Supporting Information

Performance of Electronic Structure Methods for the Description of Hückel-Möbius Interconversions in Extended π-Systems

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I. Performance of M06-2X to describe the geometry and relative stability of twisted Hückel topologies as compared to experimental data

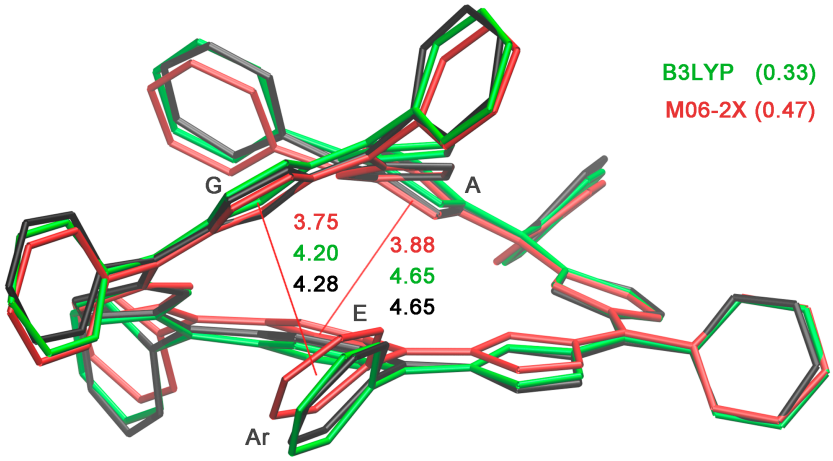

Figure S1. Comparison of B3LYP and M06-2X optimized geometries of the figure-eight conformation of neutral *meso*-C_6F_5-substituted [32]heptaphyrin, overlaid with the X-ray structure. The centroid-centroid distance (in Å) and the RMSDs (in parenthesis) are also shown.

Table S1. Geometrical descriptors of the π-π stacking interactions of the figure-eight conformation of *meso*-C_6F_5-substituted [32]heptaphyrin. Relative energies (in kcal mol^{-1}) of the figure-eight and Möbius conformers in neutral and monoprotonated states.

	$Angle_{A\text{-}E}$	$R_{c\text{-}c}$	$R_{c\text{-}plane}$	$Angle_{G\text{-}Ar}$	$R_{c\text{-}c}$	$R_{c\text{-}plane}$		**32F**	**32M**	**$[32F]^+$**	**$[32M]^+$**
RX	**25.7**	**4.65**	**3.68**	**17.3**	**4.28**	**3.86**		**x**			**x**
B3LYP	16.7	4.65	3.68	22.6	4.50	4.18		**0.00**	5.24	2.83	**0.00**
M06-2x	15.0	3.88	3.15	13.5	3.75	3.49		**0.00**	16.15	**0.00**	6.00

[a] π-π stacking interactions between pyrrole rings A and E and pyrrole ring G and a pentafluorophenyl substituent.

II. Influence of the basis set on the MP2 and DFT relative energies

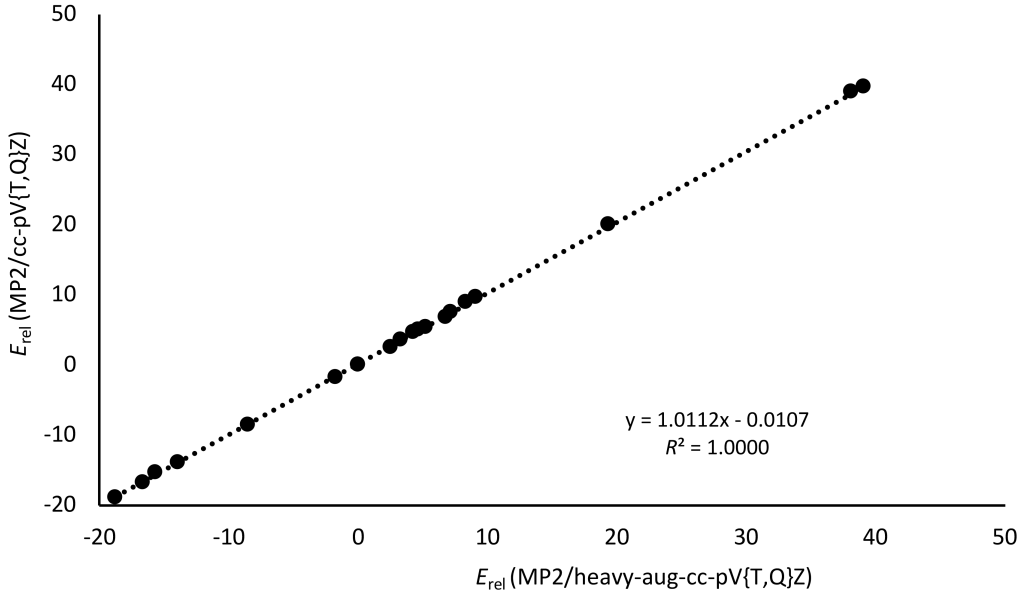

Figure S2. Influence of diffuse functions on the extrapolated MP2 relative energies to the complete basis set limit of our test set. Linear correlation between the extrapolated cc-pV{T,Q}Z and heavy-aug-cc-pV{T,Q}Z relative energies for the 21 porphyrinoid structures.

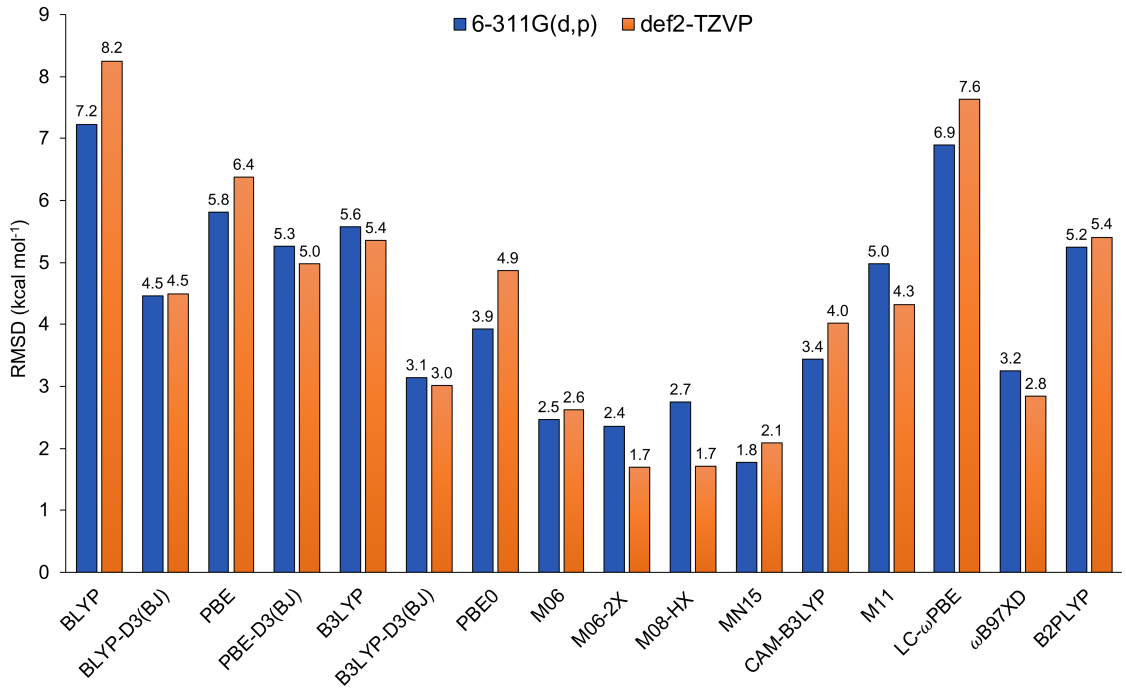

Figure S3. Basis set dependence: root-mean-square deviations (RMSDs in kcal mol^{-1}) for several exchange-correlation functionals over the relative energies of the expanded porphyrin database, relative to canonical CCSD(T)/CBS reference values. For each functional, the statistical errors obtained with the Pople 6-311G(d,p) basis set and the Weigend-Ahlrichs def2-TZVP basis set are shown.

Table S2. Relative energies (in kcal mol^{-1}) for the different minima and TSs involved in the topology interconversion of [32]heptaphyrin computed with B3LYP and B3LYP-D3 together with the reference CCSD(T)/CBS energies.

Basis set	M06-2X	M06-2X-D3(0)	B3LYP-D3(BJ)	BLYP-D3(BJ)
def2-TZVP	1.69	1.51	3.03	4.49
def2-QZVP	1.65	1.53	2.82	4.22

III. The database of Hückel and Möbius expanded porphyrins

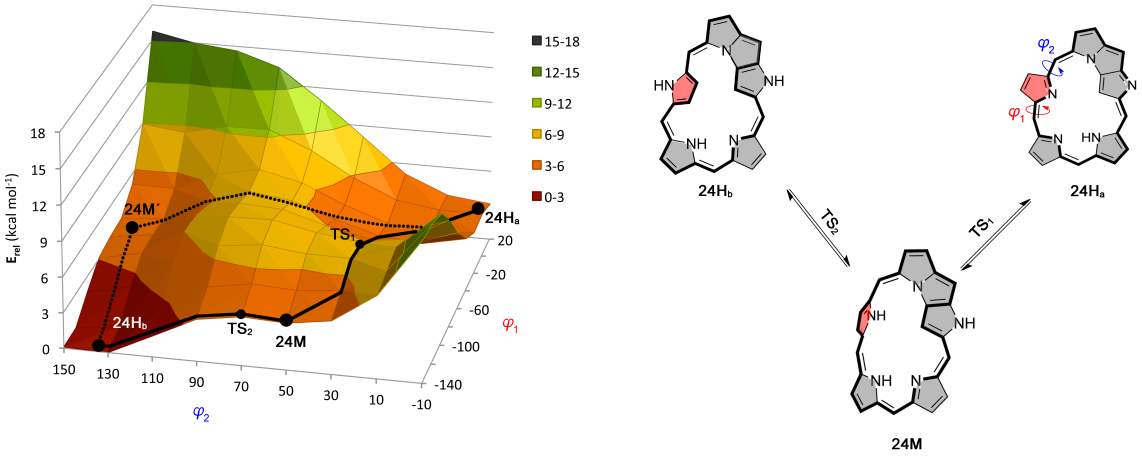

Figure S4. B3LYP/6-31G(d,p) relaxed energy potential surface computed for the Hückel-Möbius interconversions in *N*-fused [24]pentaphyrin together with the schematic geometries of the different minima.

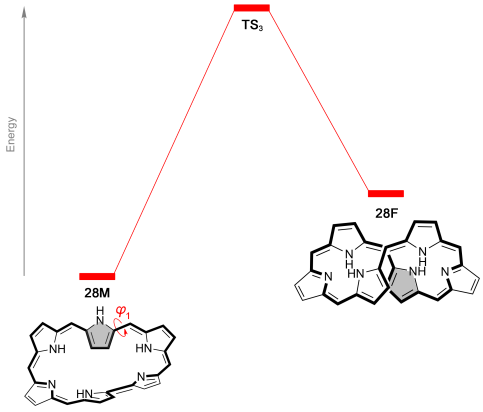

Figure S5. Schematic energetic profile for the Möbius/twisted-Hückel topology interconversion in [28]hexaphyrin.

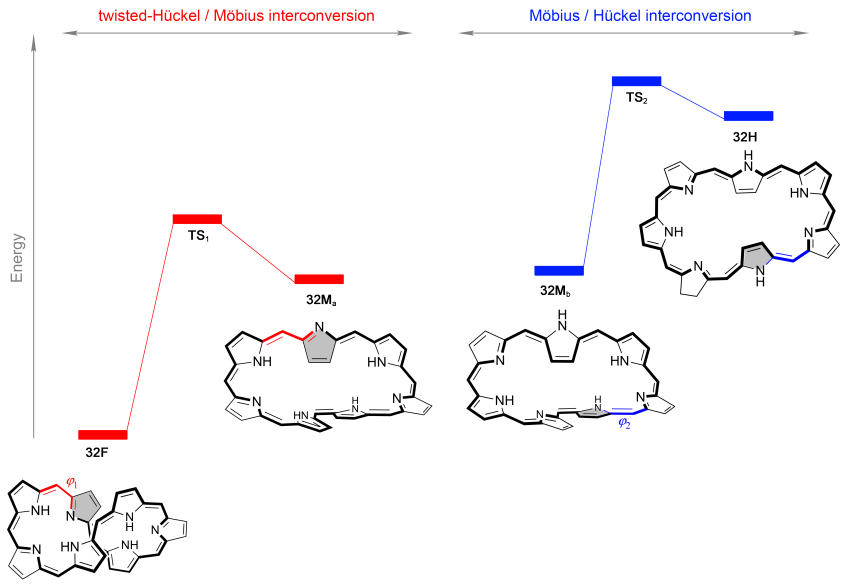

Figure S6. Schematic energetic profile for the three-level topology switching in [32]heptaphyrin, triggered by the rotation of the dihedral angles φ_1 and φ_2.

IV. Diagnostic criteria to assess the suitability of single-reference methods

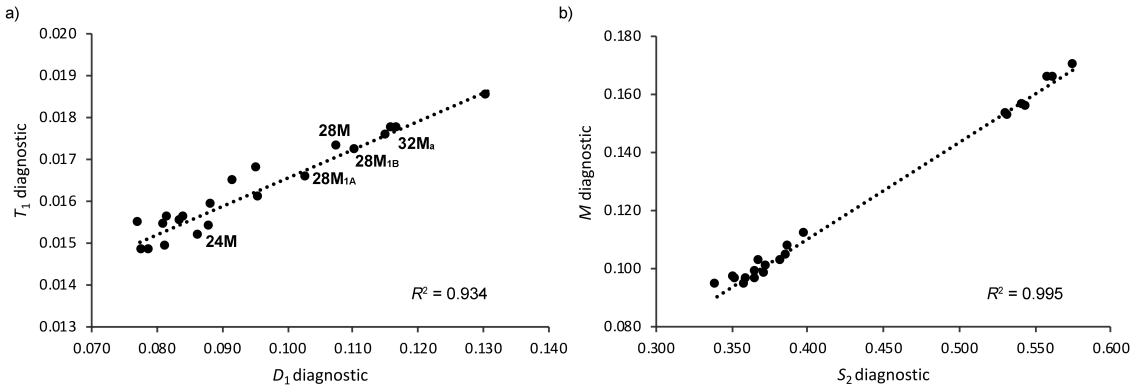

Figure S7. Relationship between several diagnostics for static correlation for our set of 21 expanded porphyrins: a) T_1 vs D_1 diagnostics and b) M vs S_2. Figure 2b shows that the structures are clustered in two groups as a function of the degree of static correlation. The Möbius structures of [26]hexaphyrin and [32]heptaphyrin exhibit the largest values for the M and S_2 diagnostics.

