SUPPORTING INFORMATION

to *Cyclic π-elelectron Delocalization in Non-planar Linear Acenes* by Michał A. Dobrowolski, Michał K. Cyrański and Zbigniew Wróbel.

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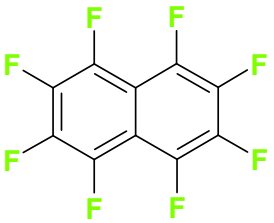
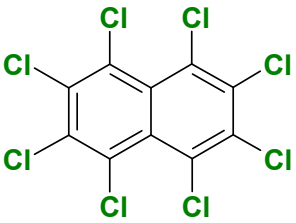
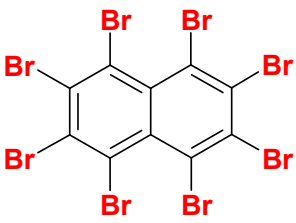
Tab. S1. Data and structure refinement for *per*-substituted naphthalenes.

Compound			
Empirical formula	$C_{10}F_8$	$C_{10}Cl_8$	$C_{10}Br_8$
Formula weight	272.10	403.70	759.30
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	$P2_1/c$	$P2_1/n$	$Pbcn$
Unit cell dimensions:			
a [Å]	13.320 (9)	9.724 (12)	11.383 (4)
b [Å]	4.879 (3)	7.174 (8)	7.811 (3)
c [Å]	19.852 (14)	18.282 (17)	16.551 (6)
α [°]	90	90	90
β [°]	100.25 (6)	98.32 (9)	90
γ [°]	90	90	90
Volume V [Å^3]	1269.6 (15)	1262.0 (2)	1471.66 (9)
Z [molecules/cell]	6	4	4
$D_{calculated}$ [Mg m^{-3}]	2.135	2.125	3.427
Absorption coefficient μ/mm^{-1}	0.249	1.756	21.775
F(000)	792	784	1360
Crystal size [mm]	0.1 x 0.1 x 0.1	0.3 x 0.15 x 0.1	0.3 x 0.2 x 0.1
Maximum θ for data collection [°]	26.0	25.0	25.0
Limiting indices			
h	-16 to 16	-11 to 11	-13 to 13
k	-6 to 4	-7 to 8	-9 to 9
l	-24 to 24	-21 to 21	-19 to 19
Reflections collected	2490	2235	1302
Data/parameters	2470/245	2214/164	1297/83
Goodness of Fit	0.934	1.031	0.864
Final R, wR^2 index	R = 0.0256 wR^2 = 0.0663	R = 0.0197 wR^2 = 0.0257	R = 0.0109 wR^2 = 0.0227
Largest diff. Peak and hole [Å^{-3}]	0.25 and -0.17	0.25 and -0.22	0.40 and -0.28

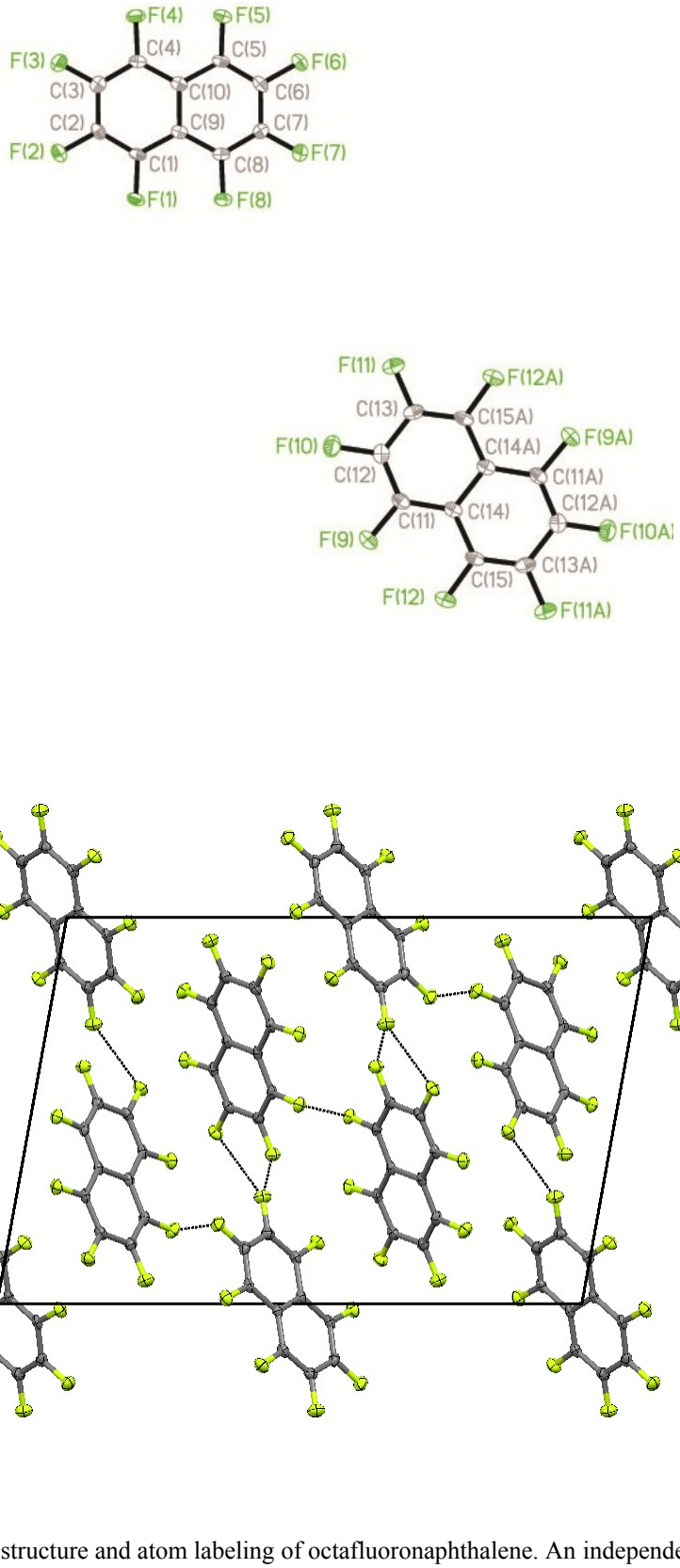


Fig. S1. The molecular structure and atom labeling of octafluoronaphthalene. An independent part of the unit cell is formed by 1.5 molecule. One of the molecules has formal C_1 symmetry, whereas the other has formal C_i

symmetry. In the latter case the presented molecule has been created by inversion. The thermal ellipsoids are drawn at 50% probability level. The crystal packing along [010] direction.

Tab. S2. Selected bond lengths [Å] and angles [º] of octafluoronaphthalene.

F(1)-C(1)	1.3391(15)	C(4)-C(3)-C(2)	119.64(14)
F(2)-C(2)	1.3372(15)	F(4)-C(4)-C(3)	117.84(13)
F(3)-C(3)	1.3285(17)	F(4)-C(4)-C(10)	120.35(13)
F(4)-C(4)	1.3460(15)	C(3)-C(4)-C(10)	121.81(13)
F(5)-C(5)	1.3398(15)	C(4)-C(10)-C(5)	123.61(13)
F(6)-C(6)	1.3383(15)	C(4)-C(10)-C(9)	118.64(13)
F(7)-C(7)	1.3272(17)	C(5)-C(10)-C(9)	117.75(13)
F(8)-C(8)	1.3462(15)	C(8)-C(9)-C(1)	123.66(13)
C(1)-C(2)	1.357(2)	C(8)-C(9)-C(10)	118.59(13)
C(1)-C(9)	1.4145(19)	C(1)-C(9)-C(10)	117.75(13)
C(2)-C(3)	1.396(2)	F(5)-C(5)-C(6)	118.38(12)
C(3)-C(4)	1.359(2)	F(5)-C(5)-C(10)	120.13(13)
C(4)-C(10)	1.404(2)	C(6)-C(5)-C(10)	121.50(13)
C(10)-C(5)	1.4167(19)	F(6)-C(6)-C(5)	120.41(13)
C(10)-C(9)	1.432(2)	F(6)-C(6)-C(7)	118.75(13)
C(9)-C(8)	1.407(2)	C(5)-C(6)-C(7)	120.85(13)
C(5)-C(6)	1.352(2)	F(7)-C(7)-C(8)	121.10(13)
C(6)-C(7)	1.400(2)	F(7)-C(7)-C(6)	119.28(13)
C(7)-C(8)	1.361(2)	C(8)-C(7)-C(6)	119.61(14)
C(11)-F(9)	1.3500(15)	F(8)-C(8)-C(7)	117.99(13)
C(11)-C(12)	1.356(2)	F(8)-C(8)-C(9)	120.31(13)
C(11)-C(14)	1.404(2)	C(7)-C(8)-C(9)	121.69(13)
C(12)-F(10)	1.3249(16)	F(9)-C(11)-C(12)	117.74(13)
C(12)-C(13)	1.405(2)	F(9)-C(11)-C(14)	120.22(12)
C(13)-F(11)	1.3339(16)	C(12)-C(11)-C(14)	122.04(13)
C(13)-C(15A	1.351(2)	F(10)-C(12)-C(11)	121.14(13)
C(14)-C(15)	1.4155(19)	F(10)-C(12)-C(13)	119.25(13)
C(14)-C(14)A	1.433(3)	C(11)-C(12)-C(13)	119.62(13)
C(15)-F(12)	1.3435(15)	F(11)-C(13)-C(15)A	121.02(13)
F(1)-C(1)-C(2)	118.49(12)	F(11)-C(13)-C(12)	118.52(13)
F(1)-C(1)-C(9)	120.18(13)	C(15)A-C(13)-C(12)	120.46(13)
C(2)-C(1)-C(9)	121.33(13)	C(11)-C(14)-C(15)	123.79(12)
F(2)-C(2)-C(1)	120.54(13)	C(11)-C(14)-C(14)A	118.39(16)
F(2)-C(2)-C(3)	118.63(13)	C(15)-C(14)-C(14)A	117.82(16)
C(1)-C(2)-C(3)	120.82(13)	F(12)-C(15)-C(13)A	118.35(12)
F(3)-C(3)-C(4)	121.08(13)	F(12)-C(15)-C(14)	119.97(12)
F(3)-C(3)-C(2)	119.28(13)	C(13)A-C(15)-C(14)	121.67(13)

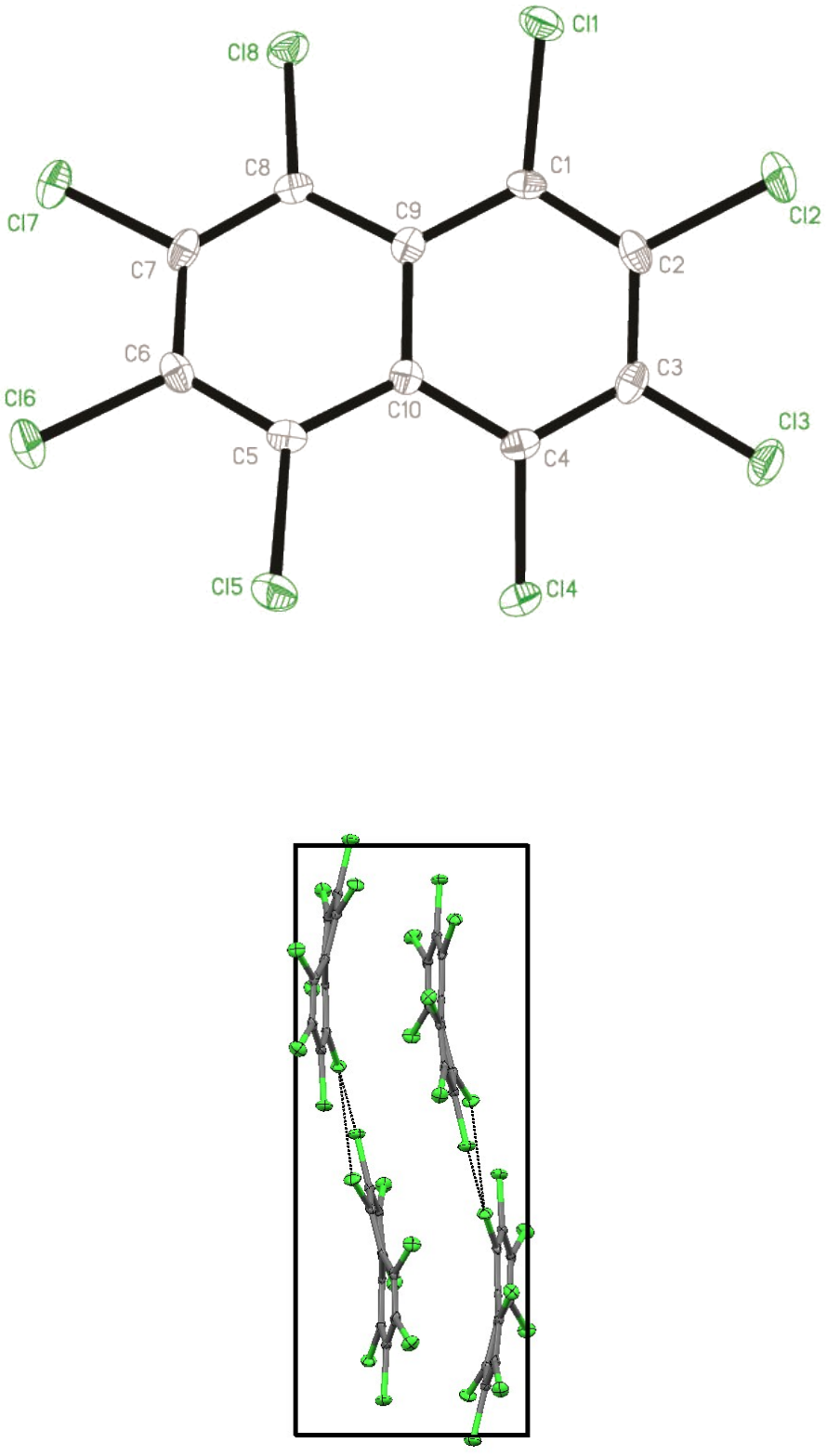


Fig. S2. The molecular structure and atom labeling of octachloronaphthalene. The thermal ellipsoids are drawn at 50% probability level. The crystal packing along [100] direction.

Tab. S3. Selected bond lengths [Å] and angles [º] of octachloronaphthalene.

