Electronic Supplementary Material (ESI) for Chemical Science.

Synthesis, Photophysical and Electronic Properties of Tetra- Donor- or Acceptor-Substituted *ortho*-Perylenes Displaying Four Reversible Oxidations or Reductions

Electronic Supporting Information

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Contents

UV-Vis Absorption and Emission Spectra

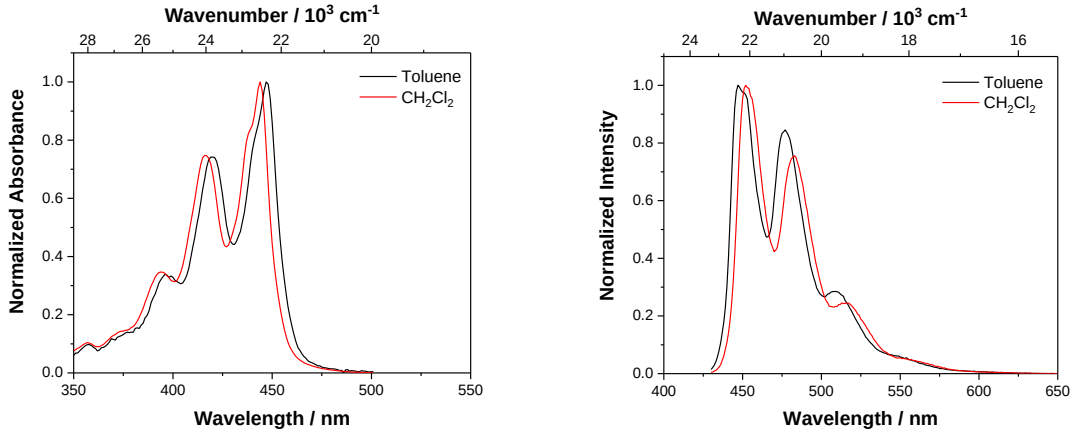

Figure S1. Left: absorption spectra; right: emission spectra of **$(Br)_4$-Per** in toluene and CH_2Cl_2.

Excitation Spectra

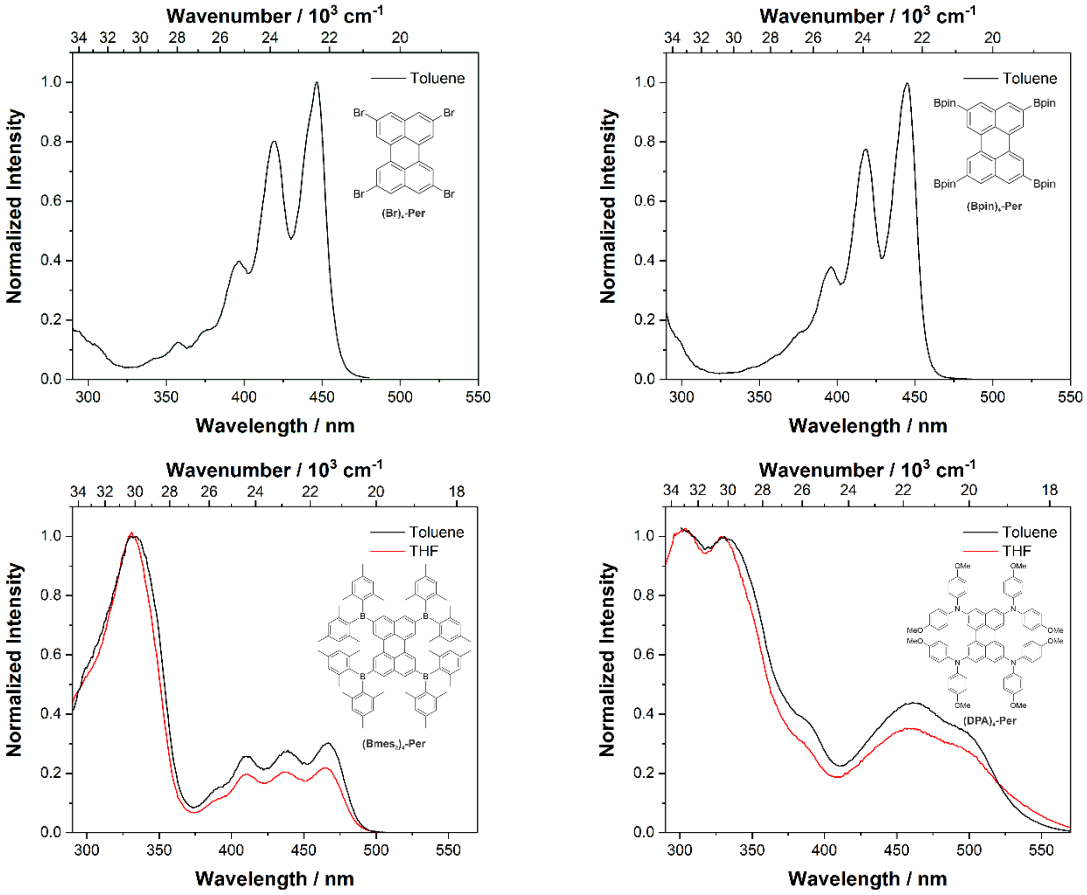

Figure S2. Excitation spectra of compounds **$(Br)_4$-Per** (top left) and **$(Bpin)_4$-Per** (top right) in toluene, **$(Bmes_2)_4$-Per** (bottom left) and **$(DPA)_4$-Per** (bottom right) in toluene and in THF.

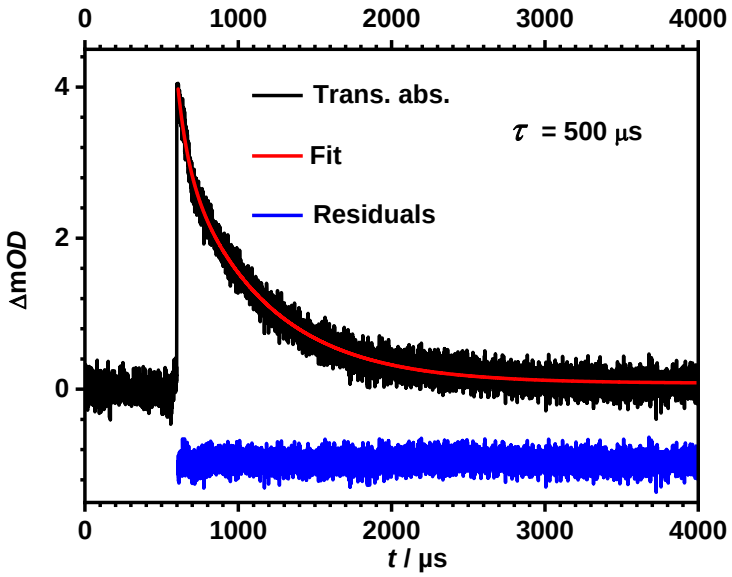

Figure S3. Transient absorption decay curve of **(DPA)$_4$-Per** at 460-550 nm and fit (red).

Spectroelectrochemistry

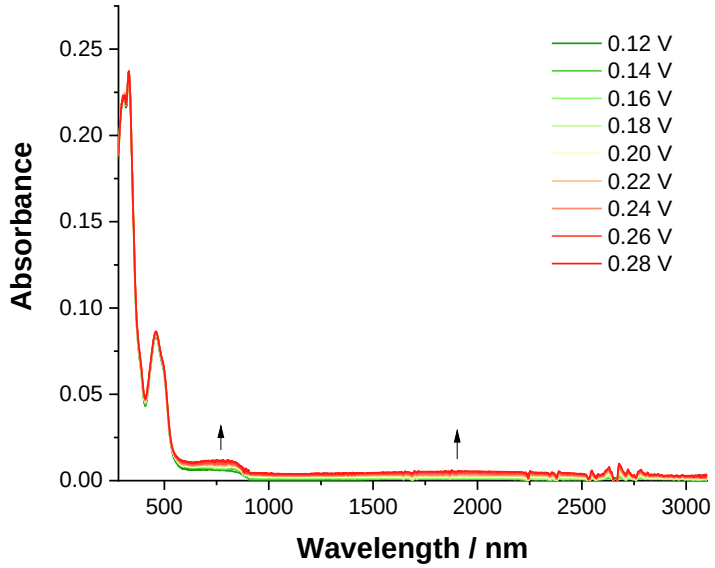

Figure S4. Absorption spectra of **(DPA)$_4$-Per** recorded by spectroelectrochemical measurements (by increasing the applied potential stepwise from 0.12-0.28 V and recording the respective absorption spectrum) in CH_2Cl_2.

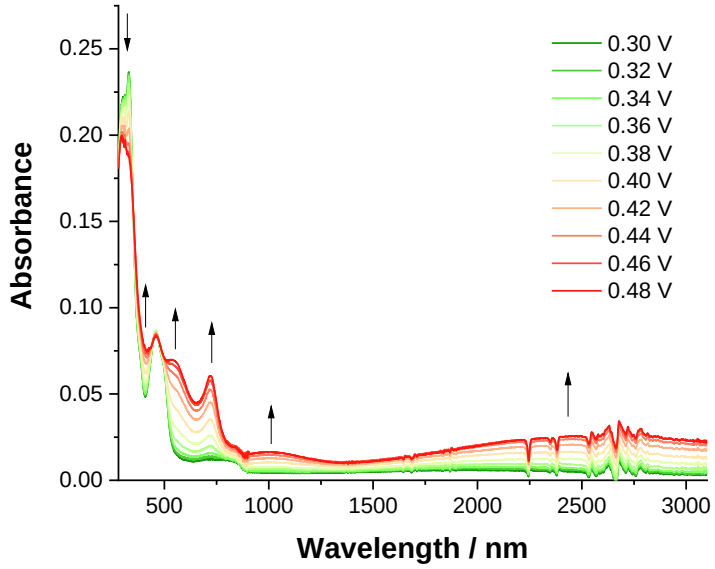

Figure S5. Absorption spectra of **$(DPA)_4$-Per** recorded by spectroelectrochemical measurements (by increasing the applied potential stepwise from 0.30-0.48 V and recording the respective absorption spectrum) in CH_2Cl_2.

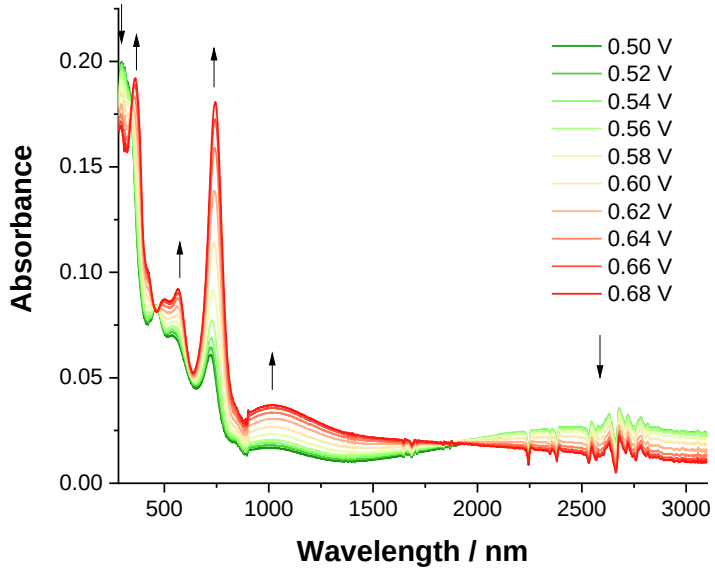

Figure S6. Absorption spectra of **$(DPA)_4$-Per** recorded by spectroelectrochemical measurements (by increasing the applied potential stepwise from 0.50-0.68 V and recording the respective absorption spectrum) in CH_2Cl_2.

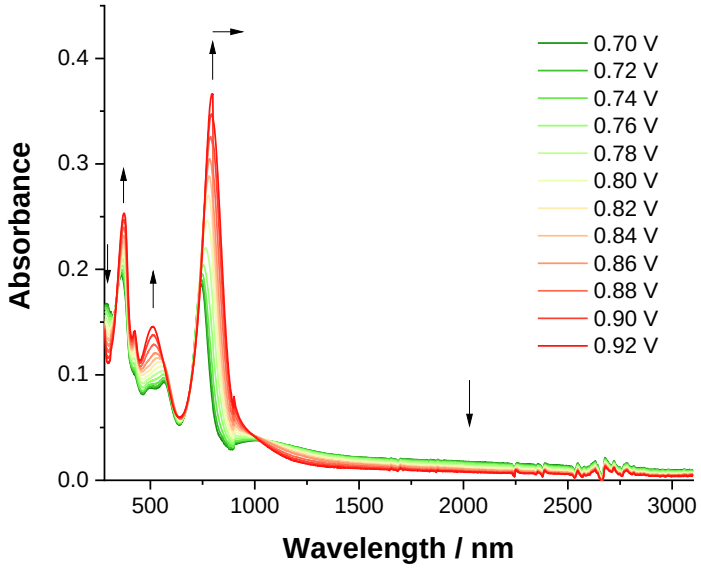

Figure S7. Absorption spectra of **$(DPA)_4$-Per** recorded by spectroelectrochemical measurements (by increasing the applied potential stepwise from 0.70-0.92 V and recording the respective absorption spectrum) in CH_2Cl_2.

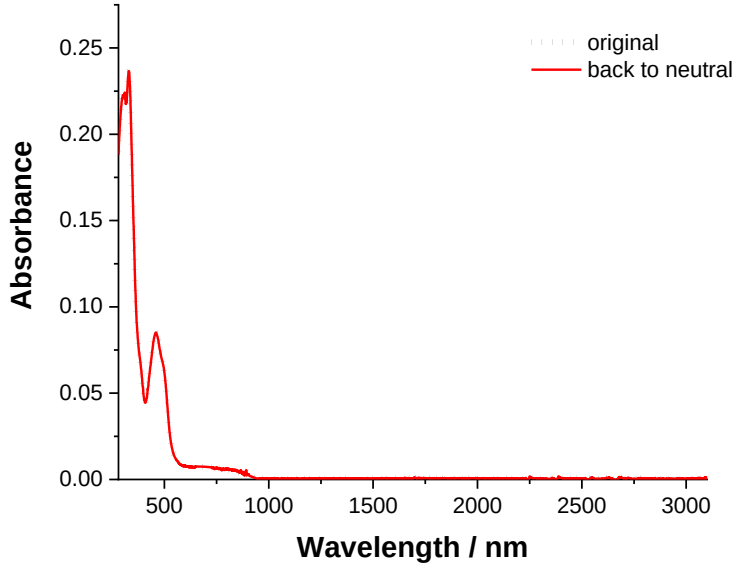

Figure S8. Control absorption spectra of **$(DPA)_4$-Per** recorded by spectroelectrochemical measurements before (dotted, black) and after (red) increasing the applied potential stepwise in CH_2Cl_2.

