Supporting Information

Understanding Molecular Switching Properties of Octaphyrins

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This PDF files includes:

I. Performance of several density functionals in geometry determination of neutral and diprotonated *meso*-octakis(pentafluorophenyl) [36]octaphyrins

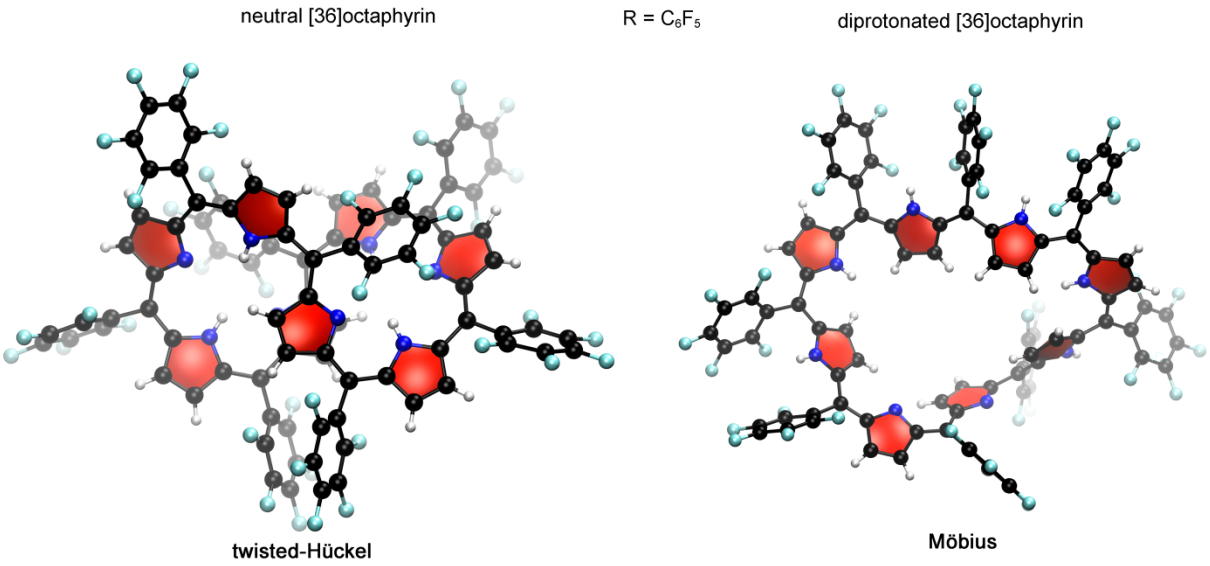


Figure S1. X-ray crystal structures of the *meso*-octakis(pentafluorophenyl) [36]octaphyrin(1.1.1.1.1.1.1.1) in the neutral and diprotonated states.

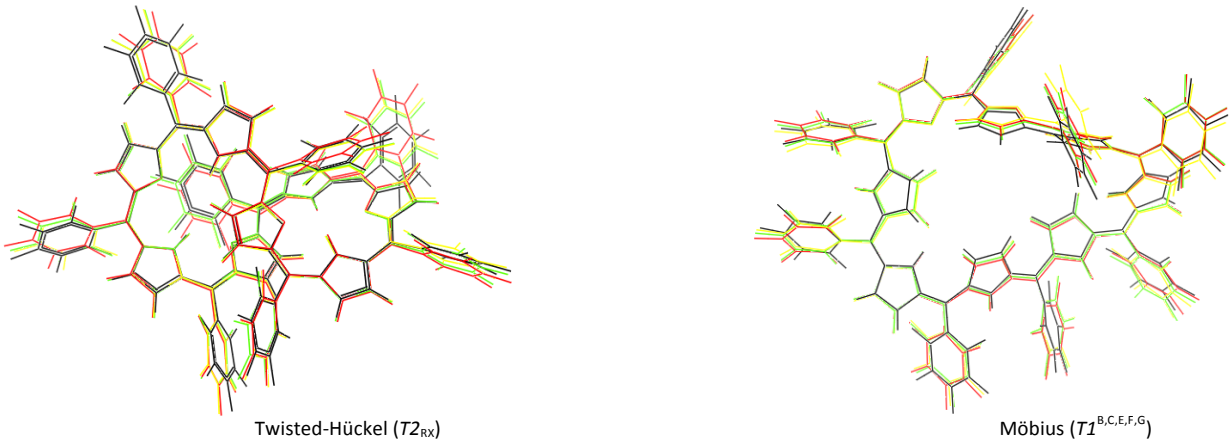


Figure S2. Comparison of the B3LYP, M06, ωB97XD optimized geometries of the figure-eight conformation and the Möbius, overlaid with the X-ray structure of the neutral and diprotonated *meso*-octakis(pentafluorophenyl) [36]octaphyrin. The all-heavy atom RMS (in Å) are displayed.

Table S1. Root-mean-square deviations (RMS in Å) and mean absolute errors (MUE) of the DFT optimized geometries relative to the X-ray structure of diprotonated *meso*-octakis(pentafluorophenyl) [36]octaphyrin.

$[36]^{2+}T1^{B,C,E,H}$	MUE_{bonds}	MUE_{angles}	$MUE_{torsions}$	RMS_{48}	RMS_{heavy}
B3LYP	0.033	1.259	3.453	0.272	0.620
PBE	0.036	1.290	3.419	0.256	0.523
M06	0.034	1.279	3.542	0.243	0.606
ωB97XD	0.036	1.322	3.766	0.332	0.887
B3LYP-D	0.033	1.322	3.488	0.270	0.583
BP86	0.037	1.282	3.526	0.263	0.590

Table S2. Torsional descriptors (Ψ_{MAX}, Ψ_{SMC} and Π) and bond-length alternation descriptors ($\Delta r_{C\text{-}N}$, $\Delta r_{C\text{-}C}$ and HOMA) and the corresponding mean unsigned error relative to the X-ray structure of the Möbius [36]octaphyrin.[a]

$[36]^{2+}T1^{B,C,E,,H}$	Ψ_{MAX}	Ψ_{SMC}	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$	HOMA	MUE $\Delta r_{C\text{-}N}$	MUE $\Delta r_{C\text{-}C}$	MUE HOMA
RX	34.638	11.353	-0.286	0.058	0.099	0.720	-	-	-
B3LYP	32.145	9.773	-0.343	0.051	0.070	0.753	0.007	0.029	0.033
PBE	32.229	9.955	-0.340	0.063	0.081	0.661	0.005	0.018	0.059
M06	32.297	9.708	-0.338	0.060	0.113	0.698	0.002	0.015	0.022
ωB97XD	43.515	9.876	-0.260	0.092	0.115	0.576	0.034	0.016	0.144
B3LYP-D	30.701	9.559	-0.349	0.062	0.101	0.697	0.004	0.002	0.023
BP86	30.984	9.786	-0.356	0.062	0.08	0.645	0.004	0.019	0.075

[a] Ψ_{MAX} and Ψ_{SMC} are given in °; $\Delta r_{C\text{-}N}$ and $\Delta r_{C\text{-}C}$ in Å.

Table S3. Root-mean-square deviations (RMS in Å) and mean absolute errors (MUE) of the DFT optimized geometries relative to the X-ray structure of the neutral *meso*-octakis(pentafluorophenyl) [36]octaphyrin.

$[36]T2_{RX}$	MUE_{bonds}	MUE_{angles}	$MUE_{torsions}$	RMS_{48}	RMS_{heavy}
B3LYP	0.037	0.951	2.926	0.206	0.724
PBE	0.041	1.313	3.110	0.174	0.665
M06	0.031	0.947	2.511	0.120	0.425
ωB97XD	0.035	0.956	2.406	0.192	0.438
B3LYP-D	0.034	1.008	2.679	0.196	0.542
BP86	0.045	1.030	2.817	0.133	0.665

Table S4. Torsional descriptors (Ψ_{MAX}, Ψ_{SMC} and Π) and bond-length alternation descriptors ($\Delta r_{C\text{-}N}$, $\Delta r_{C\text{-}C}$ and HOMA) and the corresponding mean unsigned error relative to the X-ray structure of the twisted-Hückel conformations.

$[36]T2_{RX}$	Ψ_{MAX}	Ψ_{SMC}	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$	HOMA	MUE $\Delta r_{C\text{-}N}$	MUE $\Delta r_{C\text{-}C}$	MUE HOMA
RX	20.244	7.888	0.618	0.084	0.119	0.684			
B3LYP	19.177	6.114	0.699	0.059	0.095	0.697	0.025	0.024	0.014
PBE	16.439	6.636	0.680	0.041	0.078	0.690	0.043	0.041	0.006
M06	17.883	7.275	0.655	0.067	0.094	0.743	0.017	0.025	0.059
ωB97XD	16.375	7.625	0.631	0.088	0.115	0.596	0.004	0.005	0.088
B3LYP-D	15.700	7.432	0.630	0.065	0.092	0.727	0.019	0.027	0.043
BP86	16.627	6.427	0.691	0.042	0.079	0.667	0.042	0.040	0.017

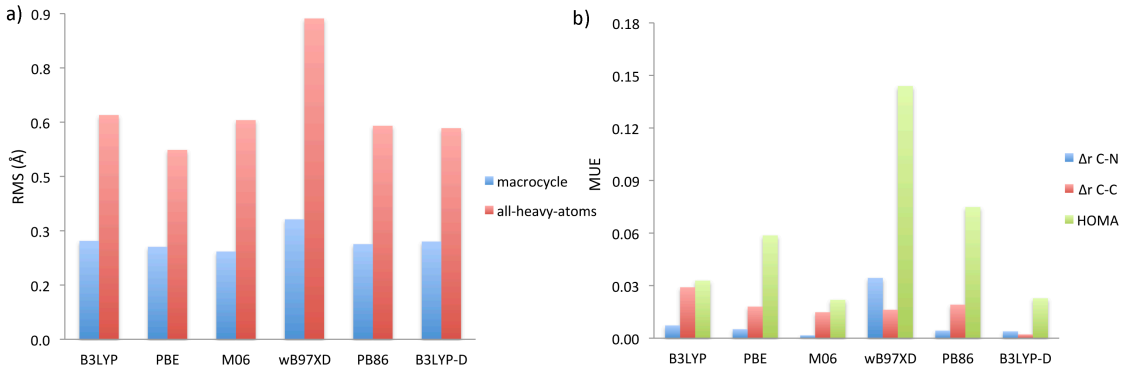


Figure S3. (a) Root-mean-square deviations (RMS) and (b) mean unsigned errors (MUE) for the bond-length alternation parameters of the DFT optimized geometries relative to the X-ray structure of the diprotonated *meso*-octakis(pentafluorophenyl) [36]octaphyrin.

Table S5. π–π stacking interactions distances of crystallographic and DFT-optimized neutral *meso*-octakis(pentafluorophenyl) [36]octaphyrin in the figure-eight conformation.

[36]$T2_{RX}$	RX	M06	B3LYP	B3LYP-D	wB97XD	BP86	PBE
phenyl-phenyl	3.13	3.13	3.22	3.06	3.20	3.27	3.59
pyrrol-pyrrol	3.41	3.33	3.71	3.06	3.52	3.61	3.23
pyrrol-phenyl	3.48	3.55	4.17	3.45	3.58	3.61	3.52
MUE	-	*0.05*	*0.36*	*0.15*	*0.09*	*0.16*	*0.23*

II. Dependence of the relative energies with the functional

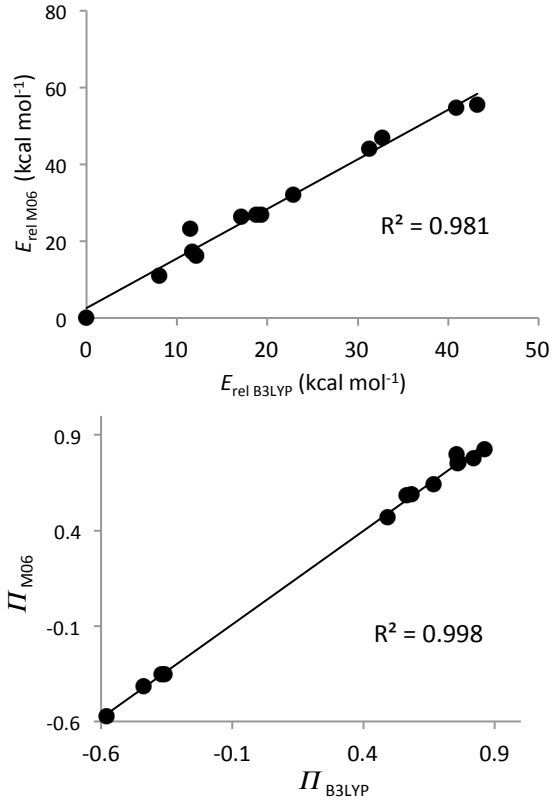


Figure S4. Correlation between the relative energies (in kcal mol^{-1}) and the extent of Π conjugation computed with B3LYP and M06 functionals for unsubstituted [36]octaphyrins.

Table S6. Relative and Gibbs free energies (in kcal mol^{-1}) together with the π-conjugation index (Π) of the different conformations of neutral unsubstituted [36]octaphyrin 1 computed with M06 and B3LYP functionals.

conf	Tn^X	M06[a]					B3LYP[b]				
		E_{rel}	ΔG_{298}	ΔG_{THF}	ΔG_{DMSO}	Π	E_{rel}	ΔG_{298}	ΔG_{THF}	ΔG_{DMSO}	Π
1a	$T0^{5,10,25,30}$	23.3	20.0	13.2	12.1	0.83	11.5	12.9	5.9	4.4	0.86
1b	$T0^{B,C,E,F,H}$	43.7	41.3	47.3	44.8	0.76	49.0	51.7	38.4	35.6	0.63
1c	$T0^{B,F,5,20,25}$	26.8	25.5	22.4	22.6	0.58	18.8	19.2	16.8	16.9	0.56
1e	$T1^{B,C,E,H}$	47.1	45.0	40.1	38.4	-0.35	40.8	42.3	30.7	28.7	-0.36
1f	$T1^{B,C,F}$	26.6	25.4	17.9	16.7	-0.57	17.1	18.3	11.6	10.4	-0.58
1g	$T2^{B,F}$	17.3	17.3	12.5	11.3	0.76	11.7	12.1	7.3	6.2	0.76
1h	$T2^{C,G}$	16.3	15.5	11.3	10.4	0.80	12.1	13.0	9.2	8.0	0.76
1i	$T2_{RX}$	0.0	0.0	0.0	0.0	0.78	0.0	0.0	0.0	0.0	0.82
	MAD						*6.3*	*5.3*	*5.6*	*5.8*	

[a] ZPE-corrected relative energies and Gibbs free energies at the M06/6-311+G(d,p)//M06/6-31G(d,p) level of theory. [b] ZPE-corrected relative energies and Gibbs free energies at the B3LYP/6-311+G(d,p)//B3LYP/6-31G(d,p) level. [c] *MAD* is the mean absolute difference of the energies computed with both functionals.

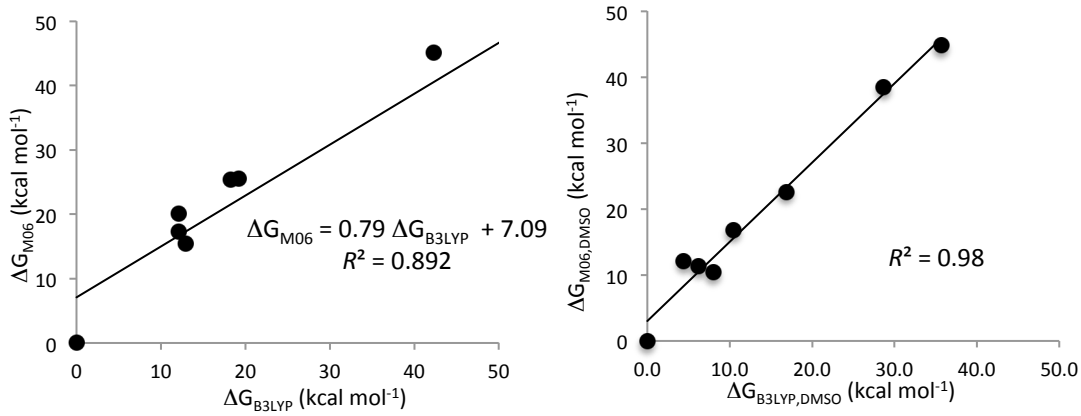


Figure S5. Correlation between the Gibbs free energy (in kcal mol^{-1}) computed with B3LYP and M06 in gas-phase and DMSO.

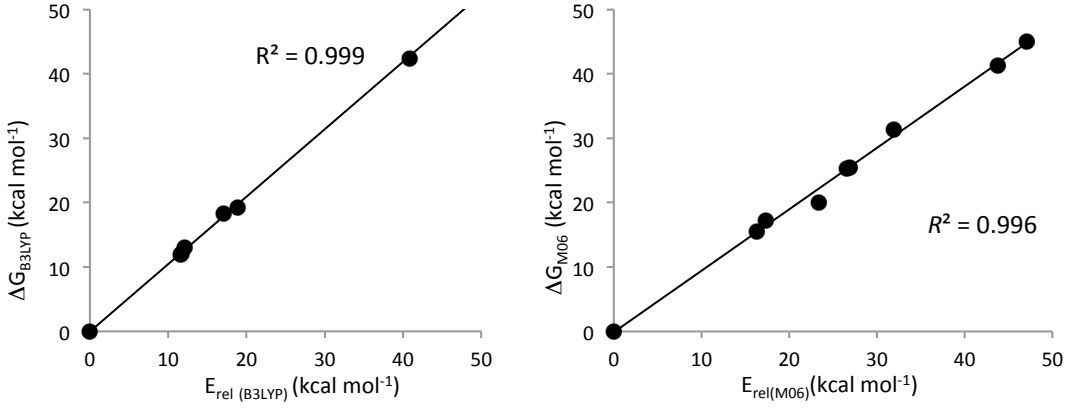


Figure S6. Correlation between the Gibbs free energy and the relative energy (in kcal mol^{-1}) computed with B3LYP and M06, respectively.

III. Conformational analysis of neutral unsubstituted [36]octaphyrin

Table S7. Relative energies (E_{rel} in kcal mol^{-1}), relative Gibbs free energies (ΔG_{298} in kcal mol^{-1}), hydrogen bonding index (N_H), p-conjugation index (Π), ring strain (Φ_p and Ψ_{SMC}) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the conformers of the neutral unsubstituted [36]octaphyrin.

conformers	E_{rel} [a]	ΔG_{298}	N_H	Ψ_{SMC}	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
1a	23.3	20.0	3	3.54	13.0	0.83	0.055	0.094
1b	43.9	41.3	1	5.23	16.9	0.76	0.063	0.100
1c	26.8	25.5	3	7.57	23.6	0.58	0.061	0.096
1d	32.0	31.4	3	8.86	27.3	0.47	0.064	0.097
1e	54.6	45.0	0	9.56	30.3	-0.35	0.058	0.089
1f	26.6	25.4	2.5	7.58	31.5	-0.57	0.062	0.098
1g	17.3	17.3	3	4.70	18.4	0.76	0.064	0.090
1h	16.3	15.5	3	4.70	15.0	0.80	0.054	0.095
1i	0.0	0.0	4	4.28	15.1	0.78	0.052	0.090
1j	26.9	26.5	3	10.36	31.5	-0.35	0.051	0.084
1k	55.6	41.8	0	6.45	34.9	0.59	0.065	0.102
1l	46.8	45.2	1	9.60	33.9	-0.42	0.091	0.115
1m	11.0	10.6	3.5	5.75	16.3	0.64	0.103	0.093

[a] ZPE-corrected relative energies and Gibbs free energies at the M06/6-311+G(d,p)//M06/6-31G(d,p) level of theory

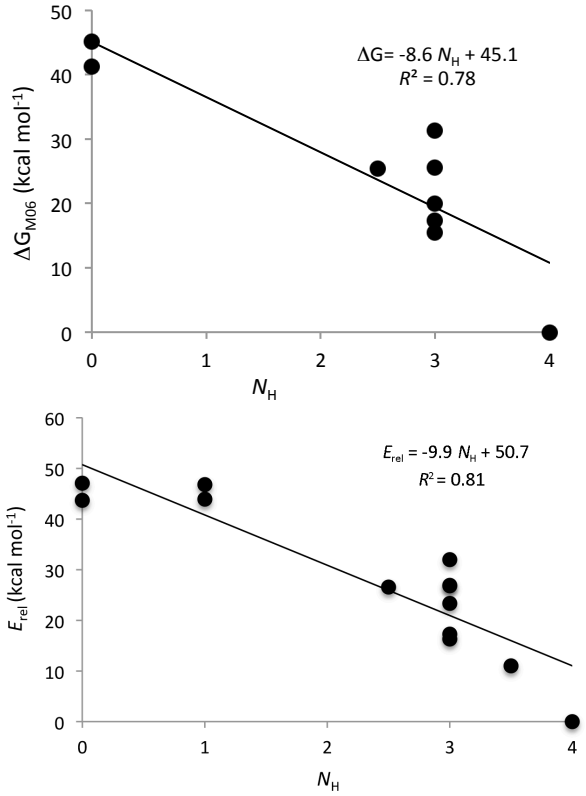


Figure S7. Relationship between the relative energy and the Gibbs free energies of neutral [36]octaphyrin conformers (**1a-m**) and the hydrogen bonding index (N_H).

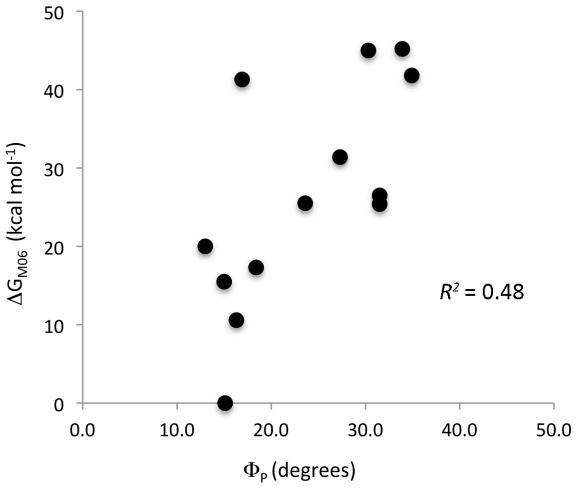


Figure S8. Relationship between the Gibbs free energies of neutral [36]octaphyrin conformers (**1a-m**) and the torsional ring strain (Φ_P).

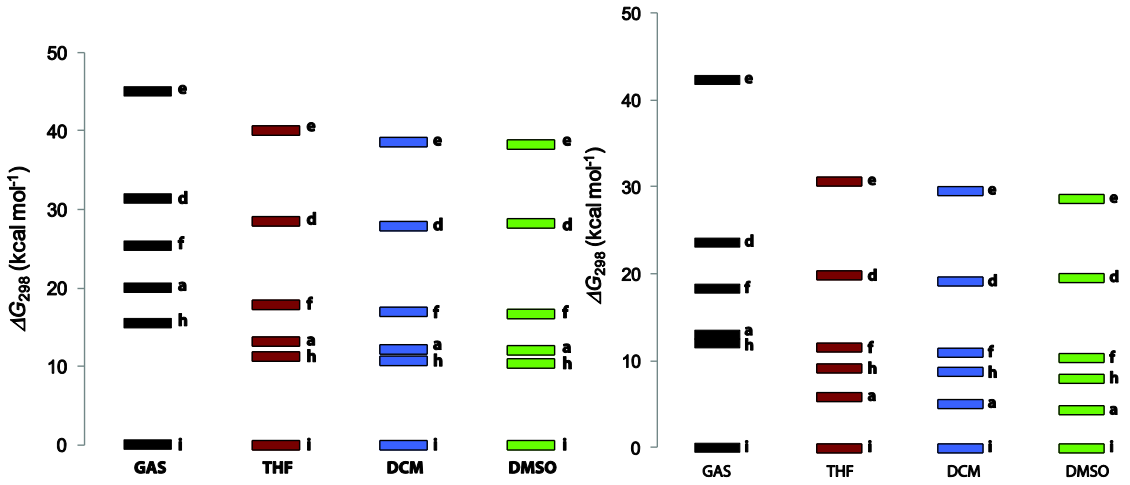


Figure S9. Evolution of the Gibbs free energy with the solvent computed at M06/6-311+G(d,p) (left) and at B3LYP/6-311+G(d,p) (right) level of theory.

Table S8. Relative and Gibbs free energies (in kcal mol^{-1}) in gas-phase and different solvents together with the hydrogen bonding index (N_H) and ring strain (Φ_p) of the different conformations of neutral unsubstituted [36]octaphyrin **1**.[a]

conf	Tn^X	E_{rel}	ΔG_{298}	N_H	Φ_p	ΔG_{THF}	ΔG_{DCM}	ΔG_{DMSO}
1a	$T0^{5,10,25,30}$	11.5	12.0	3	11.8	5.9	5.1	4.4
1b	$T0^{B,C,E,F,H}$	49.0	51.7	0	23.1	38.4	37.2	35.6
1c	$T0^{5,20,25,B,F}$	18.8	19.2	3	33.1	16.8	16.4	16.9
1d	$T0^{20,25,B,F}$	22.9	23.6	3	39.0	19.9	19.2	19.6
1e	$T1^{B,C,E,H}$	40.8	42.3	0	34.3	30.7	29.6	28.7
1f	$T1^{B,C,F}$	17.1	18.3	2.5	31.1	11.6	11.0	10.4
1g	$T2^{B,F}$	11.7	12.1	3	18.1	7.3	6.7	6.2
1h	$T2^{C,G}$	12.1	13.0	3	17.4	9.2	8.8	8.0
1i	$T2_{RX}$	0.0	0.0	4	14.6	0.0	0.0	0.0
1j	*T3*	19.3	20.5	3	30.5	17.0	16.4	16.4
1k	$T0^{B,C,E,G}$	31.3	32.2	1	18.5	23.8	22.9	22.5
1l	$T1^{B,C,E,G}$	32.7	34.4	1	33.8	25.4	24.4	24.1
1m	$T2^{B}$	8.0	8.3	3.5	19.8	6.0	5.7	5.7

[a] ZPE-corrected relative energies and Gibbs free energies at the B3LYP/6-311+G(d,p)//B3LYP/6-31G(d,p) level of theory.

Table S9. Relative energies (E_{rel} in kcal mol^{-1}), hydrogen bonding index (N_H), π–conjugation index (Π), ring strain (Φ_p and Ψ_{SMC}) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the conformers of the neutral unsubstituted [36]octaphyrin.

conformers	Tn^X	E_{rel} [a]	N_H	Ψ_{SMC}	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
1a	$T0^{5,10,25,30}$	11.5	3	3.34	11.8	0.86	0.049	0.092
1b	$T0^{B,C,E,F,H}$	49.0	0	6.38	23.1	0.63	0.010	0.063
1c	$T0^{5,20,25,B,F}$	18.8	3	7.64	33.1	0.56	0.059	0.094
1d	$T0^{20,25,B,F}$	22.9	3	8.14	39.0	0.49	0.067	0.099
1e	$T1^{B,C,E,H}$	40.8	0	9.63	34.3	-0.36	0.096	0.105
1f	$T1^{B,C,F}$	17.1	2.5	7.69	31.1	-0.58	0.044	0.080
1g	$T2^{B,F}$	11.7	3	5.21	18.1	0.76	0.103	0.090
1h	$T2^{C,G}$	12.1	3	5.23	17.4	0.76	0.052	0.118
1i	$T2_{RX}$	0.0	4	4.28	14.6	0.82	0.050	0.114
1j	*T3*	19.3	3	10.56	30.5	-0.37	0.034	0.073
1k	$T0^{B,C,E,G}$	31.3	1	5.26	18.5	0.76	0.106	0.101
1l	$T1^{B,C,E,G}$	32.7	1	9.62	33.8	-0.44	0.030	0.082
1m	$T2^{B}$	8.0	3.5	5.39	19.8	0.66	0.099	0.093

[a] E_{rel} corresponds to the sum of the electronic energy computed at the B3LYP/6-311+G(d,p) level of theory and the zero-point vibrational energy obtained at the B3LYP/6-31G(d,p) level.

IV. Interconversion pathways of neutral unsubstituted [36]octaphyrin

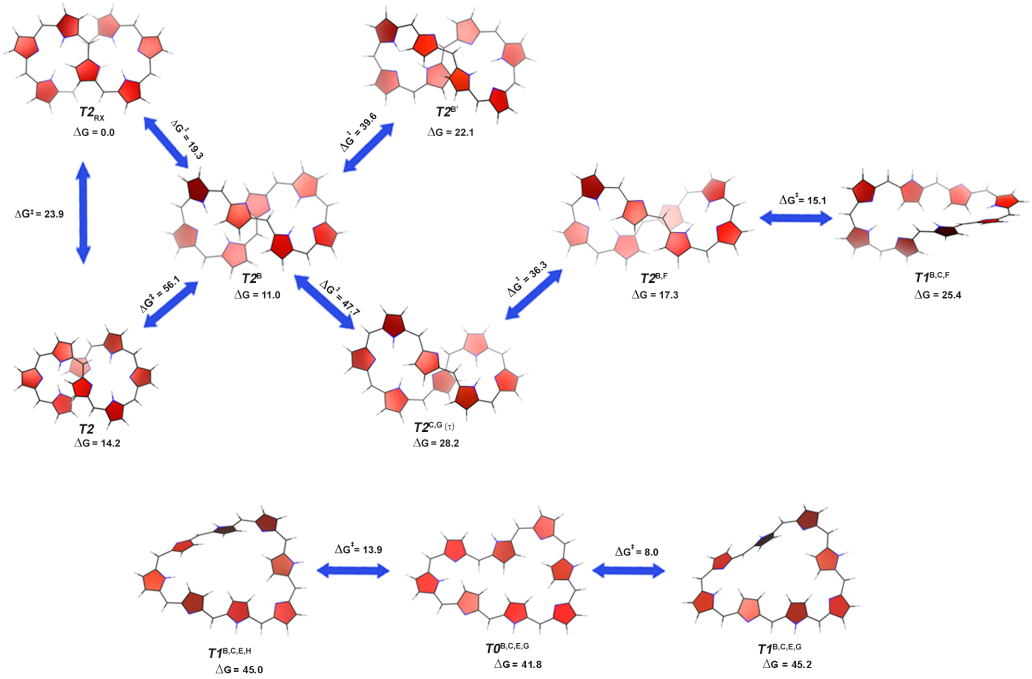


Figure S10. Activation energy barriers ($\Delta G^{\ddagger}$ in kcal mol^{-1}) for the interconversions between the most relevant conformations in **1** computed at the M06/6-311+G(d,p)//M06/6-31G(d,p) level of theory. The relative Gibbs free energies of the different conformations with respect the global minima ($T2_{RX}$) are also shown.

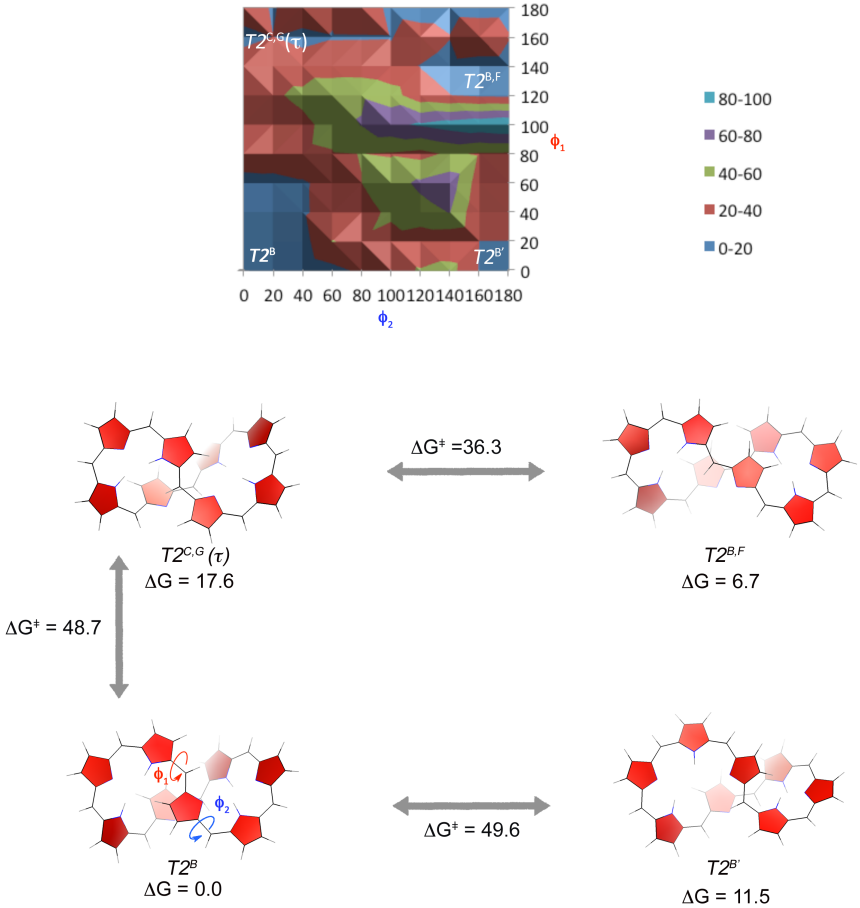


Figure S11. M06/6-31G(d,p) relaxed potential energy surface for the figure-eight conformation **1m** ($T2^{B}$) obtained by rotating the dihedral angles ϕ_1 and ϕ_2 (in °). The fully optimized geometries for the different minima and the corresponding Gibbs free energies and activation barriers ($\Delta G^{\ddagger}$ in kcal mol^{-1}) with respect to **1m** are also shown.

