
F	-2.04603400	6.01143300	-2.73945500
F	3.83647700	3.04938500	2.28267600
F	6.33968300	3.27789700	3.22278200
F	8.45653100	2.38358000	1.74921800
F	8.03023700	1.26460400	-0.70416300
F	5.53792200	1.06227400	-1.68800400
F	4.71161100	-2.24502000	1.57392800

F	7.15722100	-3.27486400	1.97502000
F	8.08697300	-5.29926200	0.38885000
F	6.52428800	-6.26132500	-1.63372400
F	4.09017900	-5.21653500	-2.08693200
F	-1.88288800	-5.56128800	1.73455500
F	-3.92850700	-7.20498400	2.27760900
F	-6.06820300	-7.36486300	0.58635200
F	-6.11364900	-5.85365300	-1.68888700
F	-4.05205400	-4.23533100	-2.28546400
F	-5.67070700	-0.71245200	-1.48864800
F	-7.98746900	-1.39187800	-0.29690400
F	-8.43585500	-0.72836900	2.31162900
F	-6.52619500	0.61292500	3.72501500
F	-4.19700800	1.28035100	2.56448300
C	-1.12250100	6.15619400	-0.56005400
C	-0.84139200	6.99374400	0.52611000
C	-1.13638900	8.35536000	0.51146300
C	-1.74945600	8.91426700	-0.60674000
C	-2.05516100	8.10941100	-1.70169800
C	-1.73929500	6.75388600	-1.66676700
C	4.57888600	2.05318600	0.24982800
C	4.84281600	2.61793600	1.50982300
C	6.13446400	2.73827800	2.01643300
C	7.21557700	2.27570600	1.27094100
C	6.99426900	1.69979700	0.02156900
C	5.69768900	1.59961400	-0.47187300
C	4.30350600	-3.67490300	-0.28970600
C	5.13781800	-3.22234500	0.73938300
C	6.40497300	-3.74431500	0.97433000
C	6.87732400	-4.77970700	0.17146700
C	6.07575000	-5.27112000	-0.85547400
C	4.81709900	-4.71704400	-1.07658100
C	-2.86832400	-4.83675800	-0.31361400
C	-2.89395300	-5.62439300	0.85065500
C	-3.95084900	-6.47743600	1.15468600
C	-5.04729000	-6.55372200	0.30009100
C	-5.07002100	-5.77699400	-0.85653700
C	-3.99594100	-4.94356800	-1.15001800
C	-4.84422100	0.32147500	0.48407900
C	-5.84737200	-0.38018600	-0.20476700
C	-7.05115400	-0.73576200	0.39615800
C	-7.28467800	-0.39343200	1.72666500
C	-6.31112800	0.29720800	2.44354400
C	-5.11172600	0.64233000	1.82443400
H	-5.08245500	3.06918400	0.33322600
H	-3.61609700	5.27687800	-0.00578900
H	1.63324300	6.24277100	-0.41615400
H	3.78398200	4.71402000	-0.11076000
H	1.59001400	0.96149800	-2.56700300
H	1.60657700	-1.73565200	-2.79143200
H	2.37760600	-5.98614100	-0.02813500
H	-0.22972000	-6.44623300	-0.05745600
H	-1.71076500	0.45479300	-2.45738600
H	0.34773900	2.21772700	-0.53273200
H	3.79087400	-0.67146400	0.63078200
H	-3.33883300	-1.97928900	0.55707800
H	0.39905600	-2.34195800	-0.85891200
H	-0.87274500	-2.10008300	-2.83698100

2f($T0^{4,D}$)

Sum of electronic and zero-point Energies= -4873.133503

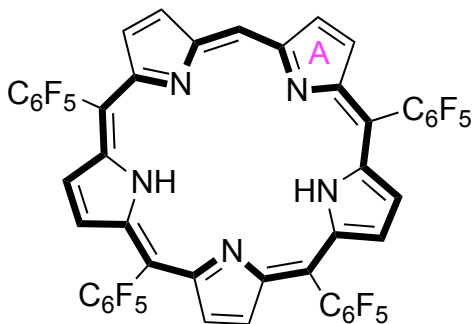
C	3.38402300	-2.70303800	0.64817700
N	2.21787800	-2.01414300	0.97263400
C	1.44868700	-2.86639000	1.63837200
C	0.10380900	-2.39625100	2.02078500
C	-1.02800400	-2.96901900	1.50610800
N	-2.26285600	-2.33936000	1.40452300
C	-3.17053800	-3.09319300	0.65894900
C	-4.30222400	-2.57304900	0.07244100
C	-4.45416000	-1.13681700	-0.14085500
C	-5.56357200	-0.30637300	-0.32971800
C	-5.09782000	0.98159200	-0.66425800
C	-3.70072000	0.94178500	-0.70201900
C	-2.69544500	1.96054000	-0.96242700

C	-1.46191400	1.62758800	-1.48621500
N	-0.30500600	2.39880100	-1.35418700
C	0.82122200	1.64909100	-1.67268100
C	2.13276700	2.04736600	-1.47326700
C	3.20054400	1.05988300	-1.39931400
C	4.53532500	1.12002900	-1.85341900
C	5.16106200	-0.07449800	-1.49936100
C	4.22093700	-0.86675000	-0.80354300
C	4.36163600	-2.13755200	-0.16699000
C	3.31505400	-4.04608800	1.18727800
C	2.09404100	-4.15471000	1.79858900
C	-2.50611000	-4.36961700	0.44530600
C	-1.22260700	-4.27073800	0.87786500
N	-3.34271700	-0.34603900	-0.36659100
C	-1.03441200	0.40690000	-2.14133900
C	0.32268400	0.40890700	-2.23037900
N	3.04164900	-0.14749600	-0.78286500
H	1.69296000	-5.00596100	2.33237400
H	4.07521200	-4.81031000	1.10020000
H	6.18412900	-0.35380300	-1.70536000
H	4.96632600	1.94226800	-2.40617600
H	0.95016200	-0.34212000	-2.68779300
H	-1.70929900	-0.34303100	-2.52845400
H	-5.70315400	1.85148300	-0.87530300
H	-6.59409100	-0.60905900	-0.21812100
H	-2.94568300	-5.20535500	-0.07825100
H	-0.44507000	-5.01514700	0.78792600
C	5.62726400	-2.88520400	-0.40880200
C	6.50037600	-3.20516100	0.63888800
C	7.68559500	-3.90430200	0.42329800
C	8.02567800	-4.30364500	-0.86662900
C	7.17965800	-4.00071400	-1.93093900
C	6.00013200	-3.30034500	-1.69378700
C	2.47736000	3.46746200	-1.25841200
C	3.32427200	3.88140000	-0.21370600
C	3.69163600	5.21065500	-0.03267100
C	3.20096600	6.18775600	-0.89605000
C	2.35070200	5.82164700	-1.93670100
C	2.00840600	4.48408400	-2.11142800
C	-2.96965600	3.34379800	-0.51148400
C	-2.85269400	4.44313800	-1.37750900
C	-3.13302900	5.74375900	-0.96691300
C	-3.54536600	5.97984500	0.34250700
C	-3.66583400	4.91426200	1.23273200
C	-3.37170500	3.62404600	0.80495700
C	-5.32594900	-3.47570900	-0.52848500
C	-6.61008900	-3.57201900	0.01892300
C	-7.60070100	-4.37636600	-0.53748000
C	-7.31570100	-5.12703600	-1.67548200
C	-6.04855000	-5.05728300	-2.24827100
C	-5.08126600	-4.23170700	-1.68014500
F	6.22081600	-2.82622900	1.89137500
F	8.50014300	-4.18696400	1.44511100
F	9.15810000	-4.97545500	-1.08235900
F	7.49862100	-4.39193300	-3.16930400
F	5.20477600	-3.04488300	-2.74077600
F	3.79114400	2.98551100	0.66687200
F	4.49397500	5.55923300	0.97937200
F	3.54080200	7.46719600	-0.72458200
F	1.88614100	6.75366200	-2.77623100
F	1.21169400	4.17875500	-3.14397100
F	-2.47237900	4.25722100	-2.64769500
F	-3.02097600	6.76375200	-1.82442900
F	-3.81824500	7.22249500	0.74561400
F	-4.03979700	5.14161600	2.49659800
F	-3.46212100	2.63323300	1.70319100
F	-6.92214500	-2.85643400	1.11139600
F	-8.81620000	-4.43895800	0.01694600
F	-8.25362100	-5.90894900	-2.21527500
F	-5.77127800	-5.77157300	-3.34512800
F	-3.87645900	-4.18491700	-2.27297400
H	-2.38775300	-0.66148300	-0.29776800
H	2.27026000	-0.47403500	-0.19329000
C	0.04009500	-1.07380400	2.70702900
C	0.28623200	-0.96325000	4.08122000
C	-0.22227400	0.11740000	2.03076100
C	0.25974700	0.26358500	4.74158900

C	-0.26330600	1.35642600	2.66020000
C	-0.01868700	1.42881800	4.02877200
F	0.55165900	-2.05973900	4.80055700
F	-0.42693600	0.07754700	0.69809800
F	-0.51245400	2.47591900	1.95965500
F	-0.04897200	2.60698500	4.65421700
F	0.48918200	0.33119800	6.05655500
H	-0.25535800	3.13883400	-0.66936900
H	-2.47596700	-1.43599700	1.79486300

tetrakis(pentafluorophenyl)-substituted pentaphyrins (8)

22PP



1a (T0)

Sum of electronic and zero-point Energies= -4144.781325

C	-1.05532400	-3.73106800	-1.96997300
N	-1.50563000	-2.77907200	-1.13353700
C	-2.60646700	-3.33156700	-0.52425600
C	-3.48665000	-2.61498000	0.29124100
C	-3.51322900	-1.20705600	0.39712700
C	-4.60824400	-0.42712600	0.86564200
C	-4.38833100	0.87311300	0.47683700
C	-3.12079900	0.93310900	-0.17226400
C	-2.54844300	2.11973200	-0.71152000
C	-1.19768600	2.44781700	-0.82517900
N	-0.15448400	1.73052300	-0.27629800
C	0.87450200	2.59546400	-0.24581300
C	2.12738600	2.40086100	0.41619100
C	2.82483000	1.20999200	0.60214000
C	4.04163200	1.07280800	1.36795100
C	4.57957400	-0.14709400	1.10695200
C	3.72750500	-0.81791000	0.15866600
C	4.03791300	-1.96955200	-0.56020000
C	3.17583000	-2.57997200	-1.51552000
N	1.84085100	-2.41283700	-1.54428000
C	1.40322600	-3.24861100	-2.54297100
C	0.13461800	-3.77328600	-2.74002500
C	0.53883300	3.87278800	-0.88495700
C	-0.74511700	3.76300700	-1.28566600
N	2.63639600	0.00359800	-0.04253600
C	2.53865400	-3.86691200	-3.23971500
C	3.64628400	-3.48845700	-2.56547000
N	-2.60925100	-0.33870900	-0.17381500
C	-1.90359600	-4.92558900	-1.93256000
C	-2.83027100	-4.70303000	-0.97087500
H	1.21148000	4.70677900	-1.02694400
H	-1.33976400	4.49315100	-1.81484700
H	1.85012000	-0.26096600	-0.62860000
H	5.49101700	-0.56100800	1.51026200
H	4.43529000	1.83333900	2.02458300
H	2.46186800	-4.54341500	-4.08120400
H	4.67400600	-3.76415000	-2.75513900
H	-1.75808600	-0.67280300	-0.62404600
H	-5.47139700	-0.81793100	1.38253700
H	-5.02790100	1.72417400	0.65447400
H	-1.75374900	-5.81948900	-2.52400300
H	-3.60892000	-5.36958800	-0.62997200
C	5.38510900	-2.57720900	-0.36389500

C	5.51767800	-3.88519600	0.12297600
C	6.57117200	-1.90237200	-0.68251300
C	6.75960100	-4.49029900	0.29607100
C	7.82461900	-2.48509300	-0.51205300
C	7.91802700	-3.78542900	-0.02214200
C	2.77586300	3.64488200	0.93031100
C	2.14321300	4.43983800	1.89705100
C	4.01188600	4.10229600	0.45213200
C	2.70907900	5.61919400	2.37404000
C	4.59779500	5.27728400	0.91595000
C	3.94211300	6.03894900	1.88043200
C	-4.57976300	-3.35257900	0.99865200
C	-4.49637100	-3.60105800	2.37234300
C	-5.72313200	-3.80909300	0.33636300
C	-5.49782000	-4.28232800	3.06055700
C	-6.73557500	-4.49607600	1.00223600
C	-6.62135700	-4.73127300	2.37051400
C	-3.55736900	3.16327200	-1.07935500
C	-4.42887900	2.95966500	-2.15685600
C	-3.70362300	4.35797700	-0.36383300
C	-5.38779400	3.90035400	-2.52235300
C	-4.65774400	5.31259300	-0.70948100
C	-5.50191900	5.08182200	-1.79302900
F	6.84773400	-5.73708400	0.77157200
F	9.11410900	-4.35409200	0.14227900
F	8.93558300	-1.81045300	-0.82844200
F	6.52572700	-0.65741200	-1.17671500
F	4.42796400	-4.59052400	0.44805700
F	4.66637800	3.41197200	-0.49151800
F	5.77651300	5.68471500	0.43233600
F	4.49465600	7.16697900	2.33087900
F	2.08168400	6.34619300	3.30446800
F	0.96288600	4.06543300	2.40257900
F	-2.92575100	4.60883900	0.69594900
F	-4.77503800	6.44137700	-0.00200300
F	-6.41827800	5.99066700	-2.13159100
F	-4.34335600	1.83643500	-2.88039800
F	-6.19457000	3.67955200	-3.56543700
F	-5.38680200	-4.50757600	4.37377000
F	-7.58693300	-5.38628100	3.01864800
F	-7.81602100	-4.92277600	0.33951200
F	-5.86739400	-3.59293800	-0.97771600
F	-3.42929300	-3.18157000	3.06299300
H	0.10401700	-4.53530400	-3.51625300

1c ($T0^A$)

Sum of electronic and zero-point Energies= -4144.772642

C	0.37309200	-3.90557000	0.66576800
N	1.71406300	-4.08491400	0.59707500
C	2.23505700	-2.93818700	1.10447900
C	3.58177000	-2.58978800	0.88509800
C	3.93489400	-1.24372900	0.66121600
C	5.22831400	-0.65407100	0.55521800
C	5.07142600	0.65890100	0.18166300
C	3.67197400	0.91303100	0.03764300
C	3.04424200	2.09264400	-0.41334200
C	1.66792500	2.36940700	-0.45588100
N	0.63139800	1.58211100	0.02029900
C	-0.46166000	2.38250000	-0.01836600
C	-1.81199200	2.20400900	0.46037300
C	-2.74405500	1.15452500	0.49632000
C	-4.12004300	1.37290500	0.88846800
C	-4.85932400	0.28874100	0.53744100
C	-3.97981700	-0.69742900	-0.01331800
C	-4.39240000	-1.95808400	-0.47362800
C	-3.53552100	-3.06878000	-0.66514500
N	-2.25575200	-3.04881800	-0.25683800
C	-1.77350700	-4.30959700	-0.47228800
C	-0.50027300	-4.71544100	-0.07958200
C	1.17817600	3.66505600	-0.90552800
C	-0.13342400	3.69361400	-0.59827800
N	3.02447900	-0.24487300	0.36562200
C	0.02516600	-2.69624300	1.41920700
C	1.19982200	-2.07747400	1.68120000

N	-2.70442900	-0.14889400	0.01463500
C	-2.78357300	-5.14302500	-1.12044000
C	-3.89712500	-4.37501600	-1.22490500
H	6.15503000	-1.17138200	0.75443400
H	5.85123900	1.38837800	0.02462700
H	-4.48722400	2.26687100	1.36376900
H	-5.91960800	0.14895100	0.68198000
H	1.76136300	4.43963900	-1.38015200
H	-0.82960800	4.49456800	-0.79266900
H	2.01503300	-0.33468000	0.30197600
H	-0.97301100	-2.40082700	1.69725900
H	1.36269900	-1.17694700	2.25749800
H	-1.88389400	-0.67806900	-0.25633600
H	-2.65392800	-6.17586700	-1.41634000
H	-4.85574600	-4.64935100	-1.64236900
C	4.58703100	-3.66131600	0.71467200
C	5.39856400	-3.77262800	-0.42400800
C	4.72982500	-4.66070400	1.69006400
C	6.31556900	-4.80790500	-0.57986900
C	5.64072500	-5.70250200	1.55351500
C	6.43637500	-5.77710000	0.41250700
C	3.98555200	3.16572400	-0.86995600
C	4.22784700	4.31034800	-0.10329400
C	4.67780300	3.05329900	-2.08052900
C	5.10856000	5.30541200	-0.52096600
C	5.56511600	4.03377200	-2.51826300
C	5.77973100	5.16446500	-1.73353300
C	-2.37367100	3.51375400	0.96133100
C	-1.94319000	4.03592800	2.18570200
C	-3.29493600	4.27902300	0.23778200
C	-2.41209900	5.25194400	2.67860000
C	-3.77490300	5.49938300	0.70535100
C	-3.33106200	5.98615300	1.93354700
C	-5.85286100	-2.14747300	-0.70376200
C	-6.60053000	-3.08565600	0.02120900
C	-6.54331400	-1.40595800	-1.67251500
C	-7.95989100	-3.28457000	-0.20576600
C	-7.90313400	-1.58413000	-1.91307300
C	-8.61341200	-2.52944700	-1.17687800
F	-8.52734900	-0.86166200	-2.84918200
F	-9.91652200	-2.70940800	-1.39944000
F	-8.64293200	-4.18397000	0.51019000
F	-6.01409400	-3.81753200	0.97707300
F	-5.89309100	-0.49576200	-2.40911100
F	-1.06053900	3.35760000	2.92830400
F	-1.98780600	5.71576200	3.85848800
F	-3.72810500	3.84934500	-0.95621800
F	-3.78667600	7.15303900	2.39349100
F	-4.65030900	6.20810400	-0.01624400
F	4.49325300	1.97861000	-2.85790800
F	6.20714900	3.89844000	-3.68312200
F	3.60283100	4.47617100	1.06899400
F	5.31724600	6.38832400	0.23509300
F	6.62705900	6.11082700	-2.14226500
F	5.29330600	-2.88648200	-1.42379500
F	7.06766300	-4.88571000	-1.68354600
F	7.31409900	-6.77219500	0.27291400
F	5.76284300	-6.62705400	2.51191800
F	3.99926200	-4.61644800	2.80892000
H	-0.11927200	-5.66987900	-0.43178300

1d ($T0^D$)

Sum of electronic and zero-point Energies= -4144.785313

C	1.35881000	-4.09868500	-0.07524100
N	2.03818900	-2.91481900	-0.11562100
C	3.36396400	-3.25696300	-0.01534200
C	4.45910400	-2.36348500	-0.00572600
C	4.36213500	-0.97106500	-0.13431900
C	5.39875400	0.02017100	-0.12418200
C	4.80611900	1.25023100	-0.24632700
C	3.39221100	1.05397300	-0.37601300
C	2.38065600	2.00885100	-0.55173200
C	1.07469100	1.63722500	-0.92532300
N	-0.00009200	2.40627500	-0.63390400

C	-1.07475600	1.63715200	-0.92548300
C	-2.38083500	2.00868800	-0.55213400
C	-3.39227900	1.05369900	-0.37642200
C	-4.80623600	1.24980000	-0.24684000
C	-5.39872000	0.01970100	-0.12450500
C	-4.36197300	-0.97142200	-0.13445100
C	-4.45881700	-2.36382500	-0.00567800
C	-3.36359100	-3.25721600	-0.01525800
N	-2.03786800	-2.91497700	-0.11563200
C	-1.35838600	-4.09880000	-0.07520800
C	0.00022100	-4.49359900	-0.08511700
C	3.54271900	-4.70026000	0.09492200
C	2.30261900	-5.22285600	0.04233500
N	3.17761400	-0.30620000	-0.29186700
C	-0.67580800	0.38722900	-1.58257600
C	0.67592400	0.38728900	-1.58251100
C	-3.54224300	-4.70052700	0.09507700
C	-2.30210600	-5.22303200	0.04249400
N	-3.17752800	-0.30643600	-0.29201500
H	4.48225600	-5.22116300	0.20168800
H	2.01825900	-6.26567500	0.09381400
H	2.29333800	-0.81228900	-0.22950500
H	5.29705000	2.21075200	-0.28846300
H	6.45464300	-0.18958800	-0.04261600
H	-1.32577800	-0.34149400	-2.04388300
H	1.32599700	-0.34139300	-2.04373500
H	-4.48173900	-5.22150100	0.20184200
H	-2.01765100	-6.26582200	0.09404400
H	-5.29726600	2.21026100	-0.28914500
H	-6.45458200	-0.19019000	-0.04292900
H	-2.29319800	-0.81243200	-0.22966800
C	2.66623300	3.44145400	-0.24928500
C	2.17103700	4.05462200	0.90635700
C	3.39989700	4.23671300	-1.13224400
C	2.39103500	5.40501600	1.16697300
C	3.63984200	5.58604700	-0.88727800
C	3.12705000	6.17207400	0.26683700
C	-2.66662800	3.44130000	-0.24994500
C	-3.40030700	4.23630900	-1.13312700
C	-2.17160400	4.05473100	0.90563000
C	-3.64043100	5.58565800	-0.88841600
C	-2.39177400	5.40514900	1.16597800
C	-3.12779900	6.17195100	0.26563100
C	-5.83794700	-2.92093600	0.14384500
C	-6.46062700	-3.62310000	-0.89403700
C	-6.57090800	-2.75110400	1.32330000
C	-7.74652700	-4.14259200	-0.76782700
C	-7.86099900	-3.25549800	1.47093600
C	-8.44953000	-3.95520700	0.42021600
C	5.83828900	-2.92050800	0.14363000
C	6.57135400	-2.75077700	1.32303200
C	6.46090800	-3.62249900	-0.89440900
C	7.86149700	-3.25509100	1.47046900
C	7.74685900	-4.14191500	-0.76839400
C	8.44996800	-3.95463300	0.41960100
F	3.90684500	3.69660200	-2.25317300
F	4.35166600	6.31836500	-1.75226500
F	3.34798500	7.46558500	0.51445700
F	1.90952000	5.96749600	2.28054600
F	1.48044100	3.34603800	1.80280800
F	-1.48101400	3.34638300	1.80227200
F	-1.91041800	5.96790300	2.27947700
F	-3.34889700	7.46548700	0.51298800
F	-4.35225200	6.31775300	-1.75359700
F	-3.90706400	3.69594100	-2.25400700
F	-5.81476500	-3.81688200	-2.05118000
F	-6.03426100	-2.08497700	2.35437200
F	-8.53335700	-3.07617600	2.61252700
F	-9.68416200	-4.44420400	0.55095300
F	-8.31120200	-4.80975100	-1.77951500
F	5.81495700	-3.81616300	-2.05151700
F	8.31147700	-4.80890500	-1.78022500
F	9.68464700	-4.44356000	0.55015400
F	8.53396400	-3.07587100	2.61201100
F	6.03476000	-2.08481800	2.35424200
H	0.00026300	-5.57919900	-0.05157600

1e ($TO^{4,D}$)