Cl(1)-C(1)	1.7244(17)	C(3)-C(2)-Cl(2)	118.73(14)
Cl(7)-C(7)	1.7194(17)	C(4)-C(3)-C(2)	119.90(16)
Cl(4)-C(4)	1.7183(18)	C(4)-C(3)-Cl(3)	120.69(14)
Cl(5)-C(5)	1.7234(18)	C(2)-C(3)-Cl(3)	119.38(13)
Cl(8)-C(8)	1.7284(18)	C(3)-C(4)-C(10)	120.43(16)
Cl(2)-C(2)	1.7223(17)	C(3)-C(4)-Cl(4)	117.51(14)
Cl(6)-C(6)	1.7150(17)	C(10)-C(4)-Cl(4)	121.71(13)
Cl(3)-C(3)	1.7197(17)	C(9)-C(10)-C(4)	118.53(15)
C(1)-C(2)	1.373(2)	C(9)-C(10)-C(5)	118.10(16)
C(1)-C(9)	1.437(2)	C(4)-C(10)-C(5)	123.36(17)
C(2)-C(3)	1.402(2)	C(10)-C(9)-C(8)	117.26(15)
C(3)-C(4)	1.375(2)	C(10)-C(9)-C(1)	117.19(15)
C(4)-C(10)	1.431(2)	C(8)-C(9)-C(1)	125.55(17)
C(10)-C(9)	1.426(2)	C(6)-C(5)-C(10)	120.77(17)
C(10)-C(5)	1.439(2)	C(6)-C(5)-Cl(5)	117.28(14)
C(9)-C(8)	1.434(2)	C(10)-C(5)-Cl(5)	121.59(14)
C(5)-C(6)	1.366(2)	C(5)-C(6)-C(7)	119.87(16)
C(6)-C(7)	1.410(2)	C(5)-C(6)-Cl(6)	121.25(15)
C(7)-C(8)	1.375(2)	C(7)-C(6)-Cl(6)	118.88(14)
		C(8)-C(7)-C(6)	120.23(16)
C(2)-C(1)-C(9)	120.71(16)	C(8)-C(7)-Cl(7)	120.78(15)
C(2)-C(1)-Cl(1)	116.76(14)	C(6)-C(7)-Cl(7)	118.98(14)
C(9)-C(1)-Cl(1)	122.37(14)	C(7)-C(8)-C(9)	121.13(17)
C(1)-C(2)-C(3)	120.79(16)	C(7)-C(8)-Cl(8)	116.26(14)
C(1)-C(2)-Cl(2)	120.47(15)	C(9)-C(8)-Cl(8)	122.40(13)

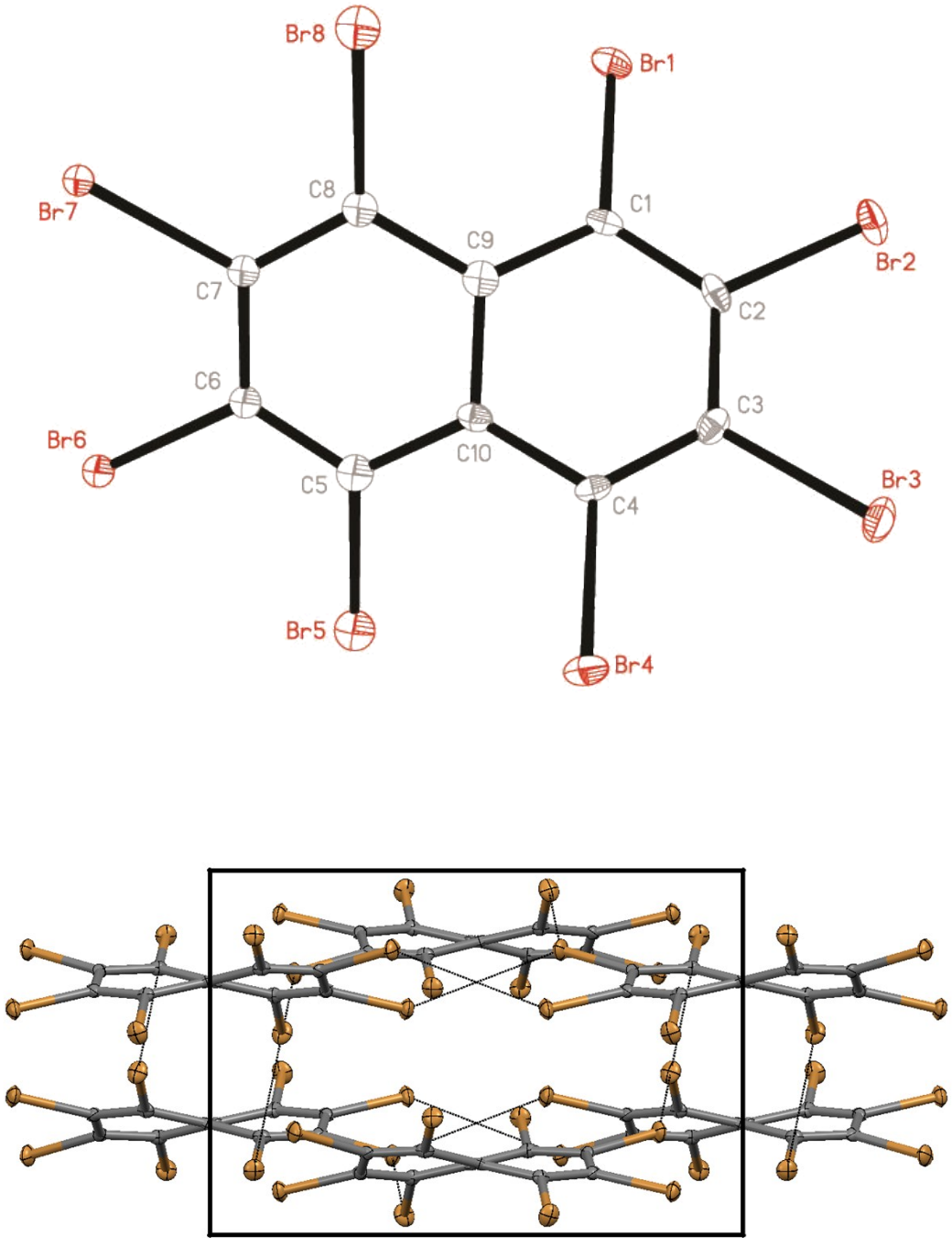
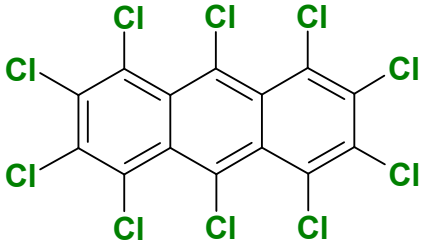


Fig. S3. The molecular structure and atom labeling of octabromonaphthalene. The thermal ellipsoids are drawn at 50% probability level. The crystal packing along [001] direction.

Tab. S4. Selected bond lengths [Å] and angles [º] of octabromonaphthalene.

Br(3)-C(3)	1.885(2)	C(3)-C(2)-Br(2)	119.37(17)
Br(4)-C(4)	1.887(2)	C(3)-C(4)-C(10)	120.7(2)
Br(2)-C(2)	1.885(2)	C(3)-C(4)-Br(4)	118.73(17)
Br(1)-C(1)	1.890(2)	C(10)-C(4)-Br(4)	119.77(16)
C(2)-C(1)	1.368(3)	C(4)-C(3)-C(2)	119.8(2)
C(2)-C(3)	1.420(3)	C(4)-C(3)-Br(3)	121.16(17)
C(4)-C(3)	1.368(3)	C(2)-C(3)-Br(3)	119.08(16)
C(4)-C(5)	1.433(3)	C(2)-C(1)-C(9)	120.6(2)
C(1)-C(9)	1.436(3)	C(2)-C(1)-Br(1)	118.65(17)
C(9)-C(10)	1.425(4)	C(10)-C(1)-Br(1)	120.09(16)
C(10)-C(5)	1.436(3)	C(9)-C(10)-C(4)	117.0(3)
		C(9)-C(10)-C(1)A	117.1(2)
C(1)-C(2)-C(3)	119.6(2)	C(4)-C(10)-C(1)A	126.0(2)
C(1)-C(2)-Br(2)	120.97(17)		

Tab. S5. Data and structure refinement for decachloroanthracene.

Compound	
Empirical formula	$C_{10}Cl_8$
Formula weight	522.64
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions:	
a [Å]	7.1558 (5)
b [Å]	9.5084 (6)
c [Å]	12.4684 (8)
α [°]	75.854 (5)
β [°]	82.701 (6)
γ [°]	87.954 (5)
Volume V [Å^3]	815.95 (9)
Z [molecules/cell]	2
$D_{calculated}$ [Mg m^{-3}]	2.127
Absorption coefficient μ/mm^{-1}	1.701
F(000)	508
Crystal size [mm]	0.2 x 0.15 x 0.1
Maximum θ for data collection [°]	25.0
Limiting indices	
h	-8 do 8
k	-11 do 11
l	-14 do 14
Reflections collected	2872
Data/parameters	2234/217
Goodness of Fit	1.036
Final R, wR^2 index	R = 0.0271
	wR^2 = 0.0678
Largest diff. Peak and hole [Å^{-3}]	0.73 and -0.40

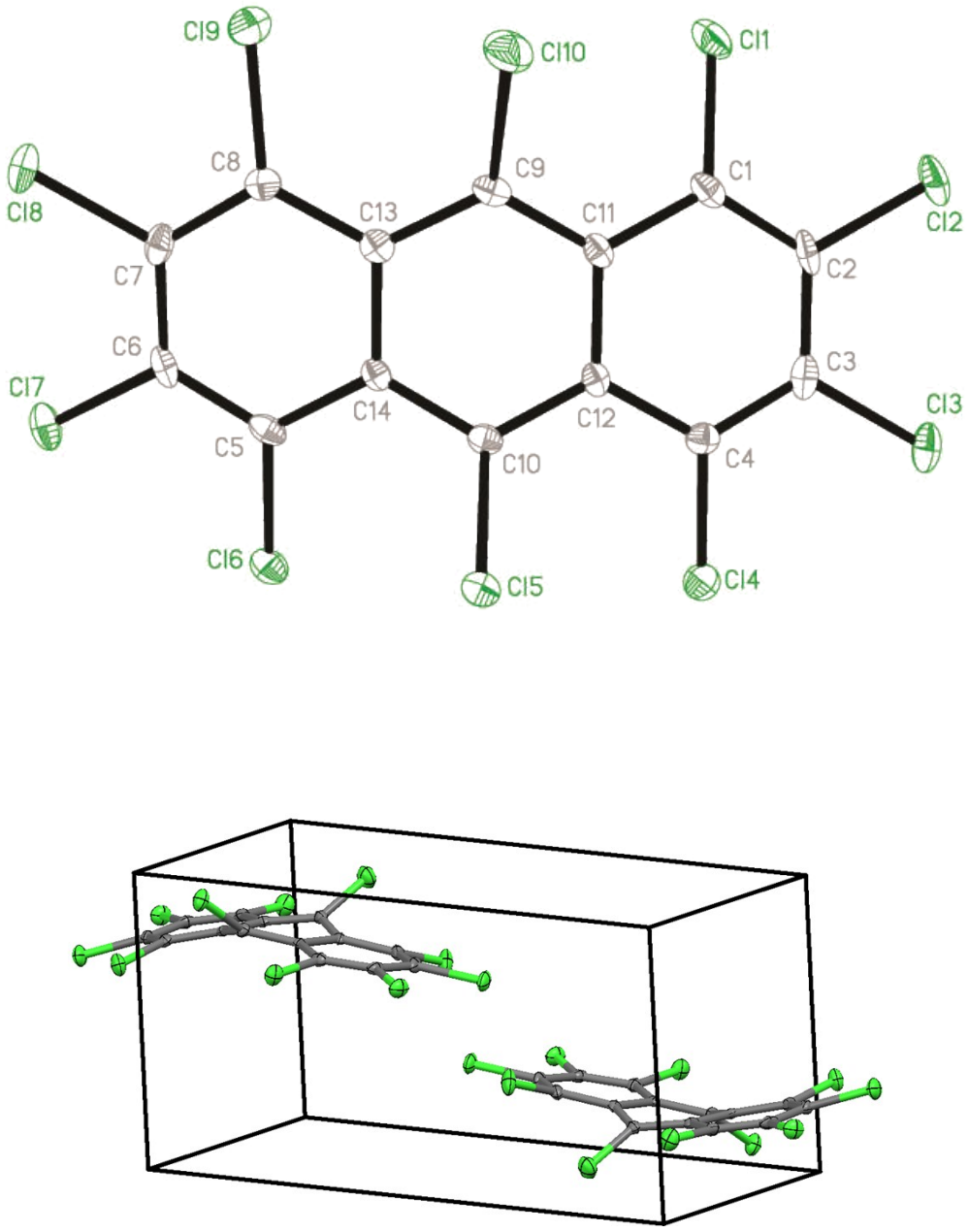


Fig. S4. The molecular structure, atom labeling and crystal packing of decachloroanthracene. The thermal ellipsoids are drawn at 50% probability level.

Tab. S6. Selected bond lengths [Å] and angles [º] of decachloroanthracene.

Cl(1)-C(1)	1.731(3)	C(2)-C(3)-Cl(3)	118.86(19)
Cl(5)-C(10)	1.717(2)	C(3)-C(4)-C(12)	120.7(2)
Cl(6)-C(5)	1.725(3)	C(3)-C(4)-Cl(4)	117.38(19)
Cl(7)-C(6)	1.721(2)	C(12)-C(4)-Cl(4)	121.61(18)
Cl(4)-C(4)	1.721(3)	C(10)-C(12)-C(4)	123.8(2)
Cl(3)-C(3)	1.721(3)	C(10)-C(12)-C(11)	117.5(2)
Cl(9)-C(8)	1.725(3)	C(4)-C(12)-C(11)	118.7(2)
Cl(8)-C(7)	1.721(2)	C(9)-C(11)-C(12)	118.0(2)
Cl(2)-C(2)	1.724(2)	C(9)-C(11)-C(1)	123.6(2)
Cl(10)-C(9)	1.722(2)	C(12)-C(11)-C(1)	118.3(2)
C(1)-C(2)	1.365(4)	C(14)-C(10)-C(12)	120.4(2)
C(1)-C(11)	1.443(3)	C(14)-C(10)-Cl(5)	117.94(18)
C(2)-C(3)	1.418(4)	C(12)-C(10)-Cl(5)	120.45(18)
C(3)-C(4)	1.368(3)	C(10)-C(14)-C(5)	122.9(2)
C(4)-C(12)	1.437(3)	C(10)-C(14)-C(13)	117.9(2)
C(12)-C(10)	1.419(3)	C(5)-C(14)-C(13)	119.2(2)
C(12)-C(11)	1.441(3)	C(9)-C(13)-C(8)	125.2(2)
C(11)-C(9)	1.415(3)	C(9)-C(13)-C(14)	117.3(2)
C(10)-C(14)	1.414(3)	C(8)-C(13)-C(14)	117.6(2)
C(14)-C(5)	1.436(3)	C(11)-C(9)-C(13)	120.8(2)
C(14)-C(13)	1.446(3)	C(11)-C(9)-Cl(10)	117.49(18)
C(13)-C(9)	1.419(3)	C(13)-C(9)-Cl(10)	121.04(19)
C(13)-C(8)	1.428(3)	C(6)-C(5)-C(14)	120.8(2)
C(5)-C(6)	1.367(3)	C(6)-C(5)-Cl(6)	117.68(19)
C(6)-C(7)	1.422(4)	C(14)-C(5)-Cl(6)	121.12(19)
C(7)-C(8)	1.375(3)	C(5)-C(6)-C(7)	120.0(2)
C(2)-C(1)-C(11)	120.7(2)	C(5)-C(6)-Cl(7)	120.8(2)
C(2)-C(1)-Cl(1)	117.25(19)	C(7)-C(6)-Cl(7)	119.04(18)
C(11)-C(1)-Cl(1)	121.60(19)	C(8)-C(7)-C(6)	120.7(2)
C(1)-C(2)-C(3)	120.7(2)	C(8)-C(7)-Cl(8)	120.6(2)
C(1)-C(2)-Cl(2)	120.3(2)	C(6)-C(7)-Cl(8)	118.61(19)
C(3)-C(2)-Cl(2)	118.92(19)	C(7)-C(8)-C(13)	121.3(2)
C(4)-C(3)-C(2)	120.7(2)	C(7)-C(8)-Cl(9)	116.03(19)
C(4)-C(3)-Cl(3)	120.3(2)	C(13)-C(8)-Cl(9)	122.51(19)

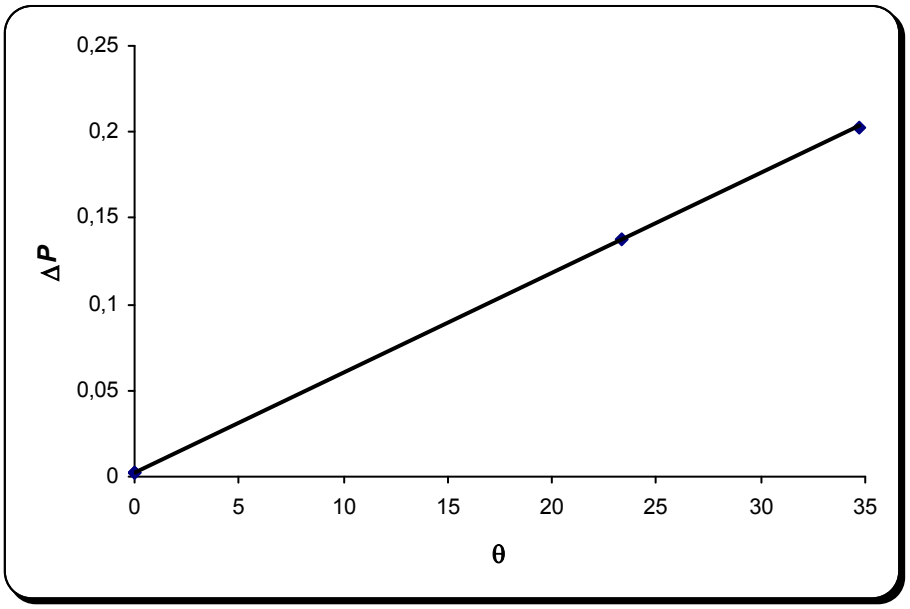


Fig. S5. The dependence of Δ*P* index on the twist angle θ for experimental *per*-substituted naphthalenes.