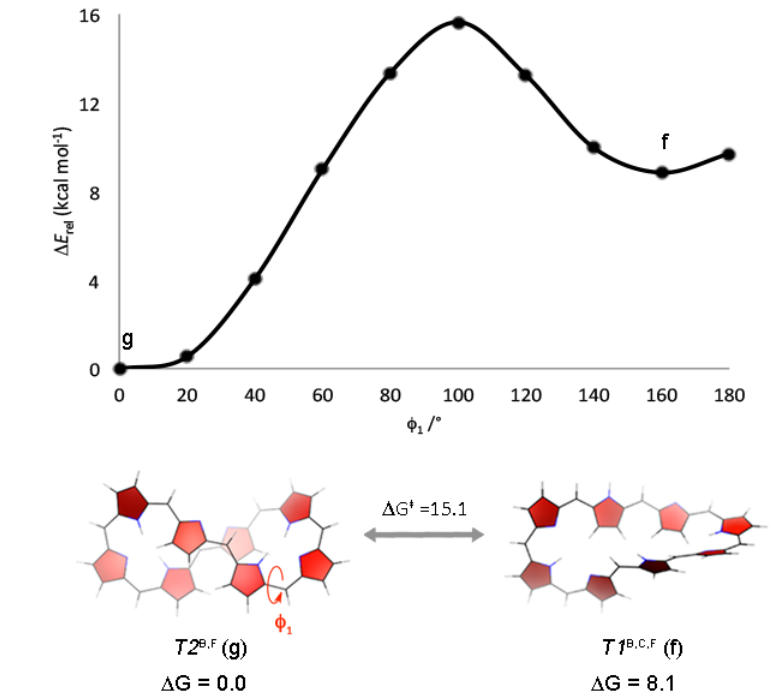


Figure S12. M06/6-31G(d,p) potential energy curve for the figure-eight/Möbius interconversion in **1** as a function of dihedral angle ϕ_1. The fully optimized geometries for the different minima and the corresponding relative Gibbs free energy and the activation barrier ($\Delta G^{\ddagger}$ in kcal mol^{-1}) with respect to **1g** are also shown.

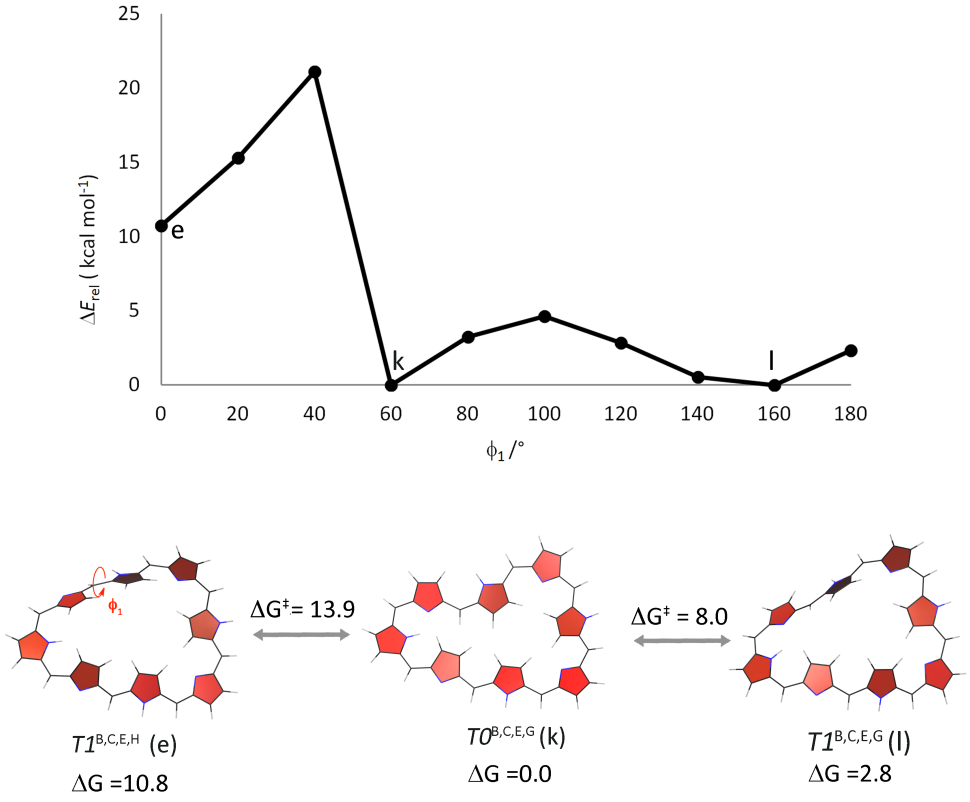


Figure S13. M06/6-31G(d,p) potential energy curve for the Hückel/Möbius interconversions in **1** as a function of dihedral angle ϕ_1. The fully optimized geometries for the different minima and the corresponding relative Gibbs free energy and the activation barrier ($\Delta G^{\ddagger}$ in kcal mol^{-1}) with respect to **1k** are also shown.

V. Substituent effect on the conformation of neutral [36]octaphyrins

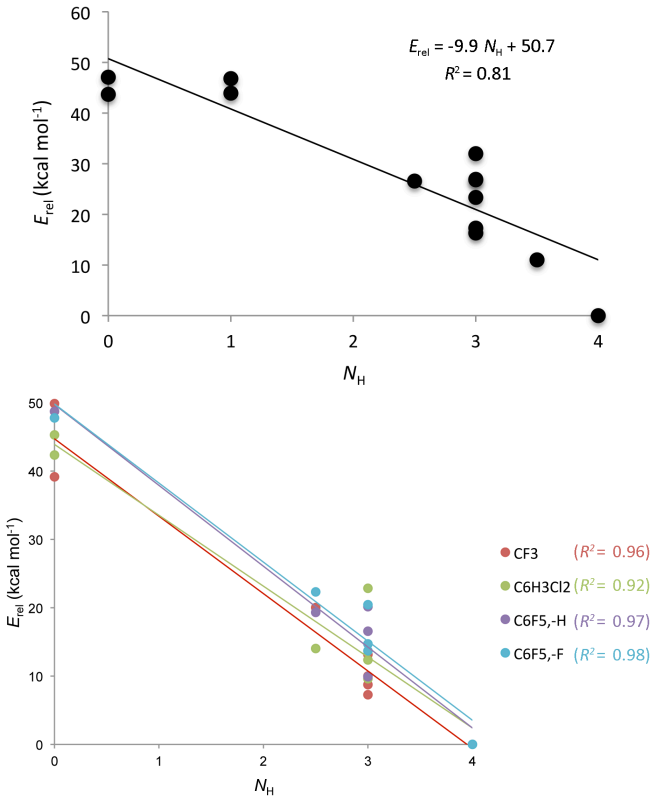


Figure S14. Dependence of the relative energy on the intramolecular hydrogen bonding index (N_H) for unsubstituted (top) and substituted [36]octaphyrins (bottom).

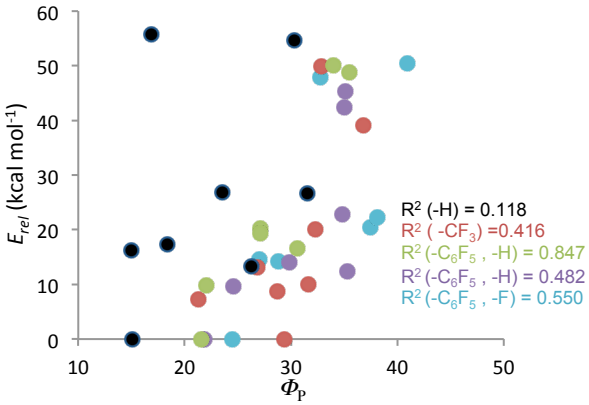


Figure S15. Dependence of the relative energy on the torsional ring strain (in degrees) for substituted [36]octaphyrins.

Table S10. Relative energies (E_{rel}), Gibbs free energies (ΔG_{298} in kcal mol^{-1}), hydrogen bonding index (N_H), ring strain (Φ_p and Ψ), π-conjugation index (Π) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the neutral *meso*-trifluoromethyl-substituted [36]octaphyrins (R = CF_3).

conformers	E_{rel}	ΔG_{298}	N_H	Φ_p	Ψ_{SMC}	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
$T0^{5,10,25,30}$	8.8	6.7	3	28.7	8.3	0.48	0.069	0.102
$T0^{B,C,E,F,H}$	49.9	41.2	0	32.9	8.8	0.35	0.068	0.109
$T0^{5,20,25,B,F}$	10.0	5.2	3	31.6	10.2	0.30	0.075	0.107
$T1^{B,C,E,H}$	20.0	30.1	2.5	36.8	9.7	-0.39	0.064	0.101
$T1^{B,C,F}$	39.2	14.8	0	32.2	9.6	-0.30	0.131	0.102
$T2^{B,F}$	13.2	10.1	3	26.8	8.4	0.46	0.076	0.104
$T2^{C,G}$	7.3	3.9	3	21.3	6.5	0.53	0.061	0.104
$T2_{RX}$	0.0	0.0	4	29.3	9.8	0.46	0.073	0.110

Table S11. Relative energies (E_{rel}), Gibbs free energies (ΔG_{298} in kcal mol^{-1}), hydrogen bonding index (N_H), ring strain (Φ_p) and π-conjugation index (Π) of the neutral *meso*-aryl-substituted [36]octaphyrins.

Conformation	-C_6F_5					-$C_6H_3Cl_2$					-C_6F_5, -F				
	E_{rel}	ΔG_{298}	N_H	Φ_p	Π	E_{rel}	ΔG_{298}	N_H	Φ_p	Π	E_{rel}	ΔG_{298}	N_H	Φ_p	Π
a $T0^{5,10,25,30}$	16.6	16.8	3	30.6	0.38	22.9	16.6	3.0	34.9	0.31	20.4	19.2	3.0	37.4	0.23
b $T0^{B,C,E,F,H}$	48.7	41.4	0	35.5	0.47	45.4	38.3	0.0	35.1	0.52	47.8	44.2	0.0	32.7	0.32
c $T0^{5,20,25,B,F}$	20.2	18.3	3	27.1	0.45	12.4	8.3	3.0	35.2	0.38	13.9	14.2	3.0	27.2	0.40
f $T1^{B,C,F}$	19.3	10.1	2.5	27.1	-0.47	14.0	7.4	2.5	29.8	-0.50	14.7	15.7	2.5	28.8	-0.36
e $T1^{B,C,E,H}$	50.1	40.6	0	33.9	-0.34	42.4	31.7	0.0	35.0	-0.35	50.4	42.4	0.0	40.9	-0.16
i $T2_{RX}$	0.0	0.0	4	21.6	0.65	0.0	0.0	4.0	21.9	0.61	0.0	0.0	4.0	24.5	0.48
h $T2^{C,G}$	9.9	5.4	3	22.0	0.60	9.6	4.0	3.0	24.6	0.50	14.7	11.6	3.0	27.2	0.23

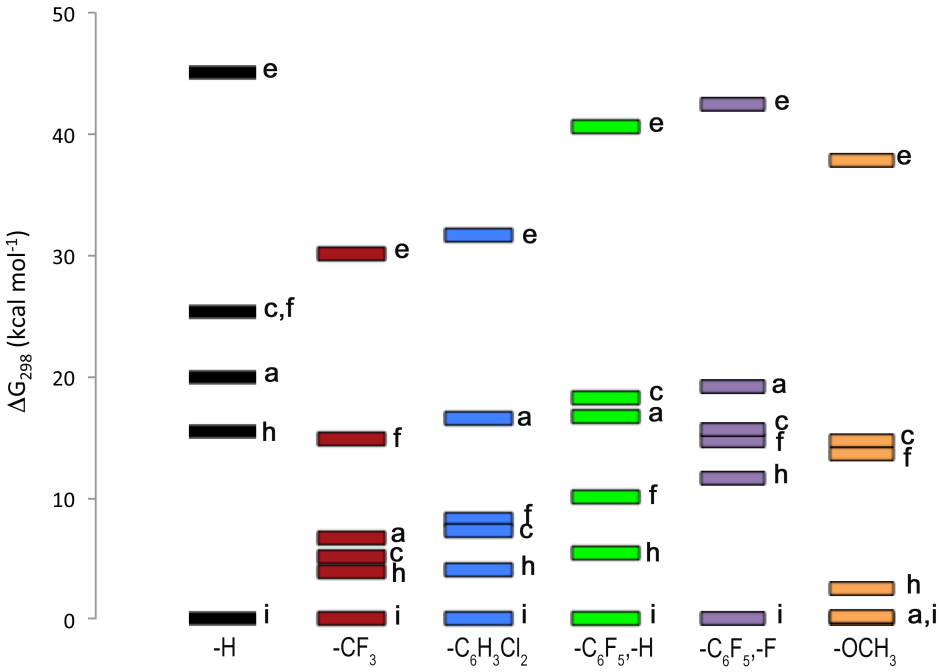


Figure S16. Evolution of the Gibbs free energy with the substituents at *meso* and *β*-positions, computed at the M06/6-311+G(d,p) level of theory.

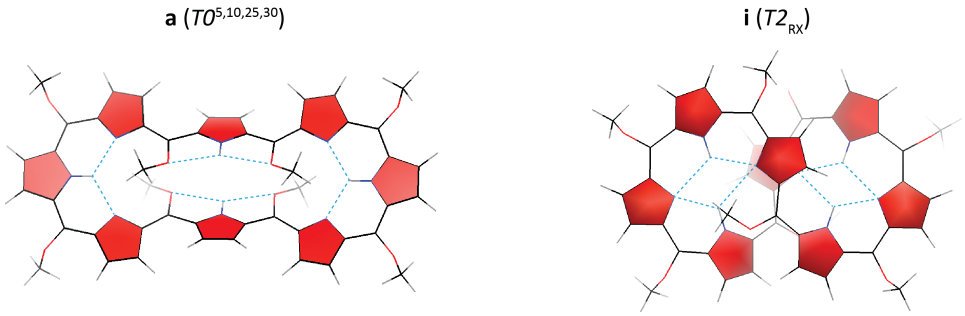


Figure S17. The most stable conformations for *meso*-octakis(methoxy) [36]octaphyrin in neutral state. Intramolecular hydrogen bonds together with the torsional descriptors and the Gibbs free energies at the M06/6-311+G(d,p)//M06/6-31G(d,p) level of theory are also shown.

VI. Conformational changes upon protonation and redox reactions

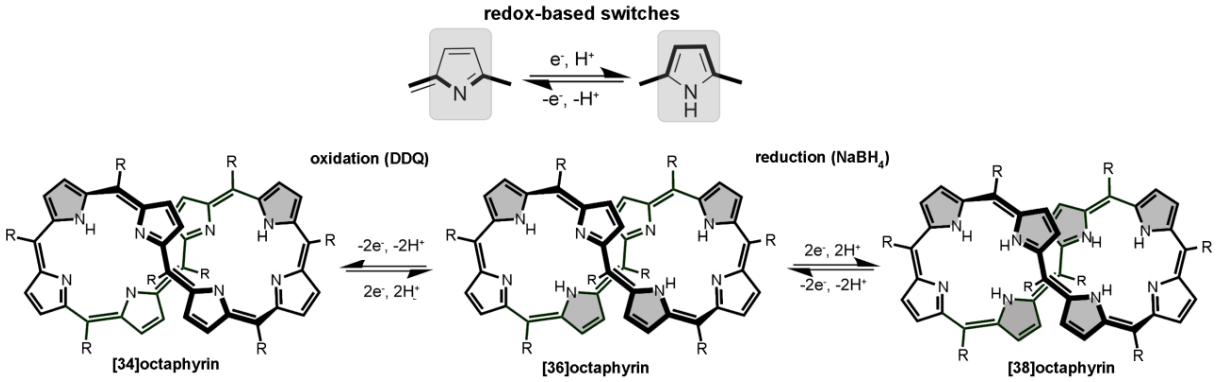


Figure S18. Oxidation states available for the regular [36]octaphyrin.

Table S12. Relative energies (E_{rel}), Gibbs free energies (ΔG_{298} in kcal mol^{-1}), hydrogen bonding index (N_H), ring strain (Φ_p and Ψ), π-conjugation index (Π) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the neutral unsubstituted [34]octaphyrins **3**.

conformers	Tn^X	E_{rel}	ΔG_{298}	N_H	Ψ_{SMC}	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
2a	$T0^{5,10,25,30}$	6.1	4.1	3	2.6	9.3	0.94	0.080	0.100
2b	$T0^{B,C,E,F,H}$	34.5	33.3	0	6.7	21.4	0.62	0.070	0.100
2c	$T0^{5,20,25,B,F}$	10.1	9.7	3	7.6	32.6	0.63	0.110	0.110
2d	$T0^{20,25,B,F}$	13.6	14.4	3	9.1	39.5	0.51	0.080	0.080
2e	$T1^{B,C,E,H}$	41.3	39.6	0	10.6	33.3	-0.33	0.080	0.100
2f	$T1^{B,C,F}$	17.1	16.6	2.5	7.7	30.8	-0.56	0.090	0.130
2g	$T2^{B,F}$	0.0	0.0	3	4.8	14.9	0.83	0.110	0.100
2h	$T2^{C,G}$	0.0	0.0	3	4.8	15.9	0.83	0.080	0.100
2i	$T2_{RX}$	6.4	6.5	3	5.4	15.9	0.79	0.050	0.090

Table S13. Relative energies (E_{rel}), Gibbs free energies (ΔG_{298} in kcal mol^{-1}), hydrogen bonding index (N_H), ring strain (Φ_p and Ψ), π-conjugation index (Π) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the neutral unsubstituted [38]octaphyrin **3**.

conformers	Tn^X	E_{rel}	ΔG_{298}	N_H	Ψ_{SMC}	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
3a	$T0^{5,10,25,30}$	17.0	14.8	3.0	4.43	14.72	0.79	0.05	0.060
3b	$T0^{B,C,E,F,H}$	50.0	48.8	0.0	5.9	22.5	0.59	0.038	0.085
3c	$T0^{5,20,25,B,F}$	16.8	16.5	3.0	6.7	34.9	0.59	0.034	0.078
3d	$T0^{20,25,B,F}$	21.0	20.4	3.0	8.0	38.8	0.51	0.034	0.079
3e	$T1^{B,C,E,H}$	53.9	39.6	0.0	9.5	35.1	-0.30	0.069	0.094
3f	$T1^{B,C,F}$	26.9	16.6	2.5	6.7	28.7	-0.56	0.110	0.100
3g	$T2^{B,F}$	7.2	7.9	3.0	5.2	20.2	0.78	0.004	0.056
3h	$T2^{C,G}$	7.0	6.8	3.0	7.9	14.9	0.81	0.050	0.070
3i	$T2_{RX}$	0.0	0.0	3.0	4.6	16.0	0.81	0.009	0.058

Table S14. Relative energies (E_{rel}), Gibbs free energies (ΔG_{298} in kcal mol^{-1}), hydrogen bonding index (N_H), ring strain (Φ_p and Ψ), π-conjugation index (Π) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the diprotonated unsubstituted [36]octaphyrin **4**.

conformers	Tn^X	E_{rel}	ΔG_{298}	N_H	Ψ_{SMC}	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
4a	$T0^{5,10,25,30}$	5.5	4.3	3	4.9	16.4	0.74	0.054	0.094
4b	$T0^{B,C,E,F,H}$	36.8	34.7	0	7.0	26.1	0.52	0.069	0.089
4c	$T0^{5,20,25,B,F}$	11.1	9.7	3	6.8	28.1	0.6	0.089	0.076
4d	$T0^{20,25,B,F}$	15.3	14.8	3	9.2	29.5	0.43	0.030	0.100
4e	$T1^{B,C,E,H}$	30.9	29.7	0	9.7	38.8	-0.39	0.100	0.100
4f	$T1^{B,C,F}$	3.6	2.7	2.5	7.7	29.5	-0.58	0.040	0.080
4g	$T2^{B,F}$	0.2	0.3	3	4.3	15.8	0.81	0.090	0.080
4h	$T2^{C,G}$	0.0	0.0	3	4.6	17.1	0.80	0.080	0.110
4i	$T2_{RX}$	1.6	3.4	3	4.9	17.4	0.73	0.069	0.087

Table S15. Relative energies (E_{rel}), Gibbs free energies (ΔG_{298} in kcal mol^{-1}), hydrogen bonding index (N_H), ring strain (Φ_p and Ψ), π-conjugation index (Π) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the diprotonated unsubstituted [38]octaphyrin **5**.

conformers	Tn^X	E_{rel}	ΔG_{298}	N_H	Ψ_{SMC}	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
5a	$T0^{5,10,25,30}$	10.9	10.2	-	4.5	16.4	0.76	0.002	0.054
5b	$T0^{B,C,E,F,H}$	6.5	4.9	-	6.6	25.1	0.56	0.004	0.064
5c	$T0^{5,20,25,B,F}$	10.7	10.5	-	7.2	28.6	0.51	0.018	0.075
5d	$T0^{20,25,B,F}$	15.5	13.7	-	7.5	35.7	0.50	0.021	0.079
5e	$T1^{B,C,E,H}$	14.4	13.0	-	10.0	33.3	-0.29	0.032	0.095
5f	$T1^{B,C,F}$	10.9	9.2	-	7.1	28.5	-0.48	0.035	0.097
5g	$T2^{B,F}$	2.9	2.2	-	6.2	17.5	0.64	0.002	0.052
5h	$T2^{C,G}$	5.1	4.6	-	6.1	20.2	0.66	0.007	0.054
5i	$T2_{RX}$	0.0	0.0	-	4.4	14.1	0.79	0.006	0.052

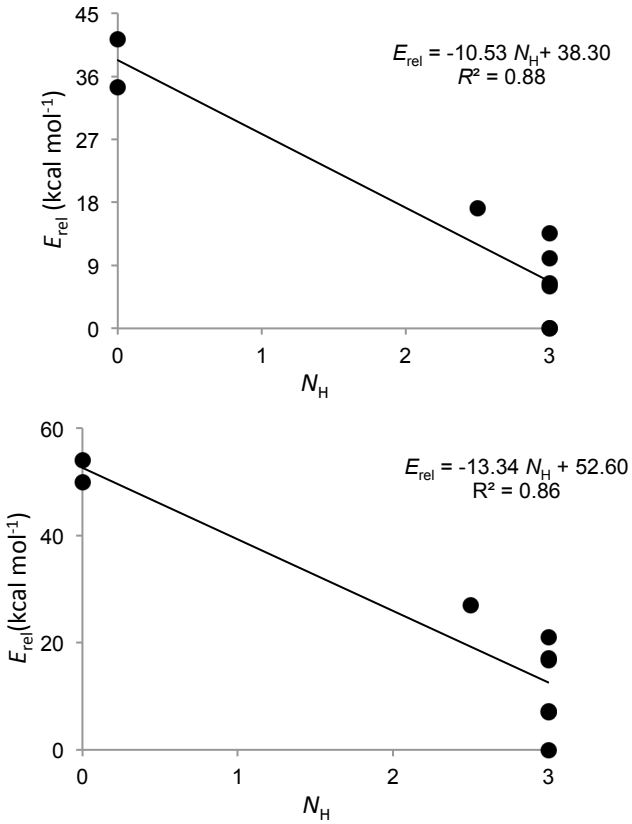


Figure S19. Dependence of the relative energy on the intramolecular hydrogen bonds of neutral unsubstituted [34] (top) and [38] octaphyrins (bottom).

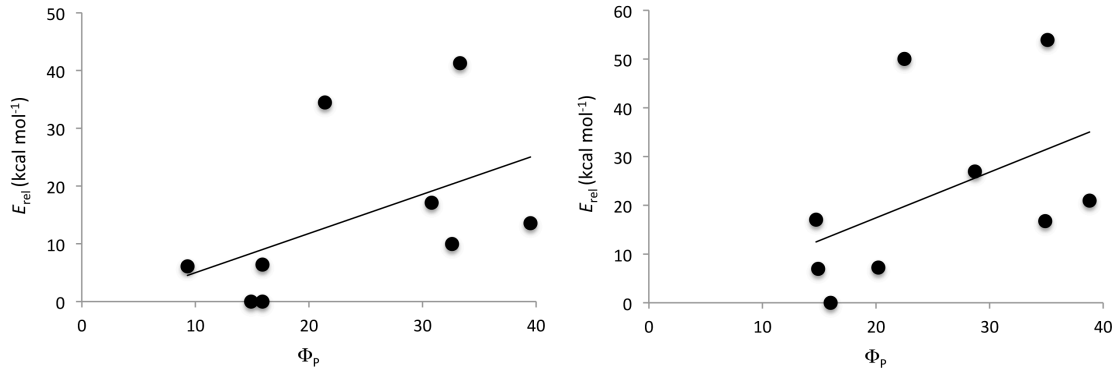


Figure S20. Dependence of the relative energy on the ring strain of neutral unsubstituted [34] (left) and [38]octaphyrins (right).

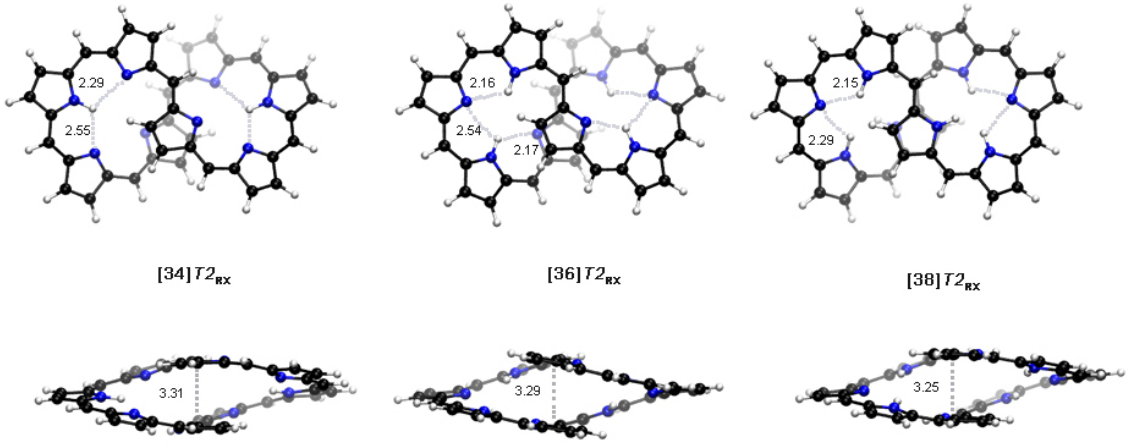


Figure S21. Structural features of the neutral unsubstituted [34], [36] and [38]octaphyrins in the figure-eight $T2_{RX}$ conformation.

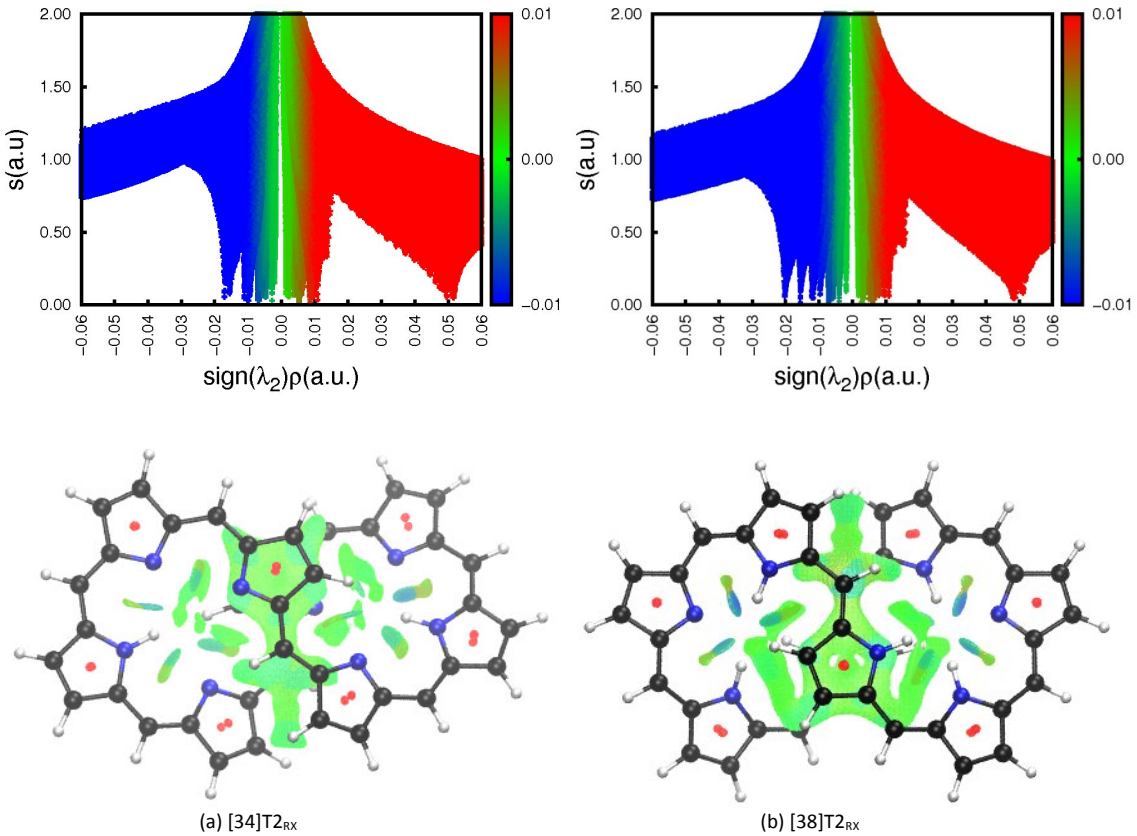


Figure S22. NCI analysis of the neutral unsubstituted [34] and [38]octaphyrins with a twisted-Hückel topology. (a) Plot of the reduced density gradient s(ρ) and (b) gradient isosurface (s = 0.5). The surfaces are coloured according to sign(λ_2)ρ over the range -0.03 to 0.03 a.u.

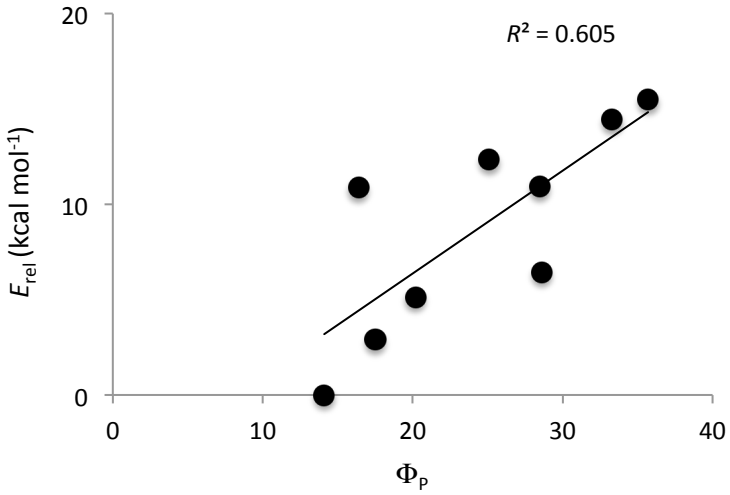


Figure S23. Dependence of the relative energy on the ring strain of diprotonated unsubstituted [38]octaphyrin **5**.

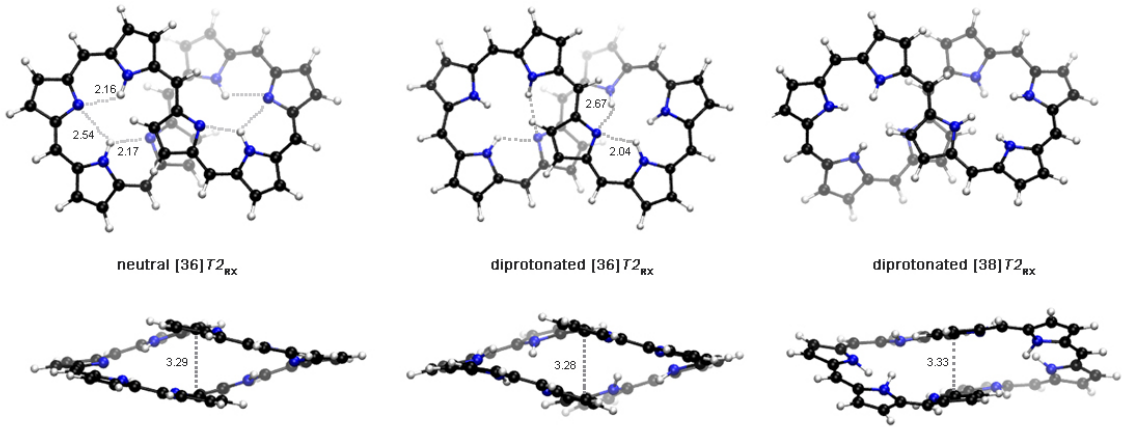
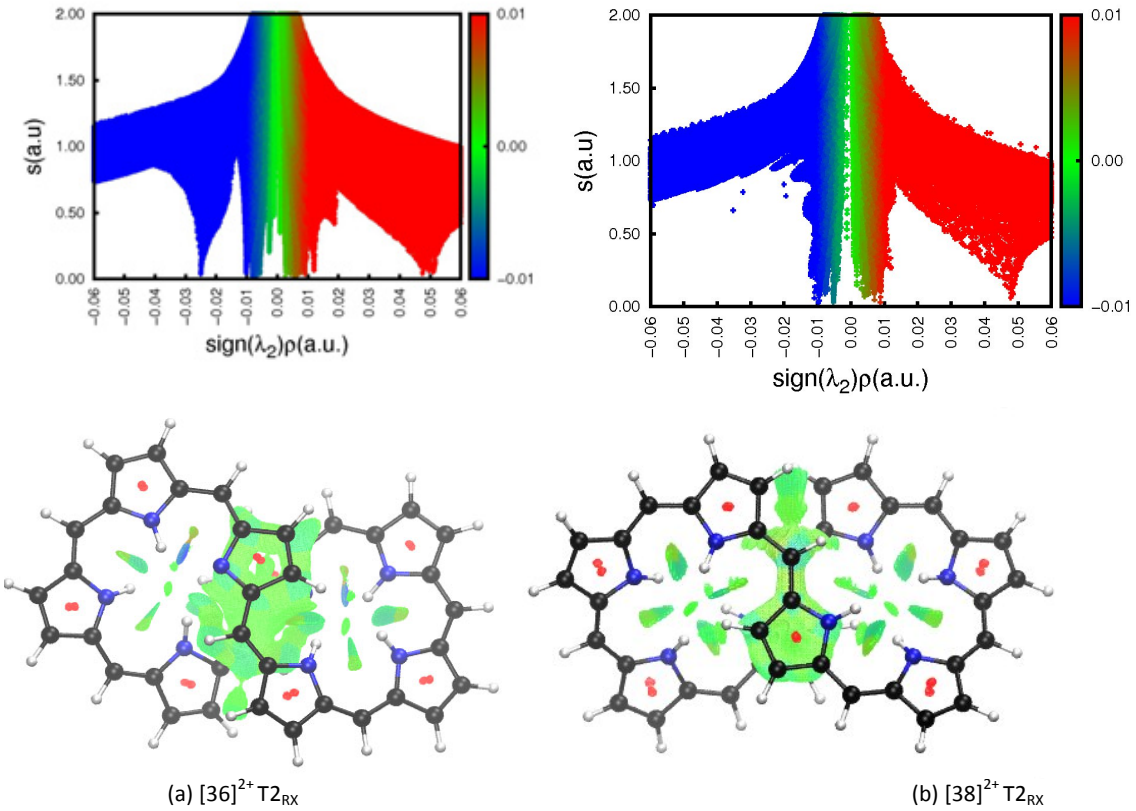


Figure S24. Structural features of neutral [36] and diprotonated [36] and [38]octaphyrins in the figure-eight conformation



(a) $[36]^{2+}T2_{RX}$ (b) $[38]^{2+}T2_{RX}$

Figure S25. NCI analysis of the diprotonated unsubstituted [36] and [38]octaphyrins with a twisted-Hückel topology. (a) Plot of the reduced density gradient $s(\rho)$ and (b) gradient isosurface (s = 0.5). The surfaces are coloured according to sign(λ_2)ρ over the range -0.03 to 0.03 a.u.