Sum of electronic and zero-point Energies= -4144.810710

C	3.49756800	-3.09622800	0.24006600
N	2.27969400	-2.52344600	0.31664500
C	1.34656700	-3.51292000	0.40412000
C	0.03091300	-3.04258300	0.41773600
C	-1.27603600	-3.53708400	0.36814100
N	-2.22182100	-2.56739100	0.22843100
C	-3.43152100	-3.16141100	0.16414000
C	-4.60554600	-2.37849200	-0.01496500
C	-4.52850200	-0.97641100	-0.18663900
C	-5.54291900	0.02329000	-0.38871100
C	-4.92173700	1.24625100	-0.47293100
C	-3.50250800	1.03860300	-0.36104400
C	-2.42815400	1.95790600	-0.42016200
C	-1.09380900	1.54207300	-0.66491200
N	-0.01758800	2.29385500	-0.32190700
C	1.07313000	1.55883400	-0.65503800
C	2.39742300	1.99345600	-0.38794100
C	3.48806300	1.09509900	-0.32383300
C	4.90546900	1.33833800	-0.37194500
C	5.55291300	0.13011600	-0.27859500
C	4.55588000	-0.89786400	-0.14160800
C	4.65964600	-2.29575500	0.05124300
C	3.35141400	-4.55233800	0.30974300
C	2.01425100	-4.80794100	0.40397000
C	-3.26384700	-4.61092500	0.29625300
C	-1.92353200	-4.84161800	0.40930400
N	-3.33203700	-0.30652500	-0.18688700
C	-0.67502700	0.29981400	-1.32424500
C	0.67951100	0.31119500	-1.31965200
N	3.34351900	-0.25832600	-0.18946500
H	1.53558800	-5.77596000	0.46608500
H	4.15214400	-5.27829900	0.26999800
H	6.62006400	-0.03354400	-0.30093400
H	5.35964100	2.30978400	-0.50188600
H	1.33833400	-0.40998600	-1.78025700
H	-1.31829700	-0.43362300	-1.78751700
H	-5.39251300	2.20341100	-0.64361700
H	-6.60236600	-0.17030400	-0.47002100
H	-4.05287500	-5.35032200	0.29585400
H	-1.43145500	-5.79842100	0.52076400
H	0.02141400	-1.95739800	0.39220500
C	6.00199000	-2.92894400	0.04955900
C	6.45838500	-3.67882600	1.14336800
C	7.70965200	-4.28902100	1.15448100
C	8.55104600	-4.15631900	0.05251300
C	8.13204900	-3.41730000	-1.05108900
C	6.87388300	-2.82157900	-1.04328800
C	2.62993900	3.43031600	-0.11595600
C	3.30686900	3.86868400	1.03199700
C	3.49940600	5.21840800	1.31078500
C	3.00374200	6.17887000	0.43359700
C	2.32355200	5.78089100	-0.71521100
C	2.14327600	4.42677600	-0.97786200
C	-2.69219700	3.39324400	-0.17431300
C	-2.20093500	4.38731900	-1.03690300
C	-2.41325700	5.74114400	-0.79795600
C	-3.13192000	6.14155400	0.32632900
C	-3.63377600	5.18382700	1.20306800
C	-3.40901400	3.83432000	0.94852600
C	-5.94137000	-3.02972400	-0.02740900
C	-6.92367000	-2.71366700	0.92092700
C	-8.17669600	-3.32102600	0.92144500
C	-8.47670400	-4.28120600	-0.04171400
C	-7.52348400	-4.62171800	-0.99844800
C	-6.27988000	-3.99606700	-0.98408400
F	5.68836600	-3.81734000	2.23071300
F	8.11244200	-4.98930200	2.21966300
F	9.75330100	-4.73452200	0.05431400
F	8.93218700	-3.29533200	-2.11541600
F	6.50379200	-2.13669900	-2.13500600
F	3.77356900	2.98181100	1.92342100
F	4.14413300	5.59609300	2.42091900

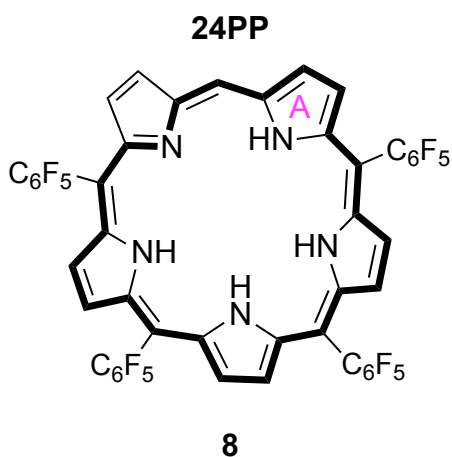
F	3.18364000	7.47621400	0.68983200
F	1.85975900	6.70326700	-1.56536700
F	1.51101300	4.09630200	-2.10721700
F	-1.53407800	4.05426500	-2.14535400
F	-1.94443500	6.66061600	-1.64845600
F	-3.34285500	7.43853200	0.55929000
F	-4.31566800	5.56449500	2.28959500
F	-3.88322100	2.95111500	1.83920800
F	-6.66957800	-1.80596800	1.87353600
F	-9.08636900	-2.99645800	1.84584800
F	-9.67293900	-4.87211300	-0.04864200
F	-7.81162000	-5.53544100	-1.93109800
F	-5.39680800	-4.34013600	-1.93216700
H	-2.48296100	-0.85995900	0.01905400
H	2.50625900	-0.82733000	0.02490300

1f ($TO^{A,D}$)

Sum of electronic and zero-point Energies= -4144.789951

C	0.39127100	-3.66380300	0.42710800
N	1.70259300	-4.00495100	0.17967000
C	2.42550200	-2.99204200	0.67456300
C	3.82606400	-2.80703500	0.38621100
C	4.25649900	-1.50349400	0.09358700
C	5.54189200	-0.85955500	-0.03171600
C	5.33741900	0.47351200	-0.28631900
C	3.91639800	0.70752900	-0.38237600
C	3.11364500	1.83024000	-0.63851400
C	1.71410800	1.61085800	-0.89743600
N	0.74488800	2.38933100	-0.39516800
C	-0.43200100	1.74397700	-0.67743900
C	-1.65987000	2.20660800	-0.17972400
C	-2.84631400	1.42986800	-0.12795800
C	-4.18226900	1.91613700	0.00151400
C	-5.04000700	0.84280000	-0.03753200
C	-4.25594300	-0.34320700	-0.16041300
C	-4.69084400	-1.68526100	-0.22061200
C	-3.83042900	-2.80029600	-0.24477400
N	-2.47757000	-2.71759600	-0.06874100
C	-2.00788400	-3.98261000	-0.22812400
C	-0.66041900	-4.39049800	-0.11601600
C	0.30262600	-2.45132100	1.23555900
C	1.57888100	-2.02915600	1.40430700
N	3.33928500	-0.51162900	-0.14373700
C	1.15203800	0.47092400	-1.63674200
C	-0.19462100	0.55582000	-1.49249400
N	-2.93902000	0.05727600	-0.21936300
C	-3.09270000	-4.90430800	-0.54808000
C	-4.23648500	-4.17477600	-0.52499700
H	-0.60981900	-2.03615400	1.63617300
H	1.93076200	-1.20423600	2.00964100
H	6.49396100	-1.35528000	0.08832000
H	6.09735300	1.22897900	-0.42171300
H	1.70534800	-0.23660500	-2.23963700
H	-0.94297600	-0.07346600	-1.95311400
H	-4.44747200	2.96054100	0.06950500
H	-6.11751600	0.87025300	0.02022700
H	-2.19560000	-0.64008700	-0.18553600
H	-2.97943200	-5.96464900	-0.73242900
H	-5.24469100	-4.51566900	-0.71236400
H	2.34082400	-0.66073900	-0.11658400
C	-6.16195500	-1.92132100	-0.27105700
C	-6.82471500	-2.60889300	0.75395800
C	-6.94634500	-1.47523900	-1.34236700
C	-8.19687500	-2.84399700	0.71979400
C	-8.32024500	-1.69492700	-1.39555800
C	-8.94720000	-2.38394900	-0.35986100
C	-1.72062300	3.59196300	0.35244000
C	-2.14402900	3.86158400	1.66080400
C	-1.31594200	4.69024900	-0.42008400
C	-2.17168700	5.15293200	2.17919200
C	-1.33616400	5.98861200	0.07905200
C	-1.76406800	6.22081000	1.38431600
C	4.71256900	-3.97389500	0.26100500
C	5.60756600	-4.14707100	-0.80809300

C	4.66868500	-5.01163000	1.20960100
C	6.41540300	-5.27308600	-0.92712000
C	5.46517400	-6.14641700	1.10608200
C	6.34349200	-6.27908300	0.03299600
C	3.62808300	3.20342300	-0.51427400
C	3.27324700	4.19009600	-1.45186800
C	4.45529000	3.61877900	0.54253800
C	3.71875600	5.50345700	-1.35191200
C	4.91377000	4.92694300	0.65817500
C	4.54331000	5.87487700	-0.29214200
F	5.69199300	-3.22656500	-1.78130900
F	7.24760200	-5.40105500	-1.96686800
F	7.11514300	-7.36219400	-0.07213700
F	5.40497200	-7.10311600	2.03818400
F	3.86470300	-4.91655400	2.27335800
F	-6.13981100	-3.05540600	1.81376700
F	-8.79727700	-3.49879200	1.71856700
F	-10.26257800	-2.60192000	-0.40205800
F	-9.03686200	-1.25837600	-2.43638100
F	-6.37748800	-0.81976900	-2.36345700
F	-2.52075500	2.85949600	2.46866000
F	-2.57577300	5.37087400	3.43599100
F	-1.78866700	7.46378700	1.86963700
F	-0.95669700	7.01567500	-0.68929400
F	-0.92203700	4.51785500	-1.68490200
F	2.50868000	3.87545100	-2.50206600
F	4.81386200	2.75530200	1.50576700
F	5.69433400	5.28169900	1.68521800
F	4.97986900	7.13132000	-0.19055500
F	3.37395100	6.40732900	-2.27453100
H	-0.40872900	-5.36602200	-0.52464900



2a (*T0*)

Sum of electronic and zero-point Energies= -4145.998912

C	0.45308200	-3.14393100	0.12567400
C	-0.22387000	-4.38814900	0.38278100
C	-1.54111100	-4.24311100	0.04741700
C	-1.76151000	-2.88612900	-0.38092300
N	-0.53303700	-2.26534600	-0.30136900
C	1.78730000	-2.78007500	0.21473400
C	-2.93869300	-2.25344400	-0.76557900
C	2.21612600	-1.58002400	-0.48047800
N	2.97811200	-0.60694800	0.10942600
C	3.28862800	0.39802200	-0.78401100
C	2.72572100	0.02354400	-2.01088500
C	2.03248500	-1.18148900	-1.81663700
C	3.99365800	1.57621300	-0.33200200
C	3.62510300	2.13307200	0.89254600
N	2.37185500	1.95213000	1.47324600
C	2.30201500	2.59906900	2.68737300
C	3.61721600	3.12735700	2.93971800
C	4.39493800	2.89611000	1.83882700
C	1.14973400	2.85586900	3.40863600
C	-3.10846300	-0.83259700	-0.81269000

N	-2.46044100	0.09987500	-0.01355400
C	-3.03213700	1.35447000	-0.18166500
C	-3.98417600	1.21593300	-1.22328400
C	-4.03917700	-0.11446700	-1.59469400
C	-2.88894600	2.46941700	0.68189100
C	-1.95797900	2.70186600	1.71289600
N	-0.68385200	2.18826800	1.84763000
C	-0.19748800	2.76350600	2.98139900
C	-1.20414000	3.57579600	3.64866200
C	-2.28048900	3.58871400	2.82669000
H	0.25849000	-5.28187300	0.75002400
H	-2.31849100	-4.98900700	0.12824100
H	3.23525300	-0.59195600	1.08432100
H	2.79496300	0.59350800	-2.92648300
H	1.50694300	-1.75681800	-2.56597800
H	3.89863500	3.65068600	3.84338900
H	5.43131600	3.16869300	1.69941800
H	-1.86069500	-0.11561900	0.77139700
H	-4.56544200	2.02603300	-1.63655500
H	-4.66535600	-0.55383900	-2.35725100
H	-1.06681400	4.10506200	4.58276500
H	-3.22058000	4.09995300	2.97571300
H	1.52407100	1.69125000	0.97960500
H	-0.32749700	-1.34959100	-0.67328900
C	-3.94873800	3.51561700	0.52243400
C	-3.62537100	4.80455900	0.07962600
C	-5.29575200	3.27008100	0.81920800
C	-4.58873900	5.79963200	-0.06989600
C	-6.27551300	4.24944200	0.67913900
C	-5.91871100	5.51985800	0.23256600
C	-4.10254700	-3.09117600	-1.14425900
C	-5.35492300	-2.94112400	-0.52584700
C	-4.01600400	-4.07299900	-2.14429000
C	-6.45748700	-3.71176400	-0.88220500
C	-5.10351700	-4.86228400	-2.50861700
C	-6.33066500	-4.67927200	-1.87657900
C	2.75740100	-3.55450500	1.00775500
C	4.05458000	-3.82078400	0.52574600
C	2.46996800	-4.04879600	2.29452700
C	4.99775400	-4.52613200	1.26538200
C	3.39469600	-4.77057300	3.04282500
C	4.66660200	-5.00979800	2.52930600
C	5.07687500	2.14762600	-1.14315500
C	5.21882000	3.53500700	-1.34206500
C	6.02182500	1.33401400	-1.79938600
C	6.23006500	4.07726900	-2.12854900
C	7.03122500	1.85764800	-2.59962800
C	7.14011000	3.23665500	-2.76437600
F	6.31882200	5.40212700	-2.29530300
F	4.34857400	4.39215200	-0.78869900
F	8.11193700	3.74850300	-3.52347300
F	7.91432900	1.04555800	-3.19213700
F	5.99025900	0.00347900	-1.64294700
F	4.41525000	-3.40242600	-0.69411100
F	1.27700200	-3.81077800	2.86245600
F	3.07540300	-5.21388400	4.26434200
F	5.56206600	-5.69578300	3.24318400
F	6.21335400	-4.76329100	0.76052600
F	-2.86294100	-4.26935100	-2.80020700
F	-5.51588000	-2.04585100	0.45626800
F	-7.63079500	-3.54436800	-0.26223200
F	-7.38026800	-5.42873200	-2.22048100
F	-4.98044600	-5.78241500	-3.47227000
F	-2.36045500	5.11091600	-0.23187000
F	-4.24630300	7.01761600	-0.50539100
F	-6.85044200	6.46635800	0.09500200
F	-7.55191600	3.98353400	0.98105200
F	-5.67601200	2.06784500	1.27096500
H	1.30420700	3.39431200	4.33862600

2b (TI)

Sum of electronic and zero-point Energies= -4145.990062

C	2.21230300	-3.34397100	-0.29496400
C	1.41605500	-4.39914200	0.18059900

C	0.33692400	-4.54417800	-0.69821300
C	0.50678800	-3.62221900	-1.75033400
C	-0.30357100	-3.47277300	-2.94883900
C	-1.61489400	-3.11030700	-2.83275600
C	-2.73283200	-3.18825900	-3.75209000
C	-3.86110400	-2.78138200	-3.10409300
C	-3.49718000	-2.33464400	-1.77313500
C	-4.23567500	-1.71605200	-0.78108800
C	-3.61561200	-0.91788200	0.25127200
C	-4.06743900	-0.58746400	1.53772300
C	-3.25943500	0.43428900	2.03472200
C	-2.29807300	0.76287200	1.05954600
C	-1.51446600	1.96224800	0.99314300
C	-0.38997800	2.28325100	0.22684500
C	-0.06579300	3.62482900	-0.18665300
C	1.09140000	3.60203900	-0.90237200
C	1.60530500	2.25801900	-0.88592300
C	2.91235400	1.88043400	-1.19102500
C	3.49230900	0.61680400	-0.85547600
N	2.79134800	-0.50073500	-0.59524700
C	3.70810400	-1.40483400	-0.07513000
C	3.38247500	-2.72308600	0.24134000
N	-2.13867700	-2.55696000	-1.67090000
N	-2.48218700	-0.13872300	0.01935600
N	0.62201400	1.47204500	-0.29263200
N	1.64476900	-2.91896900	-1.48085600
C	4.90922200	0.43648800	-0.55183700
C	5.02733200	-0.80426100	-0.00895500
H	1.60964700	-4.97339400	1.07527100
H	-0.45216200	-5.28140300	-0.65010600
H	-2.65805100	-3.55037200	-4.76829800
H	-4.85788400	-2.72207100	-3.51535600
H	-4.88651200	-1.07162300	2.04684300
H	-3.34400600	0.91101900	3.00024700
H	-0.69334600	4.48246800	0.00409400
H	1.57924500	4.44015300	-1.37584700
H	-1.61880300	-2.50165500	-0.80789000
H	-2.10981000	0.01212900	-0.90734100
H	0.83948300	0.51596900	-0.02507500
H	1.91949900	-2.04353300	-1.91123400
H	5.68691100	1.17636200	-0.68071600
H	5.92687500	-1.28808500	0.34621600
C	-2.06184600	3.08891600	1.80742600
C	-1.31538800	3.66918100	2.84338800
C	-3.34510900	3.61246900	1.58895800
C	-1.81512600	4.70730700	3.62656600
C	-3.86447000	4.64868100	2.35873000
C	-3.09486700	5.19843100	3.38232700
C	3.83360900	2.91465600	-1.74753900
C	4.34483100	2.77865800	-3.04469300
C	4.27463000	4.02344200	-1.01450600
C	5.23294800	3.69842500	-3.59599500
C	5.15678600	4.96167400	-1.54598700
C	5.63979600	4.79609500	-2.84159400
C	4.25740800	-3.52097700	1.12982500
C	4.65337200	-3.05212200	2.39351100
C	4.72426300	-4.79414400	0.76156900
C	5.46533400	-3.80068800	3.24137300
C	5.53430500	-5.55809900	1.59587100
C	5.90739200	-5.05909200	2.84165600
C	-5.72545400	-1.77602500	-0.82159700
C	-6.45822200	-2.49456100	0.12959300
C	-6.46839000	-1.10732000	-1.80146600
C	-7.84938700	-2.54373400	0.12140700
C	-7.85964400	-1.15559400	-1.84542700
C	-8.55386200	-1.87467000	-0.87621200
F	-1.07863300	5.22782700	4.61436900
F	-3.58344900	6.19417300	4.12470900
F	-5.08822800	5.13104000	2.11298500
F	-4.10739200	3.13101400	0.59847800
F	-0.08727000	3.21648500	3.12356700
F	5.55517600	6.00972500	-0.81516700
F	3.85237100	4.20965800	0.24410000
F	6.48854200	5.68806200	-3.35914800
F	5.69082800	3.53914100	-4.84337300
F	3.97176700	1.73828800	-3.80298600
F	4.23134800	-1.86212100	2.83800400

F	5.81084300	-3.32427400	4.44265900
F	6.68640400	-5.78342800	3.64768600
F	5.97039200	-6.76000800	1.20210900
F	4.42041300	-5.30407600	-0.43871600
F	-5.83964300	-0.39796900	-2.75318500
F	-8.53095400	-0.50741800	-2.80423400
F	-9.88802900	-1.92260900	-0.90297700
F	-8.50974200	-3.23997200	1.05351900
F	-5.81584000	-3.15439900	1.10878500
H	0.11334900	-3.69516200	-3.92645000

2e ($T0^{A,D}$)

Sum of electronic and zero-point Energies=

-4146.005712

C	0.48836400	-3.62575500	-0.16054600
C	0.39448100	-2.75738300	0.93298600
C	1.69506000	-2.36552700	1.28321500
C	2.59069500	-2.97496700	0.39872300
C	4.02203700	-2.67920800	0.19078100
C	4.32401800	-1.35634900	-0.06464800
C	5.57671400	-0.61069800	-0.12948100
C	5.29412100	0.70465000	-0.32352300
C	3.84936800	0.86604800	-0.42079800
C	3.03488600	1.95915700	-0.62544500
C	1.60846800	1.69902400	-0.87092900
C	1.00715900	0.80011000	-1.74979200
C	-0.38210700	0.82042300	-1.51585500
C	-0.63213800	1.73576800	-0.49197500
C	-1.89373300	2.14335600	0.10439600
C	-2.97959400	1.30024100	0.20077900
C	-4.33209700	1.64086600	0.61114300
C	-5.11288000	0.53771700	0.50582700
C	-4.29111300	-0.56789400	0.04795200
C	-4.67083200	-1.87440800	-0.21304300
C	-3.72605900	-2.90252200	-0.59258300
N	-2.40628400	-2.78547300	-0.43141300
C	-1.85459700	-3.95213600	-0.95731300
C	-0.52621200	-4.30095700	-0.89964100
N	0.59187300	2.28314400	-0.14293100
N	-3.01828600	-0.05603500	-0.10931800
C	-2.90670000	-4.79731500	-1.50459200
C	-4.07934100	-4.16509500	-1.24621500
N	3.34213900	-0.41004400	-0.27575100
N	1.84342000	-3.77182100	-0.43492100
H	-0.53530600	-2.48330300	1.40600300
H	1.98399900	-1.71185300	2.09401700
H	6.55673700	-1.04949200	-0.01653400
H	6.00741800	1.51120200	-0.40792300
H	1.52726500	0.22931900	-2.50574300
H	-1.13586400	0.28013600	-2.06907100
H	-4.64389600	2.62418200	0.92937200
H	-6.16492300	0.46285000	0.73635300
H	0.74175200	2.82126100	0.69738700
H	-2.23518500	-0.68129500	-0.28287900
H	-2.75752700	-5.75919100	-1.97852800
H	-5.07853700	-4.49208100	-1.49867800
H	2.35380100	-0.61047500	-0.24193300
H	2.21451500	-4.24592900	-1.24463800
C	3.53338400	3.34613800	-0.58561200
C	3.13145400	4.29285300	-1.54703800
C	4.38813400	3.82481900	0.42357200
C	3.54988100	5.61870800	-1.51261500
C	4.83064300	5.14358000	0.46733500
C	4.40837200	6.04826900	-0.50296500
C	-2.05308100	3.56552400	0.53594100
C	-2.88668700	4.45454300	-0.15707400
C	-1.36083200	4.09976200	1.62703700
C	-3.03711200	5.78606700	0.22533900
C	-1.47692800	5.42829900	2.02262800
C	-2.32892900	6.27621100	1.31963700
C	-6.10753700	-2.24039500	-0.12668100
C	-7.09454100	-1.61553500	-0.90283000
C	-6.54632700	-3.26704300	0.72319600
C	-8.43855800	-1.97339000	-0.83027100

C	-7.88129500	-3.65262400	0.80196400
C	-8.83383100	-2.99966100	0.02332600
C	5.02705400	-3.75140100	0.24529500
C	4.96393000	-4.76078100	1.22580000
C	6.07200100	-3.87682400	-0.68862800
C	5.86981400	-5.81452700	1.27779600
C	6.99981000	-4.91262600	-0.64320100
C	6.89899500	-5.89118900	0.34202900
F	4.01051600	-4.71900800	2.16687700
F	5.77188100	-6.74238500	2.23652000
F	7.78095600	-6.89299700	0.39014400
F	7.97284900	-4.98647100	-1.55948300
F	6.19472700	-2.98874800	-1.69134800
F	4.79598400	3.00908400	1.41058100
F	2.32808400	3.92456800	-2.55364800
F	3.15022100	6.47819800	-2.45655000
F	4.82377800	7.31651800	-0.46711200
F	5.64088600	5.55106700	1.45128000
F	-0.51062600	3.31483400	2.32768800
F	-0.78786200	5.88788700	3.07253700
F	-2.46118800	7.55150900	1.68944100
F	-3.84873700	6.59850300	-0.45866900
F	-3.57999200	4.03366600	-1.22245200
F	-5.66558200	-3.91070800	1.50181100
F	-8.25721400	-4.63377100	1.63118900
F	-10.11963400	-3.35507200	0.09660600
F	-9.34802400	-1.35007600	-1.58970000
F	-6.76086900	-0.63737400	-1.75866200
H	-0.23033400	-5.19227500	-1.45072800

