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Supporting Information

Understanding the Structures and Aromaticity of Heteroporphyrins with Computations

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We evaluate the planarity of the macrocycle based on four dihedral angles of the porphyrins, as shown in Table S1. We set the cut-off dihedral angles for planarity as 5 degree. So the porphyrins with these dihedral angles less than 5 degree are considered to be planar. The CH_2-, SiH_2-, O-, S-, and Se- substituted heteroporphines are planar. The PH-, AsH-, and Te-substituted heteroporphines are twisted from planarity.

Table S1. Dihedral Angles (deg) between the Four Five-Membered Rings in Each Macrocycle

Molecule	Dihedral AB	Dihedral BC	Dihedral CD	Dihedral DA
NHNH[Por]	-0.0	0.0	-0.0	0.0
PHNH[Por]	-6.3	1.5	-1.5	6.3
AsHNH[Por]	-6.9	1.7	-1.7	6.9
CH_2NH[Por]	0.0	-0.0	-0.0	0.0
SiH_2NH[Por]	-0.0	0.0	0.0	0.0
ONH[Por]	0.0	-0.0	0.0	-0.0
SNH[Por]	0.0	-0.0	0.0	-0.0
SeNH[Por]	0.0	-0.0	0.0	-0.0
TeNH[Por]	2.5	6.5	-6.5	-2.5
PHPH[Por]	-7.6	-7.6	7.6	7.6
AsHAsH[Por]	-10.5	-10.5	10.5	10.5
CH_2CH_2[Por]	0.0	-0.0	-0.0	0.0
SiH_2SiH_2[Por]	4.1	4.0	-4.1	-4.0
OO[Por]	0.0	0.0	0.0	0.0
SS[Por]	0.0	-0.0	0.0	-0.0
SeSe[Por]	-2.0	2.0	-2.0	2.0
TeTe[Por]	-29.8	0.1	-0.1	29.8

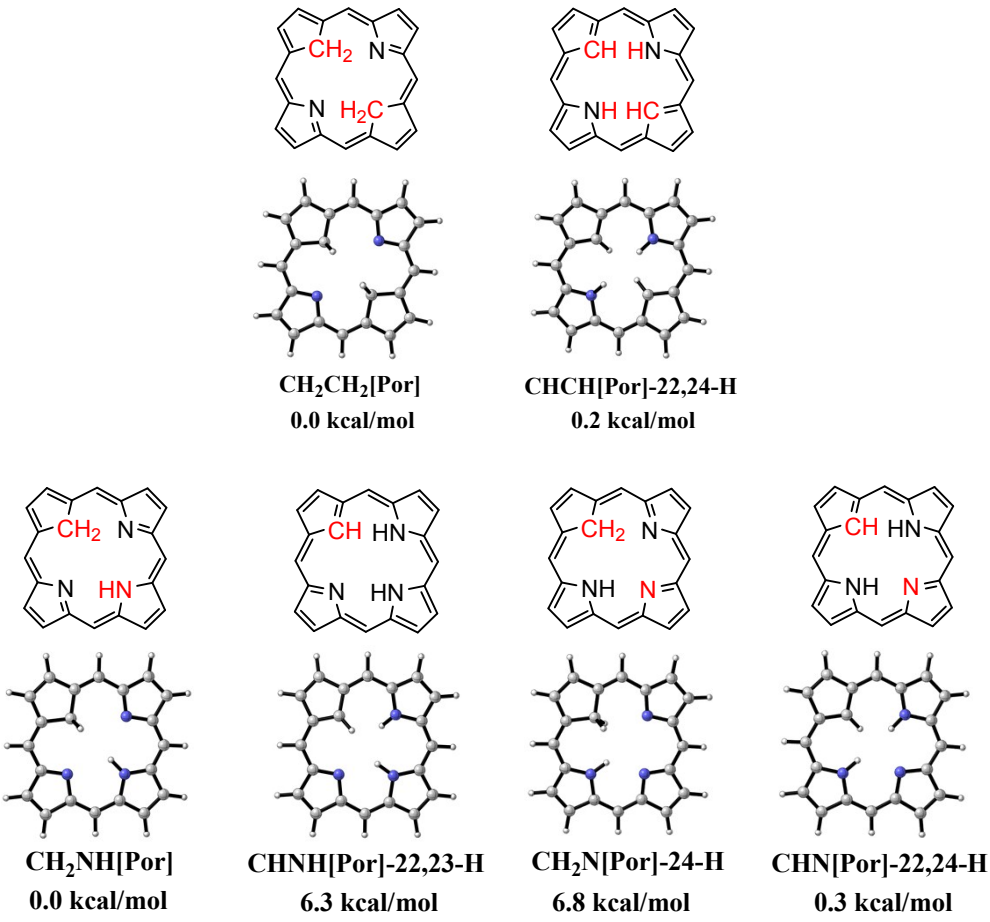
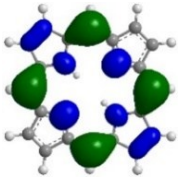
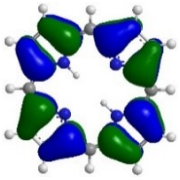
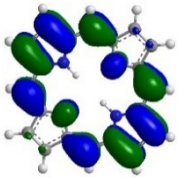
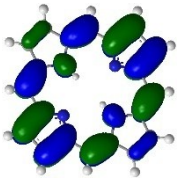
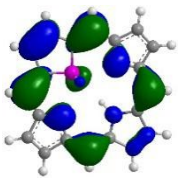
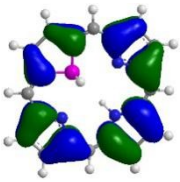
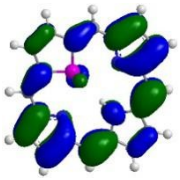
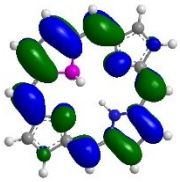
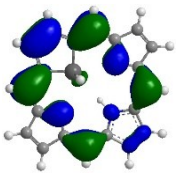
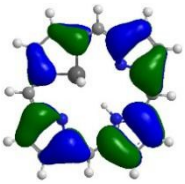
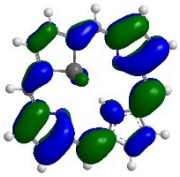
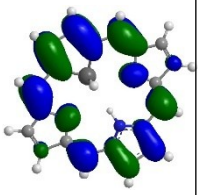
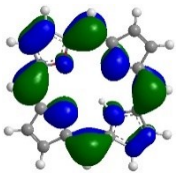
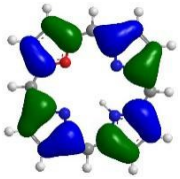
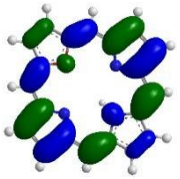
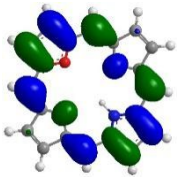
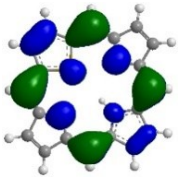
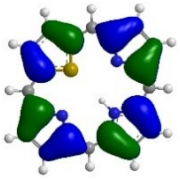
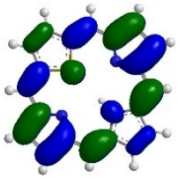
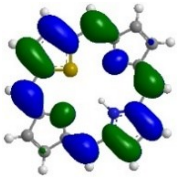
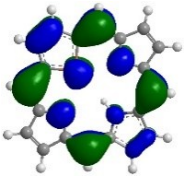
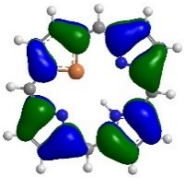
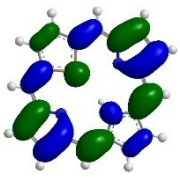
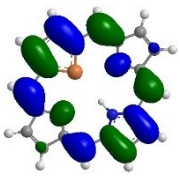
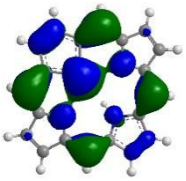
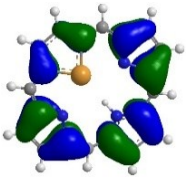
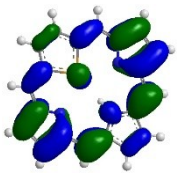
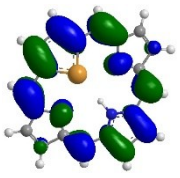
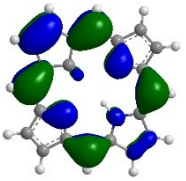
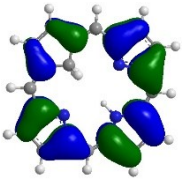
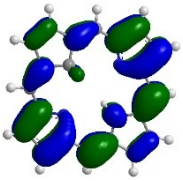
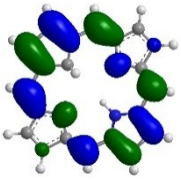
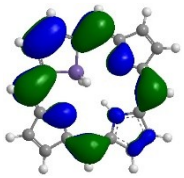
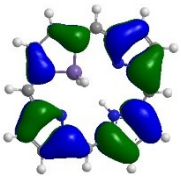
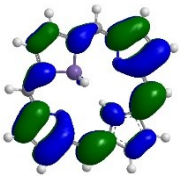
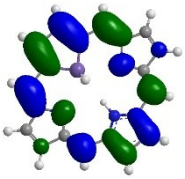
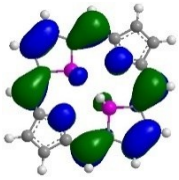
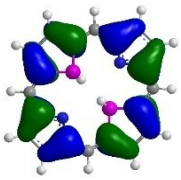
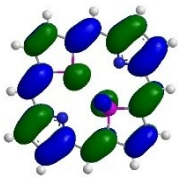
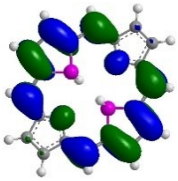
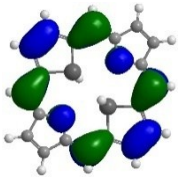
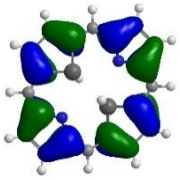
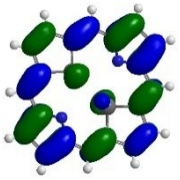
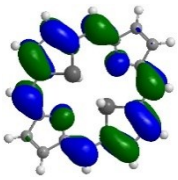
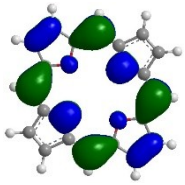
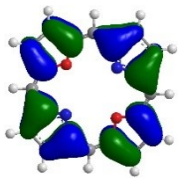
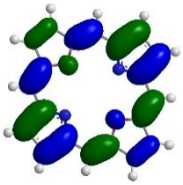
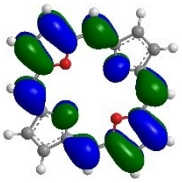
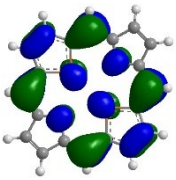
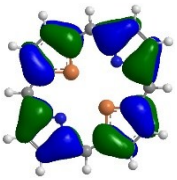
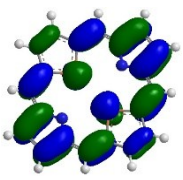
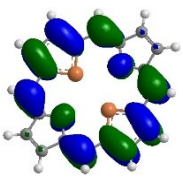
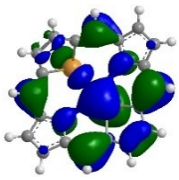
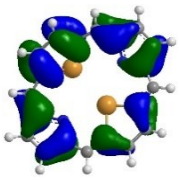
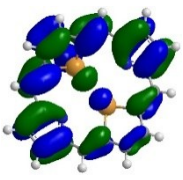
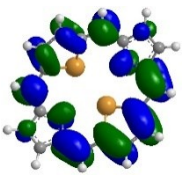
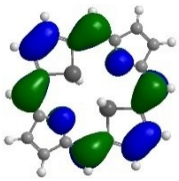
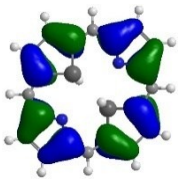
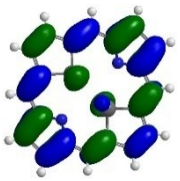
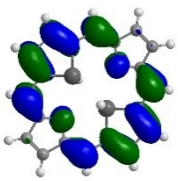