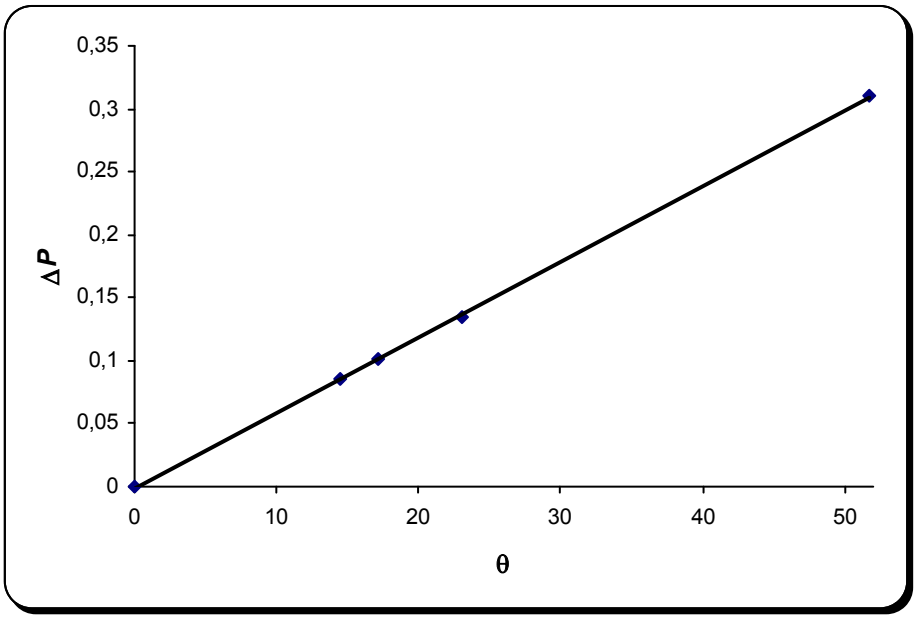


Fig. S6. The dependence of Δ*P* index on the twist angle θ for calculated *peri*-substituted naphthalenes.

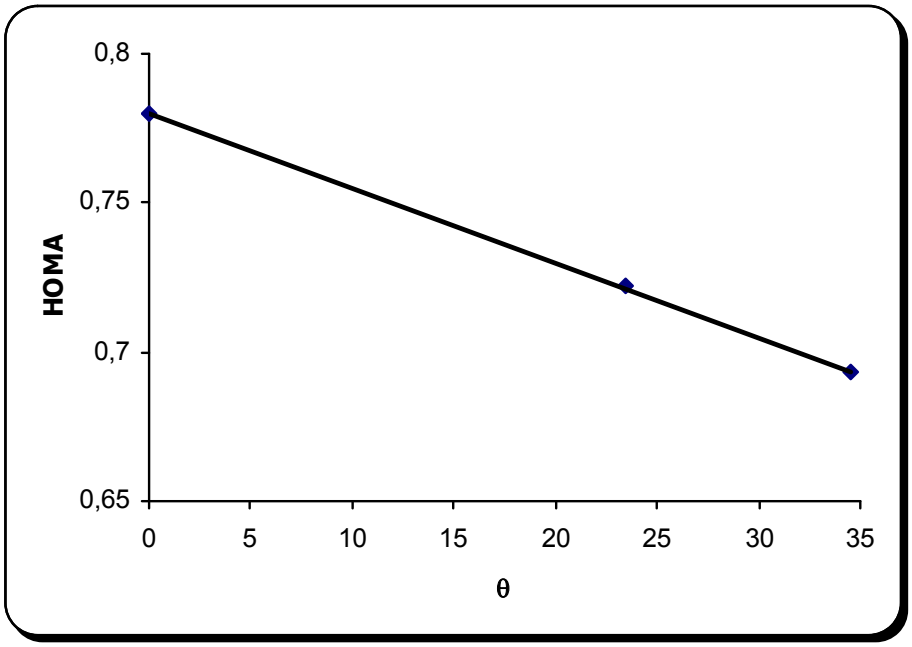


Fig. S7. The dependence of HOMA index on the twist angle θ for *per*-substituted naphthalenes.

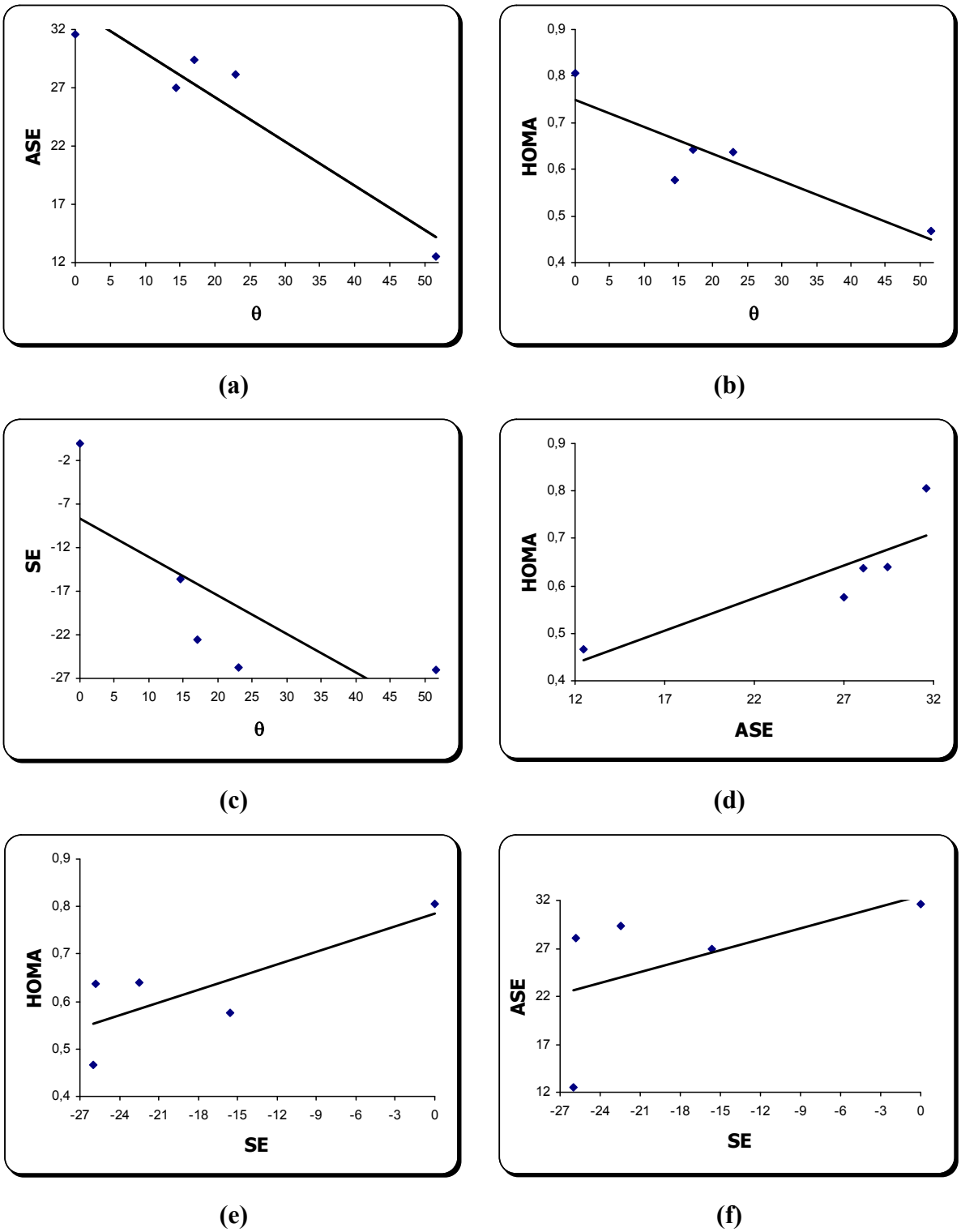


Fig. S8. The dependencies between ASE and θ, R = 0.950 (a); HOMA and θ, R = 0.896 (b); SE and θ, R = 0.769 (c); ASE and HOMA, R = 0.853 (d); SE and HOMA, R = 0.790 (e); SE and ASE, R = 0.543 (f) for *peri*-substituted naphthalene derivatives.

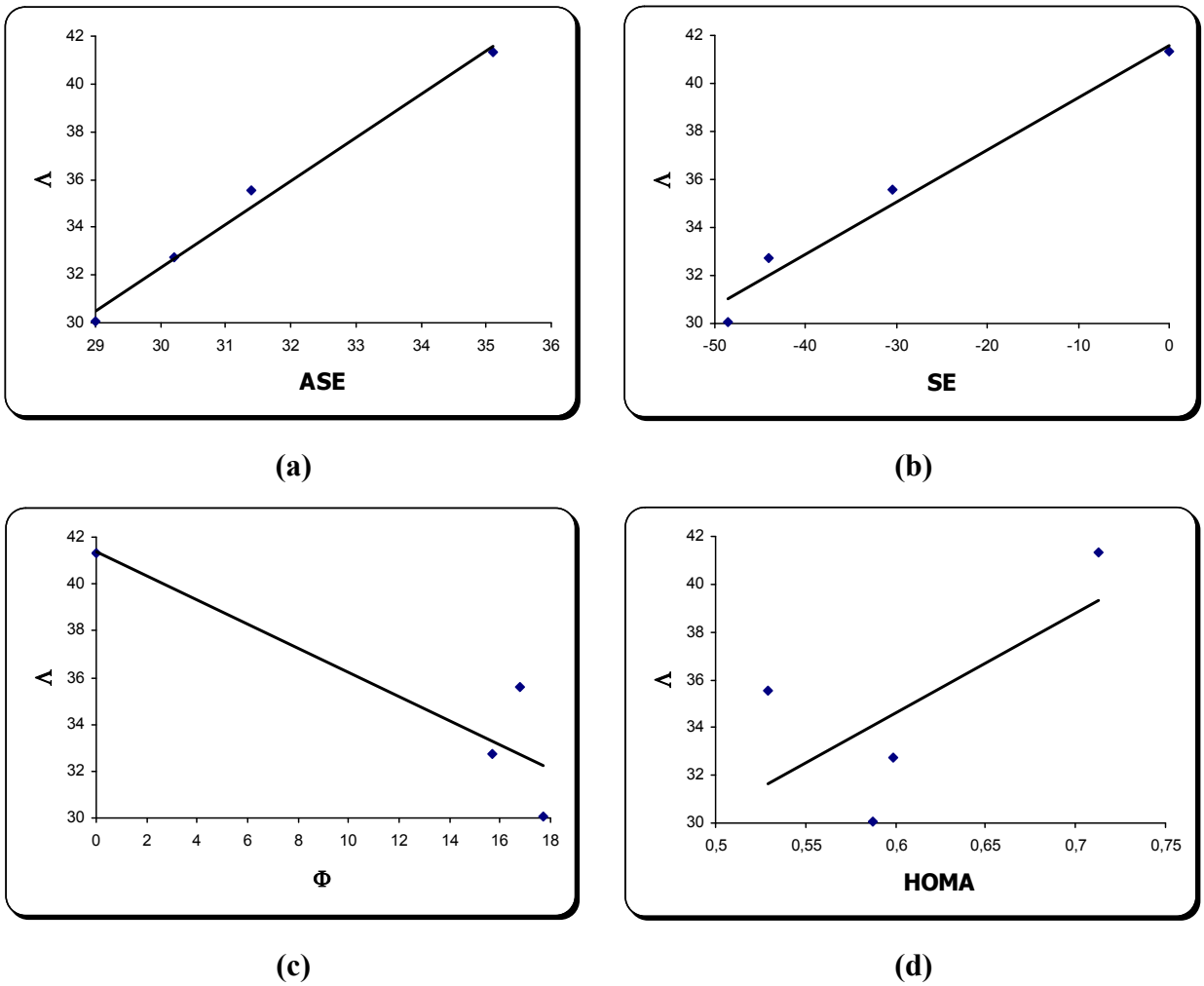


Fig. S9. The dependences between Λ and ASE, R = 0.994 (a); Λ and SE, R = 0.987 (b); Λ and Φ, R = 0.900 (c); Λ and HOMA, R = 0.668 (d) for *peri*-substituted anthracenes.