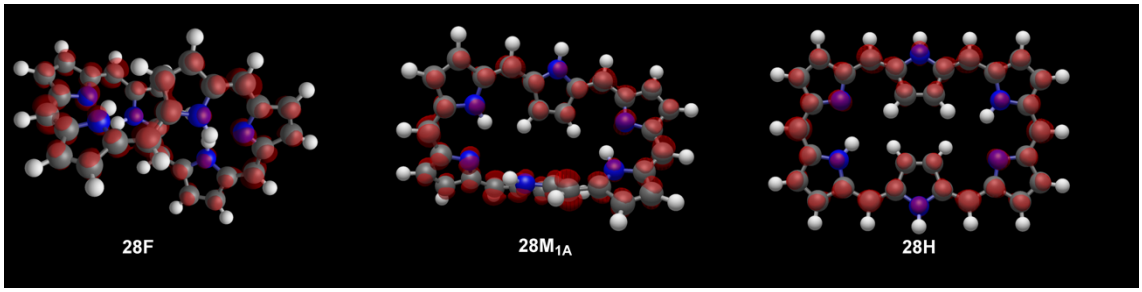

Figure S8. FOD plots at σ=0.005 e Bohr^{-3} [M06-2X/def2-TZVP (T=5000 K) level] for the twisted-Hückel, Möbius and Hückel topologies of [28]hexaphyrin.

V. Comparison between limited orbital space full CI and CCSD(T) calculations

Table S3. Relative energies for Hückel-Möbius interconversions in expanded porphyrins computed with ICE-CI and CCSD(T) methods for different orbital active spaces (in kcal mol^{-1}).

system	CCSD(T)	ICE-CI	CCSD(T)	ICE-CI	CCSD(T)	ICE-CI	CCSD(T)	ICE-CI	CCSD(T)
active space	*all orbitals*	*(12,12)*	*(12,12)*	*(18,18)*	*(18,18)*	*(24,24)*	*(24,24)*	*(30,30)*	*(30,30)*
24H$_a$	9.12	6.79	6.82	-0.53	-0.49	4.84	4.84	4.49	4.36
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24M	6.06	8.12	8.24	4.89	4.96	7.90	7.92	8.40	8.31
24TS$_1$	9.05	6.70	6.71	3.29	3.28	6.68	6.62	6.53	6.38
24TS$_2$	4.87	6.00	6.04	3.08	3.09	5.86	5.83	6.39	6.27
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28M	-0.73	10.88	11.12	8.91	9.09	9.28	9.43	7.62	7.56
28M$_{1A}$	0.46	12.60	12.87	9.91	10.12	10.39	10.54	8.55	8.48
28M$_{1B}$	1.82	13.57	13.82	11.67	11.86	10.98	11.09	11.38	11.34
28F	-0.38	7.41	7.38	9.18	9.12	5.40	5.28	4.70	4.45
28TS$_{1A}$	6.33	13.75	13.77	12.24	12.16	10.82	10.66	14.06	13.92
28TS$_{1B}$	2.86	9.14	9.12	10.02	9.97	8.72	8.60	6.56	6.16
28TS$_{2A}$	6.87	26.41	26.68	28.09	28.31	24.60	24.74	22.21	22.05
28TS$_{2B}$	9.89	30.33	30.57	31.42	31.62	28.31	28.44	26.44	26.30
28TS$_3$	5.17	15.03	15.02	14.55	14.44	13.31	13.15	12.17	11.84
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32M$_a$	16.81	18.35	18.63	10.75	10.99	13.47	13.71	12.55	12.62
32M$_b$	16.74	18.46	18.72	13.85	14.15	15.71	16.03	17.48	17.98
32H	34.60	22.91	22.90	24.75	24.74	24.18	24.17	27.23	27.49
32TS$_1$	17.49	16.64	16.64	10.69	10.67	11.23	11.22	14.13	14.39
32TS$_2$	33.79	24.28	24.22	24.71	24.65	25.40	25.37	27.58	27.74
RMSD[a]	-	0.15		0.14		0.13		0.21	
MUE[a]	-	0.10		0.10		0.09		0.16	

[a] RMSD and MUE (in kcal mol^{-1}) for the relative energies computed with ICE-CI and CCSD(T) methods for different orbital active spaces.

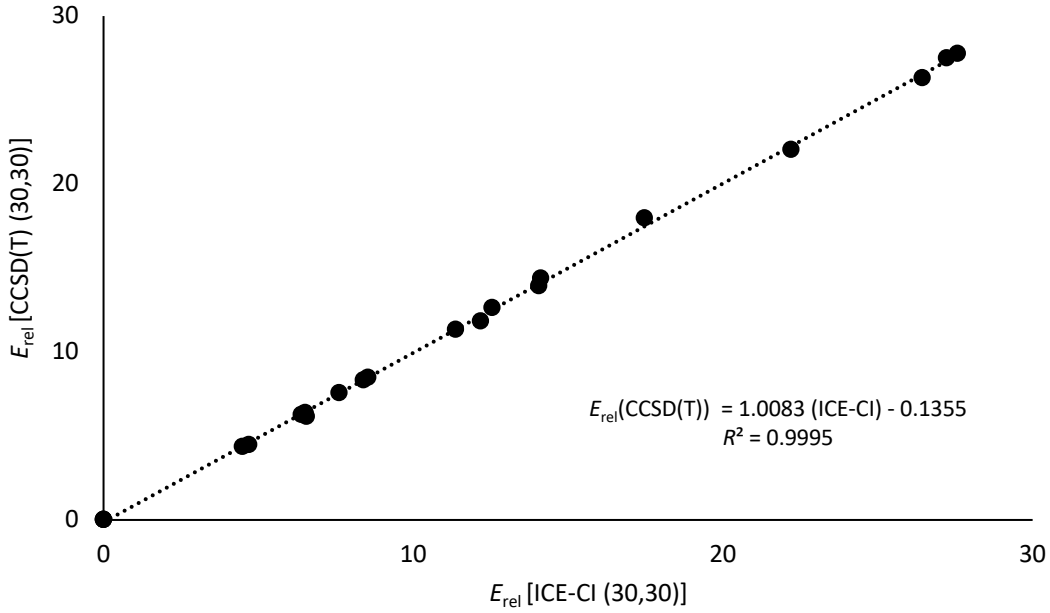

Figure S9. Reliability of the canonical CCSD(T) method for describing the relative energies of topology interconversions in expanded porphyrins. Linear correlation between the relative energies computed with CCSD(T) and the ICE-CI methods for an orbital active space (30,30).

VI. Performance of lower-level wavefunction methods

Table S4. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several coupled cluster approaches. The statistical errors (in kcal mol^{-1}) are computed with respect to canonical CCSD(T)/cc-pVDZ data.[a]

system	CCSD(T)	CCSD	SCS-CCSD	SCS(MI)-CCSD	DCSD	SCS-DCSD
24H$_a$	9.12	9.23	9.95	9.54	9.32	9.45
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00
24M	6.06	8.14	7.46	7.17	7.30	6.71
24TS$_1$	9.05	8.74	8.97	9.07	8.79	8.97
24TS$_2$	4.87	5.60	5.24	5.23	5.25	5.02
28H	0.00	0.00	0.00	0.00	0.00	0.00
28M	-0.73	7.02	4.95	3.28	4.48	2.18
28M$_{1A}$	0.46	9.73	7.42	5.43	6.80	4.17
28M$_{1B}$	1.82	11.10	9.05	6.92	8.29	5.71
28F	-0.38	0.35	-0.76	-0.57	-0.02	-0.51
28TS$_{1A}$	6.33	6.62	6.08	6.26	6.44	6.24
28TS$_{1B}$	2.86	2.76	2.22	2.47	2.68	2.54
28TS$_{2A}$	6.87	17.42	14.11	11.99	13.99	10.72
28TS$_{2B}$	9.89	19.78	16.49	14.59	16.46	13.34
28TS$_3$	5.17	5.69	4.53	4.93	5.28	4.88
32F	0.00	0.00	0.00	0.00	0.00	0.00
32M$_a$	16.81	22.02	21.89	20.56	20.27	21.65
32M$_b$	16.74	24.11	24.07	21.97	21.98	24.07
32H	34.60	31.40	33.25	33.82	32.40	33.84
32TS$_1$	17.49	15.84	16.49	16.91	16.29	- [b]
32TS$_2$	33.79	30.20	31.89	32.71	31.26	32.40
RMSD	-	5.1	3.9	2.8	3.5	2.7
MUE	-	3.5	2.6	1.8	2.3	

[a] The structures highlighted in grey exhibit energy differences larger than 4.0 kcal mol^{-1} with respect to the canonical CCSD(T) energies. [b] The SCS-DCSD calculation crashed twice for the **32TS$_1$** structure after several days.

Table S5. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several second- and third-order MP approaches. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T)/cc-pVDZ data.[a]

system	CCSD(T)	MP2	OO-MP2	SCS-MP2	S2-MP2	SOS-MP2	MP3	SCS-MP3	MP2.5	MP2.X
24H$_a$	9.12	8.53	7.53	8.71	8.73	8.80	8.71	8.75	8.62	8.66
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24M	6.06	3.18	-0.75	5.43	3.69	6.55	8.04	6.64	5.61	6.68
24TS$_1$	9.05	9.49	9.51	8.91	9.35	8.62	8.97	8.78	9.23	9.11
24TS$_2$	4.87	4.17	2.11	4.85	4.30	5.19	5.79	5.26	4.98	5.34
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28M	-0.73	-14.62	-20.44	-4.74	-12.13	0.20	5.48	0.29	-4.57	-0.15
28M$_{1A}$	0.46	-18.75	-19.37	-6.31	-15.59	-0.09	7.16	0.17	-5.79	-0.09
28M$_{1B}$	1.82	-16.34	-17.25	-4.11	-13.16	2.00	8.83	2.18	-3.75	1.78
28F	-0.38	-2.32	-5.18	-0.95	-2.15	-0.27	1.25	-0.06	-0.54	0.25
28TS$_{1A}$	6.33	8.46	1.88	8.31	8.36	8.24	7.96	8.19	8.21	8.10
28TS$_{1B}$	2.86	3.34	-0.64	3.30	3.23	3.28	3.28	3.29	3.31	3.30
28TS$_{2A}$	6.87	-13.34	-17.13	0.67	-9.89	7.67	15.66	7.92	1.16	7.54
28TS$_{2B}$	9.89	-7.58	-14.22	5.13	-4.51	11.48	18.46	11.64	5.44	11.17
28TS$_3$	5.17	5.97	-3.10	6.37	5.89	6.58	7.49	6.75	6.73	7.06
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32M$_a$	16.81	10.16	3.72	15.11	11.55	17.58	19.92	17.55	15.04	17.19
32M$_b$	16.74	4.97	4.05	12.98	7.27	16.99	21.52	17.12	13.24	16.88
32H	34.60	40.76	43.56	35.87	39.66	33.43	30.72	33.36	35.74	33.53
32TS$_1$	17.49	21.11	20.73	18.58	20.49	17.32	15.77	17.25	18.44	17.27
32TS$_2$	33.79	41.01	43.54	35.47	39.68	32.70	29.96	32.71	35.49	33.06
RMSD	-	9.5	12.0	3.0	7.9	**0.8**	4.2	**0.9**	2.8	**0.8**
MUE	-	6.4	8.9	2.0	5.3	**0.6**	3.0	**0.7**	1.9	**0.6**

[a] The structures highlighted in grey exhibit energy differences larger than 4.0 kcal mol^{-1} with respect to the canonical CCSD(T) energies.

Table S6. Breakdown of the reference CCSD(T)/cc-pVDZ relative energies for the expanded porphyrin database into the SCF, CCSD and (T) components. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T)/cc-pVDZ data.

system	SCF	CCSD	CCSD(T)	(T)[a]	MP2	CCSD-MP2	CCSD(T)-MP2
24H$_a$	6.51	9.23	9.12	-0.11	8.53	0.70	0.59
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24M	12.25	8.14	6.06	-2.08	3.18	4.96	2.88
24TS$_1$	7.36	8.74	9.05	0.31	9.49	-0.75	0.45
24TS$_2$	7.48	5.60	4.87	-0.73	4.17	1.43	0.70
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28M	21.32	7.02	-0.73	-7.75	-14.62	21.64	13.89
28M$_{1A}$	25.98	9.73	0.46	-9.28	-18.75	28.49	19.21
28M$_{1B}$	26.35	11.10	1.82	-9.28	-16.34	27.44	18.16
28F	5.55	0.35	-0.38	-0.74	-2.32	2.68	1.94
28TS$_{1A}$	8.94	6.62	6.33	-0.29	8.46	-1.84	2.13
28TS$_{1B}$	4.90	2.76	2.86	0.11	3.34	-0.58	0.47
28TS$_{2A}$	39.01	17.42	6.87	-10.55	-13.34	30.76	20.21
28TS$_{2B}$	40.78	19.78	9.89	-9.89	-7.58	27.36	17.48
28TS$_3$	10.63	5.69	5.17	-0.52	5.97	-0.28	0.81
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32M$_a$	25.71	22.02	16.81	-5.21	10.16	11.85	6.65
32M$_b$	29.12	24.11	16.74	-7.37	4.97	19.14	11.77
32H	20.71	31.40	34.60	3.21	40.76	-9.36	6.16
32TS$_1$	11.63	15.84	17.49	1.64	21.11	-5.26	3.62
32TS$_2$	19.78	30.20	33.79	3.59	41.01	-10.81	7.23
RMSD	14.66	5.14			9.54		

[a] The structures highlighted in grey exhibit energy contributions from the triple excitations (T) larger than 5.0 kcal mol^{-1}.