Figure S1. The optimized geometries and relative energies of the different tautomers of CH_2CH_2[Por] and CH_2NH[Por]. Calculations were done at B3LYP/LANL2DZ/6-31G(d) level of theory.

Table S2. The Molecular Orbitals of Monoheteroporphines and Diheteroporphines at the HF/LANL2DZ/6-31G(d) Level of Theory

Molecule	HOMO-1	HOMO	LUMO	LUMO+1
NHNH[Por]	 -6.49 eV	 -5.99 eV	 0.37 eV	 0.43 eV

PHNH[Por]	 **-6.78 eV**	 **-6.19eV**	 **0.15 eV**	 **0.53 eV**
AsHNH[Por]	 **-6.84 eV**	 **-6.23 eV**	 **0.14 eV**	 **0.54 eV**
ONH[Por]	 **-6.53 eV**	 **-6.02 eV**	 **0.35 eV**	 **0.40 eV**
SNH[Por]	 **-6.56 eV**	 **-6.15 eV**	 **0.17 eV**	 **0.33 eV**
SeNH[Por]	 **-6.66 eV**	 **-6.19 eV**	 **0.13 eV**	 **0.34 eV**
TeNH[Por]	 **-6.75 eV**	 **-6.27 eV**	 **-0.07 eV**	 **0.38 eV**
CH_2NH[Por]	 **-6.73 eV**	 **-6.08 eV**	 **0.27 eV**	 **0.66 eV**

SiH_2NH[Por]	 **-6.83 eV**	 **-6.22 eV**	 **0.11 eV**	 **0.60 eV**
PHPH[Por]	 **-6.74 eV**	 **-6.11 eV**	 **-0.35 eV**	 **0.30 eV**
AsHAsH[Por]	 **-6.79 eV**	 **-6.23 eV**	 **-0.48 eV**	 **0.24 eV**
OO[Por]	 **-6.50 eV**	 **-6.05 eV**	 **0.25 eV**	 **0.36 eV**
SeSe[Por]	 **-6.73 eV**	 **-6.29 eV**	 **-0.18 eV**	 **0.14 eV**
TeTe[Por]	 **-6.62 eV**	 **-6.54 eV**	 **-0.06 eV**	 **0.32 eV**
CH_2CH_2[Por]	 **-6.48 eV**	 **-5.83 eV**	 **-0.16 eV**	 **0.54 eV**

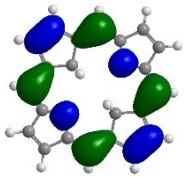
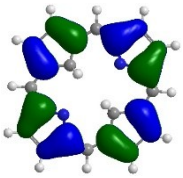
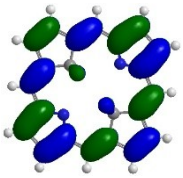
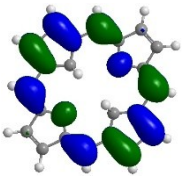
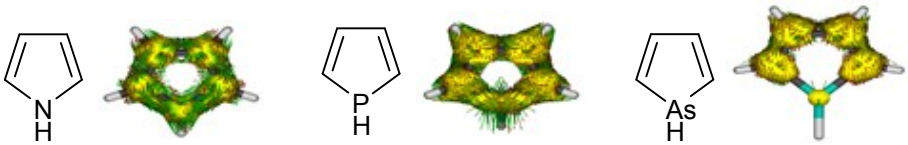
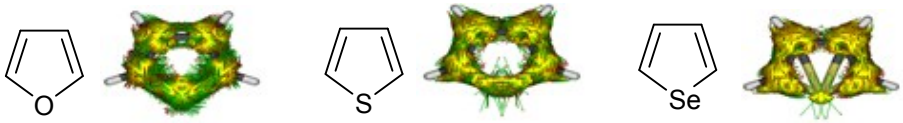
SiH_2SiH_2[Por]				
	-6.65 eV	**-6.00 eV**	**-0.57 eV**	**0.17 eV**

Table S3. The NICS(1) Value and $NICS(1)_{zz}$ Value for the Heteroporphines Calculated at the B3LYP/LANL2DZ/6-31G(d) Level of Theory

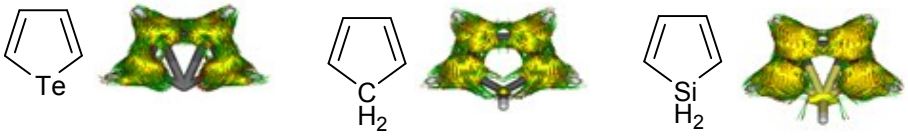
Molecule	$NICS(1)_A$/ $NICS(1)_{zz\_A}$	$NICS(1)_B$/ $NICS(1)_{zz\_B}$	$NICS(1)_C$/ $NICS(1)_{zz\_C}$	$NICS(1)_D$/ $NICS(1)_{zz\_D}$	$NICS(1)_{Macro}$/ $NICS(1)_{zz\_Macro}$
NHNH[Por]	-12.69/-31.09	-6.28/-10.70	-12.69/-31.09	-6.28/-10.70	-13.57/-36.93
PHNH[Por]	-17.29/-44.50	-5.64/-8.42	-12.89/-32.11	-5.64/-8.42	-13.90/-34.26
AsHNH[Por]	-15.68/-40.87	-5.15/-7.02	-13.44/-32.88	-5.15/-7.02	-13.84/-34.56
CH_2NH[Por]	-18.95/-49.23	-5.27/-7.53	-13.03/-32.16	-5.27/-7.53	-12.52/-32.66
SiH_2NH[Por]	-18.48/-49.88	-5.25/-7.59	-13.08/-32.33	-5.25/-7.58	-14.82/-33.45
ONH[Por]	-16.37/-42.24	-4.73/-5.95	-12.59/-30.69	-4.73/-5.95	-13.45/-36.20
SNH[Por]	-14.81/-37.19	-5.07/-6.86	-12.88/-31.70	-5.07/-6.86	-13.45/-36.04
SeNH[Por]	-14.37/-33.83	-5.35/-7.46	13.01/-31.97	-5.35/-7.46	-14.10/-36.67
TeNH[Por]	-10.97/-24.59	-4.81/-5.86	-13.73/-34.24	-4.81/-5.85	-14.07/-34.57
PHPH[Por]	-16.75/-42.71	-5.08/-7.02	-16.12/-43.00	-5.08/-7.02	-16.84/-37.27
AsHAsH[Por]	-17.11/-41.05	-4.90/-6.24	-18.15/-48.80	-4.90/-6.24	-18.21/-39.22
CH_2CH_2[Por]	-19.89/-52.09	-3.97/-3.51	-19.91/-52.15	-3.97/-3.51	-13.55/-33.84
SiH_2SiH_2[Por]	-21.45/-57.88	-4.48/-5.59	-18.72/-50.60	-4.46/-5.55	-16.23/-36.00
OO[Por]	-16.32/-42.12	-2.97/-0.42	-16.32/-42.12	-2.97/-0.42	-13.48/-35.66
SS[Por]	-14.43/-36.12	-4.59/-5.40	-14.43/-36.12	-4.59/-5.40	-14.15/-36.58
SeSe[Por]	-12.36/-27.02	-4.67/-5.24	-12.36/-27.02	-4.67/-5.24	-14.37/-35.62
TeTe[Por]	-9.67 /-17.24	-3.59/-2.47	-8.72/-18.14	-3.59/-2.47	-10.93/-25.68