VII. Conformational changes of *meso*-octakis(pentafluorophenyl) octaphyrins upon protonation and redox reactions

Table S16. Relative energies (E_{rel}) and Gibbs free energies (ΔG_{298} in kcal mol^{-1}) in gas-phase and DCM solvent, hydrogen bonding index (N_H), ring strain (Φ_p), π-conjugation index (Π) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the neutral *meso*-octakis(pentafluorophenyl)-substituted [36]octaphyrins **6**.

conformers	E_{rel}	E_{rel}^{DCM}	ΔG_{298}	ΔG_{298}^{DCM}	N_H	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
6a	16.6	14.2	16.8	14.4	3	30.6	0.38	0.062	0.113
6b	48.7	30.7	41.4	23.4	0	35.6	0.47	0.061	0.101
6c	20.2	18.0	18.3	16.2	3	27.1	0.45	0.062	0.100
6d	29.7	27.5	25.4	23.2	3	31.6	0.19	0.087	0.127
6e	50.1	33.6	40.6	24.1	0	33.9	-0.04	0.064	0.979
6f	19.3	11.0	10.1	1.8	2.5	27.1	-0.48	0.024	0.070
6h	9.9	6.23	5.4	1.2	3	22.0	0.65	0.067	0.094
6i	0.0	0.0	0.0	0.0	4	21.6	0.60	0.056	0.094

Table S17. Relative energies (E_{rel}) and Gibbs free energies (ΔG_{298} in kcal mol^{-1}) in gas-phase and DCM solvent, hydrogen bonding index (N_H), ring strain (Φ_p), π-conjugation index (Π) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the neutral *meso*-octakis(pentafluorophenyl)-substituted [38]octaphyrins **7**.

conformers	E_{rel}	ΔG_{298}	N_H	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
7a	13.1 (14.3)	16.7(17.9)	3	30.3	0.38	0.015	0.073
7b	43.1 (28.3)	39.4 (24.6)	0	31.2	0.45	0.037	0.083
7c	7.0 (7.5)	7.3 (8.7)	3	37.6	0.45	0.039	0.079
7d	17.9 (19.7)	19.5 (21.4)	3	32.4	0.25	0.045	0.118
7e	49.0 (37.0)	44.1(31.2)	0	48.1	-0.21	0.067	0.093
7f	17.4 (13.0)	12.3 (8.0)	2.5	28.6	-0.39	0.054	0.102
7h	0.0 (0.0)	0.0 (0.0)	3	24.1	0.55	0.006	0.052
7i	5.3 (6.4)	7.5 (8.6)	3	21.1	0.57	0.012	0.058

Table S18. Relative energies (E_{rel}) and Gibbs free energies (ΔG_{298} in kcal mol^{-1}) in gas-phase and TFA solvent, hydrogen bonding index (N_H), ring strain (Φ_p), π-conjugation index (Π) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the diprotonated *meso*-octakis(pentafluorophenyl)-substituted [36]octaphyrins **8**.

conformers	E_{rel}	ΔG_{298}	N_H	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
8a	2.0 (5.8)	4.9 (8.6)	3	31.3	0.34	0.104	0.104
8b	34.9 (26.0)	32.6 (23.6)	0	35.2	0.34	0.087	0.087
8c	5.1 (10.7)	8.1 (13.6)	3	39.6	0.43	0.086	0.086
8d	22.4 (24.5)	24.5 (22.8)	3	38.6	0.31	0.024	0.084
8e	32.7 (26.8)	26.8 (23.1)	0	35.5	-0.31	0.113	0.113
8f	8.1 (5.1)	3.9 (1.0)	2.5	31.2	-0.43	0.070	0.070
8h	0.0 (0.0)	0.0 (0.0)	3	24.1	0.53	0.093	0.093
8i	12.2 (7.4)	15.8 (11.1)	3	21.6	0.57	0.091	0.091

Table S19. Relative energies (E_{rel}) and Gibbs free energies (ΔG_{298} in kcal mol^{-1}) in gas-phase and TFA solvent, hydrogen bonding index (N_H), ring strain (Φ_P), π-conjugation index (Π) and bond-length alternation ($\Delta r_{C\text{-}C}$ and $\Delta r_{C\text{-}N}$) of the diprotonated *meso*-octakis(pentafluorophenyl)-substituted [38]octaphyrins **9**.

conformers	E_{rel}	ΔG_{298}	N_H	Φ_p	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$
9a	6.9 (10.0)	6.1 (8.2)	0	31.7	0.38	0.005	0.057
9b	4.0 (6.0)	1.3 (2.4)	0	31.9	0.40	0.011	0.066
9c	6.2 (12.8)	6.5 (12.1)	0	29.9	0.41	0.028	0.075
9d	17.0 (22.6)	15.6 (20.3)	0	43.0	0.25	0.025	0.096
9e	12.6 (12.1)	6.9 (5.6)	0	26.9	-0.22	0.028	0.091
9f	7.3 (10.5)	3.5 (5.7)	0	42.9	-0.33	0.038	0.086
9h	0.0(1.0)	0.0 (0.0)	0	28.5	0.49	0.006	0.052
9i	1.9 (0.0)	5.9 (3.0)	0	35.9	0.45	0.002	0.058

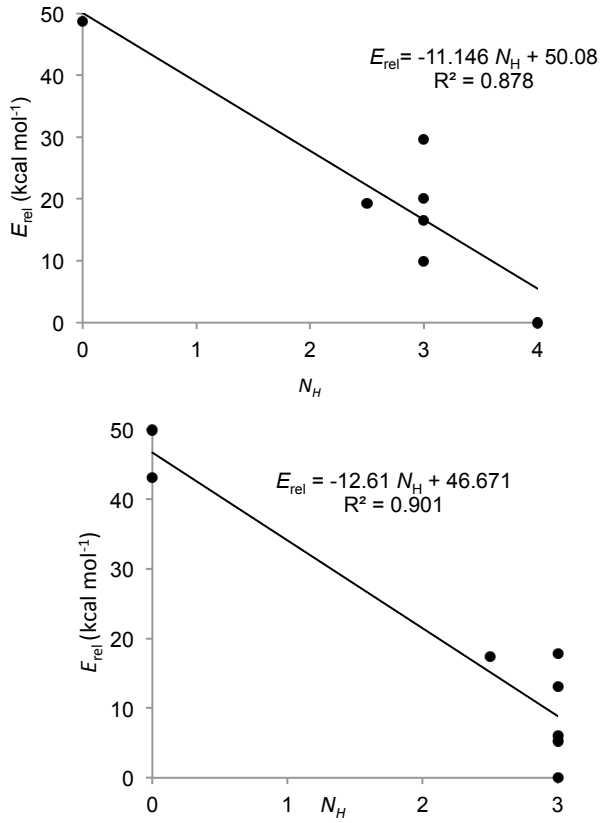


Figure S26. Dependence of the relative energy with N_H for *meso*-octakis(pentafluorophenyl) [36] (top) and [38]octaphyrins (bottom).

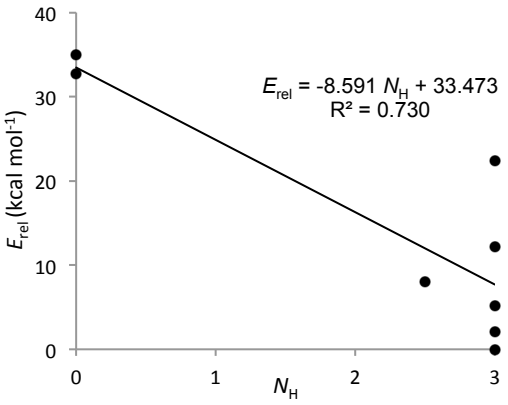


Figure S27. Dependence of the relative energy with N_H for diprotonated *meso*-octakis(pentafluorophenyl) [36]octaphyrin **8**.

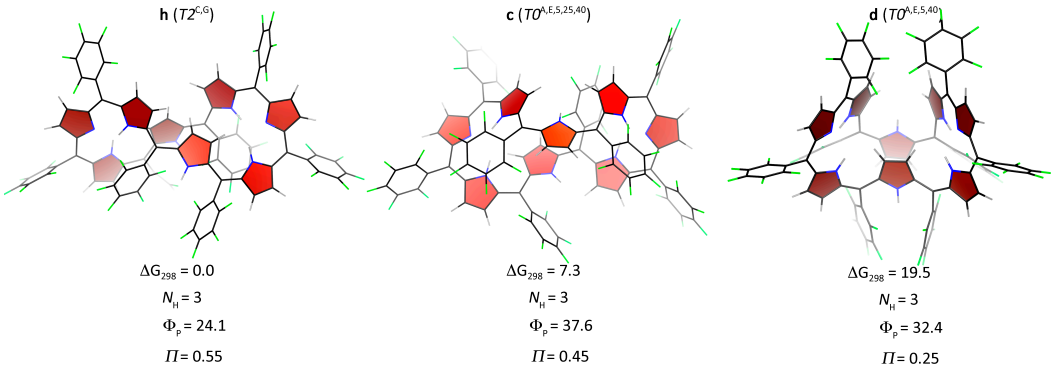


Figure S28. Plausible conformations for *meso*-octakis(pentafluorophenyl) [38]octaphyrin in neutral state.

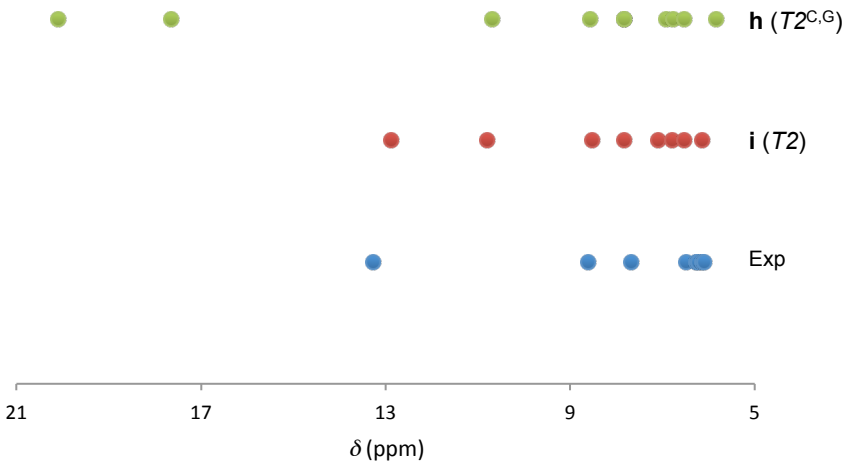


Figure S29. Experimental and computed ^{1}H NMR shifts of the NH protons and β-protons for the neutral *meso*-octakis(pentafluorophenyl) [36]octaphyrin **6** in different conformations.

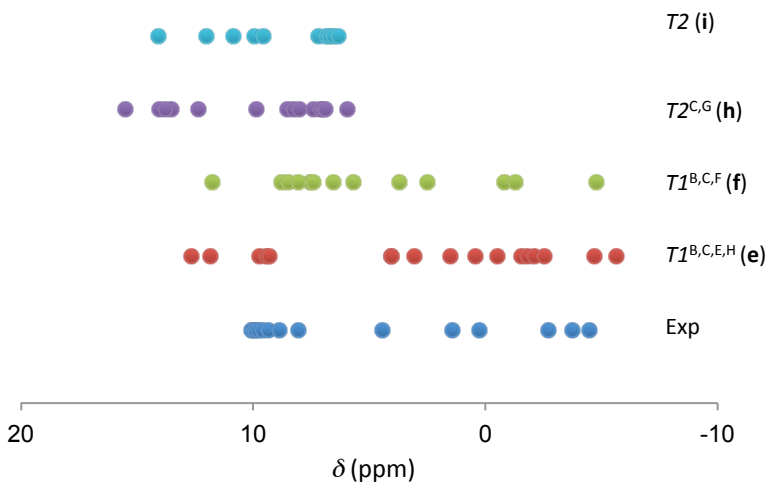


Figure S30. Experimental and computed ^{1}H NMR shifts of the NH protons and β-protons for the diprotonated *meso*-octakis(pentafluorophenyl) [36]octaphyrin **8** in different conformations

Table S20. Relative Gibbs free energies (in kcal mol^{-1}) of the different conformations of neutral and diprotonated *meso*-octakis(pentafluorophenyl) [36] and [38]octaphyrins computed with B3LYP and M06 functionals in solvent.[a]

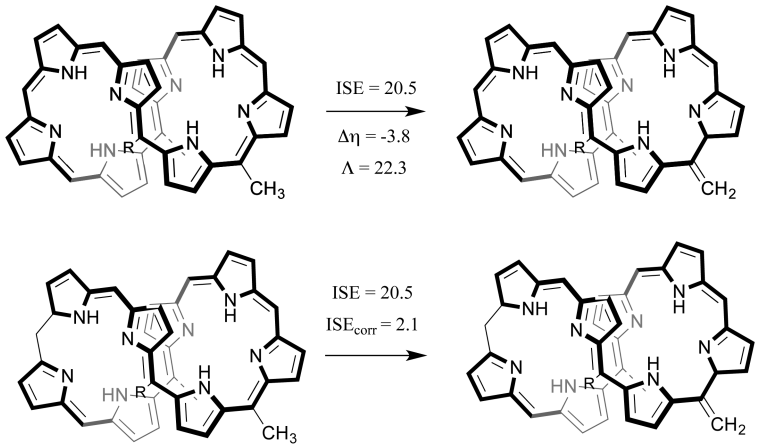
conf	Tn^{X}	[36] (**6**)	[38] (**7**)	$[36]^{2+}$ (**8**)	$[38]^{2+}$ (**9**)
a	$T0^{5,10,25,30}$	34.6 (14.4)	26.6 (17.9)	24.1 (8.6)	17.3 (8.2)
b	$T0^{B,C,E,F,H}$	12.0 (23.4)	8.8 (24.6)	12.2 (23.6)	**0.0** (2.4)[c]
c	$T0^{B,F,5,20,25}$	25.6 (16.2)	**0.0** (8.7)	21.9 (13.6)	22.2 (12.1)
d	$T0^{B,F,20,25}$	34.2 (23.2)	13.0 (21.4)	19.8 (23.6)	37.9 (20.3)
e	$T1^{B,C,E,H}$	6.2 (24.1)	4.9 (31.2)	6.1 (23.1)[c]	6.8 (5.6)
f	$T1^{B,C,F}$	**0.0** (1.8)	8.3 (8.0)	**0.0** (2.1)	17.6 (5.7)
h	$T2^{C,G}$	17.0 (1.7)	4.6 (**0.0**)	14.1 (**0.0**)	20.2 (**0.0**)
i	*T2*	26.5 (**0.0**)[c]	22.5 (8.6)	33.9 (11.1)	33.9 (3.0)
	MAD[b]	*14.2*	*10.8*	*11.8*	*12.9*

[a] Gibbs free energies at the M06/6-311+G(d,p)//M06/6-31G(d,p) level of theory in parenthesis and Gibbs free energies at the B3LYP/6-311+G(d,p)//M06/6-31G(d,p). [b] *MAD* is the mean absolute difference between the relative Gibbs free energies computed with both functionals. [c] The X-ray structure corresponds to this conformation.

In contrast to unsubstituted [36]octaphyrins, the relative Gibbs free energies of the different conformations of *meso*-octakis(pentafluorophenyl) octaphyrins in neutral and diprotonated state are strongly dependent on the functional used to evaluate the electronic energies in solvent. Whereas M06 predicts the twisted-Hückel topologies (**i** and **h**) as the most stable ones for the neutral [36] and [38]octaphyrins, B3LYP predicts that the Möbius **f** and the non-symmetric Hückel **c** for **6** and **7**, respectively. However, a doubly-twisted topology **6i** with all the pyrrolic nitrogens pointing inward was revealed by the X-ray crystallographic structure for the neutral [36]octaphyrin. In the case of neutral [38]octaphyrin, no crystallographic structure is available, but the ^{1}H-NMR spectra of the three plausible conformations (**7c**, **7d** and **7h**) (Figure 6) indicate that the most plausible structure for the neutral *meso*-octakis(pentafluorophenyl) [38]octaphyrin is the figure-eight conformation **7h** with two inverted pyrrole rings. Therefore, M06 provides relative energies in better agreement with the experimental data than B3LYP.

By contrast, in the diprotonated species, B3LYP provides relative energies in better agreement with the experimental observations than M06, although it describes the overall Hückel and Möbius structures worse. According to B3LYP, the Möbius **8f** and the Hückel **9b** are the global minima. The main difference between both functionals is related to the relative stability of the figure-eight conformations, which seems to be overstabilized by M06 in the diprotonated state, whereas B3LYP underestimates the stability of the figure-eight conformations in the neutral state. Since both M06 and B3LYP describe well the degree of π-electron delocalization in Hückel and Möbius octaphyrins, the discrepancies between the different methodologies mainly arise from an overestimation of the noncovalent interactions stabilizing the figure-eight topologies, such us the π-π staking interactions. Therefore, the selection of a functional for describing the thermochemistry of neutral and protonated *meso*-substituted octaphyrins is a complex task.

VIII. Aromaticity



Scheme S1. Example of the isomerization reaction used to evaluate the ISE and other aromaticity indices of [36]octaphyrin. *Syn-anti* correction for the ISE. ISE and $\Delta\eta$ are given in kcal mol^{-1} and Λ in ppm cgs.

Table S21. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformations of the neutral unsubstituted [36]octaphyrins computed at M06/6-311+G(d,p) level of theory.[a]

conformers	ISE	ISE$_{corr}$	$\Delta\eta$	Λ	NICS(0)	NICS$_{ZZ}$(1)	HOMA
1a	28.0	4.5	-1.6	238.4	8.6	31.5	0.75
1b	18.4	/	-6.1	458.8	8.4	26.9	0.73
1c	8.4	-2.8	-8.4	295.0	13.2	22.9	0.76
1d	18.4	1.0	-2.9	102.5	6.1	22.6	0.73
1e	20.1	20.1	-1.0	-325.1	-6.1	-13.3	0.71
1f	21.3	2.2	1.6	-299.0	-13.4	-24.6	0.82
1g	23.2	-1.0	-5.3	62.8	3.8	-22.5	0.76
1h	27.3	0.3	-3.5	92.1	4.0	-17.7	0.72
1i	20.3	-13.3	-3.5	79.1	0.8	-19.3	0.76

[a] ISE is given in kcal mol^{-1}, Λ in ppm cgs and NICS indices in ppm.

Table S22. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformations of the neutral unsubstituted [34]octaphyrins computed at B3LYP/6-311+G(d,p) level of theory.[a]

conformers	ISE	ISE$_{corr}$	$\Delta\eta$	Λ	NICS(0)	NICS$_{ZZ}$(1)	HOMA
2a	27.4	-2.8	4.1	-444.9	-15.2	-34.2	0.81
2b	20.8	1.0	-0.1	-513.7	-6.5	-15.5	0.73
2c	23.4	-2.0	0.0	272.5	-12.7	-19.9	0.82
2d	16.1	-1.3	0.5	-192.0	-21.6	-29.1	0.79
2e	17.4	-0.4	-5.1	348.6	5.4	19.6	0.71
2f	15.1	-4.7	-6.2	347.0	10.8	33.5	0.78
2g	26.1	-13.3	-1.1[b]	-127.8	-12.7	-20.9	0.86
2h	25.7	-12.6	3.6	-126.9	-12.7	-20.9	0.84
2i	23.8	11.7	-1.2[b]	-30.1	-3.2	-9.3	0.85

[a] ISE and ISE$_{corr}$ are given in kcal mol^{-1}, Λ in ppm cgs and NICS indices in ppm.
[b] The large flexibility induces topology changes in the dihydrogen derivative of the methylene adducts of these conformations during the optimization.

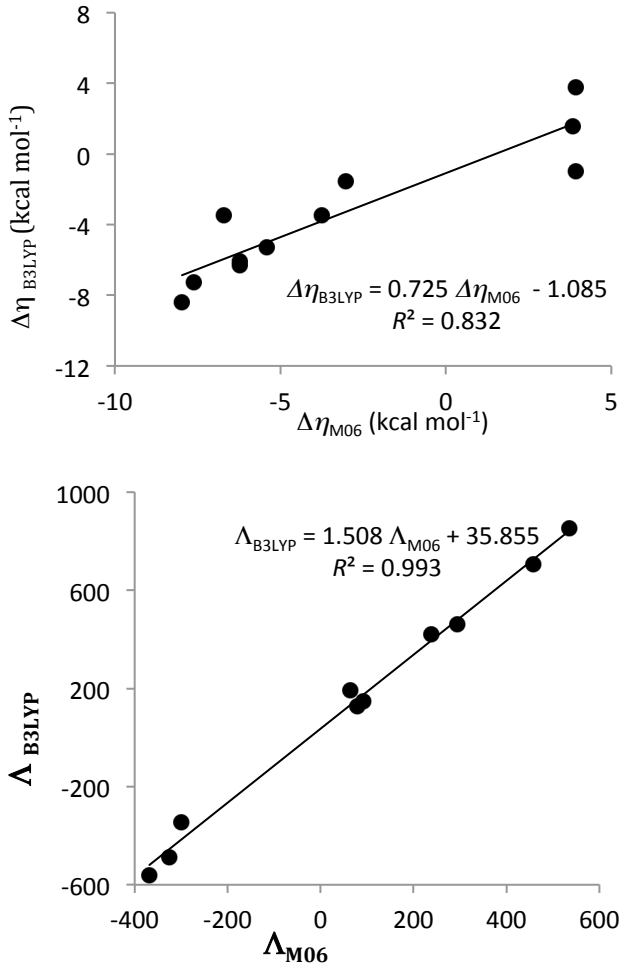


Figure S31. Correlation between the relative hardness ($\Delta\eta$) (top) and the diamagnetic susceptibility exaltation (Λ in ppm cgs) (bottom) computed with B3LYP and M06.

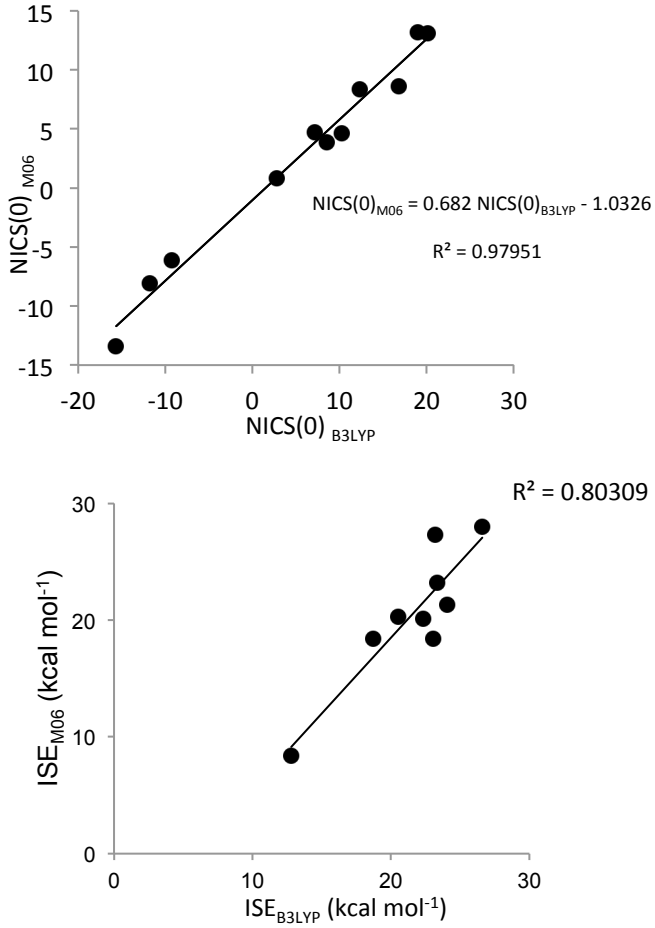


Figure S32. Correlation between the NICS(0) and ISE computed with B3LYP and M06 functionals.

Table S23. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformations of the neutral unsubstituted [38]octaphyrins computed at the B3LYP/6-311+G(d,p) level of theory.[a]

conformers	ISE	ISE_{corr}	$\Delta\eta$	Λ	NICS(0)	$NICS_{ZZ}$ (1)	HOMA
3a	29.3	-13.5[b]	1.1	-491.7	-18.2	-37.3	0.84
3b	24.2	-12.3[b]	3.7	-791.2	-9.5	-24.4	0.70
3c	33.9	-9.8[b]	9.1	-158.7	-8.6	-9.0	0.82
3d	26.6	-	5.0	-215.3	-18.2	-25.7	0.83
3e	28.5	-9.4	4.9	307.1	5.0	18.3	0.73
3f	20.8	-6.2	-3.4	325.4	10.4	34.5	0.83
3g	29.1	-10.3[b]	7.3	-136.3	-14.1	-19.1	0.81
3h	31.9	-12.1[b]	4.9	-158.2	-15.8	-41.2	0.87
3i	27.9	-9.0[b]	7.9	-107.2	-14.5	-44.1	0.88

[a] ISE and ISE_{corr} are given in kcal mol^{-1}, Λ in ppm cgs and NICS indices in ppm.
[b] The large flexibility induces topology changes in the dihydrogen derivative of the methylene adducts of these conformations during the optimization.

Table S24. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformations of the diprotonated unsubstituted [36]octaphyrins computed at the B3LYP/6-311+G(d,p) level of theory.[a]

conformers	ISE	ISE_{corr}	$\Delta\eta$	Λ	NICS(0)	$NICS_{ZZ}(1)$	HOMA
4a	22.1	-13.5	-7.3	880.7	28.4	81.7	0.69
4b	26.1	2.9[b]	-3.0	1199.1	16.1	49.3	0.76
4c	16.1	-15.5	-9.2	478.5	5.1	37.1	0.80
4d	21.9	-16.1	-9.8	469.6	9.7	37.5	0.81
4e	26.2	0.95	10.8	-558.8	-10.4	-26.0	0.80
4f	20.7	3.2	5.1	-361.1	-15.3	-30.9	0.71
4g	19.7	-1.7	-8.5	365.8	12.5	-17.9	0.79
4h	20.9	-1.5	-8.0	378.6	18.6	-17.1	0.78
4i	25.1	0.3[b]	-3.4	70.0	1.2	-25.6	0.77

[a] ISE and ISE_{corr} are given in kcal mol^{-1}, Λ in ppm cgs and NICS indices in ppm.
[b] The large flexibility induces topology changes in the dihydrogen derivative of the methylene adducts of these conformations during the optimization.

Table S25. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformations of the diprotonated unsubstituted [38]octaphyrins computed at B3LYP/6-311+G(d,p) level of theory.[a]

conformers	ISE	ISE_{corr}	$\Delta\eta$	Λ	NICS(0)	$NICS_{ZZ}$ (1)	HOMA
5a	27.7	-13.0	7.7	-638	-17.8	-39.2	0.88
5b	25.5	-7.1	9.6	-1 081	-12.1	-32.5	0.84
5c	22.1	-9.6	6.7	-277.8	-18.5	-28.0	0.86
5d	27.4	-8.9	10.1	[c]	-7.4	-15.7	0.83
5e	29.3	-14.2	-2.6	707.0	12.8	40.5	0.76
5f	15.3	-15.6	-2.7	462.1	20.8	59.2	0.76
5g	23.8	0.0	8.1	-217.6	-16.9	-21.7	0.88
5h	27.8	-2.4	8.3	-283.0	-18.0	-21.1	0.87
5i	27.6	-13.0	10.3	-183.2	-14.4	-33.5	0.88

[a] ISE and ISE_{corr} are given in kcal mol^{-1}, Λ in ppm cgs and NICS indices in ppm.
[b] The large flexibility induces topology changes in the dihydrogen derivative of the methylene adducts of these conformations during the optimization.
[c] Due to computational issues, the magnetic susceptibility exaltation of $T0^{B,F,20,25}$ is not reported.

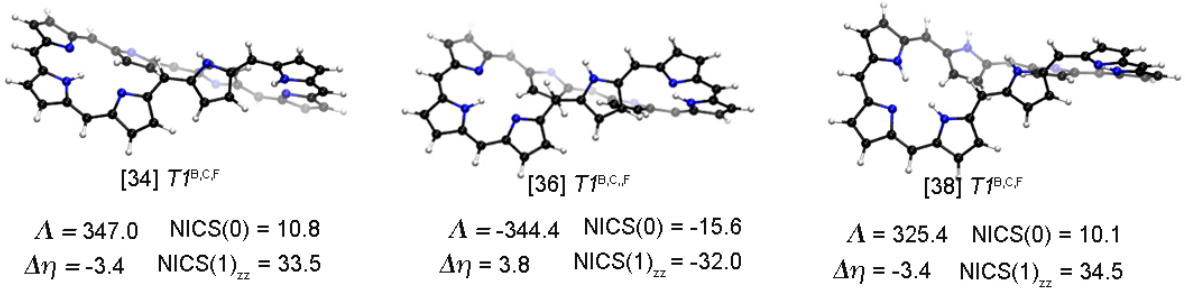


Figure S33. Evolution of magnetic and reactivity descriptors of the Möbius topology $T1^{B,C,F}$ (**f**) with the number of π-electrons.

Table S26. Correlation between several descriptors of aromaticity for unsubstituted octaphyrins (*n*=25).[a]

	$\Delta\eta$	Λ	NICS(0)	HOMA	$NICS_{zz}(1)$	ISE_{corr}
$\Delta\eta$	1					
Λ	0.75	1				
NICS(0)	0.83	0.92	1			
HOMA	0.50	0.44	0.54	1		
$NICS(1)_{zz}$	0.89[b]	0.94[b]	0.96[b]	0.49[b]	1	
ISE_{CORR}	0.01	0.04	0.07	0.04	0.03	1

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis
[b] The figure-eight topologies were left out because their $NICS_{zz}(1)$ are not associated with the macrocyclic ring current.

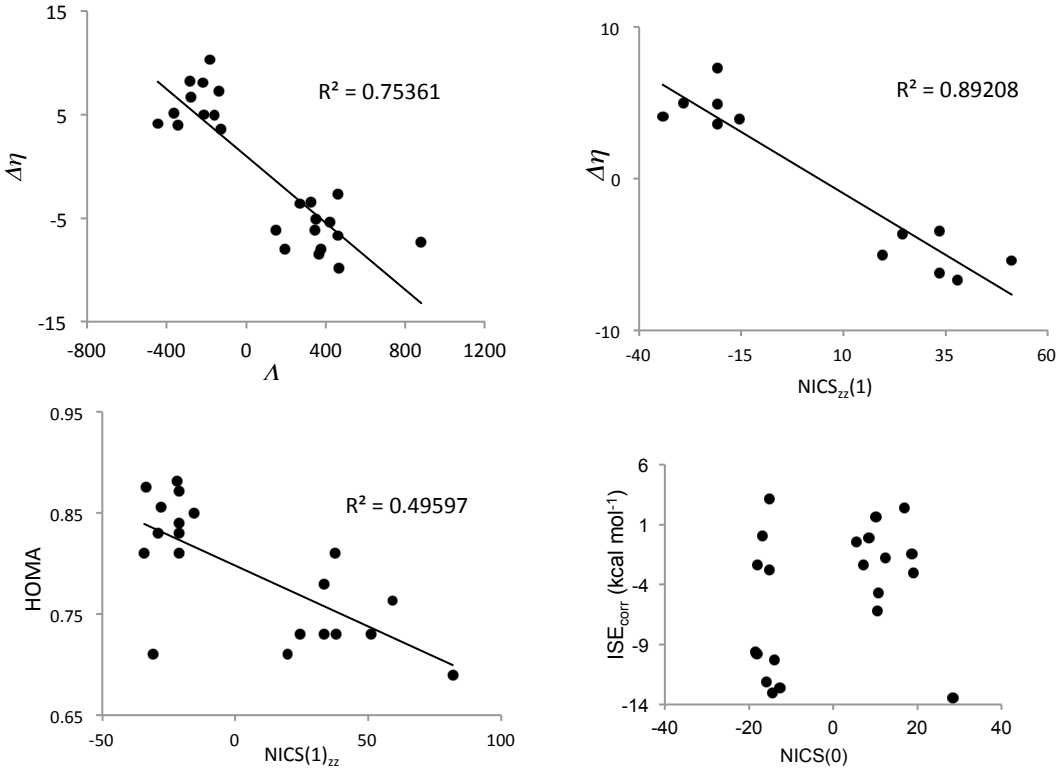


Figure S34. Correlation between several aromaticity descriptors computed for neutral and diprotonated octaphyrins (*n* = 25).