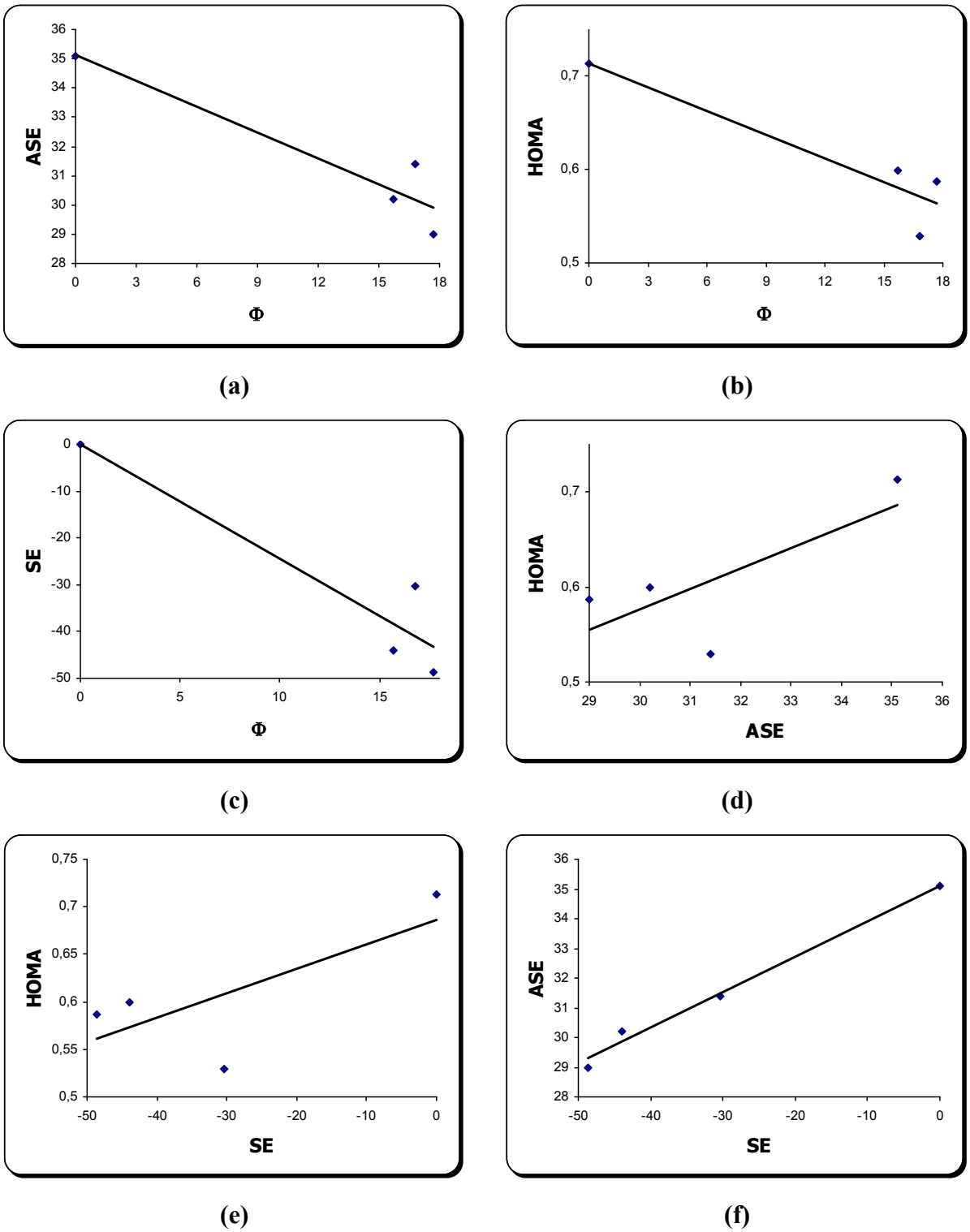
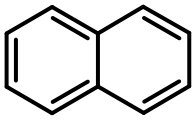
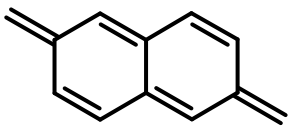


Fig. S10. The dependences between ASE and Φ, R = 0.940 (a); HOMA and Φ, R = 0.922 (b); SE and Φ, R = 0.938 (c); ASE and HOMA, R = 0.738 (d); SE and HOMA, R = 0.730 (e); SE and ASE, R = 0.995 (f) for *peri*-substituted anthracenes.



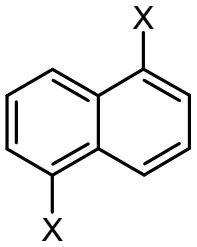
Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_{2h}	-385.9849305	-90.286

C	0.00000000	2.42943900	0.70739400
C	0.00000000	1.24351400	1.40021800
C	0.00000000	0.00000000	0.71562300
C	0.00000000	0.00000000	-0.71562300
C	0.00000000	1.24351400	-1.40021800
C	0.00000000	2.42943900	-0.70739400
H	0.00000000	-1.24180600	2.48538000
H	0.00000000	3.37227600	1.24277400
H	0.00000000	1.24180600	2.48538000
C	0.00000000	-1.24351400	1.40021800
C	0.00000000	-1.24351400	-1.40021800
H	0.00000000	1.24180600	-2.48538000
H	0.00000000	3.37227600	-1.24277400
C	0.00000000	-2.42943900	-0.70739400
C	0.00000000	-2.42943900	0.70739400
H	0.00000000	-1.24180600	-2.48538000
H	0.00000000	-3.37227600	-1.24277400
H	0.00000000	-3.37227600	1.24277400



Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-463.3591259	-75.2267

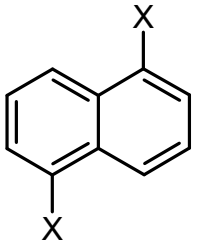
C	2.45568100	0.67107600	0.00000000
C	1.30903700	1.37901700	0.00000000
C	0.01093100	0.73191500	0.00000000
C	-0.01093100	-0.73191500	0.00000000
C	1.15727200	-1.43346500	0.00000000
C	2.45568100	-0.78805100	0.00000000
C	-1.15727200	1.43346500	0.00000000
C	-2.45568100	0.78805100	0.00000000
C	-2.45568100	-0.67107600	0.00000000
C	-1.30903700	-1.37901700	0.00000000
C	-3.61004200	1.49929000	0.00000000
C	3.61004200	-1.49929000	0.00000000
H	3.41476300	1.17808100	0.00000000
H	1.33381300	2.46406200	0.00000000
H	1.12995300	-2.51893600	0.00000000
H	-1.12995300	2.51893600	0.00000000
H	-3.41476300	-1.17808100	0.00000000
H	-1.33381300	-2.46406200	0.00000000
H	-4.57550500	1.00780200	0.00000000
H	-3.60586200	2.58275600	0.00000000
H	4.57550500	-1.00780200	0.00000000
H	3.60586200	-2.58275600	0.00000000



X = Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-1305.2248735	-130.0197

C	-0.00928200	0.71898700	0.00000000
C	1.24959700	1.38453500	0.00000000
C	2.43838300	0.70159700	0.00000000
C	2.43167600	-0.70789300	0.00000000
C	1.24959700	-1.40376600	0.00000000
C	0.00928200	-0.71898700	0.00000000
C	-1.24959700	1.40376600	0.00000000
C	-2.43167600	0.70789300	0.00000000
C	-2.43838300	-0.70159700	0.00000000
C	-1.24959700	-1.38453500	0.00000000
H	1.25284300	-2.48458700	0.00000000
H	3.37560200	-1.23975900	0.00000000
H	3.37300000	1.24683100	0.00000000
Cl	1.30539100	3.14535200	0.00000000
H	-1.25284300	2.48458700	0.00000000
H	-3.37560200	1.23975900	0.00000000
H	-3.37300000	-1.24683100	0.00000000
Cl	-1.30539100	-3.14535200	0.00000000

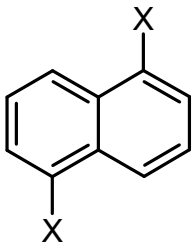


X = Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-5533.0650993	-117.2911

C	-0.00885400	0.72055400	0.00000000
C	1.25141000	1.38588700	0.00000000
C	2.44058500	0.70286000	0.00000000
C	2.43348700	-0.70716400	0.00000000
C	1.25141000	-1.40229800	0.00000000
C	0.00885400	-0.72055400	0.00000000
C	-1.25141000	1.40229800	0.00000000
C	-2.43348700	0.70716400	0.00000000
C	-2.44058500	-0.70286000	0.00000000
C	-1.25141000	-1.38588700	0.00000000
H	1.25476200	-2.48331500	0.00000000
H	3.37750700	-1.23916500	0.00000000
H	3.37805000	1.24297100	0.00000000

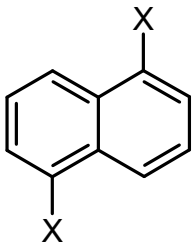
Br	1.33271400	3.30759300	0.00000000
H	-1.25476200	2.48331500	0.00000000
H	-3.37750700	1.23916500	0.00000000
H	-3.37805000	-1.24297100	0.00000000
Br	-1.33271400	-3.30759300	0.00000000



X = CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-464.6375716	-110.1561

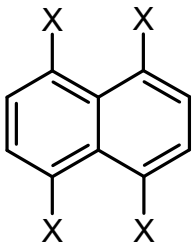
C	-2.42737600	0.70146400	0.00000000
C	-1.24583700	1.39906100	0.00000000
C	0.00041800	0.71754900	0.00000000
C	-0.00041800	-0.71754900	0.00000000
C	-1.24583700	-1.42534000	0.00000000
C	-2.42305400	-0.70900000	0.00000000
C	1.24583700	1.42534000	0.00000000
C	2.42305400	0.70900000	0.00000000
C	2.42737600	-0.70146400	0.00000000
C	1.24583700	-1.39906100	0.00000000
H	1.26347900	-2.48139800	0.00000000
C	1.27909500	2.93432300	0.00000000
C	-1.27909500	-2.93432300	0.00000000
H	-1.26347900	2.48139800	0.00000000
H	0.77972900	3.35065500	0.88079200
H	2.30889900	3.29493900	0.00000000
H	0.77972900	3.35065500	-0.88079200
H	-2.30889900	-3.29493900	0.00000000
H	-0.77972900	-3.35065500	-0.88079200
H	-0.77972900	-3.35065500	0.88079200
H	-3.37294000	1.23247000	0.00000000
H	-3.36869600	-1.24142000	0.00000000
H	3.36869600	1.24142000	0.00000000
H	3.37294000	-1.23247000	0.00000000



X = t-but

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-700.5526651	-171.435

C	-2.48731900	-0.46277600	0.00050800
C	-1.74209000	0.68805900	0.00038200
C	-0.31807500	0.65249600	0.00015800
C	0.31807500	-0.65249600	0.00015800
C	-0.48356900	-1.86248700	0.00015200
C	-1.86016500	-1.72361900	0.00036900
C	0.48356900	1.86248700	0.00015200
C	1.86016500	1.72361900	0.00036900
C	2.48731900	0.46277600	0.00050800
C	1.74209000	-0.68805900	0.00038200
H	2.26219200	-1.63373600	0.00057300
C	-0.12638800	3.29198300	-0.00006500
C	0.12638800	-3.29198300	-0.00006500
H	-2.26219200	1.63373600	0.00057300
C	-0.96817300	3.54161500	-1.28017300
C	-0.95370900	3.54799500	1.28817100
C	0.96817300	4.38609400	-0.00904700
C	0.95370900	-3.54799500	1.28817100
C	-0.96817300	-4.38609400	-0.00904700
C	0.96817300	-3.54161500	-1.28017300
H	-3.57367300	-0.40677600	0.00071100
H	-2.49855200	-2.59833800	0.00041500
H	2.49855200	2.59833800	0.00041500
H	3.57367300	0.40677600	0.00071100
H	-1.34895900	4.57062700	-1.28043800
H	-0.34203700	3.41632700	-2.17142200
H	-1.82265800	2.87178700	-1.38936800
H	-1.33484600	4.57687500	1.28744100
H	-1.80666900	2.87844500	1.41040200
H	-0.31751100	3.42746700	2.17292500
H	0.48628300	5.37034200	-0.01023600
H	1.61056200	4.33809200	0.87730200
H	1.60220600	4.33184000	-0.90103500
H	-0.48628300	-5.37034200	-0.01023600
H	-1.61056200	-4.33809200	0.87730200
H	-1.60220600	-4.33184000	-0.90103500
H	1.33484600	-4.57687500	1.28744100
H	1.80666900	-2.87844500	1.41040200
H	0.31751100	-3.42746700	2.17292500
H	1.34895900	-4.57062700	-1.28043800
H	0.34203700	-3.41632700	-2.17142200
H	1.82265800	-2.87178700	-1.38936800

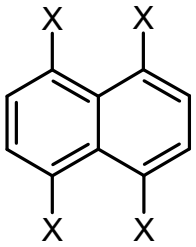


X = Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_2	-2224.4288882	-163.6355

C	0.00000000	0.00000000	-0.73243100

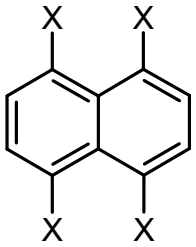
C	-0.14946000	1.26583700	-1.38766600
C	-0.10366800	2.44528900	-0.69070100
C	0.10366800	2.44528900	0.69070100
C	0.14946000	1.26583700	1.38766600
C	0.00000000	0.00000000	0.73243100
C	0.14946000	-1.26583700	-1.38766600
C	0.10366800	-2.44528900	-0.69070100
C	-0.10366800	-2.44528900	0.69070100
C	-0.14946000	-1.26583700	1.38766600
Cl	0.52996600	1.44563000	3.09444600
H	0.22041200	3.38143700	1.21941900
H	-0.22041200	3.38143700	-1.21941900
Cl	-0.52996600	1.44563000	-3.09444600
Cl	0.52996600	-1.44563000	-3.09444600
H	0.22041200	-3.38143700	-1.21941900
H	-0.22041200	-3.38143700	1.21941900
Cl	-0.52996600	-1.44563000	3.09444600



X =Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_2	-10680.1042298	-200.8569

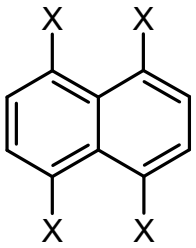
C	0.00000000	0.00000000	-0.73237900
C	-0.19845300	1.26222300	-1.38115300
C	-0.13948500	2.44215200	-0.68594200
C	0.13948500	2.44215200	0.68594200
C	0.19845300	1.26222300	1.38115300
C	0.00000000	0.00000000	0.73237900
C	0.19845300	-1.26222300	-1.38115300
C	0.13948500	-2.44215200	-0.68594200
C	-0.13948500	-2.44215200	0.68594200
C	-0.19845300	-1.26222300	1.38115300
Br	0.77005800	1.46258700	3.20424100
H	0.29636100	3.38064100	1.19957600
H	-0.29636100	3.38064100	-1.19957600
Br	-0.77005800	1.46258700	-3.20424100
Br	0.77005800	-1.46258700	-3.20424100
H	0.29636100	-3.38064100	-1.19957600
H	-0.29636100	-3.38064100	1.19957600
Br	-0.77005800	-1.46258700	3.20424100



X =CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_2	-543.2655151	-123.9587

C	-0.08830300	2.42503500	0.69408700
C	-0.12584100	1.25932300	1.42290900
C	0.00000000	0.00000000	0.72930100
C	0.00000000	0.00000000	-0.72930100
C	0.12584100	1.25932300	-1.42290900
C	0.08830300	2.42503500	-0.69408700
C	0.12584100	-1.25932300	1.42290900
C	0.08830300	-2.42503500	0.69408700
C	-0.08830300	-2.42503500	-0.69408700
C	-0.12584100	-1.25932300	-1.42290900
C	-0.38501400	-1.41417000	-2.90945400
C	0.38501400	-1.41417000	2.90945400
C	0.38501400	1.41417000	-2.90945400
C	-0.38501400	1.41417000	2.90945400
H	0.46962800	1.14734100	3.53296400
H	-0.62378000	2.45808600	3.11968400
H	-1.23591500	0.81547400	3.24042300
H	1.23591500	-0.81547400	3.24042300
H	-0.46962800	-1.14734100	3.53296400
H	0.62378000	-2.45808600	3.11968400
H	-0.46962800	1.14734100	-3.53296400
H	0.62378000	2.45808600	-3.11968400
H	1.23591500	0.81547400	-3.24042300
H	-1.23591500	-0.81547400	-3.24042300
H	0.46962800	-1.14734100	-3.53296400
H	-0.62378000	-2.45808600	-3.11968400
H	-0.18899300	3.37447700	1.20924300
H	0.18899300	3.37447700	-1.20924300
H	0.18899300	-3.37447700	1.20924300
H	-0.18899300	-3.37447700	-1.20924300