NICS(0)	-15.52	-5.52	-4.24
NICS(1)	-11.44	-5.31	-4.61
NICS(1)$_{zz}$	-30.41	-10.99	-7.28



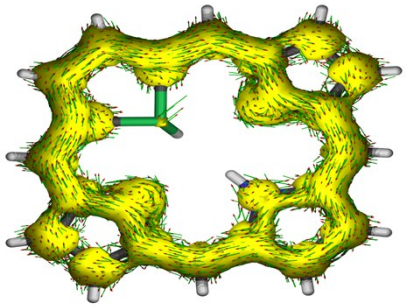
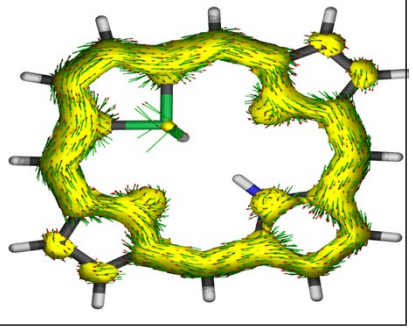
NICS(0)	-13.10	-13.47	-13.08
NICS(1)	-10.32	-10.47	-10.51
NICS(1)$_{zz}$	-26.69	-26.81	-24.06

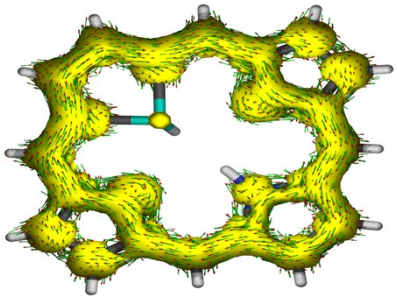
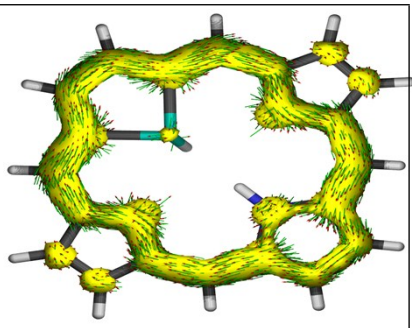
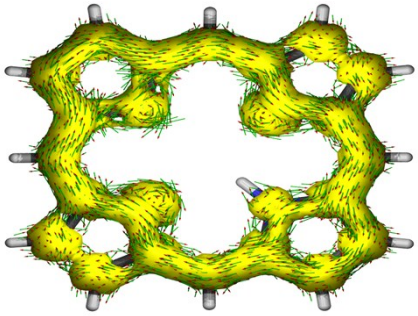
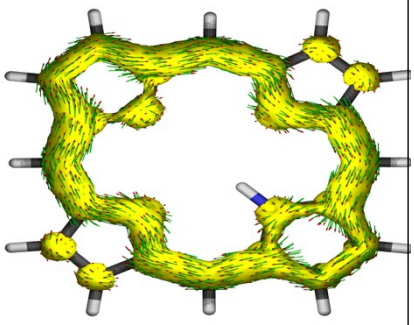
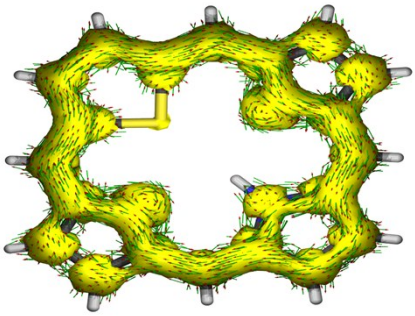
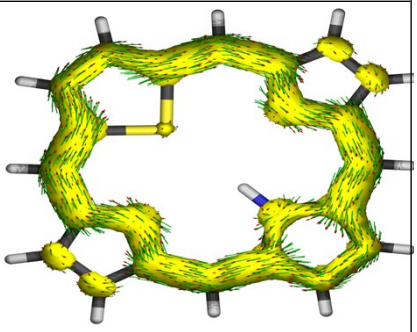
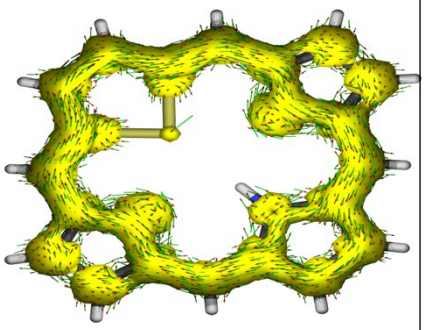
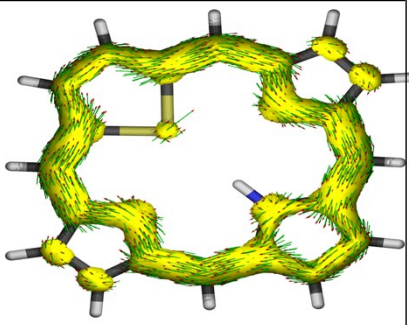
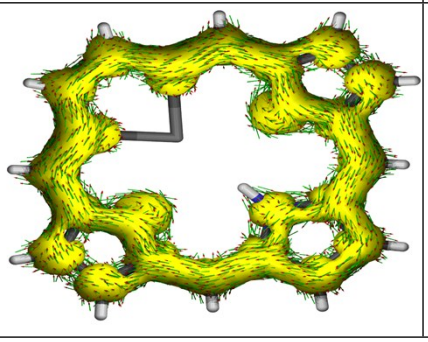
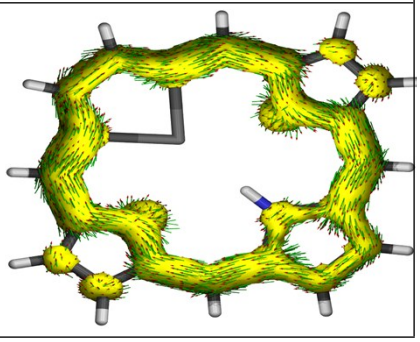


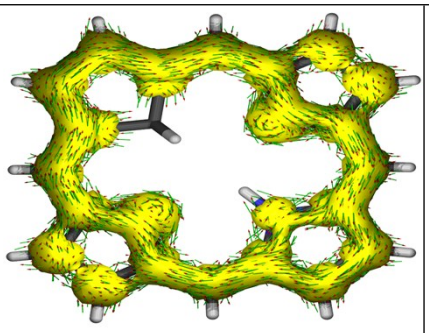
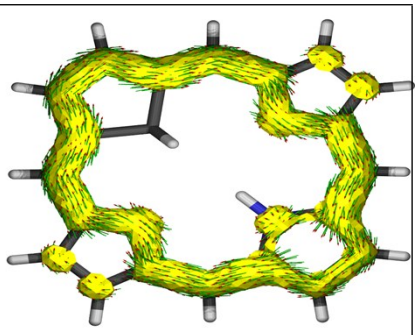
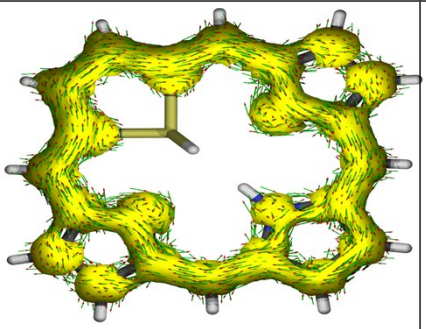
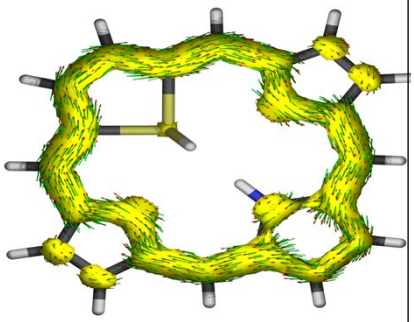
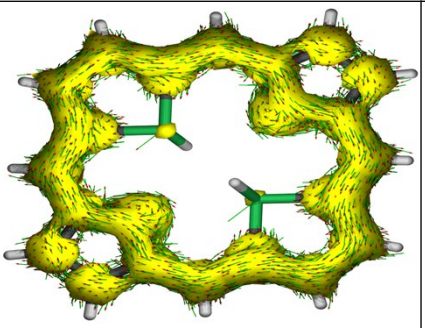
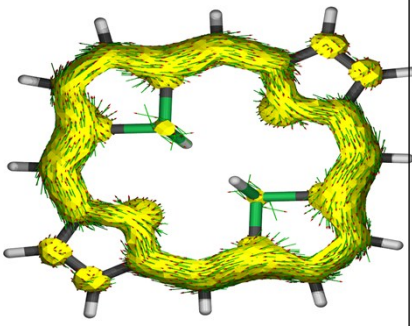
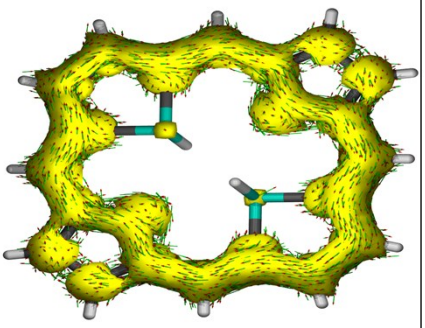
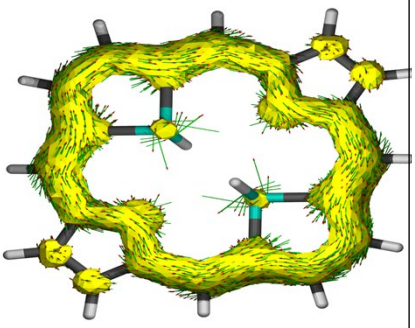
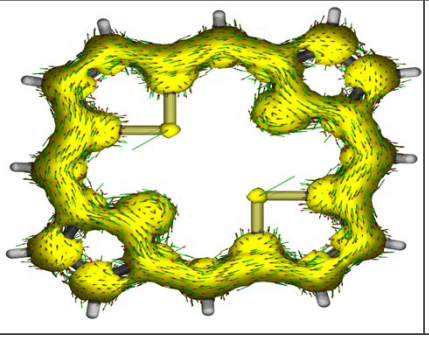
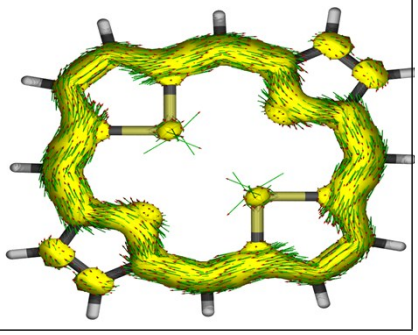
NICS(0)	-11.56	-3.40	0.91
NICS(1)	-8.98	-5.18	-0.51
NICS(1)$_{zz}$	-18.15	-10.64	2.73