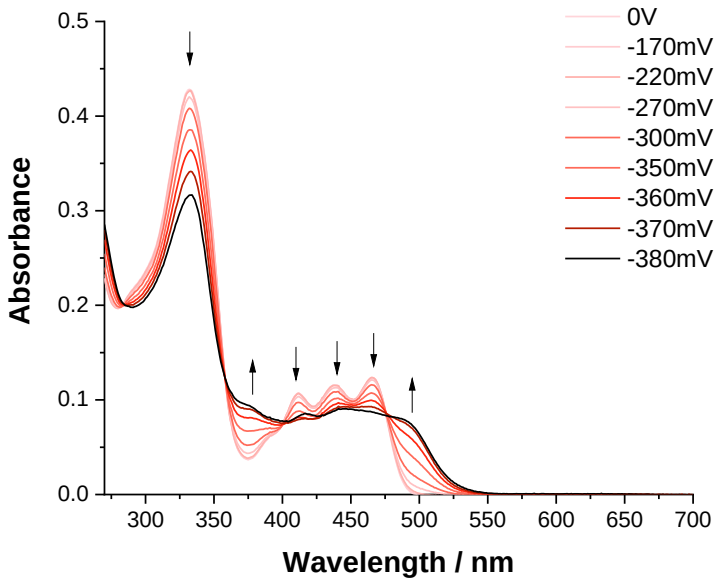

Figure S9. Absorption spectra of **$(Bmes_2)_4$-Per** recorded by spectroelectrochemical measurements (by increasing the applied potential stepwise from 0-(-0.38) V and recording the respective absorption spectrum) in THF.

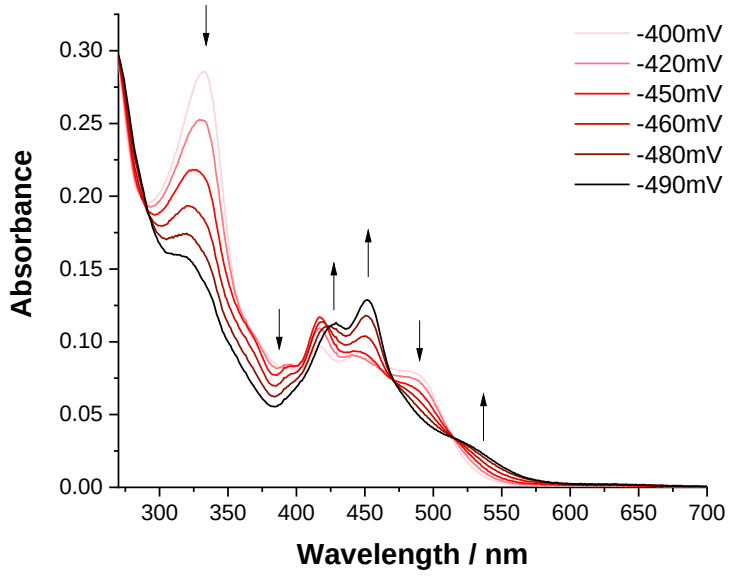

Figure S10. Absorption spectra of **$(Bmes_2)_4$-Per** recorded by spectroelectrochemical measurements (by increasing the applied potential stepwise from (-0.40)-(-0.49) V and recording the respective absorption spectrum) in THF.

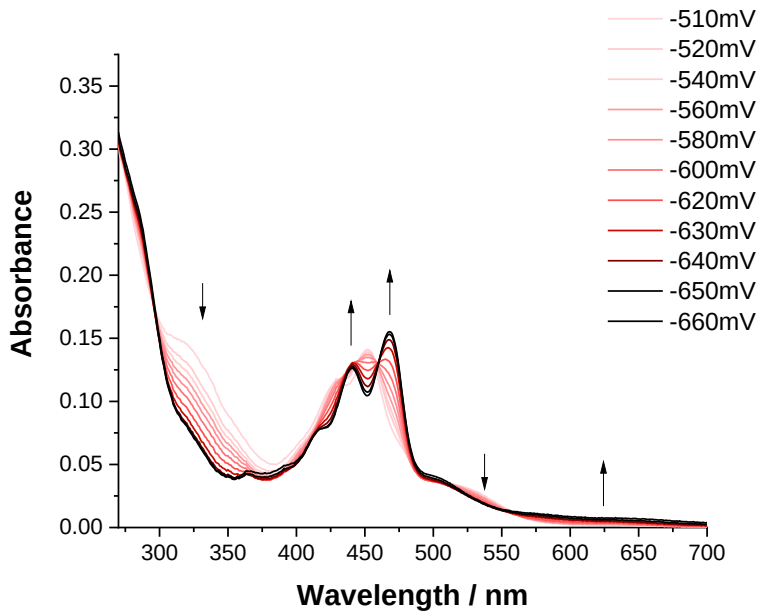

Figure S11. Absorption spectra of **$(Bmes_2)_4$-Per** recorded by spectroelectrochemical measurements (by increasing the applied potential stepwise from (-0.51)-(-0.66) V and recording the respective absorption spectrum) in THF.

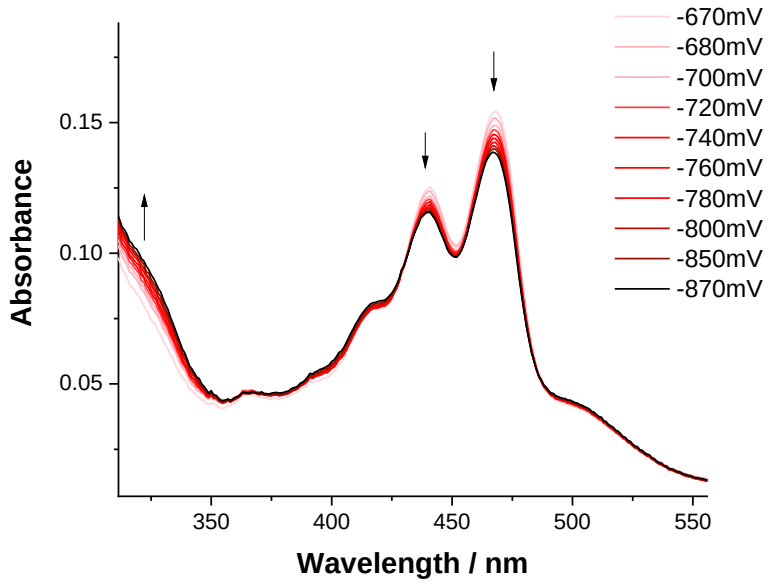

Figure S12. Absorption spectra of **$(Bmes_2)_4$-Per** recorded by spectroelectrochemical measurements (by increasing the applied potential stepwise from (-0.67)-(-0.87) V and recording the respective absorption spectrum) in THF.

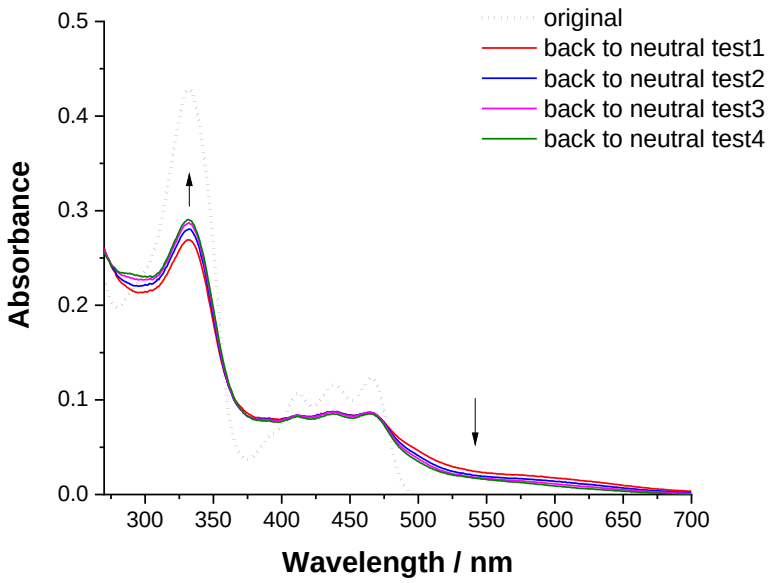

Figure S13. Control absorption spectra of **$(Bmes_2)_4$-Per** recorded by spectroelectrochemical measurements before (black dotted line) and after (solid lines) increasing the applied potential stepwise in THF.

NMR Spectra

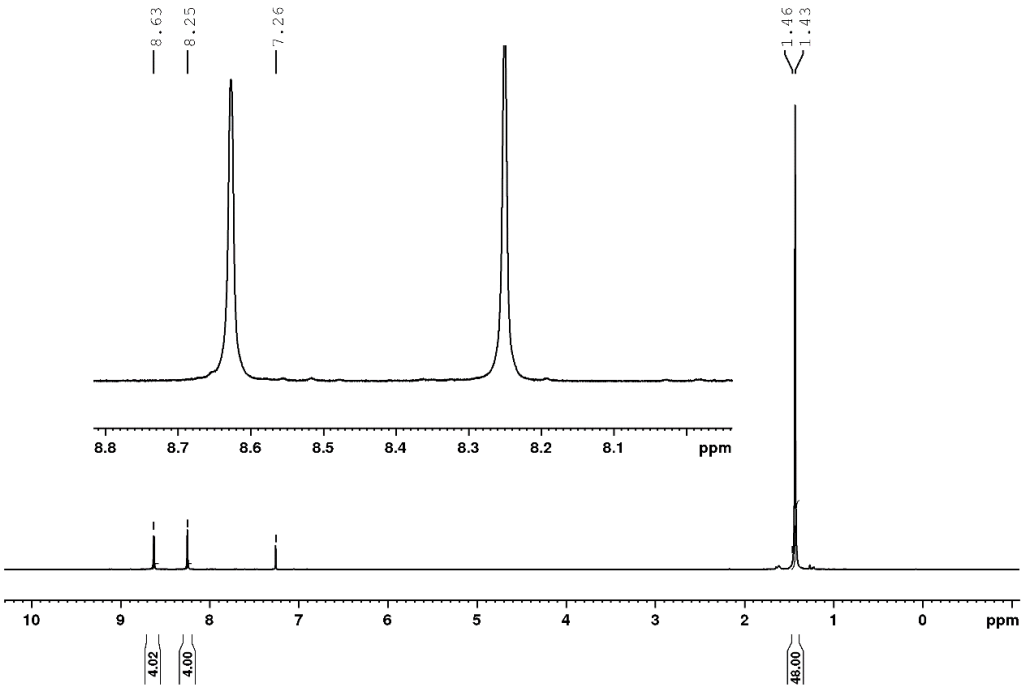

Figure S14. ^{1}H NMR spectrum of **(Bpin)$_4$-Per** in $CDCl_3$ at 300 MHz.

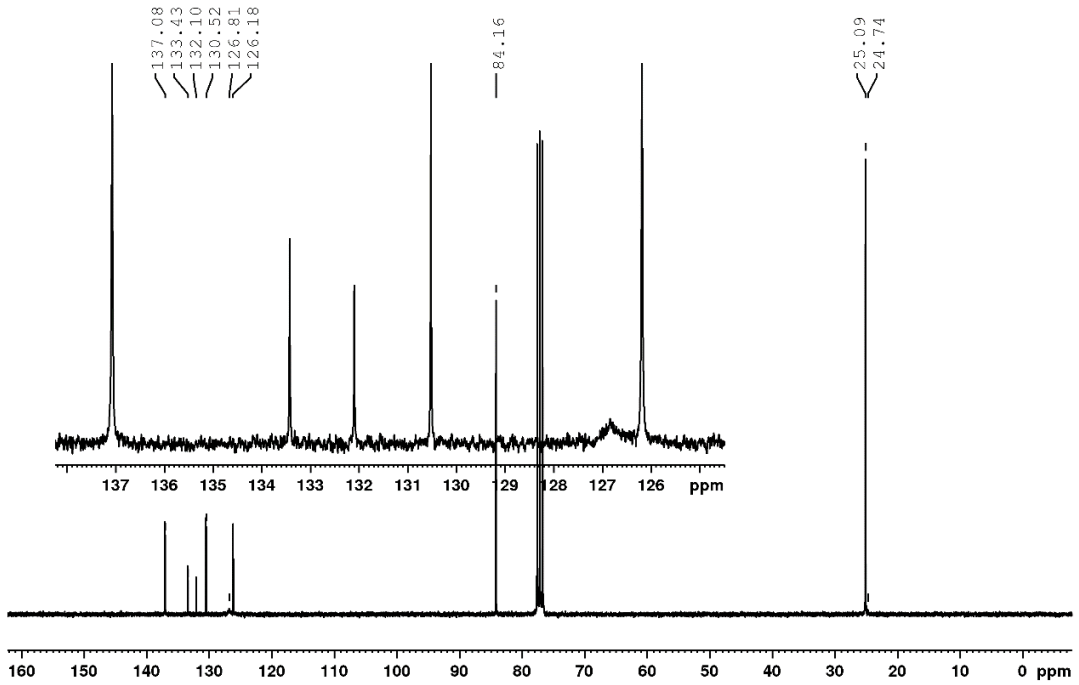

Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of **(Bpin)$_4$-Per** in $CDCl_3$ at 75 MHz.