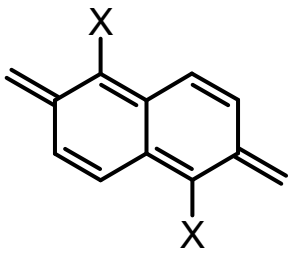


X = t-but

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_2	-1015.0483926	-248.1787

C	-0.08830300	2.42503500	0.69408700
C	-0.12584100	1.25932300	1.42290900
C	0.00000000	0.00000000	0.72930100
C	0.00000000	0.00000000	-0.72930100
C	0.12584100	1.25932300	-1.42290900
C	0.08830300	2.42503500	-0.69408700
C	0.12584100	-1.25932300	1.42290900
C	0.08830300	-2.42503500	0.69408700
C	-0.08830300	-2.42503500	-0.69408700
C	-0.12584100	-1.25932300	-1.42290900
C	-0.38501400	-1.41417000	-2.90945400

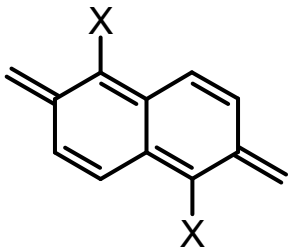
C	0.38501400	-1.41417000	2.90945400
C	0.38501400	1.41417000	-2.90945400
C	-0.38501400	1.41417000	2.90945400
H	0.46962800	1.14734100	3.53296400
H	-0.62378000	2.45808600	3.11968400
H	-1.23591500	0.81547400	3.24042300
H	1.23591500	-0.81547400	3.24042300
H	-0.46962800	-1.14734100	3.53296400
H	0.62378000	-2.45808600	3.11968400
H	-0.46962800	1.14734100	-3.53296400
H	0.62378000	2.45808600	-3.11968400
H	1.23591500	0.81547400	-3.24042300
H	-1.23591500	-0.81547400	-3.24042300
H	0.46962800	-1.14734100	-3.53296400
H	-0.62378000	-2.45808600	-3.11968400
H	-0.18899300	3.37447700	1.20924300
H	0.18899300	3.37447700	-1.20924300
H	0.18899300	-3.37447700	1.20924300
H	-0.18899300	-3.37447700	-1.20924300



X =Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-1382.5960683	-116.3654

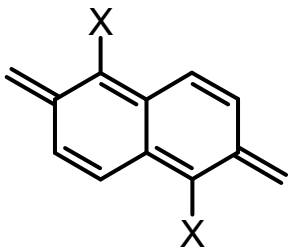
C	-0.00646000	0.73533500	0.00000000
C	-1.29532900	1.39531400	0.00000000
C	-2.44462300	0.69780400	0.00000000
C	-2.48510800	-0.75754900	0.00000000
C	-1.18465400	-1.41183000	0.00000000
C	0.00646000	-0.73533500	0.00000000
C	1.18465400	1.41183000	0.00000000
C	2.48510800	0.75754900	0.00000000
C	2.44462300	-0.69780400	0.00000000
C	1.29532900	-1.39531400	0.00000000
Cl	-1.18465400	-3.17363800	0.00000000
C	-3.67226900	-1.40873100	0.00000000
H	-3.39619700	1.21737900	0.00000000
H	-1.31822100	2.47558000	0.00000000
Cl	1.18465400	3.17363800	0.00000000
C	3.67226900	1.40873100	0.00000000
H	3.39619700	-1.21737900	0.00000000
H	1.31822100	-2.47558000	0.00000000
H	4.59756500	0.84633000	0.00000000
H	3.74230500	2.48640100	0.00000000
H	-4.59756500	-0.84633000	0.00000000
H	-3.74230500	-2.48640100	0.00000000



X =Br

	Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
	C_{2h}	-5610.4349132	-135.1255

C	-0.00647100	0.73780600	0.00000000
C	-1.29904100	1.39067700	0.00000000
C	-2.44616000	0.69095900	0.00000000
C	-2.48658700	-0.76479400	0.00000000
C	-1.18432500	-1.41670600	0.00000000
C	0.00647100	-0.73780600	0.00000000
C	1.18432500	1.41670600	0.00000000
C	2.48658700	0.76479400	0.00000000
C	2.44616000	-0.69095900	0.00000000
C	1.29904100	-1.39067700	0.00000000
Br	-1.18432500	-3.34290000	0.00000000
C	-3.68001400	-1.40488100	0.00000000
H	-3.39841300	1.20948000	0.00000000
H	-1.32570900	2.47074800	0.00000000
Br	1.18432500	3.34290000	0.00000000
C	3.68001400	1.40488100	0.00000000
H	3.39841300	-1.20948000	0.00000000
H	1.32570900	-2.47074800	0.00000000
H	4.59906600	0.83219000	0.00000000
H	3.76150300	2.48166800	0.00000000
H	-4.59906600	-0.83219000	0.00000000
H	-3.76150300	-2.48166800	0.00000000

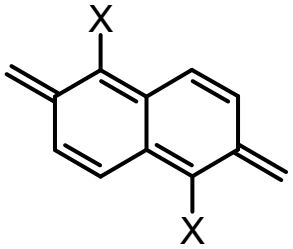


X =CH_3

	Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
	C_i	-542.0039338	-99.5223

C	-1.28400300	1.39624700	-0.07923000
C	0.00845700	0.73808600	-0.01412300
C	-0.00845700	-0.73808600	0.01412300
C	-1.19027300	-1.44632900	-0.02068400
C	-2.47492500	-0.74485100	-0.09111000
C	-2.43708100	0.70693500	-0.11521500
C	1.19027300	1.44632900	0.02068400
C	2.47492500	0.74485100	0.09111000
C	2.43708100	-0.70693500	0.11521500

C	1.28400300	-1.39624700	0.07923000
C	1.25465200	2.95302400	-0.00856200
C	3.67331700	1.38089400	0.13427300
C	-1.25465200	-2.95302400	0.00856200
C	-3.67331700	-1.38089400	-0.13427300
H	1.32726200	-2.47563200	0.09840500
H	-1.32726200	2.47563200	-0.09840500
H	1.74613300	3.33429700	0.89269100
H	1.84877700	3.29440500	-0.86250800
H	0.28235100	3.43135300	-0.07710400
H	-1.84877700	-3.29440500	0.86250800
H	-1.74613300	-3.33429700	-0.89269100
H	-0.28235100	-3.43135300	0.07710400
H	-3.38487200	1.23283200	-0.16425100
H	3.38487200	-1.23283200	0.16425100
H	4.59246000	0.80931300	0.18649900
H	3.77321300	2.45681300	0.12052900
H	-3.77321300	-2.45681300	-0.12052900
H	-4.59246000	-0.80931300	-0.18649900

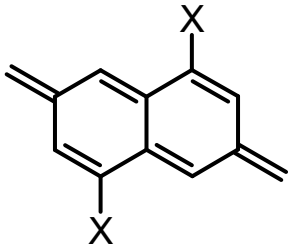


X = t-but

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-777.8773815	-154.4873

C	1.16352900	1.48004800	0.00000000
C	-0.08320200	0.74705700	0.00000000
C	0.08320200	-0.74705700	0.00000000
C	1.32084600	-1.39269400	0.00000000
C	2.54708300	-0.55497600	0.00000000
C	2.35927800	0.88000800	0.00000000
C	-1.32084600	1.39269400	0.00000000
C	-2.54708300	0.55497600	0.00000000
C	-2.35927800	-0.88000800	0.00000000
C	-1.16352900	-1.48004800	0.00000000
C	-1.58601200	2.94383400	0.00000000
C	-2.35927800	3.31788300	1.30207400
C	1.58601200	-2.94383400	0.00000000
C	2.35927800	-3.31788300	1.30207400
C	0.41499000	-3.96162700	0.00000000
C	2.35927800	-3.31788300	-1.30207400
C	-0.41499000	3.96162700	0.00000000
C	-2.35927800	3.31788300	-1.30207400
C	-3.85165000	0.94762900	0.00000000
H	-3.25620200	-1.49040900	0.00000000
H	3.25620200	1.49040900	0.00000000
H	1.15958400	2.54696200	0.00000000
C	3.85165000	-0.94762900	0.00000000
H	-1.15958400	-2.54696200	0.00000000
H	0.86432800	-4.95895600	0.00000000
H	-0.20916800	-3.90142900	0.89272100
H	-0.20916800	-3.90142900	-0.89272100

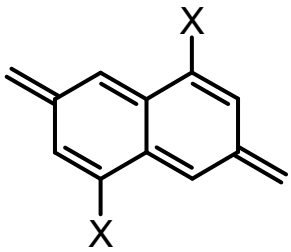
H	2.71362300	-4.35127500	1.23795200
H	3.20759700	-2.68062600	1.52742700
H	1.67632300	-3.25462800	2.15397700
H	2.71362300	-4.35127500	-1.23795200
H	1.67632300	-3.25462800	-2.15397700
H	3.20759700	-2.68062600	-1.52742700
H	-0.86432800	4.95895600	0.00000000
H	0.20916800	3.90142900	0.89272100
H	0.20916800	3.90142900	-0.89272100
H	-2.71362300	4.35127500	-1.23795200
H	-1.67632300	3.25462800	-2.15397700
H	-3.20759700	2.68062600	-1.52742700
H	-2.71362300	4.35127500	1.23795200
H	-3.20759700	2.68062600	1.52742700
H	-1.67632300	3.25462800	2.15397700
H	4.62110700	-0.18439200	0.00000000
H	4.20805200	-1.96212100	0.00000000
H	-4.62110700	0.18439200	0.00000000
H	-4.20805200	1.96212100	0.00000000



X =Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-1382.5992605	-117.1443

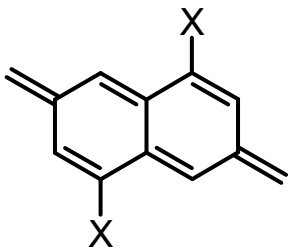
C	-0.00211700	0.73606600	0.00000000
C	1.31059100	1.37046800	0.00000000
C	2.46285500	0.67654200	0.00000000
C	2.46285500	-0.77747800	0.00000000
C	1.17138800	-1.43055800	0.00000000
C	0.00211700	-0.73606600	0.00000000
C	-1.17138800	1.43055800	0.00000000
C	-2.46285500	0.77747800	0.00000000
C	-2.46285500	-0.67654200	0.00000000
C	-1.31059100	-1.37046800	0.00000000
H	1.15314500	-2.51214600	0.00000000
C	3.62020600	-1.48318300	0.00000000
H	3.41212900	1.19714700	0.00000000
Cl	1.39011000	3.13073400	0.00000000
H	-1.15314500	2.51214600	0.00000000
C	-3.62020600	1.48318300	0.00000000
H	-3.41212900	-1.19714700	0.00000000
Cl	-1.39011000	-3.13073400	0.00000000
H	-4.58382600	0.98876100	0.00000000
H	-3.61720500	2.56623600	0.00000000
H	4.58382600	-0.98876100	0.00000000
H	3.61720500	-2.56623600	0.00000000



X =Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-5610.4394673	-135.7745

C	-0.00217800	0.73772700	0.00000000
C	1.31161400	1.37188500	0.00000000
C	2.46395400	0.67793400	0.00000000
C	2.46395400	-0.77666700	0.00000000
C	1.17310900	-1.42931800	0.00000000
C	0.00217800	-0.73772700	0.00000000
C	-1.17310900	1.42931800	0.00000000
C	-2.46395400	0.77666700	0.00000000
C	-2.46395400	-0.67793400	0.00000000
C	-1.31161400	-1.37188500	0.00000000
H	1.15518800	-2.51106800	0.00000000
C	3.62206300	-1.48105100	0.00000000
H	3.41603500	1.19304000	0.00000000
Br	1.42060200	3.29279300	0.00000000
H	-1.15518800	2.51106800	0.00000000
C	-3.62206300	1.48105100	0.00000000
H	-3.41603500	-1.19304000	0.00000000
Br	-1.42060200	-3.29279300	0.00000000
H	-4.58495300	0.98521000	0.00000000
H	-3.62058400	2.56410100	0.00000000
H	4.58495300	-0.98521000	0.00000000
H	3.62058400	-2.56410100	0.00000000

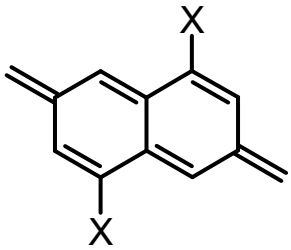


X =CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_i	-542.0135988	-97.4185

C	-0.00217800	0.73772700	0.00000000
C	1.31161400	1.37188500	0.00000000
C	2.46395400	0.67793400	0.00000000
C	2.46395400	-0.77666700	0.00000000
C	1.17310900	-1.42931800	0.00000000
C	0.00217800	-0.73772700	0.00000000
C	-1.17310900	1.42931800	0.00000000
C	-2.46395400	0.77666700	0.00000000
C	-2.46395400	-0.67793400	0.00000000

C	-1.31161400	-1.37188500	0.00000000
H	1.15518800	-2.51106800	0.00000000
C	3.62206300	-1.48105100	0.00000000
H	3.41603500	1.19304000	0.00000000
Br	1.42060200	3.29279300	0.00000000
H	-1.15518800	2.51106800	0.00000000
C	-3.62206300	1.48105100	0.00000000
H	-3.41603500	-1.19304000	0.00000000
Br	-1.42060200	-3.29279300	0.00000000
H	-4.58495300	0.98521000	0.00000000
H	-3.62058400	2.56410100	0.00000000
H	4.58495300	-0.98521000	0.00000000
H	3.62058400	-2.56410100	0.00000000

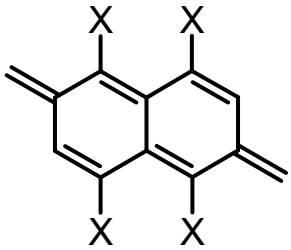


X = t-but

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-777.9103435	-156.4384

C	1.16677500	1.42314900	0.00000000
C	-0.01685400	0.74856500	0.00000000
C	0.01685400	-0.74856500	0.00000000
C	1.33376500	-1.43593700	0.00000000
C	2.45033100	-0.66786900	0.00000000
C	2.45234900	0.77473500	0.00000000
C	-1.33376500	1.43593700	0.00000000
C	-2.45033100	0.66786900	0.00000000
C	-2.45234900	-0.77473500	0.00000000
C	-1.16677500	-1.42314900	0.00000000
C	-1.62272300	2.98320400	0.00000000
C	-2.45033100	3.32202300	1.26741400
C	1.62272300	-2.98320400	0.00000000
C	2.45033100	-3.32202300	1.26741400
C	0.44210300	-3.97870600	0.00000000
C	2.45033100	-3.32202300	-1.26741400
C	-0.44210300	3.97870600	0.00000000
C	-2.45033100	3.32202300	-1.26741400
H	-3.42762400	1.13380500	0.00000000
C	-3.60760400	-1.48794900	0.00000000
C	3.60760400	1.48794900	0.00000000
H	1.19251900	2.49432000	0.00000000
H	3.42762400	-1.13380500	0.00000000
H	-1.19251900	-2.49432000	0.00000000
H	0.86057500	-4.98907900	0.00000000
H	-0.18200000	-3.89534200	0.89149600
H	-0.18200000	-3.89534200	-0.89149600
H	2.68983700	-4.38976200	1.28486500
H	3.38929700	-2.76980600	1.31408600
H	1.88212900	-3.08835700	2.17203000
H	2.68983700	-4.38976200	-1.28486500
H	1.88212900	-3.08835700	-2.17203000
H	3.38929700	-2.76980600	-1.31408600