2e' (T0^{A,D})

Sum of electronic and zero-point Energies= -4145.997613

C	-2.03070300	0.81307200	-0.79954800
C	-1.53057500	0.15393500	-1.92344600
C	-2.32208000	-0.98871000	-2.13830200
C	-3.29017400	-1.05111000	-1.12891600
C	-4.18815200	-2.15060800	-0.72938900
C	-3.60776600	-3.39555600	-0.58129800
C	-4.12064100	-4.70841700	-0.19301100
C	-3.07755100	-5.57826000	-0.11116700
C	-1.85051500	-4.87535300	-0.46017800
C	-0.53586100	-5.25156700	-0.47079100
C	0.47611600	-4.30475300	-0.90885100
C	0.42461700	-3.37462700	-1.95280700
C	1.54879900	-2.53497600	-1.85556200
C	2.30344000	-2.95907000	-0.76350300
C	3.56918100	-2.46177900	-0.26931900
C	3.90169000	-1.12111500	-0.31531900
C	5.23149900	-0.55684600	-0.21947500
C	5.14768900	0.78675100	-0.38056400
C	3.74861400	1.14790600	-0.51420700
C	3.21324200	2.42721000	-0.52975200
C	1.80820000	2.73541300	-0.44134100
N	0.80797400	1.85033900	-0.54138300
C	-0.34746400	2.55702100	-0.20461600
C	-1.63832400	2.05135400	-0.18490300
N	3.04572300	-0.03965400	-0.52315500
C	-0.01562500	3.94322400	0.10579600
C	1.31829800	4.06883000	-0.07840800
N	-3.12344200	0.07549200	-0.36073900
N	1.65223000	-4.05917000	-0.22895500
N	-2.25941800	-3.59120700	-0.77349000
H	-0.70635500	0.51114400	-2.52110800
H	-2.23558200	-1.69350300	-2.95247500
H	-5.15820100	-4.92384700	0.01307300
H	-3.12471500	-6.62408300	0.16133400
H	-0.32837100	-3.35686100	-2.72622800
H	1.83232500	-1.74440100	-2.53472500
H	6.13013000	-1.14343300	-0.09789300
H	5.96521700	1.49106400	-0.39373700
H	2.02894100	-0.04425400	-0.52757200
H	-0.71986800	4.71788200	0.37435100

H	1.92117400	4.95565700	0.05442200
H	-3.60247900	0.23631800	0.51227500
H	1.89602000	-4.48629200	0.65171000
H	-1.61302400	-2.83280400	-0.93473600
C	-2.70968800	2.83006300	0.49792500
C	-2.61473400	3.19959000	1.84900600
C	-3.88279800	3.20953800	-0.17499400
C	-3.62103100	3.91550100	2.49375800
C	-4.89966200	3.92399200	0.45128200
C	-4.76707800	4.27988500	1.79202500
C	-5.59801800	-1.86226400	-0.41377700
C	-6.24190800	-2.30351400	0.75574500
C	-6.37912200	-1.06888800	-1.27618900
C	-7.57182100	-2.00563100	1.03868800
C	-7.70319700	-0.74285900	-1.00359700
C	-8.30799400	-1.21783600	0.15836600
C	4.54906900	-3.44080000	0.25963100
C	4.89497300	-4.59896100	-0.45960800
C	5.15196200	-3.29272200	1.52102600
C	5.78194800	-5.54820700	0.03783200
C	6.05147000	-4.22528800	2.03143900
C	6.36686300	-5.35973400	1.28845300
C	4.16301000	3.57830200	-0.52173800
C	4.23463900	4.45571300	-1.61160100
C	4.99585900	3.86618600	0.56659600
C	5.08912400	5.55481900	-1.62869800
C	5.86855800	4.95219300	0.56919900
C	5.91215400	5.80225100	-0.53255700
F	-8.40643200	0.00444500	-1.86170000
F	-5.85030400	-0.61113300	-2.41929100
F	-9.58253600	-0.91985900	0.42488700
F	-8.13665800	-2.44956800	2.16856400
F	-5.56994000	-3.02937300	1.66764200
F	4.85763900	-2.23661100	2.29198100
F	4.37870500	-4.81129200	-1.67648900
F	6.09123600	-6.63045000	-0.68501100
F	7.22390800	-6.26209500	1.77077300
F	6.59706200	-4.04712400	3.23971300
F	4.97546300	3.08233000	1.65498000
F	6.65270400	5.19100500	1.62747900
F	6.74156000	6.84943900	-0.53941600
F	5.13241100	6.36711100	-2.69141100
F	3.45947500	4.24874700	-2.68493500
F	-1.54558000	2.84966600	2.57432800
F	-3.49816700	4.24213400	3.78481600
F	-4.04272500	2.90296500	-1.46728400
F	-5.99538600	4.28061300	-0.22680900
F	-5.73596600	4.96579000	2.40079600
H	-0.25608700	-6.23363700	-0.10314100

2f ($TO^{4,D}$)

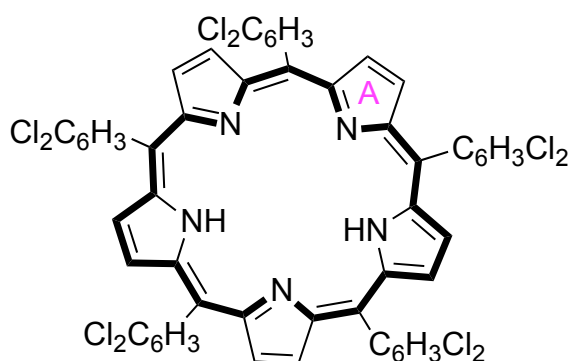
Sum of electronic and zero-point Energies= -4146.003657

C	3.51578900	-3.14517900	-0.37102900
N	2.35287400	-2.63564800	-0.76467400
C	1.39155800	-3.63671800	-0.63366800
C	0.10020100	-3.23380200	-0.86997600
C	-1.19658800	-3.72853600	-0.56884200
N	-2.23551000	-2.83341200	-0.79627400
C	-3.40784000	-3.26028600	-0.23311900
C	-4.58719800	-2.41299200	-0.17733300
C	-4.49905200	-1.03350100	-0.26607100
C	-5.54667200	-0.03095200	-0.31094300
C	-4.98091000	1.20581800	-0.37260200
C	-3.53976200	1.06242500	-0.39276900
C	-2.52520100	1.99421200	-0.48180600
C	-1.16370700	1.56698100	-0.80549900
N	-0.03443300	2.14748800	-0.26308800
C	1.11615300	1.57846800	-0.77865700
C	2.45028700	1.99755000	-0.35940700
C	3.50009800	1.10093000	-0.30684800
C	4.91356500	1.32596500	-0.02946400
C	5.55070800	0.12625900	-0.02015100
C	4.56903500	-0.91747600	-0.28218000
C	4.68983300	-2.30077700	-0.23174300

C	3.35683600	-4.56662400	-0.04034500
C	2.03205600	-4.85730700	-0.18245400
C	-3.12744700	-4.51461200	0.34068300
C	-1.76649400	-4.79878100	0.13897000
N	-3.30870700	-0.31305400	-0.36510000
C	-0.71031900	0.61125800	-1.71662500
C	0.70036000	0.62041000	-1.70315500
N	3.37948000	-0.26121600	-0.49936500
H	1.54963600	-5.81133000	-0.01638000
H	4.13829400	-5.24188000	0.27820700
H	6.59879500	-0.04905300	0.17417700
H	5.35876700	2.29531600	0.13866300
H	1.35215800	0.03410000	-2.33353400
H	-1.34397500	0.05253300	-2.39095000
H	-5.50259600	2.14882500	-0.44608600
H	-6.60295700	-0.25635400	-0.32143900
H	-3.83305600	-5.11259600	0.89905300
H	-1.22828400	-5.65609100	0.51706500
H	0.07777400	-2.21501700	-1.25226700
C	6.02380200	-2.90058900	0.02524700
C	6.30036500	-3.65765300	1.17163900
C	7.54471400	-4.23766200	1.40252400
C	8.57321400	-4.05018200	0.48274400
C	8.34219500	-3.29239500	-0.66204700
C	7.08373700	-2.73663800	-0.87833500
C	2.63889900	3.41498300	0.02638100
C	3.22438000	3.80274800	1.24430100
C	3.38358300	5.13805200	1.60582600
C	2.92938000	6.14384100	0.75733500
C	2.32281400	5.80176300	-0.44960600
C	2.18868000	4.46198600	-0.80007700
C	-2.78700400	3.43466200	-0.28002900
C	-2.25264200	4.40748300	-1.14796300
C	-2.45690500	5.77048200	-0.95832400
C	-3.22361100	6.21319000	0.11766100
C	-3.76857000	5.28401800	0.99973200
C	-3.53967900	3.92523300	0.80254100
C	-5.89323600	-3.06876900	0.05825100
C	-6.72855000	-2.73140300	1.13446200
C	-7.94538800	-3.36960000	1.36054300
C	-8.35588700	-4.39449100	0.51242300
C	-7.54820500	-4.76602000	-0.56039200
C	-6.34305800	-4.10538400	-0.77585300
F	5.34721300	-3.84383300	2.09845900
F	7.76391500	-4.95385800	2.51203300
F	9.77513500	-4.59217300	0.69884900
F	9.32585400	-3.11239200	-1.55186400
F	6.90504400	-2.02323500	-2.00015800
F	3.63992600	2.87711000	2.12221900
F	3.94632700	5.45750800	2.77690000
F	3.07001600	7.42664700	1.09908700
F	1.88847900	6.76288600	-1.27182100
F	1.61226100	4.18534800	-1.97695600
F	-1.52773700	4.03518000	-2.21012100
F	-1.93991900	6.65647100	-1.81519200
F	-3.43321700	7.51807400	0.30171600
F	-4.49001500	5.70176300	2.04582600
F	-4.05319900	3.08001200	1.71026600
F	-6.36460500	-1.77145300	1.99820900
F	-8.71116800	-3.01664100	2.39915900
F	-9.51819600	-5.01599400	0.72389900
F	-7.94371200	-5.74142400	-1.38574500
F	-5.60787700	-4.47834900	-1.83231000
H	-2.42493400	-0.66882600	-0.03045900
H	2.53824800	-0.83008600	-0.64499100
H	-0.04532300	2.82217100	0.48656000
H	-2.15912900	-2.04799200	-1.42394700

Meso-pentakis(2,6-dichlorophenyl)-substituted pentaphyrins (5)

22PP



5

1a (T0)

Sum of electronic and zero-point Energies= -6987.101377

C	-1.35443800	-3.16258800	-0.01353600
N	-1.66960300	-1.90038500	0.29333400
C	-2.70733300	-2.00040400	1.20187900
C	-3.52790400	-0.93947800	1.56819400
C	-3.48792400	0.36036400	1.00421600
C	-4.55525300	1.29560500	0.99427900
C	-4.21830000	2.30439700	0.11780500
C	-2.90131300	2.05241200	-0.35514700
C	-2.15195800	2.94693800	-1.17582700
C	-0.77672200	3.14596800	-1.17412300
N	0.13236100	2.50058300	-0.35243800
C	1.21757100	3.28935200	-0.35762100
C	2.40097300	3.11302500	0.43171100
C	2.97158100	1.91681400	0.83603100
C	4.23594600	1.80154900	1.53281500
C	4.65038800	0.51238800	1.45648800
C	3.65614000	-0.24060700	0.72661100
C	3.82271500	-1.52045200	0.22372500
C	2.83349700	-2.26173800	-0.49469700
N	1.51512300	-2.10382800	-0.34021400
C	0.94374600	-3.11532300	-1.09307000
C	-0.33761800	-3.61604500	-0.93374600
C	1.06031600	4.43789200	-1.25622700
C	-0.16288400	4.31133900	-1.81405000
N	2.61842900	0.63387500	0.46217700
C	1.97827800	-3.83525800	-1.85339300
C	3.16180200	-3.33825500	-1.43844600
N	-2.49155200	0.86957700	0.20364800
C	-2.18627600	-4.12450600	0.71808400
C	-2.98654400	-3.39281100	1.52833700
H	1.80079300	5.20164500	-1.44517000
H	-0.63377000	4.96261600	-2.53572600
H	1.76665800	0.37315600	-0.02174500
H	5.56877900	0.09267000	1.83848200
H	4.75543300	2.63186300	1.98635800
H	1.80522500	-4.63747600	-2.55593800
H	4.15566200	-3.63603500	-1.74194500
H	-1.63841800	0.35609400	-0.00198100
H	-5.47759200	1.18791900	1.54423900
H	-4.80903500	3.17097100	-0.13505400
H	-2.12271900	-5.20035000	0.64801200
H	-3.72495800	-3.74834400	2.23243100
C	-0.69329800	-4.87153700	-1.68360400
C	-0.30319600	-6.16077200	-1.27342500
C	-1.47258800	-4.80659400	-2.85445600
C	-0.65830200	-7.31045400	-1.97887400
C	-1.83534100	-5.94021700	-3.57997700

C	-1.42496600	-7.19378300	-3.13500700
C	5.16320600	-2.16564300	0.40406700
C	5.39737300	-3.10438800	1.42784400
C	6.25449500	-1.89221000	-0.44329800
C	6.63221100	-3.72685000	1.60679400
C	7.49798500	-2.50398200	-0.28754100
C	7.68088600	-3.42202100	0.74318900
C	3.15518600	4.36650500	0.77073600
C	2.77711600	5.17560000	1.85977500
C	4.25985200	4.81757800	0.02193600
C	3.45175200	6.34976300	2.19250800
C	4.94842000	5.99007400	0.33157400
C	4.53903700	6.75287900	1.42209200
C	-4.64266900	-1.20195600	2.53791000
C	-4.47233700	-0.96559600	3.91440200
C	-5.90177500	-1.68725700	2.13939800
C	-5.48380000	-1.20304900	4.84409400
C	-6.92916600	-1.93068200	3.05074700
C	-6.71284300	-1.68736300	4.40453200
C	-2.99281100	3.86622600	-2.01757300
C	-3.44821400	3.45937000	-3.28571500
C	-3.38281200	5.15305100	-1.60169200
C	-4.23048300	4.27725800	-4.09939400
C	-4.16892000	5.98795400	-2.39605400
C	-4.58877900	5.54434100	-3.64714800
H	-4.44323900	6.97026700	-2.02972300
H	-5.19883300	6.18890100	-4.27200300
H	-4.54918500	3.91790800	-5.07078400
H	3.12247900	6.93259600	3.04472100
H	5.06938100	7.66642100	1.67181000
H	5.79020500	6.29389400	-0.27953100
H	8.30390500	-2.26008800	-0.96973100
H	8.64529400	-3.90283200	0.87332600
H	6.76055400	-4.43831600	2.41408100
H	-0.33400900	-8.27955600	-1.61821900
H	-1.70382500	-8.08343400	-3.69077200
H	-7.88154700	-2.30546200	2.69460100
H	-7.50673700	-1.87553600	5.12037000
H	-5.30114500	-1.00863600	5.89441300
Cl	1.42007200	4.69963500	2.86471400
Cl	4.80310600	3.90251200	-1.37662200
Cl	6.06749600	-0.75616000	-1.77086200
Cl	4.10731300	-3.50878300	2.54583400
Cl	-2.00172200	-3.24584800	-3.45828400
Cl	0.64893400	-6.37089400	0.18876900
Cl	-6.22468500	-2.00129600	0.44250800
Cl	-2.93818800	-0.35479500	4.50741700
Cl	-2.89457100	5.75456600	-0.02545600
Cl	-3.01623600	1.87054200	-3.89389700
H	-2.43069400	-5.83168800	-4.47892700

1c ($T0^A$)

Sum of electronic and zero-point Energies= -6987.098821

C	-0.14543500	-2.98962700	-0.79986400
N	-1.47242800	-3.23929400	-0.68975500
C	-2.06849400	-2.10341900	-1.12783600
C	-3.42213100	-1.84086300	-0.84857600
C	-3.86266000	-0.53984600	-0.56969700
C	-5.19717300	-0.09148900	-0.32518000
C	-5.14341000	1.22391600	0.05821900
C	-3.76832800	1.62610400	0.06894200
C	-3.24062400	2.86958500	0.45403300
C	-1.89756400	3.29158200	0.41029500
N	-0.78739800	2.58195900	0.00269700
C	0.22138100	3.49849400	-0.04310200
C	1.59090000	3.40154500	-0.45491600
C	2.58181400	2.39670900	-0.51354200
C	3.94602100	2.72070400	-0.85804500
C	4.74311000	1.65725000	-0.57204000
C	3.91702700	0.58820800	-0.10886600
C	4.42094200	-0.66723200	0.27155300
C	3.68463200	-1.85797800	0.42539600
N	2.37793700	-1.94995500	0.10773600
C	2.05842900	-3.26880100	0.23235500

C	0.80364100	-3.78707400	-0.12846500
C	-1.56158800	4.67864600	0.70251600
C	-0.26238000	4.82241600	0.38315000
N	-3.03597800	0.54650500	-0.34098800
C	0.11210600	-1.73710900	-1.51888200
C	-1.10124600	-1.16968900	-1.70981100
N	2.60992200	1.06288400	-0.12005500
C	3.20008000	-4.03616200	0.72826600
C	4.22711500	-3.15733700	0.83207600
H	-6.07582500	-0.70915000	-0.43851200
H	-5.97312200	1.86523200	0.31364800
H	4.27121000	3.66959200	-1.24894900
H	5.81292200	1.59269000	-0.69577400
H	-2.23788100	5.43453000	1.07211300
H	0.32496700	5.72196000	0.46621600
H	-2.02075300	0.55526800	-0.33888200
H	1.07954000	-1.38493500	-1.83537900
H	-1.33117800	-0.26226500	-2.25150200
H	1.81769900	0.48533500	0.13512900
H	3.20885800	-5.09920600	0.92496800
H	5.24339100	-3.35520200	1.14264200
C	0.42148000	-5.17057400	0.28205100
C	0.04938300	-5.48470300	1.60152600
C	0.40960500	-6.23356300	-0.63824300
C	-0.31621300	-6.77394100	1.98531400
C	0.05286700	-7.53129200	-0.27806100
C	-0.31178700	-7.79536100	1.03945400
C	-4.36756000	-2.98052700	-0.66360700
C	-4.72869100	-3.46401600	0.60753400
C	-4.93317600	-3.64228900	-1.76802500
C	-5.59759600	-4.54158700	0.77219300
C	-5.80730500	-4.71814000	-1.62808100
C	-6.13498700	-5.16488800	-0.35073600
C	-4.26387600	3.86229200	0.93012200
C	-4.94259900	4.72075000	0.04550500
C	-4.61003700	3.97176200	2.28964500
C	-5.90168500	5.63562800	0.47898800
C	-5.56442800	4.87933400	2.74824500
C	-6.20812200	5.71044200	1.83527800
C	2.14029900	4.74984300	-0.88086300
C	1.93794600	5.22970300	-2.18775300
C	2.86861200	5.59397200	-0.02026800
C	2.42471400	6.46387600	-2.61894800
C	3.36094600	6.83390100	-0.42483300
C	3.13638200	7.26449900	-1.73044300
C	5.90720200	-0.75750200	0.45916300
C	6.76842600	-1.20417500	-0.56078900
C	6.51633800	-0.42054900	1.68245600
C	8.14762600	-1.30892200	-0.38291500
C	7.89209500	-0.52015600	1.88619600
C	8.70407700	-0.96565100	0.84648800
H	-6.22006900	-5.19166900	-2.51099100
H	-6.81220200	-6.00453100	-0.22983700
H	-5.83929800	-4.88415600	1.77143200
H	-6.39485900	6.27635900	-0.24251600
H	-6.95255500	6.41998500	2.18232900
H	-5.79350400	4.92605500	3.80639100
H	3.51717000	8.22757800	-2.05516500
H	2.24292900	6.78349100	-3.63829600
H	3.91027500	7.44703900	0.27994200
H	8.76793000	-1.65542000	-1.20114800
H	9.77624900	-1.04592300	0.99507200
H	8.31148000	-0.25202000	2.84878400
H	0.06471700	-8.31659400	-1.02461800
H	-0.59415400	-8.80232400	1.33032300
H	-0.60304100	-6.96388900	3.01288500
Cl	-4.06025700	-2.72692100	2.05119100
Cl	-4.56082200	-3.09599900	-3.39652600
Cl	0.00915400	-4.22689800	2.82462000
Cl	0.88399100	-5.94974600	-2.30664200
Cl	6.11207000	-1.63434700	-2.13155700
Cl	5.52832600	0.13584300	3.02274300
Cl	1.06003900	4.25116700	-3.35137400
Cl	3.16340700	5.10698400	1.64201800
Cl	-3.82475800	2.94127700	3.47393100
Cl	-4.58537800	4.66377500	-1.67282600

1d ($T0^D$)

Sum of electronic and zero-point Energies= -6987.094165

C	0.28001200	-3.36165100	0.00428500
N	1.18598900	-2.36159700	0.02284300
C	2.33961200	-2.92839900	0.54620400
C	3.61809800	-2.36025900	0.57103200
C	3.98039400	-1.07330500	0.12066800
C	5.27677100	-0.47875500	0.08098500
C	5.12953200	0.82571800	-0.33247700
C	3.74355300	1.06305300	-0.56375600
C	3.09555600	2.28389900	-0.84021100
C	1.72544000	2.32961500	-1.12392200
N	0.94863400	3.36651900	-0.69793700
C	-0.31579700	2.92230000	-0.82444700
C	-1.39786600	3.58883100	-0.19018500
C	-2.54095700	2.90461300	0.21276800
C	-3.79115800	3.44808500	0.67642800
C	-4.66738500	2.41659800	0.85905600
C	-3.98567400	1.18964400	0.53092600
C	-4.50219100	-0.09718000	0.41460900
C	-3.76395500	-1.22490300	-0.05177200
N	-2.41898300	-1.37915300	-0.04137300
C	-2.18986300	-2.62490900	-0.60156400
C	-1.05515800	-3.44712400	-0.56304200
C	2.11076000	-4.30614000	0.95176900
C	0.84780200	-4.59428700	0.57840500
N	3.09116900	-0.12593600	-0.30437300
C	-0.37050500	1.63632500	-1.52930200
C	0.91793200	1.25612300	-1.70085000
C	-4.44195800	-2.35827300	-0.67775900
C	-3.46682000	-3.19195000	-1.08345400
N	-2.70430300	1.53263000	0.18802500
H	2.82816100	-4.95822700	1.42762500
H	0.32850100	-5.52868600	0.71702700
H	2.08884200	-0.30034800	-0.29171500
H	5.90563800	1.56439500	-0.46804300
H	6.19519000	-0.98293000	0.34119800
H	-1.25320400	1.13212300	-1.89496900
H	1.28329800	0.38277600	-2.22330700
H	-5.50742100	-2.45779200	-0.82622300
H	-3.59013900	-4.11850700	-1.62100900
H	-3.98420000	4.50412800	0.79589500
H	-5.70193300	2.47980500	1.16201400
H	-1.99603200	0.81915800	0.03810000
C	3.84845600	3.55667600	-0.63769000
C	4.12072800	4.07614100	0.64131200
C	4.31509800	4.30851600	-1.73047500
C	4.81379700	5.27145600	0.82472500
C	5.01402300	5.50345600	-1.57166000
C	5.25962800	5.98105900	-0.28714500
C	-1.25735900	5.03591400	0.14394200
C	-1.41339700	6.03274700	-0.83625700
C	-0.94395800	5.48158300	1.44127100
C	-1.26891900	7.38933200	-0.55402000
C	-0.79162700	6.83301900	1.74767600
C	-0.95533300	7.78376400	0.74407600
C	-5.96259000	-0.27569300	0.69414000
C	-6.96170100	0.04061400	-0.24676300
C	-6.41490400	-0.77694800	1.93021200
C	-8.32076500	-0.12814400	0.01660300
C	-7.76761700	-0.95319100	2.21825300
C	-8.71787200	-0.62619400	1.25469100
C	-1.26683000	-4.81843400	-1.17853200
C	-1.91671500	-5.88504100	-0.52666800
C	-0.79228900	-5.09176600	-2.47531600
C	-2.08378800	-7.13685000	-1.11718800
C	-0.95331400	-6.33253100	-3.09115200
C	-1.59951200	-7.35582100	-2.40437200
C	4.74830300	-3.18933300	1.10917400
C	5.10485300	-3.15810900	2.46985400
C	5.52029700	-4.02499700	0.28157500
C	6.15774400	-3.91457500	2.98335500
C	6.57905400	-4.78915600	0.77111600
C	6.89261500	-4.72975700	2.12650600