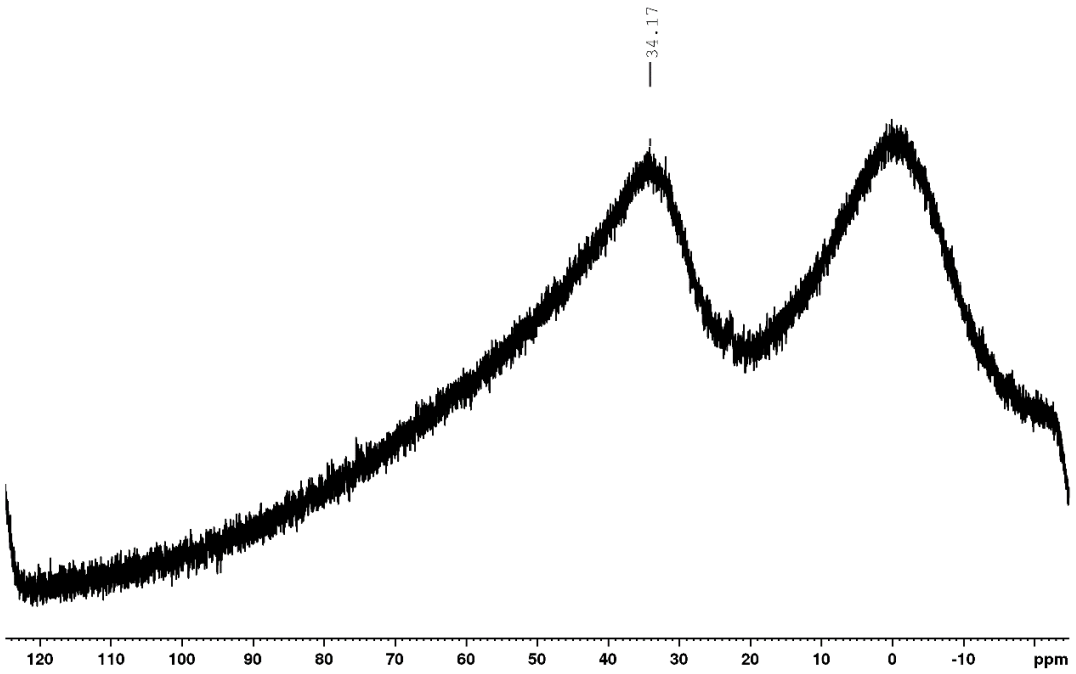

Figure S16. $^{11}B\{^{1}H\}$ NMR spectrum of **$(Bpin)_4$-Per** in $CDCl_3$ at 75 MHz.

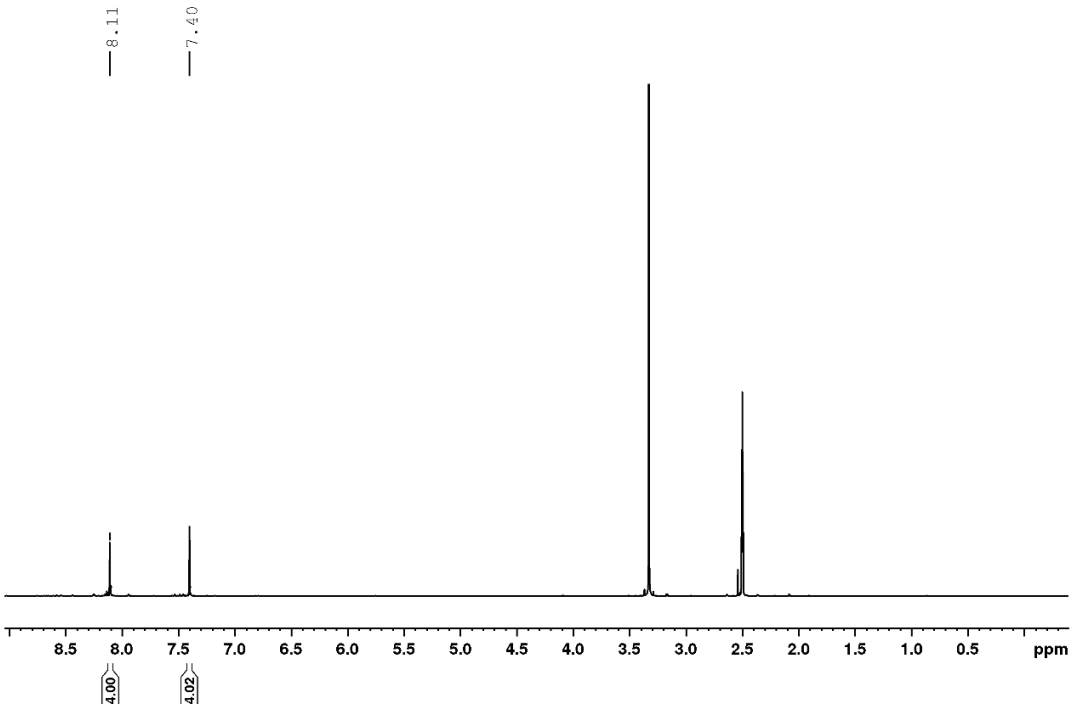

Figure S17. ^{1}H NMR spectrum of **$(BF_3K)_4$-Per** in DMSO-d_6 at 500 MHz.

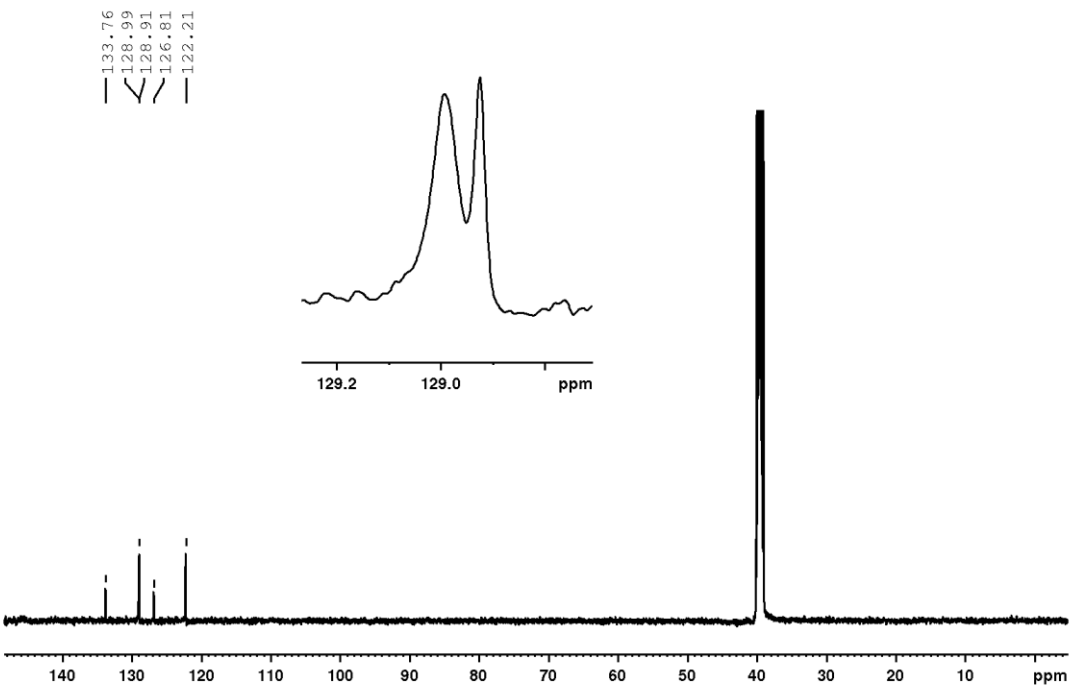

Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **$(BF_3K)_4$-Per** in DMSO-d_6 at 125 MHz.

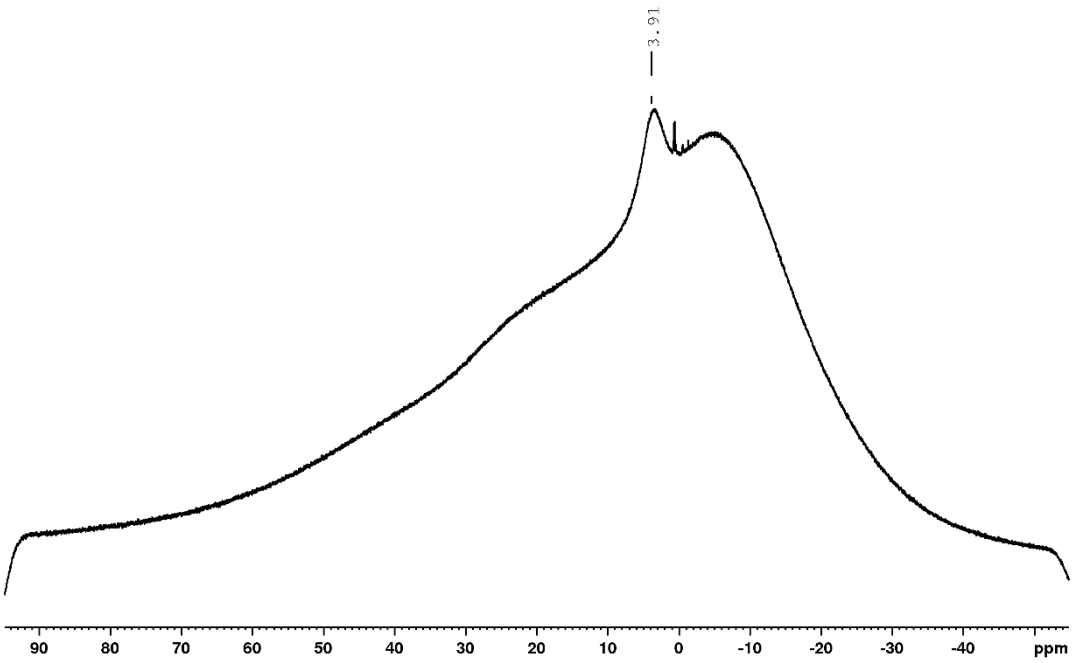

Figure S19. $^{11}B\{^{1}H\}$ NMR spectrum of **$(BF_3K)_4$-Per** in DMSO-d_6 at 160 MHz.

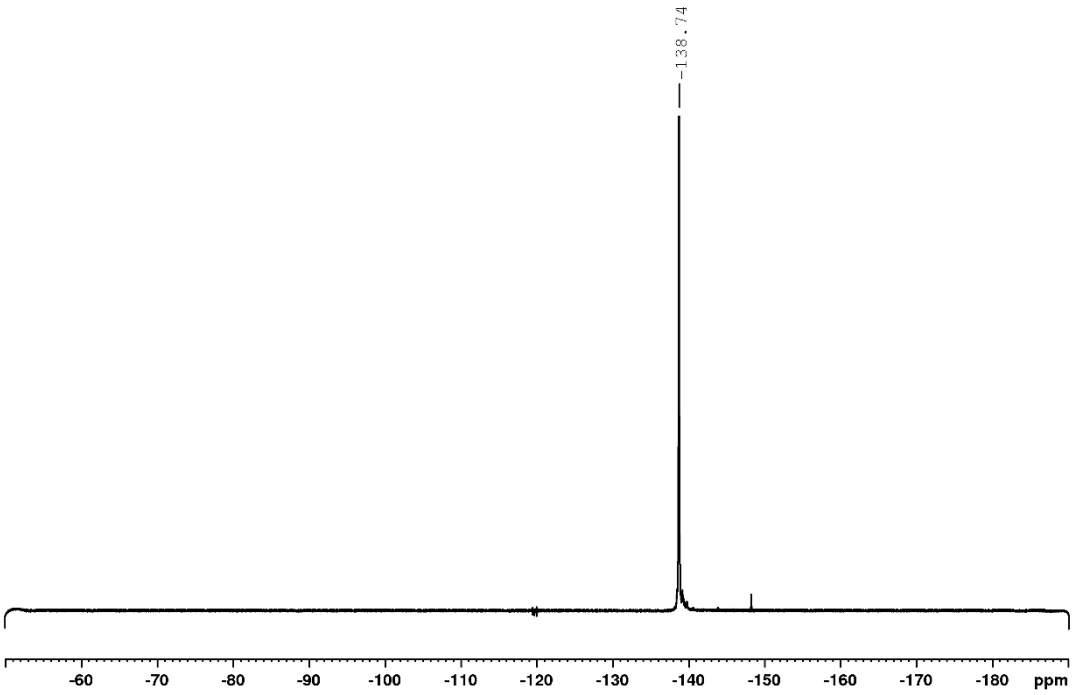

Figure S20. $^{19}F\{^{1}H\}$ NMR spectrum of **$(BF_3K)_4$-Per** in DMSO-d_6 at 470 MHz.

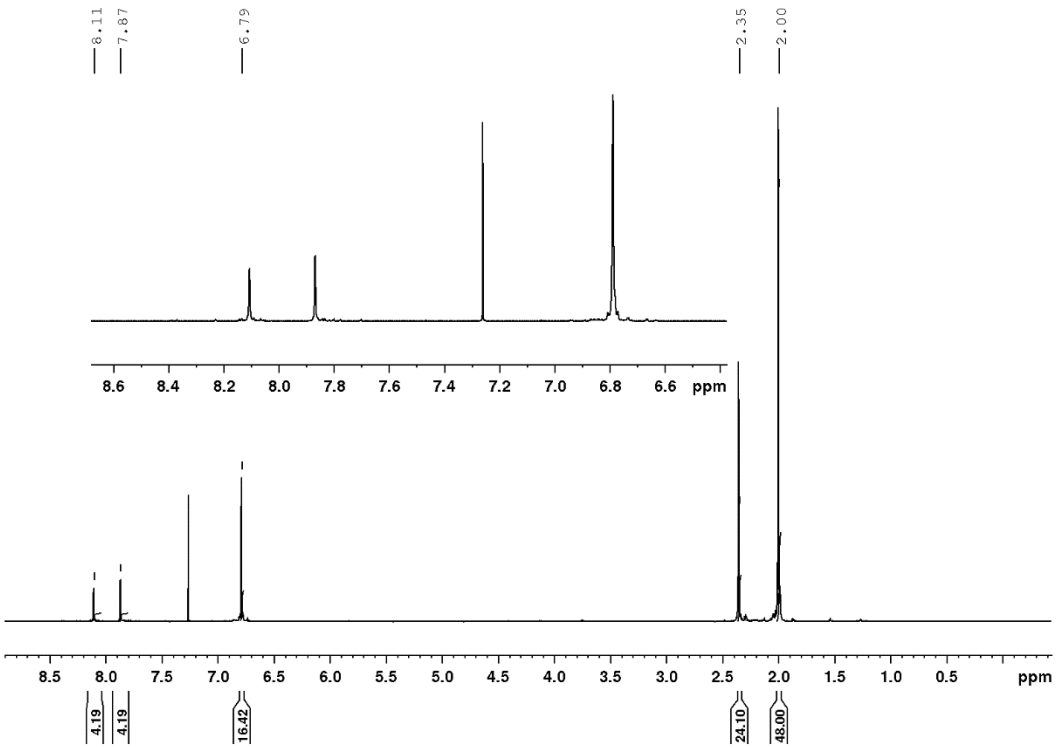

Figure S21. ^{1}H NMR spectrum of **$(Bmes_2)_4$-Per** in $CDCl_3$ at 500 MHz.

