

–Supplementary Material–
**Investigating the (poly)radicaloid nature
of real-world organic compounds by
DFT-based methods**

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1 Error estimates

When needed, the Mean Signed Error (MSE) and Mean Unsigned Error (MUE) will be used to estimate the deviations between computational (a_i) and experimental (e_i) results for energy differences:

$$\text{MSE} = \frac{1}{N} \sum_i^N (a_i - e_i), \quad (\text{S1})$$

$$\text{MUE} = \frac{1}{N} \sum_i^N |a_i - e_i|, \quad (\text{S2})$$

as well as the Minimum (MIN) and Maximum (MAX) deviations.

2 Results from the RAS-SF method

Table S1: N_U and energy difference (kcal/mol) between the low-spin (LS) and high-spin (HS) states, $\Delta E(\text{LS} - \text{HS})$, obtained at the RAS-SF level.

Compound	GS	$N_U(\text{LS})$	$N_U(\text{HS})$	$\Delta E(\text{LS} - \text{HS})$	Exp.
Diradical I	T ₀	2.03	2.08	0.28 ^a	0.50±0.02
Diradical II	T ₀	2.05	2.09	1.12 ^a	1.74±0.07
[6]CPPM-Mes	S ₀	2.54	3.43	-9.41 ^b	-6.23±0.78
[3]CPBM-Ant	D ₀	1.70	3.00	-4.19 ^c	-3.5
[4]CPBM-Ant	S ₀	2.95	3.47	-3.40 ^c	-2.8
[5]CPBM-Ant	D ₀	3.94	4.51	-3.40 ^c	-2.4
[6]CPBM-Ant	S ₀	4.61	4.98	-1.63 ^c	-2.2
MC-F3A3	D ₀	2.58	3.00	-1.66 ^a	-2.10
8MC	S ₀	4.85	5.39	-2.70 ^d	-3.08

^a Done here (see Computational Details).

^b Taken from Wu *et al.*¹

^c Taken from Wu *et al.*²

^d Taken from Wu *et al.*³

3 Radical(oid) indices

Table S2: Calculated radical indices y_i^α by the FT-DFT method at the TPSS0/def2-TZVP level.

Compound	y_0^α	y_1^α	y_2^α	y_3^α
Diradical I	0.49	0.06	0.05	0.02
Diradical II	0.49	0.07	0.02	0.02
[6]CPPM-Mes	0.31	0.29	0.10	0.03
[3]CPBM-Ant	0.37	0.13	0.13	0.13
[4]CPBM-Ant	0.32	0.27	0.11	0.11
[5]CPBM-Ant	0.35	0.33	0.12	0.12
[6]CPBM-Ant	0.37	0.33	0.27	0.11
MC-F3A3	0.52	0.12	0.12	0.12
8MC	0.37	0.37	0.30	0.30

Table S3: Calculated radical indices y_i^α by the FT-DFT method at the TPSSHH/def2-TZVP level.

Compound	y_0^α	y_1^α	y_2^α	y_3^α
Diradical I	0.48	0.08	0.07	0.03
Diradical II	0.49	0.09	0.04	0.03
[6]CPPM-Mes	0.32	0.31	0.13	0.05
[3]CPBM-Ant	0.36	0.15	0.15	0.15
[4]CPBM-Ant	0.33	0.29	0.14	0.14
[5]CPBM-Ant	0.36	0.34	0.15	0.15
[6]CPBM-Ant	0.38	0.34	0.29	0.14
MC-F3A3	0.53	0.14	0.14	0.14
8MC	0.40	0.39	0.33	0.33

4 Calculation of ZFS tensor

By default, the g-tensor is used as reference tensor for $|D| < 0.3 \text{ cm}^{-1}$, with its axes assigned depending on their magnitude:

$$|g_{min}\rangle \longrightarrow |g_x\rangle, \quad (\text{S3})$$

$$|g_{mid}\rangle \longrightarrow |g_y\rangle, \quad (\text{S4})$$

$$|g_{max}\rangle \longrightarrow |g_z\rangle, \quad (\text{S5})$$

and thus proper care should be given if previous or future calculations re-assign this ordering. The D-tensor is used as reference only if $S > 1/2$ and $|D| > 0.3 \text{ cm}^{-1}$, which is not the case here.

Table S4: Comparison between calculated and experimental EPR parameter for the triplet state of Diradical I and II, with the EPR-II basis set.

Method	Diradical I			Diradical II		
	D/hc (10^3 cm^{-1})	E/hc (10^3 cm^{-1})	g-tensor	D/hc (10^3 cm^{-1})	E/hc (10^3 cm^{-1})	g-tensor
HF	-5.03	-0.94	2.0063	12.37	2.13	2.0064
HF-PBE	-5.11	-0.93	2.0064	12.32	2.27	2.0065
TPSS	-5.42	-1.68	2.0048	12.14	3.30	2.0048
TPSS0	-5.42	-1.28	2.0052	11.87	3.25	2.0052
TPSSHH	-5.39	-1.10	2.0056	11.77	3.01	2.0056
PBE0	-5.44	-1.28	2.0053	11.90	3.34	2.0053
M06-2X	-5.53	-1.02	2.0064	11.75	3.58	2.0064
CAM-B3LYP	-5.51	-0.96	2.0054	11.58	3.57	2.0055
LC-BLYP	-5.58	-0.80	2.0054	-11.48	-3.72	2.0054
ω B97XD	-5.56	-0.83	2.0055	11.41	3.80	2.0055
Exp. values ^a	-2.32	-0.14	2.0044	-8.08	-1.17	2.0050

^a Taken from Rajca *et al.*⁴

Table S5: Comparison between calculated and experimental EPR parameter for the triplet state of Diradical I and II, with the IGLO-II basis set.

Method	Diradical I			Diradical II		
	D/hc (10^3 cm^{-1})	E/hc (10^3 cm^{-1})	g-tensor	D/hc (10^3 cm^{-1})	E/hc (10^3 cm^{-1})	g-tensor
TPSS	-5.37	-1.60	2.0049	11.81	3.26	2.0049
TPSS0	-5.37	-1.23	2.0053	11.49	3.21	2.0053
TPSSHH	-5.35	-1.06	2.0057	11.34	2.97	2.0057
PBE0	-5.39	-1.22	2.0055	11.53	3.28	2.0055
M06-2X	-5.48	-0.98	2.0065	11.35	3.52	2.0066
CAM-B3LYP	-5.47	-0.92	2.0056	11.22	3.51	2.0056
LC-BLYP	-5.54	-0.77	2.0056	-11.20	-3.59	2.0056
ω B97XD	-5.52	-0.80	2.0056	-11.13	-3.66	2.0056
Exp. values ^a	-2.32	-0.14	2.0044	-8.08	-1.17	2.0050

^a Taken from Rajca *et al.*⁴

4.1 Theoretical estimates of the exciton size

If the spin-orbit and crystal-field contributions to the ZFS are neglected, which is a reasonable assumption for organic systems,⁵ the D parameter can be formulated as:⁶

$$D = \frac{3}{4} \frac{\mu_0}{4\pi\hbar} (g_e\mu_B)^2 \left\langle \frac{1 - 3\cos^2\theta}{r^3} \right\rangle, \quad (\text{S6})$$

with r the distance between the spins of the unpaired electrons, θ the angle between the spin vectors and the dipolar z -axis, and μ_0 , g_e , and μ_B physical constants. Note that the sign of D depends on the $(1 - 3\cos^2\theta)$ term, with $D > 0$ ($D < 0$) an oblate (prolate) shape of the spin distribution. If D is given in cm^{-1} , while using \AA as length unit, one arrives to the expression:

$$|D| = 0.6495 \frac{g^2}{r_{AB}^3}, \quad (\text{S7})$$

from which we estimate the exciton size r_{AB} (or simply Δr) as that determining:

$$|D| \propto \iint \sigma_A(\mathbf{r}_A) \frac{1}{r_{AB}^3} \sigma_B(\mathbf{r}_B) d\mathbf{r}_A d\mathbf{r}_B, \quad (\text{S8})$$

in terms of spin densities around radical centers A and B .

5 Cartesian coordinates of all compounds

All the calculations were performed at the molecular geometries extracted from literature, to consistently compare FT-DFT, SF-DFT, SF-TDDFT, and RAS-SF methods. The exception was the MC-F3A3 system, for which the B97-3c composite method⁷ was used here.