H	5.35677900	6.04390000	-2.44608900
H	5.80063200	6.91232600	-0.15185800
H	4.99216400	5.63611400	1.82946300
H	-0.54224800	7.12598000	2.76071100
H	-0.83801100	8.83798600	0.97454100
H	-1.40320900	8.11833600	-1.34446600
H	-8.06244300	-1.34039000	3.18646900
H	-9.77334000	-0.76083000	1.46909900
H	-9.04923500	0.12654500	-0.74420400
H	-0.57420000	-6.48382800	-4.09504200
H	-2.58803300	-7.92331700	-0.56792400
H	-1.72728100	-8.32652200	-2.87279000
H	7.14286300	-5.41884100	0.09294900
H	7.71411900	-5.32189800	2.51709700
H	6.39100000	-3.85844400	4.04010700
Cl	4.04340700	3.73083100	-3.36810700
Cl	3.55865600	3.23018400	2.07035700
Cl	-0.70635300	4.32081800	2.73594600
Cl	-1.83140200	5.57977200	-2.48181900
Cl	-5.25195500	-1.18958400	3.17743500
Cl	-6.51092200	0.65181000	-1.83189100
Cl	0.01458200	-3.83021500	-3.39279700
Cl	-2.53568400	-5.67490200	1.10549300
Cl	5.15891400	-4.12909900	-1.43335900
Cl	4.20620000	-2.14153900	3.58293200

1e ($T0^{4,D}$)

Sum of electronic and zero-point Energies= -6987.095002

C	3.47234200	-2.53121600	-0.31056800
N	2.32690600	-2.08408400	0.32609700
C	1.45898200	-3.09384200	0.28630000
C	0.13233300	-2.87660700	0.86749100
C	-1.03092500	-3.02787300	0.14855200
N	-2.20420200	-2.38560100	0.53467000
C	-3.11218200	-2.69985600	-0.38304800
C	-4.36203800	-1.97714300	-0.51427700
C	-4.38456300	-0.60368900	-0.33579500
C	-5.47477900	0.34392400	-0.46777500
C	-4.96870200	1.60405200	-0.34808900
C	-3.52998800	1.50727700	-0.19695000
C	-2.56579500	2.50945100	-0.23879400
C	-1.19896600	2.20607600	-0.56767000
N	-0.15737100	2.93962800	-0.16172900
C	0.96292100	2.26640100	-0.60767800
C	2.25904100	2.64948000	-0.27924400
C	3.36160000	1.73993600	-0.39424800
C	4.73647600	1.99150900	-0.65615200
C	5.37504000	0.76798800	-0.78829200
C	4.41199000	-0.25275300	-0.56223600
C	4.52226700	-1.66802000	-0.63127700
C	3.30865300	-3.92102500	-0.69784400
C	2.02541000	-4.26024300	-0.36951900
C	-2.58208000	-3.65579100	-1.36512500
C	-1.25971500	-3.78260700	-1.08605400
N	-3.25132000	0.16036000	-0.13520600
C	-0.77125100	1.07412700	-1.40942100
C	0.57848100	1.11137900	-1.42864000
N	3.21594300	0.38289000	-0.32472900
H	1.53857600	-5.21755100	-0.49456100
H	4.05123400	-4.53988200	-1.18277600
H	6.41413600	0.59844300	-1.03098300
H	5.16799600	2.97253000	-0.79218200
H	1.24926300	0.47290000	-1.98445800
H	-1.42129200	0.39731300	-1.94486400
H	-5.50595100	2.53713900	-0.44059700
H	-6.50131700	0.06736300	-0.66063600
H	-3.13175200	-4.09085400	-2.18921900
H	-0.52266600	-4.36301800	-1.62268900
C	5.80650600	-2.23619200	-1.14794900
C	6.81576800	-2.68320400	-0.27536900
C	8.01842600	-3.21541800	-0.73837100
C	8.23692400	-3.31492400	-2.10979300
C	7.26609500	-2.88462800	-3.01053200
C	6.07294300	-2.35194000	-2.52455700

C	2.52962200	4.02488700	0.22805200
C	2.88142400	4.26835600	1.56927100
C	3.13534700	5.54911800	2.05531200
C	3.04991300	6.63586200	1.18949700
C	2.71454200	6.44338600	-0.14780800
C	2.45975800	5.15389200	-0.61057200
C	-2.95077400	3.91675100	0.05486100
C	-2.96985500	4.90619900	-0.94825600
C	-3.30902100	6.23190500	-0.68856100
C	-3.64542900	6.60746600	0.60947500
C	-3.64500700	5.66613400	1.63463900
C	-3.30225100	4.34512000	1.35012600
C	-5.57773200	-2.69375200	-0.99357500
C	-6.31600500	-3.53440400	-0.13519500
C	-7.44722700	-4.23100500	-0.55605400
C	-7.87383500	-4.10450900	-1.87543400
C	-7.17517800	-3.29290500	-2.76495800
C	-6.04595800	-2.60595900	-2.32051200
H	-2.38742000	-0.25650700	0.19443800
H	2.41608800	-0.15512400	0.02002500
C	0.08922100	-2.48369800	2.31739600
C	0.15333300	-3.52327600	3.26918500
C	0.00734900	-1.18608700	2.84258300
C	0.13715800	-3.29617500	4.64236000
C	-0.00881300	-0.93139000	4.21442800
C	0.05716700	-1.98915800	5.11360700
Cl	6.58499600	-2.56324300	1.45981600
Cl	4.87234900	-1.82964400	-3.69474000
Cl	2.97527500	2.93374200	2.70625300
Cl	2.08044100	4.96716800	-2.31525500
Cl	-2.59450600	4.47481200	-2.60894000
Cl	-3.28882600	3.20809100	2.68989800
Cl	-0.07427500	0.19596500	1.78360300
Cl	0.24279900	-5.20192800	2.73920000
Cl	-5.18028700	-1.62892800	-3.49952100
Cl	-5.82429400	-3.70622500	1.53963100
H	8.76667200	-3.54399400	-0.02676400
H	9.16936900	-3.72986200	-2.47910000
H	7.42289900	-2.95784600	-4.08023200
H	3.39036300	5.68368600	3.09985300
H	3.24652300	7.63755500	1.55851500
H	2.65101700	7.27911300	-0.83455200
H	-3.31172600	6.95194100	-1.49837800
H	-3.90961400	7.63851400	0.82257600
H	-3.89943300	5.94522100	2.65034200
H	-7.98168400	-4.85859000	0.14736100
H	-8.75367300	-4.64303800	-2.21301800
H	-7.49090900	-3.19245600	-3.79669700
H	0.18467800	-4.13784600	5.32321200
H	0.04490700	-1.79652400	6.18159800
H	-0.07218400	0.09394700	4.55933300

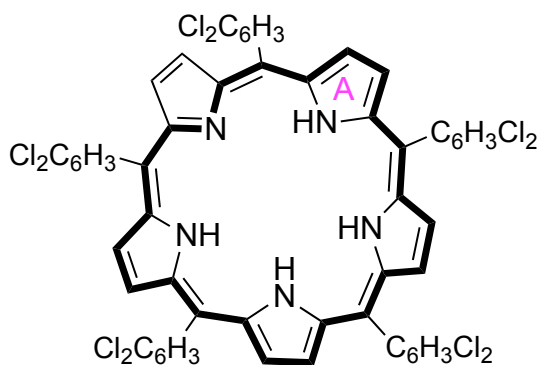
1f($T0^{A,D}$)

Sum of electronic and zero-point Energies= -6987.108600

C	0.14000300	2.75790300	0.57101300
N	-1.09983500	3.30987100	0.34232700
C	-1.97562900	2.41687900	0.82155400
C	-3.38905600	2.47457300	0.56493400
C	-4.05173600	1.27919300	0.27380200
C	-5.44048800	0.89721800	0.15319500
C	-5.49842100	-0.44551700	-0.12337700
C	-4.14760300	-0.94509300	-0.24649000
C	-3.59063500	-2.19277000	-0.53984200
C	-2.18027200	-2.25365900	-0.81244500
N	-1.37126600	-3.21374100	-0.34315600
C	-0.09502900	-2.77372500	-0.60193900
C	1.02711500	-3.44238700	-0.10602400
C	2.32771100	-2.88444900	-0.01815100
C	3.55008100	-3.60302100	0.13960400
C	4.58672800	-2.69852400	0.13938000
C	4.02897200	-1.39118900	0.02382500
C	4.70711000	-0.15374600	0.01821700
C	4.09322400	1.10837500	-0.00520300
N	2.73963800	1.30668900	0.07367000

C	2.55994700	2.64735100	-0.02008600
C	1.30636300	3.32323100	0.05543500
C	0.03549900	1.52723900	1.35227700
C	-1.29021200	1.31009200	1.51823200
N	-3.34471700	0.13479400	0.01169600
C	-1.41907200	-1.21271900	-1.52535400
C	-0.11173300	-1.53926500	-1.38396800
N	2.66469100	-1.54797200	-0.08101300
C	3.83729500	3.33493300	-0.19417900
C	4.79697100	2.37757900	-0.15109600
H	0.86964700	0.96419900	1.74104200
H	-1.76584500	0.53819100	2.10864500
H	-6.27463800	1.57026000	0.29157000
H	-6.38760000	-1.04380800	-0.26228600
H	-1.83695200	-0.40313500	-2.10855800
H	0.74018800	-1.04321500	-1.82740300
H	3.61864500	-4.67882900	0.20128400
H	5.64208700	-2.91308900	0.21677100
H	2.05276200	-0.73397000	-0.06630200
H	3.96736300	4.40326400	-0.29344300
H	5.86760400	2.50532300	-0.22562700
H	-2.33609000	0.09231700	0.01961000
C	1.22783000	4.71994400	-0.47699800
C	1.12702300	4.98099100	-1.85439100
C	1.24735100	5.84199800	0.36922700
C	1.04293900	6.27439600	-2.36601100
C	1.17055600	7.14571000	-0.11719100
C	1.06601000	7.35590200	-1.48955500
C	6.20465800	-0.21453300	0.03423600
C	6.93608800	-0.16998100	1.23548700
C	6.95702500	-0.32001500	-1.15018900
C	8.32913500	-0.22380500	1.26362200
C	8.35027700	-0.37353600	-1.14766300
C	9.03162300	-0.32481100	0.06570500
C	0.84836000	-4.83538000	0.40949100
C	0.73534100	-5.10468600	1.78468900
C	0.77619800	-5.94365800	-0.45202700
C	0.55413600	-6.39437300	2.27986000
C	0.60080400	-7.24364000	0.01875700
C	0.48794600	-7.46247400	1.38909400
C	-4.08643800	3.78166800	0.46157100
C	-4.53499800	4.30826700	-0.76618100
C	-4.31734300	4.58094200	1.59905100
C	-5.17268500	5.54429200	-0.85974600
C	-4.95353000	5.81788000	1.52974600
C	-5.38010700	6.29569600	0.29339100
C	-4.39430800	-3.43615700	-0.42453500
C	-4.70268100	-4.21853300	-1.55549500
C	-4.87438900	-3.91788100	0.80983700
C	-5.44068500	-5.39677800	-1.47426500
C	-5.61358400	-5.09497000	0.91546200
C	-5.89490300	-5.83125600	-0.23176200
Cl	-4.17938300	-3.69559600	-3.14852600
Cl	-4.51372800	-3.05750100	2.29863000
Cl	0.93486900	-5.71591800	-2.18675400
Cl	0.79661900	-3.78442800	2.94102800
Cl	6.13766600	-0.37932500	-2.70176800
Cl	6.08932800	-0.05038400	2.76841600
Cl	1.07919900	3.64506900	-2.99391100
Cl	1.39857700	5.62549300	2.10660900
Cl	-4.26253200	3.42734800	-2.26169700
Cl	-3.82754800	4.00608500	3.18464600
H	-5.95226100	-5.42698300	1.88975400
H	-6.46944500	-6.74910600	-0.15710200
H	-5.65490200	-5.95743800	-2.37645300
H	0.55434600	-8.06586300	-0.68547200
H	0.34763800	-8.47102900	1.76499100
H	0.46310800	-6.54960300	3.34841300
H	8.88454500	-0.45157500	-2.08715000
H	10.11614000	-0.36594900	0.07778900
H	8.84686900	-0.18626300	2.21479500
H	0.95779200	6.42210700	-3.43615600
H	1.19298800	7.97765800	0.57678000
H	1.00253400	8.36756000	-1.87783400
H	-5.11150900	6.39019700	2.43620300
H	-5.49056000	5.90905300	-1.82931400
H	-5.87488800	7.25958500	0.22817000

24PP



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2a (T0)

Sum of electronic and zero-point Energies= -6988.316783

C	2.74322300	2.53975900	-0.44225500
C	2.89720700	3.61957300	-1.40220700
C	1.67489900	4.11766900	-1.70047300
C	0.68104100	3.43561100	-0.88201700
N	1.36480000	2.39988300	-0.24315700
C	3.71858200	1.79686000	0.15923600
C	-0.61525400	3.79746200	-0.66434900
C	3.47811700	0.55711900	0.88515000
N	2.63599000	-0.43135100	0.40113900
C	2.82568000	-1.60642800	1.11216900
C	3.72060400	-1.30993700	2.14444600
C	4.12912700	0.02722600	1.99833700
C	2.41645400	-2.89956400	0.61777100
C	1.36954500	-3.17497600	-0.23374000
N	0.22227200	-2.40730500	-0.48377900
C	-0.62005400	-3.09348700	-1.35102700
C	0.13958000	-4.22771900	-1.84040400
C	1.28282800	-4.31804400	-1.11677900
C	-1.97677400	-2.89736300	-1.51786300
C	-1.46468200	3.18439300	0.36623900
N	-1.83339500	1.86399000	0.42536600
C	-2.70560600	1.66491300	1.48320900
C	-2.83291900	2.89652000	2.14508100
C	-2.07085600	3.83774300	1.44647000
C	-3.48999500	0.48539400	1.65473400
C	-3.40911900	-0.66103400	0.88466800
N	-2.36340500	-0.97819800	0.01112800
C	-2.78359300	-2.06113100	-0.65916400
C	-4.13521400	-2.44915800	-0.26799800
C	-4.49081100	-1.61864000	0.74416400
H	3.84839500	3.92670900	-1.81285700
H	1.44236900	4.91779000	-2.38786300
H	2.23143500	-0.40496900	-0.52402100
H	4.04700300	-2.00967100	2.89994800
H	4.82248900	0.56842600	2.62574200
H	-0.20770300	-4.90864700	-2.60282200
H	2.05404900	-5.06951600	-1.20266400
H	-1.65788900	1.13370200	-0.25867300
H	-3.43680700	3.07039400	3.02332700
H	-1.94152500	4.88356700	1.68278700
H	-4.69957900	-3.27604600	-0.67402600
H	-5.41819400	-1.61093000	1.29926000
H	-0.17312600	-1.71965600	0.15124500
H	0.99615200	1.95546800	0.58637200
C	-4.57000600	0.57092500	2.69157500
C	-4.36627100	0.08529300	3.99603600
C	-5.82721500	1.14729000	2.43153500
C	-5.34776200	0.15903300	4.98380800
C	-6.82583400	1.22883000	3.40137900

C	-6.57899700	0.73256500	4.67878000
C	-1.19226000	4.97682000	-1.37713400
C	-2.12537800	4.80814600	-2.42116500
C	-0.88694800	6.31232800	-1.04519900
C	-2.70986500	5.87821400	-3.09446300
C	-1.45392100	7.40187700	-1.70600900
C	-2.36761400	7.17863200	-2.73198600
C	5.14279900	2.23515800	0.03694200
C	5.70532400	3.19565800	0.89974300
C	6.01297700	1.69564700	-0.93024300
C	7.03946100	3.59297700	0.81574500
C	7.34896300	2.07625700	-1.03837600
C	7.85849600	3.02697800	-0.15711900
C	3.31433200	-4.04013900	0.98555900
C	2.94795300	-4.97996600	1.96932600
C	4.57808200	-4.23148400	0.39197500
C	3.77611900	-6.03912600	2.34104800
C	5.42140700	-5.28395500	0.74265300
C	5.01408500	-6.18634200	1.72247600
C	-2.70075100	-3.78154300	-2.48544200
C	-3.08578400	-5.10647600	-2.19539500
C	-3.06514800	-3.30794200	-3.76164900
C	-3.77269700	-5.90862800	-3.10688300
C	-3.75259800	-4.08729800	-4.69075700
C	-4.10378400	-5.39232600	-4.35648000
Cl	-2.82430000	-0.63554700	4.42903300
Cl	-6.18942600	1.77598200	0.83298200
Cl	0.23223500	6.66298800	0.26796400
Cl	4.71608200	3.92879300	2.15556300
Cl	5.40531200	0.51496700	-2.08141000
Cl	1.40740900	-4.82762100	2.80137300
Cl	5.12379800	-3.13560400	-0.86600800
Cl	-2.71863700	-5.80593500	-0.62465100
Cl	-2.63731100	-1.67012600	-4.23372500
H	-5.14054800	-0.22967600	5.97389400
H	-7.35033900	0.79296400	5.44004600
H	-7.78043000	1.67563100	3.14936200
H	-1.18304400	8.40800000	-1.40812600
H	-2.81604700	8.02067800	-3.24956600
H	-3.41763900	5.68705800	-3.89252200
H	7.97308600	1.63233900	-1.80504600
H	8.89837900	3.32918000	-0.23071400
H	7.42233800	4.33405000	1.50747900
H	6.37966700	-5.38998200	0.24776100
H	5.66472300	-7.00827500	2.00406900
H	3.44758900	-6.73153400	3.10714700
H	-4.04421300	-6.92063600	-2.83021200
H	-4.63914700	-6.00882000	-5.07170100
H	-4.00346300	-3.67049800	-5.65909500
Cl	-2.57144700	3.18579500	-2.92732600

2b (TI)

Sum of electronic and zero-point Energies= -6988.317374

C	2.14430600	-2.25321500	1.48759800
C	1.40624700	-3.14115300	2.28907800
C	0.37761200	-3.66693000	1.50042400
C	0.52447400	-3.15223400	0.19774100
C	-0.24487400	-3.51406600	-0.99465500
C	-1.57398200	-3.17768500	-1.02783700
C	-2.68285900	-3.66412400	-1.82295600
C	-3.82994000	-3.07845300	-1.37225400
C	-3.48913000	-2.12152400	-0.34355300
C	-4.27338200	-1.18163200	0.29804800
C	-3.74732200	0.01697800	0.88830800
C	-4.34034300	0.85627600	1.84470500
C	-3.59732100	2.03125400	1.91456900
C	-2.53389300	1.94664800	0.99167500
C	-1.75471100	3.04198400	0.50017500
C	-0.58754800	3.08994000	-0.26262500
C	-0.23587700	4.20979800	-1.10070900
C	0.96448800	3.96388000	-1.69071900
C	1.47734400	2.72328100	-1.17087200
C	2.80647900	2.31594300	-1.23829900
C	3.38646700	1.28615900	-0.43356600

N	2.68857200	0.31144400	0.17244900
C	3.58498700	-0.30686900	1.03592200
C	3.26703100	-1.42752200	1.79134000
N	-2.11997000	-2.21891100	-0.18396900
N	-2.59701800	0.67039600	0.44475100
N	0.45714300	2.17000700	-0.40148100
N	1.59159600	-2.30034900	0.22271500
C	4.78477700	1.28314800	-0.00831700
C	4.88658800	0.33193200	0.95673800
H	1.60928500	-3.35730900	3.32811000
H	-0.35899300	-4.40367200	1.78667500
H	-2.58849600	-4.40071200	-2.60799800
H	-4.83162400	-3.23043500	-1.74915200
H	-5.22301900	0.60869800	2.41629800
H	-3.79247200	2.88226300	2.54971700
H	-0.86940800	5.07021500	-1.25356900
H	1.49249400	4.59862300	-2.38610200
H	-1.61255400	-1.82450100	0.59428100
H	-2.13541000	0.42305100	-0.41925000
H	0.66529700	1.38588600	0.21044000
H	1.84395800	-1.63057700	-0.49608500
H	5.55647800	1.95429800	-0.35839200
H	5.76498000	0.04774900	1.52009100
C	-2.37533600	4.38277000	0.77925400
C	-1.90739200	5.21189100	1.81688400
C	-3.46424400	4.88109400	0.03677900
C	-2.48030100	6.45088800	2.10457300
C	-4.04929400	6.11871000	0.29881300
C	-3.55270400	6.90009300	1.33939700
C	3.73607400	3.13466100	-2.08105800
C	4.08411400	2.72756000	-3.38387400
C	4.33420400	4.32980200	-1.63412400
C	4.95611300	3.45271900	-4.19475600
C	5.21024100	5.07426700	-2.42419500
C	5.51748400	4.62975000	-3.70724700
C	4.13096900	-1.82776500	2.94104800
C	4.07742400	-1.16162300	4.18088200
C	5.03798900	-2.90220000	2.85505300
C	4.87163700	-1.53347000	5.26522900
C	5.84511100	-3.28962900	3.92302700
C	5.75597400	-2.59985000	5.12953300
C	0.39512100	-4.27802500	-2.10448400
C	0.97917900	-3.62858200	-3.20966500
C	0.47727200	-5.68436100	-2.11163900
C	1.60045000	-4.31508700	-4.25092900
C	1.08874000	-6.39828200	-3.14135700
C	1.65103500	-5.70596500	-4.21043600
C	-5.75419000	-1.36703000	0.31403000
C	-6.38548600	-2.24969000	1.21282200
C	-6.60892600	-0.66846500	-0.56250900
C	-7.76842000	-2.42630400	1.24757600
C	-7.99326700	-0.82840300	-0.54994700
C	-8.56856900	-1.71000600	0.36189800
H	-2.08502300	7.04695900	2.91868000
H	-4.00326700	7.86408400	1.55368000
H	-4.87941100	6.45864200	-0.30928100
H	5.64287100	5.98626500	-2.02981100
H	6.19837300	5.20239100	-4.32913800
H	5.18584100	3.09346000	-5.19102400
H	4.78859700	-0.99065400	6.19944100
H	6.37914000	-2.89506800	5.96780100
H	6.53284300	-4.11818600	3.80112000
H	1.12038100	-7.48063800	-3.09748500
H	2.13223000	-6.25284300	-5.01509600
H	2.03654400	-3.76224200	-5.07462900
H	-8.20306000	-3.11443700	1.96299800
H	-9.64597300	-1.84053500	0.38082100
H	-8.60364800	-0.27062700	-1.25039200
Cl	-5.92741800	0.42808600	-1.75263000
Cl	-5.42303000	-3.16218000	2.36757000
Cl	-0.22509800	-6.60688200	-0.79025000
Cl	0.95211600	-1.87015100	-3.29452200
Cl	2.95757900	0.17132500	4.41415000
Cl	5.20663100	-3.78403400	1.34520600
Cl	3.39871500	1.24991200	-4.04408400
Cl	3.99514200	4.92872500	-0.01743400
Cl	-0.56902700	4.68425800	2.82561800