Table S7. Deviations with respect to canonical CCSD(T)/cc-pVDZ relative energies (in kcal mol^{-1}) for the expanded porphyrin database obtained with DLPNO-CCSD(T) using different settings.

system	CCSD(T)	DLPNO-CCSD(T_1) ORCA	
	canonical	NormalPNO	TightPNO
24H$_a$	9.1	0.8	0.2
24H$_b$	0.0	0.0	0.0
24M	6.1	0.4	0.4
24TS$_1$	9.0	-0.1	-0.1
24TS$_2$	4.9	0.0	0.1
28F	-0.4	-1.5	-1.0
28M	0.5	1.3	1.7
28M$_{1A}$	-0.7	2.1	1.7
28M$_{1B}$	1.8	2.5	1.9
28TS$_3$	5.2	-0.9	-0.4
28R	0.0	0.0	0.0
28TS$_{1A}$	6.3	-0.3	0.1
28TS$_{1B}$	2.9	-0.8	-0.4
28TS$_{2A}$	6.9	1.8	2.2
28TS$_{2B}$	9.9	2.3	2.0
32F	0.0	0.0	0.0
32H	34.6	0.3	0.3
32TS$_2$	33.8	-0.1	0.1
32M$_a$	16.8	4.0	2.5
32M$_b$	16.7	4.7	3.3
32TS$_1$	17.5	0.1	-0.1
MUE		1.14	0.87
RMSD		1.74	1.33
Möbius (-like)		2.73	2.11
Other structures		0.59	0.33

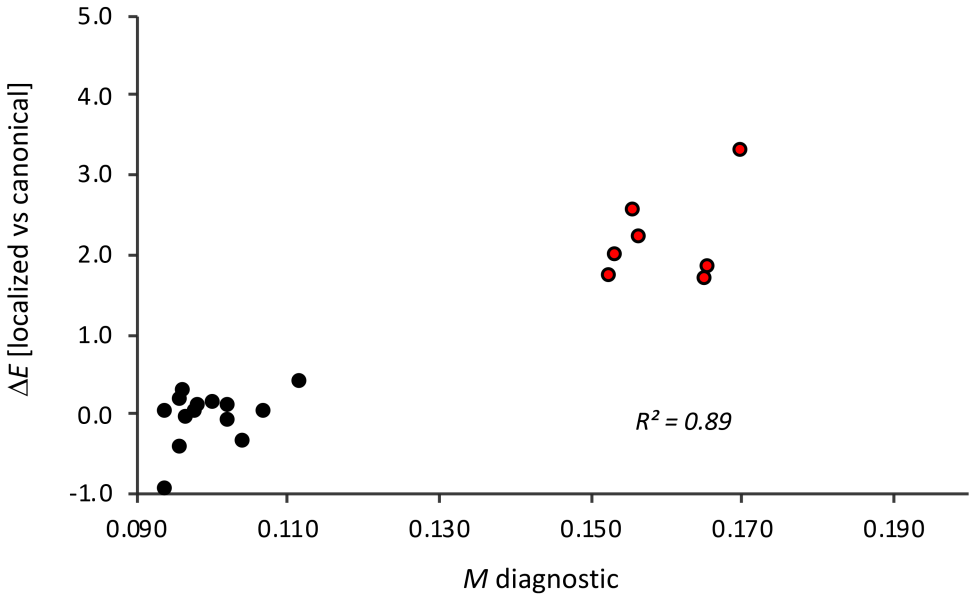

Figure S10. Relationship between the energy differences computed with localized DLPNO-CCSD(T_1) and canonical CCSD(T) methods and the *M* diagnostic for static correlation. The Möbius structures are highlighted in red.

VII. Performance of DFT methods

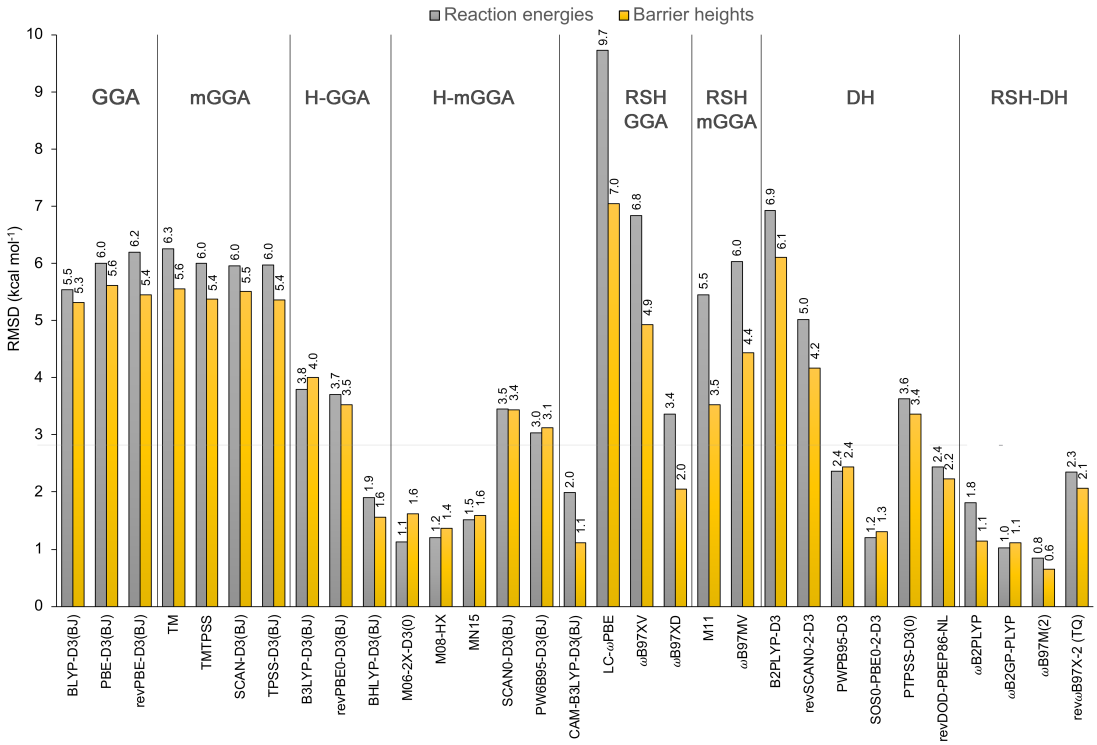

Figure S11. Root-mean-square deviations (RMSDs in kcal mol^{-1}) for DFT methods over the reaction energies and barrier heights of the topology interconversions of the expanded porphyrin database relative to canonical CCSD(T)/CBS reference values.

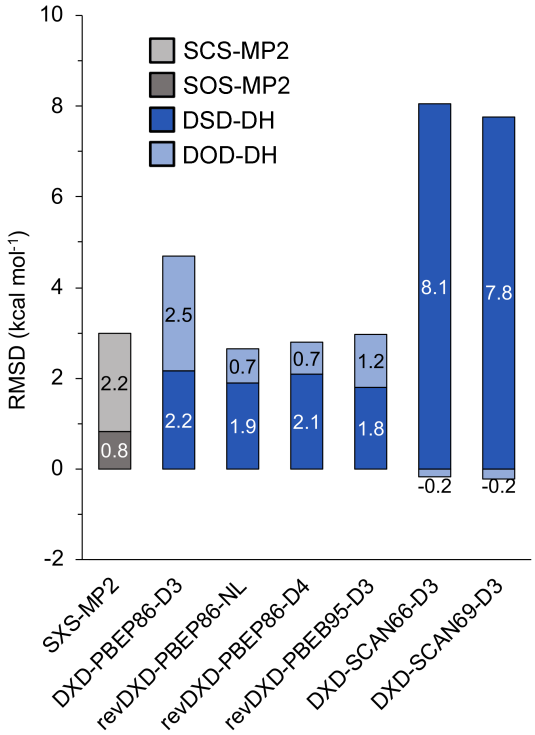

Figure S12. RMSDs values for spin-component (DSD) and spin-opposite (DOD) scaled double hybrids. The errors for SCS-MP2 and SOS-MP2 are also displayed for comparison.

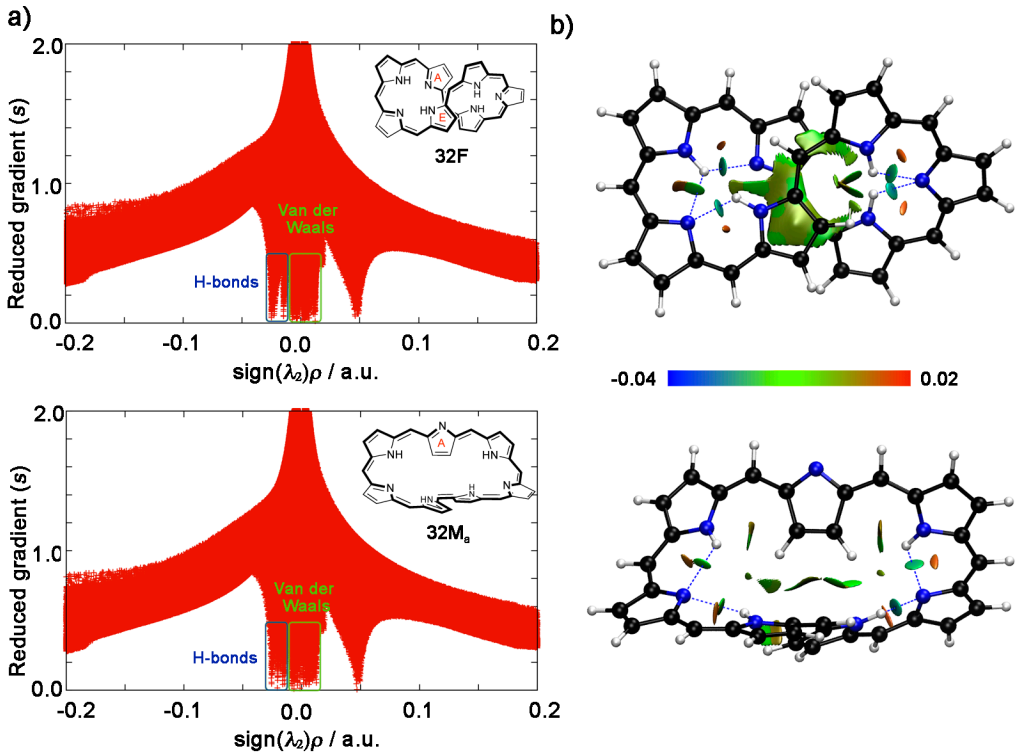

Figure S13. Noncovalent interactions in twisted-Hückel and Möbius topologies of neutral [32]heptaphyrin, as revealed by the NCI method. Reduced density gradient s(ρ)

plots (left) and gradient isosurfaces (s = 0.4 a.u., right) coloured according to values of sign(λ_2)ρ, ranging from -0.04 to 0.02 a.u.

Table S8. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several DFT approaches together with def2-TZVP basis set. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T)/CBS data.[a]

system	BLYP	BLYP-D3	PBE	PBE-D3	revPBE	revPBE-D3	TM	TMTPSS	SCAN	SCAN-D3
24H$_a$	1.53	2.38	5.31	4.33	1.22	4.88	4.55	4.49	4.32	4.97
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24M	2.87	2.06	1.81	1.46	2.31	2.19	2.81	3.05	3.10	2.99
24TS$_1$	5.68	6.65	8.20	7.90	5.42	8.12	8.74	8.67	8.33	8.70
24TS$_2$	4.01	3.81	3.99	3.74	3.31	3.63	4.13	4.28	4.27	4.22
28F	5.67	1.08	3.12	0.26	3.14	1.52	3.30	4.03	3.81	2.96
28M$_{1A}$	-2.20	-6.43	-4.76	-7.12	-3.68	-6.86	-5.83	-5.03	-4.98	-5.75
28M	-3.24	-7.53	-5.85	-8.24	-4.55	-7.94	-7.05	-6.23	-6.24	-7.04
28M$_{1B}$	-0.79	-4.67	-3.13	-5.27	-2.20	-5.12	-4.15	-3.42	-3.41	-4.10
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28TS$_{1A}$	7.84	7.18	7.35	6.94	7.43	7.11	7.78	8.10	7.89	7.71
28TS$_{1B}$	5.45	5.01	5.11	4.80	4.98	4.90	5.34	5.58	5.52	5.35
28TS$_{2A}$	3.72	-1.15	-0.51	-3.19	1.53	-2.59	0.09	2.14	-0.46	-1.37
28TS$_{2B}$	6.56	1.56	2.22	-0.52	4.39	0.26	3.01	5.12	2.49	1.56
28TS$_3$	9.08	7.78	8.28	7.26	8.75	7.08	8.96	9.58	9.39	8.51
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32H	16.47	36.10	23.12	34.13	19.48	32.21	29.56	28.61	28.95	32.43
32M$_a$	-2.92	9.25	0.58	7.39	0.28	5.81	4.17	4.06	4.33	6.14
32M$_b$	-2.83	10.60	1.09	8.62	0.50	7.09	4.98	4.75	4.94	6.97
32TS$_1$	8.61	18.26	11.95	17.14	10.65	16.09	15.96	15.64	15.67	16.99
32TS$_2$	16.95	37.67	24.20	35.71	21.55	33.79	31.40	30.50	30.84	34.07
RMSD	**8.25**	**4.49**	**6.38**	**4.97**	**6.92**	**4.97**	**4.95**	**4.78**	**4.95**	**4.64**
MUE	**5.65**	**3.78**	**4.79**	**3.81**	**5.19**	**3.66**	**3.71**	**3.60**	**3.78**	**3.52**

Table S9. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several DFT approaches together with def2-TZVP basis set. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T)/CBS data.[a]

system	TPSS	TPSS-D3	B3LYP	B3LYP-D3	PBE0	PBE0-D3	revPBE0	revPBE0-D3	BHLYP	BHLYP-D3
24H$_a$	1.61	4.05	2.80	5.90	3.61	5.26	2.74	5.92	4.55	6.85
24H$_b$	0.00	0.00	0.00	0.00	0	0.00	0.00	0.00	0.00	0.00
24M	2.71	2.49	4.51	4.09	4.9	4.43	4.63	4.50	7.69	7.53
24TS$_1$	6.42	8.01	6.48	8.55	7.33	8.36	6.39	8.70	7.38	8.91
24TS$_2$	3.69	3.73	4.51	4.54	4.54	4.55	4.45	4.71	5.93	6.02
28F	2.58	1.11	4.03	1.58	2.70	1.44	3.02	1.51	4.28	2.96
28M$_{1A}$	-4.51	-6.76	-0.89	-3.93	-1.84	-5.15	-0.74	-3.53	5.68	3.63
28M	-5.48	-7.85	-2.17	-5.30	-3.26	-3.66	-2.04	-5.00	3.82	1.66
28M$_{1B}$	-2.90	-4.95	0.54	-2.22	-0.26	-1.92	0.68	-1.87	6.98	5.12
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28TS$_{1A}$	7.60	7.23	7.69	7.14	7.32	6.93	7.42	7.11	7.74	7.42
28TS$_{1B}$	5.16	4.88	4.89	4.49	4.51	4.18	4.50	4.38	4.47	4.25
28TS$_{2A}$	1.14	-1.73	5.99	1.68	3.47	1.22	5.59	2.01	14.41	11.82
28TS$_{2B}$	3.97	1.07	9.09	4.37	6.45	4.15	8.54	4.94	17.54	14.92
28TS$_3$	8.63	6.97	9.73	8.25	8.62	7.12	8.80	7.24	9.90	8.46
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32H	23.07	32.47	21.91	35.60	23.86	32.17	21.04	32.17	22.76	31.11
32M$_a$	1.78	6.34	3.82	11.27	4.29	9.20	4.37	9.25	11.04	14.98
32M$_b$	2.11	7.33	4.00	12.41	4.70	10.04	4.40	10.20	11.28	15.81
32TS$_1$	12.57	16.52	11.90	18.14	12.56	16.30	11.50	16.23	12.51	16.01
32TS$_2$	25.18	34.06	23.50	36.92	24.61	33.08	22.47	33.15	23.51	31.41
RMSD	**6.01**	**4.76**	**5.35**	**3.01**	**4.86**	**3.11**	**5.36**	**2.90**	**5.11**	**2.67**
MUE	**4.65**	**3.56**	**3.61**	**2.56**	**3.48**	**2.31**	**3.56**	**2.18**	**4.17**	**1.95**