Table S3: Cartesian coordinates of Diradical-I

C	0.00981	-0.05729	-0.00718
C	0.00284	-0.06449	1.37993
C	1.20113	-0.04103	2.11492
C	2.42243	0.02925	1.38568
C	2.41616	-0.00199	-0.01325
C	1.21595	-0.04157	-0.73476
H	-0.93886	-0.07868	-0.52936
H	-0.92556	-0.10596	1.93970
H	3.36039	-0.00232	-0.54187
C	2.36047	-0.18945	4.09043
N	1.17170	-0.11628	3.48074
N	3.56451	-0.10235	3.51278
N	3.58599	0.08809	2.16158
C	2.37179	-0.37006	5.56780
C	3.57561	-0.39752	6.28888
C	1.15934	-0.51625	6.25773
C	3.56361	-0.57044	7.67093
H	4.51196	-0.27827	5.75644
C	1.15210	-0.68777	7.64038
H	0.23514	-0.49174	5.69237
C	2.35296	-0.71629	8.35207
H	4.50165	-0.58918	8.21842
H	0.20667	-0.80006	8.16343
H	2.34609	-0.85018	9.43010
C	4.89219	0.29299	1.62749
C	5.94886	-0.51306	2.06360
C	5.14314	1.32426	0.71516
C	7.23267	-0.31329	1.57425
H	5.75301	-1.29318	2.78934
C	6.42577	1.52984	0.22225
H	4.33926	1.98328	0.40716
C	7.49693	0.70921	0.63644
H	8.04153	-0.95039	1.90184
H	6.61616	2.33724	-0.47003
C	8.84697	0.91843	0.11301
C	10.63957	1.72245	-1.23565
C	11.21012	0.75909	-0.15065
N	9.23265	1.92103	-0.72788
N	9.93828	0.14400	0.37980
O	10.00109	-0.89755	1.11435
O	8.51489	2.85827	-1.21375
C	11.86582	1.47190	1.04612
H	12.03394	0.73688	1.83660
H	12.82701	1.90778	0.76164
H	11.22702	2.26425	1.44492
C	12.13090	-0.34686	-0.66545
H	13.05569	0.08974	-1.05377
H	12.37859	-1.01837	0.15797
H	11.66561	-0.94013	-1.45367
C	11.33315	3.07969	-1.34795
H	12.35633	2.94591	-1.71118
H	10.78729	3.70234	-2.05829
H	11.36616	3.60880	-0.39472
C	10.49862	1.09147	-2.63301
H	9.89829	1.76021	-3.25416
H	11.47676	0.95998	-3.10264
H	9.99801	0.12053	-2.59167
C	1.26185	-0.07399	-2.27387
C	1.99309	1.18532	-2.79723
H	3.02181	1.24293	-2.42969
H	2.03278	1.17454	-3.89214
H	1.47412	2.09767	-2.48584
C	2.02282	-1.33853	-2.73946
H	3.05065	-1.35752	-2.36552
H	1.52317	-2.24739	-2.38912
H	2.06643	-1.37461	-3.83370
C	-0.14564	-0.10414	-2.89948
H	-0.70852	-0.99290	-2.59651
H	-0.73146	0.78101	-2.63096
H	-0.06077	-0.12420	-3.99052

Table S4: Cartesian coordinates of Diradical-II

H	7.33160	0.14670	7.55590
H	6.75050	1.58910	5.61270
C	6.32920	0.12250	7.13850
C	6.00320	0.93070	6.04650
H	5.60640	-1.35930	8.53020
C	5.36180	-0.71900	7.68810
C	4.71830	0.91120	5.51260
H	4.43510	1.55160	4.68710
C	4.07350	-0.75520	7.15770
H	2.66250	0.40290	12.78170
C	3.75080	0.07570	6.08080
H	3.33090	-1.42220	7.57840
C	1.71180	0.92950	12.88380
O	2.26000	-0.07550	10.27990
H	1.41730	0.92760	13.93810
H	3.42750	-0.00780	1.94920
H	2.15210	0.34370	8.20710
H	1.57060	-1.71470	12.26120
N	2.44350	0.06340	5.51080
H	3.48040	-0.07330	-0.53400
N	2.43240	0.07560	4.15290
N	1.06430	0.23870	10.60120
C	0.65390	0.21590	12.04720
C	0.58960	-1.26790	12.44100
H	0.33710	-1.38110	13.49910
C	2.50540	-0.02580	1.38160
C	1.24060	0.23190	7.64600
C	2.53110	-0.07820	-0.00840
C	1.26380	0.10460	6.26180
C	-0.00450	0.40600	9.77100
C	1.24640	0.03910	3.55090
H	-0.14860	-1.81040	11.84350
C	1.28320	0.01230	2.06850
C	-0.73280	0.91790	11.97970
C	0.01360	0.27300	8.32970
H	-1.55920	0.43420	13.91590
C	1.33400	-0.09710	-0.72660
C	0.05340	0.05580	5.50840
N	-1.09290	0.71210	10.53430
H	1.35640	-0.16760	-1.81020
N	0.04320	0.00320	4.15220
C	-1.82080	0.30850	12.86040
H	-1.96730	-0.75400	12.65880
C	0.08520	0.01800	1.33950
C	-1.19610	0.19680	7.59320
C	0.11310	-0.03640	-0.05230
C	-1.16580	0.09000	6.21980
O	-2.26680	1.01130	10.13030
H	-0.85430	0.06410	1.87640
H	-2.13760	0.23900	8.12120
H	-0.81990	-0.03460	-0.60910
H	-2.08270	0.03430	5.64260
H	1.86280	1.96190	12.56350
H	0.07520	2.90900	11.57010
H	-0.47520	2.67480	13.24280
C	-0.68500	2.43730	12.19620
H	-1.65850	2.85400	11.92670
H	-2.76470	0.82200	12.66760

Table S5: Cartesian coordinates of [6]CPPM-Mes

C	13.429720	7.568790	-3.687620
C	13.256220	19.078060	-3.928700
C	12.183570	8.242740	-3.528640
C	12.030840	18.374110	-3.740860
C	14.655100	8.272740	-3.875460
C	14.502370	18.404100	-4.087670
C	10.953200	7.628620	-3.826460
C	10.782710	18.937880	-4.063350
C	15.903230	7.708970	-3.552960
C	15.732740	19.018230	-3.789850
C	9.764600	8.311330	-3.770130
C	9.615180	18.222630	-3.977740
C	17.070760	8.424220	-3.638580
C	16.921340	18.335520	-3.846180
C	9.682910	9.655600	-3.356260
C	9.573770	16.895000	-3.507900
C	17.112170	9.751850	-4.108420
C	17.003030	16.991250	-4.260060
C	10.899710	10.213990	-2.923540
C	10.806580	16.392130	-3.052950
C	15.879360	10.254720	-4.563370
C	15.786230	16.432850	-4.692780
C	12.081260	9.548810	-3.008140
C	11.967590	17.088490	-3.166070
C	14.718350	9.558360	-4.450240
C	14.604680	17.098040	-4.608170
C	8.461260	10.388140	-3.367770
C	8.374760	16.126150	-3.487960
C	18.311180	10.520700	-4.128360
C	18.224680	16.258710	-4.248550
C	8.429850	11.812670	-3.431970
C	8.386330	14.699880	-3.492450
C	18.299610	11.946970	-4.123870
C	18.256090	14.834180	-4.184350
C	9.443980	12.578100	-4.036970
C	9.423440	13.940700	-4.065520
C	17.262500	12.706150	-3.550800
C	17.241960	14.068750	-3.579340
C	7.336960	12.569490	-2.981920
C	7.316450	13.929980	-3.010420
C	19.369490	12.716870	-4.605900
C	19.348980	14.077360	-4.634390
C	13.452140	6.081650	-3.656470
C	13.233800	20.565200	-3.959850
C	13.460320	5.357380	-4.860100
C	13.220910	21.238360	-5.192750
C	13.465030	5.408490	-2.423560
C	13.225630	21.289470	-2.756210
C	13.427280	6.069390	-6.177750
C	13.210170	20.471140	-6.479420
C	13.475770	6.175710	-1.136890
C	13.258660	20.577460	-1.438560
C	13.487200	3.967590	-4.797770
C	13.205860	22.629710	-5.188670
C	13.480080	4.017130	-2.427640
C	13.198740	22.679250	-2.818550
C	13.494260	3.287580	-3.597940
C	13.191680	23.359270	-4.018370
C	13.517270	1.761650	-3.565980
C	13.168670	24.885200	-4.050340
C	7.159160	9.655990	-3.336500
C	7.051170	16.819400	-3.486550
C	19.634770	9.827450	-4.129770
C	19.526780	16.990860	-4.279820
C	6.745570	8.961560	-2.194580
C	6.616120	17.548250	-2.374450
C	20.069820	9.098590	-5.241870
C	19.940370	17.685290	-5.421730
C	7.612680	8.877560	-0.979830
C	7.479550	17.709120	-1.164820
C	19.206390	8.937730	-6.451490
C	19.073260	17.769290	-6.636480
C	5.487610	8.366860	-2.187910
C	5.340810	18.104530	-2.391880
C	21.345130	8.542310	-5.224440
C	21.198330	18.279990	-5.428410
C	4.627760	8.448430	-3.246220
C	4.484480	17.952850	-3.445300
C	22.201460	8.693990	-4.171010
C	22.058180	18.198410	-4.370100
C	3.231830	7.857680	-3.178960
C	3.071340	18.503580	-3.401960
C	23.614600	8.143270	-4.214360
C	23.454110	18.789170	-4.437350