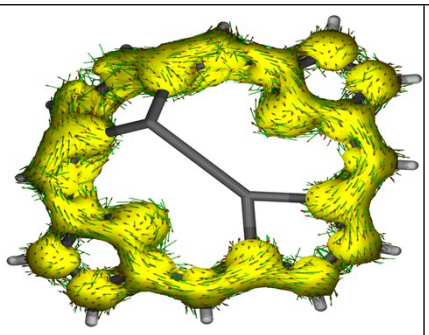
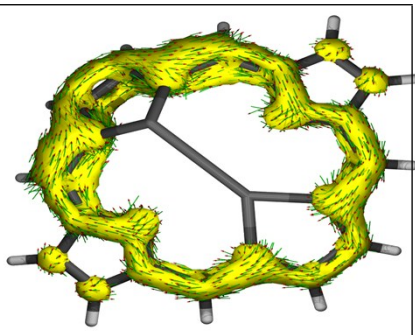
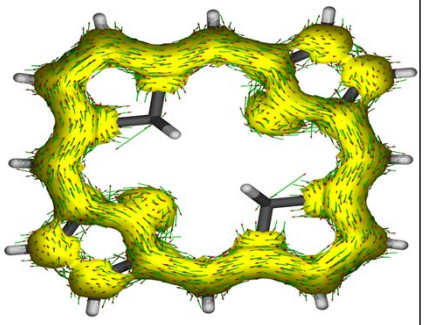
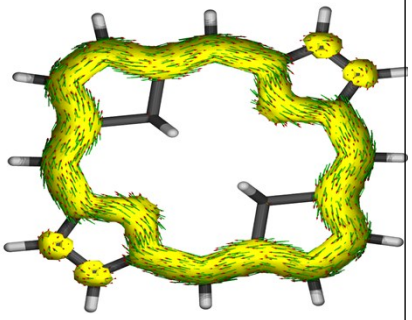
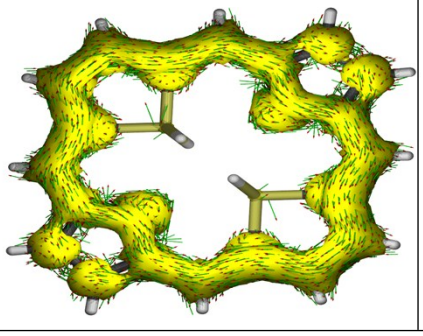
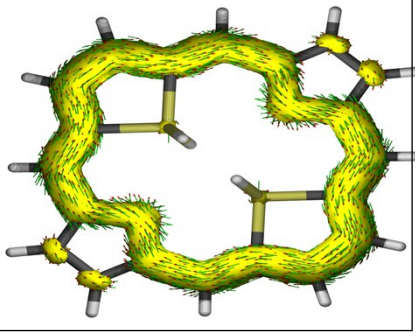
Figure S2. The NICS value and AICD plots (σ+π) (isovalue, 0.065 au) for the five-membered rings calculated at the B3LYP/LANL2DZ/6-31G(d) level of theory.

Table S4. AICD Plots (isovalue, 0.065 au) of Monoheteroporphines and Diheteroporphines at the B3LYP/LANL2DZ/6-31G(d) Level of Theory

Molecule	σ + π	π
PHNH[Por]		

AsHNH[Por]		
ONH[Por]		
SNH[Por]		
SeNH[Por]		
TeNH[Por]		

CH_2NH[Por]		
SiH_2NH[Por]		
PHPH[Por]		
AsHAsH[Por]		
SeSe[Por]		

TeTe[Por]		
CH_2CH_2[Por]		
SiH_2SiH_2[Por]		

The induced diatropic "pyrrolic" ring currents (shown in solid purple line) and "macrocyclic" ring currents (shown in dotted red line) of **NHNH[Por]** have opposite effects and offset each other at the pyrrolic NH lone pair regions, but accumulate at the pyrrolic double bond regions. For **CH_2CH_2[Por]**, the aromatic pathway is mainly contributed by 18π-[18]annulene model, and the ring currents accumulate even more at the cyclopentadiene double bond regions.

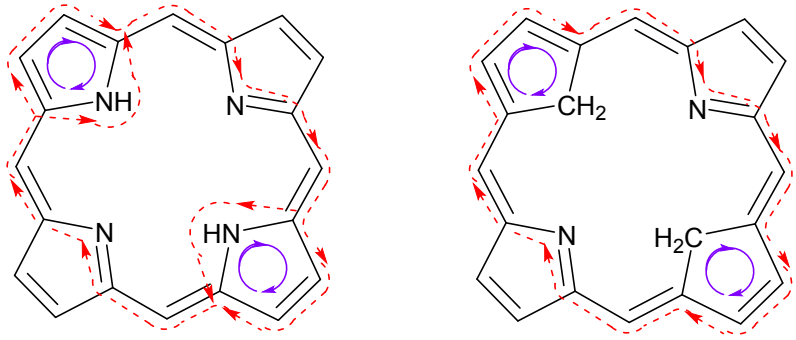


Figure S3. Schematic illustration of the local five membered ring "pyrrolic" (solid purple line) circulations and macrocyclic"porphyrin" (dotted red line) circulations in **NHNH[Por]** and **CH_2CH_2[Por]**.

Table S5. Electronic Energies, Enthalpies, and Free Energies (in Hartree) of the Structures Calculated at the B3LYP/LANL2DZ/6-31G(d) Level

Structures	ZPVE	TCE	TCH	TCG	G_{gas}	Imaginary Frequency
NHNH[Por]	0.296596	0.313570	0.314514	0.252549	-989.278145	—
PHNH[Por]	0.288725	0.306344	0.307288	0.244131	-1275.839742	—
AsHNH[Por]	0.286815	0.304813	0.305757	0.241404	-3167.896696	—
CH_2NH[Por]	0.307020	0.324162	0.325106	0.262948	-973.194725	—
CHNH[Por]-22,23-H	0.307679	0.324943	0.325887	0.263579	-973.184747	—
CH2N[Por]-24-H	0.307003	0.324098	0.325042	0.262999	-973.183902	—
CHN[Por]-22,24-H	0.308078	0.325269	0.326213	0.264041	-973.194205	—
SiH_2NH[Por]	0.296173	0.314364	0.315308	0.250437	-1224.580455	—
ONH[Por]	0.283325	0.300190	0.301134	0.239257	-1009.127731	—
SNH[Por]	0.279821	0.297185	0.298129	0.235223	-1332.102694	—
SeNH[Por]	0.278418	0.296192	0.297136	0.232768	-3332.838832	—
TeNH[Por]	0.277179	0.295114	0.296058	0.231164	-941.936196	—
PHPH[Por]	0.280761	0.298866	0.299810	0.235857	-1562.401163	—

AsHAsH[Por]	0.277206	0.296025	0.296969	0.230179	-5346.506225	—
CH_2CH_2[Por]	0.316702	0.334183	0.335127	0.272345	-957.110977	—
CHCH[Por]-22,24-H	0.319343	0.336677	0.337621	0.275452	-957.110609	—
SiH_2SiH_2[Por]	0.296192	0.315113	0.316057	0.250301	-1459.852640	—
OO[Por]	0.269602	0.286550	0.287494	0.225178	-1028.966936	—
SS[Por]	0.263299	0.280957	0.281902	0.218380	-1674.932048	—
SeSe[Por]	0.260523	0.278886	0.279830	0.213250	-5676.401018	—
TeTe[Por]	0.257567	0.276744	0.277688	0.209040	-894.586219	—

ZPVE = zero-point vibrational energy; **TCE** = thermal correction to energy; **TCH** = thermal correction to enthalpy; **TCG** = thermal correction to Gibbs free energy.

Cartesian coordinates of the structures

NHNH[Por]

C	-2.88839600	1.15085000	-0.00002400
C	-4.25628400	0.71661800	0.00014100
C	-4.26624100	-0.65595900	-0.00005100
C	-2.90475400	-1.10991300	-0.00013400
N	-2.11765200	0.01483600	-0.00013300
H	-1.10226100	0.00737800	-0.00015000
H	-5.10797100	1.38408500	0.00030300
H	-5.12751000	-1.31100800	-0.00005400
C	1.10533500	2.84825300	-0.00008000
C	0.70866600	4.25388700	0.00009200
C	-0.64797300	4.26349300	0.00011900
C	-1.06449200	2.86360000	0.00002600
N	0.01457600	2.03006100	0.00009400
H	1.38841300	5.09742700	0.00013700
H	-1.31569100	5.11658400	0.00019200
C	-1.10534700	-2.84826600	-0.00007600
C	-0.70865700	-4.25389100	0.00013700
C	0.64798600	-4.26349300	0.00017800
C	1.06450000	-2.86359100	0.00004000
N	-0.01459100	-2.03007500	0.00015200
H	-1.38840000	-5.09743300	0.00019700
H	1.31571400	-5.11657600	0.00027600
C	2.88841100	-1.15084200	-0.00004500
C	4.25628600	-0.71661100	0.00011900

C	4.26623300	0.65597500	-0.00004600
C	2.90475400	1.10991100	-0.00013900
N	2.11765500	-0.01483900	-0.00016900
H	1.10226400	-0.00740300	0.00001500
H	5.10798700	-1.38406100	0.00021800
H	5.12750000	1.31102800	-0.00007200
C	-2.40496000	2.45872200	0.00001200
C	-2.43998400	-2.42454300	-0.00018000
C	2.43996400	2.42454100	-0.00015700
C	2.40496000	-2.45872400	-0.00000100
H	-3.15673000	3.24287700	0.00006600
H	3.20274200	3.19798600	-0.00015200
H	-3.20276200	-3.19798800	-0.00024200
H	3.15673400	-3.24287500	0.00008000

PHNH[Por]