Table S27. Energetic, reactivity, magnetic and structural indices of aromaticity of the most stable conformation of *meso*-octakis(pentafluorophenyl) [36] and [38]octaphyrins upon protonation.

		$\Delta\eta$	Λ	NICS(0)	$NICS_{zz}(1)$	HOMA	σ_{TPA}[a]
[36]	*T2*	-1.2	-30	-3.2	-9.3	0.85	800
[38]	$T2^{C,G}$	4.9	-158	-15.8	-41.2	0.87	1800
$\mathbf{[36]^{2+}}$	$T1^{B,C,E,H}$	10.80	-559.00	-10.40	-26.00	0.80	5100
$\mathbf{[38]^{2+}}$	$T0^{B,C,E,F,H}$	9.60	-1081.00	-12.10	-32.10	0.84	6600

[a] $\Delta\eta$ is given in kcal mol^{-1}, Λ in ppm cgs and NICS indices in ppm. [b] Two-photon absorption cross-section in GM measured experimentally (*J. Am. Chem. Soc.* **2010**, *132*, 3105).

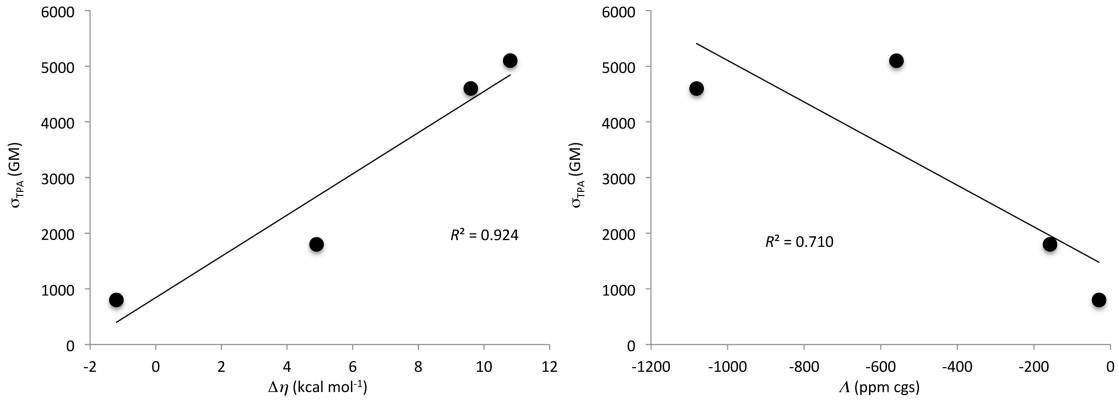


Figure S35. Correlation between the two-photon absorption cross-section values (σ_{TPA} in GM) and relative hardness and exaltation for *meso*-octakis(pentafluorophenyl) [36] and [38]octaphyrins in neutral and diprotonated states.

Table S28. Correlation between several descriptors of aromaticity for neutral unsubstituted octaphyrins (*n* = 14).

	$\Delta\eta$	Λ	NICS(0)	HOMA	$NICS_{zz}(1)$
$\Delta\eta$	1				
Λ	0.77	1			
NICS(0)	0.90	0.77	1		
HOMA	0.78	0.73	0.80	1	
$NICS_{zz}(1)$	0.89[b]	0.91[b]	0.96[b]	0.73[b]	1

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis
[b] The figure-eight topologies were left out because their $NICS_{zz}(1)$ are not associated with the macrocyclic ring current.

Table S29. Correlation between several descriptors of aromaticity for diprotonated unsubstituted octaphyrins *(n* = 11).[a]

	$\Delta\eta$	Λ	NICS(0)	HOMA	$NICS_{zz}(1)$
$\Delta\eta$	1				
Λ	0.77	1			
NICS(0)	0.82	0.91	1		
HOMA	0.37	0.42	0.48	1	
$NICS_{zz}(1)$	0.80[b]	0.96[b]	0.98[b]	0.38[b]	1

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis
[b] The figure-eight topologies were left out because their $NICS_{zz}(1)$ are not associated with the macrocyclic ring current.

Table S30. Correlation between several descriptors of aromaticity for unsubstituted [4*n* + 2] π-electrons octaphyrins (*n* = 13).[a]

	$\Delta\eta$	Λ	NICS(0)	HOMA	$NICS_{zz}(1)$
$\Delta\eta$	1				
Λ	0.67	1			
NICS(0)	0.78	0.92	1		
HOMA	0.82	0.65	0.63	1	
$NICS_{zz}(1)$	0.78[b]	0.72[b]	0.93[b]	0.73[b]	1

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis
[b] The figure-eight topologies were left out because their $NICS_{zz}(1)$ are not associated with the macrocyclic ring current.

Table S31. Correlation between several descriptors of aromaticity for unsubstituted [4*n*] π-electrons octaphyrins (*n* = 12).[a]

	$\Delta\eta$	Λ	NICS(0)	HOMA	$NICS_{zz}(1)$
$\Delta\eta$	1				
Λ	0.70	1			
NICS(0)	0.73	0.92	1		
HOMA	0.19	0.10	0.14	1	
$NICS_{zz}(1)$	0.92[b]	0.91[b]	0.87[b]	0.53[b]	1

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis

[b] The figure-eight topologies were left out because their $NICS_{zz}(1)$ are not associated with the macrocyclic ring current.

VII Cartesian coordinates of M06/6-31G(d,p) optimized geometries

1a (Hückel $T0^{5,10,25,30}$)

C	-7.63494	1.1164	-0.04268
C	-8.98048	0.69264	-0.03154
C	-8.9805	-0.69246	0.03154
C	-7.63499	-1.11628	0.04267
C	-7.11345	-2.43187	0.08176
C	-5.78244	-2.75921	0.00479
N	-4.78161	-1.82209	-0.15718
C	-3.64529	-2.50485	-0.19002
C	-2.41267	-1.81063	-0.39971
C	-1.14882	-2.27564	-0.17984
C	-0.67659	-3.50488	0.41949
C	0.67666	-3.50485	0.41943
C	1.14877	-2.27558	-0.17988
C	2.4126	-1.81052	-0.39975
C	3.64521	-2.50475	-0.19004
N	4.78156	-1.82205	-0.15726
C	5.78233	-2.75923	0.00473
C	7.11335	-2.43198	0.08173
C	7.63494	-1.11641	0.04267
C	8.98048	-0.69265	0.03153
C	8.9805	0.69245	-0.03156
C	7.63499	1.11627	-0.04268
C	7.11345	2.43187	-0.08177
C	5.78245	2.7592	-0.00481
N	4.78161	1.82208	0.15716
C	3.64529	2.50485	0.19001
C	2.41267	1.81062	0.3997
C	1.14882	2.27565	0.17985
C	0.6766	3.5049	-0.41945
C	-0.67665	3.50488	-0.41939
C	-1.14877	2.27559	0.17989
C	-2.4126	1.81052	0.39975
C	-3.64521	2.50476	0.19005
N	-4.78156	1.82204	0.15726
C	-5.78233	2.75923	-0.00473
C	-7.11335	2.43197	-0.08173
N	-6.8545	0.00005	-0.00001
C	-5.21937	-4.09369	0.06029
C	-3.87778	-3.94148	-0.05681
N	-0.00005	-1.55154	-0.47289
C	3.87758	-3.94137	-0.05658
C	5.21917	-4.09368	0.06036
N	6.8545	-0.00006	-0.00001
C	5.21938	4.09368	-0.0603
C	3.87779	3.94147	0.05681
N	0.00005	1.55155	0.4729
C	-3.87759	3.94137	0.0566
C	-5.21918	4.09367	-0.06034
H	-5.82722	-0.00001	-0.00009
H	5.82722	0.	0.00008
H	0.00008	0.70863	1.03104
H	-0.00008	-0.70867	-1.0311
H	7.83872	-3.23873	0.17635

H	7.83886	3.23858	-0.17639
H	2.53016	0.78747	0.76077
H	-2.53008	0.78737	0.76085
H	-7.83872	3.23873	-0.17634
H	-7.83886	-3.23859	0.17637
H	-2.53016	-0.78748	-0.7608
H	2.53009	-0.78738	-0.76087
H	5.7838	5.01432	-0.1592
H	3.13106	4.72416	0.11377
H	1.32408	4.25548	-0.85291
H	-1.32422	4.25543	-0.85281
H	-3.13079	4.72401	0.11337
H	-5.78355	5.01434	-0.15932
H	-9.83794	1.3536	-0.05852
H	-9.83799	-1.3534	0.05851
H	-5.78379	-5.01433	0.1592
H	-3.13105	-4.72416	-0.11376
H	-1.32408	-4.25545	0.85297
H	1.32422	-4.25539	0.85287
H	3.13078	-4.724	-0.11334
H	5.78354	-5.01434	0.15935
H	9.83794	-1.35361	0.05852
H	9.83799	1.35339	-0.05853

E(RM06) = -1977.64678429 A.U. after 14 cycles

1b (Hückel $TO^{B,C,E,F,H}$)

C	0.14091	-5.38931	3.56325
C	0.2508	-5.94639	4.89117
C	0.3072	-4.93332	5.78731
C	0.22472	-3.67658	5.07989
C	0.19376	-2.42845	5.63357
C	0.14825	-1.17956	4.94163
N	-0.12892	-0.04714	5.57391
C	-0.13703	0.92897	4.59452
C	-0.39492	2.24894	4.86019
C	-0.64369	3.20324	3.83249
C	-1.21501	2.99782	2.57018
C	-1.18488	4.20101	1.87787
C	-0.59841	5.16502	2.7077
C	-0.26212	6.52142	2.42883
C	-0.08106	6.99301	1.15257
N	-0.11995	6.15779	0.05907
C	0.1355	6.90879	-0.99758
C	0.25471	6.37078	-2.32157
C	0.32886	5.02751	-2.5807
C	0.40876	3.92513	-1.64168
C	0.468	2.76888	-2.33286
C	0.42647	3.05747	-3.75171
C	0.37202	2.19299	-4.80582
C	0.47549	0.76597	-4.68237
N	-0.0747	-0.05232	-5.56359
C	0.15358	-1.32949	-5.07593
C	-0.36864	-2.43437	-5.69378
C	-0.43226	-3.7487	-5.15739
C	-0.6559	-4.96568	-5.81206

C	-0.6687	-5.97322	-4.85063
C	-0.46958	-5.38258	-3.59502
C	-0.46072	-6.02237	-2.3309
C	-0.15703	-5.51476	-1.0931
N	-0.30697	-6.3108	0.02954
C	0.04238	-5.55807	1.06073
C	0.03384	-6.08106	2.3917
N	0.16897	-4.00815	3.72896
C	0.40229	-0.96004	3.51483
C	0.21409	0.35913	3.29916
N	-0.34363	4.54548	3.91641
C	0.20309	8.35625	0.72908
C	0.31831	8.31176	-0.62112
N	0.36163	4.44225	-3.83623
C	1.18153	0.03513	-3.62565
C	0.96968	-1.27683	-3.86997
N	-0.30619	-4.0343	-3.81567
C	0.34661	-4.20236	-0.7146
C	0.47278	-4.22493	0.63264
H	0.28783	9.21866	1.38085
H	-1.5551	4.41162	0.8854
H	-1.65982	2.06579	2.24762
H	0.37726	0.91505	2.38439
H	0.78114	-1.68458	2.80321
H	0.41497	-5.00364	6.86293
H	0.30546	-7.01035	5.08742
H	0.89784	-3.44845	1.2594
H	0.20421	4.95451	4.65954
H	-0.24481	-3.38833	3.04869
H	0.5377	9.12821	-1.3007
H	0.40065	4.07608	-0.57189
H	0.4878	1.77157	-1.91666
H	1.82403	0.46665	-2.86753
H	1.41857	-2.12181	-3.3592
H	-0.76419	-5.07567	-6.88354
H	-0.79548	-7.03644	-5.01178
H	0.63935	-3.38916	-1.37022
H	0.28997	4.95059	-4.70369
H	-0.37978	-3.32952	-3.09677
H	-0.7466	-7.07338	-2.34018
H	-0.08309	-7.15995	2.46753
H	0.15776	-2.37128	6.71918
H	-0.42351	2.5573	5.90579
H	-0.10588	7.20307	3.26559
H	0.28909	7.07224	-3.15461
H	-0.81404	-2.28334	-6.67589
H	0.16107	2.57546	-5.80368

SCF Done: E(RM06) = -1977.59152008 A.U. after 7 cycles

1c (Hückel $T0^{5,20,25,B,F}$)

C	6.07536	2.20847	0.07551
C	6.25664	3.56169	0.54861
C	5.03514	4.09412	0.78356
C	4.02542	3.09827	0.49497
C	2.67537	3.29546	0.57728

C	1.6373	2.33841	0.37365
N	0.36084	2.70782	0.31026
C	-0.33636	1.52776	0.15426
C	-1.68578	1.37769	-0.00152
C	-2.72136	2.34237	-0.08578
C	-2.79317	3.74683	0.00053
C	-4.11573	4.11162	-0.2316
C	-4.86487	2.93484	-0.45628
C	-6.21621	2.72582	-0.83584
C	-6.77577	1.47787	-1.03453
N	-6.08898	0.32294	-0.73318
C	-6.77766	-0.69455	-1.25643
C	-6.26201	-2.0275	-1.21898
C	-5.15869	-2.36261	-0.46798
C	-4.28883	-3.51956	-0.52867
C	-3.22914	-3.31346	0.29698
C	-3.42915	-2.05554	0.98523
C	-2.74078	-1.42674	1.98628
C	-1.407	-1.65967	2.43546
N	-0.46226	-2.29245	1.74825
C	0.7036	-2.04249	2.45285
C	1.96834	-2.17291	1.94865
C	2.3374	-2.64622	0.66127
C	1.6939	-3.49801	-0.2509
C	2.53728	-3.657	-1.34585
C	3.6773	-2.8656	-1.13104
C	4.81474	-2.65177	-1.9456
C	5.749	-1.66008	-1.77826
N	5.62499	-0.59057	-0.8997
C	6.76435	0.0982	-1.0275
C	7.02804	1.36215	-0.42579
N	4.72122	1.96039	0.11469
C	1.80333	0.88797	0.26859
C	0.55976	0.38158	0.14153
N	-3.98478	1.89505	-0.33938
C	-8.00275	1.13919	-1.72387
C	-7.99112	-0.21279	-1.89081
N	-4.60639	-1.54354	0.48654
C	-0.89562	-1.03937	3.65401
C	0.42803	-1.30316	3.67457
N	3.53579	-2.28537	0.10089
C	7.02083	-1.60626	-2.46661
C	7.67829	-0.53369	-1.96493
H	4.20364	-1.5942	0.43499
H	4.35292	1.1245	-0.32861
H	-4.29206	0.94407	-0.54587
H	-4.99731	-0.6229	0.6616
H	7.3605	-2.32273	-3.2062
H	8.66326	-0.16225	-2.22454
H	2.36166	-4.25855	-2.22909
H	0.72096	-3.93765	-0.07811
H	7.22409	4.03514	0.6626
H	4.79934	5.09164	1.13437
H	-1.94103	4.38251	0.20194
H	-4.5216	5.11587	-0.24626
H	-8.74466	1.84618	-2.07782
H	-8.73172	-0.82779	-2.38928

H	-2.37596	-3.95543	0.47448
H	-4.46221	-4.37253	-1.17372
H	2.72693	0.32563	0.33955
H	0.24469	-0.65619	0.07422
H	4.96444	-3.35433	-2.7642
H	8.0457	1.74259	-0.47863
H	2.34596	4.30403	0.81844
H	2.77606	-1.76217	2.55697
H	1.17215	-0.99326	4.39962
H	-1.48617	-0.46925	4.3624
H	-6.69596	-2.78179	-1.87004
H	-3.24592	-0.58083	2.45698
H	-6.81226	3.60959	-1.05592
H	-2.02293	0.34222	-0.09852

SCF Done: E(RM06) = -1977.63975611 A.U. after 7 cycles

1d (Hückel $TO^{20,25,B,F}$)

C	5.75709	1.86238	-1.01897
C	6.03336	3.20908	-0.72798
C	4.9008	3.75374	-0.14944
C	3.8973	2.76348	-0.11742
C	2.57676	3.01703	0.32199
C	1.36328	2.37404	0.22806
N	0.26313	3.09387	0.65935
C	-0.80569	2.39193	0.30472
C	-2.06738	3.0519	0.457
C	-3.32883	2.86956	-0.04407
C	-4.28354	3.95674	-0.09925
C	-5.34586	3.57469	-0.84301
C	-5.16372	2.19575	-1.21963
C	-6.03578	1.42987	-1.95183
C	-5.94293	0.02016	-2.10622
N	-5.12993	-0.71587	-1.3494
C	-5.3485	-2.03161	-1.71352
C	-4.78479	-3.08839	-1.03299
C	-4.02313	-2.93651	0.15046
C	-3.14311	-3.80793	0.81615
C	-2.51392	-3.08505	1.82656
C	-3.04154	-1.783	1.80947
C	-2.7443	-0.59859	2.55769
C	-1.48052	-0.2352	2.9159
N	-0.37714	-0.9686	2.52135
C	0.65545	-0.17083	2.71697
C	1.95854	-0.45154	2.19802
C	2.28484	-1.59332	1.51641
C	1.57423	-2.84626	1.35929
C	2.3141	-3.65824	0.56308
C	3.48419	-2.93191	0.13098
C	4.43976	-3.27586	-0.79836
C	5.38251	-2.34081	-1.29526
N	5.30867	-1.03095	-1.02274
C	6.3905	-0.4504	-1.63922
C	6.62512	0.90283	-1.58907
N	4.45433	1.62261	-0.63978
C	0.92891	1.11733	-0.36947
C	-0.42866	1.12506	-0.31949

N	-3.94089	1.80863	-0.69432
C	-6.70811	-0.80948	-3.01873
C	-6.31098	-2.08971	-2.79124
N	-3.97264	-1.73934	0.81933
C	-1.07496	1.051	3.4677
C	0.26895	1.10005	3.33366
N	3.4411	-1.72404	0.77785
C	6.53485	-2.63584	-2.13165
C	7.17814	-1.45665	-2.32329
H	4.13833	-1.01362	0.56833
H	4.03982	0.7046	-0.76887
H	-3.58905	0.86881	-0.83216
H	-4.43702	-0.9205	0.41982
H	6.81395	-3.61919	-2.49275
H	8.08326	-1.26934	-2.88981
H	2.07464	-4.66492	0.24259
H	0.61216	-3.02916	1.81651
H	6.98217	3.69546	-0.91657
H	4.75744	4.76827	0.20129
H	-4.09481	4.92651	0.3454
H	-6.21677	4.15867	-1.11434
H	-7.43181	-0.45041	-3.74172
H	-6.66035	-2.99528	-3.27451
H	-1.77415	-3.43261	2.53462
H	-2.97873	-4.84555	0.55267
H	1.56174	0.33891	-0.78421
H	-1.09841	0.34036	-0.65713
H	4.44186	-4.29052	-1.18767
H	7.55175	1.2879	-2.01114
H	2.47483	4.0049	0.77241
H	2.69729	0.34979	2.24056
H	0.93914	1.92226	3.55945
H	-1.74569	1.81694	3.84001
H	-4.92766	-4.09739	-1.41566
H	-3.55514	0.11409	2.71421
H	-6.88498	1.94472	-2.39559
H	-1.93495	4.02508	0.92893

SCF Done: E(RM06) = -1977.63063906 A.U. after 8 cycles

1e (Hückel $T1^{B,C,E,H}$)

C	7.06231700	0.39754900	0.23117300
C	8.32205900	-0.29277600	0.36582100
C	8.14818900	-1.58975900	0.00634700
C	6.76873900	-1.78799100	-0.36574900
C	6.11002400	-2.96593900	-0.59546000
C	4.52168500	1.98067600	-0.64084400
C	4.71170600	-3.06068800	-0.86911400
N	3.97969600	-4.10465900	-0.49705500
C	2.67649700	-3.75760400	-0.78916000
C	1.62757800	-4.53540500	-0.35233200
C	0.26773200	-4.15779400	-0.29382300
C	-0.35858600	-2.90245600	-0.44443200
C	-1.71036100	-3.05436600	-0.21206400
C	-1.95270000	-4.40656800	0.10535100
C	-3.15352000	-5.07176900	0.43367400

C	-4.38512500	-4.46660500	0.57918200
N	-4.58917700	-3.11756600	0.45966400
C	-5.90274200	-2.93627100	0.58002900
C	-6.53686000	-1.66732200	0.45950400
C	-5.86255300	-0.47266200	0.40250700
C	-4.47707000	-0.18650600	0.68640000
C	-4.23270200	1.11578100	0.40382800
C	-5.45046000	1.71517900	-0.08943200
C	-5.64506500	2.93849400	-0.67805500
C	-4.60397900	3.87325000	-0.95402500
N	-3.39255500	3.83939000	-0.40908400
C	-2.64716500	4.75315100	-1.11559200
C	-1.30682000	4.96909800	-0.90191500
C	-0.56982400	4.47425500	0.20248300
C	-0.99860600	4.11945900	1.49293000
C	0.12994700	3.90182600	2.27259400
C	1.26241300	4.04321600	1.45576700
C	2.61679800	3.77124000	1.77887700
C	3.57747400	3.24884500	0.94853700
N	4.85473400	2.99469400	1.41094000
C	5.41244200	2.21635700	0.49627800
C	6.72076600	1.65138300	0.65369200
N	6.17942000	-0.53195300	-0.30539500
C	3.90196100	-2.03355800	-1.52677000
C	2.62635300	-2.48012500	-1.48340700
N	-0.73188000	-5.04332000	0.04355900
C	-5.64482000	-5.15749700	0.80744900
C	-6.60314500	-4.19954100	0.78894700
N	-6.42478000	0.73475600	0.02179500
C	-4.70034900	4.88446700	-2.00468400
C	-3.45706200	5.40441600	-2.13292900
C	3.37894100	2.65240700	-0.36660600
N	0.80613400	4.40187300	0.20946600
H	1.75379700	-2.02622000	-1.93548900
H	5.18082700	-0.43126400	-0.17995200
H	-0.58537200	-6.02713200	0.21535000
H	-3.79730000	-0.93525700	1.06824100
H	-7.67399400	-4.31616300	0.91516800
H	-5.58842100	5.10965600	-2.58532000
H	4.76223700	1.41016400	-1.53184400
H	8.89046500	-2.37874300	-0.00273500
H	-5.76412300	-6.22734200	0.93936800
H	-2.03959800	4.07147700	1.78207800
H	4.27623800	-1.14796400	-2.02938900
H	-2.48967900	-2.30739600	-0.24675500
H	-3.11074500	6.16543800	-2.82349800
H	-3.31038300	1.67414800	0.49373300
H	0.15572100	-1.97345800	-0.64438900
H	2.46935200	2.67017400	-0.95586900
H	0.16339900	3.61259300	3.31558900
H	9.23379600	0.18304300	0.70601500
H	6.65247500	-3.89162400	-0.41824500
H	1.90275600	-5.50872500	0.05676800
H	-3.10788700	-6.15285200	0.57318600
H	-7.62010700	-1.66034400	0.33657900
H	-6.63130300	3.16282400	-1.08547300
H	-0.77045100	5.57340200	-1.63526900

H	2.90412900	3.89828700	2.82208700
H	7.43874300	2.19644100	1.26180600
H	-7.33734700	0.80987500	-0.40163000
H	1.40699200	4.66735600	-0.55719100

SCF Done: E(RM06) = -1977.59280402 A.U. after 7 cycles

1f (Hückel $T1^{B,C,F}$)

C	7.46686	0.07819	-0.36968
C	8.3878	0.893	-1.11113
C	7.66936	1.8542	-1.75827
C	6.27573	1.66032	-1.46343
C	5.218	2.4712	-1.81675
C	3.85831	2.22955	-1.51425
N	2.94372	3.20824	-1.50038
C	1.77995	2.60395	-1.1123
C	0.63663	3.32608	-0.82522
C	-0.61107	2.78012	-0.4733
C	-1.18805	1.50943	-0.71257
C	-2.44419	1.47805	-0.14493
C	-2.67598	2.7343	0.46823
C	-3.73956	3.21997	1.23567
C	-4.95158	2.6021	1.50419
N	-5.37385	1.40208	1.0144
C	-6.65013	1.29029	1.43058
C	-7.53943	0.28186	1.02457
C	-7.2604	-0.74748	0.14647
C	-8.21228	-1.60562	-0.4972
C	-7.53906	-2.39069	-1.38309
C	-6.14145	-2.08753	-1.27342
C	-5.11078	-2.7047	-1.95405
C	-3.73638	-2.57472	-1.69396
N	-3.20542	-1.86651	-0.68207
C	-1.86562	-2.1481	-0.71062
C	-1.01624	-1.73927	0.30673
C	0.37906	-1.90917	0.3603
C	1.34757	-2.13867	-0.64782
C	2.59771	-2.14041	-0.06247
C	2.43725	-1.93438	1.32659
C	3.38409	-2.0136	2.36363
C	4.75595	-1.89634	2.21434
N	5.38553	-1.37079	1.11988
C	6.70552	-1.47835	1.37675
C	7.71517	-0.89006	0.58861
N	6.21248	0.54269	-0.6595
C	3.27604	0.93806	-1.15929
C	1.97157	1.17502	-0.90771
N	-1.55828	3.50103	0.21678
C	-5.98805	3.24533	2.29741
C	-7.05692	2.41892	2.25451
N	-6.02498	-1.08994	-0.33964
C	-2.71916	-3.31112	-2.42831
C	-1.54433	-3.03987	-1.8176
N	1.08591	-1.78798	1.539
C	5.72434	-2.34327	3.2008
C	6.94531	-2.13539	2.65227

H	-0.73004	0.71804	-1.29239
H	-0.57215	-3.46284	-2.03663
H	-2.90423	-3.96997	-3.26976
H	-7.94277	-3.14085	-2.05202
H	-9.27837	-1.57383	-0.30865
H	-8.03436	2.54706	2.70609
H	-5.89151	4.20537	2.79279
H	1.23254	0.46452	-0.56077
H	8.04495	2.6482	-2.39232
H	9.46208	0.75571	-1.11047
H	7.9204	-2.35192	3.07437
H	5.48195	-2.79444	4.15677
H	1.12817	-2.22808	-1.70386
H	-1.40397	4.42579	0.5905
H	0.65999	-1.6349	2.4411
H	8.75334	-1.10808	0.82797
H	-8.57408	0.3669	1.35173
H	-3.61536	4.2193	1.6568
H	0.74141	4.41202	-0.82454
H	5.45525	3.41689	-2.29998
H	-1.50027	-1.27301	1.16661
H	3.01225	-2.23095	3.36604
H	-5.40539	-3.41413	-2.72535
H	3.77511	-0.02297	-1.13123
H	-3.14967	0.65546	-0.15796
H	5.41979	0.1783	-0.12835
H	-5.15129	-0.65426	-0.05007
H	3.5611	-2.29233	-0.53157

SCF Done: E(RM06) = -1977.15482365 A.U. after 19 cycles

1g (Hückel $T2^{B,F}$)

C	-6.23639	2.07606	0.47483
C	-6.33111	3.45788	0.88922
C	-5.12038	3.84081	1.36671
C	-4.22002	2.71056	1.30847
C	-2.92125	2.64205	1.71973
C	-2.11158	1.45951	1.74073
N	-0.79203	1.53655	1.72981
C	-0.34228	0.22571	1.70046
C	0.99759	-0.01838	1.55018
C	1.6773	-1.25441	1.40123
C	1.25544	-2.59807	1.35027
C	2.38131	-3.39339	1.17383
C	3.50171	-2.54778	1.09893
C	4.87482	-2.87495	0.96437
C	5.89499	-1.98061	0.75571
N	5.70723	-0.63717	0.48915
C	6.93616	-0.10586	0.40796
C	7.19564	1.24421	0.05637
C	6.23643	2.07602	-0.47511
C	6.33111	3.45779	-0.88964
C	5.12031	3.8407	-1.36699
C	4.21997	2.71046	-1.30857
C	2.92116	2.64187	-1.71969
C	2.11158	1.45928	-1.74053

N	0.79202	1.53625	-1.72957
C	0.34234	0.22537	-1.70016
C	-0.99753	-0.01869	-1.54986
C	-1.67731	-1.2547	-1.40099
C	-1.25546	-2.59835	-1.34993
C	-2.38136	-3.39366	-1.17356
C	-3.50175	-2.54802	-1.09876
C	-4.8749	-2.87511	-0.96433
C	-5.89501	-1.98069	-0.75581
N	-5.7072	-0.63725	-0.48931
C	-6.93612	-0.10585	-0.40827
C	-7.19557	1.24425	-0.05675
N	-4.9537	1.68349	0.74478
C	-2.57836	0.07112	1.78579
C	-1.46421	-0.69596	1.76762
N	3.03996	-1.26985	1.24322
C	7.31121	-2.28334	0.83051
C	7.96193	-1.10906	0.65244
N	4.95368	1.68345	-0.74484
C	2.57842	0.07092	-1.78559
C	1.46432	-0.69623	-1.76736
N	-3.03997	-1.27011	-1.24305
C	-7.31124	-2.28334	-0.83076
C	-7.96191	-1.10902	-0.65276
H	0.23318	-2.94154	1.43057
H	2.41691	-4.47349	1.10252
H	7.73096	-3.26375	1.02599
H	9.03027	-0.92467	0.64795
H	7.23241	4.0533	-0.81261
H	4.84086	4.80818	-1.76621
H	3.60303	-0.27821	-1.86613
H	1.42454	-1.7783	-1.79485
H	-0.23319	-2.94181	-1.43009
H	-2.41699	-4.47375	-1.10216
H	-7.73102	-3.26373	-1.02625
H	-9.03025	-0.92458	-0.64834
H	-7.23241	4.05338	0.81201
H	-4.84096	4.80831	1.76589
H	3.67131	-0.47402	1.20331
H	4.64652	0.7518	-0.47852
H	-3.67132	-0.47427	-1.20332
H	-4.64643	0.75192	0.47831
H	-5.1316	-3.92787	-1.06968
H	-8.20903	1.62415	-0.15482
H	-2.43266	3.56824	2.01391
H	1.61588	0.88028	1.50238
H	5.13145	-3.92773	1.06968
H	8.20914	1.62406	0.15428
H	-1.61577	0.88001	-1.50206
H	2.43248	3.568	-2.01392
H	-3.60295	-0.27807	1.86631
H	-1.42437	-1.77803	1.79496

SCF Done: E(RM06) = -1977.65391418 A.U. after 19 cycles

1h (Hückel $T2^{C,G}$)

C	-7.0665	-0.22027	-0.06575

C	-8.05398	-1.2109	-0.24351
C	-7.41691	-2.36319	-0.68115
C	-6.04343	-2.07046	-0.80155
C	-4.98641	-2.90143	-1.24057
C	-3.69302	-2.49222	-1.46053
N	-3.28748	-1.17882	-1.3329
C	-1.9956	-1.16286	-1.64022
C	-1.30121	0.08646	-1.643
C	0.0433	0.30835	-1.66598
C	1.1785	-0.58929	-1.61913
C	2.31448	0.13848	-1.52066
C	1.96474	1.5432	-1.50563
C	2.76454	2.65041	-1.39734
C	4.17249	2.62561	-1.16382
N	4.8512	1.56351	-0.74693
C	6.17768	1.94967	-0.7393
C	7.20953	1.11306	-0.39609
C	7.06653	-0.22027	0.06569
C	8.05397	-1.21096	0.24335
C	7.41689	-2.36321	0.68105
C	6.04343	-2.07042	0.80154
C	4.9864	-2.90138	1.24056
C	3.69302	-2.49217	1.46054
N	3.28746	-1.17878	1.33287
C	1.99558	-1.16282	1.64023
C	1.30117	0.08648	1.64302
C	-0.04334	0.30837	1.66607
C	-1.17855	-0.58925	1.61928
C	-2.31452	0.13852	1.52076
C	-1.96476	1.54323	1.50569
C	-2.76453	2.65046	1.39731
C	-4.17248	2.62566	1.16374
N	-4.85116	1.56355	0.74685
C	-6.17765	1.94969	0.73924
C	-7.20949	1.11307	0.39603
N	-5.87035	-0.77184	-0.41417
C	-2.58089	-3.32294	-1.87197
C	-1.50948	-2.49663	-1.97643
N	0.59135	1.58415	-1.64266
C	5.04858	3.77022	-1.39962
C	6.3071	3.33532	-1.15554
N	5.8704	-0.77176	0.41429
C	2.5809	-3.32289	1.87202
C	1.50949	-2.4966	1.9765
N	-0.59138	1.58418	1.64281
C	-5.04857	3.77025	1.39956
C	-6.30708	3.33534	1.15547
H	1.10573	-1.66898	-1.59982
H	-9.10958	-1.07437	-0.04405
H	-7.86756	-3.32101	-0.91021
H	-2.62446	-4.38967	-2.06236
H	-0.51181	-2.75747	-2.30724
H	4.72755	4.749	-1.73926
H	7.23911	3.88359	-1.23598
H	9.10956	-1.0745	0.04375
H	7.86752	-3.32105	0.91009
H	2.62449	-4.38961	2.06245