Table S5 (cont.): Cartesian coordinates of [6]CPPM-Mes

C	5.068560	9.089400	-4.388660
C	4.945110	17.278190	-4.560180
C	21.740830	9.368660	-3.056130
C	21.617380	17.557440	-3.227660
C	6.322500	9.692950	-4.461710
C	6.216710	16.710170	-4.608700
C	20.469230	9.936670	-3.007620
C	20.363450	16.953900	-3.154600
C	6.741750	10.375660	-5.738790
C	6.657150	15.987540	-5.856340
C	20.028790	10.659310	-1.759980
C	19.944190	16.271190	-1.877530
H	10.945430	6.712010	-4.076200
H	10.747480	19.842570	-4.351240
H	15.938460	6.804280	-3.265080
H	15.740510	19.934830	-3.540120
H	8.965970	7.860240	-4.018210
H	8.803480	18.638660	-4.243980
H	17.882460	8.008190	-3.372330
H	17.719970	18.786610	-3.598110
H	10.894650	11.090620	-2.557620
H	10.827690	15.531840	-2.650650
H	15.858250	11.115010	-4.965670
H	15.791290	15.556230	-5.058700
H	13.916500	9.954030	-4.771410
H	13.815320	16.665280	-4.911990
H	12.870620	9.981560	-2.704320
H	12.769440	16.692810	-2.844900
H	10.174360	12.125780	-4.442650
H	10.140120	14.397440	-4.490240
H	16.545830	12.249400	-3.126080
H	16.511580	14.521070	-3.173660
H	6.577740	12.111340	-2.641480
H	6.543550	14.378890	-2.688980
H	20.142390	12.267950	-4.927340
H	20.108200	14.535510	-4.974840
H	13.501960	3.471260	-5.607390
H	13.206170	23.091940	-6.018370
H	13.479770	3.554900	-1.597940
H	13.183980	23.175590	-2.008930
H	5.216100	7.884340	-1.415750
H	5.054400	18.610560	-1.640420
H	21.631540	8.036290	-5.975890
H	21.469840	18.762510	-6.200570
H	4.498750	9.119430	-5.148010
H	4.376940	17.199240	-5.317260
H	22.309000	9.447600	-2.299060
H	22.187190	17.527410	-2.468300
H	13.512480	5.416880	-6.903820
H	13.276130	21.094950	-7.232220
H	13.409810	5.551900	-0.384100
H	13.173460	21.229970	-0.712500
H	14.170140	6.707160	-6.222790
H	13.971940	19.854720	-6.498180
H	12.714000	6.792130	-1.118130
H	12.515800	19.939690	-1.393530
H	12.578180	6.550110	-6.268230
H	12.375990	19.961690	-6.549160
H	14.309950	6.685160	-1.067160
H	14.107760	20.096740	-1.348090
H	14.081240	1.428240	-4.294740
H	13.722810	25.204650	-4.792770
H	12.605700	1.418970	-3.675250
H	12.247270	25.195380	-4.173290
H	13.879620	1.458450	-2.707430
H	13.521180	25.234850	-3.205460
H	7.109710	8.463050	-0.247960
H	6.963850	18.138560	-0.450630
H	19.722090	8.508290	-7.165680
H	19.576230	18.183800	-7.368350
H	7.892120	9.778580	-0.715150
H	7.785840	16.828790	-0.862830
H	18.900100	9.818050	-6.753490
H	18.793820	16.868260	-6.901160
H	8.404080	8.335470	-1.180420
H	8.254380	18.265930	-1.388430
H	18.431560	8.380920	-6.227880
H	18.281860	18.311370	-6.435890
H	3.291610	6.899070	-2.985440
H	3.102080	19.470810	-3.248780
H	23.583850	7.176030	-4.367540
H	23.394330	19.747780	-4.630870
H	2.780040	7.989420	-4.039250

Table S5 (cont.): Cartesian coordinates of [6]CPPM-Mes

H	2.624270	18.322380	-4.255690
H	24.061670	8.324470	-3.360620
H	23.905900	18.657420	-3.577060
H	2.721970	8.303370	-2.471080
H	2.574690	18.072760	-2.675720
H	24.111250	8.574090	-4.940600
H	23.963970	18.343480	-5.145230
H	6.120440	10.135630	-6.457240
H	6.029340	16.178450	-6.583810
H	20.656600	10.468390	-1.032500
H	20.565500	16.511220	-1.159080
H	7.647360	10.088520	-5.980400
H	7.553850	16.291460	-6.110330
H	19.132090	10.355380	-1.505980
H	19.038580	16.558320	-1.635910
H	6.731370	11.347000	-5.608450
H	6.675950	15.022640	-5.685440
H	20.009990	11.624210	-1.930870
H	19.954580	15.299850	-2.007860

Table S6: Cartesian coordinates of [3]CPBM-Ant

C	2.35370	2.54251	-2.19211
C	3.07174	1.36823	-2.30680
C	4.24141	1.13411	-1.55923
C	4.73841	2.21904	-0.81235
C	4.04109	3.42329	-0.73384
C	2.77771	3.60520	-1.35674
C	1.87468	4.70110	-0.96618
C	0.24843	4.45367	-2.87310
C	-1.02599	4.08788	-3.16987
C	-2.06708	4.12904	-2.16880
C	-1.78848	5.00571	-1.05707
C	-0.50935	5.39461	-0.76609
C	0.61307	4.89579	-1.54195
C	2.23485	5.48772	0.26124
C	2.70801	6.81616	0.11584
C	3.06903	7.58233	1.28802
C	2.94716	7.00063	2.55258
C	2.48001	5.69301	2.71683
C	2.11309	4.91816	1.55336
C	2.35036	5.10723	4.01494
C	1.87937	3.83151	4.17032
C	1.50417	3.06829	3.02798
C	1.61408	3.59289	1.76646
C	2.87082	7.44192	-1.16259
C	3.33441	8.72647	-1.27406
C	3.67448	9.48129	-0.11494
C	3.54686	8.92096	1.12698
H	1.38388	2.57401	-2.66542
H	2.63970	0.55370	-2.87990
H	5.66345	2.10864	-0.25145
H	4.44718	4.22025	-0.11926
H	1.01677	4.40526	-3.63918
H	-1.26241	3.74029	-4.17155
H	-2.58144	5.24039	-0.35284
H	-0.31204	5.94103	0.14994
H	2.63364	5.70368	4.87910
H	1.78541	3.39738	5.16210
H	1.12589	2.05814	3.16092
H	1.32042	2.99965	0.90757
H	2.61918	6.87741	-2.05326
H	3.44753	9.17676	-2.25666
H	4.03791	10.49960	-0.22361
H	3.80786	9.48456	2.01975
C	1.34888	-3.37316	-1.96997
C	-0.01083	-3.28917	-2.18808
C	-0.92654	-4.11275	-1.50360
C	-0.38127	-5.15190	-0.72277
C	0.99164	-5.28263	-0.54802
C	1.91303	-4.32816	-1.07623
C	3.27982	-4.23832	-0.60984
C	4.22972	-2.53784	-2.25228
C	4.49505	-1.19296	-2.48127
C	4.62887	-0.28938	-1.40778
C	4.77237	-0.84557	-0.12326
C	4.51990	-2.19626	0.10519
C	4.08074	-3.03817	-0.94041
C	3.79966	-5.15926	0.44488
C	4.81066	-6.09380	0.09933
C	5.35470	-6.97484	1.10612
C	4.87476	-6.89886	2.41665
C	3.88475	-5.98276	2.78217
C	3.33787	-5.08885	1.78562
C	3.41154	-5.90167	4.12974
C	2.46299	-4.98480	4.49338
C	1.93598	-4.08697	3.52181
C	2.35747	-4.13658	2.21851
C	5.31058	-6.22166	-1.23576
C	6.28689	-7.13113	-1.54926
C	6.82916	-7.98778	-0.54960
C	6.37092	-7.91122	0.73799
H	1.97733	-2.62431	-2.42898
H	-0.39109	-2.48140	-2.80652
H	-1.04588	-5.85198	-0.22190
H	1.36485	-6.08707	0.07694
H	4.04072	-3.19382	-3.09800
H	4.50128	-0.81677	-3.50131
H	4.92802	-0.18859	0.72860
H	4.51093	-2.56477	1.12610
H	3.83171	-6.58653	4.86278
H	2.11409	-4.93245	5.52115
H	1.19204	-3.35287	3.81997
H	1.94525	-3.44400	1.49324