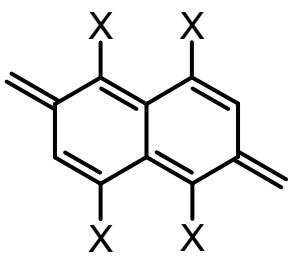
H	-0.86057500	4.98907900	0.00000000
H	0.18200000	3.89534200	0.89149600
H	0.18200000	3.89534200	-0.89149600
H	-2.68983700	4.38976200	-1.28486500
H	-1.88212900	3.08835700	-2.17203000
H	-3.38929700	2.76980600	-1.31408600
H	-2.68983700	4.38976200	1.28486500
H	-3.38929700	2.76980600	1.31408600
H	-1.88212900	3.08835700	2.17203000
H	3.60239900	2.57141100	0.00000000
H	4.57393500	0.99781600	0.00000000
H	-4.57393500	-0.99781600	0.00000000
H	-3.60239900	-2.57141100	0.00000000



X =Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-2301.8032939	-153.5008

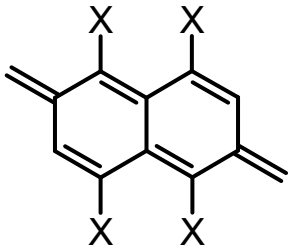
C	-0.00103600	0.74518400	0.06660300
C	1.30796300	1.35767000	0.31060100
C	2.44512700	0.68266500	0.08577500
C	2.44512700	-0.69894700	-0.36278100
C	1.16153100	-1.39135700	-0.25808600
C	0.00103600	-0.74518400	0.06660300
C	-1.16153100	1.39135700	-0.25808600
C	-2.44512700	0.69894700	-0.36278100
C	-2.44512700	-0.68266500	0.08577500
C	-1.30796300	-1.35767000	0.31060100
Cl	1.19218800	-3.09929800	-0.64051400
C	3.59660700	-1.27696100	-0.77090500
H	3.40067900	1.15691100	0.26817600
Cl	1.44742700	2.94077900	1.06300100
Cl	-1.19218800	3.09929800	-0.64051400
C	-3.59660700	1.27696100	-0.77090500
H	-3.40067900	-1.15691100	0.26817600
Cl	-1.44742700	-2.94077900	1.06300100
H	-4.51340100	0.70129300	-0.79027100
H	-3.64626600	2.30793700	-1.08742200
H	4.51340100	-0.70129300	-0.79027100
H	3.64626600	-2.30793700	-1.08742200



X =Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-10757.4794413	-135.7745

C	-0.00217800	0.73772700	0.00000000
C	1.31161400	1.37188500	0.00000000
C	2.46395400	0.67793400	0.00000000
C	2.46395400	-0.77666700	0.00000000
C	1.17310900	-1.42931800	0.00000000
C	0.00217800	-0.73772700	0.00000000
C	-1.17310900	1.42931800	0.00000000
C	-2.46395400	0.77666700	0.00000000
C	-2.46395400	-0.67793400	0.00000000
C	-1.31161400	-1.37188500	0.00000000
H	1.15518800	-2.51106800	0.00000000
C	3.62206300	-1.48105100	0.00000000
H	3.41603500	1.19304000	0.00000000
Br	1.42060200	3.29279300	0.00000000
H	-1.15518800	2.51106800	0.00000000
C	-3.62206300	1.48105100	0.00000000
H	-3.41603500	-1.19304000	0.00000000
Br	-1.42060200	-3.29279300	0.00000000
H	-4.58495300	0.98521000	0.00000000
H	-3.62058400	2.56410100	0.00000000
H	4.58495300	-0.98521000	0.00000000
H	3.62058400	-2.56410100	0.00000000

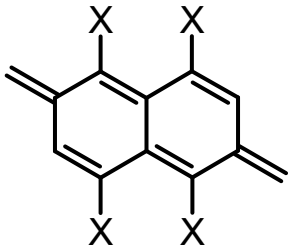


X =CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-620.6348895	-117.8687

C	1.20491500	-1.39292500	0.00005000
C	0.01165100	-0.73494000	0.00001800
C	-0.01165100	0.73494000	-0.00001800
C	1.26934500	1.44813800	-0.00001700
C	2.42750500	0.75138900	0.00001500
C	2.47708100	-0.70160700	0.00005100
C	-1.26934500	-1.44813800	0.00001700
C	-2.42750500	-0.75138900	-0.00001500
C	-2.47708100	0.70160700	-0.00005100
C	-1.20491500	1.39292500	-0.00005000
C	-1.28322000	-2.95521200	0.00005300
C	1.28322000	2.95521200	-0.00005300
H	1.23242700	-2.47578300	0.00007600
H	-1.23242700	2.47578300	-0.00007600
H	0.77529200	3.36125500	0.88076700
H	2.30773900	3.32970800	-0.00004800
H	0.77531600	3.36121300	-0.88090600
H	-2.30773900	-3.32970800	0.00004800
H	-0.77529200	-3.36125500	-0.88076700

H	-0.77531600	-3.36121300	0.88090600
C	-3.65470100	1.37405800	-0.00008300
H	-3.37408000	-1.28327900	-0.00001500
H	3.37408000	1.28327900	0.00001500
C	3.65470100	-1.37405800	0.00008300
H	3.68638800	-2.45716600	0.00010900
H	4.60354500	-0.85091600	0.00008300
H	-4.60354500	0.85091600	-0.00008300
H	-3.68638800	2.45716600	-0.00010900

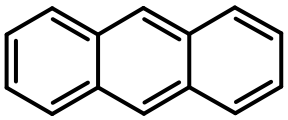


X = t-but

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-1092.419573	-238.1947

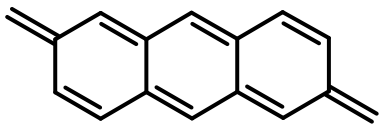
C	1.16677500	1.42314900	0.00000000
C	-0.01685400	0.74856500	0.00000000
C	0.01685400	-0.74856500	0.00000000
C	1.33376500	-1.43593700	0.00000000
C	2.45033100	-0.66786900	0.00000000
C	2.45234900	0.77473500	0.00000000
C	-1.33376500	1.43593700	0.00000000
C	-2.45033100	0.66786900	0.00000000
C	-2.45234900	-0.77473500	0.00000000
C	-1.16677500	-1.42314900	0.00000000
C	-1.62272300	2.98320400	0.00000000
C	-2.45033100	3.32202300	1.26741400
C	1.62272300	-2.98320400	0.00000000
C	2.45033100	-3.32202300	1.26741400
C	0.44210300	-3.97870600	0.00000000
C	2.45033100	-3.32202300	-1.26741400
C	-0.44210300	3.97870600	0.00000000
C	-2.45033100	3.32202300	-1.26741400
H	-3.42762400	1.13380500	0.00000000
C	-3.60760400	-1.48794900	0.00000000
C	3.60760400	1.48794900	0.00000000
H	1.19251900	2.49432000	0.00000000
H	3.42762400	-1.13380500	0.00000000
H	-1.19251900	-2.49432000	0.00000000
H	0.86057500	-4.98907900	0.00000000
H	-0.18200000	-3.89534200	0.89149600
H	-0.18200000	-3.89534200	-0.89149600
H	2.68983700	-4.38976200	1.28486500
H	3.38929700	-2.76980600	1.31408600
H	1.88212900	-3.08835700	2.17203000
H	2.68983700	-4.38976200	-1.28486500
H	1.88212900	-3.08835700	-2.17203000
H	3.38929700	-2.76980600	-1.31408600
H	-0.86057500	4.98907900	0.00000000
H	0.18200000	3.89534200	0.89149600
H	0.18200000	3.89534200	-0.89149600
H	-2.68983700	4.38976200	-1.28486500

H	-1.88212900	3.08835700	-2.17203000
H	-3.38929700	2.76980600	-1.31408600
H	-2.68983700	4.38976200	1.28486500
H	-3.38929700	2.76980600	1.31408600
H	-1.88212900	3.08835700	2.17203000
H	3.60239900	2.57141100	0.00000000
H	4.57393500	0.99781600	0.00000000
H	-4.57393500	-0.99781600	0.00000000
H	-3.60239900	-2.57141100	0.00000000



Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_{2h}	-539.6551832	-128.3796

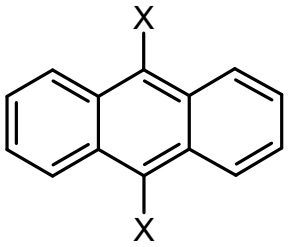
C	0.00000000	3.65457500	0.71228300
C	0.00000000	2.47656700	1.40482800
C	0.00000000	1.22177300	0.72148000
C	0.00000000	1.22177300	-0.72148000
C	0.00000000	2.47656700	-1.40482800
C	0.00000000	3.65457500	-0.71228300
C	0.00000000	0.00000000	1.40155000
C	0.00000000	0.00000000	-1.40155000
C	0.00000000	-1.22177300	-0.72148000
C	0.00000000	-1.22177300	0.72148000
C	0.00000000	-2.47656700	1.40482800
H	0.00000000	-2.47553800	2.48986700
C	0.00000000	-3.65457500	0.71228300
C	0.00000000	-3.65457500	-0.71228300
C	0.00000000	-2.47656700	-1.40482800
H	0.00000000	0.00000000	2.48741700
H	0.00000000	4.59933200	1.24414700
H	0.00000000	2.47553800	2.48986700
H	0.00000000	2.47553800	-2.48986700
H	0.00000000	4.59933200	-1.24414700
H	0.00000000	0.00000000	-2.48741700
H	0.00000000	-4.59933200	1.24414700
H	0.00000000	-4.59933200	-1.24414700
H	0.00000000	-2.47553800	-2.48986700



Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-617.0237088	-99.9061

C	3.64611000	0.83538300	0.00000000
C	2.46352400	1.48232200	0.00000000
C	1.20305500	0.76840500	0.00000000
C	1.25349500	-0.69419300	0.00000000
C	2.46352400	-1.33433900	0.00000000

C	3.72194500	-0.62208300	0.00000000
C	-0.00349700	1.40674900	0.00000000
C	0.00349700	-1.40674900	0.00000000
C	-1.20305500	-0.76840500	0.00000000
C	-1.25349500	0.69419300	0.00000000
C	-2.46352400	1.33433900	0.00000000
H	-2.49274600	2.41970300	0.00000000
C	-3.72194500	0.62208300	0.00000000
C	-3.64611000	-0.83538300	0.00000000
C	-2.46352400	-1.48232200	0.00000000
H	-0.03537100	2.49230900	0.00000000
H	4.57758500	1.39140500	0.00000000
H	2.43135600	2.56722700	0.00000000
H	2.49274600	-2.41970300	0.00000000
H	0.03537100	-2.49230900	0.00000000
H	-4.57758500	-1.39140500	0.00000000
H	-2.43135600	-2.56722700	0.00000000
C	4.91569600	-1.26963700	0.00000000
C	-4.91569600	1.26963700	0.00000000
H	5.85186600	-0.72454700	0.00000000
H	4.97095100	-2.35164200	0.00000000
H	-4.97095100	2.35164200	0.00000000
H	-5.85186600	0.72454700	0.00000000

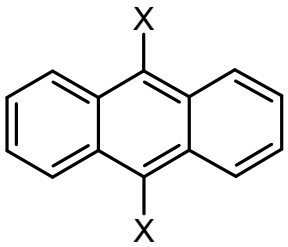


X =Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_{2h}	-1458.8904981	-167.8615

C	0.00000000	3.66778400	0.70969300
C	0.00000000	2.49025700	1.40058100
C	0.00000000	1.23205000	0.72339400
C	0.00000000	1.23205000	-0.72339400
C	0.00000000	2.49025700	-1.40058100
C	0.00000000	3.66778400	-0.70969300
C	0.00000000	0.00000000	1.39444500
C	0.00000000	0.00000000	-1.39444500
C	0.00000000	-1.23205000	-0.72339400
C	0.00000000	-1.23205000	0.72339400
C	0.00000000	-2.49025700	1.40058100
H	0.00000000	-2.49509000	2.48108900
C	0.00000000	-3.66778400	0.70969300
C	0.00000000	-3.66778400	-0.70969300
C	0.00000000	-2.49025700	-1.40058100
H	0.00000000	4.60892800	1.24722100
H	0.00000000	2.49509000	2.48108900
H	0.00000000	2.49509000	-2.48108900
H	0.00000000	4.60892800	-1.24722100
H	0.00000000	-4.60892800	1.24722100
H	0.00000000	-4.60892800	-1.24722100
H	0.00000000	-2.49509000	-2.48108900
Cl	0.00000000	0.00000000	-3.15823200

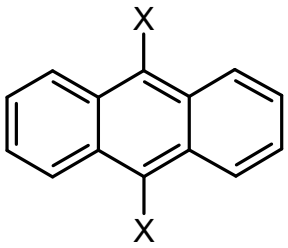
Cl	0.00000000	0.00000000	3.15823200



X =Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_{2h}	-5686.7290672	-186.9699

C	0.00000000	3.66778400	0.70969300
C	0.00000000	2.49025700	1.40058100
C	0.00000000	1.23205000	0.72339400
C	0.00000000	1.23205000	-0.72339400
C	0.00000000	2.49025700	-1.40058100
C	0.00000000	3.66778400	-0.70969300
C	0.00000000	0.00000000	1.39444500
C	0.00000000	0.00000000	-1.39444500
C	0.00000000	-1.23205000	-0.72339400
C	0.00000000	-1.23205000	0.72339400
C	0.00000000	-2.49025700	1.40058100
H	0.00000000	-2.49509000	2.48108900
C	0.00000000	-3.66778400	0.70969300
C	0.00000000	-3.66778400	-0.70969300
C	0.00000000	-2.49025700	-1.40058100
H	0.00000000	4.60892800	1.24722100
H	0.00000000	2.49509000	2.48108900
H	0.00000000	2.49509000	-2.48108900
H	0.00000000	4.60892800	-1.24722100
H	0.00000000	-4.60892800	1.24722100
H	0.00000000	-4.60892800	-1.24722100
H	0.00000000	-2.49509000	-2.48108900
Cl	0.00000000	0.00000000	-3.15823200
Cl	0.00000000	0.00000000	3.15823200

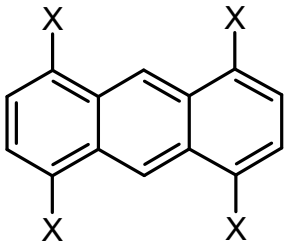


X =CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2v}	-618.2967462	-150.8098

C	0.00000000	3.66778400	0.70969300
C	0.00000000	2.49025700	1.40058100
C	0.00000000	1.23205000	0.72339400
C	0.00000000	1.23205000	-0.72339400
C	0.00000000	2.49025700	-1.40058100
C	0.00000000	3.66778400	-0.70969300