H	0.51184	-2.75745	2.30734
H	-1.10581	-1.66895	1.60006
H	-4.72755	4.74903	1.73923
H	-7.2391	3.8836	1.23591
H	0.03619	2.42494	-1.60149
H	-0.03619	2.42492	1.60107
H	5.23535	-3.94573	1.42377
H	8.22824	1.48463	-0.49573
H	2.30422	3.63055	-1.52697
H	-2.30419	3.63059	1.52691
H	1.96046	0.95174	1.54679
H	-8.2282	1.48464	0.49562
H	-5.23538	-3.94577	-1.4238
H	-1.96051	0.95171	-1.54677
H	-3.33277	-0.21196	1.42269
H	-4.97215	-0.28002	-0.42711
H	3.33273	-0.21199	-1.42256
H	4.97223	-0.27989	0.4273

1i (Hückel $T2_{RX}$)

C	4.82693	-2.28698	0.4187
C	4.93641	-3.69104	0.46872
C	3.68704	-4.20175	0.77765
C	2.81229	-3.11116	0.94104
C	1.45006	-3.14465	1.31094
C	0.64325	-2.05936	1.53526
N	1.0761	-0.74933	1.44934
C	-0.01258	-0.01016	1.64292
C	0.0578	1.41211	1.63018
C	-0.97513	2.27432	1.39508
C	-0.90343	3.71679	1.43869
C	-2.11506	4.21981	1.10022
C	-2.99741	3.11328	0.81422
C	-4.31256	3.15563	0.43605
C	-5.12744	2.01533	0.20669
N	-4.68242	0.75512	0.11355
C	-5.82415	-0.01298	-0.01407
C	-5.8775	-1.37379	-0.18469
C	-4.82679	-2.28708	-0.41878
C	-4.93621	-3.69115	-0.46873
C	-3.68684	-4.20183	-0.77771
C	-2.81209	-3.11122	-0.94099
C	-1.44986	-3.14464	-1.31088
C	-0.64313	-2.05928	-1.53512
N	-1.07612	-0.7493	-1.44911
C	0.01248	-0.01002	-1.64279
C	-0.05797	1.41222	-1.62994
C	0.97498	2.27444	-1.39495
C	0.90323	3.71691	-1.43841
C	2.11488	4.21993	-1.09999
C	2.99725	3.11339	-0.8141
C	4.31241	3.15571	-0.43594
C	5.12736	2.01542	-0.20681
N	4.6824	0.75519	-0.11361
C	5.82417	-0.01286	0.01382

C	5.8776	-1.37367	0.18446
N	3.52701	-1.96823	0.69811
C	-0.77323	-2.11397	1.83534
C	-1.19813	-0.8303	1.883
N	-2.26931	1.96596	1.02419
C	-6.57668	2.09449	0.11675
C	-7.01265	0.81875	0.01509
N	-3.52685	-1.96831	-0.69808
C	0.77332	-2.11376	-1.83536
C	1.19811	-0.83004	-1.8829
N	2.26919	1.96607	-1.02425
C	6.57661	2.09463	-0.1171
C	7.01264	0.8189	-0.01561
H	5.85188	-4.23978	0.28489
H	3.40487	-5.24028	0.89918
H	-1.35461	-3.01985	1.97044
H	-2.19896	-0.47307	2.10115
H	-0.00655	4.2581	1.71587
H	-2.41647	5.25914	1.05006
H	-7.15694	3.0094	0.15984
H	-8.03032	0.45262	-0.06342
H	-5.85169	-4.2399	-0.28494
H	-3.40464	-5.24035	-0.89926
H	1.3548	-3.01957	-1.97047
H	2.19893	-0.4727	-2.10093
H	0.00632	4.25823	-1.71549
H	2.41628	5.25926	-1.04982
H	7.15683	3.00956	-0.16024
H	8.03034	0.4528	0.06268
H	3.1261	-1.03433	0.79743
H	-2.63769	1.06431	0.72897
H	-3.12593	-1.03441	-0.79741
H	2.63769	1.06435	-0.72934
H	4.77981	4.13524	-0.36488
H	6.87018	-1.82338	0.16814
H	-1.00879	-4.13588	-1.41364
H	1.00905	-4.13592	1.4136
H	-4.77999	4.13516	0.36514
H	1.04747	1.85114	1.75176
H	-1.04767	1.85125	-1.75141
H	-6.87008	-1.82352	-0.16849

SCF Done: E(RM06) = -1977.68236697 A.U. after 22 cycles

2a (Hückel [34]$T0^{5,10,25,30}$)

C	7.55698	1.11776	-0.00852
N	6.77214	-0.00014	-0.00019
C	7.55689	-1.1181	0.00813
C	7.08556	-2.4347	0.00889
C	5.75518	-2.82015	-0.04616
N	4.71999	-1.94202	-0.14193
C	3.60758	-2.69747	-0.16145
C	2.34715	-2.0823	-0.29078
C	1.08628	-2.63603	-0.15093
N	-0.01012	-1.85998	-0.38137
C	-1.07162	-2.63114	-0.11742
C	-2.36246	-2.07769	-0.22074
C	-3.59677	-2.68909	-0.0798
N	-4.73445	-1.93326	-0.08717
C	-5.74814	-2.80357	0.02571
C	-7.10035	-2.42543	0.06372
C	-7.56047	-1.12174	0.03268
C	-8.92702	-0.68043	0.02408
C	-8.92693	0.68024	-0.02433
C	-7.56032	1.12141	-0.03287
C	-7.10022	2.42511	-0.06395
C	-5.74807	2.80343	-0.02587
N	-4.73424	1.93331	0.08737
C	-3.59671	2.68933	0.07989
C	-2.3623	2.07818	0.22112
C	-1.07151	2.63166	0.11784
C	-0.66057	3.96858	-0.32063
C	0.68855	3.9705	-0.29756
C	1.08642	2.63631	0.15124
C	2.34725	2.08239	0.29077
C	3.60773	2.69743	0.16146
N	4.72006	1.94185	0.14171
C	5.75532	2.81987	0.04601
C	7.08569	2.43437	-0.00917
C	8.91209	0.68603	-0.00949
C	8.91204	-0.68647	0.00906
C	5.27965	-4.19254	-0.02221
C	3.93076	-4.11963	-0.08759
C	-3.9226	-4.10856	0.03784
C	0.68831	-3.97001	0.29831
C	-0.6608	-3.96796	0.32148
C	-5.27031	-4.17908	0.0946
N	-6.77737	-0.00021	-0.00009
C	-5.27046	4.17899	-0.09514
C	-3.92274	4.10871	-0.03827
N	-0.01002	1.86033	0.38149
C	3.93106	4.11956	0.08788
C	5.27995	4.19233	0.02237
H	-5.75184	-0.00051	0.
H	-7.8522	-3.21018	0.11791
H	-7.85213	3.20978	-0.11824
H	-2.38465	1.01018	0.43528
H	2.3659	1.01748	0.52114
H	7.84281	3.21556	-0.05278
H	7.84268	-3.21588	0.05256
H	2.36591	-1.01746	-0.52146
H	-2.38494	-1.00967	-0.43476
H	-5.8957	5.0621	-0.16783

H	-3.22339	4.93399	-0.02451
H	-1.30507	4.77026	-0.65725
H	1.34297	4.77252	-0.61327
H	3.23043	4.94251	0.13722
H	5.90513	5.0769	-0.0265
H	9.76591	1.3521	-0.01625
H	9.76582	-1.35259	0.01581
H	5.90473	-5.07716	0.0268
H	3.23003	-4.94251	-0.13673
H	1.3427	-4.77195	0.61429
H	-1.30539	-4.76938	0.65855
H	-3.2231	-4.9337	0.0237
H	-5.8954	-5.06232	0.16697
H	-9.77996	-1.34752	0.04576
H	-9.77977	1.34746	-0.04608
H	5.74625	-0.00014	-0.00017

SCF Done: E(RM06) = -1976.38849696 A.U. after 7 cycles

2b (Hückel [34]$T0^{B,C,E,F,H}$)

C	5.07649	3.95632	-0.14994
N	3.70149	3.92503	-0.19229
C	3.32058	5.19417	-0.26485
C	1.95399	5.61766	-0.31038
C	0.85693	4.83987	-0.05636
N	-0.42696	5.33221	-0.22588
C	-1.22973	4.33045	0.09993
C	-2.64785	4.44372	-0.05388
C	-3.58543	3.5514	0.39217
N	-4.88749	3.58555	-0.09295
C	-5.44945	2.48004	0.36551
C	-6.75096	2.05183	-0.06084
C	-7.11025	0.73082	-0.11834
N	-6.20382	-0.27695	0.12947
C	-6.82239	-1.4106	-0.1457
C	-6.16405	-2.6803	-0.13424
C	-4.80182	-2.82457	-0.05777
C	-3.77667	-1.8037	-0.0159
C	-2.56782	-2.4062	-0.03176
C	-2.75154	-3.83893	-0.07425
C	-1.80824	-4.83305	-0.05845
C	-0.4095	-4.60575	-0.2205
N	0.50444	-5.46553	0.2125
C	1.72125	-4.88746	-0.08007
C	2.90719	-5.46185	0.3087
C	4.17946	-4.83835	0.28482
C	5.45868	-5.41818	0.36751
C	6.39467	-4.39609	0.3233
C	5.7065	-3.17157	0.22848
C	6.24833	-1.8738	0.19206
C	5.6053	-0.66826	-0.00435
N	6.32652	0.49901	0.09277
C	5.44692	1.47901	-0.11116
C	5.87076	2.83598	-0.07842
C	5.56113	5.32769	-0.19765
C	4.45919	6.10755	-0.29197
C	0.82538	3.45597	0.40375
C	-0.47772	3.13163	0.50006
C	-8.38656	0.16236	-0.54021

C	-3.41151	2.42392	1.30491
C	-4.57627	1.74861	1.28995
C	-8.2168	-1.17973	-0.53822
N	-4.12214	-4.03228	-0.06075
C	0.20089	-3.46253	-0.91016
C	1.5348	-3.64119	-0.82005
N	4.36458	-3.48108	0.18975
C	4.21183	-0.38074	-0.31869
C	4.10891	0.96634	-0.38386
H	-9.27535	0.72749	-0.79599
H	-4.85796	0.86347	1.84361
H	-2.54491	2.22754	1.92168
H	-0.89475	2.16923	0.76406
H	1.7025	2.85812	0.61015
H	4.39871	7.18811	-0.35634
H	6.60278	5.62681	-0.17573
H	3.24965	1.58034	-0.62026
H	-8.93775	-1.94716	-0.79835
H	-4.00731	-0.7488	0.03288
H	-1.60497	-1.91994	0.04119
H	-0.32285	-2.69629	-1.46848
H	2.30759	-3.05954	-1.31006
H	5.64656	-6.48287	0.42001
H	7.47342	-4.48915	0.33824
H	3.41551	-1.0872	-0.52519
H	-4.56458	-4.93505	-0.13989
H	3.62676	-2.81247	0.35487
H	7.3238	-1.80535	0.34956
H	6.94716	2.97742	0.0171
H	1.75818	6.6579	-0.56983
H	-3.0003	5.2867	-0.64627
H	-7.43124	2.8143	-0.43651
H	-6.78057	-3.57218	-0.24308
H	2.86061	-6.47611	0.70104
H	-2.11492	-5.86212	0.12417

SCF Done: E(RM06) = -1976.34405050 A.U. after 8 cycles

2c (Hückel [34]$T0^{5,20,25,B,F}$)

C	5.93127	2.30598	-0.13772
N	4.64986	1.94843	-0.00316
C	3.99167	3.1024	0.34849
C	2.62812	3.2801	0.46919
C	1.60148	2.32488	0.27121
N	0.31261	2.67297	0.35946
C	-0.36918	1.50029	0.14754
C	-1.7296	1.31559	0.11458
C	-2.79566	2.24756	0.10523
N	-4.02189	1.76336	-0.09225
C	-4.83951	2.84694	-0.26875
C	-6.14559	2.70499	-0.70737
C	-6.73165	1.45748	-1.03085
N	-6.11059	0.28139	-0.77063
C	-6.75719	-0.76108	-1.35974
C	-6.21272	-2.06314	-1.36306
C	-5.11351	-2.42916	-0.59872
C	-4.22366	-3.5672	-0.77848
C	-3.19834	-3.38729	0.09528
C	-3.52864	-2.18678	0.84856

C	-2.89825	-1.58042	1.96578
C	-1.59383	-1.62038	2.3959
N	-0.53347	-2.17778	1.71932
C	0.54486	-1.72299	2.36262
C	1.87705	-1.77092	1.87536
C	2.37636	-2.42939	0.77822
C	1.7935	-3.52082	0.00901
C	2.73682	-3.87886	-0.89211
C	3.85299	-2.95389	-0.70007
C	5.04018	-2.91524	-1.46667
C	5.94021	-1.87232	-1.44264
N	5.75913	-0.66637	-0.80922
C	6.83342	0.15355	-1.01977
C	6.95754	1.47118	-0.63271
C	6.14655	3.71789	0.1771
C	4.93172	4.21225	0.48894
C	1.78692	0.903	-0.02396
C	0.54465	0.38627	-0.0859
C	-7.89835	1.14737	-1.78313
C	-2.79287	3.70573	0.12846
C	-4.07663	4.07907	-0.09915
C	-7.89934	-0.21601	-2.00753
N	-4.66685	-1.63736	0.42148
C	-1.14234	-0.84369	3.54343
C	0.20441	-0.91182	3.5265
N	3.62397	-2.10601	0.30404
C	7.22452	-1.80635	-2.0901
C	7.77972	-0.60039	-1.80356
H	7.64402	-2.60983	-2.68291
H	8.73738	-0.21261	-2.12857
H	2.69263	-4.66723	-1.63552
H	0.80986	-3.93826	0.18451
H	7.10162	4.23017	0.14313
H	4.65948	5.22476	0.76477
H	-1.90884	4.31482	0.27129
H	-4.47652	5.08396	-0.17764
H	-8.61617	1.87308	-2.14461
H	-8.6273	-0.78843	-2.56876
H	-2.31796	-3.99866	0.25076
H	-4.34764	-4.35985	-1.5079
H	2.74357	0.4125	-0.14774
H	0.23424	-0.63937	-0.25871
H	5.26529	-3.75046	-2.12642
H	7.92429	1.93512	-0.81963
H	2.28053	4.28313	0.71562
H	2.58609	-1.10695	2.3708
H	0.92008	-0.4441	4.19296
H	-1.79195	-0.31172	4.22889
H	-6.63945	-2.78232	-2.06012
H	-3.55594	-0.89443	2.50164
H	-6.73033	3.59958	-0.91341
H	-2.06624	0.28416	-0.00574
H	-5.21801	0.2118	-0.26927
H	4.94516	-0.44577	-0.23701

SCF Done: E(RM06) = -1976.38427789 A.U. after 7 cycles

2d (Hückel [34]$T0^{20,25,B,F}$)

C	5.22334	2.12126	-1.12127

N	4.04644	1.73135	-0.57272
C	3.57833	2.83857	0.05969
C	2.31685	3.07699	0.61244
C	1.0783	2.42789	0.51468
N	-0.00032	3.13548	0.92538
C	-1.07893	2.42776	0.51478
C	-2.31752	3.07674	0.61263
C	-3.579	2.83823	0.0599
N	-4.047	1.73099	-0.57252
C	-5.22391	2.12084	-1.12112
C	-6.07476	1.3164	-1.89542
C	-6.00803	-0.06256	-2.01857
N	-5.18236	-0.84632	-1.27297
C	-5.3686	-2.16456	-1.56748
C	-4.68189	-3.19678	-0.92909
C	-3.82103	-2.96542	0.14783
C	-2.82464	-3.87878	0.69743
C	-2.09352	-3.15106	1.57405
C	-2.70014	-1.82403	1.59479
C	-2.33915	-0.67874	2.30283
C	-1.0665	-0.39321	2.80114
N	0.00029	-1.17915	2.55023
C	1.06715	-0.39342	2.80134
C	2.33983	-0.67908	2.30313
C	2.70075	-1.82427	1.59493
C	2.09402	-3.15125	1.57391
C	2.82514	-3.87886	0.6972
C	3.82154	-2.96543	0.14772
C	4.68235	-3.19661	-0.92928
C	5.36887	-2.16424	-1.5676
N	5.18237	-0.84603	-1.27304
C	6.00784	-0.06208	-2.01866
C	6.07431	1.3169	-1.89553
C	5.5309	3.51122	-0.82395
C	4.52361	3.9468	-0.03739
C	0.67796	1.17259	-0.12061
C	-0.67851	1.17252	-0.12056
C	-6.76664	-0.94124	-2.85934
C	-4.52436	3.9464	-0.03717
C	-5.53161	3.51075	-0.82375
C	-6.3587	-2.2211	-2.60146
N	-3.74782	-1.75801	0.74785
C	-0.67456	0.90087	3.35534
C	0.67536	0.90071	3.35554
N	3.74842	-1.75815	0.74798
C	6.35893	-2.22054	-2.60164
C	6.76663	-0.94059	-2.85946
H	6.7157	-3.13475	-3.05952
H	7.50863	-0.6125	-3.57683
H	2.6903	-4.91538	0.40899
H	1.24016	-3.44777	2.16766
H	6.41197	4.04509	-1.1619
H	4.37648	4.92887	0.39783
H	-4.37731	4.92847	0.39807
H	-6.41271	4.04456	-1.1617
H	-7.50874	-0.61331	-3.5767
H	-6.71532	-3.1354	-3.05927
H	-1.2397	-3.44753	2.16788
H	-2.68985	-4.91536	0.40941
H	1.3639	0.43255	-0.51807

H	-1.3644	0.43241	-0.51796
H	4.79712	-4.20496	-1.32025
H	6.8799	1.81794	-2.42957
H	2.21788	4.04939	1.09717
H	3.07082	0.13038	2.28809
H	1.35521	1.69689	3.63698
H	-1.35431	1.6972	3.63662
H	-4.79659	-4.20519	-1.31993
H	-3.07005	0.1308	2.28765
H	-6.88044	1.81733	-2.42942
H	-2.21861	4.04914	1.09737
H	4.55243	-0.52874	-0.52778
H	-4.55249	-0.52886	-0.52773

SCF Done: E(RM06) = -1976.37659028 A.U. after 8 cycles

2e (Möbius [34]$T1^{B,C,E,H}$)

C	-7.07529	0.13943	-0.23783
N	-6.08816	-0.70511	0.24927
C	-6.57565	-1.92365	0.1209
C	-5.77535	-3.11087	0.28532
C	-4.49558	-3.14902	0.75037
N	-3.6934	-4.27063	0.54288
C	-2.48542	-3.89615	0.91669
C	-1.34974	-4.73415	0.64075
C	-0.05904	-4.31358	0.50518
N	0.95259	-5.21003	0.16757
C	2.04185	-4.47363	0.03978
C	3.29328	-5.07072	-0.32566
C	4.46806	-4.40904	-0.55342
N	4.62357	-3.03702	-0.47411
C	5.90845	-2.80655	-0.67749
C	6.50346	-1.50647	-0.608
C	5.79266	-0.34055	-0.53474
C	4.37852	-0.10683	-0.74306
C	4.10375	1.18648	-0.46233
C	5.32864	1.83816	-0.04453
C	5.50884	3.06788	0.52331
C	4.44479	3.9661	0.8583
N	3.22312	3.91864	0.35161
C	2.47994	4.80629	1.10658
C	1.13889	5.01308	0.93966
C	0.36393	4.5287	-0.15365
C	0.74362	4.2334	-1.46979
C	-0.41648	4.01157	-2.20663
C	-1.50948	4.09725	-1.33581
C	-2.8709	3.79502	-1.60729
C	-3.77946	3.22259	-0.75779
N	-5.05928	2.92785	-1.20964
C	-5.551	2.09142	-0.31468
C	-6.8175	1.4427	-0.54726
C	-3.73511	-2.08464	1.39454
C	-8.25899	-0.62299	-0.61052
C	-7.94612	-1.92005	-0.39221
C	-2.47987	-2.55366	1.51769
C	5.74992	-5.04449	-0.84698
C	0.47993	-2.95592	0.5855
C	6.65718	-4.04638	-0.90901
C	1.79125	-3.05229	0.30284

N	6.33198	0.89424	-0.20885
C	4.55792	4.95601	1.93205
C	3.31281	5.44879	2.11341
C	-3.53912	2.59743	0.53541
N	-1.00545	4.42029	-0.09713
C	-4.64264	1.86115	0.80089
H	-1.64172	-2.07183	2.0034
H	3.70543	-0.88382	-1.07735
H	7.72311	-4.11442	-1.09721
H	5.46151	5.18426	2.48671
H	-4.84064	1.20865	1.64121
H	-8.55299	-2.79992	-0.57474
H	5.90736	-6.11044	-0.96578
H	1.77047	4.22553	-1.80855
H	-4.14343	-1.12957	1.69223
H	2.54508	-2.27915	0.26737
H	2.975	6.18698	2.83216
H	3.15824	1.71086	-0.50757
H	-0.07602	-2.05028	0.78192
H	-2.61856	2.62911	1.10645
H	-0.49042	3.75723	-3.25654
H	-9.17521	-0.2066	-1.01275
H	-6.17838	-4.04387	-0.10781
H	-1.56019	-5.7809	0.42754
H	3.28043	-6.15575	-0.41997
H	7.58982	-1.46072	-0.53212
H	6.50619	3.33297	0.87484
H	0.62368	5.61138	1.69275
H	-3.20609	3.94181	-2.63365
H	-7.552	2.00019	-1.12765
H	7.25958	1.00432	0.17234
H	-1.57475	4.63537	0.70867

SCF Done: E(RM06) = -1976.33206100 A.U. after 7 cycles

2f (Möbius [34]$T1^{B,C,F}$)

C	7.40991	0.34271	-0.56963
N	6.0895	0.74463	-0.58878
C	6.06711	1.88468	-1.27093
C	4.89809	2.69276	-1.45559
C	3.68576	2.53547	-0.847
N	2.62595	3.38382	-1.16049
C	1.59927	2.91629	-0.47964
C	0.32304	3.57673	-0.47221
C	-0.86598	2.9922	-0.15366
N	-1.99802	3.75947	0.08386
C	-2.95296	2.88851	0.35817
C	-4.22572	3.37038	0.79311
C	-5.37983	2.67835	1.02435
N	-5.62112	1.33764	0.76737
C	-6.90527	1.16435	1.06306
C	-7.6558	-0.01265	0.79758
C	-7.21368	-1.11309	0.11544
C	-8.04859	-2.16136	-0.42899
C	-7.27263	-2.96256	-1.1921
C	-5.90713	-2.49298	-1.09907
C	-4.82553	-3.05676	-1.71677
C	-3.45702	-2.74951	-1.48322
N	-3.00343	-2.01182	-0.47966
C	-1.61964	-2.10658	-0.55961

C	-0.80029	-1.70952	0.45661
C	0.63881	-1.79202	0.44056
C	1.49939	-1.63264	-0.73522
C	2.76848	-1.75452	-0.28982
C	2.66296	-2.01614	1.14258
C	3.65142	-2.35445	2.02647
C	5.05531	-2.29298	1.79568
N	5.6285	-1.4759	0.86923
C	6.99199	-1.60173	0.89852
C	7.83661	-0.75891	0.14241
C	8.23144	1.27428	-1.31153
C	7.38823	2.23888	-1.76129
C	3.2703	1.54899	0.14361
C	1.95749	1.76099	0.35601
C	-6.58213	3.33103	1.53482
C	-1.18406	1.56905	-0.04043
C	-2.49866	1.49638	0.25179
C	-7.53538	2.38142	1.57708
N	-5.92827	-1.38495	-0.28556
C	-2.37644	-3.32197	-2.28842
C	-1.22807	-2.8951	-1.73105
N	1.33268	-2.00171	1.54292
C	6.09881	-2.99178	2.43432
C	7.29591	-2.58636	1.85817
H	-0.50264	0.74849	-0.23407
H	-0.21458	-3.14926	-2.01491
H	-2.50976	-3.97131	-3.14681
H	-7.56851	-3.82918	-1.77054
H	-9.11705	-2.22349	-0.26267
H	-8.56955	2.46637	1.89158
H	-6.6472	4.37709	1.81158
H	1.30523	1.24655	1.05331
H	7.62494	3.12138	-2.34447
H	9.30296	1.19574	-1.45449
H	8.2934	-2.92766	2.10495
H	5.95864	-3.7334	3.21034
H	1.16529	-1.41295	-1.74293
H	8.90338	-0.97401	0.17266
H	-8.71617	0.01056	1.0401
H	-4.25094	4.44569	0.967
H	0.31616	4.64132	-0.70098
H	4.97978	3.53581	-2.14108
H	-1.26437	-1.36225	1.37938
H	3.32631	-2.71176	3.00258
H	-5.03779	-3.86192	-2.41747
H	3.91941	0.83836	0.63337
H	-3.11664	0.61438	0.38153
H	-5.12624	-0.80112	-0.05964
H	3.67859	-1.71009	-0.87691
H	5.21354	-0.71063	0.3313

SCF Done: E(RM06) = -1976.37180804 A.U. after 7 cycles

2g (Twisted-Hückel [34]$T2^{B,F}$)

C	-6.09689	1.93265	0.91461
N	-4.82595	1.5075	0.90989
C	-4.08509	2.57133	1.34238
C	-2.72507	2.55242	1.58845
C	-1.87195	1.42564	1.60555

N	-0.55043	1.58506	1.70662
C	-0.03195	0.31668	1.71728
C	1.33226	0.13398	1.67574
C	2.06247	-1.08007	1.74213
N	3.36208	-1.08394	1.4313
C	3.7985	-2.36083	1.66133
C	5.10814	-2.75636	1.45973
C	6.12252	-1.94137	0.92875
N	5.90855	-0.69315	0.42364
C	7.08624	-0.14107	0.01251
C	7.19723	1.1328	-0.5673
C	6.13128	1.92659	-0.956
C	6.22068	3.28408	-1.46516
C	4.94481	3.67326	-1.70078
C	4.10782	2.525	-1.37741
C	2.70579	2.49255	-1.576
C	1.8946	1.37773	-1.59132
N	0.53384	1.51746	-1.68318
C	0.04971	0.27497	-1.67261
C	-1.3451	0.06835	-1.6107
C	-2.05286	-1.11587	-1.7051
C	-1.61949	-2.43774	-2.14652
C	-2.72572	-3.21759	-2.13579
C	-3.81187	-2.37145	-1.65675
C	-5.15075	-2.77225	-1.47364
C	-6.12869	-1.95631	-0.93588
N	-5.90394	-0.71048	-0.41783
C	-7.07662	-0.13792	-0.01048
C	-7.19035	1.11948	0.55004
C	-6.2028	3.32138	1.35089
C	-4.93608	3.73141	1.58315
C	-2.25554	0.01231	1.56317
C	-1.10187	-0.68145	1.64504
C	7.51248	-2.20699	0.81897
C	1.62017	-2.39684	2.19153
C	2.71596	-3.19271	2.15375
C	8.10875	-1.09016	0.2757
N	4.83247	1.50192	-0.91176
C	2.27713	-0.0311	-1.53704
C	1.12216	-0.72594	-1.59292
N	-3.38682	-1.12411	-1.41475
C	-7.54184	-2.20181	-0.82292
C	-8.11895	-1.09142	-0.28657
H	0.63109	-2.65247	2.5495
H	2.79791	-4.23674	2.43461
H	7.98995	-3.12695	1.13253
H	9.15826	-0.94049	0.05486
H	7.13631	3.84827	-1.60136
H	4.5874	4.6212	-2.08667
H	3.29132	-0.39564	-1.44128
H	0.99713	-1.80008	-1.51782
H	-0.62623	-2.70666	-2.48312
H	-2.81485	-4.25926	-2.42408
H	-8.0278	-3.11597	-1.14103
H	-9.16699	-0.92569	-0.06936
H	-7.12466	3.88481	1.44244
H	-4.58872	4.70057	1.92275
H	-5.44578	-3.77089	-1.7881
H	-8.19519	1.49664	0.72815
H	-2.23864	3.50032	1.81665

H	1.93388	1.03402	1.54593
H	5.3921	-3.76915	1.74052
H	8.20611	1.50835	-0.72993
H	-1.94178	0.96196	-1.42391
H	2.20159	3.44243	-1.75247
H	-3.26842	-0.35231	1.45113
H	-0.97762	-1.75583	1.57853
H	4.99548	-0.22781	0.39809
H	-4.98576	-0.25663	-0.40276

SCF Done: E(RM06) = -1976.39833799 A.U. after 9 cycles

2h (Twisted-Hückel [34]$T2^{C,G}$)

C	7.08604	-0.14114	0.01179
N	5.90846	-0.69348	0.42296
C	6.12269	-1.94161	0.92811
C	5.10856	-2.75668	1.45935
C	3.79888	-2.36117	1.66114
N	3.3624	-1.08442	1.43098
C	2.06283	-1.08047	1.74214
C	1.33269	0.13356	1.67583
C	-0.03158	0.3163	1.71761
N	-0.54995	1.58466	1.70692
C	-1.87153	1.42532	1.60576
C	-2.72455	2.55208	1.58849
C	-4.08464	2.57101	1.34249
N	-4.82555	1.50726	0.91006
C	-6.09649	1.93253	0.91481
C	-7.18999	1.11949	0.55026
C	-7.07637	-0.13795	-0.01032
C	-8.1189	-1.09118	-0.28642
C	-7.54202	-2.20166	-0.82293
C	-6.12889	-1.95639	-0.9359
C	-5.15092	-2.77226	-1.47382
C	-3.81211	-2.37137	-1.65693
N	-3.38704	-1.12405	-1.41439
C	-2.05321	-1.11558	-1.70504
C	-1.34551	0.06875	-1.61047
C	0.04919	0.27539	-1.67252
C	1.12166	-0.72551	-1.59294
C	2.27659	-0.03063	-1.53693
C	1.89401	1.37817	-1.59109
C	2.70532	2.49299	-1.57569
C	4.10724	2.52538	-1.37709
N	4.83199	1.50205	-0.91185
C	6.13066	1.92674	-0.95594
C	7.1968	1.13281	-0.56767
C	8.10875	-1.09011	0.27498
C	7.51274	-2.207	0.81828
C	2.71644	-3.19305	2.15385
C	1.62063	-2.39722	2.19174
C	-4.93551	3.7312	1.58324
C	-1.10154	-0.68178	1.64555
C	-2.25519	0.012	1.56358
C	-6.20226	3.3213	1.351
N	-5.90386	-0.71062	-0.4178
C	-2.72597	-3.21716	-2.13653
C	-1.61982	-2.43719	-2.14718
N	0.53337	1.51794	-1.68301

C	4.94424	3.67375	-1.69998
C	6.22011	3.28443	-1.4646
H	-0.9773	-1.75618	1.57928
H	9.15823	-0.94028	0.05411
H	7.99038	-3.12686	1.13184
H	2.79851	-4.23704	2.43487
H	0.63162	-2.65284	2.54991
H	-4.58802	4.70033	1.9228
H	-7.12407	3.88481	1.44253
H	-9.16688	-0.92523	-0.06908
H	-8.02817	-3.11571	-1.14105
H	-2.8151	-4.2587	-2.42528
H	-0.62661	-2.70578	-2.4842
H	0.9966	-1.79965	-1.518
H	4.58679	4.62187	-2.08539
H	7.13576	3.84863	-1.60057
H	-5.44588	-3.77087	-1.78846
H	-8.1948	1.49672	0.72837
H	-2.2381	3.50002	1.81649
H	2.20119	3.44292	-1.75214
H	-1.94223	0.9623	-1.42352
H	8.20559	1.50856	-0.7305
H	5.39261	-3.76943	1.74019
H	1.93426	1.03358	1.54578
H	3.29078	-0.39512	-1.44104
H	-3.26808	-0.35259	1.45149
H	-4.98548	-0.25708	-0.40324
H	4.99532	-0.22827	0.39763

SCF Done: E(RM06) = -1976.39833799 A.U. after 8 cycles

2i (Twisted-Hückel [34]$T2_{RX}$)

C	-5.15466	-2.28751	-0.52731
N	-3.84906	-1.8879	-0.66954
C	-3.19989	-2.97671	-1.07434
C	-1.81694	-3.05066	-1.40374
C	-0.93673	-2.017	-1.58426
N	-1.27595	-0.68352	-1.60284
C	-0.11614	-0.04029	-1.64238
C	-0.112	1.37881	-1.66422
C	0.95213	2.21291	-1.43227
C	0.84369	3.66636	-1.46894
C	2.07622	4.13993	-1.19022
C	2.91429	2.95988	-0.97569
C	4.30459	3.03967	-0.72842
C	5.1775	2.00559	-0.48762
C	6.61318	2.12827	-0.51063
C	7.14582	0.89582	-0.32638
C	6.0632	-0.03013	-0.12099
C	6.1999	-1.37157	0.16284
C	5.15197	-2.23949	0.52719
N	3.89023	-1.83438	0.69134
C	3.21413	-2.9427	1.12236
C	1.89496	-2.99574	1.51382
C	0.97938	-1.92106	1.63738
N	1.31013	-0.6342	1.64755
C	0.1112	0.03431	1.65812
C	0.10257	1.40689	1.63181