Cl	-4.10813500	3.94529700	-1.30228500
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2e ($T0^{A,D}$)

Sum of electronic and zero-point Energies=	-6988.327208
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C	-0.19097400	-2.70419800	0.36249100
C	-0.17603100	-1.72691200	1.36419200
C	1.15912300	-1.51837200	1.74074400
C	1.96811000	-2.35728300	0.96727300
C	3.43768900	-2.33740600	0.83669300
C	4.00541700	-1.15483400	0.44796000
C	5.39826300	-0.72329100	0.33047000
C	5.42235700	0.57029200	-0.07897800
C	4.04725600	1.02989600	-0.27120000
C	3.52504200	2.22131600	-0.69195600
C	2.06623500	2.27886500	-0.90825900
C	1.27891300	1.47180000	-1.72804200
C	-0.07353600	1.74697400	-1.44856000
C	-0.11423300	2.72990900	-0.45694200
C	-1.23944100	3.37596900	0.18329000
C	-2.47753800	2.78518500	0.31004500
C	-3.72587700	3.43491200	0.66191200
C	-4.73151900	2.52624700	0.57130400
C	-4.16014200	1.24556400	0.20091600
C	-4.81035500	0.03669600	0.01263800
C	-4.11874100	-1.19513500	-0.25807300
N	-2.79743300	-1.35121200	-0.11739500
C	-2.52547800	-2.66428100	-0.48635300
C	-1.29359600	-3.28035300	-0.35615500
N	1.20044100	3.05678400	-0.16836800
N	-2.80610400	1.45796300	0.05065300
C	-3.75405300	-3.32169800	-0.92219200
C	-4.75370000	-2.42274900	-0.74345300
N	3.26111900	-0.05499700	0.06823600
N	1.12756100	-3.09701900	0.17021700
H	-1.06075400	-1.25739500	1.76266800
H	1.52666200	-0.84078500	2.49805700
H	6.24782900	-1.35199900	0.55807800
H	6.29557800	1.18236900	-0.25707300
H	1.66374400	0.77326500	-2.45716300
H	-0.93436000	1.32049900	-1.94139500
H	-3.81249300	4.48440100	0.90382600
H	-5.78425500	2.69377800	0.74622000
H	1.49056400	3.64959000	0.59568400
H	-2.17673800	0.66763500	-0.07025400
H	-3.83647800	-4.34419200	-1.26441900
H	-5.80868700	-2.55543100	-0.94061100
H	2.25323400	-0.04451600	0.03583300
H	1.44679300	-3.69696900	-0.57661500
C	4.38834000	3.40648600	-0.96437400
C	4.91397400	3.67307300	-2.24478800
C	4.70483900	4.35281700	0.02879600
C	5.70514800	4.78789900	-2.51824500
C	5.49293800	5.47607300	-0.21327900
C	5.99322300	5.68755000	-1.49537900
C	-1.04689400	4.76517700	0.69806300
C	-0.95298800	5.87604600	-0.16687000
C	-0.91363600	5.04716900	2.07353900
C	-0.75257900	7.17489300	0.29652800
C	-0.71446000	6.33885400	2.56134700
C	-0.63458500	7.40109200	1.66578100
C	-6.30154300	0.01122800	0.09636500
C	-7.12564600	0.38653000	-0.98352800
C	-6.97647200	-0.40849200	1.26039100
C	-8.51841100	0.35547400	-0.91698400
C	-8.36697500	-0.45108200	1.35374000
C	-9.13483700	-0.06590200	0.25800400
C	-1.08989800	-4.63866900	-0.95418500
C	-1.16439100	-5.81223000	-0.17800100
C	-0.79034900	-4.81717700	-2.31833600
C	-0.97280400	-7.08162100	-0.72072900
C	-0.59090900	-6.07678600	-2.88380400
C	-0.68616200	-7.20760600	-2.07792900
C	4.25637300	-3.54561600	1.13976900
C	4.69330400	-3.84801100	2.44538800

C	4.61667800	-4.47944900	0.14933900
C	5.44332500	-4.98415100	2.74572000
C	5.36618300	-5.62291400	0.41799000
C	5.77905600	-5.86936900	1.72476100
H	-0.47917200	8.40957000	2.03581900
H	-0.69761100	7.99275500	-0.41229700
H	-0.61851900	6.49849800	3.62883700
H	-9.10275600	0.65468800	-1.77917600
H	-10.21821200	-0.09483300	0.31982000
H	-8.83248300	-0.77958300	2.27560400
H	-1.05202900	-7.95360200	-0.08215400
H	-0.53505400	-8.19221100	-2.50901700
H	-0.36323000	-6.15916000	-3.94006500
H	5.75604500	-5.16499200	3.76745900
H	6.36241500	-6.75683900	1.94871200
H	5.61500200	-6.30523400	-0.38625900
H	6.08599800	4.94139500	-3.52116600
H	6.60782900	6.55875700	-1.69864400
H	5.70453500	6.16941200	0.59219800
Cl	4.58191500	2.56630900	-3.56712600
Cl	4.07441000	4.14039100	1.66343900
Cl	-0.96875000	3.74080900	3.25021400
Cl	-1.12431900	5.64819800	-1.89811100
Cl	-6.39887400	0.90710400	-2.49740700
Cl	-6.05205100	-0.88989700	2.67459300
Cl	-1.53737700	-5.70179100	1.53265100
Cl	-0.63289100	-3.41781400	-3.37088500
Cl	4.29898200	-2.75957200	3.76579100
Cl	4.09185600	-4.22490700	-1.51604400

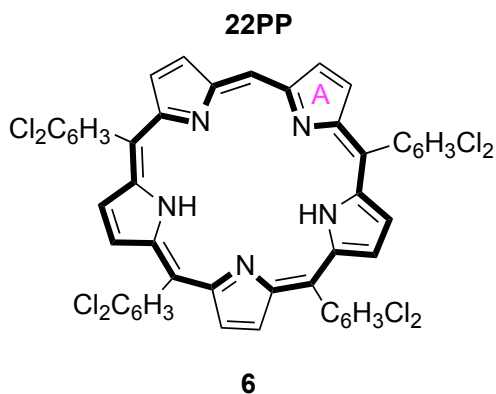
2e' (T0^{A,D})

Sum of electronic and zero-point Energies= -6988.322988

C	3.90607400	-1.60864600	-0.27943600
N	2.57790400	-1.67289300	-0.42064100
C	2.23767400	-2.99630700	-0.12925400
C	0.96091300	-3.52304900	-0.13355200
C	-0.18404200	-2.85863500	-0.69113800
N	-1.47964800	-3.08938000	-0.24727100
C	-2.37371600	-2.31691300	-0.95146400
C	-3.76400200	-2.11838400	-0.52849100
C	-4.21460100	-0.82508400	-0.40795700
C	-5.49892000	-0.25966400	-0.00513200
C	-5.38737600	1.09546500	0.03364900
C	-4.02831900	1.46476300	-0.34784600
C	-3.37381100	2.66960800	-0.41442800
C	-1.98111000	2.66853400	-0.87793200
N	-0.94570100	3.25065500	-0.17477500
C	0.27526200	2.88213200	-0.71578300
C	1.54430200	3.36642400	-0.21096000
C	2.70100400	2.62426000	-0.21366700
C	4.04342600	3.13580700	-0.00915800
C	4.92220300	2.11069500	-0.11922300
C	4.17489000	0.88338800	-0.33125900
C	4.68935000	-0.40153800	-0.31786200
C	4.48111100	-2.91552000	0.06235100
C	3.43641500	-3.76475600	0.19174600
C	-1.63336900	-1.65228300	-1.93897400
C	-0.27702800	-1.97042000	-1.76393600
N	-3.40600600	0.26731900	-0.63747800
C	-1.39804600	1.97488200	-1.94036400
C	0.00179900	2.09489400	-1.83213500
N	2.84883100	1.25238200	-0.43749700
H	3.46236900	-4.81554700	0.44476900
H	5.53002500	-3.12757300	0.21427400
H	5.99745700	2.15729300	-0.03211500
H	4.27015100	4.17767900	0.16433100
H	0.74494400	1.71858000	-2.51999900
H	-1.94665800	1.47839200	-2.72700300
H	-6.15749800	1.80452000	0.30350900
H	-6.37535200	-0.84730900	0.22951400
H	-2.05886000	-1.03460700	-2.71581700
H	0.56354600	-1.64411200	-2.35623000
C	6.17720700	-0.54189800	-0.21770600
C	6.86173600	-0.54264900	1.01385900

C	8.24590600	-0.68651100	1.10765600
C	8.99538200	-0.83938400	-0.05575600
C	8.36759000	-0.84765600	-1.29836600
C	6.98234300	-0.70100800	-1.36259600
C	1.59473200	4.77916900	0.28107500
C	1.54925900	5.09769300	1.65283200
C	1.57015300	6.41026300	2.12399100
C	1.63295300	7.45903400	1.21108300
C	1.67329900	7.19793800	-0.15642300
C	1.65133800	5.87732600	-0.60128400
C	-4.02211500	3.93529200	0.02690400
C	-4.48993900	4.88988400	-0.90069300
C	-5.08448100	6.08920900	-0.51412300
C	-5.22960300	6.37287700	0.84173500
C	-4.77915000	5.46864500	1.79929400
C	-4.18320000	4.27795900	1.38485900
C	-4.61026300	-3.28190400	-0.15219700
C	-4.92750200	-3.60278100	1.18459900
C	-5.71288000	-4.70146300	1.53276400
C	-6.20081000	-5.53541200	0.53101100
C	-5.90619600	-5.27247700	-0.80470400
C	-5.12622300	-4.16410500	-1.12636400
H	-2.41431300	0.19281300	-0.81121500
H	2.11512200	0.55001600	-0.47287200
C	0.73037200	-4.88082900	0.45913800
C	0.60368000	-6.03083600	-0.34478100
C	0.59655500	-5.07850600	1.84680600
C	0.37812200	-7.29747900	0.19106500
C	0.36629000	-6.33554700	2.40650700
C	0.26013300	-7.44375400	1.57121700
Cl	5.96163900	-0.36024700	2.51210300
Cl	6.23665400	-0.71634700	-2.95389900
Cl	1.43263500	3.80888300	2.84604000
Cl	1.72877400	5.60032100	-2.33221700
Cl	-4.35238500	4.56605900	-2.62037800
Cl	-3.58407300	3.19478200	2.63883400
Cl	0.69300600	-3.70514200	2.94039400
Cl	0.76077400	-5.89670000	-2.08690000
Cl	-4.81060400	-3.85832600	-2.82587000
Cl	-4.28795900	-2.62213600	2.50110500
H	8.72045300	-0.67976100	2.08193100
H	10.07315400	-0.95280600	0.00649800
H	8.93722600	-0.96544200	-2.21266200
H	1.53346100	6.59730300	3.19072800
H	1.65009200	8.48456900	1.56621300
H	1.72581200	8.00451800	-0.87825000
H	-5.43221200	6.78265100	-1.27085700
H	-5.69342800	7.30351100	1.15299300
H	-4.87681300	5.67928600	2.85780200
H	-5.92467400	-4.89862900	2.57711700
H	-6.81054600	-6.39466100	0.79173700
H	-6.28090700	-5.91093400	-1.59616400
H	0.29992500	-8.15184400	-0.47100700
H	0.08381200	-8.42640200	1.99718800
H	0.27200300	-6.43319800	3.48165600
H	-1.05393600	3.68400900	0.73046500
H	-1.70449600	-3.56285400	0.61531300

tetrakis(2,6-dichlorophenyl)-substituted pentaphyrins (6)



1a ($T0$)

Sum of electronic and zero-point Energies= -5836.929768

C	-1.21434900	-3.62965500	-1.81283900
N	-1.64294500	-2.64888200	-0.98981800
C	-2.81751200	-3.11698500	-0.46461400
C	-3.69013700	-2.35787300	0.32682200
C	-3.63393300	-0.95968300	0.47522500
C	-4.69255600	-0.13523300	0.95901000
C	-4.39937000	1.16020600	0.61971000
C	-3.11657000	1.17784300	-0.01022500
C	-2.49370200	2.34516800	-0.51699600
C	-1.13214900	2.61626100	-0.69016900
N	-0.08710500	1.85400000	-0.22532500
C	0.97564700	2.68917000	-0.23579800
C	2.24440200	2.45759400	0.36279700
C	2.89378200	1.25052500	0.62528600
C	4.13907200	1.14182100	1.34448300
C	4.61388400	-0.12430800	1.19492500
C	3.69390700	-0.84714400	0.35955700
C	3.95010000	-2.07192000	-0.25418900
C	3.08656000	-2.72222800	-1.16948100
N	1.76581400	-2.46033300	-1.29013500
C	1.31638500	-3.35174400	-2.22535800
C	0.01945400	-3.78882200	-2.48114900
C	0.64044700	3.99236800	-0.82160500
C	-0.66869900	3.93315800	-1.13855600
N	2.62851200	-0.00395300	0.11401500
C	2.42915500	-4.12892900	-2.78633700
C	3.52897800	-3.77505900	-2.08608000
N	-2.67205100	-0.12121900	-0.04712300
C	-2.16318200	-4.74649100	-1.85391700
C	-3.13008700	-4.45696500	-0.95240000
H	1.32540600	4.81309600	-0.97716900
H	-1.27680700	4.69956700	-1.59611700
H	1.82436200	-0.28424100	-0.44074600
H	5.53302800	-0.53281500	1.58660000
H	4.59915000	1.95315500	1.88706900
H	2.33722300	-4.88235100	-3.55824800
H	4.53602800	-4.15591000	-2.17884700
H	-1.82568800	-0.47915800	-0.48624000
H	-5.58147100	-0.49911700	1.45120100
H	-4.99917700	2.03619500	0.81170300
H	-2.04917300	-5.64248500	-2.45052100
H	-3.98962500	-5.05119800	-0.67771500
C	5.28088400	-2.70631600	0.01822200
C	5.43415100	-3.69442300	1.00916100
C	6.44141400	-2.36766600	-0.70326900
C	6.65870800	-4.30699000	1.27334000
C	7.67646500	-2.96805500	-0.46038800
C	7.77855300	-3.93898400	0.53248400
C	3.01203800	3.69283300	0.74742500
C	2.74514000	4.38812300	1.94230500
C	4.02855500	4.22930500	-0.06613800
C	3.44117400	5.53903700	2.31098800
C	4.73428200	5.38189300	0.27707300
C	4.43551400	6.03315200	1.47107600
C	-4.85879800	-3.05348700	0.95992000
C	-4.76423400	-3.59027700	2.25751600
C	-6.09603900	-3.21469300	0.30911100
C	-5.82724700	-4.24920900	2.87385800
C	-7.17311800	-3.87111300	0.90429800
C	-7.03174600	-4.38760200	2.18961400
C	-3.45024300	3.47208400	-0.80090800
C	-4.15265200	3.54212900	-2.01848500
C	-3.70261900	4.50567000	0.12107100
C	-5.04142800	4.57501900	-2.31336400
C	-4.59233900	5.54569200	-0.14783600
C	-5.25796000	5.57626000	-1.37040000
H	-4.75458500	6.31621500	0.59672500
H	-5.94944900	6.38386600	-1.58886200
H	-5.55123300	4.58604400	-3.26953200
H	3.20022900	6.03354500	3.24468000
H	4.98049100	6.93002500	1.74818300
H	5.50348800	5.75672800	-0.38787200

H	8.53933500	-2.67344500	-1.04605500
H	8.73577300	-4.41131600	0.72942500
H	6.72353100	-5.06041100	2.04953100
H	-8.10485100	-3.97135000	0.36008500
H	-7.86483200	-4.90007300	2.66017200
H	-5.70286000	-4.64504000	3.87493300
Cl	1.51326800	3.79151400	3.03991100
Cl	4.42766700	3.45375000	-1.59106900
Cl	6.35874700	-1.15602600	-1.97219500
Cl	4.04962300	-4.18366200	1.96991800
Cl	-6.32271200	-2.58166700	-1.31320400
Cl	-3.26440700	-3.43511400	3.15472400
Cl	-2.90107100	4.50216900	1.68259300
Cl	-3.90285000	2.30507300	-3.23924800
H	-0.01224600	-4.59017900	-3.21667100

1c ($T0^A$)

Sum of electronic and zero-point Energies= -5836.920380

C	-0.30409700	-3.83884500	-0.71940000
N	-1.63846100	-4.05374500	-0.58679800
C	-2.20657300	-2.90277800	-1.02051200
C	-3.53556200	-2.58003800	-0.68426200
C	-3.90115000	-1.26166000	-0.38305300
C	-5.19943700	-0.75337500	-0.06853100
C	-5.06797900	0.56099900	0.29819100
C	-3.67842400	0.90486200	0.22672800
C	-3.08250800	2.13769900	0.53976900
C	-1.73021300	2.51014200	0.40083400
N	-0.65867800	1.73867200	0.00338400
C	0.37216400	2.61852200	-0.15649700
C	1.73287500	2.44501700	-0.57100800
C	2.69136300	1.40677000	-0.54291900
C	4.07786400	1.66735500	-0.85076600
C	4.82515700	0.59024100	-0.48915200
C	3.94382100	-0.42962800	-0.01810900
C	4.38070800	-1.69342700	0.41297700
C	3.58198500	-2.84470800	0.56107800
N	2.29157800	-2.87912800	0.17496900
C	1.88916700	-4.17121400	0.34047500
C	0.62260200	-4.63003500	-0.02969200
C	-1.34649500	3.90640600	0.56138600
C	-0.06236100	3.98770700	0.16818400
N	-3.01656500	-0.21053800	-0.20634800
C	-0.02435200	-2.60218200	-1.45637700
C	-1.22491500	-2.00517800	-1.63645500
N	2.65703600	0.09345600	-0.08963800
C	2.95805600	-4.97739900	0.92507300
C	4.02980000	-4.15376000	1.04492500
H	-6.10931800	-1.33213800	-0.12813700
H	-5.85470900	1.23948500	0.59060500
H	4.45238500	2.58765200	-1.26497500
H	5.89600700	0.48378300	-0.56762500
H	-1.98654900	4.70966100	0.89348800
H	0.54642100	4.87623000	0.14318800
H	-2.00348800	-0.24699500	-0.25719100
H	0.95050400	-2.27635500	-1.78038500
H	-1.44074200	-1.09663200	-2.18208000
H	1.83456800	-0.44921900	0.14587200
H	2.89205400	-6.02962700	1.16976100
H	5.01566100	-4.39185600	1.41927200
C	-4.51898500	-3.67777900	-0.45059900
C	-4.82930100	-4.15422800	0.83643800
C	-5.17207500	-4.30892100	-1.52415600
C	-5.73282200	-5.19493700	1.04525300
C	-6.08243100	-5.34750200	-1.34028400
C	-6.35786100	-5.78784200	-0.04848300
C	-4.04122600	3.18568700	1.03245600
C	-4.75238700	4.02518400	0.15489400
C	-4.29150100	3.36891000	2.40503600
C	-5.65180800	4.99043700	0.60663400
C	-5.18526700	4.32734500	2.88195400
C	-5.86378000	5.13705600	1.97507500
C	2.32268700	3.73338800	-1.11350600
C	2.14420400	4.08986900	-2.46261500

C	3.06517600	4.63867000	-0.33066600
C	2.66482100	5.26480400	-3.00545100
C	3.59180500	5.82156400	-0.84736900
C	3.38854700	6.13001800	-2.19052500
C	5.85199200	-1.84340700	0.66328100
C	6.72994300	-2.36541600	-0.30549300
C	6.42923700	-1.49061000	1.89763100
C	8.09493900	-2.52576700	-0.06945600
C	7.79004300	-1.64471300	2.15925300
C	8.61950800	-2.16366300	1.16855300
H	-6.56291200	-5.79786300	-2.20078100
H	-7.06241600	-6.59881300	0.10672900
H	-5.93307400	-5.53358000	2.05493600
H	-6.17258200	5.61404600	-0.11047200
H	-6.56140900	5.88598900	2.33629400
H	-5.34123700	4.42936000	3.94947600
H	3.79566800	7.04811800	-2.60201300
H	2.49938400	5.48883300	-4.05269400
H	4.15080800	6.48617200	-0.19908800
H	8.72942000	-2.92880700	-0.85007300
H	9.68036900	-2.28667500	1.36223100
H	8.18435300	-1.36143600	3.12806200
Cl	-4.05114900	-3.45513100	2.24453900
Cl	-4.86364300	-3.77139300	-3.16914000
Cl	6.11498900	-2.82094800	-1.88599700
Cl	5.41766500	-0.84461100	3.17908700
Cl	1.24946400	3.02651600	-3.53591000
Cl	3.33825700	4.30524400	1.37290100
Cl	-3.46144900	2.36654400	3.58302500
Cl	-4.51276800	3.88010800	-1.57876300
H	0.29351500	-5.60579400	0.31654400

1d ($T0^D$)

Sum of electronic and zero-point Energies= -5836.937398

C	1.35565700	-3.89282600	-0.29008700
N	2.02135400	-2.70412800	-0.20636000
C	3.34981100	-3.04081100	-0.13275100
C	4.43665800	-2.14475100	-0.03928600
C	4.33827600	-0.74819000	-0.07774400
C	5.37591500	0.23652400	0.02114200
C	4.78823900	1.47378900	-0.04304000
C	3.37767100	1.29032300	-0.21511900
C	2.37878900	2.26435400	-0.34664000
C	1.07405000	1.93183600	-0.75888100
N	-0.00006500	2.67443900	-0.39986900
C	-1.07413100	1.93178900	-0.75895300
C	-2.37889400	2.26426300	-0.34681600
C	-3.37772800	1.29015000	-0.21529300
C	-4.78833100	1.47351200	-0.04343900
C	-5.37590200	0.23620200	0.02087100
C	-4.33815700	-0.74842700	-0.07781000
C	-4.43643700	-2.14499400	-0.03921200
C	-3.34953200	-3.04100000	-0.13254400
N	-2.02110600	-2.70423300	-0.20626300
C	-1.35533600	-3.89290300	-0.28987800
C	0.00016600	-4.29212000	-0.34372600
C	3.54549700	-4.48543600	-0.17257700
C	2.31100300	-5.01341200	-0.28589000
N	3.15810300	-0.07141800	-0.22187700
C	-0.67612200	0.73865400	-1.51300400
C	0.67613900	0.73869700	-1.51297200
C	-3.54512900	-4.48564200	-0.17210500
C	-2.31061300	-5.01354900	-0.28547100
N	-3.15803900	-0.07156300	-0.22190600
H	4.49482300	-4.99874000	-0.12935500
H	2.03696300	-6.05863600	-0.34803300
H	2.27087700	-0.57482300	-0.20713000
H	5.27638700	2.43679800	-0.01180400
H	6.42757700	0.01378600	0.12322000
H	-1.32924900	0.04791400	-2.02601300
H	1.32933100	0.04799300	-2.02594500
H	-4.49440200	-4.99903000	-0.12869400
H	-2.03651800	-6.05876400	-0.34750100
H	-5.27656600	2.43647800	-0.01232700