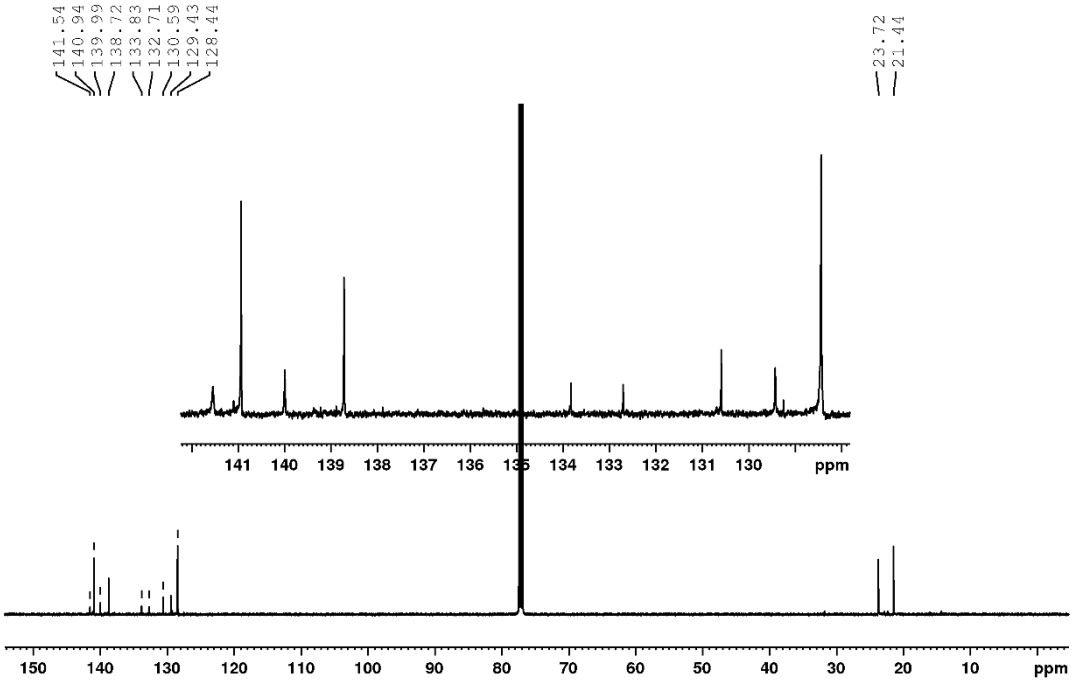

Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of **$(Bmes_2)_4$-Per** in $CDCl_3$ at 125 MHz.

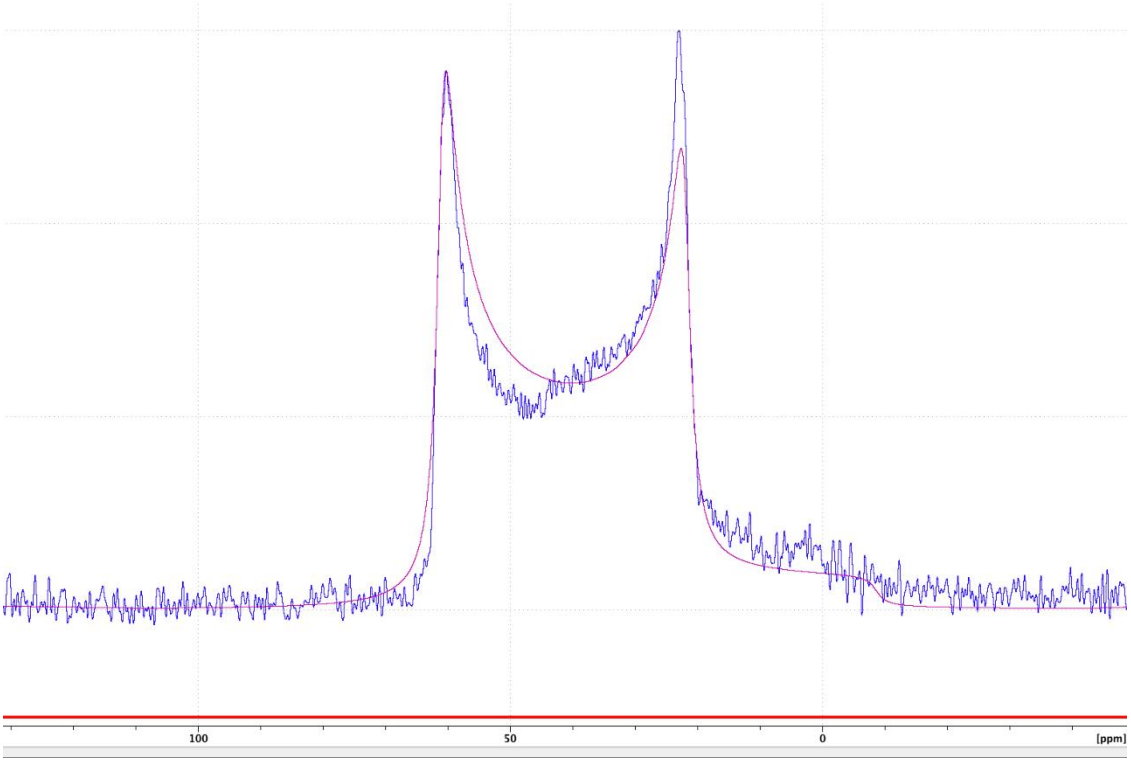

Figure S23. Observed (blue) and simulated (red) solid state $^{11}B\{^{1}H\}$ NMR spectrum of **$(Bmes_2)_4$-Per** at 128 MHz. The isotropic chemical shift (δ_{iso}) is 72.7 ppm, quadrupolar coupling constant C_Q = 4.63 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

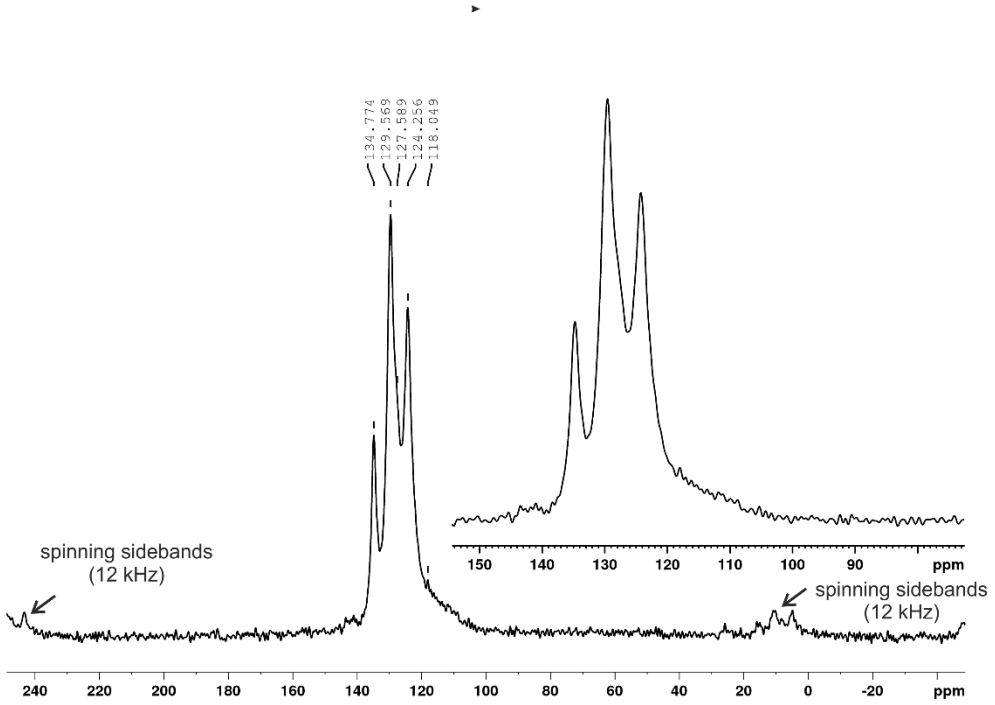

Figure S24. Solid state $^{13}C\{^{1}H\}$-CP spectrum of **$(Br)_4$-Per** at 100 MHz. Measured at 12 kHz rotation.

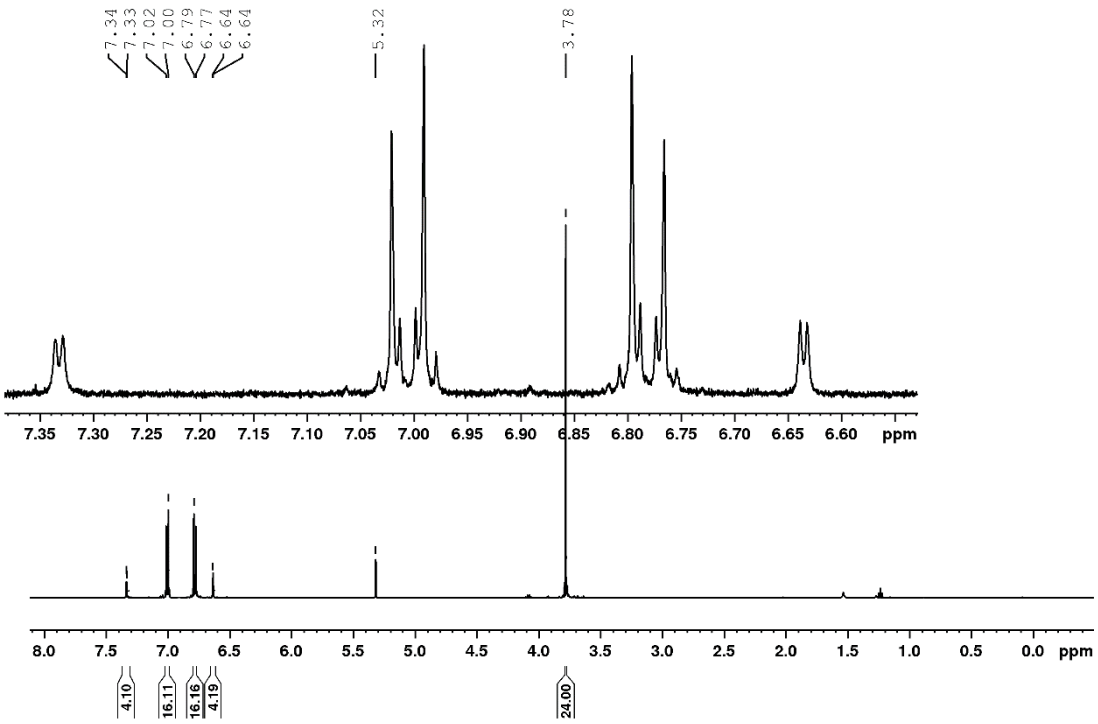

Figure S25. ^{1}H NMR spectrum of **$(DPA)_4$-Per** in CD_2Cl_2 at 500 MHz.

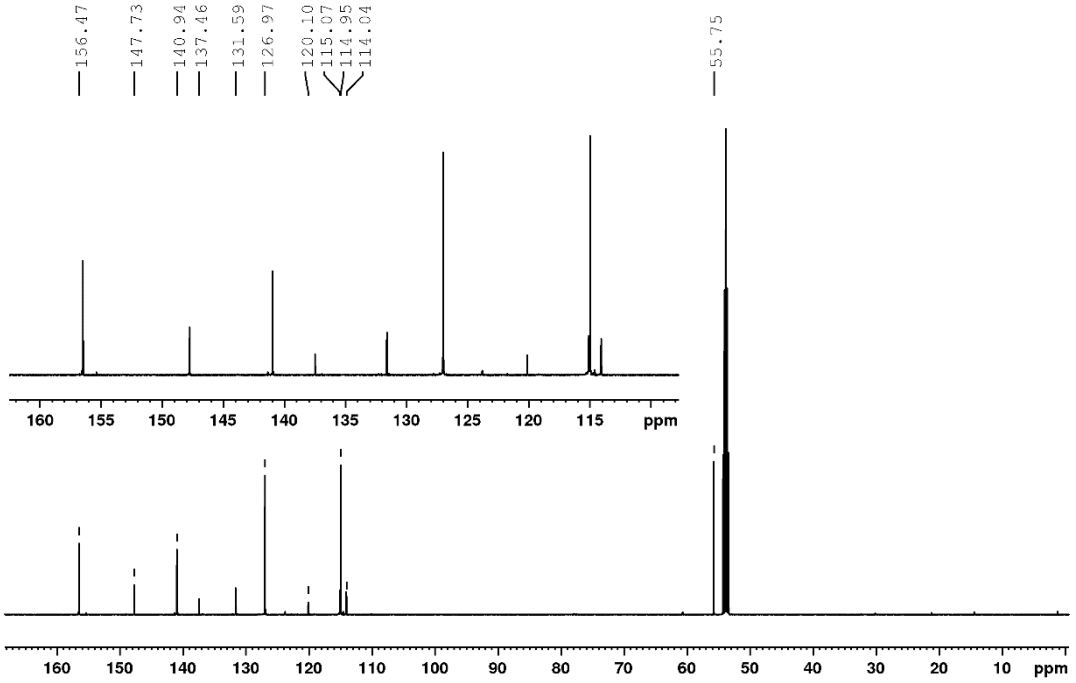

Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of **$(DPA)_4$-Per** in CD_2Cl_2 at 125 MHz.

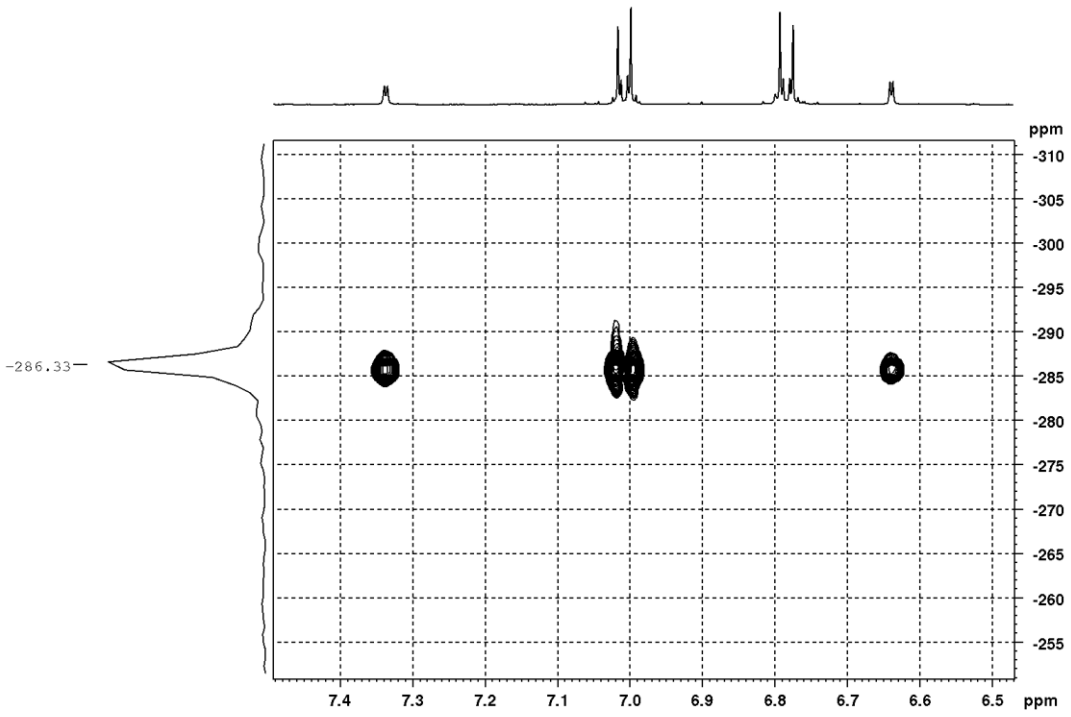

Figure S27. ^{15}N, ^{1}H HMBC NMR spectrum of **$(DPA)_4$-Per** in CD_2Cl_2 at 500 MHz.