Table S6 (cont.): Cartesian coordinates of [3]CPBM-Ant

H	4.89679	-5.58357	-2.00906
H	6.64931	-7.20519	-2.57110
H	7.60200	-8.70386	-0.81568
H	6.77233	-8.56485	1.50904
C	-3.61600	0.82512	-2.59305
C	-2.94975	1.96606	-2.91134
C	-3.11952	3.18692	-2.16884
C	-4.26170	3.20485	-1.29000
C	-5.00416	2.08475	-1.04288
C	-4.62224	0.77561	-1.54989
C	-5.08246	-0.40703	-0.96294
C	-3.99711	-2.17628	-2.47332
C	-2.96481	-3.09967	-2.59505
C	-2.32604	-3.63098	-1.45728
C	-2.93799	-3.38607	-0.21465
C	-3.96265	-2.45279	-0.09246
C	-4.41387	-1.70968	-1.20676
C	-6.10031	-0.37137	0.13983
C	-7.41510	-0.82659	-0.13369
C	-8.40802	-0.83578	0.91530
C	-8.05816	-0.39476	2.19478
C	-6.76742	0.05335	2.48759
C	-5.76329	0.06479	1.44649
C	-6.41532	0.49509	3.80197
C	-5.14616	0.91744	4.09056
C	-4.14925	0.91775	3.07324
C	-4.44612	0.50652	1.80019
C	-7.81772	-1.26753	-1.43467
C	-9.09578	-1.69822	-1.67829
C	-10.06817	-1.71366	-0.63817
C	-9.73077	-1.29154	0.61951
H	-3.32062	-0.08217	-3.09630
H	-2.15791	1.90201	-3.64965
H	-4.54289	4.13640	-0.80605
H	-5.85474	2.15266	-0.37346
H	-4.44713	-1.76727	-3.37309
H	-2.60055	-3.36444	-3.58473
H	-2.51066	-3.82119	0.68507
H	-4.32167	-2.19839	0.89888
H	-7.18463	0.48330	4.57072
H	-4.89187	1.24908	5.09367
H	-3.14174	1.24783	3.31209
H	-3.67550	0.51113	1.03744
H	-7.08923	-1.25069	-2.23799
H	-9.37467	-2.02831	-2.67546
H	-11.07711	-2.05712	-0.85004
H	-10.46589	-1.29293	1.42110
H	3.22048	7.58067	3.43189
H	5.28584	-7.56600	3.17184
H	-8.80888	-0.40181	2.98268

Table S7: Cartesian coordinates of [4]CPBM-Ant

C	5.91347	1.82002	0.50953
C	6.08769	3.26105	0.50608
H	7.08988	3.65634	0.37330
C	5.04353	4.12669	0.67217
H	5.25463	5.19188	0.67012
C	3.68522	3.67979	0.86357
C	3.51937	2.24971	0.88365
H	2.52453	1.83022	0.96225
C	4.54939	1.38117	0.72090
H	4.32858	0.32267	0.68631
C	-2.55843	-4.53198	-0.95055
C	-1.25060	-3.99770	-1.23581
H	-1.15286	-2.98043	-1.59449
C	-0.11585	-4.72958	-1.09974
H	0.83627	-4.27052	-1.33905
C	-0.13170	-6.12073	-0.70050
C	-1.45215	-6.71108	-0.62421
H	-1.53257	-7.77094	-0.40158
C	-2.58828	-5.95532	-0.71597
H	-3.54402	-6.44525	-0.55587
C	1.04970	-6.80499	-0.40864
C	2.26517	-6.01370	-0.10371
C	3.52662	-6.25482	-0.68324
H	3.65882	-7.11717	-1.33114
C	4.58799	-5.36638	-0.49759
H	5.53261	-5.55750	-1.00080
C	4.44916	-4.22164	0.30859
C	3.22171	-4.04768	0.97507
H	3.07593	-3.17715	1.60698
C	2.16169	-4.91345	0.77207
H	1.21582	-4.72290	1.26987
C	5.43233	-3.11332	0.39161
C	6.11983	-2.64374	-0.74188
H	6.08328	-3.21583	-1.66526
C	6.73319	-1.39029	-0.74548
H	7.17983	-1.01792	-1.66342
C	6.65372	-0.54303	0.37445
C	6.11968	-1.08936	1.55718
H	6.10490	-0.48789	2.46236
C	5.53325	-2.34734	1.56811
H	5.09452	-2.72093	2.48912
C	6.94197	0.91444	0.25849
C	1.44952	-8.28260	2.10510
H	1.31455	-7.20787	2.12337
C	1.67787	-8.95738	3.27649
H	1.72899	-8.40917	4.21344
C	1.84194	-10.37103	3.28217
H	2.02437	-10.88915	4.21975
C	1.75719	-11.07107	2.10890
H	1.86725	-12.15300	2.09877
C	1.39740	-11.11939	-0.32838
C	1.02964	-11.22374	-2.76033
H	1.12772	-12.30572	-2.71032
C	0.80684	-10.59674	-3.95584
H	0.72151	-11.17401	-4.87248
C	0.69523	-9.17819	-4.00084
H	0.53165	-8.68466	-4.95518
C	0.79699	-8.42857	-2.85768
H	0.71591	-7.34942	-2.91445
C	1.13100	-8.29244	-0.37522
C	1.37501	-8.96744	0.85090
C	1.51497	-10.40487	0.86725
C	1.14532	-10.47941	-1.54441
C	1.01085	-9.03932	-1.57929
C	9.34067	0.64978	1.91768
H	8.36164	0.43577	2.32983
C	10.45933	0.46694	2.68882
H	10.35969	0.09898	3.70648
C	11.75290	0.76270	2.17404
H	12.62919	0.61077	2.79840
C	11.88561	1.24733	0.90061
H	12.86667	1.49024	0.49890
C	10.87035	1.97319	-1.22542
C	9.90117	2.71866	-3.36263
H	10.90168	2.96788	-3.70855
C	8.81448	2.90660	-4.17269
H	8.93789	3.31083	-5.17375
C	7.51440	2.56213	-3.70528
H	6.65699	2.70282	-4.35809
C	7.33272	2.05377	-2.44526
H	6.33605	1.79469	-2.10750
C	8.28481	1.32765	-0.24236
C	9.43043	1.13153	0.57367

Table S7 (cont.): Cartesian coordinates of [4]CPBM-Ant

C	10.74297	1.45458	0.06633
C	9.75716	2.18772	-2.04229
C	8.43677	1.85648	-1.55281
C	-5.91347	-1.82002	-0.50953
C	-6.08769	-3.26105	-0.50608
H	-7.08988	-3.65634	-0.37330
C	-5.04353	-4.12669	-0.67217
H	-5.25463	-5.19188	-0.67012
C	-3.68522	-3.67979	-0.86357
C	-3.51937	-2.24971	-0.88365
H	-2.52453	-1.83022	-0.96225
C	-4.54939	-1.38117	-0.72090
H	-4.32858	-0.32267	-0.68631
C	2.55843	4.53198	0.95055
C	1.25060	3.99770	1.23581
H	1.15286	2.98043	1.59449
C	0.11585	4.72958	1.09974
H	-0.83627	4.27052	1.33905
C	0.13170	6.12073	0.70050
C	1.45215	6.71108	0.62421
H	1.53257	7.77094	0.40158
C	2.58828	5.95532	0.71597
H	3.54402	6.44525	0.55587
C	-1.04970	6.80499	0.40864
C	-2.26517	6.01370	0.10371
C	-3.52662	6.25482	0.68324
H	-3.65882	7.11717	1.33114
C	-4.58799	5.36638	0.49759
H	-5.53261	5.55750	1.00080
C	-4.44916	4.22164	-0.30859
C	-3.22171	4.04768	-0.97507
H	-3.07593	3.17715	-1.60698
C	-2.16169	4.91345	-0.77207
H	-1.21582	4.72290	-1.26987
C	-5.43233	3.11332	-0.39161
C	-6.11983	2.64374	0.74188
H	-6.08328	3.21583	1.66526
C	-6.73319	1.39029	0.74548
H	-7.17983	1.01792	1.66342
C	-6.65372	0.54303	-0.37445
C	-6.11968	1.08936	-1.55718
H	-6.10490	0.48789	-2.46236
C	-5.53325	2.34734	-1.56811
H	-5.09452	2.72093	-2.48912
C	-6.94197	-0.91444	-0.25849
C	-1.44952	8.28260	-2.10510
H	-1.31455	7.20787	-2.12337
C	-1.67787	8.95738	-3.27649
H	-1.72899	8.40917	-4.21344
C	-1.84194	10.37103	-3.28217
H	-2.02437	10.88915	-4.21975
C	-1.75719	11.07107	-2.10890
H	-1.86725	12.15300	-2.09877
C	-1.39740	11.11939	0.32838
C	-1.02964	11.22374	2.76033
H	-1.12772	12.30572	2.71032
C	-0.80684	10.59674	3.95584
H	-0.72151	11.17401	4.87248
C	-0.69523	9.17819	4.00084
H	-0.53165	8.68466	4.95518
C	-0.79699	8.42857	2.85768
H	-0.71591	7.34942	2.91445
C	-1.13100	8.29244	0.37522
C	-1.37501	8.96744	-0.85090
C	-1.51497	10.40487	-0.86725
C	-1.14532	10.47941	1.54441
C	-1.01085	9.03932	1.57929
C	-9.34067	-0.64978	-1.91768
H	-8.36164	-0.43577	-2.32983
C	-10.45933	-0.46694	-2.68882
H	-10.35969	-0.09898	-3.70648
C	-11.75290	-0.76270	-2.17404
H	-12.62919	-0.61077	-2.79840
C	-11.88561	-1.24733	-0.90061
H	-12.86667	-1.49024	-0.49890
C	-10.87035	-1.97319	1.22542
C	-9.90117	-2.71866	3.36263
H	-10.90168	-2.96788	3.70855
C	-8.81448	-2.90660	4.17269
H	-8.93789	-3.31083	5.17375
C	-7.51440	-2.56213	3.70528
H	-6.65699	-2.70282	4.35809
C	-7.33272	-2.05377	2.44526