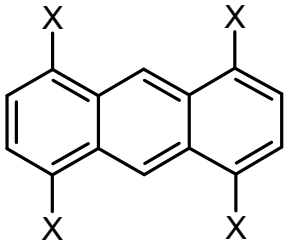
C	0.00000000	0.00000000	1.39444500
C	0.00000000	0.00000000	-1.39444500
C	0.00000000	-1.23205000	-0.72339400
C	0.00000000	-1.23205000	0.72339400
C	0.00000000	-2.49025700	1.40058100
H	0.00000000	-2.49509000	2.48108900
C	0.00000000	-3.66778400	0.70969300
C	0.00000000	-3.66778400	-0.70969300
C	0.00000000	-2.49025700	-1.40058100
H	0.00000000	4.60892800	1.24722100
H	0.00000000	2.49509000	2.48108900
H	0.00000000	2.49509000	-2.48108900
H	0.00000000	4.60892800	-1.24722100
H	0.00000000	-4.60892800	1.24722100
H	0.00000000	-4.60892800	-1.24722100
H	0.00000000	-2.49509000	-2.48108900
Cl	0.00000000	0.00000000	-3.15823200
Cl	0.00000000	0.00000000	3.15823200



X =Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_{2h}	-2378.1332412	-210.6356

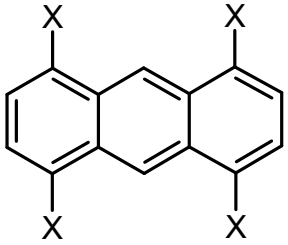
C	0.00000000	3.66778400	0.70969300
C	0.00000000	2.49025700	1.40058100
C	0.00000000	1.23205000	0.72339400
C	0.00000000	1.23205000	-0.72339400
C	0.00000000	2.49025700	-1.40058100
C	0.00000000	3.66778400	-0.70969300
C	0.00000000	0.00000000	1.39444500
C	0.00000000	0.00000000	-1.39444500
C	0.00000000	-1.23205000	-0.72339400
C	0.00000000	-1.23205000	0.72339400
C	0.00000000	-2.49025700	1.40058100
H	0.00000000	-2.49509000	2.48108900
C	0.00000000	-3.66778400	0.70969300
C	0.00000000	-3.66778400	-0.70969300
C	0.00000000	-2.49025700	-1.40058100
H	0.00000000	4.60892800	1.24722100
H	0.00000000	2.49509000	2.48108900
H	0.00000000	2.49509000	-2.48108900
H	0.00000000	4.60892800	-1.24722100
H	0.00000000	-4.60892800	1.24722100
H	0.00000000	-4.60892800	-1.24722100
H	0.00000000	-2.49509000	-2.48108900
Cl	0.00000000	0.00000000	-3.15823200
Cl	0.00000000	0.00000000	3.15823200



X =Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_{2h}	-10833.8138094	-248.8135

C	0.00000000	3.66672700	0.70959200
C	0.00000000	2.48958200	1.39884800
C	0.00000000	1.22430700	0.72394400
C	0.00000000	1.22430700	-0.72394400
C	0.00000000	2.48958200	-1.39884800
C	0.00000000	3.66672700	-0.70959200
C	0.00000000	0.00000000	1.39453400
C	0.00000000	0.00000000	-1.39453400
C	0.00000000	-1.22430700	-0.72394400
C	0.00000000	-1.22430700	0.72394400
C	0.00000000	-2.48958200	1.39884800
C	0.00000000	-3.66672700	0.70959200
C	0.00000000	-3.66672700	-0.70959200
C	0.00000000	-2.48958200	-1.39884800
H	0.00000000	0.00000000	2.47433400
H	0.00000000	4.61120000	1.23727700
H	0.00000000	4.61120000	-1.23727700
H	0.00000000	0.00000000	-2.47433400
H	0.00000000	-4.61120000	1.23727700
H	0.00000000	-4.61120000	-1.23727700
Br	0.00000000	2.56693200	3.31439100
Br	0.00000000	-2.56693200	3.31439100
Br	0.00000000	-2.56693200	-3.31439100
Br	0.00000000	2.56693200	-3.31439100

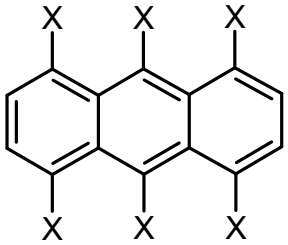


X =CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_{2h}	-696.9620812	-168.8455

C	3.64402600	0.71005900	0.00000000
C	2.48251100	1.43486200	0.00000000
C	1.23066100	0.72119500	0.00000000
C	1.23066100	-0.72119500	0.00000000
C	2.48251100	-1.43486200	0.00000000
C	3.64402600	-0.71005900	0.00000000
C	0.00000000	1.38868100	0.00000000
C	0.00000000	-1.38868100	0.00000000

C	-1.23066100	-0.72119500	0.00000000
C	-1.23066100	0.72119500	0.00000000
C	-2.48251100	1.43486200	0.00000000
C	-3.64402600	0.71005900	0.00000000
C	-3.64402600	-0.71005900	0.00000000
C	-2.48251100	-1.43486200	0.00000000
H	0.00000000	2.46976100	0.00000000
H	4.59688000	1.22966800	0.00000000
H	4.59688000	-1.22966800	0.00000000
H	0.00000000	-2.46976100	0.00000000
H	-4.59688000	1.22966800	0.00000000
H	-4.59688000	-1.22966800	0.00000000
C	-2.51726500	2.94202900	0.00000000
H	-2.01831200	3.35947500	0.88080400
H	-2.01831200	3.35947500	-0.88080400
H	-3.54785900	3.30051000	0.00000000
C	2.51726500	2.94202900	0.00000000
H	2.01831200	3.35947500	-0.88080400
H	2.01831200	3.35947500	0.88080400
H	3.54785900	3.30051000	0.00000000
C	2.51726500	-2.94202900	0.00000000
H	2.01831200	-3.35947500	0.88080400
H	2.01831200	-3.35947500	-0.88080400
H	3.54785900	-3.30051000	0.00000000
C	-2.51726500	-2.94202900	0.00000000
H	-2.01831200	-3.35947500	-0.88080400
H	-2.01831200	-3.35947500	0.88080400
H	-3.54785900	-3.30051000	0.00000000

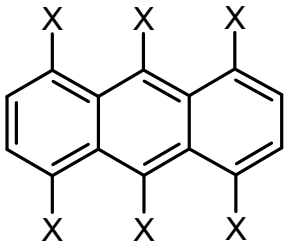


X =Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2v}	-3297.2985065	-237.0527

Cl	0.00000000	2.89779700	1.15828700
Cl	2.60433500	3.11072800	-0.50665500
Cl	-2.60433500	3.11072800	-0.50665500
Cl	2.60433500	-3.11072800	-0.50665500
Cl	-2.60433500	-3.11072800	-0.50665500
Cl	0.00000000	-2.89779700	1.15828700
C	1.23014600	-0.73140000	0.05439300
C	0.00000000	-1.38172300	0.28817500
C	-2.48709700	-1.39865300	-0.13585600
C	-3.66143900	-0.70229000	-0.20761600
C	3.66143900	-0.70229000	-0.20761600
C	0.00000000	1.38172300	0.28817500
C	3.66143900	0.70229000	-0.20761600
C	-2.48709700	1.39865300	-0.13585600
C	-1.23014600	0.73140000	0.05439300
C	1.23014600	0.73140000	0.05439300
C	2.48709700	1.39865300	-0.13585600
C	2.48709700	-1.39865300	-0.13585600

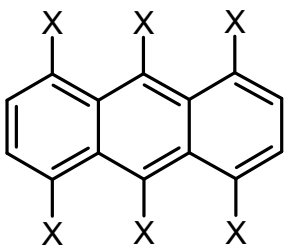
C	-3.66143900	0.70229000	-0.20761600
C	-1.23014600	-0.73140000	0.05439300
H	-4.58934900	1.23606800	-0.36235000
H	-4.58934900	-1.23606800	-0.36235000
H	4.58934900	-1.23606800	-0.36235000
H	4.58934900	1.23606800	-0.36235000



X =Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2v}	-15980.8102779	-290.4166

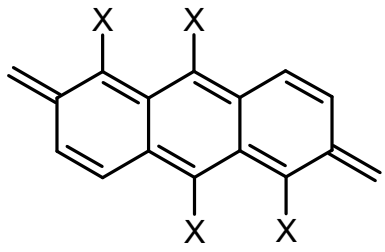
C	-1.22829900	0.73415500	0.03718300
C	0.00000000	1.37920800	0.29476400
C	2.48029100	1.39914400	-0.17739500
C	3.65460400	0.70283100	-0.26693900
C	-3.65460400	0.70283100	-0.26693900
C	0.00000000	-1.37920800	0.29476400
C	-3.65460400	-0.70283100	-0.26693900
C	2.48029100	-1.39914400	-0.17739500
C	1.22829900	-0.73415500	0.03718300
C	-1.22829900	-0.73415500	0.03718300
C	-2.48029100	-1.39914400	-0.17739500
C	-2.48029100	1.39914400	-0.17739500
C	3.65460400	-0.70283100	-0.26693900
C	1.22829900	0.73415500	0.03718300
H	4.58244700	-1.23015000	-0.44221900
H	4.58244700	1.23015000	-0.44221900
H	-4.58244700	1.23015000	-0.44221900
H	-4.58244700	-1.23015000	-0.44221900
Br	2.61378100	-3.25596700	-0.64355600
Br	0.00000000	-2.94016800	1.40144500
Br	-2.61378100	-3.25596700	-0.64355600
Br	-2.61378100	3.25596700	-0.64355600
Br	0.00000000	2.94016800	1.40144500
Br	2.61378100	3.25596700	-0.64355600



X =CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2v}	-775.5550327	-181.4266

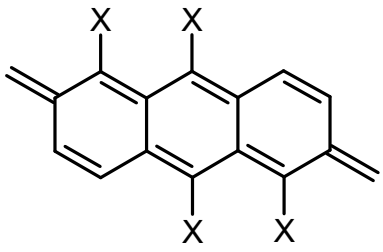
C	-2.47353300	1.43176900	-0.11937500
C	-1.22319400	0.72859100	0.07750600
C	-1.22319400	-0.72859100	0.07750600
C	-2.47353300	-1.43176900	-0.11937500
C	-3.63024100	-0.70407900	-0.22855900
C	-3.63024100	0.70407900	-0.22855900
C	0.00000000	-1.40793600	0.30013800
C	1.22319400	-0.72859100	0.07750600
C	1.22319400	0.72859100	0.07750600
C	0.00000000	1.40793600	0.30013800
C	2.47353300	1.43176900	-0.11937500
C	3.63024100	0.70407900	-0.22855900
C	3.63024100	-0.70407900	-0.22855900
C	2.47353300	-1.43176900	-0.11937500
C	2.57092900	-2.92129200	-0.38419900
C	2.57092900	2.92129200	-0.38419900
C	0.00000000	-2.75583000	1.00312600
C	0.00000000	2.75583000	1.00312600
C	-2.57092900	-2.92129200	-0.38419900
C	-2.57092900	2.92129200	-0.38419900
H	4.56603500	-1.22287400	-0.40968800
H	4.56603500	1.22287400	-0.40968800
H	-4.56603500	-1.22287400	-0.40968800
H	-4.56603500	1.22287400	-0.40968800
H	1.78188400	3.25963500	-1.05937100
H	2.51026900	3.53183100	0.51958100
H	3.52822000	3.14189200	-0.85988900
H	0.87276200	2.82599900	1.65098900
H	0.00000000	3.63305100	0.35268200
H	-0.87276200	2.82599900	1.65098900
H	-2.51026900	3.53183100	0.51958100
H	-1.78188400	3.25963500	-1.05937100
H	-3.52822000	3.14189200	-0.85988900
H	2.51026900	-3.53183100	0.51958100
H	1.78188400	-3.25963500	-1.05937100
H	3.52822000	-3.14189200	-0.85988900
H	0.00000000	-3.63305100	0.35268200
H	0.87276200	-2.82599900	1.65098900
H	-0.87276200	-2.82599900	1.65098900
H	-1.78188400	-3.25963500	-1.05937100
H	-2.51026900	-3.53183100	0.51958100
H	-3.52822000	-3.14189200	-0.85988900



X =Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-2455.4626137	-176.7035

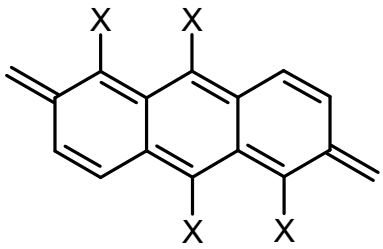
C	-2.47353300	1.43176900	-0.11937500
C	-1.22319400	0.72859100	0.07750600
C	-1.22319400	-0.72859100	0.07750600
C	-2.47353300	-1.43176900	-0.11937500
C	-3.63024100	-0.70407900	-0.22855900
C	-3.63024100	0.70407900	-0.22855900
C	0.00000000	-1.40793600	0.30013800
C	1.22319400	-0.72859100	0.07750600
C	1.22319400	0.72859100	0.07750600
C	0.00000000	1.40793600	0.30013800
C	2.47353300	1.43176900	-0.11937500
C	3.63024100	0.70407900	-0.22855900
C	3.63024100	-0.70407900	-0.22855900
C	2.47353300	-1.43176900	-0.11937500
C	2.57092900	-2.92129200	-0.38419900
C	2.57092900	2.92129200	-0.38419900
C	0.00000000	-2.75583000	1.00312600
C	0.00000000	2.75583000	1.00312600
C	-2.57092900	-2.92129200	-0.38419900
C	-2.57092900	2.92129200	-0.38419900
H	4.56603500	-1.22287400	-0.40968800
H	4.56603500	1.22287400	-0.40968800
H	-4.56603500	-1.22287400	-0.40968800
H	-4.56603500	1.22287400	-0.40968800
H	1.78188400	3.25963500	-1.05937100
H	2.51026900	3.53183100	0.51958100
H	3.52822000	3.14189200	-0.85988900
H	0.87276200	2.82599900	1.65098900
H	0.00000000	3.63305100	0.35268200
H	-0.87276200	2.82599900	1.65098900
H	-2.51026900	3.53183100	0.51958100
H	-1.78188400	3.25963500	-1.05937100
H	-3.52822000	3.14189200	-0.85988900
H	2.51026900	-3.53183100	0.51958100
H	1.78188400	-3.25963500	-1.05937100
H	3.52822000	-3.14189200	-0.85988900
H	0.00000000	-3.63305100	0.35268200
H	0.87276200	-2.82599900	1.65098900
H	-0.87276200	-2.82599900	1.65098900
H	-1.78188400	-3.25963500	-1.05937100
H	-2.51026900	-3.53183100	0.51958100
H	-3.52822000	-3.14189200	-0.85988900



X =Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-10911.1359915	-214.1006

C	-0.00196000	1.42776400	-0.14609100
C	-1.21234900	0.67938800	-0.45405700
C	-2.44924300	-1.46742300	-0.62505500
C	-2.50214100	-2.75864200	-0.26111200
C	1.37105900	3.44234800	0.34894000
C	1.21234900	-0.67938800	-0.45405700
C	2.50214100	2.75864200	-0.26111200
C	-0.11029500	-2.70312600	0.35545100
C	0.00196000	-1.42776400	-0.14609100
C	1.24514200	0.68840000	-0.43445000
C	2.44924300	1.46742300	-0.62505500
C	0.11029500	2.70312600	0.35545100
C	-1.37105900	-3.44234800	0.34894000
C	-1.24514200	-0.68840000	-0.43445000
H	-3.42157300	-3.32192200	-0.37243600
H	3.42157300	3.32192200	-0.37243600
C	-1.53649000	-4.69479700	0.83668400
C	1.53649000	4.69479700	0.83668400
H	-0.73772700	-5.24541900	1.31009700
H	-2.50157700	-5.17949900	0.75646700
H	2.50157700	5.17949900	0.75646700
H	0.73772700	5.24541900	1.31009700
H	3.32527800	0.97024600	-1.01537200
H	-3.32527800	-0.97024600	-1.01537200
Br	-2.74363500	1.62016000	-1.14318500
Br	-1.37105900	3.58660600	1.18888200
Br	2.74363500	-1.62016000	-1.14318500
Br	1.37105900	-3.58660600	1.18888200