Table S10. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several DFT approaches together with def2-TZVP basis set. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T)/CBS data.[a]

system	M06	M06-2X	M06-2X-D3(0)	M08-HX	MN15	SCAN0	SCAN0-D3	PW6B95	PW6B95-D3
24H$_a$	7.91	8.04	7.85	6.19	5.05	5.78	4.15	5.36	7.91
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24M	7.32	7.28	7.93	6.27	5.17	5.05	4.92	4.76	7.32
24TS$_1$	9.48	9.52	10.02	9.23	8.51	8.92	7.84	8.56	9.48
24TS$_2$	5.94	5.90	5.37	5.39	5.11	5.06	4.79	4.74	5.94
28F	2.29	1.63	2.38	3.77	3.45	2.57	3.30	2.19	2.29
28M$_{1A}$	2.45	2.20	1.71	1.15	-1.66	-2.47	-1.11	-2.36	2.45
28M	0.47	0.22	-0.26	-0.56	-3.25	-4.10	-2.59	-3.89	0.47
28M$_{1B}$	4.00	3.78	3.41	2.66	-0.15	-0.89	0.49	-0.64	4.00
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28TS$_{1A}$	6.63	6.57	6.39	7.38	7.66	7.47	7.67	7.40	6.63
28TS$_{1B}$	3.36	3.28	3.33	4.33	4.83	4.65	4.75	4.50	3.36
28TS$_{2A}$	7.90	7.65	8.54	7.60	4.02	3.05	5.86	4.33	7.90
28TS$_{2B}$	10.86	10.60	11.62	10.30	7.03	6.04	8.77	7.21	10.86
28TS$_3$	7.59	7.03	8.14	8.73	9.19	8.25	9.16	7.91	7.59
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32H	30.26	31.69	33.77	29.42	28.29	31.95	25.44	30.91	30.26
32M$_a$	14.22	14.92	16.32	12.38	7.55	9.50	7.01	9.86	14.22
32M$_b$	14.92	15.72	17.11	12.97	7.96	10.11	7.28	10.46	14.92
32TS$_1$	15.72	16.04	18.77	16.09	15.27	16.69	14.18	16.39	15.72
32TS$_2$	34.49	35.76	34.50	30.29	29.56	32.95	26.90	32.00	34.49
RMSD	**1.69**	**1.51**	**1.73**	**2.1**	**3.38**	**2.72**	**3.85**	**2.51**	**1.69**
MUE	**1.40**	**1.19**	**1.40**	**1.60**	**2.46**	**2.03**	**2.66**	**1.90**	**1.40**

Table S11. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several DFT approaches together with def2-TZVP basis set. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T)/CBS data.[a]

system	TPSSh	TPSSh-D3	CAM-B3LYP	CAM-B3LYP-D3	LC-wPBE	CAM-QTP00	CAM-QTP00-D3	CAM-QTP01	CAM-QTP01-D3
24H$_a$	2.21	4.59	5.14	6.96	6.48	6.69	8.00	7.08	7.93
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24M	3.59	3.35	7.32	7.09	12.05	10.10	9.90	9.24	9.10
24TS$_1$	6.75	8.27	7.28	8.39	7.80	8.26	9.01	8.21	8.68
24TS$_2$	4.11	4.12	5.51	5.46	5.44	6.76	6.67	6.20	6.13
28F	2.56	1.03	2.41	0.97	0.87	2.95	1.55	1.21	0.13
28M$_{1A}$	-3.35	-5.59	5.09	3.27	13.86	13.85	12.43	11.58	10.61
28M	-4.50	-6.85	3.21	1.30	10.54	10.66	9.17	8.46	7.46
28M$_{1B}$	-1.79	-3.82	6.61	4.95	15.32	15.17	13.88	13.11	12.24
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28TS$_{1A}$	7.63	7.24	6.59	6.21	5.71	6.74	6.41	5.77	5.54
28TS$_{1B}$	5.00	4.69	3.44	3.10	2.36	3.34	3.02	2.47	2.24
28TS$_{2A}$	2.74	-0.09	11.67	9.40	19.60	22.02	20.30	17.42	16.27
28TS$_{2B}$	5.65	2.78	14.60	12.30	21.70	24.61	22.85	19.83	18.67
28TS$_3$	8.67	6.92	7.82	6.15	6.13	8.19	6.63	6.39	5.24
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32H	23.37	32.81	24.03	31.92	21.87	25.09	31.49	26.89	31.28
32M$_a$	3.08	7.75	12.65	16.73	17.89	20.64	24.08	20.78	23.15
32M$_b$	3.35	8.66	13.26	17.82	21.54	22.94	26.72	23.31	25.91
32TS$_1$	12.69	16.66	12.60	15.88	10.87	13.23	15.81	13.64	15.35
32TS$_2$	25.18	34.07	24.39	31.77	20.81	24.74	30.69	26.36	30.43
RMSD	**5.41**	**3.97**	**4.02**	**1.78**	**7.63**	**7.76**	**6.99**	**6.10**	**5.65**
MUE	**4.08**	**3.01**	**3.20**	**1.33**	**5.40**	**5.62**	**4.62**	**4.37**	**3.68**

Table S12. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several DFT approaches together with def2-TZVP basis set. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T)/CBS data.[a]

system	ωB97XV	ωB97XD	M11	ωB97MV	B2LYP	B2LYP-D3	SCAN0-2	revSCAN0-2	revSCAN0-2-D3
24H$_a$	8.68	7.91	8.97	8.92	4.96	6.52	7.04	7.31	7.60
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24M	8.54	8.62	10.25	8.33	3.46	3.00	4.69	5.06	5.55
24TS$_1$	8.72	8.73	9.92	8.88	7.74	8.74	9.19	8.89	8.98
24TS$_2$	5.84	5.00	5.56	5.79	4.27	4.22	4.81	4.85	5.04
28F	-1.28	1.30	1.04	-0.82	1.82	-0.34	-0.15	-0.02	0.08
28M$_{1A}$	9.38	4.78	7.30	8.04	-7.27	-9.08	-12.20	-9.26	-6.95
28M	6.47	2.84	4.78	5.24	-8.30	-10.14	-11.01	-8.48	-6.60
28M$_{1B}$	10.95	6.61	9.05	9.67	-5.67	-7.32	-10.17	-7.27	-5.00
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28TS$_{1A}$	5.14	6.11	5.43	4.77	6.67	6.34	6.57	6.49	6.48
28TS$_{1B}$	1.81	2.86	1.96	1.42	3.74	3.48	3.08	2.98	2.98
28TS$_{2A}$	15.38	10.32	12.78	14.19	-1.77	-3.77	-7.25	-3.95	-1.39
28TS$_{2B}$	17.73	12.76	15.05	16.58	1.19	-0.84	-2.77	0.29	2.66
28TS$_3$	4.41	6.72	6.18	4.00	7.55	6.78	6.04	5.84	5.83
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32H	31.16	34.20	34.20	31.51	29.55	38.05	35.15	33.92	33.87
32M$_a$	23.05	19.73	22.79	22.38	4.27	9.60	8.15	9.68	11.34
32M$_b$	25.39	21.87	25.20	24.49	3.66	9.51	3.75	6.20	8.63
32TS$_1$	15.43	17.01	18.05	15.51	15.33	19.42	18.06	17.35	17.27
32TS$_2$	30.25	34.26	34.17	30.58	30.39	39.28	35.67	34.17	33.97
RMSD	**5.15**	**2.84**	**4.33**	**4.50**	**5.41**	**5.45**	**6.69**	**5.08**	**3.80**
MUE	**3.41**	**2.13**	**3.10**	**3.00**	**3.95**	**4.12**	**4.49**	**3.37**	**2.56**

Table S13. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several DFT approaches together with def2-TZVP basis set. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T)/CBS data.[a]

system	PWPB95	PWPB95-D3	SOS0-PBE0-2-D3	PTPSS-D3	ωB2PLYP	ωB2GP-PLYP	ωB97M(2)	revωB97X-2 (TQ)	dRPA75-D3
24H$_a$	5.64	6.56	7.88	6.82	7.51	7.56	8.12	7.64	7.47
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24M	5.44	5.32	6.86	5.43	7.61	7.12	6.58	6.28	4.91
24TS$_1$	8.23	8.78	9.08	9.23	8.88	9.06	8.85	8.68	8.91
24TS$_2$	4.93	4.90	5.52	5.17	5.73	5.61	5.20	5.21	4.78
28F	1.81	0.96	0.14	1.75	0.29	0.17	-1.14	0.33	0.47
28M$_{1A}$	-1.26	-2.19	-1.05	-3.23	2.06	-1.00	-0.83	-3.77	-7.62
28M	-2.74	-3.71	-1.74	-4.57	0.92	-1.38	-1.98	-3.24	-7.61
28M$_{1B}$	0.42	-0.43	0.80	-1.48	4.00	1.03	1.11	-1.77	-5.79
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28TS$_{1A}$	6.96	6.75	6.49	6.99	5.82	6.02	5.16	6.07	6.40
28TS$_{1B}$	3.95	3.76	3.03	4.14	2.50	2.60	1.98	2.55	3.19
28TS$_{2A}$	5.12	3.98	5.02	3.00	7.30	4.37	4.89	1.87	-2.00
28TS$_{2B}$	8.02	6.86	8.61	6.15	10.78	8.26	8.18	6.05	1.74
28TS$_3$	7.47	6.52	5.77	7.35	5.77	5.83	4.04	5.67	5.98
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32H	28.24	32.33	33.60	33.20	31.81	33.04	33.55	32.44	34.67
32M$_a$	9.47	11.61	15.65	9.80	17.47	16.26	16.31	14.59	10.31
32M$_b$	9.83	12.20	14.77	10.46	17.73	15.68	16.05	13.24	8.12
32TS$_1$	15.17	16.83	16.90	16.76	16.12	16.79	16.70	16.52	17.46
32TS$_2$	29.01	32.81	33.33	33.65	31.54	32.88	33.10	32.35	34.94
RMSD	**2.63**	**1.85**	**0.87**	**2.58**	**1.28**	**0.78**	**0.63**	**1.83**	**4.28**
MUE	**1.89**	**1.41**	**0.64**	**1.94**	**0.97**	**0.61**	**0.48**	**1.17**	**2.99**

Table S14. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several DFT approaches together with def2-TZVP basis set. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T) data.[a]

system	DSD-PBE86	DSD-PBE86-D3	xrevDSD-PBE86-D3	DOD-PBE86-D3	revDSD-PBE86-NL	revDOD-PBE86-NL	revDSD-PBE86-D4	revDOD-PBE86-D4
24H$_a$	7.17	7.28	7.30	7.71	7.12	7.24	7.27	7.40
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24M	4.26	4.82	5.56	5.73	5.53	5.90	5.54	5.85
24TS$_1$	8.97	8.96	8.76	9.05	8.52	8.59	8.75	8.77
24TS$_2$	4.50	4.75	4.98	5.10	4.90	5.05	4.99	5.11
28F	-0.64	0.13	0.57	0.42	0.17	0.21	0.89	0.99
28M$_{1A}$	-11.32	-8.52	-5.20	-4.55	-5.13	-2.77	-5.29	-4.09
28M	-11.18	-8.04	-4.31	-3.35	-4.28	-3.83	-4.46	-3.11
28M$_{1B}$	-9.36	-6.18	-2.52	-1.56	-2.49	-0.99	-2.68	-1.33
28H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28TS$_{1A}$	6.19	6.35	6.38	6.35	6.27	6.27	6.46	6.47
28TS$_{1B}$	2.90	3.14	3.20	3.23	3.00	3.00	3.23	3.24
28TS$_{2A}$	-6.52	-2.77	1.45	2.40	1.42	2.91	1.11	2.58
28TS$_{2B}$	-2.68	0.76	4.83	5.58	4.78	6.18	4.50	5.90
28TS$_3$	5.24	5.80	6.03	5.85	5.67	5.68	6.25	6.29
32F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32H	36.37	34.89	33.37	34.44	33.15	33.06	33.43	33.20
32M$_a$	8.19	9.12	11.12	12.33	11.40	12.59	11.27	12.27
32M$_b$	5.44	7.66	10.46	12.41	10.53	12.10	10.36	11.66
32TS$_1$	18.28	17.58	16.85	17.25	16.71	16.67	17.11	16.99
32TS$_2$	36.72	35.19	33.44	34.48	33.19	33.01	33.55	33.24
RMSD	**6.39**	**4.69**	**2.73**	**2.21**	**2.68**	**1.85**	**2.83**	**2.13**
MUE	**4.39**	**3.25**	**1.92**	**1.64**	**1.85**	**1.33**	**2.02**	**1.54**

Table S15. Relative energies for the different minima and TSs involved in the topology interconversions of several expanded porphyrins computed with several DFT approaches together with def2-TZVP basis set. The statistical errors (in kcal mol^{-1}) are computed with respect canonical CCSD(T) data.[a]

system	revDSD-PBEB95-D3	revDOD-PBEB95-D3	DSD-SCAN$_{66}$-D3	DOD-SCAN$_{66}$-D3	DSD-SCAN$_{69}$-D3	DOD-SCAN$_{69}$-D3
24H$_a$	7.13	7.33	12.37	12.72	11.98	12.61
24H$_b$	0.00	0.00	0.00	0.00	0.00	0.00
24M	5.32	5.85	5.12	5.28	5.13	5.44
24TS$_1$	8.92	8.95	12.33	12.54	12.04	12.41
24TS$_2$	4.89	5.09	5.29	5.37	5.25	5.40
28F	0.64	0.74	-2.49	-2.65	-2.37	-2.64
28M$_{1A}$	-5.71	-3.72	-9.35	-8.86	-9.63	-8.61
28M	-4.72	-2.50	-10.48	-10.10	-10.50	-9.71
28M$_{1B}$	-2.95	-0.75	-7.18	-6.68	-7.46	-6.42
28H	0.00	0.00	0.00	0.00	0.00	0.00
28TS$_{1A}$	6.56	6.58	5.87	5.82	5.91	5.83
28TS$_{1B}$	3.37	3.37	2.85	2.82	2.81	2.75
28TS$_{2A}$	1.35	3.77	-4.94	-4.47	-5.15	-4.14
28TS$_{2B}$	4.62	6.93	-1.67	-1.24	-1.74	-0.83
28TS$_3$	6.17	6.18	2.94	2.75	3.13	2.80
32F	0.00	0.00	0.00	0.00	0.00	0.00
32H	32.99	32.60	51.45	52.42	50.06	51.70
32M$_a$	10.38	12.10	18.89	19.97	18.16	20.12
32M$_b$	9.83	11.99	19.53	20.86	18.19	20.65
32TS$_1$	16.97	16.77	24.49	24.88	23.93	24.57
32TS$_2$	33.28	32.74	50.71	51.57	49.39	50.84
RMSD	**2.99**	**1.86**	**7.88**	**8.05**	**7.55**	**7.77**
MUE	**2.09**	**1.28**	**5.53**	**5.68**	**5.26**	**5.49**

Table S16. D3BJ parameters and RMSD (in kcal mol^{-1}) for selected functionals with and without DFT-D3BJ atom-pairwise dispersion correction.