H	-6.42755000	0.01336900	0.12288300
H	-2.27077100	-0.57490200	-0.20726500
C	2.68224700	3.66924000	0.05402500
C	2.74134400	4.06573000	1.40241600
C	2.91140900	4.67369400	-0.90314300
C	3.00850700	5.38051700	1.78014500
C	3.18480600	5.99351100	-0.55004700
C	3.23035700	6.34143600	0.79741700
C	-2.68253900	3.66912600	0.05374000
C	-2.91167800	4.67348400	-0.90353800
C	-2.74194900	4.06571400	1.40210200
C	-3.18540200	5.99327700	-0.55059000
C	-3.00945100	5.38046800	1.77967200
C	-3.23130200	6.34128300	0.79683600
C	-5.81824200	-2.70954500	0.09662400
C	-6.63011400	-2.96630800	-1.02385700
C	-6.38140800	-3.00420700	1.35231100
C	-7.91847900	-3.48750400	-0.91096500
C	-7.66732100	-3.52536700	1.49160600
C	-8.43206400	-3.76566300	0.35309400
C	5.81849300	-2.70921600	0.09656200
C	6.38159200	-3.00397500	1.35226800
C	6.63045200	-2.96580200	-1.02388400
C	7.66753800	-3.52504000	1.49158400
C	7.91884700	-3.48692600	-0.91096900
C	8.43237300	-3.76516700	0.35309300
H	3.35866900	6.73029000	-1.32536300
H	3.43960000	7.36752400	1.08306200
H	3.03511900	5.63918900	2.83208000
H	-3.03629800	5.63919800	2.83158800
H	-3.44081900	7.36734300	1.08238000
H	-3.35924300	6.72995600	-1.32600500
H	-8.05495100	-3.73624000	2.48134000
H	-9.43384700	-4.17168900	0.45131300
H	-8.50273400	-3.66989200	-1.80523500
H	8.50316200	-3.66920300	-1.80522200
H	9.43418100	-4.17112600	0.45134600
H	8.05514900	-3.73597700	2.48131200
Cl	2.88354600	4.27279900	-2.61355300
Cl	2.44649200	2.89346100	2.67425200
Cl	-2.44702600	2.89355400	2.67400300
Cl	-2.88340000	4.27251100	-2.61393700
Cl	-5.45244600	-2.71255200	2.81273400
Cl	-6.02051400	-2.63301500	-2.63690400
Cl	6.02094200	-2.63239600	-2.63693900
Cl	5.45250900	-2.71256100	2.81264600
H	0.00019100	-5.37587000	-0.42149300

1e ($T0^{4,D}$)

Sum of electronic and zero-point Energies= -5836.954222

C	3.46913300	-2.95474600	0.07559100
N	2.24475800	-2.39046100	0.11263700
C	1.31659100	-3.38569700	0.17764400
C	0.00009600	-2.91470600	0.19943900
C	-1.31634900	-3.38576700	0.17756600
N	-2.24456600	-2.39056900	0.11234300
C	-3.46889500	-2.95486900	0.07550100
C	-4.63072000	-2.14403500	-0.02293000
C	-4.53652800	-0.74080300	-0.13495700
C	-5.54429000	0.28469400	-0.18156100
C	-4.90694000	1.50212900	-0.22153600
C	-3.48609400	1.26682300	-0.23649600
C	-2.41143400	2.18072500	-0.27902200
C	-1.08335900	1.79051000	-0.57215400
N	-0.00007600	2.53325600	-0.22375900
C	1.08329900	1.79052500	-0.57197600
C	2.41128200	2.18075700	-0.27861200
C	3.48603600	1.26692500	-0.23611200
C	4.90684200	1.50237300	-0.22105300
C	5.54430600	0.28497300	-0.18119400
C	4.53663900	-0.74059000	-0.13476200
C	4.63088800	-2.14386400	-0.02283700
C	3.33218100	-4.41128000	0.13372700
C	1.99360200	-4.67633500	0.18988800

C	-3.33191900	-4.41141200	0.13392900
C	-1.99333800	-4.67642600	0.19007400
N	-3.32968000	-0.09124600	-0.18447100
C	-0.67623400	0.56663800	-1.27562600
C	0.67630600	0.56666200	-1.27556200
N	3.32973000	-0.09114600	-0.18424100
H	1.51976600	-5.64763300	0.23959600
H	4.14263600	-5.12809800	0.12366600
H	6.61014400	0.10701200	-0.18157900
H	5.36652100	2.47878300	-0.27142300
H	1.32733200	-0.14247000	-1.76505700
H	-1.32718000	-0.14251300	-1.76520300
H	-5.36671400	2.47848900	-0.27204400
H	-6.61011100	0.10664400	-0.18198200
H	-4.14237600	-5.12822700	0.12412300
H	-1.51946000	-5.64770000	0.23987100
C	5.98411100	-2.77551100	-0.00976800
C	6.66702000	-3.04871700	1.19046700
C	7.92721700	-3.64478500	1.21440100
C	8.54215200	-3.98649700	0.01281800
C	7.90575700	-3.73571300	-1.19998600
C	6.64599600	-3.13846200	-1.19790500
C	2.68435500	3.60987100	0.05626300
C	2.84709700	4.04644300	1.38335200
C	3.09126800	5.38052100	1.70465900
C	3.18455600	6.32178700	0.68308100
C	3.03493300	5.93463800	-0.64606100
C	2.78693700	4.59569900	-0.94141300
C	-2.68464600	3.60987300	0.05554800
C	-2.78682100	4.59555400	-0.94232700
C	-3.03496400	5.93453200	-0.64728400
C	-3.18515800	6.32189000	0.68173600
C	-3.09228000	5.38078700	1.70349800
C	-2.84794000	4.04666300	1.38249700
C	-5.98389900	-2.77577600	-0.00972100
C	-6.66702400	-3.04827600	1.19055000
C	-7.92717300	-3.64444200	1.21461500
C	-8.54182700	-3.98699500	0.01312800
C	-7.90521000	-3.73693600	-1.19971000
C	-6.64551100	-3.13955500	-1.19775600
H	-2.48305300	-0.66608200	-0.04166300
H	2.48316000	-0.66610900	-0.04143900
Cl	5.92897800	-2.62768700	2.72648600
Cl	5.87656500	-2.84324400	-2.74884900
Cl	2.71897700	2.89702600	2.70403200
Cl	2.62781100	4.14678000	-2.63254900
Cl	-2.62702300	4.14639500	-2.63333300
Cl	-2.72027400	2.89748000	2.70343600
Cl	-5.87581900	-2.84515100	-2.74872000
Cl	-5.92929500	-2.62628500	2.72646300
H	8.41194200	-3.83372600	2.16497100
H	9.52312100	-4.45093600	0.02157900
H	8.37271800	-3.99761400	-2.14209900
H	3.20085700	5.66881800	2.74346900
H	3.37499600	7.36293900	0.92392200
H	3.10892100	6.65579600	-1.45150900
H	-3.10862600	6.65556300	-1.45287500
H	-3.37572200	7.36307600	0.92232800
H	-3.20230300	5.66923600	2.74222000
H	-8.41206700	-3.83282100	2.16521000
H	-9.52275300	-4.45152600	0.02198500
H	-8.37196200	-3.99948700	-2.14174600
H	0.00008600	-1.82934200	0.18979100

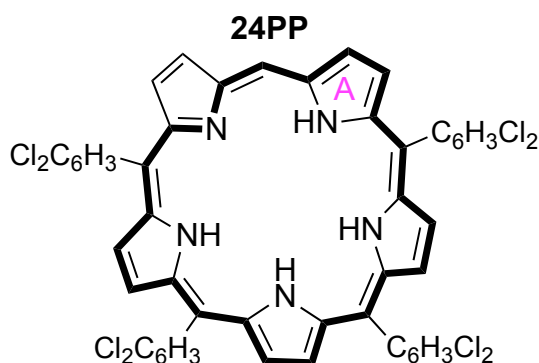
1f($TO^{A,D}$)

Sum of electronic and zero-point Energies= -5836.931034

C	0.35659600	-3.55307100	0.33705700
N	1.66716900	-3.88556800	0.07390000
C	2.39079000	-2.88682500	0.60053300
C	3.78283000	-2.67462900	0.31371400
C	4.21036800	-1.36254300	0.08633500
C	5.50160000	-0.72698800	-0.03953900
C	5.30636000	0.61760700	-0.23660100
C	3.88456500	0.86714200	-0.30286100

C	3.09842400	2.00444700	-0.51796800
C	1.69692200	1.81751500	-0.77142800
N	0.73121600	2.59385700	-0.25660600
C	-0.44687700	1.94524400	-0.53571900
C	-1.67097800	2.38324300	-0.01914800
C	-2.85293900	1.60272400	0.02646500
C	-4.18682500	2.08357600	0.19886400
C	-5.04628700	1.01240800	0.12398100
C	-4.26366900	-0.16758900	-0.05439200
C	-4.70331100	-1.50261600	-0.16408500
C	-3.85641200	-2.62173500	-0.25060100
N	-2.49728300	-2.55944700	-0.10957900
C	-2.04859200	-3.82599900	-0.30630700
C	-0.70365200	-4.25336800	-0.22374400
C	0.26952300	-2.37120800	1.19146700
C	1.54456600	-1.95402400	1.37124000
N	3.29992600	-0.35285700	-0.09097500
C	1.12809200	0.68984200	-1.53012200
C	-0.21506900	0.77034000	-1.37426600
N	-2.94760100	0.23426600	-0.11504600
C	-3.15386100	-4.72720800	-0.61701100
C	-4.28799600	-3.98465800	-0.54536800
H	-0.64212200	-1.97281000	1.61041000
H	1.89808500	-1.15314400	2.00699200
H	6.44807000	-1.24245400	0.04103500
H	6.06787500	1.37476100	-0.35805600
H	1.67878900	-0.00259000	-2.15247500
H	-0.96694300	0.15148500	-1.84312100
H	-4.44695900	3.12470700	0.31864700
H	-6.12406200	1.03292700	0.18740900
H	-2.20402600	-0.46264000	-0.12464800
H	-3.05924800	-5.78559400	-0.82272000
H	-5.30810600	-4.30782400	-0.69804600
H	2.30091700	-0.49467100	-0.05846400
C	-6.18425300	-1.72400300	-0.20700300
C	-6.92399800	-2.02357100	0.95206100
C	-6.91298700	-1.64835900	-1.40857700
C	-8.30139200	-2.23835900	0.92442600
C	-8.28994700	-1.86057300	-1.46188700
C	-8.97955300	-2.15609600	-0.28883900
C	-1.74139200	3.76287600	0.55426600
C	-1.68274700	3.99159100	1.94011300
C	-1.86218900	4.90112100	-0.26175100
C	-1.73413400	5.27161500	2.48824400
C	-1.92094900	6.19117600	0.26215600
C	-1.85418100	6.37022200	1.64130300
C	4.69704400	-3.82535100	0.09981800
C	5.17724100	-4.18537600	-1.17513500
C	5.11537500	-4.63941400	1.17105200
C	6.02000800	-5.27750000	-1.37460400
C	5.95900000	-5.73361300	0.99637500
C	6.40915900	-6.04871300	-0.28310300
C	3.66504600	3.36694400	-0.35141900
C	3.80077800	4.24377100	-1.44645300
C	4.08277400	3.86825100	0.89766700
C	4.31966400	5.52973400	-1.31744900
C	4.60366300	5.15205800	1.05094400
C	4.72069800	5.97956100	-0.06215600
C1	3.34203100	3.71033100	-3.05576500
C1	3.91871400	2.88718300	2.34601200
C1	-1.97039200	4.72037900	-2.00581600
C1	-1.51465400	2.63470400	3.04246600
C1	-6.08124300	-1.28666900	-2.91217900
C1	-6.10934800	-2.12742800	2.50351000
C1	4.68421000	-3.27777900	-2.59673600
C1	4.59599300	-4.26476700	2.80682000
H	4.90243600	5.49316500	2.03510800
H	5.12460900	6.98085700	0.04923100
H	4.40858100	6.16146600	-2.19335700
H	-2.01755900	7.03698700	-0.40828200
H	-1.89584500	7.37149400	2.05829200
H	-1.67633900	5.39640800	3.56311000
H	-8.80533200	-1.79475300	-2.41281000
H	-10.05155800	-2.32290200	-0.32042700
H	-8.82604700	-2.46559600	1.84489800
H	6.25617500	-6.32316200	1.85557900
H	6.35408200	-5.51839800	-2.37685500

H	7.06440200	-6.90137000	-0.43044700
H	-0.46551800	-5.21701500	-0.66742700



6

2a (T0)

Sum of electronic and zero-point Energies= -5838.141244

C	2.87066000	1.45333300	0.51842800
C	3.98486000	1.22392900	1.42478500
C	4.41655400	-0.04841800	1.27161200
C	3.62591400	-0.68993700	0.23241400
N	2.61980600	0.22098300	-0.09798100
C	2.21898900	2.62464600	0.27313300
C	3.87580300	-1.88692100	-0.37766800
C	1.00579500	2.74566600	-0.53979300
N	-0.14310800	2.02580800	-0.26117300
C	-1.21061200	2.53657600	-0.98284700
C	-0.69355900	3.52995700	-1.81540700
C	0.68104200	3.66182200	-1.53599800
C	-2.58810100	2.25608600	-0.64028600
C	-3.07242300	1.10184500	-0.07225100
N	-2.48483000	-0.17137000	-0.06419700
C	-3.33673800	-1.07737800	0.55301700
C	-4.39974500	-0.29164200	1.15234100
C	-4.28379900	0.98553500	0.71331600
C	-3.31865600	-2.45025200	0.41568700
C	3.09440500	-2.44286100	-1.47383100
N	1.71860800	-2.48652500	-1.54075500
C	1.32773600	-3.18722600	-2.67109300
C	2.49719500	-3.52104900	-3.37118800
C	3.58924900	-3.07083600	-2.62503500
C	0.03047000	-3.70221400	-2.90978900
C	-1.11988700	-3.60104200	-2.16217900
N	-1.37429600	-2.71930000	-1.10926300
C	-2.52553100	-3.15057500	-0.56912900
C	-3.02516600	-4.35091400	-1.23536900
C	-2.18288700	-4.58279300	-2.27315900
H	4.37097100	1.97134600	2.10265300
H	5.22617700	-0.53417400	1.79645100
H	-0.25500700	1.46769700	0.57298300
H	-1.26882000	4.10003200	-2.53050200
H	1.37814800	4.34424300	-2.00041900
H	-5.17819000	-0.69965500	1.77946600
H	-4.93357600	1.81801300	0.94105400
H	1.06719500	-2.27972900	-0.79205300
H	2.52085100	-4.05957200	-4.30853900
H	4.63646000	-3.16019800	-2.87359800
H	-3.92195100	-4.89307200	-0.97300500
H	-2.22741000	-5.37647500	-3.00823300
H	-1.80197500	-0.51154600	-0.73608000
H	2.12767000	0.17001000	-0.97946800
C	5.08833800	-2.66717300	0.01476500
C	4.98204400	-3.84010800	0.79028300
C	6.39357600	-2.31409300	-0.38283600
C	6.08629000	-4.60591300	1.15658300
C	7.51624400	-3.06219600	-0.02754600

C	7.35622800	-4.20950100	0.74386600
C	2.74689200	3.88888300	0.87390800
C	3.78938000	4.62594200	0.27897300
C	2.21278400	4.43398100	2.05783900
C	4.26825600	5.82109000	0.81431500
C	2.67184300	5.62526900	2.61558400
C	3.70264900	6.31797900	1.98521200
C	-3.54563700	3.39039500	-0.82762500
C	-4.46737000	3.41253700	-1.89338500
C	-3.56988800	4.50902000	0.02923000
C	-5.35528500	4.46902200	-2.09644900
C	-4.44949600	5.57460800	-0.14987700
C	-5.34202500	5.54927500	-1.21910500
C	-4.34260400	-3.24425900	1.16552600
C	-5.67970700	-3.39087300	0.74383900
C	-4.00218300	-3.92230600	2.35310500
C	-6.61526400	-4.14602300	1.45149500
C	-4.91606700	-4.68462400	3.07899000
C	-6.22656000	-4.79218300	2.62159200
Cl	6.65646100	-0.89560100	-1.38978600
Cl	4.52774800	4.05108000	-1.21098700
Cl	0.93151400	3.57912900	2.90693900
Cl	-4.50956800	2.08790500	-3.04823400
Cl	-2.48282800	4.57255400	1.40637500
Cl	-6.22402900	-2.61821600	-0.73883100
Cl	-2.36167200	-3.81266400	2.97419500
H	8.49727400	-2.74586800	-0.36200200
H	8.22407900	-4.79845900	1.02321800
H	5.94580300	-5.49524900	1.75966700
H	2.22630200	5.99598900	3.53125700
H	4.06723200	7.24804300	2.40960400
H	5.07088000	6.34903600	0.31293800
H	-4.43199400	6.40599800	0.54504800
H	-6.03002100	6.37545800	-1.36837800
H	-6.04097300	4.43779100	-2.93499300
H	-7.63043100	-4.22431600	1.08031200
H	-6.94734900	-5.38296100	3.17807800
H	-4.59759300	-5.18164400	3.98777400
Cl	3.40250100	-4.36744700	1.34956100
H	-0.01319100	-4.39700200	-3.74456700

2b (TI)

Sum of electronic and zero-point Energies= -5838.136132

C	2.13760900	-3.24613200	0.00283600
C	1.37394200	-4.30051000	0.53143200
C	0.27818200	-4.49442800	-0.31779800
C	0.40725200	-3.60666400	-1.40407200
C	-0.42645000	-3.52613100	-2.59571200
C	-1.72855500	-3.13160200	-2.48018400
C	-2.86973000	-3.26813200	-3.36358900
C	-3.97732800	-2.79634900	-2.72172900
C	-3.57440700	-2.24825400	-1.44458700
C	-4.29367000	-1.52363700	-0.51274200
C	-3.67973200	-0.62162900	0.42230400
C	-4.18977000	-0.12600200	1.63265600
C	-3.36519800	0.91061000	2.06191300
C	-2.33361000	1.08628800	1.11550800
C	-1.49387500	2.23605700	0.98328300
C	-0.36371000	2.48012600	0.20041000
C	0.01940000	3.79482400	-0.24808700
C	1.16415200	3.69994800	-0.97747200
C	1.61908300	2.33558600	-0.92778300
C	2.91554100	1.91509100	-1.21425100
C	3.47692200	0.66296900	-0.81296200
N	2.75788100	-0.42731600	-0.49524700
C	3.65986700	-1.31431900	0.08176400
C	3.31672500	-2.60071900	0.47887100
N	-2.21535800	-2.47442000	-1.35574100
N	-2.49951000	0.07831700	0.17293800
N	0.60554500	1.60752900	-0.30886700
N	1.53364900	-2.86943000	-1.18182600
C	4.89164300	0.47618400	-0.49793700
C	4.98778400	-0.73000300	0.12118700
H	1.60262700	-4.84215900	1.43809000

H	-0.49659200	-5.24285600	-0.22789500
H	-2.82286900	-3.71036100	-4.34934600
H	-4.98770500	-2.75719300	-3.10414000
H	-5.07315000	-0.50316100	2.12736900
H	-3.48558300	1.50353600	2.95619400
H	-0.56026000	4.68688000	-0.06504700
H	1.69456700	4.50259100	-1.46697900
H	-1.68018800	-2.37601200	-0.50578500
H	-2.07412800	0.11188400	-0.74268500
H	0.79928800	0.66313300	0.01268800
H	1.79508800	-2.00995100	-1.65244200
H	5.68130900	1.19371400	-0.67114900
H	5.87552700	-1.20531700	0.51584700
C	-1.98419600	3.42661300	1.75902100
C	-1.38885300	3.80314800	2.97888600
C	-3.06431800	4.22256800	1.32986600
C	-1.83406600	4.89271100	3.72725100
C	-3.52333900	5.32094900	2.05524000
C	-2.90360200	5.65014100	3.25830600
C	3.84603000	2.92008500	-1.82166300
C	4.08965000	2.93759400	-3.20895600
C	4.54643800	3.88243100	-1.06724100
C	4.95831600	3.84506200	-3.81343800
C	5.42174400	4.80166200	-1.64598400
C	5.62363000	4.77835000	-3.02322700
C	4.20482700	-3.36363800	1.40423800
C	4.24453300	-3.09752600	2.78701000
C	5.04310800	-4.40097800	0.95046600
C	5.06233300	-3.81045900	3.66321500
C	5.87198100	-5.12459400	1.80570700
C	5.87597500	-4.82431800	3.16555400
C	-5.78226800	-1.61440200	-0.51383900
C	-6.46385800	-2.72635600	0.02111200
C	-6.59795900	-0.59324800	-1.04318000
C	-7.85512600	-2.82105800	0.03632700
C	-7.98966000	-0.66347200	-1.04058300
C	-8.61426200	-1.78296700	-0.49624000
H	-1.34384500	5.13560900	4.66265500
H	-3.25554300	6.50179200	3.83191200
H	-4.35270800	5.90544300	1.67455500
H	5.93525500	5.51996800	-1.01767400
H	6.30317900	5.48950300	-3.48226300
H	5.10494700	3.81380400	-4.88668100
H	5.05206900	-3.56904200	4.71959800
H	6.51688300	-5.38304400	3.84027200
H	6.50470400	-5.90679500	1.40302700
H	-8.32787700	-3.69665600	0.46542300
H	-9.69778700	-1.84690800	-0.48859300
H	-8.56787200	0.14821300	-1.46620900
Cl	-5.85782800	0.82087100	-1.77570500
Cl	-5.55634000	-4.05451300	0.73261500
Cl	3.21527900	-1.84986300	3.47173400
Cl	5.09658300	-4.79602600	-0.76063000
Cl	3.26951100	1.78215900	-4.25006500
Cl	4.34166700	3.94881300	0.67664100
Cl	-0.04814700	2.86956700	3.62491300
Cl	-3.86145400	3.86594800	-0.19393500
H	-0.03714400	-3.83644600	-3.56085700

2e ($T0^{A,D}$)

Sum of electronic and zero-point Energies= -5838.148527

C	0.21950000	-3.47910300	-0.18865400
C	0.14372000	-2.64885500	0.93551700
C	1.45455400	-2.33316700	1.32593800
C	2.33754700	-2.95133300	0.43498500
C	3.78475900	-2.69802900	0.27698500
C	4.14981200	-1.40698200	0.00601500
C	5.45234600	-0.74530900	-0.07367500
C	5.25752500	0.57586300	-0.31733800
C	3.82265000	0.82722200	-0.43695600
C	3.10453700	1.96651100	-0.67871700
C	1.65322300	1.82451500	-0.88391200
C	0.98142100	0.97924900	-1.76665600
C	-0.39454400	1.04463500	-1.47871600