Single-crystal X-ray diffraction

Table S1: Single-crystal X-ray diffraction data and structure refinement of **$(DPA)_4$-Per**.

Compound	4N-Per
CCDC	1881912
Formula	$C_{76}H_{64}N_4O_8$
ρ_x/ g cm^{-3}	1.305
F(000)	1224
Crystal size/mm^3	0.132×0.302×0.39
Crystal color, habit	orange plate
μ/mm^{-1}	0.085
M_r/g·mol^{-1}	1161.31
T/K	100
λ/Å, radiation	0.71073, MoKα
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.025(7)
b/Å	11.576(7)
c/Å	18.285(9)
α/°	90
β/°	95.45(2)
γ/°	90
V/Å^3	2955(3)
Z	2
θ_{max}/°	26.511
Reflections collected	23828
Unique refls.	6104
Parameters	401
GooF on F^2	1.016
R_1 [I>2σ(I)]	0.0470
wR_2 (all data)	0.1182
Max./min. residual electron density/e·Å^{-3}	0.271/-0.214

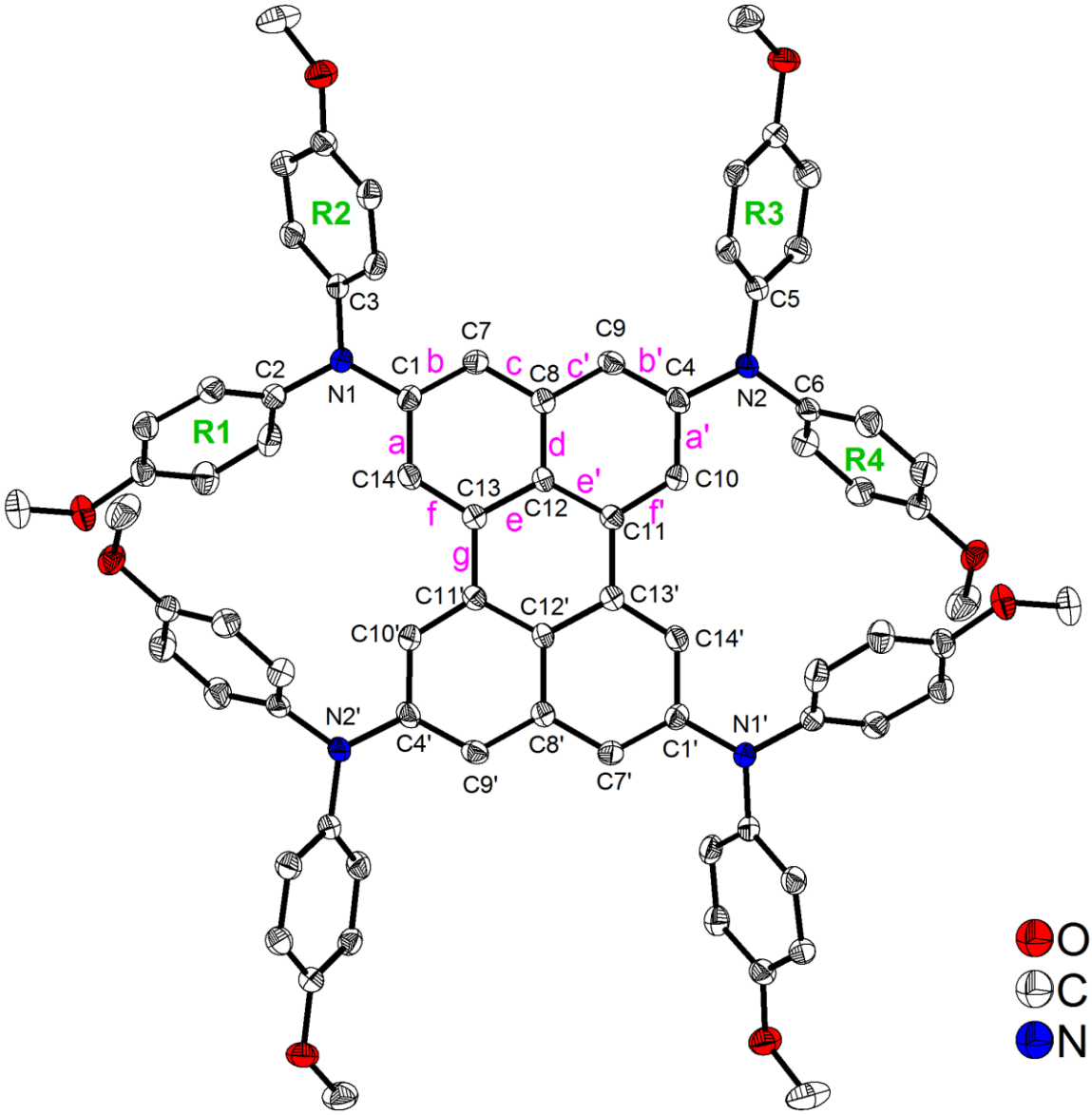

Figure S28. Solid state molecular structure of **(DPA)$_4$-Per** from single-crystal X-ray diffraction at 100 K. Atomic displacement ellipsoids are drawn at the 50% probability level, and hydrogen atoms are omitted for clarity. Terminal aryl rings bonded to nitrogen are labelled R1 and R2 if bonded to N1 and R3 and R4 if bonded to N2, respectively.

Table S2. Selected bond lengths (Å) and angles (°) of compound **$(DPA)_4$-Per**. Bonds are labelled according to the scheme in Figure S28.

	$(DPA)_4$-Per this study	**β-perylene[1]**
a, a’	1.412(3), 1.412(3)	1.407(1), 1.409(1)
b, b’	1.372(3), 1.378(3)	1.370(1), 1.371(1)
c, c’	1.412(3), 1.416(3)	1.417(1), 1.418(1)
d	1.426(3)	1.429(1)
e, e’	1.424(3), 1.422(2)	1.430(1), 1.429(1)
f, f’	1.380(3), 1.371(3)	1.389(1), 1.387(1)
g	1.479(2)	1.474(1)
N1–C1	1.406(2)	
N1–C2	1.429(2)	
N1–C3	1.422(2)	
N2–C4	1.399(2)	
N2–C5	1.413(2)	
N2–C6	1.432(2)	
∠ $N1C_3$-R1	42.90(8)	
∠ $N1C_3$-R2	43.99(9)	
∠ $N2C_3$-R3	44.15(7)	
∠ $N2C_3$-R4	66.00(9)	
Sum ∠ CN1C	359.8(2)	
Sum ∠ CN2C	359.2(2)	

Table S3. Intra- and intermolecular interaction distances (Å) of compound **$(DPA)_4$-Per** at 100 K. Aryl rings are labelled according to the scheme in Figure S28. '(m)' denotes that the methoxy group of the respective aryl ring is involved in the interaction.

	H···O/C/π	C···O/C/π	Aryl / (m)···Aryl / (m)
Intramolecular contact			
C20-H20C···O4'	2.5064(18)	3.246(3)	R1(m)···R4′(m), R1′(m)···R4(m)
Intermolecular contacts			
C24-H24···π(R3)	2.8207(14)	2.8419(13)	R2···π(R3)
C32-H32A···O4	2.5422(17)	3.287(3)	R3(m)···R4(m)
C33-H33···O2	2.6568(16)	3.378(3)	R4(m)···R2
C16-H16···C29	2.714(2)	3.395(3)	R1···R3
C32-H32B···C8	2.6230(19)	3.445(3)	R3(m)···perylene
C30-H30···O2	2.6986(17)	3.499(3)	R3···R2(m)
C38-H38B···C13	2.675(2)	3.540(3)	R4(m)···perylene
C32-H32C···O1	2.6826(17)	3.616(3)	R3(m)···R1(m)
C21-H21···C9	2.773(2)	3.630(3)	R2···perylene
C16-H16···O3	2.7954(17)	3.676(3)	R1···R3(m)
C38-H38B···C14	2.745(2)	3.685(3)	R4(m)···perylene
C7-H7···π(R1)	2.800(2)	3.695(3)	perylene···π(R1)
C35···O3		3.175(3)	R3···R4(m)
C20···O2		3.526(3)	R1(m)···R2(m)

Note: For the intramolecular contact the notation of the aryl rings distinguishes between the inversion symmetric rings, i.e. R1 and R1′ as well as R4 and R4′, respectively.

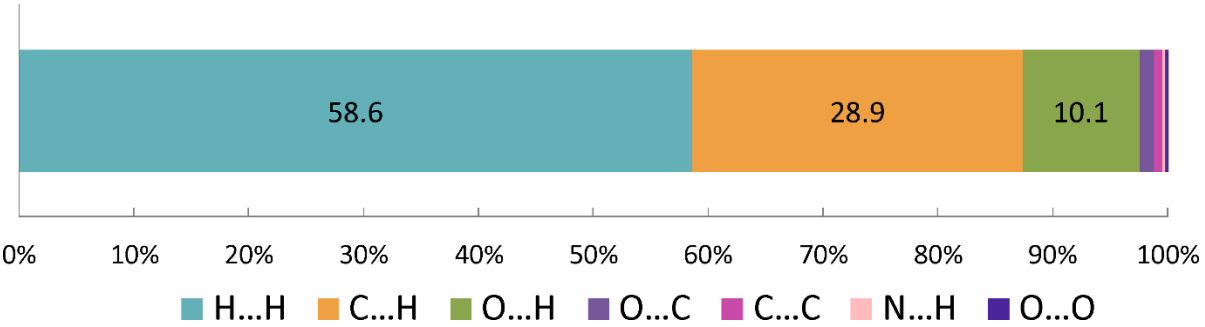

Figure S29. Percentage contributions to the Hirshfeld surface area for the various close intermolecular contacts in **(DPA)$_4$-Per** at 100 K.

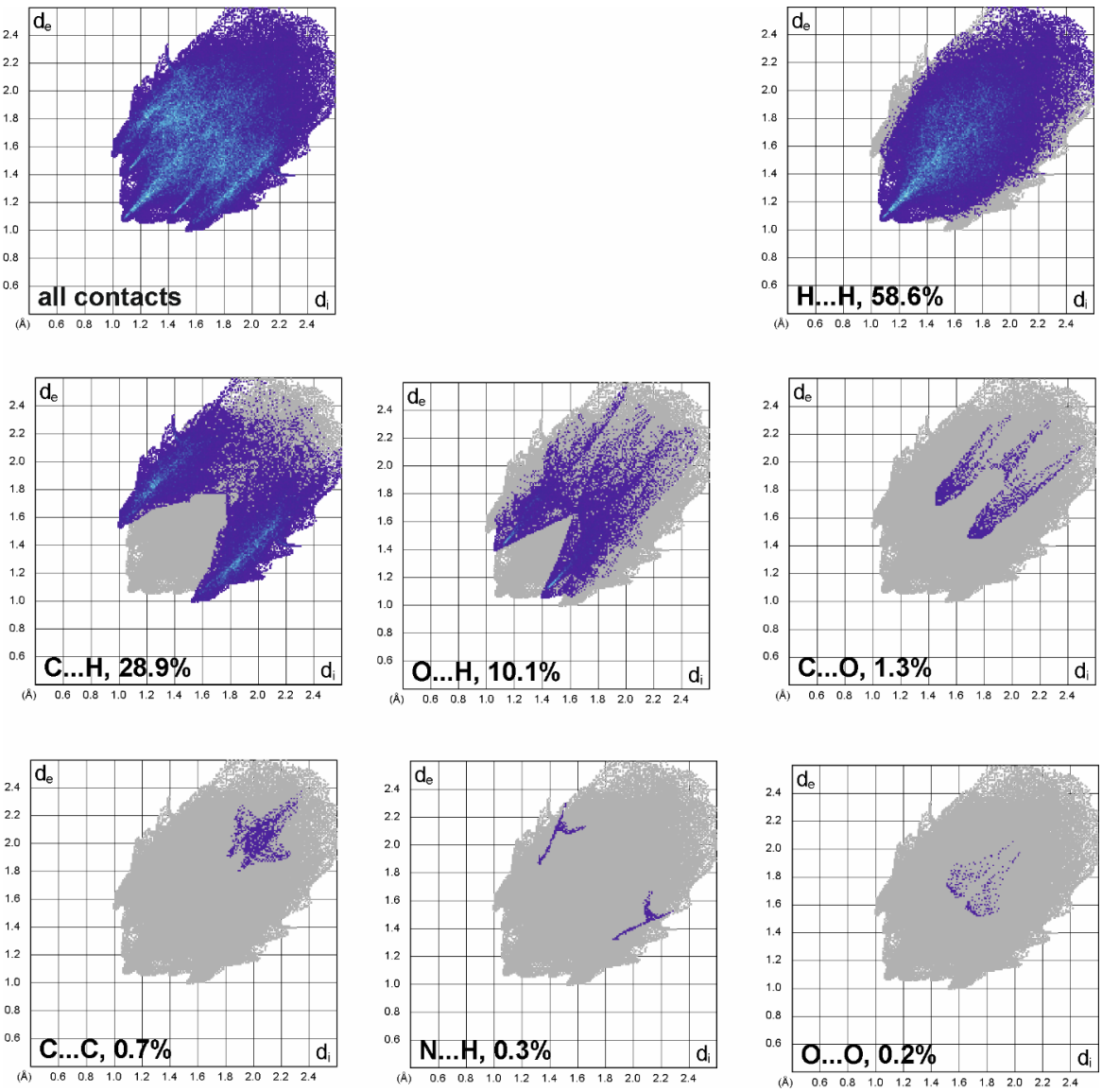

Figure S30. Two-dimensional fingerprint plots of **(DPA)$_4$-Per** calculated from the Hirshfeld surface at 100 K. The top left figure shows the complete fingerprint plot, while the other plots indicate the contributions of the individual intermolecular interactions within the grey area of all contributions.