	BLYP	PBE	TPSS	SCAN	
RMSD (no D3BJ)	8.25	6.38	6.01	4.95	
RMSD (with D3BJ)	4.49	4.97	4.76	4.64	
Improvement RMSD	**3.76**	**1.40**	**1.25**	**0.31**	
s_6	1.0000	1.0000	1.0000	1.00	
s_8	2.6996	0.7875	1.9435	0.00	
a_1	0.4298	0.4289	0.4535	0.54	
a_2	4.2359	4.4407	4.4752	5.42	
	B3LYP	PBE0	TPSSh	SCAN0	PW6B95
RMSD (no D3BJ)	5.35	4.86	5.41	3.38	3.85
RMSD (with D3BJ)	3.01	3.11	3.97	2.72	2.51
Improvement RMSD	**2.34**	**1.76**	**1.45**	**0.66**	**1.34**
s_6	1.0000	1.0000	1.0000	1.0000	0.0000
s_8	1.9889	1.2177	2.2382	0.0000	0.7257
a_1	0.3981	0.4145	0.4529	0.0000	0.2076
a_2	4.4211	4.8593	4.6550	7.9042	6.3750
	BHLYP	PWPB95	CAM-B3LYP	M06-2X, GRID4	DSD-PBEP86
RMSD (no D3BJ)	5.11	2.63	4.02	1.67	6.39
RMSD (with D3BJ)	2.67	1.85	1.78	1.32	4.68
Improvement RMSD	**2.44**	**0.78**	**2.24**	**0.35**	**1.70**
s_6	1.0000	0.8200	1.0000	1.00	0.418
s_8	1.0354	0.2904	2.0674	0.00	0.000
a_1	0.2793	0.0000	0.3708	$s_{r,6}$=1.619	0.000
a_2	4.9615	7.3141	5.4743	using D3(0)	5.650

[a] All D3BJ parameters taken from Table S3 in Goerigk, L.; Hansen, A.; Bauer, C.; Ehrlich, S.; Najibi, A.; Grimme, S., A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. *Phys. Chem. Chem. Phys.* **2017**, *19*, 32184-32215, except for SCAN-D3BJ (Brandenburg, J. G.; Bates, J. E.; Sun, J.; Perdew, J. P. Benchmark tests of a strongly constrained semilocal functional with a long-range dispersion correction. *Phys. Rev. B - Condens. Matter Mater. Phys.* **2016**, *94*, 17–19) and SCAN0-D3BJ (Table 1 of Santra, G.; Sylvetsky, N.; Martin, J. M. L. Minimally empirical double-hybrid functionals trained against the GMTKN55 database: RevDSD-PBEP86-D4, RevDOD-PBE-D4, and DOD-SCAN-D4. *J. Phys. Chem. A* **2019**, *123*, 5129–5143).

VIII. Cartesian coordinates of B3LYP/6-311G(d,p) optimized geometries

[24]pentaphyrin

$24H_a$

N	-2.3974	-1.69516	0.17754
N	-2.85222	1.05377	-0.22313
N	0.55579	2.24403	0.02974
N	3.3491	-0.37177	-0.14791
N	1.71473	-3.39258	-0.11812
C	-1.95446	-2.99437	0.36053
C	-3.08718	-3.90403	0.46301
C	-4.20026	-3.14635	0.31355
C	-3.73335	-1.77608	0.12567
C	-4.59162	-0.67057	-0.13088
C	-4.16415	0.61814	-0.30506
C	-4.97456	1.78974	-0.55751
C	-4.15886	2.86726	-0.58408
C	-2.79026	2.43315	-0.34356
C	-1.76293	3.32265	-0.21087
C	-0.36957	3.27619	0.11011
C	0.32064	4.4075	0.56063
C	1.65763	4.06432	0.72491
C	1.81913	2.71972	0.3705
C	3.1219	2.1381	0.30099
C	3.75823	0.95808	0.05897
C	5.21589	0.92958	-0.09491
C	5.63812	-0.31975	-0.39912
C	4.48247	-1.17303	-0.41481
C	4.14187	-2.50688	-0.50953
C	2.74554	-2.52582	-0.26178
C	2.25023	-1.22095	-0.03242
C	0.87186	-1.30996	0.23591
C	0.54459	-2.68039	0.16993
C	-0.6515	-3.41865	0.34172
H	-3.01856	-4.97251	0.61181
H	-5.23346	-3.46294	0.31129
H	-6.04634	1.76477	-0.68296
H	-4.4335	3.90031	-0.73713
H	-0.13912	5.36529	0.7478
H	2.45964	4.70425	1.05945
H	5.8234	1.81803	-0.00623
H	6.64959	-0.64508	-0.58611
H	0.16674	-0.55289	0.53126
H	-2.12306	0.37689	-0.01584
H	0.38848	1.36307	-0.43083

H	1.7465	-4.3842	-0.28499
H	-5.6561	-0.85614	-0.19733
H	-0.51685	-4.49502	0.42177
H	4.81171	-3.33006	-0.69341
H	3.85396	2.92224	0.46637
H	-2.09924	4.35045	-0.29338

24H_b

N	2.11631	3.05588	0.07431
N	3.4877	-0.09248	-0.09436
N	0.44333	-3.14709	-0.24578
N	-3.05301	-1.05898	0.00959
N	-2.22391	1.65492	0.018
C	0.86066	2.42839	0.0598
C	1.06967	1.0361	-0.01667
C	2.45866	0.84738	-0.03985
C	3.09141	2.11181	-0.00131
C	4.50231	1.97058	-0.08305
C	4.70728	0.60367	-0.16357
H	2.25422	4.0519	0.10101
C	5.74184	-0.36839	-0.40817
H	0.48783	-3.62662	-1.13078
C	5.15639	-1.58792	-0.51198
H	-2.22979	-0.47203	0.11203
C	3.71568	-1.46988	-0.28551
H	0.27471	0.31682	-0.0655
C	2.8387	-2.50146	-0.20566
H	6.79294	-0.14051	-0.49867
C	1.49355	-2.42986	0.30091
H	5.64634	-2.53621	-0.67495
C	0.97587	-1.70943	1.36995
H	1.55494	-1.08598	2.0312
C	-0.41151	-1.9469	1.4216
H	-1.11452	-1.54443	2.13311
C	-0.73722	-2.82071	0.3888
H	-4.85166	-3.75181	-0.62381
C	-2.03597	-3.28394	-0.05103
H	-6.25135	-1.4746	-0.6631
C	-3.09671	-2.43668	-0.15332
H	-4.85336	3.71844	-0.12531
C	-4.48524	-2.74974	-0.45774
H	-2.49498	5.00689	0.07818
C	-5.19579	-1.59593	-0.47048
C	-4.28646	-0.49335	-0.20733
C	-4.53996	0.85317	-0.21156
C	-3.54578	1.87001	-0.07671

C	-3.86096	3.2952	-0.06202
C	-2.67525	3.94145	0.04248
C	-1.64314	2.91218	0.07691
C	-0.30363	3.23178	0.10324
H	3.21677	-3.47281	-0.51281
H	5.26067	2.73542	-0.11177
H	-0.10679	4.30129	0.14336
H	-5.56414	1.17049	-0.36236
H	-2.18108	-4.32721	-0.30863

24M

N	-2.42991	1.34997	0.44046
N	-2.81643	-1.21307	-0.15898
N	1.08938	-2.26765	-0.16485
N	3.33229	0.05248	-0.32282
N	1.58297	3.01661	-0.57485
C	-1.97166	2.63529	0.52834
C	-3.09224	3.55298	0.70696
C	-4.21938	2.79765	0.67199
C	-3.78206	1.42284	0.46295
C	-4.63344	0.34515	0.1127
C	-4.1366	-0.88108	-0.30013
C	-4.72956	-1.91969	-1.11086
C	-3.73086	-2.75227	-1.53251
C	-2.49393	-2.31475	-0.92564
C	-1.2109	-2.80132	-0.98864
C	-0.25753	-2.46624	0.02944
C	-0.45693	-2.47243	1.42305
C	0.78828	-2.35176	2.043
C	1.75414	-2.18767	1.0433
C	3.16311	-1.95749	1.13051
C	3.86627	-1.05343	0.38889
C	5.29367	-0.98901	0.18673
C	5.60016	0.10223	-0.58215
C	4.39307	0.81076	-0.85002
C	3.96823	2.10976	-1.14915
C	2.63084	2.15744	-0.72719
C	2.22147	0.89953	-0.2086
C	0.89748	0.98909	0.2198
C	0.49801	2.33728	-0.00199
C	-0.6742	3.06314	0.29243
H	-3.01191	4.62605	0.81113
H	-5.24671	3.12656	0.73841
H	-5.77696	-1.97439	-1.36793
H	-3.82704	-3.62047	-2.16727
H	-1.4147	-2.61288	1.89711

H	0.99162	-2.33885	3.10264
H	5.97581	-1.74286	0.55029
H	6.5831	0.41043	-0.90523
H	0.27823	0.24749	0.69418
H	-2.16625	-0.47347	0.13244
H	1.53769	-2.17587	-1.06248
H	1.53274	3.95825	-0.92444
H	-5.69468	0.53533	0.0165
H	-0.55856	4.14401	0.24916
H	4.58541	2.90351	-1.53749
H	3.726	-2.55093	1.8431
H	-0.93458	-3.48624	-1.78227

24TS$_1$

C	2.66262	2.38542	-0.52885
C	2.21466	1.09563	-0.14799
C	0.87697	1.18281	0.25813
C	0.5214	2.54753	0.15164
C	-0.65185	3.27525	0.45836
C	-1.94898	2.83976	0.59536
N	-2.39399	1.55123	0.37694
C	-3.73232	1.62403	0.36441
C	-4.57642	0.54567	-0.03709
C	-4.10282	-0.68663	-0.39803
C	-4.81013	-1.77698	-1.04781
C	-3.92133	-2.75745	-1.32194
C	-2.61855	-2.36947	-0.7817
C	-1.51743	-3.15629	-0.71736
C	-0.34033	-2.97489	0.14156
C	-0.04408	-3.73256	1.26706
C	1.27347	-3.43777	1.65506
C	1.77801	-2.47662	0.78203
C	3.14531	-2.05937	0.70629
C	3.79134	-0.99222	0.16843
C	5.23088	-0.94943	-0.05089
C	5.58121	0.22903	-0.63001
C	4.39601	1.02774	-0.74832
C	4.01849	2.35163	-0.92327
N	1.63804	3.25189	-0.31863
N	3.30802	0.24368	-0.31574
N	0.76005	-2.18294	-0.11603
N	-2.79603	-1.10277	-0.25485
C	-4.19683	2.97597	0.65476
C	-3.08057	3.73363	0.79887
H	1.62519	4.22646	-0.56783
H	0.86744	-1.61096	-0.93929

H	-2.09189	-0.43852	0.0582
H	0.2288	0.42053	0.65305
H	6.57054	0.54315	-0.92515
H	5.87971	-1.78227	0.17667
H	1.82532	-3.86747	2.47729
H	-0.72019	-4.4382	1.72334
H	-4.10949	-3.70704	-1.80021
H	-5.86613	-1.76074	-1.27286
H	-5.23008	3.28847	0.70541
H	-3.01289	4.79431	0.99613
H	3.82166	-2.7891	1.14069
H	4.65969	3.1642	-1.22212
H	-0.51779	4.35251	0.52974
H	-5.63575	0.73752	-0.15048
H	-1.59925	-4.12686	-1.19668

24TS$_2$

C	2.77253	2.1848	-0.54172
C	2.30684	0.90219	-0.16409
C	0.94889	0.99102	0.16935
C	0.59595	2.3556	0.02439
C	-0.5856	3.10192	0.25821
C	-1.90123	2.7159	0.40437
N	-2.40777	1.44175	0.30666
C	-3.74997	1.56987	0.28765
C	-4.64805	0.5086	-0.00617
C	-4.21394	-0.76894	-0.2968
C	-4.89926	-1.87522	-0.93577
C	-3.97913	-2.83582	-1.22505
C	-2.69286	-2.40434	-0.71152
C	-1.47719	-3.02461	-0.7139
C	-0.40715	-2.58606	0.14965
C	-0.46275	-2.22059	1.49649
C	0.85804	-2.05335	1.95979
C	1.713	-2.26739	0.88948
C	3.16733	-2.19571	0.77912
C	3.86821	-1.2005	0.19484
C	5.31266	-1.19236	-0.04126
C	5.68004	-0.00404	-0.58569
C	4.50933	0.81769	-0.69882
C	4.14082	2.14125	-0.88959
N	-2.91469	-1.16674	-0.1337
N	0.9278	-2.59854	-0.19373
N	3.41014	0.04853	-0.27817
N	1.73481	3.05348	-0.40113
C	-2.99384	3.6781	0.52589

C	-4.14443	2.96622	0.4533
H	-2.87583	4.74825	0.62454
H	-5.16113	3.3319	0.47869
H	-5.95373	-1.88663	-1.16814
H	-4.15112	-3.78377	-1.71283
H	-1.37184	-2.12893	2.06855
H	1.17003	-1.77287	2.95348
H	5.94518	-2.03929	0.17722
H	6.67616	0.30096	-0.86936
H	0.28113	0.2245	0.52128
H	-2.20944	-0.46093	0.09462
H	1.28605	-2.7791	-1.1177
H	1.73556	4.02552	-0.65935
H	-5.69972	0.73772	-0.11895
H	-0.43612	4.17968	0.26129
H	4.79004	2.94702	-1.1911
H	3.75197	-3.01173	1.19483
H	-1.33869	-3.90679	-1.32937