C	-0.56823400	1.93612700	-0.41725600
C	-1.77170900	2.36168000	0.26514600
C	-2.91020800	1.58913600	0.33267100
C	-4.24041100	2.01330500	0.72955400
C	-5.10159400	0.97901000	0.54516100
C	-4.34926400	-0.16438900	0.06252800
C	-4.81057900	-1.43008100	-0.25842500
C	-3.93346600	-2.50240800	-0.65556600
N	-2.60641600	-2.46525000	-0.49558000
C	-2.12305200	-3.65582500	-1.02894900
C	-0.81726200	-4.08299300	-0.96185700
N	0.68937100	2.42100100	-0.09703300
N	-3.04095000	0.25783400	-0.04766100
C	-3.22378700	-4.43435000	-1.58361000
C	-4.35891000	-3.73956500	-1.31588700
N	3.23033700	-0.40738500	-0.24627600
N	1.57056500	-3.67892000	-0.44497800
H	-0.78184000	-2.34660500	1.39963700
H	1.75938900	-1.71876800	2.16108500
H	6.39795200	-1.25031600	0.06633700
H	6.01690800	1.33792400	-0.42472700
H	1.45566100	0.40102700	-2.54663000
H	-1.18954400	0.54168900	-2.00854200
H	-4.48085000	3.01238700	1.06358700
H	-6.16738800	0.97485600	0.72165400
H	0.89510000	2.98495900	0.71460300
H	-2.30359100	-0.41959600	-0.22986100
H	-3.13040900	-5.40049500	-2.06361500
H	-5.37745500	-4.00827400	-1.56090300
H	2.23162200	-0.54536000	-0.21950900
H	1.94368500	-4.12336400	-1.27122000
C	3.76250000	3.30235700	-0.76152000
C	4.18697200	3.85376300	-1.98727300
C	3.97309800	4.10999500	0.37235000
C	4.78845700	5.10789100	-2.08129000
C	4.57185100	5.36681600	0.31011100
C	4.98003400	5.86109300	-0.92591700
C	-1.78052000	3.71995600	0.88750300
C	-1.88977500	4.89442800	0.11349700
C	-1.64816300	3.91279200	2.27790700
C	-1.87912300	6.16929900	0.67624700
C	-1.63641700	5.17825800	2.86502700
C	-1.75252100	6.30526100	2.05668800
C	-6.27890800	-1.69346700	-0.20184500
C	-7.15780700	-1.30942400	-1.23480100
C	-6.87455000	-2.36438200	0.88549900
C	-8.52864600	-1.56313500	-1.19359000
C	-8.24097300	-2.63309500	0.95149100
C	-9.06569000	-2.22770900	-0.09454000
C	4.78755100	-3.78577900	0.45751400
C	5.35579000	-4.08599700	1.71229100
C	5.20631200	-4.60781000	-0.60627900
C	6.27930200	-5.11434300	1.89623900
C	6.12583900	-5.64323700	-0.45484300
C	6.66208600	-5.89115000	0.80616900
H	-1.74420200	7.29423700	2.50389100
H	-1.97554600	7.03775700	0.03519300
H	-1.53214600	5.26860800	3.93988200
H	-9.15719300	-1.24561800	-2.01728600
H	-10.13114400	-2.43131700	-0.05341800
H	-8.64457900	-3.14949800	1.81453900
H	6.68643300	-5.29821500	2.88360100
H	7.37916800	-6.69483400	0.93982000
H	6.41141100	-6.24079200	-1.31253300
H	5.10024100	5.48113700	-3.04974100
H	5.44719500	6.83875200	-0.98928600
H	4.70986100	5.94319000	1.21735500
Cl	3.97347200	2.93866500	-3.47045200
Cl	3.44693600	3.53753500	1.95604300
Cl	-1.46295600	2.52568900	3.34372100
Cl	-2.07837700	4.77392000	-1.62669000
Cl	-6.53014600	-0.48899800	-2.65778700
Cl	-5.87870100	-2.88140400	2.23752300
Cl	4.90252200	-3.13887600	3.12024800
Cl	4.54562400	-4.34168000	-2.22256100
H	-0.56307300	-4.98038100	-1.52374200

2e' (T0^{A,D})

Sum of electronic and zero-point Energies= -5838.141506

C	2.02619400	-1.14974500	-0.67911700
C	1.56974700	-0.40695900	-1.76899900
C	2.44709900	0.67693400	-1.94547100
C	3.42461400	0.62145600	-0.94271100
C	4.38483200	1.64293800	-0.49953300
C	3.91237900	2.92348800	-0.33472200
C	4.52789100	4.15085200	0.16546900
C	3.56655700	5.10841100	0.27184400
C	2.29473900	4.54946600	-0.17061300
C	1.01639300	5.03641900	-0.16993400
C	-0.06772800	4.20539200	-0.66908200
C	-0.07904500	3.31925800	-1.75168100
C	-1.26584200	2.56422400	-1.69633500
C	-1.99513800	3.00000800	-0.59289900
C	-3.29868900	2.57838300	-0.12489900
C	-3.72717900	1.27293700	-0.16595100
C	-5.09111500	0.81012400	0.00779500
C	-5.11522900	-0.53737500	-0.13325400
C	-3.75467100	-1.00461600	-0.33680300
C	-3.33147500	-2.32192900	-0.34622000
C	-1.95808400	-2.75456500	-0.29576700
N	-0.88891600	-1.96149800	-0.42615200
C	0.21023600	-2.76926600	-0.12090100
C	1.53429000	-2.37491000	-0.11322700
N	-2.96572600	0.12595200	-0.40493300
C	-0.23357200	-4.12232300	0.19885800
C	-1.57800000	-4.12907800	0.05097300
N	3.18256100	-0.52665900	-0.22596000
N	-1.26974800	4.02886400	-0.01136000
N	2.60018700	3.26414200	-0.58282100
H	0.71488000	-0.67439600	-2.37053900
H	2.41452700	1.41795700	-2.73070500
H	5.57215600	4.24406400	0.42867200
H	3.69529500	6.12125800	0.62986900
H	0.67821900	3.27448700	-2.52004000
H	-1.60410500	1.82558200	-2.40826600
H	-5.93096800	1.46601300	0.18552000
H	-5.97584400	-1.18671300	-0.07224700
H	-1.95251200	0.05386000	-0.43398200
H	0.40966200	-4.95097300	0.46038900
H	-2.25577600	-4.95845500	0.19543700
H	3.63734500	-0.74853700	0.64738300
H	-1.47641500	4.41301400	0.89845500
H	1.88747200	2.57384700	-0.77262500
C	2.55452300	-3.27966000	0.51167800
C	2.76310100	-3.32001900	1.90357200
C	3.38327100	-4.11549800	-0.26232300
C	3.72008100	-4.14494000	2.49515300
C	4.34278700	-4.95172700	0.30560100
C	4.50678400	-4.96220200	1.68874100
C	5.77662000	1.26312400	-0.13951500
C	6.23251800	1.16704400	1.19224200
C	6.73094300	0.94009900	-1.12903600
C	7.53702400	0.80136900	1.52285200
C	8.03725700	0.56305800	-0.82632900
C	8.43809800	0.49919500	0.50603700
C	-4.23460900	3.63570600	0.37077600
C	-4.97613600	4.45111800	-0.50816100
C	-4.40039000	3.90673000	1.74300800
C	-5.83352800	5.45417700	-0.05899900
C	-5.25161600	4.90347700	2.21935000
C	-5.96855800	5.67538000	1.30949000
C	-4.38947300	-3.38036600	-0.28589500
C	-4.88052900	-3.99889200	-1.45236600
C	-4.94566800	-3.83616300	0.92584200
C	-5.85614300	-4.99495700	-1.42651500
C	-5.92286400	-4.82991000	0.98130300
C	-6.37512000	-5.40720100	-0.20220500
H	0.81356200	6.00906100	0.26693900
H	8.72743200	0.33279400	-1.62953000
H	9.45489300	0.21009400	0.75222000
H	7.82996200	0.74578000	2.56472800

H	4.94685000	-5.58408100	-0.33442300
H	5.25208700	-5.60980100	2.13957300
H	3.83964200	-4.13832900	3.57216900
H	-6.19805000	-5.43480000	-2.35605400
H	-7.13472500	-6.18198500	-0.17005100
H	-6.31595100	-5.14178400	1.94188800
H	-5.34219200	5.06708900	3.28679600
H	-6.63458600	6.45384600	1.66792800
H	-6.38687600	6.04672100	-0.77815200
Cl	5.12194600	1.47330800	2.52670700
Cl	6.28624700	1.03694500	-2.82463200
Cl	1.81660800	-2.28270300	2.96202500
Cl	3.20208800	-4.14620700	-2.00704000
Cl	-4.40298400	-3.14713300	2.44884100
Cl	-4.25767400	-3.51227500	-3.02183200
Cl	-4.85409400	4.19805700	-2.24017700
Cl	-3.48389900	2.98400700	2.93084500

2f($TO^{4,D}$)

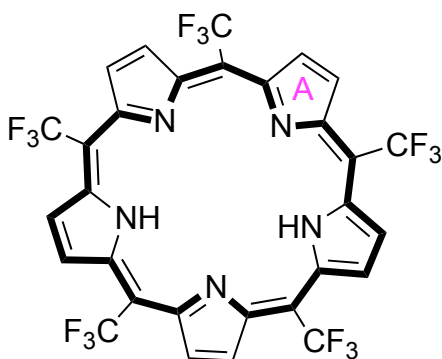
Sum of electronic and zero-point Energies= -5838.146630

C	3.50638800	-2.94704600	-0.02721000
N	2.31288100	-2.42687900	0.23100100
C	1.36453300	-3.43260800	0.06836400
C	0.06791000	-3.02221500	0.26542900
C	-1.24382000	-3.51955000	0.03923300
N	-2.25939600	-2.61321000	0.31813700
C	-3.47796900	-3.05573700	-0.11663800
C	-4.65117200	-2.19705700	-0.04235100
C	-4.53156000	-0.82123300	-0.03912100
C	-5.53079000	0.20432200	0.21517100
C	-4.93253900	1.42594100	0.18370000
C	-3.51941100	1.25578600	-0.10735900
C	-2.50846700	2.18216900	-0.20832300
C	-1.14849600	1.79272700	-0.56112900
N	-0.02400400	2.40843200	-0.03848600
C	1.13117000	1.77116400	-0.45905300
C	2.47273300	2.19592600	-0.07884100
C	3.51282100	1.29411500	-0.00387400
C	4.94993400	1.52241300	0.07505900
C	5.58264200	0.31798000	0.03952400
C	4.57382900	-0.73087100	-0.02396700
C	4.69379200	-2.11364800	-0.04353300
C	3.37409200	-4.37521400	-0.33719800
C	2.04033600	-4.66546800	-0.29633600
C	-3.25142700	-4.32952500	-0.66816600
C	-1.87498800	-4.61239400	-0.57587600
N	-3.34520500	-0.11963500	-0.22935700
C	-0.68074700	0.76193200	-1.38239000
C	0.72480800	0.74297600	-1.31268000
N	3.36348900	-0.07702000	-0.05939700
H	1.57269800	-5.62517600	-0.47302800
H	4.18569000	-5.05353500	-0.56666700
H	6.64876900	0.14109100	0.05786600
H	5.41025100	2.49989400	0.10664500
H	1.38727100	0.09355000	-1.86413000
H	-1.28701400	0.16005000	-2.04534100
H	-5.40347700	2.38325400	0.35615700
H	-6.56771500	-0.00629400	0.43462700
H	-4.00645200	-4.94716600	-1.13300500
H	-1.37308300	-5.48713600	-0.96432300
C	6.03993100	-2.74776400	-0.09459000
C	6.62493500	-3.34862600	1.03947200
C	7.87495200	-3.96466000	1.00946600
C	8.59089100	-3.99489100	-0.18435300
C	8.05985200	-3.41744900	-1.33427100
C	6.80482200	-2.81191700	-1.27772100
C	2.71947600	3.64180600	0.18622300
C	2.93599600	4.14549900	1.48668900
C	3.15659900	5.49865600	1.74408800
C	3.15646000	6.40314900	0.68627900
C	2.93925400	5.95921500	-0.61600100
C	2.72582500	4.60207600	-0.84876300
C	-2.79291000	3.62070800	0.07166500
C	-2.94600600	4.56142400	-0.96799300

C	-3.19232000	5.91202000	-0.72906600
C	-3.29070100	6.36599400	0.58413900
C	-3.14195600	5.47940100	1.64682500
C	-2.89372700	4.13273600	1.38097100
C	-5.99172500	-2.83756500	0.02176600
C	-6.42869000	-3.52648500	1.17323100
C	-7.66710900	-4.15903400	1.25095100
C	-8.52384400	-4.11518600	0.15362800
C	-8.14276400	-3.44787000	-1.00685700
C	-6.89469800	-2.82783200	-1.06214000
H	-2.50075800	-0.52815900	-0.59097900
H	2.51371600	-0.63682300	0.06949500
Cl	5.77332700	-3.31567300	2.57611700
Cl	6.17225400	-2.12764700	-2.76940500
Cl	2.90185700	3.05819400	2.86941300
Cl	2.49558600	4.09046000	-2.51128600
Cl	-2.85326000	4.03103000	-2.63737000
Cl	-2.67819500	3.06081700	2.76114400
Cl	-6.45558300	-2.03821200	-2.57114600
Cl	-5.40162500	-3.57649100	2.59846600
H	8.27629000	-4.40636000	1.91404400
H	9.56593200	-4.47069800	-0.21872900
H	8.60250400	-3.43770400	-2.27206500
H	3.31818000	5.82965500	2.76328200
H	3.32641700	7.45812100	0.87685800
H	2.94314700	6.65059800	-1.45059200
H	-3.30918400	6.59089700	-1.56569600
H	-3.48343700	7.41605600	0.77984200
H	-3.21034800	5.81932400	2.67354200
H	-7.95214500	-4.66903900	2.16362000
H	-9.49198500	-4.60330200	0.20347200
H	-8.79633200	-3.41122200	-1.87048800
H	0.05633200	-1.98825000	0.60729500
H	-0.04792500	3.12604600	0.67040700
H	-2.13270400	-1.81136000	0.91731200

Meso-pentakis(trifluoromethyl)-substituted pentaphyrins (9)

22PP



9

1a (*T0*)

Sum of electronic and zero-point Energies= -2921.330254

C	-0.62835400	-3.20447600	-0.11999900
N	-1.19967500	-2.08253700	0.28414900
C	-2.04369700	-2.44748000	1.33238300
C	-3.02153800	-1.58650800	1.80950600
C	-3.36368400	-0.35030600	1.18475300
C	-4.60005000	0.34865600	1.21006000
C	-4.55827800	1.30538800	0.21163700
C	-3.26930400	1.25683400	-0.38000900
C	-2.71976600	2.15392100	-1.35602600
C	-1.43035300	2.65212700	-1.34268500
N	-0.49442200	2.31587700	-0.36078000

C	0.39350600	3.30204200	-0.38327200
C	1.49690900	3.45330400	0.54397500
C	2.38758700	2.47159200	0.91909400
C	3.64788200	2.67704700	1.62160300
C	4.37475100	1.54139300	1.54454900
C	3.60450700	0.54957800	0.80767800
C	4.02096400	-0.67832800	0.33078400
C	3.21004700	-1.52882900	-0.50555800
N	1.89358700	-1.62934900	-0.38570100
C	1.51821500	-2.62242600	-1.29262000
C	0.34441800	-3.32829000	-1.19682200
C	0.11977700	4.27729400	-1.44872400
C	-0.98430100	3.83627600	-2.08774700
N	2.39142100	1.14782000	0.51585400
C	2.68328600	-3.03283900	-2.10194300
C	3.74556900	-2.39876200	-1.56933300
N	-2.57887300	0.25663800	0.23722200
C	-1.06503600	-4.35941400	0.66828100
C	-1.90070000	-3.87430200	1.61804800
H	0.71137200	5.15439600	-1.66775900
H	-1.48960300	4.29183100	-2.92397300
H	1.62536600	0.66086600	0.06174800
H	5.37112100	1.38693500	1.91999600
H	3.95108500	3.60831200	2.06943200
H	2.67845700	-3.75530200	-2.90214900
H	4.78304000	-2.47759400	-1.85897200
H	-1.67130800	-0.12667300	-0.02447700
H	-5.42918900	0.13154100	1.86362000
H	-5.33599400	2.00576100	-0.04931600
H	-0.74258900	-5.38034500	0.52140000
H	-2.41165600	-4.42768200	2.38923400
C	1.79198600	4.87580200	0.97916200
C	-3.71151600	2.75962500	-2.34105300
C	-3.94619400	-2.04710400	2.92526900
C	0.11552000	-4.52036800	-2.11227000
C	5.44040600	-1.14970300	0.54414800
F	0.71022000	5.67049700	0.86152900
F	2.78052500	5.44613100	0.24185500
F	2.18223200	4.95165800	2.27429500
F	-3.17723800	2.87875600	-3.57738400
F	-4.11150300	3.99398000	-1.95799700
F	-4.82101500	2.00744300	-2.47565000
F	-4.38635600	-1.00778300	3.66735500
F	-5.03721400	-2.67693100	2.43548700
F	-3.34213900	-2.89449300	3.78274500
F	-1.19231100	-4.83928500	-2.17900800
F	0.52252100	-4.28630100	-3.37923400
F	0.77166400	-5.62656500	-1.68057100
F	6.25048600	-0.80698200	-0.49205100
F	5.49686300	-2.49588600	0.64508100
F	6.01551700	-0.66109000	1.66563700

1c ($T0^A$)

Sum of electronic and zero-point Energies= -2921.319094

C	1.09465400	2.66262700	1.00512800
N	0.00873700	3.45945400	0.85004700
C	-1.04844200	2.65431800	1.09043200
C	-2.34201600	3.02288200	0.65092900
C	-3.21256900	2.09457000	0.07089600
C	-4.50734400	2.29994900	-0.52273200
C	-4.91375600	1.12599700	-1.09199300
C	-3.89736800	0.13602400	-0.84497100
C	-3.88510800	-1.24356800	-1.10239800
C	-2.96782300	-2.15076400	-0.51946800
N	-1.74083100	-1.83302200	0.00061500
C	-1.33766300	-2.94593700	0.67440000
C	-0.06525900	-3.27705500	1.20907200
C	1.24285900	-2.98325500	0.75053800
C	2.28887200	-3.97043800	0.76469300
C	3.32674000	-3.51185000	0.00640100
C	3.02375600	-2.17358200	-0.39826600
C	3.93153200	-1.26871300	-0.98707200
C	3.89111100	0.13081100	-0.82115800
N	2.86014200	0.74424900	-0.19354700

C	3.20933400	2.05665600	-0.08425000
C	2.34926600	3.02210700	0.47537900
C	-3.33053500	-3.53161400	-0.21260400
C	-2.36925900	-3.99346700	0.61431100
N	-2.90072500	0.76605900	-0.14933100
C	0.72543100	1.35497400	1.56169900
C	-0.62731900	1.34672400	1.61269200
N	1.73949700	-1.90598000	0.04720100
C	4.52152100	2.29292700	-0.69343000
C	4.94389000	1.09831200	-1.16418000
H	-5.04420500	3.23377300	-0.50737300
H	-5.84107300	0.94642400	-1.60915400
H	2.21331200	-4.94229800	1.22288700
H	4.24502900	-4.03185000	-0.21015600
H	-4.22796100	-4.04188800	-0.52433700
H	-2.31065900	-4.97397700	1.05868500
H	-2.03714600	0.27770900	0.07838400
H	1.41951000	0.60189000	1.89944600
H	-1.26896900	0.58056200	2.02638700
H	1.31958500	-0.98561300	-0.03554900
H	5.03660800	3.23898900	-0.73925500
H	5.87415500	0.88415000	-1.66402500
C	-0.09566700	-4.35252500	2.29984300
C	-5.05251800	-1.83813000	-1.86750400
C	-2.69765100	4.49833900	0.55884100
C	2.70616200	4.49141700	0.30885800
C	5.14780000	-1.88912500	-1.65704800
F	0.95094700	-4.23237600	3.14407400
F	-0.05930200	-5.62239300	1.81183000
F	-1.20437300	-4.25752300	3.05953500
F	-4.68198100	-2.92299200	-2.57975400
F	-6.05731700	-2.22951500	-1.04650400
F	-5.58537000	-0.96755900	-2.75373400
F	-4.01026300	4.69432200	0.86982600
F	-1.99142400	5.25019600	1.40731800
F	-2.51873200	4.98130200	-0.68715200
F	1.95939300	5.30740800	1.05706500
F	3.99925800	4.70524200	0.68066800
F	2.60198700	4.88491300	-0.97867400
F	6.15353400	-2.10774200	-0.77722100
F	4.86258200	-3.07887200	-2.23207200
F	5.64087100	-1.11050800	-2.64221100

1d ($T0^D$)

Sum of electronic and zero-point Energies= -2921.318148

C	-1.07949000	-2.96661500	0.40961800
N	-1.69776600	-1.85463200	0.00900200
C	-2.85066300	-2.28852600	-0.64649100
C	-3.91746300	-1.46392900	-1.00753500
C	-4.05287500	-0.09950000	-0.63224300
C	-5.16051200	0.79930200	-0.71607300
C	-4.76527400	2.00751000	-0.18955800
C	-3.40313500	1.89277800	0.21953900
C	-2.50137300	2.88905100	0.66219000
C	-1.18566800	2.58977100	1.02771600
N	-0.15281900	3.43063800	0.70853600
C	0.95591500	2.70243300	0.87926900
C	2.20982700	3.14186800	0.34454200
C	3.11731800	2.25190600	-0.20937400
C	4.42036700	2.48647000	-0.80025400
C	4.93303600	1.29611100	-1.21163300
C	3.98155400	0.25522500	-0.87636100
C	4.10353100	-1.13161500	-0.92690000
C	3.20027000	-2.01288400	-0.25303000
N	1.90480100	-1.75461200	0.00251000
C	1.47518000	-2.78511700	0.82005700
C	0.17460000	-3.17505600	1.12067400
C	-2.88037400	-3.74752200	-0.71431000
C	-1.82133900	-4.17191800	0.00580400
N	-3.02693800	0.59372500	-0.05020000
C	0.66464100	1.40249100	1.49588200
C	-0.68672000	1.32708500	1.57388900
C	3.65013700	-3.25160500	0.39451300
C	2.61564700	-3.67304600	1.14555600

N	2.90494800	0.88490700	-0.31138300
H	-3.63462200	-4.35318200	-1.18959700
H	-1.52410300	-5.18945000	0.21018900
H	-2.11596500	0.15225100	0.08260000
H	-5.36206000	2.89950800	-0.09880200
H	-6.13377600	0.56086500	-1.10793500
H	1.38163800	0.68669900	1.87258200
H	-1.27538900	0.53892200	2.02226300
H	4.63715500	-3.68315100	0.32778900
H	2.58498200	-4.54877600	1.77277200
H	4.89046500	3.45250000	-0.87156200
H	5.89289600	1.12777800	-1.67059900
H	2.06205900	0.36014800	-0.08591500
C	0.03664000	-4.24294500	2.21067200
C	-5.07125100	-2.13024100	-1.74671100
C	-2.92584900	4.34205300	0.49931100
C	2.41961400	4.63928800	0.19706800
C	5.36673000	-1.73929000	-1.48772200
F	-1.21183900	-4.26524600	2.71792100
F	0.30571000	-5.50470400	1.77668700
F	0.86610500	-4.00411600	3.24907200
F	5.13506300	-2.95887400	-2.01865200
F	6.32750400	-1.90294200	-0.54176500
F	5.91282400	-0.98695100	-2.46989700
F	3.73958100	4.97088300	0.23303400
F	1.83381200	5.32413300	1.18784900
F	1.93609000	5.09676800	-0.97415700
F	-2.15741000	5.19008200	1.18531100
F	-4.19682300	4.51571100	0.95957400
F	-2.92524300	4.71767700	-0.79545200
F	-5.90807600	-1.24924300	-2.33254600
F	-5.81703400	-2.89460500	-0.91782500
F	-4.62548500	-2.93362800	-2.73711800

1e ($T0^{4,D}$)