Table S7 (cont.): Cartesian coordinates of [4]CPBM-Ant

H	-6.33605	-1.79469	2.10750
C	-8.28481	-1.32765	0.24236
C	-9.43043	-1.13153	-0.57367
C	-10.74297	-1.45458	-0.06633
C	-9.75716	-2.18772	2.04229
C	-8.43677	-1.85648	1.55281
H	1.50257	-12.20242	-0.31138
H	11.86098	2.21839	-1.60338
H	-1.50257	12.20242	0.31138
H	-11.86098	-2.21839	1.60338

Table S8: Cartesian coordinates of [5]CPBM-Ant

C	-0.29969	7.66957	0.10883
C	-0.47474	6.30902	0.56541
C	-1.70075	5.73210	0.68444
C	-2.91913	6.41747	0.34222
C	-2.75568	7.80651	-0.00232
C	-1.52970	8.40256	-0.09589
C	-4.16600	5.74306	0.31902
C	-4.24465	4.31394	0.46766
C	-5.41197	3.62209	0.36801
C	-6.67511	4.26975	0.09013
C	-6.60263	5.71167	-0.02444
C	-5.42750	6.39758	0.08722
C	-7.85325	3.55471	-0.13285
C	-9.04858	4.20342	-0.75074
C	-10.24449	4.35101	0.00013
C	-11.40822	4.95240	-0.60865
C	-11.34190	5.38853	-1.93501
C	-10.17790	5.24944	-2.69540
C	-9.00802	4.63908	-2.10317
C	-10.34469	3.95488	1.37158
C	-11.50914	4.11290	2.07769
C	-12.65818	4.68990	1.46675
C	-12.60334	5.10049	0.16218
C	-10.12540	5.69055	-4.05502
C	-8.99432	5.52893	-4.80803
C	-7.84873	4.90265	-4.24014
C	-7.85602	4.47229	-2.93877
C	-7.92228	2.09900	0.12218
C	-7.43753	1.52443	1.31524
C	-7.35247	0.14634	1.47236
C	-7.73014	-0.72686	0.43718
C	-8.30167	-0.15985	-0.71590
C	-8.41749	1.21885	-0.86108
C	-7.39736	-2.16770	0.52643
C	-7.56399	-2.91142	1.70824
C	-7.07553	-4.20984	1.81783
C	-6.35148	-4.80806	0.76655
C	-6.25689	-4.08783	-0.44263
C	-6.77662	-2.80541	-0.56218
C	-5.68451	-6.11600	0.94293
C	-6.46127	-7.19867	1.62260
C	-6.16632	-7.55019	2.96652
C	-6.94407	-8.57531	3.62683
C	-7.98098	-9.20538	2.93359
C	-8.28948	-8.87114	1.61186
C	-7.51997	-7.85040	0.93933
C	-5.13772	-6.90695	3.72968
C	-4.88478	-7.26137	5.02931
C	-5.64159	-8.28481	5.66706
C	-6.64281	-8.91855	4.98232
C	-9.34614	-9.52620	0.90565
C	-9.63156	-9.20769	-0.39463
C	-8.86637	-8.21319	-1.06717
C	-7.84601	-7.56186	-0.42394
C	-4.35542	-6.31135	0.56724
C	-3.46900	-5.21634	0.23720
C	-2.14730	-5.40494	-0.02638
C	-1.53250	-6.70593	-0.05050
C	-2.42302	-7.80363	0.22534
C	-3.73774	-7.62049	0.54313
C	-0.14784	-6.86981	-0.30640
C	0.46271	-8.14582	-0.57874
C	1.79066	-8.27853	-0.86568
C	2.70078	-7.15297	-0.85706
C	2.08906	-5.87811	-0.54935
C	0.75447	-5.74903	-0.31765
C	4.05275	-7.27286	-1.17527
C	4.60556	-8.49801	-1.82756
C	5.51613	-9.32852	-1.12299
C	6.10939	-10.46912	-1.78141
C	5.76863	-10.74997	-3.10756
C	4.86508	-9.95453	-3.81708
C	4.27032	-8.80306	-3.17445
C	5.85635	-9.10474	0.24881
C	6.73694	-9.92187	0.90923
C	7.33727	-11.03017	0.24765
C	7.02562	-11.29546	-1.05857
C	4.52490	-10.25200	-5.17406
C	3.65647	-9.46110	-5.87602
C	3.08293	-8.31493	-5.25597
C	3.38146	-7.99586	-3.95675
C	4.99123	-6.14870	-0.94945
C	5.04227	-5.47379	0.28687

Table S8 (cont.): Cartesian coordinates of [5]CPBM-Ant

C	5.84552	-4.35506	0.46734
C	6.61459	-3.83624	-0.58919
C	6.61313	-4.54060	-1.80558
C	5.84053	-5.68656	-1.97395
C	7.28869	-2.52718	-0.42462
C	8.02698	-2.20887	0.72962
C	8.48421	-0.91667	0.96038
C	8.17469	0.13631	0.07071
C	7.50745	-0.20854	-1.12767
C	7.09106	-1.50946	-1.37522
C	8.46225	1.52945	0.42343
C	9.71963	1.84364	1.15354
C	9.67847	2.24746	2.51748
C	10.90945	2.52735	3.22150
C	12.13055	2.38961	2.55581
C	12.19592	1.98857	1.21836
C	10.97431	1.71183	0.49861
C	8.45737	2.34760	3.25887
C	8.44985	2.72264	4.57758
C	9.66397	3.02109	5.25796
C	10.85733	2.92098	4.59566
C	13.45003	1.85642	0.54442
C	13.50933	1.48697	-0.77221
C	12.30796	1.23628	-1.49351
C	11.08646	1.34912	-0.88147
C	7.47603	2.55953	0.18549
C	6.10041	2.24373	0.02019
C	5.14278	3.22750	-0.12891
C	5.47534	4.59840	-0.13524
C	6.83944	4.92330	0.02044
C	7.80682	3.94175	0.18074
C	4.40267	5.60480	-0.24248
C	3.20774	5.29694	-0.92413
C	2.12069	6.15354	-0.89964
C	2.16135	7.38211	-0.20244
C	3.39487	7.74149	0.38210
C	4.47854	6.86904	0.37561
C	0.96350	8.23140	-0.09745
C	1.14660	9.71142	-0.20635
C	1.03567	10.52929	0.94876
C	1.24625	11.95621	0.83992
C	1.56022	12.51236	-0.40293
C	1.67577	11.72431	-1.55179
C	1.46544	10.29806	-1.45838
C	0.75306	9.99928	2.24951
C	0.66201	10.81378	3.34808
C	0.85111	12.22023	3.23083
C	1.13759	12.77020	2.01092
C	1.98739	12.30210	-2.82207
C	2.07869	11.52818	-3.94744
C	1.85465	10.12466	-3.86435
C	1.55581	9.53304	-2.66450
H	0.39976	5.74552	0.86882
H	-1.74731	4.72555	1.08322
H	-3.63219	8.40047	-0.23992
H	-1.46544	9.44342	-0.39678
H	-3.33519	3.74087	0.60245
H	-5.37997	2.54122	0.42867
H	-7.52291	6.26123	-0.19331
H	-5.45786	7.47964	0.00878
H	-9.47705	3.52078	1.85479
H	-11.55711	3.79971	3.11726
H	-13.57235	4.80753	2.04237
H	-13.47014	5.55196	-0.31493
H	-11.01279	6.15520	-4.47865
H	-8.96754	5.86715	-5.84039
H	-6.95941	4.76235	-4.84888
H	-6.97643	3.99275	-2.52550
H	-7.09618	2.17368	2.11678
H	-6.92377	-0.26137	2.38387
H	-8.64653	-0.81057	-1.51536
H	-8.84116	1.62802	-1.77358
H	-8.07633	-2.46096	2.55462
H	-7.20503	-4.75355	2.74890
H	-5.74888	-4.53794	-1.29098
H	-6.64733	-2.26165	-1.49413
H	-4.55214	-6.12297	3.26319
H	-4.09817	-6.75479	5.58225
H	-5.42429	-8.55329	6.69733
H	-7.23565	-9.69635	5.45837
H	-9.91825	-10.29000	1.42743
H	-10.43663	-9.71447	-0.91993
H	-9.09288	-7.97369	-2.10270