[28]hexaphyrin

28H

C	1.17129	2.92911	0.12886
C	0.69215	1.63073	0.56406
C	-0.66747	1.63671	0.55523
C	-1.12919	2.93656	0.11235
C	-2.38728	3.43672	-0.08156
C	-3.64434	2.75413	-0.03976
N	-3.85103	1.43578	0.02407
C	-5.23505	1.27593	0.01588
C	-5.89161	0.06713	0.01648
C	-5.31116	-1.21836	0.01186
C	-5.94198	-2.47336	0.04797
C	-4.94605	-3.44578	0.06421
C	-3.6955	-2.79302	0.02681
C	-2.42612	-3.43998	0.05488
C	-1.17129	-2.92911	-0.12885
C	-0.69215	-1.63073	-0.56406
C	0.66747	-1.63671	-0.55523
C	1.12919	-2.93656	-0.11234
C	2.38728	-3.43672	0.08156
C	3.64434	-2.75413	0.03976
N	3.85103	-1.43578	-0.02407
C	5.23505	-1.27593	-0.01588
C	5.89161	-0.06713	-0.01648
C	5.31116	1.21836	-0.01186
C	5.94198	2.47336	-0.04797
C	4.94605	3.44578	-0.06421

C	3.6955	2.79302	-0.02681
C	2.42612	3.43999	-0.05488
N	0.02236	3.68768	-0.07426
C	-4.90367	3.49257	-0.09283
C	-5.8932	2.56641	-0.04575
N	-3.94892	-1.44766	-0.00937
N	-0.02236	-3.68767	0.07426
C	4.90367	-3.49257	0.09283
C	5.8932	-2.56641	0.04574
N	3.94892	1.44766	0.00937
H	0.02761	4.57886	-0.54208
H	1.32267	0.82351	0.90185
H	-1.33567	0.85182	0.86532
H	-2.45507	4.49673	-0.31044
H	-4.99566	4.56805	-0.14846
H	-6.96216	2.72404	-0.0625
H	-6.97593	0.09143	0.01288
H	-3.30494	-0.66313	0.01841
H	-7.01006	-2.6267	0.06486
H	-5.07475	-4.51684	0.0891
H	-2.48746	-4.50167	0.27469
H	-0.02761	-4.57886	0.54208
H	-1.32267	-0.82351	-0.90185
H	1.33567	-0.85182	-0.86532
H	2.45507	-4.49673	0.31045
H	4.99567	-4.56805	0.14846
H	6.96216	-2.72404	0.0625
H	6.97593	-0.09143	-0.01289
H	3.30494	0.66313	-0.0184
H	7.01006	2.6267	-0.06486
H	5.07475	4.51684	-0.08911
H	2.48745	4.50167	-0.27469

28M

C	5.27508	0.2316	-0.26339
C	6.18464	1.23384	-0.74045
C	5.44242	2.26055	-1.2699
C	4.04996	1.92453	-1.14038
C	2.93774	2.74541	-1.30314
C	1.61577	2.36996	-1.00704
C	0.99602	1.09193	-0.95981
C	-0.2988	1.24394	-0.50907
C	-0.52769	2.62399	-0.24614
C	-1.5934	3.30513	0.35219
C	-2.80837	2.79701	0.80199
C	-3.8345	3.53055	1.48572

C	-4.89736	2.69211	1.70589
C	-4.57413	1.41428	1.14925
C	-5.39356	0.31046	0.93396
C	-5.01514	-0.80729	0.17015
N	-3.73108	-1.07666	-0.19132
C	-3.80146	-2.03421	-1.16656
C	-2.67617	-2.55596	-1.80811
C	-1.36861	-2.46572	-1.32422
C	-0.13626	-2.73216	-1.98924
C	0.88994	-2.54336	-1.09388
C	0.32053	-2.21816	0.17834
C	0.94367	-2.21354	1.43408
C	2.32113	-2.06117	1.61885
N	3.1305	-1.4704	0.69744
C	4.40006	-1.55855	1.1714
C	5.47348	-0.84522	0.59995
N	4.01552	0.66137	-0.60976
N	0.63954	3.2735	-0.62431
N	-3.28685	1.51535	0.66241
C	-5.93679	-1.67733	-0.54215
C	-5.18348	-2.39918	-1.41715
N	-1.04154	-2.14797	-0.02234
C	3.11161	-2.54006	2.74327
C	4.41399	-2.28467	2.43395
H	7.25869	1.18646	-0.64325
H	5.80995	3.18881	-1.68096
H	1.44625	0.16271	-1.26577
H	-1.00618	0.44252	-0.38328
H	-3.75245	4.57146	1.76043
H	-5.83474	2.93126	2.18444
H	-7.01173	-1.6807	-0.42975
H	-5.51906	-3.13039	-2.13872
H	-0.05571	-3.03232	-3.02303
H	1.94756	-2.67192	-1.25119
H	2.72468	-3.04689	3.61598
H	5.29178	-2.51477	3.02126
H	3.21754	0.12977	-0.24794
H	0.83335	4.23759	-0.40654
H	-2.90666	0.73586	0.13066
H	-1.74455	-1.85304	0.64334
H	6.47966	-1.03459	0.95272
H	3.13543	3.78613	-1.53704
H	-1.46316	4.37101	0.51155
H	-6.42654	0.39312	1.24952
H	-2.8157	-3.08399	-2.74429
H	0.32718	-2.4066	2.30667

28M$_{1A}$

N	-3.31081	1.48577	0.68381
H	-2.91857	0.71418	0.14903
C	-4.59238	1.35642	1.18029
C	-4.93302	2.62187	1.75194
H	-5.87079	2.84094	2.23929
C	-3.88495	3.48076	1.5332
H	-3.81872	4.52023	1.81725
C	-2.85302	2.77162	0.83366
C	-1.64793	3.30385	0.37761
N	0.58075	3.31078	-0.60222
H	0.77159	4.26755	-0.35149
C	1.56598	2.41836	-0.99455
C	0.94889	1.1366	-0.98772
H	1.42812	0.23387	-1.32117
C	-0.34636	1.27057	-0.54419
H	-1.05561	0.46606	-0.45061
C	-0.58163	2.64675	-0.2409
C	2.88719	2.79242	-1.26159
N	3.93079	0.70616	-0.57987
C	3.99973	1.95513	-1.10488
C	5.39285	2.36895	-1.22897
H	5.73509	3.31494	-1.62445
C	6.14301	1.35768	-0.71347
H	7.21707	1.31764	-0.60008
C	5.2024	0.33757	-0.26971
C	5.48415	-0.74834	0.57764
N	3.17135	-1.46575	0.75297
H	2.91076	-0.69518	0.12654
C	4.48502	-1.53619	1.15477
C	4.50588	-2.37362	2.31506
H	5.39753	-2.66132	2.85152
C	3.20454	-2.69491	2.63239
H	2.86511	-3.31393	3.44916
C	2.35164	-2.13737	1.62646
C	0.97423	-2.27344	1.4312
N	-0.99756	-2.13376	-0.03901
H	-1.70536	-1.86104	0.63094
C	-1.31812	-2.42015	-1.35291
C	-0.08003	-2.66306	-2.01634
H	0.00977	-2.93539	-3.05697
C	0.93926	-2.49938	-1.10998
H	1.99385	-2.64322	-1.27894
C	0.36102	-2.21701	0.17169
C	-2.61844	-2.51217	-1.84656
N	-3.70385	-1.0969	-0.19521

C	-3.75752	-2.03201	-1.19039
C	-5.13063	-2.42054	-1.44611
H	-5.45294	-3.14224	-2.18313
C	-5.89761	-1.73338	-0.55323
H	-6.97211	-1.7613	-0.44007
C	-4.9939	-0.86072	0.17521
C	-5.39101	0.23889	0.9552
H	-1.52955	4.36852	0.55321
H	3.08722	3.84262	-1.45379
H	6.50487	-0.90012	0.90625
H	0.36126	-2.51752	2.29176
H	-2.7447	-3.00728	-2.80238
H	-6.42416	0.29692	1.27594

28M$_{1B}$

C	-5.11517	-0.79915	0.19826
N	-3.82756	-1.08437	-0.20819
C	-3.83307	-2.11647	-1.12828
C	-5.1879	-2.55089	-1.2419
C	-5.95992	-1.78029	-0.40076
C	-2.68943	-2.58818	-1.77547
C	-1.37725	-2.4445	-1.31846
N	-1.01305	-2.18427	-0.00847
C	0.36318	-2.22825	0.14477
C	0.89293	-2.43377	-1.16737
C	-0.1566	-2.60421	-2.03763
C	1.0222	-2.30165	1.3742
C	2.40771	-2.15154	1.53312
N	3.18661	-1.48659	0.64067
C	4.47163	-1.6006	1.07539
C	4.52132	-2.41785	2.27737
C	3.22767	-2.7083	2.59702
C	5.52595	-0.84279	0.53022
C	5.30676	0.2823	-0.2651
N	4.03719	0.72572	-0.55563
C	4.05558	2.004	-1.04391
C	5.44198	2.35091	-1.19089
C	6.20058	1.3057	-0.71976
C	2.93292	2.82274	-1.17268
C	1.61721	2.43539	-0.88439
N	0.62153	3.32879	-0.53536
C	-0.54515	2.66606	-0.17481
C	-0.28764	1.28323	-0.40342
C	1.013	1.14309	-0.8241
C	-1.64683	3.3212	0.36812
C	-2.87727	2.77903	0.76581

N	-3.29783	1.49723	0.59866
C	-4.58731	1.46059	1.04811
C	-4.98679	2.75746	1.56971
C	-3.92504	3.58293	1.38293
C	-5.45136	0.36922	0.8794
H	-5.9534	2.99425	1.99092
H	-3.84614	4.63355	1.62491
H	0.7894	4.30433	-0.34963
H	1.48447	0.21649	-1.10307
H	-1.00886	0.50255	-0.24825
H	5.79703	3.29511	-1.57564
H	7.27694	1.25746	-0.65354
H	5.41463	-2.68301	2.82511
H	2.86577	-3.28292	3.4379
H	-1.672	-2.1134	0.75146
H	-0.10163	-2.81569	-3.09472
H	1.94846	-2.4944	-1.37276
H	-5.51344	-3.37628	-1.85691
H	-7.0248	-1.8545	-0.23963
H	-1.5474	4.39398	0.512
H	3.12371	3.86982	-1.38273
H	6.54058	-1.04947	0.84776
H	0.43425	-2.55162	2.25253
H	-2.82672	-3.12455	-2.70637
H	-6.48362	0.48632	1.18657
H	-3.13885	-0.32929	-0.13709
H	3.25004	0.17336	-0.20348

28F

N	3.73912200	0.62468100	-0.40325500
C	3.90976100	1.26413100	-1.61573700
C	2.82619100	1.83225300	-2.26099300
C	1.54898200	1.99695200	-1.66880600
C	0.29448400	2.26731800	-2.24979900
C	-0.65783400	2.29809300	-1.23246400
C	0.01295700	2.09588400	-0.00245500
C	-0.45763200	2.24770900	1.34916300
C	-1.74986100	2.03203300	1.74660700
C	-2.43317800	2.45753700	2.95848300
C	-3.73912200	2.08946300	2.87113300
C	-3.92940200	1.34620200	1.63716400
C	-5.02965900	0.68313600	1.14694900
C	-4.92868100	-0.15673600	-0.01854100
N	-3.73912200	-0.62468100	-0.40325500
C	-3.90976100	-1.26413100	-1.61573700
C	-2.82619100	-1.83225300	-2.26099300

C	-1.54898200	-1.99695200	-1.66880600
C	-0.29448400	-2.26731800	-2.24979900
C	0.65783400	-2.29809300	-1.23246400
C	-0.01295700	-2.09588400	-0.00245500
C	0.45763200	-2.24770900	1.34916300
C	1.74986100	-2.03203300	1.74660700
C	2.43317800	-2.45753700	2.95848300
C	3.73912200	-2.08946300	2.87113300
C	3.92940200	-1.34620200	1.63716400
C	5.02965900	-0.68313600	1.14694900
C	4.92868100	0.15673600	-0.01854100
C	5.95070200	0.53686100	-0.98115400
C	5.30581100	1.19620900	-1.99261500
N	1.32909600	1.90300100	-0.30496000
N	-2.70530100	1.38656200	0.99471500
C	-5.95070200	-0.53686100	-0.98115400
C	-5.30581100	-1.19620900	-1.99261500
N	-1.32909600	-1.90300100	-0.30496000
N	2.70530100	-1.38656200	0.99471500
H	7.00232300	0.29620600	-0.91813000
H	5.74159600	1.61222900	-2.88987800
H	2.94142600	2.17768300	-3.28258400
H	2.07113500	1.59612400	0.31597400
H	0.12073700	2.41492000	-3.30485700
H	-1.70981400	2.51057100	-1.33232300
H	0.24349300	2.62352900	2.08518200
H	-2.53395000	0.76155000	0.21248800
H	-1.96397100	3.02275600	3.75000300
H	-4.52086400	2.27973100	3.59134500
H	-5.98228100	0.80656000	1.64567500
H	-7.00232300	-0.29620600	-0.91813000
H	-5.74159600	-1.61222900	-2.88987800
H	-2.94142600	-2.17768300	-3.28258400
H	-2.07113500	-1.59612400	0.31597400
H	-0.12073700	-2.41492000	-3.30485700
H	1.70981400	-2.51057100	-1.33232300
H	-0.24349300	-2.62352900	2.08518200
H	2.53395000	-0.76155000	0.21248800
H	1.96397100	-3.02275600	3.75000300
H	4.52086400	-2.27973100	3.59134500
H	5.98228100	-0.80656000	1.64567500