Sum of electronic and zero-point Energies= -2921.340584

C	3.33536100	-2.48869700	0.08891200
N	2.27813900	-1.89784000	0.68853100
C	1.26397300	-2.80189200	0.70710700
C	0.00801700	-2.38728900	1.19211400
C	-1.24876000	-2.82427700	0.71173100
N	-2.26138800	-1.92723900	0.67252600
C	-3.32219500	-2.53384100	0.08268000
C	-4.45812600	-1.77205700	-0.27607300
C	-4.42582200	-0.35942900	-0.33135500
C	-5.44228100	0.60612900	-0.65350000
C	-4.87732100	1.85578700	-0.59384800
C	-3.47865900	1.70213100	-0.28610400
C	-2.40637200	2.61953400	-0.24774600
C	-1.07418500	2.21663200	-0.48913800
N	0.00382100	2.94075400	-0.09760600
C	1.08562100	2.22432500	-0.48010100
C	2.41780200	2.63836100	-0.23466500
C	3.49430300	1.73067000	-0.26488200
C	4.89408100	1.89731200	-0.56963800
C	5.46940500	0.65503100	-0.63772300
C	4.46049200	-0.32597500	-0.32127800
C	4.48436200	-1.73583000	-0.26217600
C	3.01200500	-3.88456400	-0.23154700
C	1.70487100	-4.05707700	0.09838700
C	-2.98983500	-3.93454700	-0.20693900
C	-1.68279900	-4.09423000	0.13238700
N	-3.27488300	0.35432100	-0.12078800
C	-0.66185700	1.02129900	-1.24442600
C	0.68746500	1.02608200	-1.23919100
N	3.30369000	0.38023100	-0.10435000
H	1.12463600	-4.96190500	-0.00717600
H	3.67926600	-4.60777400	-0.67594200
H	6.49156500	0.43274400	-0.89602400
H	5.36828000	2.84121500	-0.78165800
H	1.34967800	0.34155100	-1.74766700
H	-1.31536900	0.33219800	-1.75800300
H	-5.35936400	2.79476700	-0.80996500
H	-6.46410700	0.36963000	-0.90481900

H	-3.64839000	-4.67205600	-0.63825000
H	-1.10028700	-5.00032100	0.05170000
H	-2.46702800	-0.12679300	0.29235900
H	2.49865300	-0.10768800	0.30796900
C	-5.72818000	-2.43667600	-0.75432900
C	-0.00265400	-1.20469700	2.16790600
C	2.64715200	4.10386800	0.08805800
C	5.70134600	-2.47971700	-0.75833100
C	-2.64921200	4.07904300	0.09392900
F	-5.88475800	-2.30948400	-2.09242200
F	-5.77011300	-3.75385900	-0.47149500
F	-6.82212800	-1.88112300	-0.18063400
F	-1.07832300	-1.24799700	2.97490300
F	-0.01388200	0.00085100	1.54645400
F	1.07258000	-1.22735300	2.97589000
F	5.61125700	-2.75112400	-2.08208100
F	5.85716900	-3.66387100	-0.12725900
F	6.84808600	-1.78943400	-0.57320300
F	3.96726300	4.42171700	0.10584800
F	2.06630100	4.90856500	-0.81807600
F	2.15656100	4.41617300	1.29905000
F	-2.05587600	4.90134700	-0.78733900
F	-3.97127200	4.38872100	0.09063200
F	-2.18410700	4.37357900	1.31950300

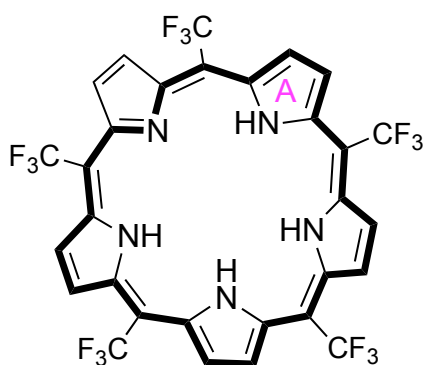
1f ($TO^{A,D}$)

Sum of electronic and zero-point Energies= -2921.321451

C	-0.17445600	-2.77571700	-0.41821500
N	-1.48790300	-3.17252700	-0.21759400
C	-2.23113300	-2.26403100	-0.83118700
C	-3.67076000	-2.18965100	-0.69937300
C	-4.23927300	-0.95926200	-0.40915400
C	-5.59756900	-0.44772800	-0.30157000
C	-5.53948600	0.87843800	0.01343100
C	-4.14297400	1.25730200	0.16971900
C	-3.47075300	2.41664400	0.52627400
C	-2.04503200	2.35146700	0.75679200
N	-1.18650700	3.24634000	0.28140900
C	0.07069900	2.74075700	0.54909000
C	1.24904600	3.32556400	0.09238000
C	2.51044600	2.66325400	0.01768100
C	3.78914700	3.27504400	-0.12641500
C	4.73975600	2.28555300	-0.18450100
C	4.07428900	1.02741800	-0.10043400
C	4.65135300	-0.27219400	-0.13516200
C	3.95345900	-1.48068000	-0.03295100
N	2.56958900	-1.53529800	-0.01466900
C	2.25311100	-2.83348800	0.15767900
C	0.91717600	-3.37340400	0.19079000
C	-0.12078500	-1.61088700	-1.31376000
C	-1.40613700	-1.28093100	-1.56992800
N	-3.43481600	0.11507800	-0.11517400
C	-1.35451200	1.25602200	1.46532400
C	-0.02952600	1.49884400	1.32383500
N	2.73088900	1.29893100	0.03587300
C	3.45575400	-3.65534300	0.28756400
C	4.51046200	-2.82455500	0.13473400
H	0.78217300	-1.16681600	-1.70211200
H	-1.77569200	-0.51572700	-2.24005500
H	-6.48432500	-1.03859500	-0.46588700
H	-6.37159500	1.54927700	0.15487700
H	-1.82282100	0.47519600	2.04988100
H	0.78626600	0.95184900	1.77504500
H	3.96233500	4.33772300	-0.15305700
H	5.80367000	2.42470800	-0.27471100
H	2.05321800	0.53873200	0.03688800
H	3.47768700	-4.72300100	0.43606900
H	5.55097100	-3.09422500	0.16251500
H	-2.42674800	0.06818300	-0.10243000
C	1.28198000	4.78058400	-0.37844900
C	6.17070800	-0.24124100	-0.28389100
C	0.79291800	-4.71772900	0.90597200
C	-4.47385700	-3.46231700	-0.66323900
C	-4.14594700	3.76285000	0.49239400

F	-5.48635600	3.65266600	0.69011600
F	-3.97539400	4.38037500	-0.69335700
F	-3.67180700	4.57892500	1.44882500
F	0.10249000	5.38837500	-0.42352500
F	2.07069700	5.50896100	0.46129300
F	1.83702100	4.87174800	-1.61027400
F	6.52325200	0.45033900	-1.39379900
F	6.74927700	0.38010900	0.76989400
F	6.75668700	-1.44477900	-0.39390300
F	1.49182200	-4.69792600	2.06846200
F	1.34034300	-5.69919100	0.13770200
F	-0.44701100	-5.09395200	1.20325300
F	-4.02955900	-4.35030300	-1.56966300
F	-4.42551800	-4.05552500	0.54553500
F	-5.78511300	-3.23187300	-0.93817300

24PP



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2a (T0)

Sum of electronic and zero-point Energies= -2922.555479

C	2.72107200	2.45537500	-0.65014100
C	2.86585000	3.44842700	-1.71276300
C	1.64438200	3.93009300	-2.03164100
C	0.65243500	3.32561600	-1.14233600
N	1.34923500	2.36675100	-0.41550800
C	3.63912300	1.71058300	0.03259900
C	-0.65521000	3.64131200	-0.91629300
C	3.26407900	0.56482300	0.86854800
N	2.57191900	-0.50365700	0.33138900
C	2.57359800	-1.57158700	1.21495500
C	3.20245800	-1.12176100	2.37875500
C	3.63331700	0.20049500	2.16006200
C	2.24461800	-2.91032500	0.75609400
C	1.29299400	-3.20482700	-0.19282800
N	0.19786400	-2.38857600	-0.51344600
C	-0.59549000	-3.00258000	-1.46500500
C	0.15269700	-4.16083600	-1.92747100
C	1.22728200	-4.32375600	-1.11852100
C	-1.92549300	-2.70772300	-1.70673200
C	-1.40474600	3.09185200	0.22496300
N	-1.79580000	1.78640900	0.34055500
C	-2.54056200	1.61237100	1.49541400
C	-2.57122600	2.86000900	2.14690500
C	-1.87363500	3.77483800	1.35205600
C	-3.30314200	0.42484500	1.73730500
C	-3.30063200	-0.68968700	0.91454800
N	-2.29157700	-0.93619500	-0.02819700
C	-2.73365900	-1.95535900	-0.77229700
C	-4.06896000	-2.37978200	-0.36572900
C	-4.38647500	-1.64325600	0.72814500
H	3.80495700	3.71494800	-2.16834300
H	1.41420200	4.66961800	-2.78060900
H	2.34757600	-0.58892800	-0.64915100

H	3.34599900	-1.70730100	3.27251100
H	4.17019900	0.83123600	2.85197400
H	-0.16001200	-4.80901500	-2.72977500
H	1.95978200	-5.11197200	-1.17081100
H	-1.67836800	1.02420500	-0.32368200
H	-3.06856200	3.06623600	3.08045200
H	-1.71601500	4.82512600	1.54627600
H	-4.64571700	-3.17250000	-0.81811100
H	-5.29440100	-1.69527000	1.30678000
H	-0.20916600	-1.68532100	0.09924300
H	0.97723400	1.94995400	0.42621700
C	-2.66027200	-3.49395100	-2.75833100
C	-4.29020900	0.52892900	2.88796600
C	-1.35567600	4.74898200	-1.64901600
C	5.12061600	1.94374200	-0.07293700
C	3.18253900	-3.98339300	1.26102100
F	-2.64747700	4.43564300	-1.88098900
F	-1.36046600	5.90629100	-0.93478300
F	-0.79927700	5.03903400	-2.84928400
F	5.45220100	3.02097100	-0.82061600
F	5.75707700	0.87849800	-0.61183800
F	5.66831900	2.14186900	1.15160300
F	3.21451000	-3.99080500	2.61739900
F	2.83058000	-5.23290000	0.88741700
F	4.45178400	-3.78804400	0.84168200
F	-1.88553200	-3.76581900	-3.83695300
F	-3.12009200	-4.69315100	-2.30652800
F	-3.73779300	-2.81832600	-3.21288000
F	-4.84080000	-0.65031800	3.23643700
F	-5.30307600	1.37647900	2.60552700
F	-3.67765100	1.00002800	4.00155000

2d (TI^A)

Sum of electronic and zero-point Energies= -2922.570180

C	0.25755600	-2.62900900	0.16461100
C	0.11829300	-2.50782300	1.55585200
C	1.39604800	-2.32393900	2.10932600
C	2.31875100	-2.29156800	1.06043200
N	1.60325000	-2.46857000	-0.10522100
C	-0.71297600	-3.06077800	-0.81791600
C	3.74681900	-1.97155900	1.04062600
C	-2.05790900	-2.74449300	-0.74750900
N	-2.56905100	-1.64646400	-0.06712500
C	-3.94504600	-1.63225500	-0.10639800
C	-4.33693700	-2.85261300	-0.78696400
C	-3.21259400	-3.47987900	-1.22490300
C	-4.70717400	-0.55070100	0.33763000
C	-4.14551000	0.74734300	0.57890600
N	-2.85582400	1.04124700	0.35693500
C	-2.71248600	2.40121600	0.58940800
C	-3.99453900	2.95364600	1.04133500
C	-4.88576900	1.93659300	1.01289000
C	-1.53527100	3.08321900	0.30620300
C	4.18975000	-0.87324300	0.34435000
N	3.29498700	-0.01418800	-0.27542800
C	3.89931900	1.16985100	-0.66410100
C	5.32385000	0.95582800	-0.44021100
C	5.49591100	-0.25247000	0.15863000
C	3.15056500	2.26359100	-1.03552100
C	1.69835300	2.14298000	-1.07922600
N	0.85977800	2.95943500	-0.36543800
C	-0.44344200	2.48942900	-0.41722000
C	-0.42293300	1.36571500	-1.26241800
C	0.89797300	1.14764400	-1.66343800
H	-0.81490700	-2.59295700	2.09313000
H	1.64180700	-2.19603900	3.15288300
H	-2.06820200	-0.79074800	0.18063000
H	-5.35320000	-3.16791400	-0.95036200
H	-3.16482200	-4.40814000	-1.77042000
H	-4.19635500	3.98145400	1.29084400
H	-5.93476300	1.97854800	1.26129900
H	2.29710200	-0.07240600	-0.12918000
H	6.09475200	1.66490600	-0.69433100
H	6.42886300	-0.68935300	0.47544700

H	-1.29926400	0.81111000	-1.55283300
H	1.25370300	0.38349600	-2.33970800
H	1.17532900	3.72386100	0.21287000
H	2.01365200	-2.59398200	-1.01819500
C	-1.33602700	4.53344900	0.69056100
C	3.72764700	3.62936400	-1.22629400
C	-6.20263800	-0.66400100	0.47096900
C	-0.20099400	-4.02254800	-1.85704200
C	4.62530000	-2.79492700	1.92964800
F	-2.31487300	5.07221400	1.43377400
F	-0.18955100	4.68020100	1.42951300
F	-1.18022900	5.31503200	-0.39979100
F	3.34115900	4.18051600	-2.39585200
F	3.29087600	4.48343900	-0.24739700
F	5.07559300	3.66371300	-1.19159400
F	4.28538000	-2.64483700	3.23679200
F	5.93721600	-2.48145600	1.82856600
F	4.51107900	-4.11376100	1.65648100
F	0.29535300	-5.15526300	-1.31638700
F	-1.11260000	-4.38051900	-2.77879700
F	0.83759100	-3.45429100	-2.55554400
F	-6.86236500	0.12399700	-0.41375600
F	-6.67335500	-1.91960800	0.29889400
F	-6.61560900	-0.27386800	1.70493900

2e ($T0^{A,D}$)

Sum of electronic and zero-point Energies= -2922.569669

C	-0.19945200	-2.66681000	-0.26480500
C	-0.09296000	-1.80616200	-1.36615200
C	-1.39086800	-1.51050100	-1.81166300
C	-2.29341300	-2.18639500	-0.98625300
C	-3.75896200	-2.03624200	-0.88777700
C	-4.24338400	-0.81679600	-0.49976400
C	-5.58461000	-0.23858700	-0.36907800
C	-5.46668500	1.05223500	0.02883800
C	-4.04617700	1.36518700	0.20487200
C	-3.35461200	2.47570800	0.61226700
C	-1.90766700	2.36042600	0.82887900
C	-1.19716000	1.40247300	1.55619700
C	0.17319300	1.62397700	1.34060200
C	0.30365500	2.72120300	0.48109700
C	1.50565000	3.30069200	-0.08073000
C	2.67532100	2.59536500	-0.26770700
C	3.98233000	3.13840800	-0.59926200
C	4.88023300	2.12688900	-0.64499500
C	4.18558800	0.87829900	-0.35753200
C	4.67250000	-0.41646900	-0.25443300
C	3.86182800	-1.54899100	0.13449500
N	2.52851500	-1.56826200	0.08782600
C	2.13983200	-2.82024400	0.57963300
C	0.83771500	-3.28446900	0.52658400
N	-0.97972700	3.15504300	0.20236000
N	2.86679200	1.22314400	-0.13664800
C	3.33044400	-3.56756800	0.99697500
C	4.39720800	-2.80188000	0.67947000
N	-3.38672500	0.19960400	-0.13063600
N	-1.55536000	-2.89111000	-0.07391500
H	0.84163900	-1.46593400	-1.78098500
H	-1.66651300	-0.88027900	-2.64527400
H	-6.49727300	-0.77306200	-0.57918800
H	-6.26913500	1.74860000	0.21324900
H	-1.63950100	0.64943800	2.19232000
H	0.98864900	1.07833600	1.79085300
H	4.18666800	4.18692300	-0.74500800
H	5.93419800	2.21370900	-0.84116500
H	-1.21263100	3.95074600	-0.37020500
H	2.16325800	0.49794600	-0.01133000
H	3.34988800	-4.56099600	1.41184300
H	5.43976200	-3.03944400	0.82323300
H	-2.38116200	0.11669000	-0.15209700
H	-1.95057000	-3.46440500	0.65540800
C	1.56155100	4.77984400	-0.39548400
C	-3.97706000	3.81792200	0.80735100
C	-4.60260700	-3.23802500	-1.14014900

C	0.42922300	-4.56857400	1.22384600
C	6.13710300	-0.71295600	-0.44859700
F	-5.30101200	3.84649400	0.54690300
F	-3.39561000	4.73841400	-0.02413600
F	-3.80219200	4.28970400	2.06001600
F	0.33549500	5.36171200	-0.39017700
F	2.09378000	5.03079500	-1.61450100
F	2.31273200	5.46533500	0.49857700
F	6.82346400	0.26511900	-1.08106600
F	6.77695400	-0.92874800	0.73230000
F	6.31906000	-1.83518800	-1.18604300
F	0.10370500	-5.53162600	0.33706000
F	-0.68998200	-4.35715000	1.98874600
F	1.34023500	-5.08307000	2.06400300
F	-4.28454200	-4.23447800	-0.26131400
F	-4.40976800	-3.75375900	-2.37356800
F	-5.92768400	-3.00632700	-1.00401300

2e' (T0^{A,D})

Sum of electronic and zero-point Energies= -2922.567471

C	0.00516900	-2.82397300	-0.30762800
C	0.09756700	-2.02382000	-1.45406300
C	1.45765900	-1.81833300	-1.72766100
C	2.20251400	-2.47439500	-0.73833600
C	3.63936300	-2.40741300	-0.44239500
C	4.23709600	-1.17361300	-0.37175000
C	5.58766800	-0.70496400	-0.05354300
C	5.57785800	0.65141400	-0.00021700
C	4.22200500	1.12470300	-0.28594800
C	3.61012600	2.35303200	-0.27535900
C	2.18646600	2.43805800	-0.61980900
C	1.48466000	1.82728900	-1.66285900
C	0.11278900	2.05813700	-1.45901000
C	-0.02325400	2.82523300	-0.29881400
C	-1.22281500	3.40812100	0.26972800
C	-2.46742700	2.82921900	0.15155600
C	-3.77647600	3.45582100	0.24147300
C	-4.72106900	2.54165700	-0.08075500
C	-4.07005700	1.25681500	-0.29409600
C	-4.65508700	0.00582000	-0.43435400
C	-3.96745600	-1.24170200	-0.19485300
N	-2.64166800	-1.39714300	-0.19576300
C	-2.41504200	-2.70222000	0.25815200
C	-1.18037500	-3.31844500	0.34174400
N	-2.71731800	1.49631800	-0.18949300
C	-3.69215100	-3.34845400	0.56731200
C	-4.65861500	-2.46576700	0.24027600
N	1.30516000	-3.09541300	0.08896400
N	1.25264300	3.05040000	0.18189600
N	3.50330600	-0.02128500	-0.55934200
H	-0.75110500	-1.67024600	-2.01741900
H	1.87732100	-1.28614000	-2.56868800
H	6.43154000	-1.35193200	0.12404600
H	6.41329200	1.29428700	0.22575600
H	1.93598200	1.31060300	-2.49685900
H	-0.69821400	1.76101600	-2.10696400
H	-3.94243800	4.49455900	0.47104100
H	-5.78434800	2.70469600	-0.12511500
H	-2.05258900	0.72503700	-0.18707400
H	-3.82212700	-4.35472100	0.93366700
H	-5.72574900	-2.59885000	0.32474300
H	1.56498400	-3.64805000	0.89015000
H	1.47107800	3.57291200	1.01660600
H	2.49822000	-0.02480900	-0.66295800
C	-1.13560300	-4.65868300	1.05973700
C	4.33198000	-3.68375300	-0.10055300
C	-6.14524700	-0.09109700	-0.64270600
C	-1.04937600	4.77674200	0.87884400
C	4.28990000	3.61166000	0.15158400
F	-1.68807700	-5.64441000	0.31786900
F	0.12998100	-5.06151400	1.34920500
F	-1.79530200	-4.63291900	2.23668000
F	4.21137500	-4.60410300	-1.08072500
F	3.77989900	-4.25535300	1.01712300

F	5.64872200	-3.53727000	0.15546100
F	-6.83249900	-0.29372700	0.51328000
F	-6.45916900	-1.12578600	-1.45802100
F	-6.68046000	1.01185200	-1.21774100
F	-0.64810600	5.69176500	-0.02855400
F	-2.14553600	5.26670500	1.48675700
F	-0.07529100	4.74535100	1.84265900
F	4.23184000	4.56782100	-0.79974900
F	5.58877300	3.44598700	0.47701400
F	3.67747800	4.14548600	1.25552400

2f($TO^{4,D}$)

Sum of electronic and zero-point Energies= -2922.558930

C	3.26164600	-2.67571400	0.09229100
N	2.30185100	-2.10976500	0.93313100
C	1.09273900	-2.79097300	0.86916000
C	-0.07092400	-2.34979900	1.45038500
C	-1.40016900	-2.77455900	0.99646700
N	-2.24955700	-1.83346400	0.62153100
C	-3.41909800	-2.47159300	0.20435900
C	-4.46369600	-1.70833200	-0.31042300
C	-4.38765700	-0.29531900	-0.52363300
C	-5.35046200	0.64305100	-0.97043900
C	-4.74898900	1.89909500	-0.98683200
C	-3.40633700	1.74151200	-0.57210400
C	-2.31485800	2.68584400	-0.43138800
C	-1.00740000	2.31715600	-0.68904300
N	0.13448200	3.00092200	-0.29987900
C	1.28192700	2.28103600	-0.61904500
C	2.57230200	2.58457800	-0.22676500
C	3.63231400	1.59509700	-0.26106000
C	5.02491800	1.67186400	-0.40997700
C	5.53774000	0.36388400	-0.39592100
C	4.46768800	-0.52759800	-0.22662400
C	4.38015400	-1.97444600	-0.30807400
C	2.63821200	-3.87957600	-0.43401800
C	1.34163500	-3.91394400	-0.02298600
C	-3.24469100	-3.90914800	0.36100700
C	-1.97915600	-4.09725400	0.84367600
N	-3.22814700	0.41737700	-0.29991100
C	-0.53791600	1.15958500	-1.42981000
C	0.81713400	1.14676600	-1.40039400
N	3.33293400	0.25708400	-0.13310700
H	0.58773700	-4.62891600	-0.31800900
H	3.11296400	-4.55472100	-1.12830800
H	6.57124000	0.07666500	-0.51084700
H	5.59002900	2.58261200	-0.53115200
H	1.46744300	0.46457600	-1.92727900
H	-1.18540200	0.47912100	-1.96141200
H	-5.20221000	2.83095000	-1.28814400
H	-6.36696300	0.41314400	-1.24902900
H	-3.97171800	-4.67227000	0.13672500
H	-1.51030300	-5.03567300	1.10810800
H	-2.43839000	-0.05973400	0.15222100
H	2.40286500	-0.09802300	0.02303600
C	-5.77817800	-2.33562300	-0.73663300
C	-0.02589900	-1.09768600	2.27989200
C	2.85836100	3.96971300	0.28816500
C	5.49622500	-2.66216300	-1.04622600
C	-2.60101700	4.09558400	0.00319800
F	-5.98264900	-2.17137600	-2.06325700
F	-5.86509400	-3.65522100	-0.48532300
F	-6.82064100	-1.75131700	-0.10184600
F	-1.08859200	-0.95122100	3.07652000
F	0.07150600	0.04048100	1.52205900
F	1.07899300	-1.07086200	3.09191600
F	5.56591400	-2.28325200	-2.34199200
F	5.38218900	-4.00916400	-1.03152000
F	6.69903200	-2.36831800	-0.49226500
F	4.09601000	4.09929100	0.79402500
F	2.71536600	4.90693800	-0.67705700
F	1.98737300	4.32530200	1.28265700
F	-2.37852400	4.99110900	-0.98824300
F	-3.86663300	4.26778400	0.42000300

F	-1.78753900	4.47807600	1.03596500
H	0.12192500	3.74622600	0.38025100
H	2.52016600	-1.44952200	1.66347900