C	-1.01466	2.25634	1.4235
N	-2.24368	1.85302	1.08578
C	-2.97036	3.00707	0.96327
C	-4.31849	3.05148	0.68533
C	-5.20638	1.98839	0.4398
N	-4.89884	0.67346	0.20486
C	-6.05795	-0.04671	0.08241
C	-6.16961	-1.42396	-0.19285
C	-5.31655	-3.69918	-0.83051
C	-4.08169	-4.13966	-1.16046
C	0.51182	-2.18913	-1.68617
C	1.03907	-0.94887	-1.67045
N	2.23388	1.82334	-1.10877
N	4.89451	0.68271	-0.23811
C	5.32351	-3.66196	0.82126
C	4.09937	-4.10734	1.17023
C	-0.47227	-2.12273	1.70963
C	-1.02281	-0.89294	1.68031
C	-0.9164	3.70827	1.50358
C	-2.1518	4.18093	1.22148
C	-6.61526	2.10215	0.45355
C	-7.13988	0.84332	0.2597
H	-6.24905	-4.25077	-0.79374
H	-3.77689	-5.1358	-1.46231
H	1.03297	-3.14062	-1.69416
H	2.07612	-0.63805	-1.66527
H	-0.06827	4.21412	-1.67926
H	2.41295	5.16924	-1.13144
H	7.13131	3.06254	-0.68957
H	8.19097	0.61234	-0.30793
H	6.25559	-4.21226	0.7574
H	3.80074	-5.10493	1.47304
H	-0.97674	-3.08357	1.72474
H	-2.06538	-0.60299	1.66491
H	-0.01386	4.25903	1.74438
H	-2.49713	5.20826	1.18863
H	-7.14926	3.02867	0.62445
H	-8.18222	0.55174	0.22704
H	-4.78981	4.03407	0.70629
H	-7.1841	-1.8199	-0.16541
H	1.49846	-3.9885	1.73298
H	-1.41019	-4.05835	-1.50424
H	4.75923	4.02619	-0.80534
H	-1.09019	1.83658	-1.81375
H	1.07923	1.88597	1.71193
H	7.21319	-1.76794	0.15138
H	3.97004	0.27987	-0.06497
H	-3.96443	0.2809	0.06003

SCF Done: E(RM06) = -1976.38919013 A.U. after 10 cycles

3a (Hückel [38]$T0^{5,10,25,30}$)

C	7.66055	1.08529	0.04721
C	9.04896	0.67811	0.03934
C	9.04895	-0.67817	-0.03934
C	7.66053	-1.08533	-0.04721
C	7.19952	-2.40394	-0.08215
C	5.86021	-2.77149	0.01884
C	5.24659	-4.04511	-0.12587

C	3.88788	-3.88614	0.00765
C	3.61977	-2.50762	0.25754
C	2.42903	-1.80915	0.47199
C	1.1427	-2.27844	0.2185
C	0.68648	-3.43303	-0.47313
C	-0.68653	-3.43304	-0.47312
C	-1.14274	-2.27845	0.21851
C	-2.42907	-1.80916	0.472
C	-3.61981	-2.50762	0.25756
N	-4.84334	-1.883	0.27077
C	-5.86025	-2.77147	0.01885
C	-7.19956	-2.40391	-0.08215
C	-7.66055	-1.0853	-0.04722
C	-9.04896	-0.67812	-0.03935
C	-9.04895	0.67817	0.03933
C	-7.66053	1.08532	0.0472
C	-7.19953	2.40393	0.08214
C	-5.86022	2.77148	-0.01884
C	-5.24659	4.04511	0.12587
C	-3.88789	3.88614	-0.00765
C	-3.61977	2.50762	-0.25754
C	-2.42903	1.80916	-0.47198
C	-1.1427	2.27845	-0.2185
C	-0.68649	3.43305	0.47312
C	0.68653	3.43305	0.47312
C	1.14274	2.27846	-0.2185
C	2.42907	1.80916	-0.47199
C	3.61981	2.50762	-0.25755
N	4.84334	1.883	-0.27076
C	5.86026	2.77147	-0.01884
C	7.19956	2.4039	0.08215
N	6.84023	-0.00001	0.
N	4.8433	-1.883	0.27075
N	-0.00002	-1.58778	0.58574
C	-3.88793	-3.88614	0.00765
C	-5.24663	-4.0451	-0.12587
N	-6.84023	0.00001	0.
N	-4.8433	1.883	-0.27075
N	0.00002	1.58779	-0.58573
C	3.88794	3.88614	-0.00764
C	5.24664	4.0451	0.12587
H	0.00002	0.77522	-1.18652
H	-0.00002	-0.77522	1.18655
H	-7.92684	-3.20324	-0.20709
H	-7.9268	3.20327	0.20707
H	-2.52019	0.78764	-0.84873
H	2.52023	0.78764	-0.84875
H	7.92685	3.20324	0.20709
H	7.9268	-3.20328	-0.20709
H	2.52019	-0.78764	0.84875
H	-2.52023	-0.78764	0.84876
H	-5.78493	4.96737	0.3069
H	-3.14082	4.66847	0.0053
H	-1.33123	4.13455	0.98538
H	1.33127	4.13455	0.98538
H	3.14087	4.66847	0.00531
H	5.78498	4.96737	0.30691
H	9.89939	1.35018	0.07043
H	9.89937	-1.35025	-0.07042
H	5.78492	-4.96738	-0.30691

H	3.14081	-4.66847	-0.00529
H	1.33123	-4.13453	-0.9854
H	-1.33128	-4.13453	-0.98539
H	-3.14086	-4.66846	-0.0053
H	-5.78497	-4.96737	-0.30691
H	-9.89939	-1.35018	-0.07044
H	-9.89937	1.35024	0.07041
H	5.0644	-0.90613	0.44702
H	-5.0644	0.90613	-0.44702
H	5.06443	0.90612	-0.44703
H	-5.06444	-0.90612	0.44703

SCF Done: E(RM06) = -1978.88937663 A.U. after 8 cycles

3b (Hückel [38]$TO^{B,C,E,F,H}$)

C	5.14502	3.93851	-0.11212
C	5.62977	5.24925	-0.27116
C	4.54694	6.10841	-0.36231
C	3.36775	5.34664	-0.2433
C	2.03961	5.82267	-0.2187
C	0.88698	5.0682	-0.21522
C	0.68298	3.66335	-0.41967
C	-0.64373	3.38512	-0.28453
C	-1.34579	4.60097	0.00671
C	-2.69729	4.79	0.20582
C	-3.55661	3.70287	0.50038
C	-3.24645	2.48342	1.12877
C	-4.37712	1.68514	1.11576
C	-5.41319	2.3974	0.48788
C	-6.72475	1.98149	0.16531
C	-7.08082	0.64962	0.05504
N	-6.16209	-0.35884	0.13894
C	-6.82834	-1.49545	-0.0511
C	-6.19578	-2.76789	-0.11758
C	-4.82849	-2.94132	-0.12546
C	-3.78642	-1.94665	-0.107
C	-2.58519	-2.57383	-0.13869
C	-2.79638	-3.99526	-0.18925
C	-1.85746	-4.99666	-0.21395
C	-0.47449	-4.74086	-0.42927
C	0.16161	-3.70592	-1.12472
C	1.54001	-3.86647	-0.9903
C	1.77475	-5.01654	-0.22188
C	2.98767	-5.61174	0.21133
C	4.18251	-4.94488	0.32292
C	5.47594	-5.47766	0.6462
C	6.36774	-4.45117	0.69101
C	5.68002	-3.22087	0.41054
C	6.22366	-1.96207	0.41519
C	5.61021	-0.71061	0.14236
N	6.30187	0.42059	0.3128
C	5.4484	1.44121	-0.01192
C	5.8824	2.7564	0.0347
N	3.75998	4.03198	-0.12245
N	-0.38152	5.59664	-0.01525
N	-4.8985	3.65059	0.18907
C	-8.40616	0.10545	-0.19492
C	-8.254	-1.24296	-0.23991
N	-4.17333	-4.16338	-0.16057

N	0.53299	-5.54771	0.06492
N	4.36359	-3.58086	0.15044
C	4.26187	-0.4358	-0.33919
C	4.16082	0.9157	-0.42735
H	-9.31899	0.68116	-0.30353
H	-4.50699	0.69883	1.53688
H	-2.29765	2.26705	1.60277
H	-1.13377	2.43547	-0.45433
H	1.44619	2.9699	-0.74879
H	4.56642	7.18079	-0.51238
H	6.68027	5.50353	-0.34068
H	3.32504	1.47867	-0.82949
H	-5.35807	4.31393	-0.41715
H	3.1694	3.30493	0.25326
H	-9.0146	-1.99652	-0.41545
H	-4.00204	-0.88914	-0.05898
H	-1.60792	-2.11414	-0.0818
H	-0.34974	-2.96904	-1.73031
H	2.3093	-3.29389	-1.49467
H	5.67143	-6.53212	0.79957
H	7.43019	-4.50587	0.89598
H	3.50569	-1.15204	-0.64372
H	-4.63862	-5.05361	-0.24236
H	3.58975	-2.93569	0.21483
H	7.27517	-1.89815	0.68922
H	6.94831	2.88571	0.21891
H	1.93858	6.90649	-0.17617
H	-3.1103	5.79703	0.13786
H	-7.47637	2.74122	-0.05187
H	-6.83511	-3.64838	-0.18277
H	2.98018	-6.66271	0.49567
H	-2.17573	-6.02832	-0.05609
H	-0.54314	6.53616	0.31307
H	0.38282	-6.28756	0.7346

SCF Done: E(RM06) = -1978.83305137 A.U. after 7 cycles

3c (Hückel [38]$TO^{5,20,25,B,F}$)

C	6.21226	2.04882	-0.02097
C	6.328	3.38943	0.4736
C	5.07348	3.85707	0.73177
C	4.12238	2.83837	0.38625
C	2.74872	2.95737	0.41408
C	1.79067	2.03796	-0.05603
C	1.90154	0.8132	-0.74702
C	0.62592	0.30517	-0.93085
C	-0.30058	1.20967	-0.38618
C	-1.70098	1.07317	-0.39846
C	-2.70566	2.01713	-0.32005
C	-2.73556	3.45319	-0.30316
C	-4.03564	3.85796	-0.45022
C	-4.87008	2.69301	-0.55445
C	-6.22053	2.56553	-0.86676
C	-6.83168	1.30064	-1.0344
N	-6.20301	0.17746	-0.65292
C	-6.92536	-0.88901	-1.12042
C	-6.45824	-2.18846	-0.96275
C	-5.30716	-2.48422	-0.19136
C	-4.38574	-3.55443	-0.2043

C	-3.31451	-3.21703	0.62149
C	-3.59333	-1.95646	1.1983
C	-2.95605	-1.08577	2.11466
C	-1.63162	-0.92338	2.42578
C	-1.1138	0.04355	3.35123
C	0.24305	0.01981	3.28826
C	0.63885	-0.96099	2.32095
C	1.91683	-1.18473	1.88269
C	2.33828	-2.08628	0.88144
C	1.7342	-3.21728	0.28073
C	2.62068	-3.72625	-0.65905
C	3.76631	-2.90463	-0.66797
C	4.93802	-2.95063	-1.44244
C	5.91351	-1.96625	-1.43672
N	5.76943	-0.75435	-0.80026
C	6.94964	-0.11816	-0.94407
C	7.19402	1.19173	-0.47519
N	4.86536	1.75524	-0.02625
N	0.43321	2.26433	0.11176
N	-4.02348	1.6242	-0.40545
C	-8.06374	0.9627	-1.72572
C	-8.10388	-0.39768	-1.80486
N	-4.80701	-1.57468	0.70464
N	-0.53252	-1.56836	1.87663
N	3.56	-1.94317	0.29087
C	7.2312	-2.07159	-2.01917
C	7.8923	-0.93286	-1.68113
H	4.24811	-1.20352	0.42893
H	4.55839	0.85164	-0.3722
H	-4.38661	0.68496	-0.57496
H	-5.2251	-0.64736	0.76901
H	7.60231	-2.92282	-2.57916
H	8.9091	-0.64791	-1.92747
H	2.4804	-4.59836	-1.28583
H	0.7869	-3.65359	0.57507
H	7.26897	3.90933	0.60454
H	4.7954	4.83598	1.10398
H	-1.86218	4.093	-0.2571
H	-4.39817	4.87684	-0.51566
H	-8.77273	1.67067	-2.14062
H	-8.8641	-1.01091	-2.27603
H	-2.45439	-3.83486	0.85289
H	-4.49433	-4.46124	-0.78668
H	2.81403	0.36126	-1.11723
H	0.35818	-0.61196	-1.44305
H	5.09228	-3.83012	-2.06456
H	8.21156	1.5735	-0.51618
H	2.37302	3.89622	0.82048
H	2.67508	-0.51003	2.28055
H	0.94841	0.6243	3.84603
H	-1.74271	0.67055	3.97172
H	-6.94725	-3.00189	-1.4941
H	-3.61337	-0.34772	2.57528
H	-6.78335	3.47038	-1.0814
H	-2.03864	0.05647	-0.60983
H	0.05607	2.96508	0.73225
H	-0.58368	-2.03911	0.9828

SCF Done: E(RM06) = -1978.88616480 A.U. after 7 cycles

3d (Hückel [38]$TO^{20,25,B,F}$)

C	5.47985	1.95154	-1.23663
C	5.73836	3.32463	-0.91509
C	4.65994	3.81649	-0.24919
C	3.64842	2.79553	-0.18269
C	2.37375	3.02769	0.28072
C	1.14369	2.33416	0.16821
C	0.69903	1.08861	-0.31626
C	-0.69899	1.08864	-0.31644
C	-1.14374	2.33415	0.16803
C	-2.37383	3.02767	0.28039
C	-3.64846	2.79556	-0.18316
C	-4.66	3.8165	-0.2497
C	-5.73836	3.32465	-0.91574
C	-5.47984	1.95155	-1.23721
C	-6.30968	1.06431	-1.8894
C	-6.06571	-0.32448	-1.98027
N	-5.09497	-0.92015	-1.27269
C	-5.18003	-2.26333	-1.5547
C	-4.41764	-3.20642	-0.89128
C	-3.584	-2.90143	0.20394
C	-2.61718	-3.67161	0.87268
C	-2.00674	-2.85959	1.82278
C	-2.62212	-1.58691	1.76901
C	-2.37733	-0.38286	2.49104
C	-1.13552	-0.03717	2.95117
C	-0.68054	1.17839	3.57025
C	0.68164	1.17806	3.5703
C	1.13604	-0.03772	2.95122
C	2.37771	-0.38392	2.49108
C	2.62212	-1.58777	1.76869
C	2.00616	-2.86024	1.82153
C	2.61654	-3.672	0.8712
C	3.58386	-2.90185	0.20314
C	4.41738	-3.20656	-0.89224
C	5.17996	-2.26335	-1.55525
N	5.0951	-0.92025	-1.27258
C	6.06572	-0.32437	-1.98012
C	6.30973	1.0644	-1.88892
N	4.21071	1.67358	-0.75629
N	-0.00005	3.02781	0.50021
N	-4.2107	1.67363	-0.75684
C	-6.79986	-1.29197	-2.77141
C	-6.22477	-2.50011	-2.52591
N	-3.57567	-1.65999	0.79917
N	0.0001	-0.78758	2.70175
N	3.57589	-1.66075	0.79903
C	6.22446	-2.49976	-2.52678
C	6.79966	-1.29157	-2.77179
H	4.17166	-0.9201	0.42637
H	3.79825	0.7597	-0.90936
H	-3.7982	0.75979	-0.91003
H	-4.17138	-0.9194	0.42637
H	6.50121	-3.46728	-2.93073
H	7.62834	-1.06599	-3.43371
H	2.39611	-4.71106	0.65949
H	1.26234	-3.15939	2.5497
H	6.65967	3.83813	-1.16099
H	4.52073	4.81847	0.13965

H	-4.5209	4.81848	0.13918
H	-6.65963	3.83819	-1.16166
H	-7.62862	-1.06657	-3.43328
H	-6.50169	-3.4678	-2.92934
H	-1.2631	-3.15855	2.55122
H	-2.39719	-4.71088	0.66157
H	1.33746	0.26645	-0.62123
H	-1.33736	0.26656	-0.62176
H	4.46438	-4.24543	-1.21292
H	7.22367	1.4661	-2.32043
H	2.26983	4.03017	0.70034
H	3.17674	0.35212	2.5617
H	1.34352	1.95868	3.92637
H	-1.34208	1.9593	3.92631
H	-4.46498	-4.24543	-1.21147
H	-3.17606	0.35351	2.5615
H	-7.22364	1.46591	-2.32098
H	-2.26993	4.03013	0.70006
H	-0.00007	4.00685	0.74481
H	-0.00002	-1.48016	1.95983

SCF Done: E(RM06) = -1978.87909867 A.U. after 8 cycles

3e (Möbius [38]$T1^{B,C,E,H}$)

C	-7.077	-0.4918	0.1762
C	-8.3461	0.1907	0.3138
C	-8.1884	1.4846	-0.0543
C	-6.8079	1.6953	-0.4285
C	-6.1543	2.8671	-0.6662
C	-4.7458	2.94	-0.9272
C	-3.874	2.0369	-1.5344
C	-2.5748	2.5636	-1.4567
C	-2.6393	3.7803	-0.7842
C	-1.6201	4.697	-0.3727
C	-0.3259	4.3433	-0.1254
C	0.2789	3.0322	-0.0647
C	1.6046	3.1645	0.1747
C	1.9151	4.572	0.2923
C	3.1236	5.1863	0.4895
C	4.3829	4.5155	0.545
N	4.5466	3.1983	0.5404
C	5.9073	2.9954	0.4476
C	6.4892	1.7621	0.3121
C	5.7999	0.5211	0.3739
C	4.607	0.1565	1.0002
C	4.378	-1.1974	0.7435
C	5.415	-1.6718	-0.0757
C	5.6134	-2.8871	-0.793
C	4.6777	-3.8554	-1.0187
C	4.7747	-4.9752	-1.9225
C	3.5617	-5.5765	-2.0091
C	2.6506	-4.9023	-1.1168
C	1.3313	-5.152	-0.8795
C	0.6002	-4.5839	0.2152
C	1.0359	-4.2381	1.5013
C	-0.092	-3.9471	2.2737
C	-1.2168	-4.0458	1.4562
C	-2.57	-3.7452	1.77
C	-3.5308	-3.2462	0.932

N	-4.8162	-2.9991	1.3946
C	-5.3941	-2.2732	0.4562
C	-6.7261	-1.7376	0.5952
N	-6.2082	0.4436	-0.3806
N	-3.9765	4.009	-0.5193
N	0.7075	5.2334	0.1455
C	5.6624	5.2226	0.5079
C	6.6154	4.2655	0.4269
N	6.2904	-0.6212	-0.2288
N	3.3927	-3.9026	-0.4978
N	-0.7633	-4.4291	0.2079
C	-3.3512	-2.6873	-0.3986
C	-4.5127	-2.0524	-0.6901
H	-1.6796	2.1473	-1.8999
H	-5.204	0.3633	-0.2709
H	0.625	6.2338	0.0563
H	4.0148	0.8326	1.6018
H	7.6914	4.3859	0.3629
H	5.683	-5.2425	-2.4495
H	-4.7694	-1.5108	-1.5949
H	-8.9385	2.2666	-0.0585
H	5.7872	6.3004	0.5069
H	2.0646	-4.2916	1.8367
H	-4.1776	1.1388	-2.059
H	2.3618	2.3996	0.2839
H	3.2908	-6.4365	-2.6094
H	3.5778	-1.7898	1.1711
H	-0.2809	2.1108	-0.157
H	-2.4414	-2.6987	-0.9883
H	-0.1158	-3.651	3.3152
H	-9.2483	-0.2894	0.6733
H	-6.7199	3.7915	-0.5632
H	-1.9032	5.7442	-0.2499
H	3.1448	6.2751	0.5423
H	7.5596	1.7315	0.1007
H	6.5611	-3.0074	-1.3163
H	0.828	-5.8682	-1.5268
H	-2.8618	-3.8592	2.8139
H	-7.4449	-2.3033	1.1829
H	7.0591	-0.6246	-0.883
H	-1.3694	-4.6747	-0.5614
H	-4.3107	4.7338	0.0985
H	2.9392	-3.0908	-0.1012

SCF Done: E(RM06) = -1978.82570394 A.U. after 6 cycles

3f (Möbius [38]$T1^{B,C,F}$)

C	7.4926	0.06196	-0.36018
C	8.37423	0.81902	-1.15329
C	7.64004	1.83957	-1.74351
C	6.29898	1.71727	-1.31775
C	5.20034	2.57377	-1.60917
C	3.88979	2.33952	-1.28645
C	3.2583	1.15891	-0.74412
C	1.94036	1.40324	-0.56365
C	1.65447	2.75646	-0.97583
C	0.4798	3.43983	-0.87762
C	-0.75384	2.81721	-0.48975

C	-1.26688	1.5441	-0.7366
C	-2.51117	1.44524	-0.09975
C	-2.7691	2.65551	0.54676
C	-3.81187	3.08974	1.41072
C	-4.96276	2.42299	1.71757
N	-5.41008	1.22133	1.1936
C	-6.65829	0.91412	1.6912
C	-7.45789	-0.09857	1.22965
C	-7.1321	-0.94162	0.13224
C	-8.13316	-1.66175	-0.63059
C	-7.48343	-2.20143	-1.69161
C	-6.08836	-1.86752	-1.52311
C	-5.08156	-2.33382	-2.3348
C	-3.69694	-2.28702	-2.08023
C	-2.63693	-2.72674	-2.88225
C	-1.46179	-2.60126	-2.14997
C	-1.7904	-2.08733	-0.88108
C	-1.00513	-1.86885	0.28977
C	0.36054	-1.91268	0.37385
C	1.37606	-1.97146	-0.65436
C	2.59867	-1.99913	-0.0686
C	2.43266	-1.96675	1.36485
C	3.375	-2.09424	2.34722
C	4.79178	-2.05132	2.13766
N	5.38342	-1.37642	1.14787
C	6.73759	-1.62819	1.28392
C	7.71533	-1.00082	0.5304
N	6.24583	0.63048	-0.50186
N	2.8643	3.26344	-1.43294
N	-1.69458	3.47698	0.26629
C	-5.96486	2.83863	2.66782
C	-6.97173	1.93028	2.66549
N	-5.90487	-1.08471	-0.39406
N	-3.14837	-1.89195	-0.87955
N	1.06324	-1.89198	1.57124
C	5.75667	-2.74707	2.96
C	6.97405	-2.51368	2.39545
H	-0.79877	0.78757	-1.35641
H	-0.47698	-2.91904	-2.4624
H	-2.74445	-3.11565	-3.88739
H	-7.88799	-2.80223	-2.4988
H	-9.19077	-1.69948	-0.39421
H	-7.87993	1.94137	3.25555
H	-5.88202	3.73656	3.26907
H	1.2035	0.72862	-0.14508
H	8.00199	2.60678	-2.41683
H	9.4334	0.62228	-1.26522
H	7.94492	-2.87464	2.71708
H	5.52202	-3.36059	3.82287
H	1.17029	-1.95682	-1.71631
H	-1.55887	4.39183	0.66921
H	0.62694	-1.90141	2.47959
H	8.74937	-1.30718	0.68189
H	-8.45962	-0.1725	1.64676
H	-3.67795	4.05141	1.90548
H	0.47283	4.51218	-1.08073
H	5.45306	3.51477	-2.0962
H	-1.55972	-1.71429	1.21682
H	3.03355	-2.27544	3.36729
H	-5.37485	-2.85024	-3.24807

H	3.7497	0.21988	-0.53029
H	-3.15175	0.57341	-0.10848
H	5.48198	0.27384	0.07266
H	3.5706	-2.05613	-0.54227
H	3.0026	4.21366	-1.7377
H	-3.74179	-1.57245	-0.11709
H	-5.07805	0.73687	0.36317

SCF Done: E(RM06) = -1978.87103986 A.U. after 7 cycles

3g (Twisted-Hückel [38]$T2^{B,F}$)

C	-6.0908	2.14861	0.51474
C	-6.02851	3.54697	0.77235
C	-4.72216	3.87394	1.03691
C	-3.93926	2.68213	0.98694
C	-2.57927	2.56065	1.26103
C	-1.83669	1.38848	1.42465
C	-2.20985	0.02044	1.55517
C	-1.07023	-0.73342	1.71031
C	0.0564	0.12874	1.65673
C	1.43173	-0.09026	1.64089
C	2.0957	-1.30343	1.47566
C	1.65044	-2.6572	1.38353
C	2.74729	-3.45725	1.16242
C	3.89572	-2.62414	1.06876
C	5.22146	-2.93423	0.7695
C	6.19403	-1.97031	0.48571
N	5.89813	-0.6536	0.29641
C	7.08439	-0.02466	0.08967
C	7.18068	1.34007	-0.21249
C	6.09083	2.14861	-0.51487
C	6.02854	3.54698	-0.77244
C	4.72218	3.87398	-1.03691
C	3.93926	2.68219	-0.98689
C	2.57925	2.56073	-1.26088
C	1.83667	1.38855	-1.42442
C	2.20983	0.02051	-1.55484
C	1.07022	-0.73336	-1.71002
C	-0.05642	0.1288	-1.65654
C	-1.43175	-0.09021	-1.64078
C	-2.0957	-1.30338	-1.47559
C	-1.65042	-2.65714	-1.38344
C	-2.74727	-3.45721	-1.16239
C	-3.89572	-2.62413	-1.06879
C	-5.22147	-2.93423	-0.76961
C	-6.19404	-1.97031	-0.48587
N	-5.89812	-0.65361	-0.29657
C	-7.08437	-0.02464	-0.08989
C	-7.18065	1.34009	0.21227
N	-4.80311	1.67249	0.64892
N	-0.46127	1.40715	1.54626
N	3.45477	-1.3444	1.29308
C	7.6185	-2.18778	0.38148
C	8.17861	-0.96549	0.16775
N	4.80313	1.67251	-0.64899
N	0.46124	1.40721	-1.54606
N	-3.45478	-1.34437	-1.29307
C	-7.61853	-2.18775	-0.38173
C	-8.17862	-0.96544	-0.16803

H	0.62448	-2.98719	1.47731
H	2.75933	-4.53393	1.04358
H	8.11762	-3.14445	0.48913
H	9.22766	-0.72177	0.04113
H	6.88356	4.21133	-0.74865
H	4.32238	4.85017	-1.28408
H	3.22626	-0.35614	-1.58114
H	1.03674	-1.80445	-1.8556
H	-0.62445	-2.98711	-1.47716
H	-2.7593	-4.5339	-1.04356
H	-8.11765	-3.1444	-0.48942
H	-9.22767	-0.7217	-0.04148
H	-6.88351	4.21133	0.74852
H	-4.32236	4.85012	1.28413
H	4.10335	-0.56392	1.21199
H	4.62073	0.6861	-0.47924
H	-4.10337	-0.5639	-1.21197
H	-4.62072	0.68608	0.47911
H	-5.50496	-3.98442	-0.75781
H	-8.16667	1.79843	0.24638
H	-2.04856	3.50354	1.39677
H	2.06469	0.8003	1.63004
H	5.50495	-3.98441	0.75768
H	8.16671	1.79839	-0.24664
H	-2.06472	0.80035	-1.62997
H	2.04854	3.50362	-1.3966
H	-3.22628	-0.35622	1.58153
H	-1.03674	-1.80451	1.85593
H	0.11262	2.22109	1.38185
H	-0.11265	2.22116	-1.38169

SCF Done: E(RM06) = -1978.90164996 A.U. after 17 cycles

3h (Twisted-Hückel [38]$T2^{C,G}$)

C	-7.16579	-0.06458	-0.01355
C	-8.26351	-0.98094	-0.21603
C	-7.71112	-2.15396	-0.62952
C	-6.28886	-1.92221	-0.72268
C	-5.33994	-2.83314	-1.19807
C	-4.01899	-2.50196	-1.4841
C	-2.91742	-3.32569	-1.84435
C	-1.80515	-2.5276	-1.97013
C	-2.19279	-1.17706	-1.71752
C	-1.48186	0.02213	-1.71333
C	-0.09829	0.17296	-1.67678
C	0.97137	-0.75485	-1.5612
C	2.15302	-0.05835	-1.46687
C	1.86593	1.3358	-1.53538
C	2.6707	2.47624	-1.53093
C	4.04237	2.57304	-1.31379
N	4.89022	1.58252	-0.88976
C	6.19291	2.03634	-0.84386
C	7.27139	1.24567	-0.47008
C	7.1658	-0.06458	0.01354
C	8.26351	-0.98095	0.21602
C	7.71112	-2.15396	0.62952
C	6.28886	-1.9222	0.72267
C	5.33994	-2.83313	1.19807
C	4.01899	-2.50193	1.48411

C	2.91742	-3.32566	1.84438
C	1.80515	-2.52756	1.97016
C	2.19279	-1.17703	1.71752
C	1.48187	0.02216	1.71332
C	0.09829	0.173	1.6768
C	-0.97137	-0.75482	1.56126
C	-2.15302	-0.05832	1.46693
C	-1.86593	1.33583	1.5354
C	-2.6707	2.47627	1.53092
C	-4.04237	2.57306	1.31377
N	-4.89021	1.58253	0.88976
C	-6.19291	2.03635	0.84384
C	-7.27138	1.24567	0.47006
N	-5.98143	-0.65361	-0.32935
N	0.49565	1.4205	-1.67645
N	-3.53599	-1.21675	-1.44339
C	4.8534	3.72866	-1.5202
C	6.1583	3.39714	-1.25695
N	5.98143	-0.6536	0.32934
N	3.53599	-1.21672	1.44338
N	-0.49565	1.42053	1.67646
C	-4.85341	3.72869	1.52016
C	-6.1583	3.39716	1.2569
H	0.85748	-1.82819	-1.48224
H	-9.30937	-0.75671	-0.03758
H	-8.21343	-3.08159	-0.88075
H	-2.97468	-4.39794	-1.98743
H	-0.81567	-2.84194	-2.27445
H	4.46882	4.68237	-1.86136
H	7.03025	4.03537	-1.32972
H	9.30938	-0.75672	0.03756
H	8.21342	-3.08159	0.88076
H	2.97468	-4.3979	1.98747
H	0.81567	-2.84189	2.27449
H	-0.85748	-1.82817	1.48232
H	-4.46883	4.6824	1.8613
H	-7.03025	4.03539	1.32966
H	-0.01792	2.28687	-1.73089
H	0.01793	2.28691	1.73084
H	5.64839	-3.86184	1.372
H	8.26422	1.67699	-0.57994
H	2.1784	3.4218	-1.75998
H	-2.1784	3.42183	1.75994
H	2.07769	0.93393	1.62785
H	-8.26422	1.67699	0.57991
H	-5.6484	-3.86185	-1.37198
H	-2.07769	0.9339	-1.62789
H	-3.13914	-0.49863	1.37152
H	3.13914	-0.49865	-1.37144
H	-4.154	-0.45104	-1.18244
H	4.154	-0.45102	1.1824
H	-4.68958	0.62451	0.61669
H	4.68958	0.6245	-0.61668

SCF Done: E(RM06) = -1978.90146269 A.U. after 16 cycles

3i (Twisted-Hückel [38]$T2_{RX}$)

C	4.91939	-2.40036	0.43763
C	4.95221	-3.79853	0.70127

C	3.69776	-4.1902	1.08317
C	2.84297	-3.04853	1.0837
C	1.50782	-3.036	1.45608
C	0.64482	-1.94944	1.59334
C	-0.76086	-1.9993	1.76835
C	-1.25333	-0.71615	1.76846
C	-0.15873	0.17979	1.61858
C	-0.09651	1.56445	1.52116
C	-1.1708	2.42125	1.28926
C	-1.14721	3.84167	1.24572
C	-2.4053	4.28414	0.90334
C	-3.23252	3.14766	0.71724
C	-4.58264	3.06276	0.40317
C	-5.32116	1.89046	0.23697
N	-4.82716	0.61176	0.17223
C	-5.93432	-0.18059	0.09757
C	-5.96711	-1.56918	-0.08443
C	-4.91935	-2.40048	-0.43782
C	-4.95218	-3.79868	-0.7013
C	-3.69769	-4.19044	-1.08302
C	-2.84287	-3.04881	-1.08356
C	-1.50769	-3.03631	-1.45579
C	-0.64471	-1.94973	-1.59295
C	0.76099	-1.9995	-1.76788
C	1.25336	-0.71631	-1.76801
C	0.15869	0.17955	-1.61809
C	0.09638	1.5642	-1.52065
C	1.17064	2.42108	-1.28895
C	1.14697	3.84149	-1.24538
C	2.40511	4.28404	-0.90329
C	3.23244	3.1476	-0.71736
C	4.58262	3.06277	-0.40355
C	5.32118	1.89049	-0.23746
N	4.82718	0.6118	-0.17256
C	5.93435	-0.18055	-0.09807
C	5.96714	-1.56913	0.08402
N	3.62648	-1.98394	0.67678
N	-2.44817	2.04223	0.96081
N	0.97413	-0.61377	1.53166
C	-6.76392	1.89889	0.18378
N	-0.97411	-0.61409	-1.53114
C	-7.14941	0.60027	0.13951
N	-3.6264	-1.98413	-0.67691
N	2.44812	2.04213	-0.96083
C	6.76396	1.89891	-0.18455
C	7.14944	0.60029	-0.14025
H	5.84235	-4.40999	0.61919
H	3.37306	-5.18038	1.37949
H	-1.32812	-2.91896	1.85025
H	-2.28919	-0.43291	1.91736
H	-0.26668	4.43478	1.46185
H	-2.73956	5.30839	0.79315
H	-7.38121	2.79003	0.21161
H	-8.15275	0.19083	0.09964
H	-5.84234	-4.41011	-0.61925
H	-3.37299	-5.18067	-1.3792
H	1.3283	-2.91912	-1.84978
H	2.2892	-0.43297	-1.91688
H	0.26635	4.43455	-1.46129
H	2.73934	5.3083	-0.79316

H	7.38124	2.79005	-0.21254
H	8.15278	0.19085	-0.10053
H	3.3498	-1.04532	0.41272
H	-2.83334	1.11174	0.83093
H	-3.34971	-1.04547	-0.413
H	2.83339	1.11166	-0.8311
H	5.12519	4.00362	-0.3317
H	6.94394	-2.04506	0.01651
H	-1.06365	-4.01152	-1.64491
H	1.06381	-4.0112	1.64525
H	-5.12523	4.00359	0.33121
H	0.88376	2.03977	1.57132
H	-0.88394	2.03945	-1.57064
H	-6.94393	-2.04509	-0.01701
H	1.91073	-0.23679	1.55342
H	-1.91074	-0.23718	-1.55284