28TS$_{1A}$

N	-3.73098	1.49538	0.45978
H	-3.18934	0.69443	0.14187
C	-5.06315	1.33018	0.74297

C	-5.57179	2.62891	1.11382
H	-6.59366	2.82153	1.40224
C	-4.5505	3.52374	1.0113
H	-4.58425	4.58563	1.2048
C	-3.36267	2.82372	0.58586
C	-2.13401	3.39141	0.35229
N	0.22722	3.51508	-0.20468
H	0.29539	4.50152	-0.0125
C	1.30447	2.70626	-0.49545
C	0.7989	1.39367	-0.56458
H	1.38784	0.53603	-0.8218
C	-0.56271	1.42688	-0.29086
H	-1.21225	0.56595	-0.2844
C	-0.92682	2.769	-0.03855
C	2.61294	3.2224	-0.666
N	3.9186	1.16935	-0.33656
C	3.79329	2.51281	-0.61337
C	5.11627	3.13005	-0.70808
H	5.30474	4.17225	-0.92452
C	6.01525	2.15304	-0.44827
H	7.09243	2.22852	-0.40271
C	5.23691	0.93796	-0.19328
C	5.78386	-0.28082	0.26914
N	3.66792	-1.4862	0.4013
H	3.15353	-0.65726	0.10502
C	5.02045	-1.38122	0.61704
C	5.41662	-2.57398	1.32903
H	6.43193	-2.79952	1.61796
C	4.29811	-3.3073	1.584
H	4.2371	-4.2553	2.0978
C	3.16529	-2.64362	0.98085
C	1.88058	-3.11033	0.89923
N	-0.4576	-3.05902	0.14591
H	-0.8335	-3.55761	0.93652
C	-1.21129	-2.64621	-0.92457
C	-0.35844	-1.95253	-1.77436
H	-0.64574	-1.51862	-2.71872
C	0.92513	-1.94577	-1.19224
H	1.82603	-1.54058	-1.6238
C	0.8601	-2.65219	0.01385
C	-2.59478	-3.11173	-1.08824
N	-3.85092	-1.22381	-0.12949
C	-3.73151	-2.4941	-0.68293
C	-5.06195	-3.12634	-0.7682
H	-5.25351	-4.11335	-1.16456
C	-5.93509	-2.25186	-0.23961
H	-7.0037	-2.3598	-0.11668

C	-5.15468	-1.05491	0.12605
C	-5.74508	0.13401	0.6096
H	-2.09544	4.46621	0.50176
H	2.70224	4.29886	-0.78489
H	6.85052	-0.33152	0.44629
H	1.64709	-3.97195	1.51695
H	-2.71313	-4.08044	-1.56959
H	-6.80642	0.13286	0.82063

28TS$_{1B}$

C	-5.23908	-0.91392	0.1034
N	-3.92025	-1.22665	-0.15908
C	-3.81272	-2.49219	-0.71551
C	-5.17636	-3.01655	-0.76324
C	-6.01469	-2.08885	-0.25097
C	-2.69449	-3.13828	-1.12794
C	-1.30981	-2.68358	-0.9537
N	-0.58646	-3.04302	0.15395
C	0.73279	-2.62991	0.04332
C	0.8295	-1.97179	-1.18978
C	-0.43257	-2.01208	-1.80593
C	1.72309	-3.03143	0.97825
C	3.02632	-2.59835	1.04848
N	3.54963	-1.51708	0.36428
C	4.86628	-1.5162	0.62085
C	5.23828	-2.63587	1.48163
C	4.08312	-3.27978	1.78496
C	5.75533	-0.48653	0.19824
C	5.33226	0.73879	-0.26191
N	4.00807	1.10675	-0.38083
C	3.89238	2.45765	-0.63877
C	5.24708	2.94831	-0.78949
C	6.10872	1.91979	-0.5694
C	2.73796	3.20115	-0.66451
C	1.41849	2.70647	-0.48229
N	0.37318	3.52249	-0.1245
C	-0.80317	2.79691	0.01431
C	-0.4797	1.46636	-0.31611
C	0.87541	1.40865	-0.61519
C	-1.99592	3.41555	0.43815
C	-3.24118	2.85651	0.63965
N	-3.59577	1.53682	0.43667
C	-4.90933	1.46916	0.69965
C	-5.44274	2.76337	1.10877
C	-4.39853	3.62826	1.06975
C	-5.70439	0.29695	0.53975

H	-6.47053	2.96387	1.37576
H	-4.39591	4.68487	1.29801
H	0.47321	4.49376	0.12303
H	1.40992	0.53751	-0.94709
H	-1.1854	0.65578	-0.34284
H	5.49226	3.97374	-1.02265
H	7.1877	1.94961	-0.58431
H	6.23815	-2.86048	1.82491
H	3.95046	-4.15479	2.40569
H	-0.97562	-3.54439	0.9367
H	-0.69831	-1.61767	-2.77399
H	1.75065	-1.57405	-1.58095
H	-5.42339	-3.99855	-1.1379
H	-7.08583	-2.15925	-0.13349
H	-1.93122	4.4835	0.63353
H	2.86122	4.27255	-0.7819
H	6.81877	-0.63447	0.33737
H	1.44019	-3.81944	1.67198
H	-2.84041	-4.09855	-1.61413
H	-6.76872	0.38279	0.72072
H	-3.20576	-0.5093	-0.08804
H	3.28578	0.44631	-0.10037

28TS$_{2A}$

N	-3.34239	1.49443	0.62851
H	-2.94455	0.71591	0.1085
C	-4.63261	1.37551	1.10324
C	-4.98402	2.65244	1.64091
H	-5.9304	2.88152	2.10649
C	-3.93079	3.50665	1.42556
H	-3.86877	4.55102	1.69206
C	-2.88547	2.78296	0.76309
C	-1.6663	3.29982	0.32637
N	0.58344	3.25678	-0.61482
H	0.77465	4.22588	-0.41814
C	1.56228	2.34143	-0.96607
C	0.94144	1.06641	-0.90267
H	1.41373	0.14216	-1.18276
C	-0.35718	1.22791	-0.47839
H	-1.06977	0.43262	-0.35192
C	-0.58911	2.61633	-0.24223
C	2.88143	2.69063	-1.27211
N	3.98692	0.60899	-0.57212
C	3.99308	1.85707	-1.12912
C	5.36963	2.25708	-1.3315
H	5.68045	3.19559	-1.76748

C	6.16514	1.26645	-0.82892
H	7.24368	1.2464	-0.77607
C	5.28406	0.25313	-0.30595
C	5.55948	-0.8062	0.56932
N	3.2162	-1.31054	0.74389
H	3.23874	-0.27501	0.00665
C	4.50401	-1.4955	1.1815
C	4.47554	-2.26479	2.39727
H	5.3418	-2.58708	2.95629
C	3.15704	-2.45581	2.71666
H	2.75647	-2.99392	3.56357
C	2.36834	-1.89511	1.64592
C	0.98916	-2.03668	1.45715
N	-0.99089	-2.08015	-0.0013
H	-1.70371	-1.78331	0.65319
C	-1.30919	-2.46535	-1.28812
C	-0.06748	-2.72959	-1.93971
H	0.02328	-3.07337	-2.95894
C	0.95113	-2.47543	-1.05418
H	2.01089	-2.59041	-1.2116
C	0.37154	-2.10711	0.20401
C	-2.61042	-2.60671	-1.76847
N	-3.71484	-1.11611	-0.19275
C	-3.75396	-2.09974	-1.14106
C	-5.12291	-2.51174	-1.3864
H	-5.43374	-3.27153	-2.08926
C	-5.90153	-1.78743	-0.53504
H	-6.97654	-1.8184	-0.42774
C	-5.00975	-0.87393	0.15817
C	-5.42341	0.24875	0.89413
H	-1.54794	4.36883	0.47268
H	3.0886	3.72807	-1.51598
H	6.57926	-0.99275	0.87915
H	0.37526	-2.213	2.33465
H	-2.73411	-3.16221	-2.6908
H	-6.46156	0.31057	1.19749

28TS$_{2B}$

C	-5.09649	-0.83122	0.20487
N	-3.79217	-0.93905	-0.22212
C	-3.76844	-1.85748	-1.24931
C	-5.10484	-2.34925	-1.45933
C	-5.91221	-1.7619	-0.52279
C	-2.61744	-2.28556	-1.91159
C	-1.31924	-2.24836	-1.40057
N	-0.99587	-2.08725	-0.0671

C	0.36756	-2.19064	0.12947
C	0.93665	-2.38462	-1.16776
C	-0.08565	-2.45419	-2.08327
C	0.99373	-2.29667	1.37713
C	2.37288	-2.14649	1.56346
N	3.16544	-1.48104	0.68093
C	4.44001	-1.57929	1.13974
C	4.47442	-2.38642	2.35134
C	3.17865	-2.68861	2.6473
C	5.49634	-0.81867	0.60125
C	5.27857	0.28782	-0.21964
N	4.01313	0.70889	-0.55784
C	4.03132	1.98827	-1.05005
C	5.418	2.35214	-1.15558
C	6.17368	1.32	-0.65586
C	2.90614	2.79406	-1.20782
C	1.58551	2.37981	-0.96731
N	0.5824	3.23888	-0.55857
C	-0.57696	2.53828	-0.24622
C	-0.31663	1.18578	-0.593
C	0.99104	1.08766	-1.01832
C	-1.66149	3.14749	0.38339
C	-2.86526	2.60192	0.83383
N	-3.36224	1.33312	0.67377
C	-4.62315	1.31204	1.2255
C	-4.9137	2.58915	1.81649
C	-3.83751	3.38719	1.56359
C	-5.48638	0.23053	1.02445
H	-5.82901	2.84623	2.32852
H	-3.70531	4.42479	1.83489
H	0.75394	4.18636	-0.26282
H	1.47335	0.19533	-1.3778
H	-1.03344	0.38782	-0.53143
H	5.77266	3.29878	-1.53468
H	7.24783	1.28601	-0.55416
H	5.35949	-2.63874	2.91825
H	2.80635	-3.26056	3.48542
H	-1.68457	-1.91029	0.64922
H	-0.00338	-2.63183	-3.1448
H	1.9937	-2.50306	-1.33521
H	-5.37772	-3.09487	-2.19198
H	-6.97148	-1.91259	-0.3752
H	-1.55249	4.20846	0.59135
H	3.08877	3.84773	-1.39051
H	6.50694	-1.00435	0.94329
H	0.38362	-2.55672	2.23674
H	-2.73946	-2.74264	-2.88669

H	-6.50552	0.28923	1.38303
H	-3.2346	0.17764	0.06693
H	3.22067	0.15577	-0.21606

28TS$_3$

N	-2.83069500	1.55643400	0.82934800
H	-2.58849100	0.78403100	0.21570400
C	-4.08347100	1.60839100	1.39337500
C	-4.06763800	2.74106700	2.29397500
H	-4.91065400	3.05473000	2.89093700
C	-2.83362500	3.31399500	2.23979600
H	-2.49582800	4.19040100	2.77306800
C	-2.02862000	2.59443900	1.27670300
C	-0.77983200	2.92793300	0.82088000
N	1.26404900	2.65299300	-0.50271300
H	1.87432000	3.07636700	0.17814700
C	1.71076000	2.09701100	-1.67441900
C	0.62013500	1.47421800	-2.26652000
H	0.63929100	0.94941800	-3.20827400
C	-0.49164900	1.64124200	-1.41601200
H	-1.49661000	1.30489400	-1.61468400
C	-0.08199100	2.38426600	-0.30238000
C	3.12559300	2.22048900	-2.06642100
N	3.84376400	0.51051400	-0.52024800
C	4.10075800	1.48715600	-1.47092400
C	5.55694300	1.67565300	-1.59276000
H	6.04529200	2.36500700	-2.26677600
C	6.12309300	0.87263300	-0.66922200
H	7.17422000	0.75906500	-0.44227500
C	5.01976000	0.14693800	-0.00798500
C	5.14322900	-0.77398500	1.06344600
N	2.81684300	-1.47748500	0.96878200
H	2.63681500	-0.82568000	0.20102600
C	4.04920300	-1.46036000	1.57011300
C	3.90580400	-2.19107000	2.81157000
H	4.71346400	-2.38915500	3.50003400
C	2.59265100	-2.52351600	2.95901000
H	2.14285800	-3.06787500	3.77622000
C	1.87799900	-2.10044200	1.77546200
C	0.56588300	-2.32718000	1.44591300
N	-1.33477600	-2.14661100	-0.10217200
H	-2.02546700	-1.73585100	0.51701200
C	-1.64232400	-2.41191300	-1.41642900
C	-0.43257100	-2.76556900	-2.04701300
H	-0.33501200	-3.06190800	-3.08030300
C	0.59014000	-2.65928300	-1.10667500

H	1.63354000	-2.88881400	-1.25250200
C	0.00980100	-2.29427700	0.12919400
C	-2.97044400	-2.33319600	-1.92127300
N	-3.77231200	-0.77191600	-0.25208000
C	-3.99298800	-1.64866700	-1.29917100
C	-5.41963700	-1.72301700	-1.57695200
H	-5.88080700	-2.32884600	-2.34420200
C	-6.03406700	-0.92675700	-0.66302700
H	-7.09265600	-0.73528600	-0.55761700
C	-4.97286900	-0.30113800	0.12408100
C	-5.12362700	0.75608400	1.05937400
H	-0.28563900	3.73290200	1.35618800
H	3.40217300	2.97168200	-2.80080000
H	6.10252600	-0.89694800	1.54858100
H	-0.09380100	-2.63698200	2.25041900
H	-3.18045500	-2.86528900	-2.84226900
H	-6.10558700	0.96977400	1.46167000

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32F

C	-0.25482	-2.17261	-1.85021
C	-0.90368	-0.97952	-1.8653
C	0.06316	0.07422	-1.59519
C	-0.07501	1.43864	-1.53083
C	-1.29972	2.15824	-1.43805
C	-1.53602	3.54264	-1.62608
C	-2.88946	3.78208	-1.40971
C	-3.49506	2.55509	-1.05787
C	-4.82074	2.2354	-0.70662
C	-5.24725	0.99425	-0.25863
N	-4.37933	-0.04869	0.02666
C	-5.14255	-1.11273	0.32697
C	-4.59757	-2.38222	0.70168
C	-3.28367	-2.57797	1.0451
C	-2.57274	-3.81054	1.32279
C	-1.2684	-3.51008	1.5518
C	-1.09945	-2.06816	1.47906
C	0.06013	-1.36163	1.65452
C	0.21502	0.05953	1.66566
N	1.41072	0.6107	1.47141
C	1.24042	1.98297	1.55993
C	2.27473	2.87929	1.39071
C	3.59998	2.51659	1.03053
C	4.77969	3.29206	0.91965