TD-DFT Results

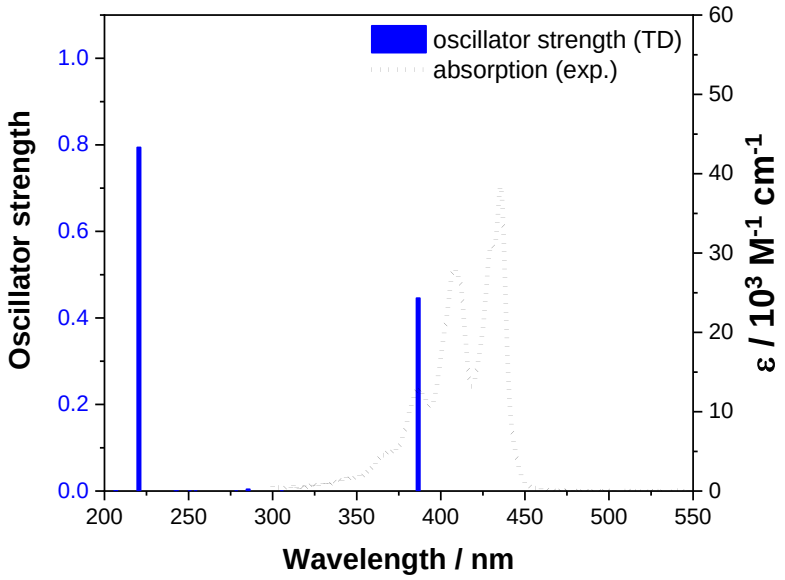

Figure S31. TD-DFT calculated singlet electronic transitions of **perylene** in the gas phase using CAM-B3LYP/6-31+G (d,p) and the experimental absorption in toluene.

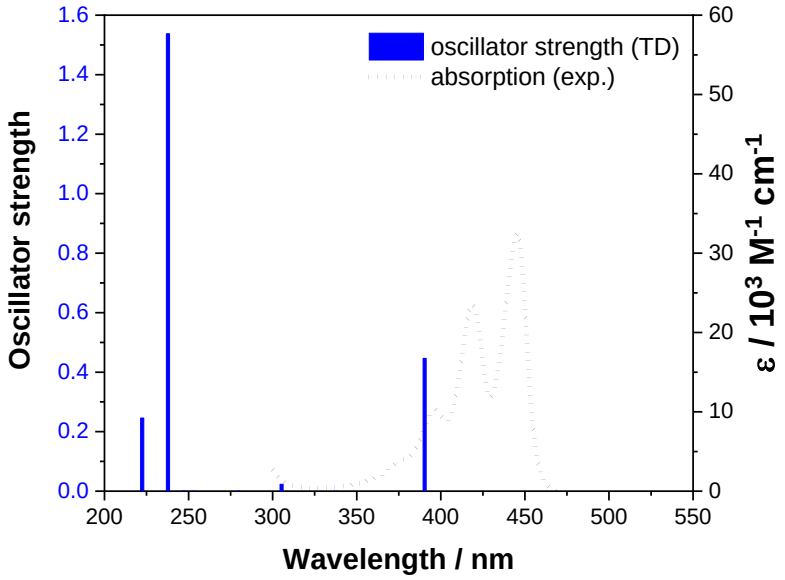

Figure S32. TD-DFT calculated singlet electronic transitions of **(Bpin$_4$)-Per** in the gas phase using CAM-B3LYP/6-31+G (d,p) and the experimental absorption in toluene.

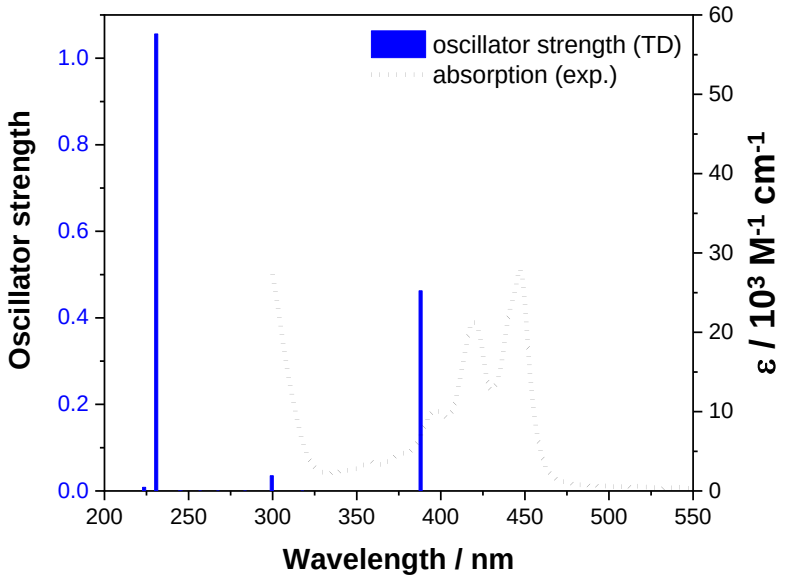

Figure S33. TD-DFT calculated singlet electronic transitions of **$(Br)_4$-Per** in the gas phase using CAM-B3LYP/6-31+G (d,p) and the experimental absorption in toluene.

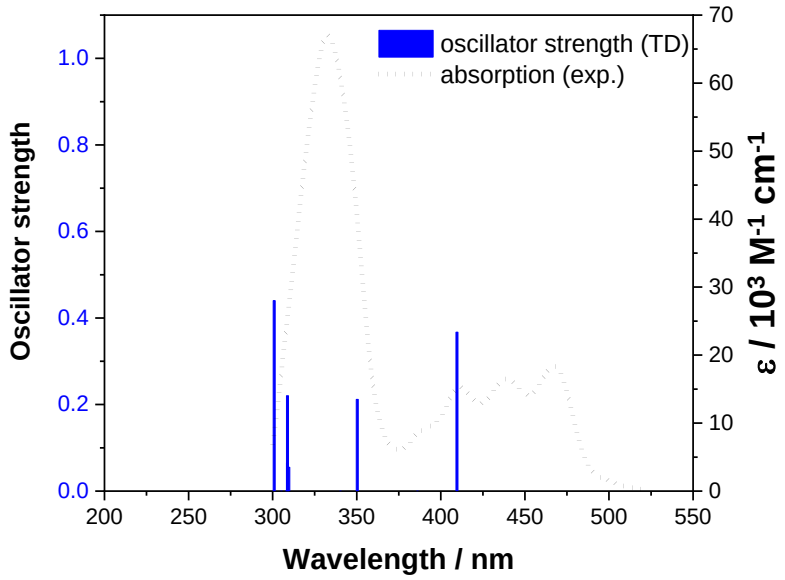

Figure S34. TD-DFT calculated singlet electronic transitions of **$(Bmes_2)_4$-Per** in the gas phase using CAM-B3LYP/6-31+G (d,p) and the experimental absorption in toluene.

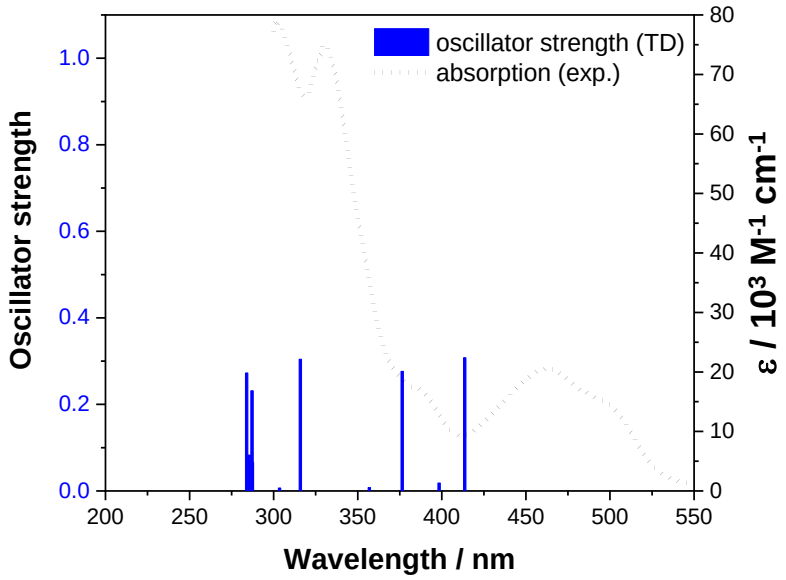

Figure S35. TD-DFT calculated singlet electronic transitions of **$(DPA)_4$-Per** in the gas phase using CAM-B3LYP/6-31+G (d,p) and the experimental absorption in toluene.

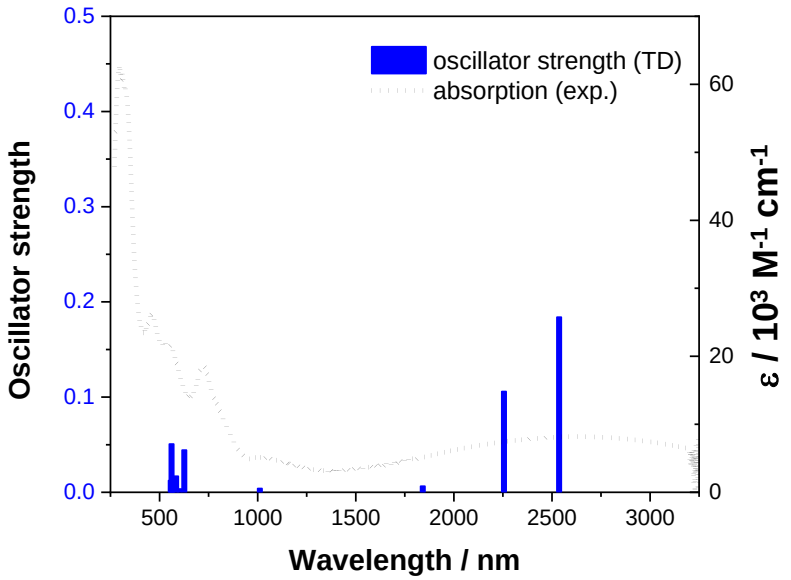

Figure S36. TD-DFT calculated singlet electronic transitions of **$(DPA)_4$-Per$^+$** in dichloromethane using ublyp/svp and the experimental absorption in dichloromethane.

Table S4. Lowest energy singlet electronic transitions of **$(DPA)_4$-Per^+** (TD-DFT) using ublyp with 35% exact exchange admixture, a SVP basis set and a polarizable continuum model accounting for solvent effects (CH_2Cl_2).

FC-S_n	E [eV] (E [nm])	f	Configuration (major contributions > 10%)
S_1	0.49 (2536)	0.184	β-H→ β-L (89%)
S_2	0.55 (2256)	0.106	β-H-1→ β-L (82%)
S_3	0.67 (1842)	0.006	β-H-2→ β-L (87%)
S_4	1.23 (1011)	0.004	β-H-3→ β-L (97%)
S_5	1.98 (626)	0.044	α-H-1→ α-L (63%), β-H-8→ β-L (19%), α-H-4→ α-L (19%)

Orbital Depictions

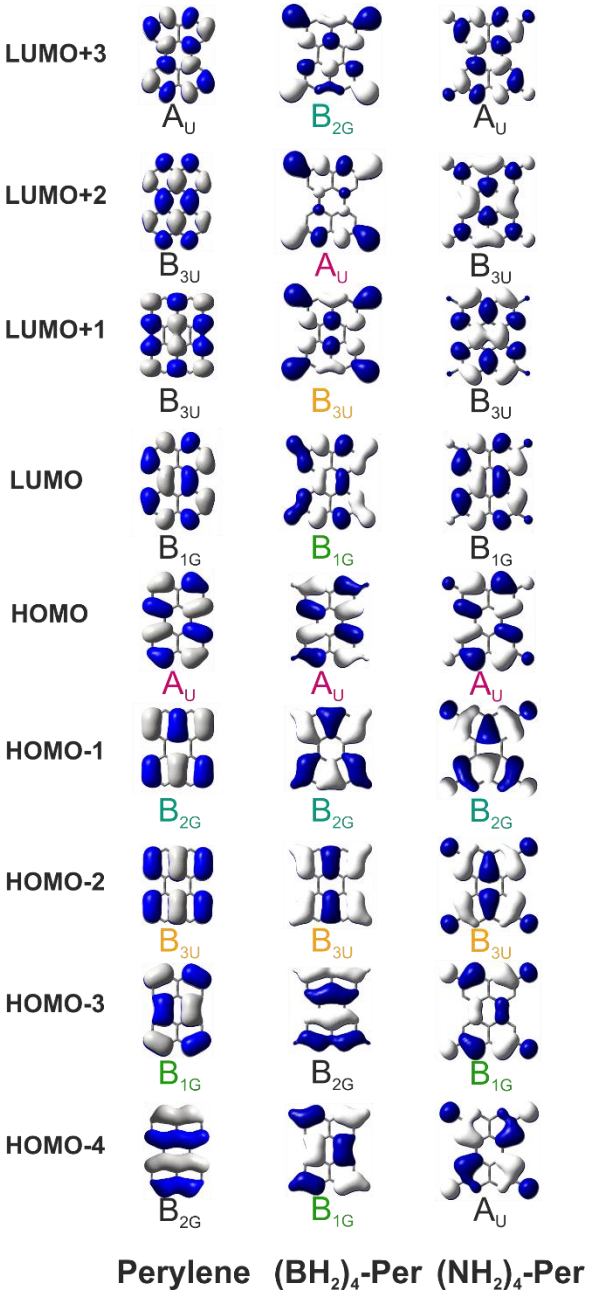

Figure S37. Depiction of the orbitals LUMO+3 to HOMO-4 of the model compounds **$(BH_2)_4$-Per** and **$(NH_2)_4$-Per**.