C	-1.29910400	-2.70884400	0.00583000
C	-0.69334100	-3.99987400	-0.03573500
C	0.69334200	-3.99987300	-0.03573500
C	1.29910500	-2.70884300	0.00583100
H	-1.27775100	-4.91677500	-0.07976300
H	1.27775300	-4.91677500	-0.07976300
C	-3.00531200	1.11579700	0.01814400
C	-4.42831200	0.77408000	0.00129900
C	-4.49285700	-0.58494600	0.02727200
C	-3.10997400	-1.05856200	0.05901400
N	-2.25126500	-0.01795400	0.06436100
H	-5.24791500	1.48170200	-0.03457700
H	-5.37738500	-1.21035600	0.02237200
C	3.10997500	-1.05856100	0.05901400
C	4.49285700	-0.58494500	0.02727300
C	4.42831200	0.77408200	0.00129800
C	3.00531100	1.11579700	0.01814400
N	2.25126600	-0.01795400	0.06436000
H	5.37738600	-1.21035400	0.02237200
H	5.24791500	1.48170300	-0.03457900
C	1.13424300	2.82050800	-0.01632900
C	0.68734400	4.17901900	-0.01687400
C	-0.68734500	4.17901900	-0.01687400
C	-1.13424400	2.82050800	-0.01632900
N	0.00000000	2.03617800	-0.01155300
H	-0.00000100	1.02318500	-0.07330900
H	1.34790700	5.03597300	-0.01239900

H	-1.34790700	5.03597300	-0.01240000
C	-2.64918600	-2.40014800	0.05967800
C	2.64918700	-2.40014800	0.05968000
C	-2.47893600	2.40640400	-0.01070000
C	2.47893500	2.40640400	-0.01069900
H	3.19657300	3.22267300	-0.03168500
H	3.38928800	-3.19871200	0.09905000
H	-3.38928800	-3.19871300	0.09904900
H	-3.19657400	3.22267300	-0.03168500
P	0.00000000	-1.43490700	-0.19075400
H	-0.00000100	-0.85172500	1.08923400

AsHNH[Por]

C	-1.13626000	2.93587200	0.00423500
C	-0.68801300	4.29396300	-0.00619400
C	0.68803000	4.29396100	-0.00619500
C	1.13627200	2.93586900	0.00423500
H	-1.34708200	5.15201400	-0.01936800
H	1.34710100	5.15201100	-0.01936800
C	-3.14797000	-0.94602600	-0.07792800
C	-4.52634000	-0.45804000	-0.05077600
C	-4.44986500	0.90119700	-0.01850900
C	-3.02370800	1.23294400	-0.02821100
N	-2.28500600	0.08908000	-0.07404400
H	-5.41762900	-1.07378500	-0.05394800
H	-5.26488600	1.61427600	0.01553300
C	3.02371300	1.23293400	-0.02821100
C	4.44986900	0.90118100	-0.01850900
C	4.52633900	-0.45805500	-0.05077600
C	3.14796600	-0.94603700	-0.07792800
N	2.28500700	0.08907300	-0.07404400
H	5.26489200	1.61425700	0.01553300
H	5.41762500	-1.07380400	-0.05394800
C	1.33971100	-2.59575700	-0.03772300
C	0.69561900	-3.86597800	-0.03673700
C	-0.69563300	-3.86597600	-0.03673700
C	-1.33972100	-2.59575300	-0.03772300
H	1.25907200	-4.79842600	-0.03063300
H	-1.25908900	-4.79842200	-0.03063300
C	-2.48363300	2.51893200	0.00011800
C	2.48364400	2.51892400	0.00011900
C	-2.68846200	-2.29465200	-0.09277700
C	2.68845300	-2.29466000	-0.09277700

H	3.43270500	-3.08915700	-0.15563600
H	3.19753100	3.33877200	0.01811300
H	-3.19751700	3.33878300	0.01811300
H	-3.43271700	-3.08914600	-0.15563600
As	-0.00000300	-1.20458100	0.20344000
H	-0.00000200	-0.68452800	-1.21988300
N	0.00000300	2.15538900	0.00565500
H	0.00000000	1.14447500	0.08927700

CH_2NH[Por]

C	-1.19051100	-2.85332900	-0.00003900
C	-0.69382800	-4.18670800	0.00011300
C	0.69396100	-4.18668800	-0.00009600
C	1.19060500	-2.85329500	0.00005000
H	-1.31809700	-5.07487900	0.00018100
H	1.31825700	-5.07484100	-0.00016000
C	-2.93115400	1.07865700	-0.00010900
C	-4.33897800	0.68481100	-0.00022200
C	-4.34526700	-0.67331600	-0.00009200
C	-2.94106300	-1.09102000	-0.00006400
N	-2.11773200	-0.01918200	-0.00014200
H	-5.18530400	1.36114000	-0.00031600
H	-5.20002900	-1.33915700	-0.00005200
C	2.94110000	-1.09093200	0.00006300
C	4.34528900	-0.67318200	0.00006300
C	4.33895400	0.68494500	0.00020300
C	2.93111700	1.07874400	0.00010800
N	2.11773200	-0.01912200	0.00011500
H	5.20007300	-1.33899500	0.00001200
H	5.18525800	1.36130200	0.00029200
C	1.13044400	2.83007400	0.00007500
C	0.68782500	4.18910700	-0.00019200
C	-0.68795800	4.18908700	0.00020500
C	-1.13053600	2.83004100	-0.00006300
N	-0.00003500	2.04514300	0.00000300
H	-0.00001900	1.02777500	0.00000100
H	1.34913700	5.04550800	-0.00033200
H	-1.34929500	5.04546900	0.00034800
C	-2.50924800	-2.44192700	-0.00003000
C	2.50932900	-2.44185300	0.00003800
C	-2.46460100	2.39019700	-0.00010100
C	2.46452200	2.39027000	0.00011100
H	3.20942300	3.18173500	0.00010200

H	3.28752100	-3.20320600	-0.00004500
H	-3.28741700	-3.20330400	0.00005400
H	-3.20952600	3.18163900	-0.00009000
C	0.00003400	-1.93610500	0.00000500
H	0.00006900	-1.26176600	-0.86164700
H	-0.00001900	-1.26176700	0.86165800

CHNH[Por]-22,23-H

C	-2.34056500	2.08707900	-0.03196000
C	-2.48915600	3.52459100	0.27342500
C	-1.25763600	4.09366700	0.28694700
C	-0.25662600	3.05196800	-0.01383800
H	-3.43504900	4.00704400	0.49261400
H	-1.01898500	5.12673500	0.51359200
C	-2.13338200	-2.24676200	0.01950600
C	-3.53037600	-2.49361400	-0.16399100
C	-4.18520100	-1.28057300	-0.21158300
C	-3.21999500	-0.23995700	-0.06682400
N	-1.99389500	-0.87646100	0.06305500
H	-3.96631100	-3.47827800	-0.26965200
H	-5.24274200	-1.11505200	-0.37033100
C	2.11689300	2.21865700	-0.08644800
C	3.54690100	2.50549500	-0.09315900
C	4.18474800	1.30407600	-0.10547500
C	3.13559300	0.29447400	-0.09114900
N	1.90112900	0.86920200	-0.09204700
H	3.98555600	3.49619800	-0.09031500
H	5.25019900	1.10835700	-0.10493800
C	2.37366500	-2.07649100	0.04149000
C	2.51786500	-3.49832700	0.12605100
C	1.26275900	-4.04944500	0.16655200
C	0.29016900	-2.99150500	0.10644100
N	1.01503300	-1.81760200	0.04181800
H	0.72221200	-0.84615200	-0.05178900
H	3.46692000	-4.01728200	0.15143500
H	1.00544700	-5.09847100	0.23254400
C	-3.38274000	1.14935200	-0.05186000
C	1.13132000	3.22145900	-0.02452900
C	-1.09465500	-3.18149600	0.08992900
C	3.35645300	-1.09376400	-0.03231400
H	4.38626000	-1.43899300	-0.02873900
H	1.50839200	4.23851800	0.07315400
H	-4.40806100	1.51013000	-0.01708000

H	-1.40924800	-4.22048500	0.09847500
C	-0.96187600	1.85433600	-0.22728100
H	-0.49037400	0.97127200	-0.61953600
H	-1.19503900	-0.38884100	0.44121100

CH_2N[Por]-24-H

C	-2.22684800	-2.21819600	-0.00002100
C	-2.22388000	-3.63998500	0.00000300
C	-0.92464000	-4.12778000	0.00001900
C	0.00859800	-3.05478500	0.00002500
H	-3.11911700	-4.25391600	0.00000100
H	-0.65193200	-5.17839600	0.00003400
C	-2.30120700	2.01206500	-0.00008800
C	-3.75315600	2.23581200	-0.00014700
C	-4.32468900	1.00380400	-0.00008600
C	-3.21246300	0.04635000	-0.00007800
N	-2.02517300	0.68014700	-0.00007900
H	-4.24459100	3.20161600	-0.00018700
H	-5.37935100	0.75509200	-0.00007800
C	2.30894900	-2.06979100	0.00006800
C	3.73514000	-2.18882400	0.00006900
C	4.27819700	-0.92320500	0.00011300
C	3.20035200	0.01214200	0.00009200
N	2.03330800	-0.72270800	0.00010600
H	4.26431300	-3.13264900	0.00005600
H	5.32641800	-0.65519300	0.00013400
C	2.13069200	2.26409700	0.00005300
C	2.19483500	3.72048200	-0.00003600
C	0.90471200	4.14481400	0.00004900
C	0.06831100	2.94230300	-0.00005200
N	0.83633200	1.82531500	-0.00002400
H	3.10017000	4.31529400	-0.00005700
H	0.53457200	5.16318100	0.00008800
C	-3.31733700	-1.36860600	-0.00005100
C	1.38688100	-3.14111800	0.00004700
C	-1.34289100	3.02325900	-0.00007600
C	3.23924700	1.40998500	0.00008900
H	4.22604300	1.86462300	0.00009000
H	1.83885400	-4.13068400	0.00004900
H	-4.31533000	-1.80301400	-0.00005000
H	-1.73540200	4.03862100	-0.00007800
C	-0.78565300	-1.77584800	-0.00001000
H	-0.57645000	-1.13864100	-0.86696700