C	5.81149	2.43792	0.54174
C	5.26321	1.14076	0.38414
C	5.87082	-0.07148	-0.04146
C	5.18134	-1.19203	-0.45357
N	3.81172	-1.2175	-0.6317
C	3.49127	-2.45977	-1.01069
C	2.16561	-2.84016	-1.36361
C	1.14121	-1.93166	-1.54344
N	-2.4966	1.60288	-1.10071
C	-6.61256	0.54575	-0.0997
C	-6.55125	-0.77576	0.23699
N	-2.34784	-1.56956	1.17184
C	-0.80065	1.09152	1.91373
C	-0.15526	2.28368	1.85227
N	3.93737	1.23503	0.69618
C	5.73619	-2.50818	-0.74994
C	4.6849	-3.30685	-1.06642
N	1.27813	-0.57096	-1.44902
H	-1.84302	0.93146	2.14347
H	-0.57548	3.27016	1.98502
H	4.84563	4.35294	1.10659
H	6.84265	2.70005	0.36098
H	6.7818	-2.77577	-0.69517
H	4.70348	-4.35188	-1.34142
H	-0.68021	-3.14897	-2.025
H	-1.94562	-0.82261	-2.09266
H	-0.78222	4.25883	-1.91388
H	-3.40493	4.72748	-1.48446
H	-7.49455	1.15054	-0.2551
H	-7.37288	-1.45089	0.42815
H	-3.033	-4.78717	1.32162
H	-0.4644	-4.19241	1.78278
H	-2.69613	0.65927	-0.7841
H	-2.59632	-0.62	0.93143
H	-5.56134	3.01881	-0.82261
H	-5.25922	-3.2391	0.72068
H	1.94949	-3.88757	-1.53077
H	0.82855	2.03505	-1.48506
H	6.95449	-0.10287	-0.04376
H	2.07331	3.93526	1.52991
H	0.97553	-1.93464	1.73714
H	2.14359	-0.17787	-1.08923
H	3.27196	0.46286	0.76301

32M$_A$

C	-0.33038	-1.98331	-0.44338
C	0.55801	-1.93685	-1.56338
H	1.6215	-2.11006	-1.52388
C	-0.19616	-1.72425	-2.69919

H	0.16243	-1.66598	-3.71542
C	-1.5608	-1.60023	-2.3108
C	-2.72286	-1.4214	-3.07224
C	-3.98734	-1.21516	-2.52042
C	-5.25999	-1.34233	-3.20833
H	-5.38643	-1.56813	-4.2575
C	-6.22656	-1.16527	-2.26707
H	-7.29849	-1.19188	-2.40125
C	-5.53755	-0.8507	-1.02407
C	-6.15562	-0.38486	0.15089
C	-5.5144	0.343	1.14655
C	-6.10131	1.02827	2.26278
H	-7.13126	0.92226	2.5679
C	-5.14908	1.8431	2.81032
H	-5.26076	2.51562	3.64728
C	-3.92524	1.67632	2.07599
C	-2.76382	2.41908	2.21602
C	-1.54283	2.23953	1.53334
C	-1.06059	1.01218	0.898
H	-1.56175	0.06153	0.89891
C	0.14909	1.30819	0.36326
H	0.78067	0.65497	-0.2185
C	0.37354	2.72369	0.64828
C	1.35081	3.55979	0.11749
C	2.49036	3.23317	-0.6249
C	3.19875	4.11617	-1.48986
H	2.91815	5.14394	-1.66244
C	4.22975	3.418	-2.0724
H	4.95335	3.7834	-2.7849
C	4.22969	2.10025	-1.53108
C	5.2496	1.15253	-1.64754
C	5.42752	0.00565	-0.87549
C	6.72431	-0.63823	-0.71959
H	7.61002	-0.40653	-1.29373
C	6.59941	-1.49741	0.32299
H	7.35543	-2.13247	0.76204
C	5.20827	-1.43383	0.74057
C	4.66212	-2.21337	1.77119
C	3.30734	-2.41212	1.9933
C	2.65414	-3.10336	3.06249
H	3.16692	-3.55979	3.89519
C	1.30433	-3.06718	2.8307
H	0.52139	-3.50585	3.43036
C	1.07837	-2.40219	1.58065
C	-0.12919	-2.29243	0.90859
N	-1.58701	-1.75948	-0.94736
H	-2.46588	-1.6576	-0.44355
N	-4.19434	-0.91432	-1.19721
N	-4.18562	0.70877	1.12001
H	-3.61997	0.4844	0.30732

N	-0.65433	3.23831	1.38902
N	3.1344	2.0114	-0.69962
H	3.03104	1.23101	-0.06123
N	4.51501	-0.52864	-0.00789
N	2.31509	-1.99757	1.13129
H	2.53296	-1.38816	0.35181
H	6.06668	1.43056	-2.30342
H	5.34825	-2.73297	2.42911
H	-2.82666	3.29063	2.85798
H	1.16505	4.62132	0.2421
H	-7.23143	-0.48076	0.23364
H	-2.63043	-1.48942	-4.14937
H	-1.01332	-2.52613	1.49199

32M$_B$

C	-0.36649	-1.9632	-0.28045
C	0.52811	-1.96023	-1.402
H	1.59507	-2.0675	-1.30262
C	-0.22347	-1.83419	-2.54438
H	0.13456	-1.81891	-3.56262
C	-1.59996	-1.71993	-2.16877
C	-2.75226	-1.62542	-2.94811
C	-4.03351	-1.41407	-2.42145
C	-5.29627	-1.63785	-3.09891
H	-5.41107	-1.96104	-4.12366
C	-6.2746	-1.40265	-2.17942
H	-7.34454	-1.47058	-2.31534
C	-5.6022	-0.96107	-0.97029
C	-6.2257	-0.39846	0.15566
C	-5.59175	0.42292	1.08206
C	-6.17763	1.20723	2.1245
H	-7.20689	1.1297	2.44025
C	-5.22451	2.0751	2.5932
H	-5.33847	2.82159	3.3646
C	-4.00723	1.84391	1.87295
C	-2.83869	2.59927	1.94693
C	-1.62047	2.33766	1.3097
C	-1.07103	1.12179	0.80233
H	-1.5563	0.16654	0.86865
C	0.18759	1.37317	0.30681
H	0.88324	0.67222	-0.12376
C	0.44728	2.76676	0.44618
C	1.4644	3.57159	-0.05774
C	2.65172	3.19472	-0.6971
C	3.45898	4.16192	-1.43724
H	3.22881	5.21167	-1.55394
C	4.50401	3.46935	-1.94796
H	5.32035	3.83453	-2.55483
C	4.35805	2.10256	-1.45475

C	5.3855	1.1597	-1.57473
C	5.5428	-0.02841	-0.86791
C	6.76472	-0.76449	-0.72716
H	7.6687	-0.54891	-1.27621
C	6.58153	-1.7068	0.24917
H	7.30314	-2.41364	0.62953
C	5.22405	-1.62448	0.69663
C	4.62045	-2.3853	1.6945
C	3.25036	-2.45686	1.96133
C	2.65427	-3.09195	3.13314
H	3.19836	-3.55221	3.94567
C	1.31245	-2.95699	2.98987
H	0.53031	-3.30421	3.65013
C	1.1078	-2.30734	1.69627
C	-0.13948	-2.18961	1.0775
N	-1.62843	-1.79268	-0.79657
H	-2.51116	-1.70854	-0.29996
N	-4.25321	-1.00407	-1.13549
N	-4.26115	0.79598	1.01492
H	-3.69449	0.48301	0.23066
N	-0.6578	3.2986	1.09787
N	3.21541	1.95773	-0.73251
N	4.63103	-0.61332	-0.02473
N	2.29307	-1.97711	1.12691
H	6.23675	1.45026	-2.18032
H	5.28501	-2.98542	2.30556
H	-2.91754	3.52023	2.51562
H	1.30056	4.64441	0.0088
H	-7.30025	-0.50018	0.25006
H	-2.64595	-1.76137	-4.01756
H	-1.01377	-2.36487	1.69776
H	3.68101	-0.28372	0.11285
H	-0.7907	4.2809	1.27579

32H

C	-5.98204	-1.1585	1.05164
C	-6.61772	-2.44756	1.22329
H	-7.62663	-2.57999	1.58358
C	-5.75086	-3.40509	0.80912
H	-5.90963	-4.47287	0.78294
C	-4.51136	-2.76681	0.4141
C	-3.40061	-3.398	-0.06942
C	-2.09754	-2.85018	-0.26884
C	-1.40586	-1.79869	0.36543
H	-1.83732	-1.14513	1.10523
C	-0.06785	-1.8493	-0.03735
H	0.75302	-1.23348	0.28909
C	0.07138	-2.91035	-0.94538
C	1.17646	-3.49991	-1.60629

C	2.51999	-3.34892	-1.36865
C	3.49558	-4.30678	-1.87899
H	3.29811	-5.06716	-2.62152
C	4.63294	-4.09025	-1.17937
H	5.57152	-4.62257	-1.23961
C	4.35502	-2.95244	-0.30104
C	5.4681	-1.22197	1.17554
C	6.55449	-0.84702	2.0629
H	7.27143	-1.55216	2.45575
C	6.50907	0.48797	2.25712
H	7.18325	1.09917	2.83795
C	5.40235	1.0272	1.48645
C	5.22016	2.36216	1.25269
C	4.30573	3.00986	0.36919
C	4.62608	4.31051	-0.22678
H	5.52529	4.88075	-0.04204
C	3.59759	4.60471	-1.05222
H	3.4617	5.48072	-1.67079
C	2.62284	3.52955	-0.88176
C	1.33386	3.66622	-1.33228
C	0.16226	2.9632	-0.95722
C	-0.08414	1.85052	-0.12857
H	0.69794	1.26033	0.31866
C	-1.46387	1.7239	0.02226
H	-2.00875	1.01549	0.61935
C	-2.0856	2.76433	-0.70027
C	-3.42099	3.23559	-0.75755
C	-4.56271	2.66056	-0.25576
C	-5.83942	3.36482	-0.1763
H	-6.01779	4.37431	-0.51908
C	-6.70451	2.52028	0.43099
H	-7.74454	2.68457	0.67414
C	-5.96245	1.28134	0.66764
C	-6.56708	0.08268	1.13069
N	-4.6928	-1.40897	0.63013
H	-4.12288	-0.64159	0.27841
N	-1.18452	-3.48097	-1.07302
N	3.10982	-2.50087	-0.44039
N	4.75298	-0.05982	0.9279
N	3.12311	2.54835	-0.03629
N	-1.07165	3.47244	-1.3032
H	-1.20909	4.30242	-1.85741
N	-4.68525	1.3886	0.27243
C	5.33345	-2.46096	0.61809
H	-7.60172	0.12525	1.44665
H	-3.51966	-4.45477	-0.28737
H	0.92378	-4.2801	-2.32109
H	6.12554	-3.15868	0.86774
H	5.95908	3.00838	1.71345
H	1.16492	4.52983	-1.97171

H	-3.55316	4.21493	-1.21129
H	3.96871	0.00869	0.29276
H	-1.39149	-4.28374	-1.64511

32TS$_1$

C	-0.01234	0.30498	-1.77508
C	-0.9367	-0.75679	-1.95667
H	-2.00697	-0.65781	-2.03672
C	-0.21305	-1.93321	-2.09496
H	-0.60933	-2.92136	-2.27059
C	1.16023	-1.61848	-1.97859
C	2.30383	-2.43693	-2.11925
C	3.59945	-2.01708	-1.897
C	4.81624	-2.70917	-2.28661
H	4.86117	-3.67582	-2.76771
C	5.84769	-1.8856	-1.96366
H	6.90537	-2.05592	-2.10524
C	5.25712	-0.72259	-1.30764
C	5.98894	0.28422	-0.62217
C	5.45826	1.06059	0.38418
C	6.17513	1.92178	1.30974
H	7.21605	2.18739	1.2001
C	5.33608	2.26458	2.31518
H	5.55718	2.86833	3.18258
C	4.03563	1.66069	2.06067
C	2.94929	1.61901	2.86462
C	1.68597	0.97432	2.46981
C	0.65983	1.60192	1.64001
H	0.70607	2.59356	1.21466
C	-0.34049	0.68926	1.51886
H	-1.25945	0.81745	0.97126
C	0.1041	-0.49154	2.23798
C	-0.43162	-1.7498	2.33364
C	-1.64496	-2.29517	1.8503
C	-2.03185	-3.64859	1.96869
H	-1.41603	-4.41866	2.40724
C	-3.30696	-3.78557	1.43962
H	-3.9029	-4.68315	1.38169
C	-3.7239	-2.5131	0.99136
C	-4.99631	-2.1357	0.49818
C	-5.38264	-0.878	0.08894
C	-6.76529	-0.45625	-0.10065
H	-7.63005	-1.09951	-0.02193
C	-6.73217	0.87917	-0.32741
H	-7.56306	1.5495	-0.49443
C	-5.3227	1.26088	-0.34913
C	-4.84518	2.55403	-0.65972
C	-3.52567	2.82245	-0.97737
C	-2.87425	4.07503	-1.26966

H	-3.36898	5.03412	-1.26228
C	-1.56019	3.81868	-1.53201
H	-0.79126	4.5303	-1.79283
C	-1.34294	2.39473	-1.45174
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H	2.1335	0.18297	-1.60548
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H	3.5182	0.32121	0.45856
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N	-2.689	-1.64225	1.23226
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H	-2.7959	0.88662	-0.87833
H	-5.75526	-2.90922	0.5237
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C	-4.28172122	-0.28921061	5.16609397
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C	-2.54120520	-1.00265497	-3.99513292
C	-2.61724913	-0.49318523	-2.62680155
C	-1.47337515	-0.30774350	-1.88506461
C	-1.27985340	-0.09082466	-0.49998675
C	-2.13991687	-0.08711246	0.61898678
C	-1.35611597	-0.04236129	1.76784222
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C	-1.01870205	-1.90777991	8.28682815
N	-4.75973206	0.98878371	5.08688849
N	-6.69443135	2.27937546	1.26422496
C	-8.36499457	0.25663839	-3.27645356
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N	-3.93687541	-0.33851433	-2.23699427
H	3.63021849	-0.97278655	5.85391622
H	3.78503876	-0.12909071	3.30121433
H	-1.70045943	-0.03438258	2.78737085
H	-3.21323179	-0.13677991	0.55074679
H	-1.62773256	-1.20394738	-4.53687452
H	-4.17175733	-1.59094472	-5.33640726
H	-8.76617596	-0.25505304	-4.13818195
H	-9.94807402	1.62671370	-2.64038489
H	-8.59441316	5.01586087	0.94348233
H	-7.07335994	5.03555621	3.16776841
H	-5.22038378	0.03866084	1.99905208
H	-4.11630298	-1.84773663	3.62137197
H	-3.09503435	-1.96502504	8.96710824
H	-0.44281001	-2.25144618	9.13310396
H	-4.78635017	1.62867528	5.86492549
H	1.61178749	-1.68415878	7.45942043
H	2.10706735	0.18400045	1.44687717
H	-0.55306455	-0.42788717	-2.45258299
H	-6.44580966	-1.16973308	-4.34213175
H	-9.22633126	3.14041471	-0.75516120
H	-5.68434691	3.27436640	4.33859990
H	-4.72871639	-0.96855342	7.18784166
H	0.83268656	-0.04566457	-0.56555576
H	-1.30892800	-0.80608580	5.26269075
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