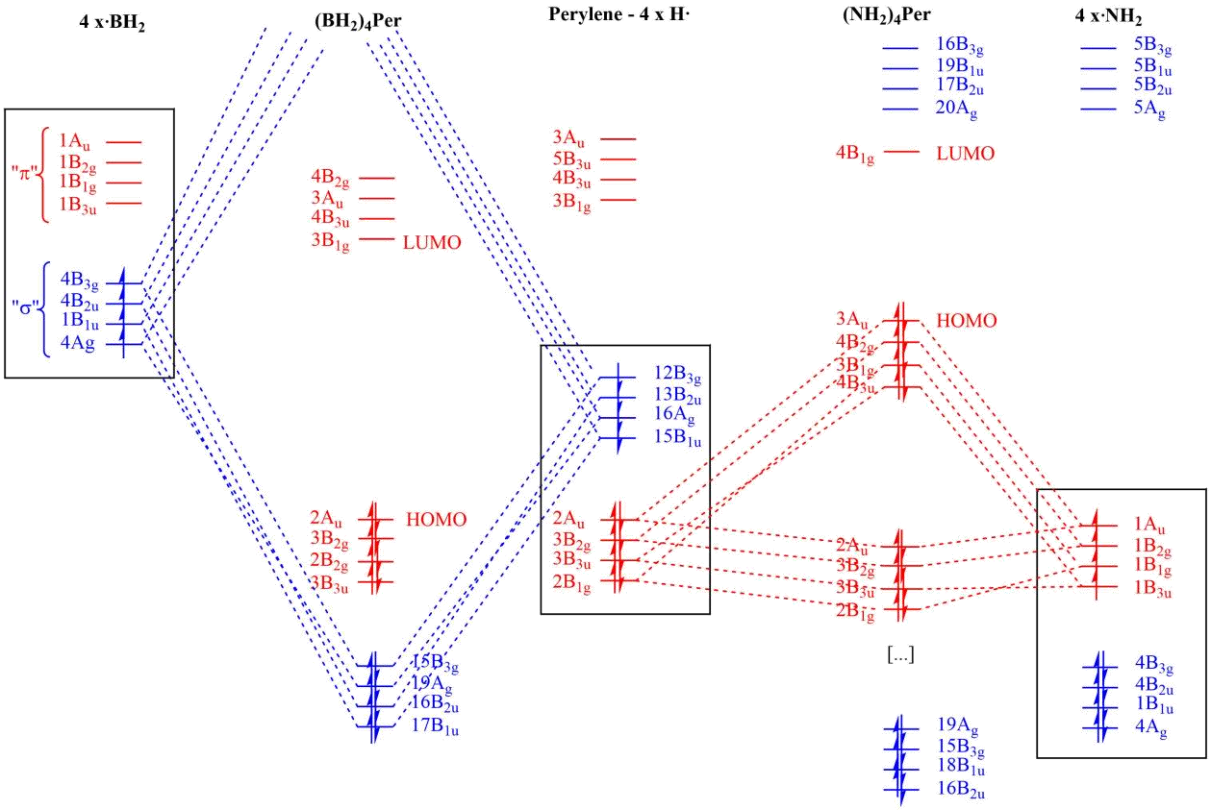

Figure S38. Schematic representation of the fragmentation of the model compounds **$(BH_2)_4$-Per** and **$(NH_2)_4$-Per**.

Cartesian Coordinates

Compound Perylene (DFT B3LYP/6-31+G(d,p), S_0)

Total energy: -482867.30 kcal mol^{-1}

Dipole moment: 0 D

Symbol	X/Å	Y/Å	Z/Å
C	-2.881740	2.421287	0.000006
C	-1.476137	2.426109	0.000000
C	-0.737075	1.248466	0.000001
C	-1.437288	-0.000014	0.000003
C	-2.871146	0.000001	0.000005
C	-3.571300	1.231791	0.000009
C	-0.737085	-1.248494	-0.000002
C	-1.476195	-2.426128	-0.000017
C	2.881794	-2.421270	0.000013
C	-3.571327	-1.231757	-0.000001
C	0.737074	1.248462	-0.000001
C	1.437291	-0.000012	-0.000002
C	0.737083	-1.248499	0.000005
C	2.871147	0.000008	-0.000006
C	3.571330	-1.231759	-0.000000
C	-2.881789	-2.421273	-0.000014
C	1.476194	-2.426126	0.000018
C	1.476138	2.426109	0.000001
C	2.881733	2.421290	-0.000006
C	3.571298	1.231790	-0.000010
H	-3.416808	3.365822	0.000007
H	-0.971928	3.384539	-0.000003
H	-4.657190	1.216550	0.000013
H	-0.972024	-3.384570	-0.000029
H	3.416892	-3.365789	0.000020
H	-4.657217	-1.216503	0.000001
H	4.657220	-1.216497	-0.000004
H	-3.416894	-3.365788	-0.000025
H	0.972032	-3.384573	0.000032
H	0.971923	3.384537	0.000006
H	3.416809	3.365821	-0.000006
H	4.657188	1.216556	-0.000016

Compound $(Bpin)_4$-Per (DFT B3LYP/6-31+G(d,p), S_0)

Total energy: -1513850 kcal mol^{-1}

Dipole moment: 0.0015 D

Symbol	X/Å	Y/Å	Z/Å
C	-2.43893700	-2.89298300	-0.01232800
C	-2.42342000	-1.47737000	-0.00775800
C	-1.24912900	-0.73765400	-0.00403400
C	0.00012200	-1.43625800	-0.00733700
C	0.00010300	-2.87013000	-0.01126400
C	-1.23100200	-3.56784800	-0.01331100
C	1.24938200	-0.73764500	-0.00665100
C	2.42366100	-1.47739700	-0.00651400
C	2.43911100	2.89304100	-0.00171600
C	1.23119600	-3.56786200	-0.01261200
C	-1.24912900	0.73761200	0.00248400
C	0.00011400	1.43623700	0.00185200
C	1.24937500	0.73765200	-0.00430500
C	0.00008700	2.87010200	0.00782300
C	1.23116600	3.56785400	0.00524900
C	2.43914100	-2.89302500	-0.00927600
C	2.42364400	1.47741800	-0.00632800
C	-2.42341200	1.47730400	0.01068200
C	-2.43893800	2.89291300	0.01641500
C	-1.23101600	3.56779800	0.01428100
H	-3.38235900	-0.97342200	-0.00828600
H	-1.21587000	-4.65421100	-0.01516200
H	3.38260800	-0.97347100	-0.00329900
H	1.21605000	-4.65422000	-0.01649600
H	1.21601100	4.65421500	0.00833600
H	3.38259000	0.97350300	-0.01127900
H	-3.38233500	0.97333800	0.01410000
H	-1.21588800	4.65415900	0.01748700
C	-5.26452800	5.37989500	-0.13898500
C	-6.01780600	4.04559300	0.21397900
O	-3.87778400	5.02889800	0.12052500
O	-5.00570400	3.03925900	-0.06112300
C	-5.63478200	6.57688200	0.72749500
H	-5.04856500	7.44726200	0.42106000
H	-6.69522500	6.82320200	0.61302400
H	-5.43113300	6.38581700	1.78185300
C	-5.35471400	5.74706300	-1.62290900
H	-6.35688300	6.09192800	-1.89235900
H	-4.64367900	6.55031700	-1.83125100
H	-5.09736600	4.89344000	-2.25539600
C	-7.24312900	3.75128000	-0.64196000
H	-7.68384300	2.79869800	-0.33619700
H	-7.99928700	4.53266800	-0.51562900
H	-6.98498500	3.68081400	-1.69934100
C	-6.36392000	3.92462700	1.70076900
H	-7.17407200	4.60299100	1.98252600
H	-6.68212800	2.89957100	1.90614400
H	-5.49363600	4.14133400	2.32569500

O	5.00537400	3.03965700	-0.09500800
C	5.26286700	5.38008500	-0.18483800
O	3.87764800	-5.03002100	0.07622500
C	5.26431800	-5.37901200	-0.18641500
C	6.01787900	-4.04801200	0.17819600
O	-5.00537400	-3.03948400	0.07535600
C	-6.01853800	-4.04585600	-0.19565900
C	-5.26368500	-5.38015700	0.15395500
O	3.87799300	5.02972200	0.08523100
O	-3.87806400	-5.02901000	-0.11129200
O	5.00594100	-3.03906400	-0.08765400
C	6.01897500	4.04749900	0.16866300
C	6.37540700	3.93316300	1.65355100
H	6.69566500	2.90917600	1.86112000
H	7.18713600	4.61313000	1.92676700
H	5.50935700	4.15211400	2.28355800
C	7.23844800	3.74985000	-0.69444400
H	7.99521900	4.53199100	-0.57669600
H	7.68153500	2.79866400	-0.38778600
H	6.97301100	3.67470400	-1.74967700
C	5.63839200	6.58079400	0.67420400
H	6.69794900	6.82703800	0.55166100
H	5.04980300	7.44966900	0.36805000
H	5.44181700	6.39406000	1.73068500
C	6.36432300	-3.94043800	1.66596000
H	7.17431300	-4.62153400	1.94151600
H	6.68299000	-2.91736800	1.88037600
H	5.49408700	-4.16240700	2.28911100
C	5.63435400	-6.58359800	0.66957500
H	5.04787300	-7.45111500	0.35562500
H	6.69471500	-6.82919900	0.55283500
H	5.43088400	-6.40167100	1.72559200
C	7.24308600	-3.74626000	-0.67532400
H	7.68388400	-2.79639200	-0.36136900
H	7.99921800	-4.52878600	-0.55602100
H	6.98474400	-3.66638700	-1.73197200
C	5.35440700	-5.73320100	-1.67347900
H	6.35648300	-6.07598700	-1.94590400
H	4.64313100	-6.53438400	-1.88883900
H	5.09733400	-4.87400300	-2.29847600
C	-5.63746600	-6.57704100	-0.71115500
H	-5.04991900	-7.44742400	-0.40728800
H	-6.69740400	-6.82345300	-0.59229300
H	-5.43824500	-6.38580500	-1.76633200
C	-6.37090800	-3.92468400	-1.68096100
H	-7.18218800	-4.60306700	-1.95940800
H	-6.69006100	-2.89962200	-1.88483600
H	-5.50324700	-4.14122300	-2.30958200
C	-7.24027900	-3.75180200	0.66546700
H	-7.68239900	-2.79923100	0.36170300
H	-7.99686200	-4.53327000	0.54221100
H	-6.97769200	-3.68145900	1.72175900
C	-5.34763900	-5.74757200	1.63818400
H	-6.34865300	-6.09253400	1.91177500

H	-4.63568400	-6.55080500	1.84342900
H	-5.08768400	-4.89404000	2.26972500
C	5.34315300	5.74113200	-1.67083200
H	4.63053200	6.54333900	-1.87778000
H	6.34342900	6.08512100	-1.94831400
H	5.08187700	4.88484200	-2.29807600
B	-3.78278400	3.66100100	0.02515400
B	3.78282800	3.66141400	-0.00401100
B	3.78289500	-3.66132800	-0.00734300
B	-3.78277300	-3.66112800	-0.01595900

Compound $(Br)_4$-Per (DFT B3LYP/6-31+G(d,p), S_0)

Total energy: -6936347.82 kcal mol^{-1}

Dipole moment: 0 D

Symbol	X/Å	Y/Å	Z/Å
C	-2.870519	-2.405753	-0.000006
C	-1.467131	-2.428014	-0.000005
C	-0.736740	-1.247265	-0.000001
C	-1.434915	0.000002	-0.000000
C	-2.866741	-0.000001	-0.000000
C	-3.574357	-1.227674	-0.000003
C	-0.736743	1.247272	0.000001
C	-1.467143	2.428017	0.000006
C	2.870526	2.405754	-0.000006
C	-3.574363	1.227667	0.000003
C	0.736742	-1.247264	0.000001
C	1.434914	0.000004	-0.000000
C	0.736741	1.247273	-0.000001
C	2.866740	0.000003	0.000000
C	3.574361	1.227673	-0.000003
C	-2.870530	2.405750	0.000007
C	1.467139	2.428019	-0.000005
C	1.467135	-2.428012	0.000004
C	2.870522	-2.405749	0.000005
C	3.574359	-1.227669	0.000003
H	-0.976278	-3.390972	-0.000007
H	-4.657739	-1.224680	-0.000003
H	-0.976297	3.390978	0.000009
H	-4.657745	1.224669	0.000004
H	4.657743	1.224676	-0.000003
H	0.976292	3.390979	-0.000008
H	0.976283	-3.390971	0.000006
H	4.657740	-1.224674	0.000003
Br	3.802752	-4.070220	0.000009
Br	3.802759	4.070223	-0.000011

Br	-3.802766	4.070218	0.000012
Br	-3.802746	-4.070226	-0.000010

Compound ($Bmes_2)_4$-Per (DFT B3LYP/6-31+G(d,p), S_0)

Total energy: -2299118.34 kcal mol^{-1}

Dipole moment: 0.00028 D

Symbol	X/Å	Y/Å	Z/Å
C	2.447730	2.893775	0.017218
C	2.418076	1.475385	0.013540
C	1.244958	0.738065	0.007485
C	-0.001316	1.437479	-0.000417
C	-0.002563	2.872403	0.000026
C	1.232973	3.567376	0.017815
C	-1.246351	0.735853	-0.008789
C	-2.420781	1.471105	-0.014849
C	-2.447693	-2.894699	0.016406
C	-1.239315	3.565179	-0.017393
C	1.246288	-0.736701	-0.008571
C	0.001276	-1.438348	-0.000861
C	-1.245012	-0.738936	0.006935
C	0.002592	-2.873284	-0.000840
C	-1.232928	-3.568278	0.016770
C	-2.452911	2.889449	-0.017616
C	-2.418106	-1.476296	0.012806
C	2.420734	-1.471914	-0.014261
C	2.452925	-2.890249	-0.017656
C	1.239375	-3.566031	-0.018230
H	3.373864	0.965004	0.008162
H	1.216825	4.655292	0.025918
H	-3.375683	0.959048	-0.010142
H	-1.225098	4.653121	-0.024689
H	-1.216771	-4.656193	0.024749
H	-3.373923	-0.965954	0.007468
H	3.375606	-0.959827	-0.008738
H	1.225197	-4.653978	-0.025987
B	3.826397	-3.633003	0.019017
B	3.819863	3.639082	-0.019174
B	-3.826145	3.632678	0.018508
B	-3.819817	-3.640015	-0.019092
C	5.056493	2.863514	-0.607771
C	6.237161	2.696481	0.157047
C	5.002562	2.267613	-1.894546
C	7.299979	1.940050	-0.349788
C	6.093884	1.540831	-2.377191
C	7.250881	1.353954	-1.615324
H	8.189659	1.805788	0.261044
H	6.039104	1.106467	-3.374764
C	3.921449	5.102863	0.537794
C	4.477303	6.142156	-0.252994
C	3.468777	5.421869	1.842006