H	1.13810400	-0.22844400	0.00013700
H	-0.57646500	-1.13860600	0.86692400

CHN[Por]-22,24-H

C	1.14872000	-2.85537900	-0.04600400
C	0.67779000	-4.20742800	0.30173200
C	-0.67915400	-4.20724300	0.30165600
C	-1.14967100	-2.85503800	-0.04601900
H	1.33127400	-5.03253900	0.56154000
H	-1.33289000	-5.03217300	0.56140400
C	2.95809400	1.13503600	-0.03025100
C	4.31945200	0.69604100	-0.09998500
C	4.31975200	-0.68000500	-0.12532000
C	2.96213200	-1.13643000	-0.08039700
N	2.18460400	0.00245500	-0.03357100
H	5.17687300	1.35540600	-0.12455700
H	5.17885700	-1.33555600	-0.18274400
C	-2.96251300	-1.13552000	-0.08041600
C	-4.31998100	-0.67864500	-0.12532500
C	-4.31921600	0.69739900	-0.09992500
C	-2.95770500	1.13594400	-0.03026000
N	-2.18459800	0.00310100	-0.03354800
H	-5.17930700	-1.33390700	-0.18274200
H	-5.17641800	1.35705100	-0.12444200
C	-1.08938500	2.80890700	0.07779000
C	-0.67703100	4.20821200	0.12710600
C	0.67839100	4.20800700	0.12716500
C	1.09031800	2.80858000	0.07779200
N	0.00034200	1.97854000	0.05573300
H	-1.35070500	5.05617400	0.15140100
H	1.35232300	5.05576400	0.15150800
C	2.49004600	-2.45320900	-0.05003200
C	-2.49086600	-2.45245000	-0.05006400
C	2.43970800	2.43036500	0.03611500
C	-2.43889500	2.43110800	0.03610400
H	-3.16810700	3.23591500	0.04675800
H	-3.25556300	-3.22130200	0.03293600
H	3.25449300	-3.22230600	0.03298800
H	3.16917700	3.23494100	0.04675700
C	-0.00036100	-2.06872000	-0.27985000
H	-0.00022600	-1.10296600	-0.76093900
H	1.18465000	0.05966500	0.11007100
H	-1.18462300	0.05997300	0.11009600

SiH_2NH[Por]

C	-1.34484900	-2.71748500	0.00002700
C	-0.69986200	-3.98642800	0.00013500
C	0.69940400	-3.98649000	0.00005500
C	1.34450400	-2.71760400	-0.00010400
H	-1.25514700	-4.92486000	0.00028500
H	1.25460400	-4.92497300	0.00019300
C	-2.99607100	1.09407200	-0.00012900
C	-4.42429500	0.77357200	-0.00049000
C	-4.51217800	-0.58420100	-0.00014500
C	-3.13891500	-1.08098900	-0.00007100
N	-2.26133200	-0.05726700	-0.00004000
H	-5.23136700	1.49642000	-0.00073300
H	-5.40648300	-1.19529200	-0.00012200
C	3.13876400	-1.08130400	0.00000300
C	4.51209900	-0.58470600	0.00007400
C	4.42440700	0.77307800	0.00049000
C	2.99622700	1.09377400	0.00019700
N	2.26132400	-0.05746100	0.00007800
H	5.40631800	-1.19592300	0.00000300
H	5.23157900	1.49581400	0.00074700
C	1.13520500	2.82230900	0.00017500
C	0.68896200	4.18004200	0.00028800
C	-0.68848000	4.18010000	0.00004800
C	-1.13484100	2.82240500	0.00002600
N	0.00014900	2.04464000	0.00004600
H	0.00012400	1.03475400	-0.00004000
H	1.34802100	5.03810900	0.00042300
H	-1.34746500	5.03822300	0.00000300
C	-2.69606800	-2.43673900	0.00004500
C	2.69575400	-2.43699900	-0.00007000
C	-2.47477100	2.38705000	-0.00009100
C	2.47509100	2.38681700	0.00025100
H	3.20299300	3.19426100	0.00038900
H	3.45162200	-3.22375700	0.00000800
H	-3.45202500	-3.22341100	0.00014500
H	-3.20258300	3.19457500	-0.00017600
Si	-0.00011600	-1.38612300	-0.00035200
H	-0.00024500	-0.65494400	-1.28375600
H	0.00016900	-0.65431600	1.28269800

ONH[Por]

C	-2.90177700	-1.10824800	-0.00004000
C	-4.25702600	-0.68821300	-0.00004600
C	-4.25708000	0.68788100	-0.00003500
C	-2.90186600	1.10802400	-0.00002900
H	-5.10976300	-1.35378800	-0.00005300
H	-5.10987000	1.35338900	-0.00003100
C	1.10293000	-2.87790300	0.00001100
C	0.67382100	-4.27747700	-0.00003600
C	-0.68163200	-4.24680700	-0.00004800
C	-1.05698300	-2.82806800	-0.00003300
N	0.03769100	-2.03234600	-0.00005100
H	1.32851400	-5.14061300	-0.00004000
H	-1.37339600	-5.08082200	-0.00006400
C	-1.05720300	2.82798600	-0.00000900
C	-0.68196200	4.24675400	-0.00002200
C	0.67348800	4.27753000	-0.00000800
C	1.10270600	2.87798900	0.00003300
N	0.03753200	2.03234900	-0.00004200
H	-1.37379100	5.08071700	-0.00003500
H	1.32811300	5.14071700	-0.00000900
C	2.88120200	1.12730000	0.00006200
C	4.24586100	0.68598300	0.00003500
C	4.24591700	-0.68565200	0.00005200
C	2.88129400	-1.12707900	0.00005200
N	2.09495600	0.00008000	0.00015800
H	1.07142400	0.00003600	0.00027300
H	5.10090400	1.34913800	0.00000300
H	5.10101400	-1.34873700	0.00003300
C	-2.39338200	-2.39861900	-0.00003800
C	-2.39357000	2.39843400	-0.00001500
C	2.43249500	-2.45067900	0.00002800
C	2.43230200	2.45086600	0.00004800
H	3.20628900	3.21338400	0.00002300
H	-3.15180900	3.17714900	-0.00001300
H	-3.15156100	-3.17739300	-0.00004400
H	3.20653800	-3.21313900	0.00000300
O	-2.10013400	-0.00008100	-0.00003400

SNH[Por]

C	-1.26281000	-2.72286500	0.00004100
C	-0.69017000	-4.02844700	0.00007400
C	0.68847900	-4.02867300	0.00007100
C	1.26158900	-2.72329000	0.00003800

H	-1.29969400	-4.92685000	0.00009200
H	1.29769500	-4.92728300	0.00008600
C	-2.99579200	1.13328000	-0.00001100
C	-4.41640700	0.77597800	-0.00005900
C	-4.46398100	-0.58323700	-0.00001000
C	-3.07354700	-1.03948100	0.00000500
N	-2.22681700	0.01665200	-0.00003800
H	-5.24513700	1.47381400	-0.00009100
H	-5.34045300	-1.22000500	-0.00000100
C	3.07310400	-1.04063200	-0.00001100
C	4.46374600	-0.58501300	-0.00004900
C	4.41680000	0.77423000	-0.00009400
C	2.99635000	1.13217300	-0.00003000
N	2.22687600	0.01589500	-0.00006000
H	5.33992500	-1.22218200	-0.00005200
H	5.24584600	1.47169100	-0.00013400
C	1.13484500	2.83698700	-0.00000300
C	0.68647500	4.19873200	-0.00001900
C	-0.68472900	4.19897300	0.00001400
C	-1.13359400	2.83739000	0.00000200
N	0.00048400	2.05127800	0.00003700
H	0.00028700	1.03544900	0.00007000
H	1.34846800	5.05464600	-0.00004300
H	-1.34641600	5.05512400	0.00001700
C	-2.61207000	-2.37040900	0.00003300
C	2.61100300	-2.37135300	0.00002400
C	-2.47598100	2.43122000	-0.00000700
C	2.47708000	2.43032100	-0.00002200
H	3.19547200	3.24597900	-0.00004900
H	3.34651900	-3.17294700	0.00003100
H	-3.34792600	-3.17169400	0.00004600
H	-3.19404900	3.24716200	-0.00002300
S	-0.00041700	-1.50406100	0.00003500

SeNH[Por]

C	1.31540700	2.59086400	0.00002200
C	0.69063400	3.87414400	0.00004900
C	-0.69056300	3.87415500	0.00004400
C	-1.31535600	2.59088400	0.00001200
H	1.27615800	4.78996200	0.00007200
H	-1.27607300	4.78998200	0.00006200
C	3.02394900	-1.24534900	0.00000100
C	4.44888000	-0.90613900	0.00001600

C	4.51760700	0.45385600	0.00003900
C	3.13624000	0.93344600	0.00002100
N	2.27878200	-0.11139000	-0.00000700
H	5.26851700	-1.61465800	0.00001900
H	5.40547700	1.07455100	0.00006100
C	-3.13622300	0.93349800	-0.00000500
C	-4.51760000	0.45393600	0.00000000
C	-4.44890100	-0.90606100	-0.00002300
C	-3.02397700	-1.24530000	-0.00002500
N	-2.27878800	-0.11135600	-0.00002800
H	-5.40545700	1.07464900	0.00001300
H	-5.26855200	-1.61456400	-0.00002800
C	-1.13697400	-2.94157400	-0.00002700
C	-0.68640900	-4.30197700	-0.00003700
C	0.68632900	-4.30198700	-0.00002700
C	1.13691600	-2.94159200	-0.00001700
N	-0.00002300	-2.15939700	-0.00001500
H	-0.00001500	-1.14604500	0.00000800
H	-1.34647400	-5.15937000	-0.00005000
H	1.34638100	-5.15939100	-0.00003100
C	2.66944500	2.26879100	0.00003100
C	-2.66940100	2.26883400	0.00000900
C	2.48289300	-2.53518700	-0.00000800
C	-2.48294400	-2.53514800	-0.00002900
H	-3.19403200	-3.35741800	-0.00003600
H	-3.40164700	3.07447300	0.00002400
H	3.40170600	3.07441700	0.00005200
H	3.19396600	-3.35747000	-0.00000800
Se	0.00001600	1.23274500	-0.00000300