Table S8 (cont.): Cartesian coordinates of [5]CPBM-Ant

H	-7.26538	-6.81340	-0.95125
H	-3.85782	-4.20536	0.25087
H	-1.54885	-4.52825	-0.24528
H	-2.03304	-8.81632	0.22444
H	-4.35537	-8.48471	0.76567
H	-0.15644	-9.03707	-0.59467
H	2.19168	-9.26205	-1.08889
H	2.70732	-4.98852	-0.55249
H	0.37314	-4.75585	-0.11048
H	5.39905	-8.27250	0.77132
H	6.97714	-9.72675	1.95098
H	8.03432	-11.66617	0.78654
H	7.46652	-12.14639	-1.57283
H	4.97872	-11.12514	-5.63722
H	3.40676	-9.69844	-6.90659
H	4.42598	-5.82748	1.10877
H	5.83494	-3.83606	1.42204
H	7.22373	-4.18229	-2.63049
H	5.85225	-6.20520	-2.92829
H	8.22965	-2.98651	1.46150
H	9.03191	-0.69499	1.87148
H	7.29621	0.56870	-1.85620
H	6.54210	-1.73213	-2.28650
H	7.52290	2.11909	2.76023
H	7.50651	2.79005	5.11297
H	9.63741	3.31819	6.30286
H	11.79487	3.13165	5.10501
H	14.35901	2.06142	1.10521
H	14.46850	1.39088	-1.27380
H	12.36286	0.95865	-2.54278
H	10.18066	1.16718	-1.44814
H	5.78173	1.20895	0.07122
H	4.09990	2.93120	-0.18391
H	7.14824	5.96499	-0.00557
H	8.84709	4.23316	0.29012
H	3.13647	4.37377	-1.49128
H	1.21771	5.88132	-1.43736
H	3.47781	8.69167	0.90157
H	5.38162	7.14890	0.91106
H	0.61243	8.92982	2.35752
H	0.44628	10.38284	4.32213
H	0.77291	12.84976	4.11307
H	1.29326	13.84161	1.90731
H	2.14664	13.37674	-2.87350
H	2.31490	11.97992	-4.90709
H	1.91782	9.51893	-4.76439
H	1.37896	8.46466	-2.61833
H	-12.21915	5.84661	-2.38769
H	-8.56369	-9.97572	3.43518
H	6.21624	-11.61137	-3.59952
H	13.05388	2.59608	3.09354
H	1.71821	13.58646	-0.47893
H	2.40287	-7.68459	-5.82279
H	2.93888	-7.11682	-3.50285

Table S9: Cartesian coordinates of [6]CPBM-Ant

C	6.90630	6.24644	-0.96826
C	5.71842	5.46204	-0.71827
C	4.46331	5.97215	-0.86253
C	4.21307	7.31596	-1.30976
C	5.39530	8.09358	-1.57622
C	6.65665	7.60338	-1.39761
C	2.89805	7.83145	-1.45339
C	1.73169	7.06634	-1.09965
C	0.46449	7.55422	-1.20992
C	0.18643	8.87443	-1.72976
C	1.35605	9.63097	-2.11770
C	2.62306	9.14725	-1.96835
C	-1.10790	9.36757	-1.90298
C	-1.35625	10.57583	-2.75176
C	-1.73260	11.80326	-2.14916
C	-1.99640	12.95901	-2.97500
C	-1.87823	12.85276	-4.36394
C	-1.51133	11.65272	-4.97887
C	-1.24488	10.48786	-4.16432
C	-1.83391	11.96281	-0.73035
C	-2.18885	13.16292	-0.17129
C	-2.46168	14.29498	-0.99066
C	-2.36374	14.19261	-2.35215
C	-1.39999	11.55104	-6.40127
C	-1.05747	10.36973	-7.00132
C	-0.81044	9.21491	-6.20568
C	-0.90225	9.27151	-4.83929
C	-2.29002	8.70474	-1.32074
C	-2.29701	8.21069	0.00188
C	-3.39812	7.53989	0.51944
C	-4.54258	7.30719	-0.26371
C	-4.55918	7.83981	-1.56555
C	-3.47203	8.54115	-2.07325
C	-5.65418	6.47658	0.25051
C	-6.13615	6.60535	1.56571
C	-7.12659	5.76210	2.05688
C	-7.65101	4.71367	1.27227
C	-7.19222	4.61455	-0.05946
C	-6.22926	5.48094	-0.55938
C	-8.64051	3.76972	1.82306
C	-9.70873	4.33449	2.70394
C	-9.66710	4.10515	4.10541
C	-10.69105	4.67037	4.95570
C	-11.70609	5.44502	4.38785
C	-11.76035	5.68974	3.01263
C	-10.74741	5.12689	2.15010
C	-8.62341	3.35391	4.73712
C	-8.60753	3.15356	6.09293
C	-9.63195	3.69271	6.92174
C	-10.64004	4.43230	6.36519
C	-12.80641	6.47782	2.43882
C	-12.86704	6.69756	1.08917
C	-11.88112	6.13113	0.23248
C	-10.86200	5.37049	0.74438
C	-8.55972	2.39246	1.59545
C	-7.36491	1.75119	1.09544
C	-7.26820	0.39758	0.96739
C	-8.36015	-0.48981	1.25743
C	-9.56432	0.14648	1.71527
C	-9.65052	1.49599	1.90697
C	-8.23259	-1.89520	1.10236
C	-6.94557	-2.52638	1.00384
C	-6.79797	-3.86433	0.79253
C	-7.92678	-4.74872	0.60850
C	-9.21749	-4.12737	0.80745
C	-9.35667	-2.78885	1.04386
C	-7.79688	-6.10507	0.28537
C	-8.97727	-7.02101	0.39570
C	-9.42580	-7.45974	1.66778
C	-10.56029	-8.35207	1.75945
C	-11.19721	-8.77713	0.59037
C	-10.76634	-8.36118	-0.67286
C	-9.63659	-7.46646	-0.77780
C	-8.78213	-7.07535	2.88866
C	-9.23513	-7.51883	4.10379
C	-10.36455	-8.38225	4.18914
C	-11.00295	-8.78658	3.04812
C	-11.42605	-8.79460	-1.86528
C	-11.00885	-8.36995	-3.09793
C	-9.90463	-7.47735	-3.20610
C	-9.24604	-7.03906	-2.08687
C	-6.52731	-6.69702	-0.15656
C	-6.18210	-8.02846	0.17322