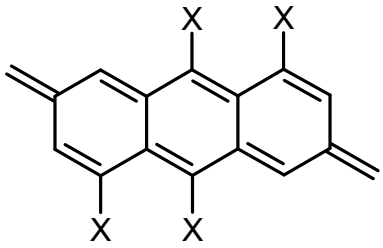


X =CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-774.2913787	-144.9802

C	-3.61398400	0.88452800	-0.19327800
C	-2.43979700	1.47310500	-0.48001700
C	-1.18411200	0.76424200	-0.33953000
C	-1.25352900	-0.68472100	-0.10188600
C	-2.43979700	-1.25712400	0.32098700
C	-3.68594800	-0.48635700	0.28388400
C	0.02146600	1.42468400	-0.37148300
C	-0.02146600	-1.42468400	-0.37148300
C	1.18411200	-0.76424200	-0.33953000
C	1.25352900	0.68472100	-0.10188600
C	2.43979700	1.25712400	0.32098700
C	3.68594800	0.48635700	0.28388400
C	3.61398400	-0.88452800	-0.19327800

C	2.43979700	-1.47310500	-0.48001700
H	-4.54280800	1.43846100	-0.27933000
H	4.54280800	-1.43846100	-0.27933000
C	0.07563300	2.87867200	-0.80434600
H	-0.59431500	3.04275900	-1.65087000
H	-0.22098800	3.58079100	-0.01800900
H	1.07527600	3.15262500	-1.13439800
C	-0.07563300	-2.87867200	-0.80434600
H	0.22098800	-3.58079100	-0.01800900
H	0.59431500	-3.04275900	-1.65087000
H	-1.07527600	-3.15262500	-1.13439800
C	4.89369300	1.00097100	0.63533800
C	-4.89369300	-1.00097100	0.63533800
H	5.02542400	2.01129300	0.99516100
H	5.78832100	0.39530200	0.55269100
H	-5.78832100	-0.39530200	0.55269100
H	-5.02542400	-2.01129300	0.99516100
C	2.53076000	2.64873200	0.89993000
H	3.04580100	3.35333200	0.23651800
H	1.55713800	3.05913000	1.14824200
H	3.10700900	2.61249800	1.82876000
C	-2.53076000	-2.64873200	0.89993000
H	-3.04580100	-3.35333200	0.23651800
H	-1.55713800	-3.05913000	1.14824200
H	-3.10700900	-2.61249800	1.82876000
H	2.42636600	-2.51346500	-0.77635000
H	-2.42636600	2.51346500	-0.77635000

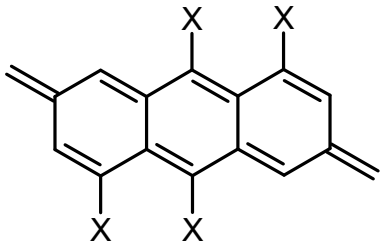


X =Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-2455.4659839	-178.4403

Cl	-2.77242600	1.49930800	-0.25377500
Cl	-1.17248800	3.81530200	1.07444400
Cl	1.17248800	-3.81530200	1.07444400
Cl	2.77242600	-1.49930800	-0.25377500
C	1.21935300	0.73133400	-0.18493100
C	1.20726800	-0.72150000	-0.10316900
C	-0.08366300	-2.88940100	0.25711600
C	-1.21935300	-3.55618800	-0.02484100
C	2.40342900	2.87126200	-0.50237800
C	-1.20726800	0.72150000	-0.10316900
C	1.21935300	3.55618800	-0.02484100
C	-2.35436400	-1.43101600	-0.47752200
C	-1.21935300	-0.73133400	-0.18493100
C	-0.05492200	1.44742900	0.02456100
C	0.08366300	2.88940100	0.25711600
C	2.35436400	1.43101600	-0.47752200
C	-2.40342900	-2.87126200	-0.50237800
C	0.05492200	-1.44742900	0.02456100
H	-1.27343000	-4.62112200	0.16211800

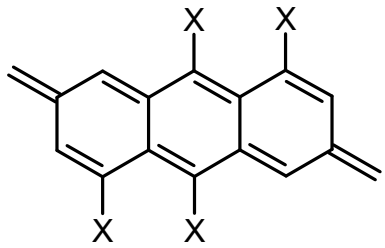
H	1.27343000	4.62112200	0.16211800
C	-3.51722600	-3.54762700	-0.87932300
C	3.51722600	3.54762700	-0.87932300
H	-4.40967000	-3.02467400	-1.20036900
H	-3.54844000	-4.63018100	-0.87450000
H	3.54844000	4.63018100	-0.87450000
H	4.40967000	3.02467400	-1.20036900
H	3.26722400	0.89695100	-0.69569800
H	-3.26722400	-0.89695100	-0.69569800



X =Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-10911.1402212	-215.6564

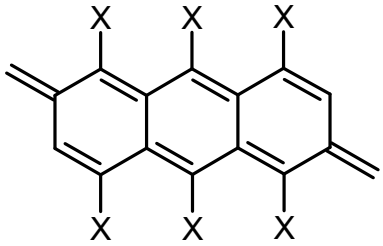
C	-1.37655100	-0.33722600	-0.40639000
C	-0.94139900	1.04727900	-0.29924300
C	0.94139900	2.71454100	0.14317200
C	2.19966000	3.04024400	-0.20753700
C	-3.09208000	-2.06378000	-0.80598400
C	0.94139900	-1.04727900	-0.29924300
C	-2.19966000	-3.04024400	-0.20753700
C	2.64031100	0.69388500	-0.77579100
C	1.37655100	0.33722600	-0.40639000
C	-0.37151400	-1.39307300	-0.14332000
C	-0.94139900	-2.71454100	0.14317200
C	-2.64031100	-0.69388500	-0.77579100
C	3.09208000	2.06378000	-0.80598400
C	0.37151400	1.39307300	-0.14332000
H	2.58946700	4.02423700	0.01966600
H	-2.58946700	-4.02423700	0.01966600
C	4.31466500	2.41025000	-1.27826300
C	-4.31466500	-2.41025000	-1.27826300
H	4.99238100	1.66769700	-1.68141900
H	4.65058500	3.43990400	-1.27172700
H	-4.65058500	-3.43990400	-1.27172700
H	-4.99238100	-1.66769700	-1.68141900
H	-3.35014700	0.07304300	-1.04993600
H	3.35014700	-0.07304300	-1.04993600
Br	2.31091400	-2.37560800	-0.49743800
Br	-0.03117600	-3.99364700	1.25811100
Br	-2.31091400	2.37560800	-0.49743800
Br	0.03117600	3.99364700	1.25811100



X =CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-774.2965139	-142.2557

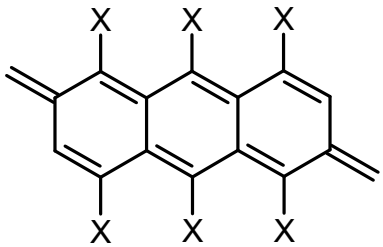
C	-1.30651600	3.49252600	0.21293900
C	-0.10132400	2.88467500	0.30902600
C	0.02260700	1.44380900	0.00832400
C	-1.23306200	0.68859800	-0.14086300
C	-2.41749900	1.36612400	-0.26360200
C	-2.52270600	2.79902900	-0.15682000
C	1.21007200	0.77109400	-0.17044000
C	-1.21007200	-0.77109400	-0.17044000
C	-0.02260700	-1.44380900	0.00832400
C	1.23306200	-0.68859800	-0.14086300
C	2.41749900	-1.36612400	-0.26360200
C	2.52270600	-2.79902900	-0.15682000
C	1.30651600	-3.49252600	0.21293900
C	0.10132400	-2.88467500	0.30902600
H	-1.39192300	4.54397700	0.47043300
H	1.39192300	-4.54397700	0.47043300
C	2.52270600	1.46674500	-0.45146200
H	2.38408200	2.50552400	-0.72401500
H	3.22335500	1.41905400	0.38948600
H	3.01154200	0.98750200	-1.30304200
C	-2.52270600	-1.46674500	-0.45146200
H	-3.22335500	-1.41905400	0.38948600
H	-2.38408200	-2.50552400	-0.72401500
H	-3.01154200	-0.98750200	-1.30304200
C	3.70040900	-3.45230500	-0.33222600
C	-3.70040900	3.45230500	-0.33222600
H	4.60934000	-2.91908900	-0.58432500
H	3.76860900	-4.52870800	-0.22988000
H	-3.76860900	4.52870800	-0.22988000
H	-4.60934000	2.91908900	-0.58432500
C	-1.04230400	-3.70903200	0.87265100
H	-1.68877800	-3.11711900	1.52228300
H	-1.67214700	-4.15804700	0.09997200
H	-0.63441200	-4.52867300	1.46706200
C	1.04230400	3.70903200	0.87265100
H	1.68877800	3.11711900	1.52228300
H	1.67214700	4.15804700	0.09997200
H	0.63441200	4.52867300	1.46706200
H	3.33980500	-0.82864200	-0.43312600
H	-3.33980500	0.82864200	-0.43312600



X =Cl

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-3374.6715005	-215.4191

Cl	-3.07109600	0.15382800	-0.75588600
Cl	-2.59435500	-2.81634600	-1.75444700
Cl	-2.69824400	2.23363800	1.59242600
Cl	2.69824400	-2.23363800	1.59242600
Cl	2.59435500	2.81634600	-1.75444700
Cl	3.07109600	-0.15382800	-0.75588600
C	0.67755600	-1.20370700	0.07073200
C	1.39771000	0.02283000	-0.28798100
C	1.29053300	2.55281100	-0.60952300
C	0.74911000	3.63132300	-0.02093300
C	0.42045100	-3.53775900	0.84022600
C	-1.39771000	-0.02283000	-0.28798100
C	-0.74911000	-3.63132300	-0.02093300
C	-1.16715000	2.28271500	0.75021800
C	-0.67755600	1.20370700	0.07073200
C	-0.74911000	-1.21971200	-0.33679000
C	-1.29053300	-2.55281100	-0.60952300
C	1.16715000	-2.28271500	0.75021800
C	-0.42045100	3.53775900	0.84022600
C	0.74911000	1.21971200	-0.33679000
H	1.17496100	4.61148600	-0.19214200
H	-1.17496100	-4.61148600	-0.19214200
C	-0.79606900	4.59479700	1.59302600
C	0.79606900	-4.59479700	1.59302600
H	-1.67107800	4.57122300	2.22545700
H	-0.21283700	5.50687000	1.57724500
H	0.21283700	-5.50687000	1.57724500
H	1.67107800	-4.57122300	2.22545700

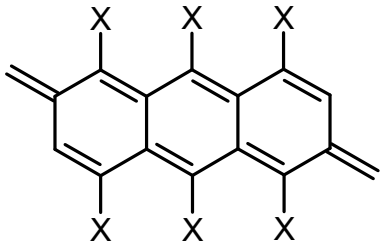


X =Br

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-16058.1843359	-271.6301

C	1.31659400	-0.35026700	0.21377500
C	0.95852200	1.01661200	-0.19234000
C	-0.95852200	2.68590100	-0.53659400
C	-2.05640300	3.06178100	0.13798300

C	2.71124600	-2.17994100	1.10118000
C	-0.95852200	-1.01661200	-0.19234000
C	2.05640300	-3.06178100	0.13798300
C	-2.36136300	0.76087900	0.98540100
C	-1.31659400	0.35026700	0.21377500
C	0.34808700	-1.38648900	-0.24659300
C	0.95852200	-2.68590100	-0.53659400
C	2.36136300	-0.76087900	0.98540100
C	-2.71124600	2.17994100	1.10118000
C	-0.34808700	1.38648900	-0.24659300
H	-2.49993300	4.03410200	-0.03324200
H	2.49993300	-4.03410200	-0.03324200
C	-3.62808900	2.68232600	1.95471900
C	3.62808900	-2.68232600	1.95471900
H	-4.15587200	2.06271800	2.66483100
H	-3.85597400	3.74097100	1.94506300
H	3.85597400	-3.74097100	1.94506300
H	4.15587200	-2.06271800	2.66483100
Br	-3.41351300	-0.46739400	2.00503000
Br	-0.33961600	3.84362400	-1.93385300
Br	2.38707000	2.13530800	-0.78780100
Br	3.41351300	0.46739400	2.00503000
Br	0.33961600	-3.84362400	-1.93385300
Br	-2.38707000	-2.13530800	-0.78780100



X =CH_3

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_2	-852.9244187	-161.4103

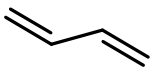
C	1.31659400	-0.35026700	0.21377500
C	0.95852200	1.01661200	-0.19234000
C	-0.95852200	2.68590100	-0.53659400
C	-2.05640300	3.06178100	0.13798300
C	2.71124600	-2.17994100	1.10118000
C	-0.95852200	-1.01661200	-0.19234000
C	2.05640300	-3.06178100	0.13798300
C	-2.36136300	0.76087900	0.98540100
C	-1.31659400	0.35026700	0.21377500
C	0.34808700	-1.38648900	-0.24659300
C	0.95852200	-2.68590100	-0.53659400
C	2.36136300	-0.76087900	0.98540100
C	-2.71124600	2.17994100	1.10118000
C	-0.34808700	1.38648900	-0.24659300
H	-2.49993300	4.03410200	-0.03324200
H	2.49993300	-4.03410200	-0.03324200
C	-3.62808900	2.68232600	1.95471900
C	3.62808900	-2.68232600	1.95471900
H	-4.15587200	2.06271800	2.66483100
H	-3.85597400	3.74097100	1.94506300
H	3.85597400	-3.74097100	1.94506300
H	4.15587200	-2.06271800	2.66483100

Br	-3.41351300	-0.46739400	2.00503000
Br	-0.33961600	3.84362400	-1.93385300
Br	2.38707000	2.13530800	-0.78780100
Br	3.41351300	0.46739400	2.00503000
Br	0.33961600	-3.84362400	-1.93385300
Br	-2.38707000	-2.13530800	-0.78780100

$CH_2=CH_2$

Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
D_{2h}	-78.6139783	-16.2679

C	0.00000000	0.00000000	0.66347700
H	0.00000000	0.92251300	1.23466300
H	0.00000000	-0.92251300	1.23466300
C	0.00000000	0.00000000	-0.66347700
H	0.00000000	-0.92251300	-1.23466300
H	0.00000000	0.92251300	-1.23466300



Point Group	Total Energy [Hartree]	Magnetic susceptibility [cgs-ppm]
C_{2h}	-156.0385032	-29.098

C	0.60104400	1.74765600	0.00000000
H	1.52250800	2.31733600	0.00000000
H	-0.32522900	2.31382500	0.00000000
C	0.60104400	0.41079900	0.00000000
H	0.32522900	-2.31382500	0.00000000
C	-0.60104400	-1.74765600	0.00000000
H	-1.52250800	-2.31733600	0.00000000
C	-0.60104400	-0.41079900	0.00000000
H	1.54951700	-0.12277400	0.00000000
H	-1.54951700	0.12277400	0.00000000