SCF Done: E(RM06) = -1978.91268275 A.U. after 19 cycles

4a (Hückel $[36]^{2+}$*T0*^{5,10,25,30})

C	7.62914	-1.07413	-0.08311
C	9.01444	-0.67757	-0.06409
C	9.01444	0.67755	0.06411
C	7.62915	1.07412	0.08312
C	7.15441	2.39465	0.154
C	5.82998	2.77928	0.02456
N	4.80553	1.90648	-0.29083
C	3.61289	2.55032	-0.29509
C	2.41058	1.85462	-0.60214
C	1.14199	2.28497	-0.32185
C	0.67646	3.40873	0.46111
C	-0.67644	3.40873	0.46112
C	-1.14198	2.28497	-0.32184
C	-2.41057	1.85461	-0.60212
C	-3.61288	2.55031	-0.29508
N	-4.80552	1.90647	-0.29082
C	-5.82996	2.77928	0.02456
C	-7.1544	2.39466	0.154
C	-7.62914	1.07413	0.08311
C	-9.01444	0.67757	0.06409
C	-9.01445	-0.67755	-0.06411
C	-7.62915	-1.07412	-0.08312
C	-7.15441	-2.39465	-0.15401
C	-5.82998	-2.77927	-0.02456
N	-4.80553	-1.90647	0.29083
C	-3.61289	-2.55032	0.29509
C	-2.41058	-1.85462	0.60213
C	-1.14199	-2.28497	0.32185
C	-0.67646	-3.40873	-0.46112
C	0.67645	-3.40873	-0.46112
C	1.14198	-2.28497	0.32185
C	2.41057	-1.85461	0.60213
C	3.61288	-2.55031	0.29508
N	4.80552	-1.90648	0.29083
C	5.82996	-2.77928	-0.02456
C	7.1544	-2.39466	-0.154
N	6.80106	-0.00001	0.
C	5.23045	4.05323	0.19933
C	3.87399	3.91427	0.01533

N	0.	1.61398	-0.72491
C	-3.87397	3.91427	0.01534
C	-5.23043	4.05323	0.19934
N	-6.80106	0.00001	0.
C	-5.23045	-4.05323	-0.19933
C	-3.87399	-3.91427	-0.01533
N	0.	-1.61398	0.72491
C	3.87397	-3.91427	-0.01534
C	5.23043	-4.05323	-0.19934
H	0.	-0.88379	1.4235
H	0.	0.88379	-1.4235
H	-7.88025	3.1869	0.32865
H	-7.88027	-3.18688	-0.32865
H	-2.5204	-0.88782	1.09667
H	2.52039	-0.88782	1.09666
H	7.88025	-3.1869	-0.32865
H	7.88027	3.18688	0.32864
H	2.5204	0.88782	-1.09667
H	-2.52039	0.88781	-1.09665
H	-5.77031	-4.96157	-0.43588
H	-3.13895	-4.70717	-0.02713
H	-1.32127	-4.08188	-1.00999
H	1.32125	-4.08188	-1.01
H	3.13893	-4.70717	-0.02714
H	5.77029	-4.96158	-0.43588
H	9.86479	-1.34632	-0.11953
H	9.8648	1.3463	0.11955
H	5.77031	4.96157	0.43588
H	3.13895	4.70717	0.02712
H	1.32127	4.08188	1.00999
H	-1.32125	4.08188	1.01
H	-3.13893	4.70717	0.02714
H	-5.77029	4.96158	0.43589
H	-9.86479	1.34632	0.11953
H	-9.8648	-1.3463	-0.11955
H	5.01252	-0.93354	0.50522
H	-5.01252	0.93353	-0.50522
H	-5.01253	-0.93353	0.50522
H	5.01253	0.93354	-0.50523

SCF Done: E(RM06) = -1978.41818064 A.U. after 17 cycles

4b (Hückel $[36]^{2+}$*TO*^{B,C,E,F,H})

C	5.19751400	3.89685000	-0.24402400
C	5.60578300	5.24568100	-0.51512000
C	4.48825100	6.01479300	-0.61508800
C	3.33493800	5.18653500	-0.39621000
C	2.02809100	5.57492400	-0.37827500
C	0.86456500	4.76214700	-0.19518100
N	-0.31925900	5.34248500	-0.06810600
C	-1.21743500	4.31284900	0.12954900
C	-2.55979900	4.55526000	0.27687800
C	-3.49949900	3.55663100	0.65623300
C	-3.30350300	2.40741800	1.42913000
C	-4.50839100	1.71279800	1.47689300
C	-5.45434900	2.43467900	0.73363900
C	-6.80603900	2.07884100	0.40832000
C	-7.17458300	0.78390800	0.18979000
N	-6.27333900	-0.27430700	0.13163600

C	-6.90038100	-1.44973600	-0.13968100
C	-6.25915500	-2.67658800	-0.29851900
C	-4.87518700	-2.80760700	-0.45648800
C	-3.90590000	-1.80933800	-0.84018200
C	-2.68009700	-2.38824300	-0.87249800
C	-2.81110200	-3.77192000	-0.51224600
C	-1.85265600	-4.72073700	-0.29681500
C	-0.44121500	-4.53960200	-0.45949800
N	0.39070800	-5.35033400	0.18040700
C	1.65142200	-4.85482900	-0.07322600
C	2.76061800	-5.43489300	0.49936100
C	4.05738000	-4.87425800	0.54892500
C	5.28711600	-5.49516000	0.81830100
C	6.27010600	-4.51662600	0.80148500
C	5.65056900	-3.27966700	0.54545200
C	6.26678900	-2.00881500	0.51994200
C	5.71095100	-0.80237100	0.17199800
N	6.37676100	0.41173500	0.32667500
C	5.60130500	1.46159600	-0.06802000
C	6.02304600	2.79044200	-0.05242000
N	3.82932100	3.89087600	-0.20493800
C	0.76596300	3.30396000	-0.13214600
C	-0.53963700	3.02625100	0.07890800
N	-4.83248700	3.57701500	0.30012000
C	-8.46697900	0.19690300	-0.06375000
C	-8.30808900	-1.14329600	-0.23008900
N	-4.17955500	-3.96654400	-0.30147100
C	0.26848200	-3.53070400	-1.24064500
C	1.58405000	-3.72365000	-0.98559400
N	4.31136400	-3.53019700	0.36059900
C	4.44439500	-0.46458500	-0.40909100
C	4.37263500	0.88773200	-0.55016500
H	-9.39228900	0.75795400	-0.10464600
H	-4.72889200	0.84572500	2.08851700
H	-2.39359900	2.17447700	1.96579500
H	-1.01151500	2.05271100	0.11775300
H	1.54906000	2.57641300	-0.31175500
H	4.43378700	7.07165100	-0.84609100
H	6.63542100	5.55261200	-0.64696000
H	3.59088500	1.44598100	-1.04966900
H	-5.24071700	4.24264100	-0.34335600
H	3.30884900	3.18240400	0.29159600
H	-9.07514900	-1.87559700	-0.44738100
H	-4.13674600	-0.79479100	-1.13622700
H	-1.74705000	-1.89996800	-1.11305300
H	-0.15823800	-2.84980300	-1.96678500
H	2.42411400	-3.24152100	-1.47353700
H	5.42126100	-6.55772700	0.97433400
H	7.33430000	-4.65412400	0.94576900
H	3.70996900	-1.17655100	-0.76449000
H	-4.58833800	-4.83958300	0.00399700
H	3.58402000	-2.83385700	0.43894300
H	7.30981000	-2.00729700	0.83500900
H	7.08068500	2.99601300	0.09628100
H	1.83055200	6.63874600	-0.49446200
H	-2.90292200	5.57244600	0.08569400
H	-7.56190600	2.85444000	0.30212100
H	-6.87853100	-3.56986300	-0.28370700
H	2.61794300	-6.39995800	0.98313500
H	-2.14720800	-5.69061000	0.10382700

H	7.28173000	0.51093400	0.76651400
H	-5.29373000	-0.17444100	0.34940400

SCF Done: E(RM06) = -1978.36842618 A.U. after 7 cycles

4c (Hückel $[36]^{2+}$*T0*^{5,20,25,B,F})

C	6.22054	2.11078	0.13528
C	6.3841	3.41064	0.7173
C	5.14394	3.92092	0.95468
C	4.1684	2.95743	0.52153
C	2.778	3.14834	0.55754
C	1.7969	2.25537	0.16942
N	0.45287	2.56015	0.20683
C	-0.31365	1.47984	-0.19259
C	-1.66615	1.36161	-0.34798
C	-2.72594	2.30461	-0.27219
C	-2.8267	3.70317	-0.07744
C	-4.15932	4.05519	-0.22453
C	-4.89429	2.87784	-0.49671
C	-6.2598	2.68187	-0.7925
C	-6.83393	1.43305	-1.00473
N	-6.10985	0.29249	-0.78368
C	-6.86602	-0.72718	-1.21197
C	-6.34131	-2.05498	-1.15636
C	-5.2352	-2.38347	-0.4055
C	-4.38468	-3.53672	-0.4303
C	-3.32635	-3.31033	0.41041
C	-3.53295	-2.03812	1.04552
C	-2.86918	-1.36338	2.09144
C	-1.55346	-1.45029	2.48508
N	-0.50353	-2.04187	1.82162
C	0.69769	-1.72196	2.45559
C	1.95943	-1.89023	1.97754
C	2.33845	-2.4692	0.73106
C	1.71475	-3.42107	-0.10164
C	2.55484	-3.65068	-1.18484
C	3.67837	-2.81823	-1.04155
C	4.81463	-2.68209	-1.85961
C	5.79701	-1.71994	-1.72157
N	5.68566	-0.62474	-0.88697
C	6.87189	-0.00195	-0.98574
C	7.15883	1.24981	-0.36385
N	4.85264	1.88033	0.06568
C	1.88291	0.8959	-0.30344
C	0.6247	0.43274	-0.49909
N	-3.98693	1.85002	-0.50149
C	-8.12481	1.09798	-1.56264
C	-8.13221	-0.25648	-1.72418
N	-4.66934	-1.52682	0.52713
C	-1.00172	-0.82353	3.66145
C	0.33882	-1.00493	3.65294
N	3.51515	-2.12496	0.13617
C	7.08864	-1.75034	-2.36467
C	7.78289	-0.69427	-1.86652
H	4.21052	-1.45068	0.45146
H	4.52423	1.03321	-0.38988
H	-4.29518	0.90459	-0.73364
H	-5.06823	-0.60757	0.70126
H	7.42445	-2.50427	-3.0665

H	8.79678	-0.38805	-2.09391
H	2.40017	-4.3471	-1.99921
H	0.80605	-3.96268	0.1332
H	7.34092	3.87649	0.91699
H	4.89444	4.88466	1.38021
H	-2.01062	4.38742	0.11504
H	-4.58142	5.04933	-0.14934
H	-8.90413	1.80107	-1.83053
H	-8.9255	-0.87182	-2.13032
H	-2.52981	-4.00306	0.65338
H	-4.56367	-4.41811	-1.03385
H	2.78701	0.32725	-0.47622
H	0.34008	-0.54438	-0.874
H	4.93778	-3.42415	-2.64681
H	8.1961	1.5776	-0.3424
H	2.45894	4.12221	0.92373
H	2.755	-1.46037	2.5843
H	1.05843	-0.67537	4.39238
H	-1.6019	-0.31748	4.4071
H	-6.79883	-2.83316	-1.76345
H	-3.47424	-0.66087	2.66254
H	-6.87651	3.57185	-0.90172
H	-1.98053	0.35637	-0.63408
H	0.09066	3.44367	0.53346
H	-0.55589	-2.36522	0.86577

SCF Done: E(RM06) = -1978.40834564 A.U. after 10 cycles

4d (Hückel $[36]^{2+}$*TO*^{20,25,B,F})

C	5.59376	1.94523	-1.0937
C	5.89115	3.27126	-0.71897
C	4.79467	3.77212	-0.05196
C	3.78417	2.7803	-0.05349
C	2.48179	3.02593	0.4373
C	1.2659	2.39472	0.31234
N	0.11575	3.04703	0.74555
C	-1.0234	2.42043	0.31385
C	-2.2452	3.07209	0.43871
C	-3.50821	2.86829	-0.13573
C	-4.46519	3.93759	-0.23759
C	-5.51878	3.50299	-0.97754
C	-5.29719	2.1261	-1.29907
C	-6.13818	1.28966	-1.9819
C	-5.98551	-0.12092	-2.0979
N	-5.12377	-0.78738	-1.32394
C	-5.28918	-2.11512	-1.65871
C	-4.65019	-3.13012	-0.97291
C	-3.86656	-2.9304	0.18263
C	-2.96216	-3.78279	0.8366
C	-2.33667	-3.04481	1.83855
C	-2.89598	-1.75084	1.82576
C	-2.60372	-0.57901	2.6044
C	-1.33567	-0.22923	2.93929
N	-0.20616	-0.92506	2.51321
C	0.9259	-0.21213	2.78491
C	2.18682	-0.51476	2.30606
C	2.48756	-1.67507	1.57177
C	1.8572	-2.96968	1.53122
C	2.54648	-3.74831	0.64352

C	3.58829	-2.9519	0.07085
C	4.46126	-3.22747	-0.95409
C	5.31938	-2.2492	-1.52525
N	5.19149	-0.94525	-1.22871
C	6.22629	-0.32352	-1.87439
C	6.44047	1.0377	-1.75183
N	4.30506	1.67676	-0.67287
C	0.79106	1.1896	-0.31378
C	-0.57518	1.20054	-0.31168
N	-4.05488	1.78786	-0.75527
C	-6.72457	-1.00118	-2.9737
C	-6.26284	-2.25398	-2.71722
N	-3.8235	-1.72135	0.83809
C	-0.84218	0.93804	3.62958
C	0.51147	0.94978	3.53729
N	3.52421	-1.72332	0.70622
C	6.43432	-2.48886	-2.4162
C	7.02077	-1.27911	-2.61413
H	4.17035	-0.98091	0.43615
H	3.87762	0.7769	-0.86482
H	-3.69619	0.8428	-0.84645
H	-4.36885	-0.93172	0.49145
H	6.74023	-3.4529	-2.80391
H	7.89504	-1.04796	-3.2104
H	2.35881	-4.78539	0.39434
H	1.05326	-3.29034	2.18203
H	6.83215	3.76986	-0.91312
H	4.68014	4.75925	0.37803
H	-4.30723	4.92642	0.17417
H	-6.39881	4.06108	-1.2721
H	-7.47779	-0.6978	-3.69054
H	-6.57563	-3.18772	-3.16878
H	-1.63649	-3.41148	2.5799
H	-2.7934	-4.82226	0.58544
H	1.4229	0.4123	-0.72899
H	-1.2232	0.4376	-0.72649
H	4.48868	-4.24246	-1.34394
H	7.35348	1.45716	-2.17078
H	2.42942	3.99442	0.93716
H	2.96395	0.23756	2.42755
H	1.19933	1.68199	3.94218
H	-1.47762	1.65603	4.13371
H	-4.75238	-4.15113	-1.33596
H	-3.41278	0.10424	2.85616
H	-7.01267	1.74888	-2.43888
H	-2.17983	4.04368	0.92873
H	-0.26275	-1.63865	1.7966
H	0.12004	4.00187	1.07825

SCF Done: E(RM06) = -1978.40266700 A.U. after 7 cycles

4e (Möbius $[36]^{2+}$*T1*^{B,C,E,H})

C	-7.03768	0.09192	-0.29562
C	-8.26396	-0.65458	-0.31323
C	-8.00915	-1.90595	0.1608
C	-6.60945	-2.00072	0.47058
C	-5.87208	-3.11732	0.78305
C	-4.65316	1.8915	0.51952
C	-4.47155	-3.11097	0.98933

N	-3.67806	-4.21089	0.76658
C	-2.34515	-3.88059	0.89752
C	-1.2877	-4.77202	0.62917
C	-0.02144	-4.34636	0.27845
C	0.40398	-3.05832	-0.17201
C	1.73642	-3.11572	-0.4574
C	2.20026	-4.44538	-0.19827
C	3.4685	-5.00721	-0.34892
C	4.65078	-4.30498	-0.55795
N	4.80374	-2.94041	-0.51001
C	6.14382	-2.6008	-0.66061
C	6.64535	-1.32437	-0.55643
C	5.8503	-0.16157	-0.45588
C	4.51711	0.06949	-0.87731
C	4.16174	1.34995	-0.51276
C	5.26598	1.93395	0.15034
C	5.37721	3.14299	0.85842
C	4.34038	4.02459	1.11196
N	3.08722	3.88999	0.58378
C	2.33362	4.75344	1.27142
C	0.92853	4.83412	1.09089
C	0.24604	4.51314	-0.06437
C	0.77865	4.43485	-1.42013
C	-0.29935	4.3145	-2.22793
C	-1.45285	4.22572	-1.33684
C	-2.76842	3.91514	-1.77551
C	-3.71026	3.27352	-1.00621
N	-4.95873	2.87288	-1.47353
C	-5.53545	1.99729	-0.60487
C	-6.76387	1.34572	-0.81454
N	-6.0824	-0.7391	0.24839
C	-3.60572	-2.06549	1.37915
C	-2.30763	-2.53772	1.32595
N	1.10052	-5.15664	0.21063
C	5.94662	-4.85324	-0.82374
C	6.84565	-3.82823	-0.87765
N	6.28437	1.00408	0.11676
C	4.38055	5.07118	2.12532
C	3.10329	5.49377	2.26451
C	-3.56501	2.6816	0.28907
N	-1.11873	4.37468	-0.05602
H	-1.41471	-2.02018	1.65106
H	-5.09334	-0.59008	0.0966
H	1.13662	-6.11107	0.54169
H	3.93558	-0.61998	-1.47686
H	7.90815	-3.89485	-1.07581
H	5.2594	5.38823	2.67437
H	-4.88699	1.3422	1.42327
H	-8.71622	-2.71595	0.2905
H	6.14195	-5.90903	-0.96283
H	1.82409	4.52825	-1.68395
H	-3.92439	-1.10952	1.77558
H	2.31958	-2.33286	-0.92291
H	2.71022	6.24402	2.93996
H	3.22767	1.87176	-0.67228
H	-0.26186	-2.22364	-0.34563
H	-2.70991	2.87469	0.92378
H	-0.32806	4.26596	-3.31046
H	-9.21474	-0.25576	-0.64324
H	-6.39584	-4.07111	0.77495

H	-1.48572	-5.84321	0.6768
H	3.56247	-6.08933	-0.28606
H	7.72831	-1.22523	-0.506
H	6.33407	3.35628	1.33611
H	0.32462	5.16959	1.93451
H	-3.0019	4.10753	-2.8233
H	-7.50674	1.79495	-1.46955
H	7.17681	1.11632	0.5793
H	-5.32437	3.09025	-2.39081
H	4.15329	-2.32671	-0.03873
H	-4.01275	-5.07458	0.36038

SCF Done: E(RM06) = -1978.37780916 A.U. after 7 cycles

4f (Möbius $[36]^{2+}$*T1*^{B,C,F})

C	7.41057	0.25929	-0.34381
C	8.35484	1.16523	-0.98657
C	7.61095	2.16428	-1.50577
C	6.22271	1.84401	-1.18692
C	5.15562	2.71355	-1.46242
C	3.82154	2.44767	-1.19676
N	2.81414	3.38742	-1.21675
C	1.6126	2.82487	-0.84728
C	0.44756	3.53859	-0.63257
C	-0.7948	2.9464	-0.35265
C	-1.29504	1.64637	-0.6369
C	-2.56749	1.55249	-0.12977
C	-2.89591	2.79061	0.48849
C	-3.99139	3.20447	1.24232
C	-5.14765	2.5022	1.55155
N	-5.54265	1.27603	1.07485
C	-6.76638	0.94876	1.59626
C	-7.51861	-0.14915	1.1802
C	-7.14167	-1.05178	0.19261
C	-8.09009	-1.9148	-0.49238
C	-7.41602	-2.45704	-1.52954
C	-6.04508	-1.99125	-1.40105
C	-5.00882	-2.42458	-2.23846
C	-3.65555	-2.33717	-1.97028
N	-3.0972	-1.90954	-0.7888
C	-1.73212	-2.10888	-0.80144
C	-0.91984	-1.91676	0.30652
C	0.48249	-2.00518	0.31236
C	1.4322	-1.9283	-0.74335
C	2.69193	-2.02566	-0.20168
C	2.56416	-2.17734	1.20473
C	3.5373	-2.47157	2.16457
C	4.90717	-2.30765	2.00421
N	5.51493	-1.51538	1.05813
C	6.87502	-1.61631	1.1712
C	7.77295	-0.82381	0.45337
N	6.12647	0.67914	-0.5094
C	3.2034	1.21188	-0.83595
C	1.88027	1.43397	-0.61827
N	-1.80424	3.61154	0.29149
C	-6.16266	2.94076	2.45599
C	-7.14369	1.98874	2.49302
N	-5.89222	-1.13969	-0.35794
C	-2.5782	-2.78502	-2.79627

C	-1.41751	-2.6392	-2.0988
N	1.21132	-2.14322	1.47015
C	5.95018	-2.95729	2.73417
C	7.14761	-2.5713	2.19614
H	-0.77515	0.89107	-1.21351
H	-0.43332	-2.95234	-2.41815
H	-2.70389	-3.19457	-3.7907
H	-7.77822	-3.13531	-2.29269
H	-9.13462	-2.02978	-0.22887
H	-8.05776	1.99913	3.07257
H	-6.12335	3.87191	3.00753
H	1.15487	0.71262	-0.26502
H	7.94285	3.042	-2.04756
H	9.43106	1.04283	-1.00383
H	8.13856	-2.89435	2.48862
H	5.78457	-3.67048	3.532
H	1.19445	-1.77622	-1.78809
H	-1.72011	4.54415	0.67281
H	0.80705	-2.27772	2.38681
H	8.83182	-1.02902	0.5916
H	-8.52234	-0.23475	1.59015
H	-3.93835	4.20068	1.68012
H	0.50362	4.62724	-0.62222
H	5.4159	3.69491	-1.85744
H	-1.41264	-1.73507	1.26255
H	3.21369	-2.91603	3.10499
H	-5.28527	-2.9376	-3.15703
H	3.74648	0.28302	-0.76513
H	-3.21411	0.68728	-0.2121
H	3.63034	-2.05337	-0.74221
H	5.12892	-0.72128	0.5428
H	-5.16385	0.71944	0.31071
H	-3.68169	-1.63479	-0.00336
H	2.95112	4.36798	-1.42053

SCF Done: E(RM06) = -1978.42150412 A.U. after 7 cycles

4g (Twisted-Hückel $[36]^{2+}$*T2*^{B,F})

C	6.39518	2.00872	-0.60935
C	6.51797	3.34541	-1.1295
C	5.30091	3.72498	-1.60204
C	4.38285	2.62706	-1.41824
C	3.03161	2.59233	-1.75845
C	2.22585	1.45551	-1.71363
N	0.86114	1.49875	-1.76206
C	0.30839	0.22012	-1.683
C	-1.04353	0.00815	-1.63452
C	-1.74085	-1.21867	-1.4971
C	-1.32802	-2.56827	-1.45017
C	-2.46065	-3.35521	-1.31703
C	-3.57691	-2.50003	-1.25357
C	-4.94538	-2.8331	-1.1339
C	-5.97827	-1.95883	-0.88806
N	-5.80041	-0.62823	-0.5538
C	-7.04096	-0.13926	-0.41879
C	-7.32283	1.18716	0.03352
C	-6.39518	2.00872	0.60934
C	-6.51797	3.34542	1.12948
C	-5.30091	3.72499	1.60202

C	-4.38285	2.62707	1.41824
C	-3.03161	2.59234	1.75844
C	-2.22585	1.45552	1.71365
N	-0.86114	1.49876	1.76206
C	-0.30839	0.22013	1.68301
C	1.04353	0.00817	1.63451
C	1.74085	-1.21866	1.49709
C	1.32802	-2.56826	1.45017
C	2.46065	-3.3552	1.31704
C	3.57691	-2.50002	1.25356
C	4.94538	-2.83309	1.1339
C	5.97827	-1.95883	0.88805
N	5.80041	-0.62823	0.5538
C	7.04096	-0.13926	0.41878
C	7.32283	1.18716	-0.03353
N	5.08002	1.62973	-0.81871
C	2.57618	0.06252	-1.6306
C	1.43044	-0.67153	-1.61387
N	-3.10589	-1.22003	-1.36941
C	-7.38709	-2.28657	-0.95418
C	-8.05527	-1.13618	-0.69655
N	-5.08003	1.62973	0.81871
C	-2.57618	0.06252	1.63066
C	-1.43044	-0.67152	1.61392
N	3.10589	-1.22002	1.36938
C	7.38708	-2.28656	0.95418
C	8.05527	-1.13618	0.69655
H	-0.31283	-2.92909	-1.54202
H	-2.50618	-4.43581	-1.26895
H	-7.79349	-3.26159	-1.19467
H	-9.12543	-0.9721	-0.66153
H	-7.43616	3.91926	1.13233
H	-5.03713	4.66358	2.07277
H	-3.58272	-0.33759	1.64522
H	-1.37329	-1.75077	1.568
H	0.31283	-2.92908	1.54203
H	2.50618	-4.43579	1.26897
H	7.79349	-3.26159	1.19468
H	9.12543	-0.97211	0.66153
H	7.43616	3.91925	-1.13236
H	5.03713	4.66356	-2.07281
H	-3.73602	-0.42276	-1.36705
H	-4.76217	0.7363	0.44669
H	3.73602	-0.42275	1.367
H	4.76217	0.7363	-0.44668
H	5.19344	-3.88493	1.26496
H	8.34698	1.54531	0.03788
H	2.58203	3.53648	-2.05855
H	-1.67494	0.89806	-1.68632
H	-5.19344	-3.88494	-1.26495
H	-8.34698	1.54531	-0.03789
H	1.67494	0.89807	1.68629
H	-2.58203	3.53649	2.05853
H	3.58273	-0.33759	-1.64513
H	1.37329	-1.75078	-1.56794
H	0.32406	2.34767	-1.86864
H	-0.32406	2.34769	1.86861

SCF Done: E(RM06) = -1978.42664075 A.U. after 20 cycles

4h (Twisted-Hückel $[36]^{2+}$*T2*^{C,G})

C	7.12758	-0.13536	0.28173
C	8.17457	-1.08594	0.61465
C	7.54322	-2.20073	1.04725
C	6.1246	-1.89645	1.02635
C	5.1338	-2.73561	1.46687
C	3.7658	-2.39976	1.62332
N	3.27982	-1.12796	1.5346
C	1.92201	-1.11853	1.75131
C	1.19308	0.08802	1.74061
C	-0.17361	0.24139	1.71103
C	-1.23489	-0.69118	1.50319
C	-2.42331	-0.01649	1.53026
C	-2.14902	1.37286	1.75428
C	-3.00288	2.47316	1.90667
C	-4.3587	2.50034	1.62259
N	-5.08534	1.53551	0.99496
C	-6.41085	1.91846	0.88308
C	-7.37402	1.14468	0.30298
C	-7.12761	-0.13532	-0.28182
C	-8.17458	-1.08588	-0.61484
C	-7.54319	-2.20062	-1.04753
C	-6.12458	-1.89633	-1.02654
C	-5.13376	-2.73543	-1.46712
C	-3.76576	-2.39955	-1.62352
N	-3.2798	-1.12775	-1.53463
C	-1.92199	-1.11826	-1.75136
C	-1.19309	0.08829	-1.74054
C	0.17361	0.24168	-1.71095
C	1.23489	-0.69088	-1.50314
C	2.42331	-0.01618	-1.53014
C	2.149	1.37317	-1.75413
C	3.00286	2.47348	-1.90648
C	4.35867	2.5006	-1.62239
N	5.08529	1.53566	-0.9949
C	6.41081	1.91856	-0.88296
C	7.37397	1.1447	-0.30295
N	5.90563	-0.61679	0.53805
C	2.67803	-3.24244	1.92708
C	1.54132	-2.45659	1.99692
N	-0.79134	1.48362	1.83701
C	-5.27523	3.57713	1.92534
C	-6.51157	3.21883	1.49803
N	-5.90564	-0.61671	-0.53811
C	-2.67798	-3.24218	-1.92735
C	-1.54127	-2.4563	-1.99708
N	0.79132	1.48392	-1.83687
C	5.27523	3.57739	-1.92504
C	6.51156	3.21901	-1.49776
H	-1.10351	-1.75051	1.3198
H	9.2379	-0.91377	0.5001
H	7.97737	-3.13538	1.38128
H	2.74927	-4.31023	2.08989
H	0.54871	-2.78834	2.27061
H	-4.98872	4.48671	2.43813
H	-7.43183	3.78269	1.58463
H	-9.23791	-0.91373	-0.50031
H	-7.97731	-3.13525	-1.38165
H	-2.74919	-4.30995	-2.09029

H	-0.54865	-2.788	-2.27079
H	1.10353	-1.75023	-1.31979
H	4.98876	4.48704	-2.43773
H	7.43184	3.78285	-1.5843
H	-0.31006	2.33715	2.08468
H	0.31003	2.33746	-2.08448
H	-5.41256	-3.74965	-1.74613
H	-8.39814	1.50881	0.32115
H	-2.57486	3.40027	2.28253
H	2.57484	3.40061	-2.28228
H	-1.78803	1.00459	-1.76022
H	8.39809	1.50883	-0.32109
H	5.41262	-3.74986	1.74576
H	1.78801	1.00432	1.76035
H	3.40495	-0.46543	-1.4428
H	-3.40494	-0.46577	1.44294
H	4.78573	0.66517	-0.56293
H	-4.78581	0.66507	0.56286
H	3.89699	-0.34336	1.3391
H	-3.89699	-0.34318	-1.33903

SCF Done: E(RM06) = -1978.42701832 A.U. after 20 cycles

4i (Twisted-Hückel $[36]^{2+}T2_{RX}$)

C	5.25963700	2.17663800	-0.27408900
C	5.44302700	3.57405400	-0.22358200
C	4.21801000	4.16940200	-0.46687400
C	3.28322100	3.13905500	-0.69104600
C	1.93691300	3.22653400	-1.09867300
C	1.11227700	2.16036700	-1.37511200
N	1.49845900	0.83169300	-1.28840600
C	0.41071300	0.13455600	-1.61793800
C	0.44774400	-1.29248800	-1.70675600
C	-0.60920200	-2.14104000	-1.57891800
C	-0.60358800	-3.55995500	-1.81055600
C	-1.83699500	-4.04448800	-1.53127000
C	-2.66927700	-2.95410200	-1.09005300
C	-3.98562800	-3.10117500	-0.69885400
C	-4.94012400	-2.14124200	-0.34576900
N	-4.77684600	-0.78080000	-0.28205400
C	-6.01240800	-0.17896800	-0.00449600
C	-6.23321500	1.16681300	0.14765900
C	-5.25966100	2.17659900	0.27404300
C	-5.44301400	3.57402300	0.22360300
C	-4.21798000	4.16932100	0.46692700
C	-3.28322900	3.13893600	0.69108700
C	-1.93693200	3.22637400	1.09876800
C	-1.11230800	2.16020400	1.37524400
N	-1.49848900	0.83152400	1.28861600
C	-0.41071800	0.13439800	1.61809500
C	-0.44771200	-1.29264900	1.70690400
C	0.60925000	-2.14117300	1.57900300
C	0.60369300	-3.56008900	1.81063900
C	1.83709400	-4.04458800	1.53126900
C	2.66931800	-2.95417800	1.09000200
C	3.98564800	-3.10121600	0.69872100
C	4.94011000	-2.14126300	0.34559900
N	4.77682100	-0.78081700	0.28195100
C	6.01236500	-0.17896600	0.00433600

C	6.23317300	1.16682300	-0.14777300
N	3.93032000	1.94259600	-0.52654600
C	-0.26791100	2.26240300	-1.79453900
C	-0.72043300	0.99204900	-1.92860300
N	-1.90887600	-1.80522800	-1.17293600
C	-6.29948200	-2.42311100	-0.01767900
C	-6.95368100	-1.23707400	0.15351300
N	-3.93034600	1.94250300	0.52645600
C	0.26787200	2.26225700	1.79469500
C	0.72040000	0.99190900	1.92880300
N	1.90888700	-1.80532800	1.17292500
C	6.29945200	-2.42311000	0.01743400
C	6.95363400	-1.23706200	-0.15374900
H	6.38439100	4.06561000	-0.01341300
H	3.99810600	5.22872600	-0.50263500
H	-0.79899700	3.18891400	-1.98176800
H	-1.69034000	0.66258900	-2.28344000
H	0.25414900	-4.10389900	-2.18725200
H	-2.19129500	-5.06283800	-1.63346000
H	-6.70860000	-3.42219400	0.06160800
H	-7.99394800	-1.08886400	0.41616900
H	-6.38436200	4.06561500	0.01344700
H	-3.99804600	5.22863700	0.50273800
H	0.79894500	3.18877600	1.98192100
H	1.69030400	0.66246900	2.28366500
H	-0.25400300	-4.10405700	2.18739400
H	2.19143000	-5.06292700	1.63343500
H	6.70857400	-3.42218700	-0.06190200
H	7.99388900	-1.08883800	-0.41644700
H	3.48079700	1.08263200	-0.84616400
H	-2.05485400	-0.98786900	-0.58518600
H	-3.48083100	1.08249700	0.84597600
H	2.05480300	-0.98797000	0.58515600
H	4.35403900	-4.12405100	0.70554700
H	7.27182100	1.48431200	-0.21124500
H	-1.53075100	4.22946600	1.21790300
H	1.53074300	4.22963300	-1.21778600
H	-4.35399700	-4.12401700	-0.70571400
H	1.42064400	-1.74728500	-1.89346300
H	-1.42059300	-1.74747100	1.89365100
H	-7.27186100	1.48431300	0.21112000
H	-4.05316000	-0.28567300	-0.78874900
H	4.05318100	-0.28572300	0.78874500