Table S9 (cont.): Cartesian coordinates of [6]CPBM-Ant

C	-4.94297	-8.56252	0.16179
C	-3.98123	-7.79975	-0.84999
C	-4.35596	-6.50590	-1.26046
C	-5.59461	-5.97608	-0.93883
C	-2.61246	-8.28710	-1.11205
C	-2.32819	-9.59952	-1.53398
C	-1.02770	-9.99926	-1.82037
C	0.06802	-9.11954	-1.65942
C	-0.22527	-7.80967	-1.20991
C	-1.52470	-7.40624	-0.95577
C	1.43303	-9.49156	-2.03687
C	1.61746	-10.41723	-3.19281
C	2.15431	-11.71618	-2.97381
C	2.32701	-12.61920	-4.08995
C	1.95644	-12.20672	-5.37233
C	1.42272	-10.93667	-5.61020
C	1.24975	-10.01973	-4.50690
C	2.50402	-12.20222	-1.67261
C	3.01153	-13.46268	-1.49188
C	3.20330	-14.33703	-2.59881
C	2.86486	-13.92437	-3.85882
C	1.05918	-10.52236	-6.92936
C	0.56364	-9.26851	-7.16522
C	0.41260	-8.35263	-6.08626
C	0.74734	-8.71331	-4.80644
C	2.55625	-8.95252	-1.37749
C	2.51026	-8.47674	-0.01961
C	3.59236	-7.89451	0.58322
C	4.79999	-7.62284	-0.13292
C	4.86937	-8.14137	-1.46472
C	3.82955	-8.82652	-2.03519
C	5.83092	-6.81252	0.43769
C	6.02391	-6.70253	1.85135
C	6.92450	-5.82853	2.39865
C	7.63625	-4.87557	1.58988
C	7.49650	-5.04269	0.16710
C	6.67723	-5.99648	-0.37607
C	8.38565	-3.83222	2.17175
C	8.89514	-3.96794	3.56989
C	8.34612	-3.17772	4.61622
C	8.87004	-3.29496	5.95742
C	9.90724	-4.19641	6.21412
C	10.45407	-4.99272	5.20453
C	9.94667	-4.88090	3.85499
C	7.24904	-2.28136	4.41166
C	6.73308	-1.53670	5.44073
C	7.27123	-1.63731	6.75452
C	8.30717	-2.49695	7.00213
C	11.51478	-5.91170	5.48031
C	12.06397	-6.67625	4.48722
C	11.58434	-6.55495	3.15217
C	10.56773	-5.68745	2.84719
C	8.59708	-2.55301	1.49751
C	7.62908	-2.01954	0.61131
C	7.72050	-0.72658	0.12778
C	8.79010	0.12535	0.47518
C	9.78953	-0.42335	1.30609
C	9.69117	-1.71167	1.81214
C	8.77946	1.54280	0.06363
C	8.00200	1.98002	-1.02895
C	7.83483	3.32712	-1.30787
C	8.45713	4.32680	-0.52744
C	9.32893	3.88629	0.49074
C	9.46620	2.53691	0.79043
C	8.19788	5.75898	-0.74546
C	9.36256	6.69026	-0.63937
C	9.48731	7.55435	0.48132
C	10.63659	8.42550	0.59069
C	11.61664	8.40005	-0.40508
C	11.51589	7.55337	-1.51281
C	10.37054	6.68219	-1.63873
C	8.53148	7.58505	1.54832
C	8.68460	8.42489	2.62076
C	9.80756	9.29539	2.71154
C	10.75528	9.28957	1.72435
C	12.52094	7.53794	-2.52975
C	12.40864	6.72052	-3.62195
C	11.27279	5.87373	-3.76111
C	10.28886	5.85880	-2.80664
H	5.82969	4.45088	-0.34519
H	3.63019	5.32526	-0.61356
H	5.29410	9.11740	-1.91938
H	7.50842	8.24196	-1.60884

Table S9 (cont.): Cartesian coordinates of [6]CPBM-Ant

H	1.84595	6.05282	-0.73354
H	-0.36712	6.91019	-0.94848
H	1.21488	10.63175	-2.51271
H	3.44702	9.78778	-2.26351
H	-1.62103	11.11156	-0.09388
H	-2.25987	13.25597	0.90915
H	-2.74152	15.23821	-0.52932
H	-2.56130	15.05182	-2.98898
H	-1.59956	12.43910	-6.99657
H	-0.97758	10.30538	-8.08312
H	-0.54791	8.27825	-6.69023
H	-0.71294	8.38342	-4.24721
H	-1.42273	8.36085	0.62861
H	-3.35837	7.15250	1.53419
H	-5.44419	7.71000	-2.18301
H	-3.51755	8.93917	-3.08258
H	-5.73478	7.38683	2.20556
H	-7.48111	5.88827	3.07549
H	-7.60660	3.84717	-0.70685
H	-5.88379	5.36318	-1.58298
H	-7.83310	2.94024	4.12155
H	-7.80260	2.57883	6.54331
H	-9.60412	3.52001	7.99419
H	-11.42387	4.85963	6.98642
H	-13.55801	6.89752	3.10352
H	-13.66779	7.29785	0.66578
H	-11.94216	6.30182	-0.83902
H	-10.12363	4.93834	0.07854
H	-6.49959	2.36206	0.86600
H	-6.33554	-0.01558	0.59852
H	-10.42572	-0.46507	1.96436
H	-10.57597	1.92123	2.28165
H	-6.05223	-1.93478	1.17453
H	-5.80008	-4.28596	0.81087
H	-10.10579	-4.74308	0.71443
H	-10.36050	-2.38336	1.12319
H	-7.91825	-6.42167	2.83832
H	-8.72747	-7.21115	5.01405
H	-10.71090	-8.72106	5.16181
H	-11.86166	-9.45207	3.09893
H	-12.27279	-9.47023	-1.76810
H	-11.51897	-8.70635	-3.99646
H	-9.58570	-7.13824	-4.18811
H	-8.41261	-6.35244	-2.18386
H	-6.88197	-8.62869	0.74633
H	-4.69285	-9.56884	0.16411
H	-3.66933	-5.92210	-1.86710
H	-5.86055	-4.99361	-1.31423
H	-3.14470	-10.30213	-1.67939
H	-0.84510	-11.00962	-2.17444
H	0.58210	-7.09237	-1.10571
H	-1.70902	-6.38956	-0.62010
H	2.35940	-11.55336	-0.81708
H	3.26750	-13.80185	-0.49167
H	3.60959	-15.33168	-2.43636
H	2.99439	-14.58506	-4.71298
H	1.19206	-11.22975	-7.74465
H	0.29207	-8.96470	-8.17256
H	0.03243	-7.35364	-6.28278
H	0.63299	-7.99818	-4.00006
H	1.59692	-8.61467	0.54997
H	3.49879	-7.55656	1.61095
H	5.78909	-8.02205	-2.03031
H	3.93531	-9.21951	-3.04140
H	5.46278	-7.35726	2.51159
H	7.04850	-5.79148	3.47605
H	8.07956	-4.40621	-0.49056
H	6.60741	-6.07324	-1.45716
H	6.82031	-2.19652	3.42025
H	5.90021	-0.86394	5.25433
H	6.85056	-1.03701	7.55671
H	8.72065	-2.59468	8.00327
H	11.87701	-5.98532	6.50311
H	12.86970	-7.37073	4.70928
H	12.03462	-7.15538	2.36616
H	10.21996	-5.60359	1.82423
H	6.74741	-2.60506	0.37299
H	6.90026	-0.34528	-0.47193
H	10.65979	0.17186	1.56693
H	10.46965	-2.08330	2.47181
H	7.52162	1.25210	-1.67514
H	7.22068	3.62094	-2.15433
H	9.84886	4.62200	1.09697

Table S9 (cont.): Cartesian coordinates of [6]CPBM-Ant

H	10.07375	2.25530	1.64511
H	7.67148	6.92721	1.49984
H	7.94211	8.42574	3.41441
H	9.91016	9.95506	3.56892
H	11.62446	9.94060	1.78476
H	13.37941	8.19584	-2.41520
H	13.17922	6.71823	-4.38824
H	11.18515	5.23654	-4.63709
H	9.42629	5.21465	-2.93361
H	-2.07712	13.72646	-4.98157
H	-12.47369	5.86906	5.03244
H	-12.05037	-9.44861	0.66549
H	2.08819	-12.89161	-6.20776
H	10.29603	-4.28257	7.22694
H	12.48161	9.05445	-0.31496