TeNH[Por]

C	-1.37635600	-2.53256900	0.01634700
C	-0.69381700	-3.77910500	0.18886400
C	0.69313900	-3.77918800	0.18885200
C	1.37585700	-2.53274600	0.01633300
H	-1.24873900	-4.70028300	0.36056600
H	1.24794200	-4.70043300	0.36056800
C	-3.04306500	1.30305400	0.06577200
C	-4.46043900	0.98635900	0.25129800
C	-4.55359300	-0.37392000	0.29283600
C	-3.19889800	-0.88762200	0.11165100
N	-2.33906100	0.14300200	-0.03667800
H	-5.25889200	1.70948600	0.36695400

H	-5.44663200	-0.97129800	0.43135600
C	3.19877000	-0.88813300	0.11141100
C	4.55351400	-0.37469200	0.29294000
C	4.46061200	0.98561200	0.25150600
C	3.04333300	1.30258300	0.06574800
N	2.33916700	0.14265700	-0.03709900
H	5.44640500	-0.97225800	0.43159900
H	5.25915300	1.70860500	0.36738700
C	1.14162000	3.01540300	0.02170300
C	0.68855900	4.37270400	-0.05675400
C	-0.68780100	4.37277400	-0.05678500
C	-1.14103700	3.01552700	0.02165300
N	0.00024600	2.24295200	0.06075200
H	0.00022400	1.24756200	0.25682800
H	1.34453000	5.23108400	-0.11913800
H	-1.34368600	5.23121800	-0.11921200
C	-2.72916700	-2.23217100	0.13229600
C	2.72875800	-2.23257300	0.13211100
C	-2.48602700	2.58917200	0.05317900
C	2.48654300	2.58880600	0.05329600
H	3.20042300	3.40823900	0.08998100
H	3.45634800	-3.02631600	0.30265000
H	-3.45687800	-3.02580100	0.30286200
H	-3.19974200	3.40876100	0.08963200
Te	-0.00011500	-0.99547100	-0.30685400

PHPH[Por]

C	-1.29969400	2.76615700	-0.00297300
C	-0.69710200	4.05750000	0.03675100
C	0.69710200	4.05750000	0.03675100
C	1.29969400	2.76615700	-0.00297300
H	-1.27806600	4.97728900	0.06234600
H	1.27806600	4.97728900	0.06234600
C	-3.13966300	-1.09258000	-0.04001400
C	-4.54254700	-0.68037500	-0.03034100
C	-4.54250100	0.68036100	0.03104300
C	-3.13957800	1.09252100	0.03996300
N	-2.33246400	-0.00006700	-0.00026000
H	-5.39737900	-1.34530700	-0.05949500
H	-5.39729700	1.34531600	0.06067200
C	3.13957800	1.09252100	0.03996300
C	4.54250100	0.68036000	0.03104300
C	4.54254700	-0.68037500	-0.03034100

C	3.13966300	-1.09258000	-0.04001400
N	2.33246400	-0.00006700	-0.00026000
H	5.39729700	1.34531600	0.06067200
H	5.39737800	-1.34530700	-0.05949500
C	1.29971100	-2.76614500	0.00283100
C	0.69711300	-4.05748700	-0.03623100
C	-0.69711300	-4.05748700	-0.03623100
C	-1.29971100	-2.76614500	0.00283100
H	1.27804400	-4.97731700	-0.06110600
H	-1.27804500	-4.97731700	-0.06110600
C	-2.65157000	2.42143600	0.06646000
C	2.65157000	2.42143600	0.06646000
C	-2.65158400	-2.42151500	-0.06645500
C	2.65158400	-2.42151500	-0.06645500
H	3.39209200	-3.21600500	-0.15971600
H	3.39208700	3.21588000	0.16000100
H	-3.39208700	3.21588000	0.16000100
H	-3.39209200	-3.21600500	-0.15971600
P	0.00000000	1.54384300	-0.29958800
P	0.00000000	-1.54363400	0.29872200
H	0.00000000	-0.81607500	-0.90335500
H	0.00000000	0.81566400	0.90217100

AsHAsH[Por]

C	-1.34033700	2.81122400	0.02775100
C	-0.70144700	4.07243500	0.18263400
C	0.70144100	4.07243600	0.18263300
C	1.34033200	2.81122600	0.02775000
H	-1.25914600	4.99826500	0.32190300
H	1.25913900	4.99826600	0.32190300
C	-3.15575300	-1.09608500	-0.06833500
C	-4.55794400	-0.67945000	-0.05230700
C	-4.55791300	0.67909200	0.05429400
C	-3.15575300	1.09587600	0.06861700
N	-2.35085100	-0.00022400	-0.00051400
H	-5.41416300	-1.34168700	-0.09904100
H	-5.41411400	1.34127200	0.10228500
C	3.15575100	1.09588000	0.06861700
C	4.55791200	0.67909900	0.05429400
C	4.55794500	-0.67944400	-0.05230600
C	3.15575500	-1.09608100	-0.06833500
N	2.35085100	-0.00022100	-0.00051400
H	5.41411200	1.34128000	0.10228500

H	5.41416500	-1.34167900	-0.09904000
C	1.34019200	-2.81116800	-0.02729700
C	0.70135000	-4.07297200	-0.17918700
C	-0.70134400	-4.07297300	-0.17918700
C	-1.34018700	-2.81117000	-0.02729700
H	1.25918200	-4.99914700	-0.31558600
H	-1.25917500	-4.99914900	-0.31558600
C	-2.68169300	2.43700400	0.13059500
C	2.68168900	2.43700800	0.13059400
C	-2.68154800	-2.43746600	-0.12956900
C	2.68155200	-2.43746200	-0.12956900
H	3.43722800	-3.20647600	-0.29820000
H	3.43724700	3.20575000	0.30104000
H	-3.43725200	3.20574500	0.30104000
H	-3.43722300	-3.20648100	-0.29820000
As	0.00000100	-1.51226800	0.42024300
H	0.00000100	-0.83039100	-0.92494400
As	-0.00000100	1.51306500	-0.42327500
H	-0.00000100	0.82919100	0.92107000

CH_2CH_2[Por]

C	-1.19236700	-2.79258900	-0.00030500
C	-0.69743500	-4.11784400	-0.00015800
C	0.69744200	-4.11784300	0.00015500
C	1.19237200	-2.79258700	0.00030400
H	-1.32037500	-5.00701700	-0.00029700
H	1.32038400	-5.00701500	0.00029400
C	-3.00837400	1.08540900	0.00007100
C	-4.41781700	0.67959200	0.00027400
C	-4.41770100	-0.67949500	-0.00014400
C	-3.00806200	-1.08495300	-0.00041300
N	-2.19688700	-0.00011900	0.00007300
H	-5.27036400	1.34838600	0.00058200
H	-5.27012400	-1.34842900	-0.00016500
C	3.00806500	-1.08494800	0.00041300
C	4.41770200	-0.67948700	0.00014700
C	4.41781600	0.67959900	-0.00027100
C	3.00837200	1.08541300	-0.00007100
N	2.19688700	-0.00011600	-0.00007000
H	5.27012700	-1.34842000	0.00016900
H	5.27036200	1.34839500	-0.00057600
C	1.19226200	2.79280800	-0.00041900
C	0.69780100	4.11742300	-0.00043300

C	-0.69780800	4.11742200	0.00043000
C	-1.19226700	2.79280600	0.00041800
H	1.32036600	5.00687700	-0.00096400
H	-1.32037400	5.00687500	0.00096100
C	-2.53172800	-2.41138400	-0.00044900
C	2.53173300	-2.41138000	0.00044800
C	-2.53212300	2.41113100	0.00021300
C	2.53211900	2.41113400	-0.00021300
H	3.27994100	3.20281200	-0.00066000
H	3.27976900	-3.20281900	0.00041600
H	-3.27976300	-3.20282400	-0.00041700
H	-3.27994600	3.20280700	0.00065900
C	0.00000200	-1.87170300	-0.00000100
H	0.00021200	-1.19233400	-0.85774300
H	-0.00020900	-1.19233400	0.85774300
C	-0.00000200	1.87171600	-0.00000100
H	-0.00081900	1.19262000	-0.85798300
H	0.00081600	1.19262000	0.85798200

CHCH[Por]-22,24-H

C	-1.15438700	-2.80217900	0.06322700
C	-0.67829100	-4.13644500	0.46328700
C	0.67879700	-4.13632100	0.46342800
C	1.15473800	-2.80207900	0.06311700
H	-1.33050000	-4.95375000	0.75002600
H	1.33109800	-4.95351600	0.75026900
C	-3.01755500	1.14122500	-0.13174700
C	-4.36637600	0.68986800	-0.27966500
C	-4.36629500	-0.69033800	-0.27959300
C	-3.01740800	-1.14151900	-0.13173800
N	-2.24369600	-0.00009100	-0.07663500
H	-5.22237600	1.34340200	-0.38544000
H	-5.22221700	-1.34398100	-0.38532200
C	3.01753900	-1.14121200	-0.13196900
C	4.36634400	-0.68986800	-0.28001000
C	4.36626300	0.69034500	-0.27998800
C	3.01739300	1.14151900	-0.13203100
N	2.24369400	0.00010100	-0.07684400
H	5.22233300	-1.34340800	-0.38582900
H	5.22217400	1.34398800	-0.38580400
C	1.15440600	2.80220300	0.06307000
C	0.67833400	4.13641600	0.46330800
C	-0.67875300	4.13634500	0.46334300

C	-1.15471400	2.80205100	0.06319900
H	1.33054700	4.95371500	0.75005500
H	-1.33104900	4.95356600	0.75012000
C	-2.50730900	-2.44174200	-0.01470600
C	2.50760200	-2.44150800	-0.01488500
C	-2.50761100	2.44151000	-0.01474900
C	2.50729700	2.44175800	-0.01498700
H	3.24815300	3.23338600	0.06826100
H	3.24853300	-3.23305400	0.06845200
H	-3.24814600	-3.23337800	0.06860600
H	-3.24851600	3.23307900	0.06856700
C	0.00012900	-2.01445100	-0.17941800
C	-0.00013500	2.01441500	-0.17934900
H	-0.00008100	1.08691600	-0.73138200
H	0.00005400	-1.08701100	-0.73154800
H	-1.29798200	-0.00004900	0.27940000
H	1.29793400	0.00007700	0.27905600