C	4.538959	7.445772	0.246404
C	3.576286	6.733190	2.319637
C	4.094002	7.764575	1.533609
H	4.955966	8.232420	-0.380423
H	3.249142	6.953125	3.334758
C	-3.929081	5.097092	-0.536653
C	-4.486511	6.134548	0.255268
C	-3.476236	5.418401	-1.840294
C	-4.549687	7.438797	-0.242469
C	-3.585273	6.730133	-2.316252
C	-4.104641	7.759855	-1.529015
H	-4.967937	8.224091	0.385205
H	-3.258050	6.951803	-3.330986
C	5.061574	-2.855193	0.607760
C	6.242131	-2.686212	-0.156769
C	5.006367	-2.259397	1.894547
C	7.303652	-1.928149	0.350386
C	6.096408	-1.530917	2.377492
C	7.253325	-1.342213	1.615932
H	8.193259	-1.792449	-0.260230
H	6.040694	-1.096650	3.375055
C	-5.056853	-2.864621	-0.607031
C	-6.236844	-2.697134	0.158679
C	-5.003927	-2.269343	-1.894151
C	-7.300088	-1.940967	-0.347692
C	-6.095659	-1.542887	-2.376316
C	-7.252054	-1.355613	-1.613597
H	-8.189197	-1.806337	0.263876
H	-6.041690	-1.109016	-3.374144
C	-3.921163	-5.103656	0.538347
C	-4.477863	-6.143077	-0.251595
C	-3.467537	-5.422326	1.842379
C	-4.539401	-7.446543	0.248320
C	-3.574940	-6.733419	2.320527
C	-4.093460	-7.765003	1.535219
H	-4.957097	-8.233310	-0.377884
H	-3.247093	-6.953057	3.335496
C	-5.062696	2.855403	0.604954
C	-5.009446	2.257043	1.890619
C	-6.243201	2.690106	-0.160608
C	-6.101119	1.529508	2.371431
C	-7.306433	1.933145	0.344467
C	-7.257993	1.344674	1.608949
H	-6.046739	1.093060	3.368114
H	-8.195943	1.800303	-0.266934
C	3.930966	-5.096636	-0.537803
C	4.489019	-6.134701	0.252972
C	3.479050	-5.416619	-1.842097
C	4.553542	-7.438200	-0.246462
C	3.589465	-6.727653	-2.319740
C	4.109359	-7.757949	-1.533660
H	4.972208	-8.223953	0.380370
H	3.262895	-6.948272	-3.334904
C	6.379478	3.291919	1.542202

H	7.347214	3.024751	1.979165
H	6.304690	4.383725	1.523258
H	5.600410	2.931245	2.224135
C	3.794788	2.405537	-2.800968
H	3.062552	1.610550	-2.615055
H	3.269070	3.354083	-2.662077
H	4.095640	2.339249	-3.852236
C	8.411159	0.557559	-2.159248
H	8.089546	-0.439713	-2.482552
H	8.859325	1.052570	-3.030436
H	9.195996	0.431694	-1.406465
C	-5.003537	-5.884220	-1.648038
H	-5.857191	-5.199018	-1.635413
H	-4.243695	-5.431697	-2.295314
H	-5.323338	-6.819030	-2.119781
C	-2.898901	-4.378247	2.784644
H	-3.070528	-4.671533	3.826142
H	-1.817608	-4.259227	2.647924
H	-3.342382	-3.389905	2.637688
C	-4.157341	-9.182600	2.049477
H	-3.290764	-9.764378	1.707010
H	-4.159556	-9.211294	3.144383
H	-5.056102	-9.698085	1.692306
C	2.900994	4.377989	2.784997
H	3.344834	3.389764	2.638297
H	3.072926	4.671813	3.826292
H	1.819695	4.258443	2.648785
C	4.158517	9.182361	2.047274
H	3.298331	9.767659	1.694887
H	4.149197	9.212019	3.142092
H	5.063339	9.693613	1.699320
C	5.001756	5.882890	-1.649822
H	5.855112	5.197316	-1.637821
H	4.241172	5.430605	-2.296416
H	5.321564	6.817502	-2.121950
C	3.798565	-2.399242	2.800637
H	3.065000	-1.605565	2.614356
H	3.274520	-3.348719	2.661779
H	4.098985	-2.332226	3.851982
C	8.412260	-0.544101	2.160204
H	8.088889	0.452288	2.484469
H	8.861625	-1.039034	3.030824
H	9.196641	-0.416141	1.407301
C	6.385742	-3.281256	-1.541962
H	6.312920	-4.373195	-1.523158
H	5.606137	-2.921894	-2.223974
H	7.353066	-3.012301	-1.978743
C	-5.011437	5.872714	1.651451
H	-4.251663	5.417781	2.297095
H	-5.330043	6.806653	2.125731
H	-5.865802	5.188388	1.637674
C	-2.906616	4.376451	-2.784317
H	-1.825078	4.258808	-2.648300
H	-3.348560	3.387246	-2.638490

H	-3.079183	4.670914	-3.825328
C	-4.169961	9.178231	-2.040944
H	-3.299589	9.757937	-1.704611
H	-4.18063	9.20837	-3.135777
H	-5.064926	9.694886	-1.676094
C	5.013023	-5.874336	1.649767
H	5.865929	-5.188188	1.637506
H	4.252078	-5.422217	2.296019
H	5.33343	-6.80848	2.122421
C	4.176576	-9.175585	-2.047384
H	5.077229	-9.688392	-1.691101
H	3.31208	-9.759655	-1.703574
H	4.177539	-9.204742	-3.142275
C	2.909103	-4.373927	-2.785103
H	3.351469	-3.384958	-2.638914
H	3.080987	-4.667783	-3.826392
H	1.827693	-4.256026	-2.648374
C	-3.796713	-2.407591	-2.801256
H	-3.063431	-1.613729	-2.6147
H	-3.27207	-3.356948	-2.663696
H	-4.097905	-2.339716	-3.852319
C	-6.37799	-3.291646	1.54435
H	-6.303295	-4.38347	1.526095
H	-5.598287	-2.930547	2.225335
H	-7.345309	-3.024068	1.981982
C	-8.412791	-0.559562	-2.157042
H	-8.091193	0.437021	-2.482458
H	-8.862551	-1.055815	-3.026709
H	-9.19641	-0.432094	-1.403266
C	-3.802284	2.393195	2.798155
H	-4.104142	2.326372	3.849104
H	-3.070588	1.597682	2.612351
H	-3.275575	3.34135	2.660451
C	-6.385154	3.288254	-1.544644
H	-6.312988	4.3802	-1.523168
H	-5.604435	2.931035	-2.226457
H	-7.351757	3.019804	-1.983336
C	-8.419559	0.549241	2.15153
H	-8.096943	-0.443282	2.488026
H	-8.876932	1.051749	3.013662
H	-9.197749	0.412711	1.393736

Compound $(DPA)_4$-Per (DFT B3LYP/6-31+G(d,p), S_0)

Total energy: -2356809.05 kcal mol^{-1}

Dipole moment: 2.6740 D

Symbol	X/Å	Y/Å	Z/Å
C	2.60953800	2.70118900	-0.31451100
C	2.51545800	1.30566500	-0.09412100
C	1.29588800	0.64924800	-0.09917300
C	0.09334500	1.40702700	-0.21147400
C	0.17815100	2.81909700	-0.42534700
C	1.44919400	3.43327100	-0.52053500
C	-1.18950000	0.80601700	-0.05695200
C	-2.32006000	1.60511700	-0.07876500
C	-2.58126200	-2.70395400	0.39116600
C	-1.00851500	3.58364500	-0.52860700
C	1.20729800	-0.81331300	0.04950100
C	-0.07423700	-1.41639300	0.21670200
C	-1.27671600	-0.64988800	0.15173300
C	-0.15467200	-2.83489800	0.39224100
C	-1.42486000	-3.45702800	0.48612300
C	-2.24939800	2.99601300	-0.32910500
C	-2.49410700	-1.30075700	0.24264100
C	2.33380700	-1.61615900	-0.02356700
C	2.26505500	-3.01668900	0.16863100
C	1.03165000	-3.60486600	0.41107400
H	3.42427700	0.75582600	0.10455000
H	1.50234200	4.50009500	-0.70149400
H	-3.29051700	1.17327600	0.11286600
H	-0.93072400	4.64719200	-0.72069100
H	-1.48237900	-4.53494900	0.58946500
H	-3.42196600	-0.75102500	0.16465000
H	3.29320400	-1.17865700	-0.26002100
H	0.95784400	-4.67504200	0.56250600
N	-3.43440400	3.75930200	-0.34700300
N	-3.86968200	-3.28941000	0.38999200
N	3.43597200	-3.79280900	0.07972800
N	3.86953700	3.32936900	-0.29127400
C	3.35992400	-5.16593100	-0.29148800
C	4.02391300	-6.13618900	0.47304200
C	2.65201900	-5.57010600	-1.42528000
C	3.98199400	-7.47358900	0.10834900
H	4.57927600	-5.82562600	1.35147500
C	2.58486100	-6.91599300	-1.78730400
H	2.13682100	-4.82503900	-2.02152900
C	3.25618800	-7.87548200	-1.02160700
H	4.49280200	-8.23148300	0.69222600
H	2.02161200	-7.19778300	-2.66812000
C	4.72962100	-3.22573700	0.23665100
C	5.74889600	-3.56058000	-0.65840400
C	5.02716700	-2.35078900	1.29509700
C	7.04401700	-3.07285800	-0.49197100
H	5.52900600	-4.22702700	-1.48487300

C	6.30707700	-1.83559800	1.44798800
H	4.24719500	-2.07945400	1.99790800
C	7.33280300	-2.21219600	0.57083000
H	7.80985900	-3.36476200	-1.19895600
H	6.54307800	-1.16183500	2.26427400
O	3.26513000	-9.21516300	-1.28884700
C	2.53844400	-9.66769500	-2.41835600
H	2.66732900	-10.75033600	-2.44741300
H	1.46976300	-9.43278800	-2.33232000
H	2.92482100	-9.23276200	-3.34915600
C	3.97622700	4.70707500	0.05392400
C	4.72176600	5.57716600	-0.75477600
C	3.36629000	5.21320100	1.20373100
C	4.85380900	6.91612000	-0.41807400
H	5.20133000	5.18733800	-1.64614300
C	3.47377600	6.56352000	1.53810200
H	2.78863100	4.54604600	1.83397500
C	4.22439400	7.42213700	0.72763300
H	5.42823600	7.59689200	-1.03680500
H	2.98203200	6.92630900	2.43200900
C	5.07579900	2.60655500	-0.49439900
C	6.16968800	2.82881900	0.34603200
C	5.21426800	1.68397800	-1.54526300
C	7.38631600	2.18294400	0.13264500
H	6.07209400	3.53077000	1.16658100
C	6.41314900	1.01288400	-1.74377400
H	4.37467300	1.49864300	-2.20603300
C	7.51743000	1.27543600	-0.92227000
H	8.21449100	2.39053300	0.79790500
H	6.52606900	0.30103000	-2.55401400
C	-3.41564000	5.13919400	0.00090700
C	-4.14081900	6.05610100	-0.76164600
C	-2.71348200	5.60179400	1.12548200
C	-4.17744000	7.40872900	-0.41983200
H	-4.68980300	5.70197500	-1.62764300
C	-2.72664100	6.94740200	1.46012600
H	-2.15000800	4.89709400	1.72665800
C	-3.46094300	7.86218200	0.69212400
H	-4.75239500	8.09256600	-1.03165400
H	-2.18525500	7.31501900	2.32512500
C	-4.70625300	3.12504600	-0.44268800
C	-5.67373300	3.34056000	0.54051500
C	-5.00908500	2.26608500	-1.51165300
C	-6.91790600	2.71347200	0.47368600
H	-5.44894300	4.00540600	1.36729100
C	-6.23633200	1.62040600	-1.57717200
H	-4.26362400	2.09338700	-2.28029800
C	-7.19715600	1.84076400	-0.58105200
H	-7.64500400	2.90108000	1.25378300
H	-6.47329200	0.94854600	-2.39386800
C	-4.16119800	-4.43209200	1.17125300
C	-4.96301300	-5.46768100	0.66287400
C	-3.66563500	-4.55121500	2.47422500
C	-5.26317900	-6.57724600	1.43961900

H	-5.35271600	-5.39190300	-0.34587300
C	-3.94406600	-5.67590300	3.25061400
H	-3.04739900	-3.75892700	2.88105900
C	-4.75237300	-6.69567200	2.73821900
H	-5.88334200	-7.37826400	1.05177900
H	-3.53741400	-5.73506300	4.25260400
C	-4.82004900	-2.80336400	-0.54903900
C	-6.14207400	-2.55001700	-0.17485100
C	-4.43152600	-2.54305100	-1.87302300
C	-7.06570000	-2.05119000	-1.09483200
H	-6.44798200	-2.74207900	0.84806000
C	-5.33660300	-2.02614700	-2.78631200
H	-3.40787700	-2.73868000	-2.17208000
C	-6.66209900	-1.77976500	-2.40616700
H	-8.07735100	-1.84249500	-0.77207100
H	-5.04323200	-1.81658000	-3.80927200
O	8.57851600	-1.71659000	0.84385200
O	-7.46839300	-1.26038700	-3.38093200
O	-5.09694300	-7.83384300	3.41612200
O	4.40191000	8.75604500	0.96425400
O	8.67931700	0.62592900	-1.23951300
O	-8.38101400	1.16379800	-0.72361400
O	-3.41432600	9.16249000	1.11073500
C	-8.85495100	-1.12413600	-3.09343800
H	-9.02278600	-0.37890600	-2.31077500
H	-9.31990300	-0.79036400	-4.02230200
H	-9.29306500	-2.08541300	-2.79536800
C	-4.59670700	-7.99086500	4.73142900
H	-4.94932900	-7.19273300	5.39791400
H	-4.97581600	-8.94945100	5.08838200
H	-3.49904300	-8.00771700	4.74869200
C	3.77156400	9.31331700	2.10460600
H	4.13577000	8.85512900	3.03324600
H	4.02673500	10.37375100	2.10376100
H	2.68046200	9.20367900	2.05756000
C	9.83831200	0.99312400	-0.50898900
H	9.75024200	0.70618300	0.54509300
H	10.66800900	0.44978200	-0.96257800
H	10.03124800	2.07074000	-0.58142000
C	-9.35176300	1.30401500	0.29906800
H	-10.19018300	0.66823000	0.01057600
H	-8.96369900	0.97315700	1.27048500
H	-9.70058300	2.34067000	0.38731600
C	-4.13363800	10.12317000	0.35743200
H	-3.96583600	11.08197200	0.84960100
H	-3.77171100	10.17961200	-0.67726100
H	-5.20966300	9.90616300	0.34651100
C	9.65136500	-2.21434200	0.06067200
H	9.55656400	-1.90262900	-0.98563900
H	10.56052100	-1.78572200	0.48390700
H	9.71018300	-3.30862600	0.11407500

[1] A. Ranganathan, G. U. Kulkarni, *Proc. Indian Acad. Sci. (Chem. Sci.)* **2003**, *115*, 637.