Table S10: Cartesian coordinates of MC-F3A3

C	-2.23867	3.55090	-0.49160
C	-1.33400	4.58631	-0.43697
C	0.03801	4.30805	-0.34049
C	0.47370	2.94311	-0.32033
C	-0.42340	1.91625	-0.37916
C	-1.81167	2.19926	-0.46122
C	1.17853	5.15716	-0.28761
C	2.33402	4.32867	-0.22941
C	1.92247	2.95617	-0.24129
C	2.83743	1.94564	-0.17506
C	3.70082	4.63146	-0.13293
C	4.62344	3.61251	-0.06924
C	4.22033	2.25339	-0.09206
C	5.10375	1.18435	-0.03070
C	-2.67647	1.11457	-0.51147
C	-3.28108	0.05115	-0.53106
C	5.73479	0.13639	-0.01663
C	-3.76666	-1.24752	-0.56448
C	6.24639	-1.15245	0.01252
H	-3.29728	3.75626	-0.56142
H	-1.67809	5.61122	-0.46004
H	4.02685	5.66239	-0.11611
H	5.67811	3.83687	0.00163
C	-5.14489	-1.57507	-0.64198
C	-2.80864	-2.29666	-0.51887
C	-3.22534	-3.59436	-0.53966
C	-5.56494	-2.88362	-0.66811
C	-4.62039	-3.92256	-0.60631
C	-4.75962	-5.33063	-0.64247
C	-3.43917	-5.90247	-0.59146
C	-2.48617	-4.84577	-0.51882
C	-2.99836	-7.22607	-0.55664
C	-1.14533	-5.10934	-0.43370
C	-0.69640	-6.45018	-0.41677
C	-1.64301	-7.49263	-0.47563
C	0.68670	-6.66104	-0.33886
C	1.90209	-6.64963	-0.27141
C	3.28061	-6.41322	-0.18636
H	-5.86482	-0.77057	-0.68489
H	-6.61950	-3.11510	-0.72891
H	-3.70954	-8.03941	-0.60101
H	-1.29267	-8.51457	-0.45435
C	3.70322	-5.06403	-0.15669
C	5.03937	-4.77503	-0.08251
C	6.01410	-5.81320	-0.03520
C	5.59707	-7.14490	-0.04722
C	4.24697	-7.43731	-0.12756
C	5.75164	-3.50944	-0.02076
C	7.15053	-3.81048	0.08164
C	7.31982	-5.21591	0.07144
C	5.31034	-2.22021	-0.05410
C	7.63007	-1.45312	0.09839
C	8.07538	-2.75326	0.12805
H	3.91597	-8.46578	-0.14327
H	6.32354	-7.94459	-0.00235
H	8.33447	-0.63482	0.13814
H	9.13393	-2.96394	0.19480
C	1.16477	6.61770	-0.29066
C	0.55997	7.31990	0.77368
C	0.53674	8.75806	0.75640
C	1.13545	9.43899	-0.29725
C	1.74873	8.76575	-1.34745
C	1.75566	7.32729	-1.35783
C	2.35264	9.46649	-2.42368
C	2.91718	8.79907	-3.46916
C	2.89249	7.38684	-3.50116
C	2.32540	6.67636	-2.48358
C	-0.08187	9.45102	1.82927
C	-0.63188	8.77702	2.87824
C	-0.57692	7.36585	2.91737
C	0.00477	6.66260	1.90303
H	-0.99322	6.83956	3.76598
H	-1.09783	9.31831	3.69084
H	-0.10076	10.53323	1.79960
H	1.12393	10.52263	-0.29995
H	2.34856	10.54898	-2.39934
H	3.37176	9.34607	-4.28437
H	3.32039	6.86534	-4.34694
H	2.29925	5.59843	-2.53068
H	0.05390	5.58574	1.95546
C	-6.00931	-6.07759	-0.71231
C	-6.95610	-5.97399	0.33095
C	-8.18829	-6.71143	0.24841

Table S10 (cont.): Cartesian coordinates of MC-F3A3

C	-8.42018	-7.53622	-0.84625
C	-7.49588	-7.66071	-1.87726
C	-6.27060	-6.91043	-1.82258
C	-7.74470	-8.49632	-2.99664
C	-5.38978	-7.00055	-2.93175
C	-5.66702	-7.81333	-3.99251
C	-6.85286	-8.57975	-4.02393
C	-9.13407	-6.59654	1.30006
C	-8.88238	-5.81888	2.39045
C	-7.65620	-5.12550	2.49406
C	-6.72276	-5.20645	1.50184
H	-7.45254	-4.53167	3.37507
H	-9.61085	-5.74242	3.18653
H	-10.06135	-7.14977	1.22049
H	-9.34628	-8.09656	-0.89758
H	-8.66734	-9.06233	-3.02123
H	-7.05644	-9.21827	-4.87311
H	-4.97697	-7.86475	-4.82406
H	-4.48901	-6.40617	-2.93327
H	-5.78401	-4.68448	1.60544
C	8.58301	-5.93745	0.16143
C	9.39296	-5.80648	1.31160
C	10.64183	-6.51621	1.38595
C	11.02302	-7.34250	0.33511
C	10.23375	-7.49491	-0.79914
C	8.99506	-6.77199	-0.90087
C	8.25790	-6.88957	-2.10789
C	10.63476	-8.33245	-1.87190
C	9.87648	-8.44317	-2.99904
C	8.67942	-7.70340	-3.11925
C	9.00178	-5.03842	2.43925
C	9.80541	-4.93063	3.53698
C	11.05031	-5.59582	3.58887
C	11.44996	-6.37355	2.54364
H	9.48261	-4.33715	4.38188
H	11.67467	-5.49809	4.46685
H	12.39203	-6.90577	2.58196
H	11.96054	-7.88186	0.40175
H	11.56549	-8.87771	-1.77876
H	10.19546	-9.08290	-3.81097
H	8.09682	-7.77615	-4.02785
H	7.35141	-6.31564	-2.22445
H	8.04594	-4.53799	2.42415
H	-1.75964	-2.03848	-0.47158
H	-0.41535	-4.31375	-0.37628
H	2.95693	-4.28237	-0.19103
H	4.25838	-1.98265	-0.13276
H	-0.10373	0.88321	-0.36561
H	2.53570	0.90714	-0.18141

Table S11: Cartesian coordinates of 8MC

C	1.21051	-5.96070	-0.27010
C	1.18945	-4.73658	0.52615
C	0.00000	-4.16538	0.95788
C	-1.18945	-4.73658	0.52615
C	-1.21051	-5.96070	-0.27010
C	0.00000	-6.59001	-0.62294
C	-2.55273	-6.16745	-0.68738
C	2.55273	-6.16745	-0.68738
C	2.50821	-4.19186	0.53144
C	-2.50821	-4.19186	0.53144
C	3.35594	-5.06653	-0.26082
C	4.65393	-4.65393	-0.61725
C	5.06653	-3.35594	-0.26083
C	4.19186	-2.50821	0.53144
C	2.94189	-2.94189	0.95297
C	-2.94189	-2.94189	0.95297
C	-4.19186	-2.50821	0.53144
C	-5.06653	-3.35594	-0.26083
C	-4.65393	-4.65393	-0.61725
C	-3.35594	-5.06653	-0.26082
C	5.96070	1.21052	-0.27012
C	4.73658	1.18945	0.52614
C	4.16538	0.00000	0.95788
C	4.73658	-1.18945	0.52614
C	5.96070	-1.21052	-0.27012
C	6.59001	0.00000	-0.62295
C	6.16744	-2.55273	-0.68739
C	6.16744	2.55273	-0.68739
C	-1.21051	5.96070	-0.27010
C	-1.18945	4.73658	0.52615
C	0.00000	4.16538	0.95788
C	1.18945	4.73658	0.52615
C	1.21051	5.96070	-0.27010
C	0.00000	6.59001	-0.62294
C	2.55273	6.16745	-0.68738
C	-2.55273	6.16745	-0.68738
C	-2.50821	4.19186	0.53144
C	2.50821	4.19186	0.53144
C	-3.35594	5.06653	-0.26082
C	-4.65393	4.65393	-0.61725
C	-5.06653	3.35594	-0.26083
C	-4.19186	2.50821	0.53144
C	-2.94189	2.94189	0.95297
C	2.94189	2.94189	0.95297
C	4.19186	2.50821	0.53144
C	5.06653	3.35594	-0.26083
C	4.65393	4.65393	-0.61725
C	3.35594	5.06653	-0.26082
C	-5.96070	-1.21052	-0.27012
C	-4.73658	-1.18945	0.52614
C	-4.16538	0.00000	0.95788
C	-4.73658	1.18945	0.52614
C	-5.96070	1.21052	-0.27012
C	-6.59001	0.00000	-0.62295
C	-6.16744	2.55273	-0.68739
C	-6.16744	-2.55273	-0.68739
H	0.00000	-3.23301	1.51594
H	0.00000	-7.48114	-1.24527
H	5.28248	-5.28248	-1.24311
H	2.27957	-2.27957	1.50427
H	-2.27957	-2.27957	1.50427
H	-5.28248	-5.28248	-1.24311
H	3.23301	0.00000	1.51593
H	7.48113	0.00000	-1.24529
H	0.00000	3.23301	1.51594
H	0.00000	7.48114	-1.24527
H	-5.28248	5.28248	-1.24311
H	-2.27957	2.27957	1.50427
H	2.27957	2.27957	1.50427
H	5.28248	5.28248	-1.24311
H	-3.23301	0.00000	1.51593
H	-7.48113	0.00000	-1.24529
H	2.89474	6.98369	-1.31343
H	-6.98368	2.89474	-1.31345
H	-6.98368	-2.89474	-1.31345
H	-2.89474	-6.98369	-1.31343
H	6.98368	-2.89474	-1.31345
H	6.98368	2.89474	-1.31345
H	-2.89474	6.98369	-1.31343
H	2.89474	-6.98369	-1.31343

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