SiH_2SiH_2[Por]

C	-1.36902400	2.80815100	0.03796900
C	-0.72230600	4.06664100	-0.05966400
C	0.69760500	4.06980600	-0.05983900
C	1.34998800	2.81421900	0.03783500
H	-1.26395800	5.00809900	-0.16410900
H	1.23498300	5.01368000	-0.16463100
C	-3.15126300	-1.10609000	0.01989000
C	-4.55439300	-0.69346400	0.01964300
C	-4.55949200	0.66685000	-0.02038300
C	-3.15948800	1.08980700	-0.01890500
N	-2.34534400	-0.00504600	0.00121500
H	-5.40600000	-1.36303400	0.03135700
H	-5.41609200	1.32998300	-0.03344500
C	3.15114600	1.10591600	-0.02007700
C	4.55430000	0.69340300	-0.01929300
C	4.55947900	-0.66691900	0.02119300
C	3.15956600	-1.08996900	0.01935400
N	2.34530500	0.00486900	-0.00116900
H	5.40585000	1.36304400	-0.03093200
H	5.41612200	-1.32999200	0.03464100
C	1.36895200	-2.80804400	-0.03831600
C	0.72228100	-4.06651200	0.05953800
C	-0.69765900	-4.06972200	0.05967800
C	-1.34995800	-2.81415600	-0.03792300

H	1.26400300	-5.00787600	0.16442900
H	-1.23500900	-5.01360800	0.16452000
C	-2.71376600	2.44392100	-0.02738400
C	2.69663700	2.45711900	-0.02824600
C	-2.69668800	-2.45722000	0.02774900
C	2.71373900	-2.44402100	0.02782200
H	3.49551200	-3.20215000	0.10730400
H	3.47411400	3.21977500	-0.10702000
H	-3.49568800	3.20196400	-0.10635900
H	-3.47408500	-3.21999700	0.10617100
Si	-0.00691000	1.55324800	0.20424100
H	-0.00497000	1.04078000	1.58520000
H	-0.00342700	0.78152300	-1.02851900
Si	0.00711700	-1.55297200	-0.20464300
H	0.00388100	-0.78206600	1.02867000
H	0.00419800	-1.04103300	-1.58580600

OO[Por]

C	-2.92032700	1.10636700	0.00003200
C	-4.27548500	0.68880100	0.00004400
C	-4.27548200	-0.68882800	0.00003600
C	-2.92032200	-1.10638800	0.00002200
H	-5.12833100	1.35427400	0.00005600
H	-5.12832300	-1.35430600	0.00004100
C	1.07653200	2.82505000	0.00000000
C	0.67693800	4.24216100	0.00001400
C	-0.67696600	4.24215700	0.00003400
C	-1.07655200	2.82504400	0.00002300
N	-0.00000800	2.00695500	0.00001100
H	1.35013700	5.09136100	0.00001100
H	-1.35017000	5.09135300	0.00005000
C	-1.07653200	-2.82504900	0.00000100
C	-0.67693800	-4.24216100	0.00000400
C	0.67696500	-4.24215700	-0.00001600
C	1.07655200	-2.82504400	-0.00002100
N	0.00000700	-2.00695500	-0.00000100
H	-1.35013700	-5.09136100	0.00001400
H	1.35016900	-5.09135300	-0.00002400
C	2.92032800	-1.10636700	-0.00003800
C	4.27548600	-0.68880100	-0.00005000
C	4.27548200	0.68882800	-0.00005100
C	2.92032200	1.10638800	-0.00003000
H	5.12833100	-1.35427400	-0.00006100

H	5.12832300	1.35430700	-0.00006100
C	-2.41257600	2.40149600	0.00003400
C	-2.41255900	-2.40151100	0.00001300
C	2.41255900	2.40151200	-0.00001900
C	2.41257600	-2.40149700	-0.00003600
H	3.17254600	-3.17882600	-0.00004700
H	-3.17252200	-3.17884800	0.00001900
H	-3.17254500	3.17882600	0.00004600
H	3.17252200	3.17884800	-0.00002600
O	-2.12072500	-0.00000700	0.00001800
O	2.12072500	0.00000700	-0.00002500

SS[Por]

C	1.26166300	2.74151200	0.00004100
C	0.68996900	4.04830500	0.00008300
C	-0.68915200	4.04840700	0.00007900
C	-1.26106100	2.74170600	0.00003300
H	1.29968400	4.94657600	0.00011300
H	-1.29872600	4.94677400	0.00010500
C	3.12846400	-1.08995800	-0.00001500
C	4.53520500	-0.68104000	-0.00000700
C	4.53536200	0.68019300	0.00001200
C	3.12871500	1.08942300	0.00000900
N	2.32502300	-0.00017500	-0.00002900
H	5.39007200	-1.34660400	-0.00000700
H	5.39038000	1.34556400	0.00002900
C	-3.12846500	1.08995800	-0.00001100
C	-4.53520400	0.68104000	-0.00001900
C	-4.53536200	-0.68019300	-0.00003400
C	-3.12871500	-1.08942400	-0.00003400
N	-2.32502300	0.00017600	-0.00004400
H	-5.39007200	1.34660400	-0.00000900
H	-5.39038000	-1.34556400	-0.00003900
C	-1.26166200	-2.74151200	-0.00002600
C	-0.68996800	-4.04830500	-0.00000900
C	0.68915200	-4.04840700	-0.00000400
C	1.26106000	-2.74170500	-0.00001800
H	-1.29968400	-4.94657600	-0.00000400
H	1.29872700	-4.94677300	0.00000600
C	2.61997000	2.40229700	0.00003600
C	-2.61943300	2.40272600	0.00002000
C	2.61943300	-2.40272500	-0.00001600
C	-2.61997000	-2.40229700	-0.00003300

H	-3.33568000	-3.22216100	-0.00003500
H	-3.33498300	3.22272900	0.00003600
H	3.33568100	3.22216100	0.00005700
H	3.33498200	-3.22272900	-0.00001400
S	0.00021100	1.52654600	0.00000800
S	-0.00021100	-1.52654600	-0.00002300

SeSe[Por]

C	1.31634800	2.78698600	0.01660000
C	0.69243200	4.06728800	0.14684600
C	-0.69243800	4.06728800	0.14684200
C	-1.31635200	2.78698400	0.01659200
H	1.27509900	4.97739500	0.26413700
H	-1.27510700	4.97739400	0.26412800
C	3.16052100	-1.09644400	0.02083900
C	4.55905000	-0.68150500	0.12234900
C	4.55904900	0.68150900	0.12236600
C	3.16051900	1.09644700	0.02086300
N	2.36106400	0.00000200	-0.05236100
H	5.41240300	-1.34510600	0.19436400
H	5.41240100	1.34511000	0.19439800
C	-3.16052100	1.09644400	0.02084400
C	-4.55905100	0.68150300	0.12233800
C	-4.55905000	-0.68151100	0.12232200
C	-3.16051900	-1.09644800	0.02082000
N	-2.36106400	-0.00000100	-0.05237500
H	-5.41240500	1.34510200	0.19436400
H	-5.41240300	-1.34511400	0.19433200
C	-1.31634800	-2.78698600	0.01653100
C	-0.69243200	-4.06729200	0.14675100
C	0.69243800	-4.06729100	0.14675600
C	1.31635200	-2.78698400	0.01653900
H	-1.27510000	-4.97740100	0.26401700
H	1.27510600	-4.97739900	0.26402500
C	2.66780500	2.42447100	0.04828600
C	-2.66780900	2.42446800	0.04826900
C	2.66780800	-2.42446900	0.04823200
C	-2.66780500	-2.42447300	0.04821600
H	-3.40533700	-3.22129100	0.13507400
H	-3.40534200	3.22128400	0.13514500
H	3.40533600	3.22128700	0.13516700
H	3.40534100	-3.22128600	0.13509500
Se	-0.00000100	1.46532400	-0.14934100

Se	0.00000200	-1.46532000	-0.14937400

TeTe[Por]

C	1.37649400	2.64472800	0.42326400
C	0.70009300	3.48133300	1.33858000
C	-0.69905700	3.48150500	1.33862000
C	-1.37572500	2.64509100	0.42332700
H	1.25420600	3.97690700	2.13334800
H	-1.25300100	3.97722200	2.13341800
C	3.25358700	-1.27819600	0.12932400
C	4.60618300	-0.87231000	0.51005100
C	4.57993000	0.48309700	0.63254900
C	3.21717600	0.90639200	0.30622000
N	2.47167400	-0.19304400	-0.04319800
H	5.43842200	-1.54026400	0.69712100
H	5.38545700	1.14017100	0.93776400
C	-3.21689600	0.90726500	0.30627800
C	-4.57966300	0.48427900	0.63298300
C	-4.60648900	-0.87104100	0.50969500
C	-3.25393400	-1.27730300	0.12924000
N	-2.47168000	-0.19237100	-0.04312800
H	-5.38493000	1.14152100	0.93852500
H	-5.43898200	-1.53876100	0.69647600
C	-1.37543500	-2.88241500	0.05586200
C	-0.69266400	-4.12981500	0.24388400
C	0.69147800	-4.12999400	0.24394000
C	1.37459800	-2.88277700	0.05595300
H	-1.24926000	-5.04561000	0.43998500
H	1.24781800	-5.04593500	0.44007900
C	2.70732800	2.19044800	0.56094800
C	-2.70667800	2.19116800	0.56103700
C	2.73309700	-2.60909500	0.12566900
C	-2.73385700	-2.60836200	0.12550500
H	-3.44674500	-3.42122600	0.26841100
H	-3.38664900	2.85539700	1.09725000
H	3.38751000	2.85451800	1.09709000
H	3.44573700	-3.42215600	0.26868700
Te	0.00027700	1.93631900	-0.97725000
Te	-0.00021800	-1.33012500	-0.22393100