SCF Done: E(RM06) = -1978.42096839 A.U. after 19 cycles

5a (Hückel $[38]^{2+}$*T0*^{5,10,25,30})

C	7.62317	-1.26098	-0.14857
C	8.95199	-0.9007	-0.48497
C	9.0548	0.47109	-0.4561
C	7.78807	1.00613	-0.11962
C	7.38795	2.32803	0.04415
C	6.06244	2.75176	0.12227
C	5.53482	3.99784	0.54698
C	4.16363	3.9412	0.46967
C	3.79182	2.6678	-0.04059
C	2.57353	2.0634	-0.34607
C	1.28395	2.55404	-0.17141
C	0.78202	3.7736	0.36342

C	-0.58689	3.73593	0.32799
C	-0.9918	2.48931	-0.2279
C	-2.25621	1.94057	-0.41701
C	-3.46929	2.62647	-0.33843
N	-4.67193	1.95245	-0.22917
C	-5.72508	2.84779	-0.15105
C	-7.0668	2.52937	0.04265
C	-7.62317	1.26098	0.14851
C	-8.95199	0.90072	0.48492
C	-9.0548	-0.47107	0.45611
C	-7.78807	-1.00614	0.11968
C	-7.38795	-2.32804	-0.04403
C	-6.06244	-2.75178	-0.12213
C	-5.53483	-3.99788	-0.54679
C	-4.16364	-3.94124	-0.4695
C	-3.79182	-2.66782	0.04072
C	-2.57352	-2.06342	0.34616
C	-1.28395	-2.55403	0.17144
C	-0.78202	-3.77353	-0.36353
C	0.58689	-3.73585	-0.32813
C	0.99181	-2.48928	0.22788
C	2.25622	-1.94057	0.41702
C	3.46929	-2.62647	0.33836
N	4.67193	-1.95245	0.22913
C	5.72507	-2.8478	0.15092
C	7.0668	-2.52938	-0.04277
N	6.91313	-0.07434	0.02719
N	4.97267	1.95938	-0.20183
N	0.17186	1.79411	-0.49145
C	-3.79041	4.00887	-0.40477
C	-5.15315	4.13975	-0.29612
N	-6.91312	0.07434	-0.02718
N	-4.97267	-1.9594	0.20195
N	-0.17186	-1.79411	0.49151
C	3.7904	-4.00888	0.40459
C	5.15313	-4.13976	0.29591
H	6.21564	-0.01306	0.76245
H	-6.21563	0.01302	-0.76243
H	-0.20687	-0.9504	1.04821
H	0.20689	0.95031	-1.04802
H	-7.74835	3.37007	0.14476
H	-8.16296	-3.08598	-0.12048
H	-2.64153	-1.0534	0.75995
H	2.30582	-0.87296	0.64563
H	7.74834	-3.37007	-0.14494
H	8.16295	3.08597	0.12063
H	2.64153	1.05337	-0.75982
H	-2.3058	0.87294	-0.64553
H	-6.1335	-4.82546	-0.90616
H	-3.48215	-4.73234	-0.74942
H	-1.38455	-4.57446	-0.7685
H	1.26179	-4.48468	-0.7212
H	3.07884	-4.80188	0.59348
H	5.72891	-5.05538	0.34854
H	9.72955	-1.60824	-0.74496
H	9.929	1.06568	-0.6897
H	6.13349	4.8254	0.90638
H	3.48214	4.73228	0.74964
H	1.38455	4.57459	0.76829
H	-1.2618	4.48481	0.72097

H	-3.07885	4.80186	-0.5937
H	-5.72893	5.05536	-0.34882
H	-9.72955	1.60826	0.74486
H	-9.92901	-1.06566	0.68973
H	5.06723	1.19967	-0.86438
H	-5.06723	-1.19966	0.86446
H	4.72358	-1.00548	-0.11522
H	-4.72357	1.00551	0.11524

SCF Done: E(RM06) = -1979.63837571 A.U. after 8 cycles

5b (Hückel $[38]^{2+}TO^{B,C,E,F,H}$)

C	5.16773	3.93505	-0.17192
C	5.62692	5.28035	-0.3073
C	4.54029	6.10437	-0.36331
C	3.36072	5.30637	-0.2483
C	2.05225	5.76836	-0.20234
C	0.89513	4.98778	-0.17803
C	0.70811	3.59166	-0.40256
C	-0.62178	3.30394	-0.25924
C	-1.31583	4.50819	0.05793
C	-2.67624	4.70278	0.25315
C	-3.53487	3.63525	0.55498
C	-3.22079	2.39798	1.15859
C	-4.36946	1.63798	1.20941
C	-5.42736	2.38904	0.63969
C	-6.77058	2.0143	0.40196
C	-7.15374	0.70233	0.21158
N	-6.26907	-0.34599	0.09487
C	-6.91647	-1.53818	-0.11283
C	-6.27534	-2.75136	-0.28787
C	-4.88016	-2.87614	-0.45029
C	-3.92108	-1.90602	-0.85479
C	-2.67637	-2.48059	-0.8165
C	-2.81466	-3.83044	-0.40676
C	-1.84409	-4.79257	-0.12787
C	-0.47746	-4.63791	-0.35364
C	0.23951	-3.71188	-1.15699
C	1.58344	-3.91074	-0.96002
C	1.74589	-4.98565	-0.04288
C	2.92269	-5.56557	0.4563
C	4.15165	-4.9319	0.48971
C	5.42833	-5.49786	0.79998
C	6.35872	-4.50214	0.76399
C	5.69869	-3.27016	0.45183
C	6.26793	-2.01815	0.4003
C	5.64412	-0.79647	0.08035
N	6.2907	0.4058	0.24945
C	5.48667	1.46274	-0.10901
C	5.93492	2.79645	-0.0674
N	3.77852	3.99277	-0.17258
N	-0.35695	5.50482	0.05755
N	-4.89648	3.61517	0.31504
C	-8.46035	0.12243	0.06017
C	-8.31938	-1.2242	-0.10577
N	-4.17347	-4.02845	-0.2192
N	0.48369	-5.42783	0.25749
N	4.36498	-3.5866	0.24805
C	4.37019	-0.48064	-0.44622

C	4.27267	0.8944	-0.55563
H	-9.38437	0.68551	0.09612
H	-4.48766	0.69847	1.73583
H	-2.26248	2.16119	1.6018
H	-1.1085	2.35734	-0.45232
H	1.47215	2.91162	-0.75516
H	4.53374	7.17991	-0.4874
H	6.67027	5.56016	-0.38392
H	3.46143	1.44632	-1.01372
H	-5.38978	4.31801	-0.21894
H	3.21469	3.264	0.24169
H	-9.10691	-1.95325	-0.24895
H	-4.14337	-0.90999	-1.21466
H	-1.74079	-1.9858	-1.03117
H	-0.20878	-3.04412	-1.87996
H	2.39516	-3.44304	-1.50389
H	5.59451	-6.54962	0.9955
H	7.4255	-4.59166	0.92802
H	3.63545	-1.19562	-0.79432
H	-4.58639	-4.88953	0.11179
H	3.62191	-2.90675	0.32538
H	7.32423	-1.97941	0.66208
H	7.00476	2.96145	0.05243
H	1.93778	6.85014	-0.17057
H	-3.0876	5.70791	0.16041
H	-7.53403	2.78373	0.31177
H	-6.88822	-3.64969	-0.26518
H	2.88029	-6.57506	0.85986
H	-2.17177	-5.71351	0.35628
H	-0.52832	6.46085	0.33687
H	0.28404	-6.12062	0.96595
H	7.2076	0.50354	0.66379
H	-5.27158	-0.24943	0.1855

SCF Done: E(RM06) = -1979.64498137 A.U. after 7 cycles

5c (Hückel $[38]^{2+}$*T0*^{5,20,25,B,F})

C	6.29995	2.13376	0.18737
C	6.50485	3.30092	0.9822
C	5.28502	3.81924	1.31174
C	4.26831	3.00356	0.72804
C	2.90468	3.19604	0.77062
C	1.92066	2.31777	0.28022
C	2.00578	0.98762	-0.19663
C	0.73633	0.56901	-0.52709
C	-0.16817	1.61865	-0.26027
C	-1.55055	1.5309	-0.45962
C	-2.59525	2.41582	-0.27854
C	-2.74085	3.74629	0.21079
C	-4.06054	4.1113	0.10923
C	-4.79804	3.0144	-0.42461
C	-6.1598	2.89528	-0.70619
C	-6.78904	1.67597	-0.96842
N	-6.20451	0.46184	-0.72113
C	-6.98842	-0.58288	-1.18632
C	-6.56886	-1.8979	-1.17896
C	-5.39946	-2.3355	-0.51195
C	-4.44877	-3.30613	-0.86679
C	-3.37563	-3.20997	0.01457

C	-3.68059	-2.22792	0.97559
C	-3.05512	-1.82074	2.1755
C	-1.73296	-1.91604	2.52874
C	-1.17292	-1.56915	3.8018
C	0.17932	-1.672	3.71963
C	0.52623	-2.0715	2.38681
C	1.8069	-2.13288	1.8814
C	2.21246	-2.50154	0.58879
C	1.55935	-3.19605	-0.45659
C	2.46915	-3.40194	-1.47711
C	3.68929	-2.79372	-1.11808
C	4.86149	-2.69027	-1.86956
C	5.88803	-1.77205	-1.70411
N	5.83557	-0.63739	-0.90681
C	7.00104	0.0819	-1.01941
C	7.24636	1.31493	-0.396
N	4.91896	1.94932	0.08789
N	0.58454	2.6604	0.23228
N	-3.88242	1.99716	-0.61653
C	-8.05375	1.38959	-1.57388
C	-8.15773	0.0341	-1.73515
N	-4.8976	-1.68907	0.60844
N	-0.66644	-2.27652	1.71542
N	3.49236	-2.228	0.13866
C	7.15696	-1.74557	-2.34325
C	7.84464	-0.64245	-1.90241
H	4.25361	-2.079	0.79003
H	4.52858	1.58391	-0.77381
H	-4.01692	1.30409	-1.34266
H	-5.49129	-1.19471	1.26357
H	7.49843	-2.49485	-3.04648
H	8.83806	-0.32584	-2.193
H	2.29406	-3.91072	-2.41703
H	0.54877	-3.58396	-0.41907
H	7.47834	3.66856	1.28161
H	5.08728	4.68701	1.92901
H	-1.95144	4.36068	0.62526
H	-4.50171	5.05073	0.41774
H	-8.76312	2.14285	-1.89186
H	-8.97477	-0.50814	-2.19432
H	-2.49437	-3.84042	0.02498
H	-4.5339	-3.96942	-1.71829
H	2.89829	0.37813	-0.23722
H	0.45506	-0.39883	-0.92723
H	4.96741	-3.38467	-2.7003
H	8.27537	1.66458	-0.3919
H	2.57156	4.12416	1.23209
H	2.58404	-1.79653	2.56633
H	0.90627	-1.49207	4.50178
H	-1.76516	-1.29289	4.66536
H	-7.12005	-2.61499	-1.78189
H	-3.69148	-1.34151	2.9192
H	-6.75865	3.8006	-0.73606
H	-1.84834	0.55213	-0.84123
H	0.23523	3.57679	0.46993
H	-0.74058	-2.30375	0.7085
H	5.08234	-0.39261	-0.28129
H	-5.33633	0.34128	-0.22189

SCF Done: E(RM06) = -1979.63325195 A.U. after 7 cycles

5d (Hückel $[38]^{2+}$*T0*^{20,25,B,F})

C	5.56619	2.58911	-0.51752
C	5.90571	3.77787	0.19462
C	4.78593	4.2409	0.81125
C	3.68391	3.39343	0.4711
C	2.38692	3.67681	0.81856
C	1.13896	3.073	0.54469
C	0.69542	1.87539	-0.05445
C	-0.69546	1.87538	-0.05444
C	-1.13901	3.07299	0.5447
C	-2.38697	3.6768	0.81857
C	-3.68396	3.3934	0.47111
C	-4.78599	4.24087	0.81126
C	-5.90576	3.77783	0.19463
C	-5.56623	2.58907	-0.51751
C	-6.44399	1.83521	-1.27445
C	-6.31132	0.52273	-1.73711
N	-5.37765	-0.39239	-1.3243
C	-5.57701	-1.60804	-1.97249
C	-4.84656	-2.76181	-1.77445
C	-3.91017	-3.00597	-0.7616
C	-2.86459	-3.94298	-0.75232
C	-2.11676	-3.7473	0.39767
C	-2.72512	-2.72187	1.15177
C	-2.40463	-2.20088	2.42932
C	-1.13504	-2.19217	2.95042
C	-0.68001	-1.69412	4.22056
C	0.68004	-1.69412	4.22056
C	1.13508	-2.19218	2.95043
C	2.40467	-2.2009	2.42933
C	2.72516	-2.72189	1.15179
C	2.11681	-3.74732	0.39768
C	2.86465	-3.94298	-0.75232
C	3.91022	-3.00596	-0.76159
C	4.8466	-2.76179	-1.77444
C	5.57703	-1.608	-1.97249
N	5.37765	-0.39235	-1.32431
C	6.3113	0.52277	-1.73712
C	6.44396	1.83526	-1.27446
N	4.21066	2.34359	-0.28981
N	-0.00003	3.75037	0.90737
N	-4.2107	2.34356	-0.2898
C	-7.14833	-0.13814	-2.68022
C	-6.68216	-1.41362	-2.84794
N	-3.79503	-2.26782	0.41144
N	0.00002	-2.55933	2.25125
N	3.79508	-2.26783	0.41147
C	6.68217	-1.41357	-2.84794
C	7.14832	-0.13808	-2.68022
H	4.56794	-1.76461	0.82835
H	3.64938	1.88867	-0.99905
H	-3.64941	1.88864	-0.99904
H	-4.56789	-1.76459	0.82832
H	7.08248	-2.18206	-3.49742
H	7.988	0.33038	-3.17738
H	2.6806	-4.66263	-1.54027
H	1.27793	-4.34586	0.72951
H	6.90762	4.18524	0.24381

H	4.69953	5.10663	1.45666
H	-4.69959	5.1066	1.45668
H	-6.90768	4.18518	0.24382
H	-7.98801	0.33031	-3.17737
H	-7.08245	-2.18211	-3.49743
H	-1.27787	-4.34584	0.72951
H	-2.68053	-4.66263	-1.54028
H	1.33182	1.07713	-0.41588
H	-1.33186	1.07711	-0.41586
H	4.9994	-3.56049	-2.4972
H	7.39067	2.31678	-1.50825
H	2.3119	4.60191	1.39104
H	3.18547	-1.71478	3.01089
H	1.3391	-1.38136	5.02082
H	-1.33907	-1.38134	5.02081
H	-4.99936	-3.56051	-2.49721
H	-3.18543	-1.71476	3.01086
H	-7.39071	2.31671	-1.50824
H	-2.31196	4.6019	1.39104
H	-0.00003	4.68054	1.30328
H	0.00002	-2.66009	1.24444
H	4.64085	-0.20271	-0.66091
H	-4.64086	-0.20274	-0.6609

SCF Done: E(RM06) = -1979.62877659 A.U. after 7 cycles

5e (Möbius $[38]^{2+}$*T1*^{B,C,E,H})

C	7.16154	0.32585	0.15993
C	8.40823	-0.4089	0.20906
C	8.17192	-1.68322	-0.18231
C	6.76085	-1.82351	-0.47782
C	6.05596	-2.97131	-0.72994
C	4.64481	-2.99985	-0.90238
C	3.7463	-1.98373	-1.30862
C	2.46083	-2.48099	-1.20852
C	2.53452	-3.80983	-0.74433
C	1.50889	-4.71484	-0.45061
C	0.21553	-4.32293	-0.13887
C	-0.26816	-3.06008	0.29312
C	-1.61572	-3.16624	0.5311
C	-2.01511	-4.50557	0.25113
C	-3.27573	-5.12819	0.32204
C	-4.48876	-4.48238	0.43576
N	-4.70734	-3.12393	0.44045
C	-6.0769	-2.85479	0.42499
C	-6.63246	-1.6168	0.31539
C	-5.89088	-0.39369	0.34732
C	-4.70519	-0.06344	1.0164
C	-4.41128	1.27198	0.73734
C	-5.40177	1.7671	-0.12308
C	-5.54853	2.99151	-0.82873
C	-4.59273	3.94756	-1.02588
C	-4.66743	5.09603	-1.88429
C	-3.43095	5.65873	-1.97037
C	-2.54189	4.9164	-1.12347
C	-1.17844	5.08634	-0.9323
C	-0.46895	4.54795	0.1518
C	-0.93752	4.22961	1.46753
C	0.15071	3.97069	2.25519

C	1.31923	4.00901	1.44106
C	2.58581	3.6025	1.79199
C	3.60063	3.16068	0.91914
N	4.86977	2.82608	1.36514
C	5.55286	2.14228	0.40304
C	6.86935	1.58504	0.58466
N	6.21823	-0.56304	-0.34433
N	3.88641	-4.10346	-0.62833
N	-0.88107	-5.17566	-0.11157
C	-5.78753	-5.10447	0.52276
C	-6.7343	-4.13402	0.50409
N	-6.30358	0.73873	-0.30334
N	-3.28982	3.92466	-0.53421
N	0.88595	4.36698	0.16686
C	3.51688	2.69984	-0.40587
C	4.71103	2.0608	-0.71774
H	1.54757	-1.99435	-1.52566
H	5.22783	-0.41323	-0.20211
H	-0.87502	-6.12706	-0.45309
H	-4.19309	-0.70931	1.71942
H	-7.80857	-4.25905	0.56018
H	-5.57579	5.42737	-2.37275
H	4.99255	1.61571	-1.66422
H	8.88749	-2.49254	-0.2589
H	-5.9388	-6.17471	0.5876
H	-1.97026	4.30882	1.78381
H	4.03615	-1.03658	-1.74593
H	-2.24395	-2.40786	0.97955
H	-3.14053	6.53336	-2.53801
H	-3.61442	1.84785	1.19257
H	0.36296	-2.20385	0.49203
H	2.64045	2.76309	-1.03783
H	0.15501	3.73238	3.31209
H	9.3543	0.02367	0.50964
H	6.60038	-3.91192	-0.69719
H	1.74196	-5.7809	-0.44997
H	-3.3146	-6.21267	0.24814
H	-7.71115	-1.56669	0.17862
H	-6.49147	3.15585	-1.34828
H	-0.64465	5.69267	-1.66078
H	2.77015	3.51642	2.86288
H	7.63504	2.15272	1.10785
H	-7.08742	0.77412	-0.94115
H	1.50284	4.65169	-0.58174
H	4.25357	-4.94367	-0.20213
H	-2.86429	3.0869	-0.16372
H	-4.03995	-2.45489	0.08097
H	5.22187	3.00755	2.29527

SCF Done: E(RM06) = -1979.63108000 A.U. after 9 cycles

5f (Möbius $[38]^{2+}$*T1*^{B,C,F})

C	7.51937	0.39255	-0.38933
C	8.35695	1.23579	-1.19599
C	7.58957	2.23064	-1.71918
C	6.23657	2.04741	-1.27607
C	5.13751	2.83163	-1.48
C	3.8212	2.47808	-1.06571
C	3.25205	1.2162	-0.82643

C	1.92323	1.39799	-0.46272
C	1.65457	2.77229	-0.47951
C	0.48913	3.50711	-0.13836
C	-0.7752	2.99799	-0.00964
C	-1.3271	1.72003	-0.37108
C	-2.65375	1.71874	-0.07486
C	-3.0029	2.99696	0.49697
C	-4.20015	3.5107	0.95942
C	-5.43906	2.86482	1.05573
N	-5.70294	1.53384	0.81908
C	-7.05997	1.27923	1.07259
C	-7.71882	0.08578	0.8813
C	-7.27735	-1.09553	0.27437
C	-8.02117	-2.26806	0.08384
C	-7.27815	-3.13439	-0.70742
C	-6.05902	-2.51342	-0.99311
C	-4.99462	-2.99292	-1.81247
C	-3.66507	-2.73563	-1.67283
C	-2.60787	-3.22561	-2.52341
C	-1.4165	-2.91493	-1.96668
C	-1.65459	-2.2259	-0.7154
C	-0.78065	-1.89026	0.27677
C	0.64307	-2.06128	0.20653
C	1.53827	-2.01756	-0.87306
C	2.82684	-2.19498	-0.37175
C	2.7407	-2.35304	1.01976
C	3.72596	-2.65503	1.98972
C	5.06589	-2.37692	1.89924
N	5.65978	-1.55846	0.94032
C	7.00966	-1.47195	1.15294
C	7.8924	-0.66267	0.42462
N	6.23135	0.87464	-0.51498
N	2.82402	3.39731	-0.85585
N	-1.84413	3.72842	0.49283
C	-6.66713	3.48326	1.41112
C	-7.64181	2.52047	1.43695
N	-6.04089	-1.29099	-0.34679
N	-3.03786	-2.04096	-0.63482
N	1.39562	-2.26767	1.33059
C	6.12544	-2.80089	2.75911
C	7.301	-2.28732	2.28969
H	-0.77934	0.92372	-0.86048
H	-0.43723	-3.18586	-2.33769
H	-2.78422	-3.76977	-3.44331
H	-7.55634	-4.12758	-1.03483
H	-9.00524	-2.44323	0.50099
H	-8.69685	2.65865	1.63991
H	-6.78087	4.54271	1.60147
H	1.23065	0.61529	-0.17835
H	7.90967	3.02689	-2.37998
H	9.41765	1.0751	-1.34143
H	8.28969	-2.40428	2.7142
H	5.98511	-3.43071	3.62899
H	1.26756	-1.83645	-1.90542
H	-1.76675	4.65952	0.8767
H	1.01558	-2.36812	2.2616
H	8.95518	-0.83533	0.56667
H	-8.7597	0.07472	1.19957
H	-4.20732	4.55413	1.26892
H	0.61854	4.57319	0.05441

H	5.29311	3.79017	-1.97163
H	-1.18847	-1.5181	1.21814
H	3.40571	-3.15746	2.90233
H	-5.27205	-3.68905	-2.60046
H	3.74156	0.2661	-0.995
H	-3.34817	0.92105	-0.30982
H	5.55696	0.7723	0.23561
H	-5.51665	-0.51731	-0.73986
H	3.72833	-2.30189	-0.96499
H	2.93918	4.39767	-0.94456
H	-3.49753	-1.94449	0.26227
H	-4.99774	0.82429	0.96413
H	5.19412	-1.23514	0.10527

SCF Done: E(RM06) = -1979.63647973 A.U. after 10 cycles

5g (Twisted-Hückel $[38]^{2+}$*T2*^{B,F})

C	-6.29652	1.884	1.14427
C	-6.2562	3.26815	1.44569
C	-4.94946	3.62505	1.66492
C	-4.13573	2.46611	1.5542
C	-2.76427	2.39849	1.74512
C	-1.91145	1.29549	1.64679
C	-2.12234	-0.0836	1.35839
C	-0.9183	-0.739	1.44684
C	0.08997	0.20921	1.77176
C	1.47607	0.10315	1.89052
C	2.22472	-1.06861	1.87663
C	1.86522	-2.4395	1.99348
C	3.01161	-3.1961	1.97507
C	4.12146	-2.33265	1.79228
C	5.45321	-2.67848	1.58883
C	6.4265	-1.87005	1.00605
N	6.16823	-0.66494	0.38896
C	7.3262	-0.1185	-0.11593
C	7.38772	1.11479	-0.76637
C	6.29652	1.88394	-1.14436
C	6.2562	3.26808	-1.44583
C	4.94945	3.62498	-1.66505
C	4.13573	2.46605	-1.55427
C	2.76427	2.39842	-1.74518
C	1.91146	1.29541	-1.64679
C	2.12239	-0.08367	-1.35836
C	0.91834	-0.73908	-1.44671
C	-0.08994	0.20909	-1.77172
C	-1.47604	0.10301	-1.89049
C	-2.2247	-1.06874	-1.87657
C	-1.86524	-2.43964	-1.99341
C	-3.01164	-3.19623	-1.97495
C	-4.12147	-2.33274	-1.79222
C	-5.45324	-2.67855	-1.58876
C	-6.42652	-1.87008	-1.00602
N	-6.16824	-0.66495	-0.38898
C	-7.32621	-0.11848	0.1159
C	-7.38772	1.11483	0.7663
N	-4.97464	1.4155	1.19149
N	-0.5576	1.42191	1.87174
N	3.60679	-1.04194	1.72715
C	7.82303	-2.09818	0.8654

C	8.37182	-1.0261	0.20553
N	4.97464	1.41545	-1.19153
N	0.55761	1.4218	-1.87174
N	-3.60678	-1.04204	-1.72713
C	-7.82305	-2.09819	-0.86538
C	-8.37184	-1.02608	-0.20554
H	0.85873	-2.81055	2.13097
H	3.08479	-4.27461	2.04229
H	8.33979	-2.97102	1.24369
H	9.41169	-0.87782	-0.05624
H	7.12129	3.91935	-1.43573
H	4.56951	4.61727	-1.87517
H	3.06191	-0.54226	-1.07416
H	0.75084	-1.78692	-1.23581
H	-0.85877	-2.81072	-2.13091
H	-3.08485	-4.27473	-2.04214
H	-8.33982	-2.97103	-1.24365
H	-9.4117	-0.87779	0.05624
H	-7.12129	3.91942	1.43556
H	-4.56952	4.61734	1.87501
H	4.14512	-0.23453	2.01716
H	4.80004	0.49056	-1.56888
H	-4.14509	-0.23464	-2.01718
H	-4.80005	0.49063	1.56888
H	-5.74682	-3.69116	-1.85372
H	-8.37547	1.53356	0.94104
H	-2.30258	3.34604	2.02113
H	2.0344	1.04058	1.92797
H	5.74677	-3.69109	1.85381
H	8.37547	1.5335	-0.94114
H	-2.03437	1.04044	-1.92798
H	2.30257	3.34595	-2.02122
H	-3.06185	-0.54223	1.07418
H	-0.75077	-1.78686	1.23601
H	-0.1168	2.27417	2.18807
H	0.11679	2.27404	-2.18811
H	-5.26375	-0.22328	-0.32485
H	5.26374	-0.22326	0.32482

SCF Done: E(RM06) = -1979.64782513 A.U. after 7 cycles

5h (Twisted-Hückel $[38]^{2+}$*T2*^{C,G})

C	7.30984	0.0081	0.10072
C	8.37455	-0.63506	0.77528
C	7.86782	-1.71423	1.46792
C	6.4688	-1.74723	1.27395
C	5.49717	-2.61089	1.77683
C	4.1367	-2.32073	1.81775
C	3.03754	-3.17975	2.08701
C	1.88299	-2.4383	2.0451
C	2.22689	-1.07875	1.78967
C	1.47803	0.09319	1.7541
C	0.08824	0.20301	1.72729
C	-0.94317	-0.75729	1.53648
C	-2.15188	-0.10775	1.55521
C	-1.91877	1.27976	1.78956
C	-2.7884	2.33671	2.06657
C	-4.17281	2.35187	1.94735
N	-4.93506	1.43158	1.24485

C	-6.28438	1.76264	1.34958
C	-7.35155	1.11469	0.74218
C	-7.30985	0.0081	-0.10066
C	-8.37456	-0.63502	-0.77526
C	-7.86782	-1.71412	-1.468
C	-6.46879	-1.7471	-1.27405
C	-5.49715	-2.61071	-1.77702
C	-4.13669	-2.32052	-1.81794
C	-3.03753	-3.1795	-2.08731
C	-1.88299	-2.43804	-2.04535
C	-2.2269	-1.07852	-1.78976
C	-1.47804	0.09342	-1.75409
C	-0.08825	0.20322	-1.72734
C	0.94315	-0.75712	-1.5367
C	2.15186	-0.10759	-1.55538
C	1.91877	1.27996	-1.78952
C	2.78841	2.33693	-2.06639
C	4.17282	2.35207	-1.94715
N	4.93506	1.43172	-1.24472
C	6.28438	1.76277	-1.34939
C	7.35154	1.11477	-0.74203
N	6.14298	-0.66007	0.45843
N	-0.55006	1.41955	1.85608
N	3.59783	-1.0609	1.60882
C	-5.07986	3.26631	2.54674
C	-6.35413	2.8943	2.20659
N	-6.14298	-0.66	-0.45846
N	-3.59783	-1.06071	-1.60886
N	0.55006	1.41977	-1.856
C	5.07989	3.26657	-2.54643
C	6.35415	2.89451	-2.20629
H	-0.78792	-1.81395	1.36144
H	9.40437	-0.30084	0.75174
H	8.41675	-2.39695	2.10414
H	3.12619	-4.24171	2.27962
H	0.88391	-2.80226	2.24298
H	-4.78485	4.07667	3.20145
H	-7.28094	3.3522	2.5291
H	-9.40438	-0.30082	-0.75167
H	-8.41675	-2.39679	-2.10427
H	-3.12617	-4.24144	-2.28004
H	-0.8839	-2.80197	-2.2433
H	0.78789	-1.8138	-1.36179
H	4.78489	4.077	-3.20106
H	7.28097	3.35244	-2.52873
H	-0.08262	2.28065	2.10215
H	0.08262	2.28091	-2.10195
H	-5.82067	-3.56543	-2.18306
H	-8.33556	1.53021	0.94518
H	-2.35186	3.24117	2.48878
H	2.35188	3.24145	-2.48849
H	-2.04002	1.02974	-1.72484
H	8.33554	1.53031	-0.94496
H	5.82069	-3.56565	2.18277
H	2.04001	1.02951	1.72499
H	3.1285	-0.56864	-1.47762
H	5.41114	-0.79637	-0.23014
H	-3.12852	-0.56877	1.47736
H	-5.41111	-0.79632	0.23007
H	4.15976	-0.22407	1.70351

H	-4.15978	-0.22387	-1.70343
H	4.54826	0.95141	-0.44448
H	-4.54829	0.95134	0.44456

SCF Done: E(RM06) = -1979.64484814 A.U. after 7 cycles

5i (Twisted-Hückel $[38]^{2+}T2_{RX}$)

C	-5.303	-2.09145	-0.99202
C	-5.53775	-3.33211	-1.64335
C	-4.33735	-3.84487	-2.05618
C	-3.31436	-2.92795	-1.70149
C	-1.95092	-3.06393	-1.90768
C	-0.97632	-2.07643	-1.77017
C	0.42953	-2.24083	-1.71439
C	1.00415	-0.99903	-1.57573
C	-0.02353	-0.01971	-1.5692
C	-0.00932	1.37188	-1.52206
C	1.07841	2.22825	-1.40293
C	1.02778	3.64692	-1.37862
C	2.31103	4.12744	-1.28283
C	3.19381	3.02176	-1.21852
C	4.58101	3.03067	-1.18805
C	5.4293	1.95511	-0.94648
N	5.04573	0.72585	-0.40235
C	6.18134	-0.06152	-0.23212
C	6.27049	-1.30328	0.38867
C	5.30301	-2.09146	0.99195
C	5.53779	-3.33213	1.64327
C	4.3374	-3.84491	2.05611
C	3.3144	-2.92801	1.70144
C	1.95095	-3.06401	1.90765
C	0.97633	-2.07653	1.77017
C	-0.42951	-2.24095	1.71441
C	-1.00415	-0.99916	1.57576
C	0.02352	-0.01981	1.56924
C	0.00929	1.37177	1.52211
C	-1.07843	2.22815	1.403
C	-1.02778	3.64682	1.3787
C	-2.31103	4.12736	1.28291
C	-3.19382	3.02169	1.21858
C	-4.58102	3.03063	1.18808
C	-5.42932	1.95508	0.94648
N	-5.04574	0.72582	0.40234
C	-6.18135	-0.06154	0.23208
C	-6.2705	-1.30329	-0.38873
N	-3.93751	-1.83521	-1.09222
N	2.40692	1.86935	-1.23441
N	-1.21905	-0.72299	-1.64346
C	6.81933	1.88543	-1.19756
N	1.21905	-0.72308	1.64349
C	7.26945	0.65518	-0.78861
N	3.93751	-1.83527	1.09216
N	-2.40695	1.86927	1.23447
C	-6.81935	1.8854	1.19753
C	-7.26947	0.65515	0.78857
H	-6.52101	-3.76375	-1.78393
H	-4.16611	-4.76703	-2.59722
H	0.93391	-3.19864	-1.75354
H	2.06759	-0.80782	-1.49816

H	0.11069	4.22078	-1.43998
H	2.62735	5.16237	-1.24519
H	7.39317	2.67332	-1.66909
H	8.27728	0.26576	-0.86154
H	6.52106	-3.76375	1.78384
H	4.16619	-4.76707	2.59714
H	-0.93388	-3.19877	1.75355
H	-2.0676	-0.80797	1.49819
H	-0.11069	4.22067	1.44009
H	-2.62733	5.1623	1.24528
H	-7.39319	2.67328	1.66907
H	-8.2773	0.26574	0.86148
H	-3.44123	-1.31223	-0.38083
H	2.78621	1.01463	-1.62095
H	3.44122	-1.3123	0.38077
H	-2.78626	1.01455	1.62098
H	-5.06276	3.98255	1.39915
H	-7.27543	-1.71886	-0.42026
H	1.60535	-4.04679	2.21903
H	-1.60529	-4.04669	-2.21906
H	5.06275	3.98259	-1.39913
H	-0.97351	1.87682	-1.58885
H	0.97348	1.87671	1.58891
H	7.27543	-1.71884	0.42019
H	-2.08003	-0.29718	-1.96339
H	2.08001	-0.29726	1.96341
H	4.27462	0.69307	0.25392
H	-4.27462	0.69304	-0.25392

SCF Done: E(RM06) = -1979.65223320 A.U. after 18 cycles