Supporting Information for

Aromaticity and Antiaromaticity in 4-, 6-, 8- and 10-Membered Conjugated Hydrocarbon Rings

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Contents

Table S1. Cartesian coordinates (in Å), point-group symmetry, total energy relative to ADF's basic atoms and number of imaginary frequencies (Nimag) of species occurring in this study, optimized at BP86/TZ2P.

C_6H_6 (D_{6h})	–1728.98 kcal/mol			Nimag = 0
C	0.000000	1.397664	0.000000	
H	0.000000	2.487887	0.000000	
C	0.000000	-1.397664	0.000000	
H	0.000000	-2.487887	0.000000	
C	1.210412	0.698832	0.000000	
H	2.154573	1.243944	0.000000	
C	1.210412	-0.698832	0.000000	
H	2.154573	-1.243944	0.000000	
C	-1.210412	-0.698832	0.000000	
H	-2.154573	-1.243944	0.000000	
C	-1.210412	0.698832	0.000000	
H	-2.154573	1.243944	0.000000	

C_4H_4 (D_{2h})	–1058.45 kcal/mol			Nimag = 0
C	0.669158	0.790718	0.000000	
H	1.440025	1.557704	0.000000	
C	0.669158	-0.790718	0.000000	
H	1.440025	-1.557704	0.000000	
C	-0.669158	-0.790718	0.000000	
H	-1.440025	-1.557704	0.000000	
C	-0.669158	0.790718	0.000000	
H	-1.440025	1.557704	0.000000	

$C_4H_4^{¨}$ (D_{4h})	–1053.26 kcal/mol			Nimag = 0
C	1.021041	0.000000	0.000000	
H	2.106901	0.000000	0.000000	
C	0.000000	1.021041	0.000000	
H	0.000000	2.106901	0.000000	
C	-1.021041	0.000000	0.000000	
H	-2.106901	0.000000	0.000000	
C	0.000000	-1.021041	0.000000	
H	0.000000	-2.106901	0.000000	

C_8H_8 (D_{4h})	–2245.86 kcal/mol			Nimag = 1 (*i*146 cm^{-1})
C	0.674787	-1.718083	0.000000	
C	1.718083	-0.674787	0.000000	
H	2.719144	-1.113031	0.000000	
C	-0.674787	-1.718083	0.000000	
H	1.113031	-2.719144	0.000000	
C	-1.718083	-0.674787	0.000000	
H	-1.113031	-2.719144	0.000000	
H	-2.719144	-1.113031	0.000000	
C	-1.718083	0.674787	0.000000	
C	0.674787	1.718083	0.000000	
H	1.113031	2.719144	0.000000	
C	1.718083	0.674787	0.000000	
H	2.719144	1.113031	0.000000	
H	-2.719144	1.113031	0.000000	
C	-0.674787	1.718083	0.000000	
H	-1.113031	2.719144	0.000000	

C_8H_8 (D_{2d})	–2255. 53 kcal/mol			Nimag = 0
C	1.586822	-0.635770	0.370496	
C	1.586822	0.635770	-0.370496	
H	2.512127	0.852781	-0.914076	
C	0.635770	-1.586822	0.370496	
H	2.512127	-0.852781	0.914076	
C	-0.635770	-1.586822	-0.370496	
H	0.852781	-2.512127	0.914076	
H	-0.852781	-2.512127	-0.914076	
C	-1.586822	-0.635770	-0.370496	
C	-0.635770	1.586822	0.370496	
H	-0.852781	2.512127	0.914076	
C	0.635770	1.586822	-0.370496	
H	0.852781	2.512127	-0.914076	
H	-2.512127	-0.852781	-0.914076	
C	-1.586822	0.635770	0.370496	
H	-2.512127	0.852781	0.914076	

$C_8H_8^{\cdot\cdot}$ (D_{8h})	–2243.53 kcal/mol			Nimag = 0
C	0.703723	1.698938	0.000000	
C	1.698938	0.703723	0.000000	
H	2.708407	1.121859	0.000000	
C	-0.703723	1.698938	0.000000	
H	1.121859	2.708407	0.000000	
C	-1.698938	0.703723	0.000000	
H	-1.121859	2.708407	0.000000	
H	-2.708407	1.121859	0.000000	
C	-1.698938	-0.703723	0.000000	
C	0.703723	-1.698938	0.000000	
H	1.121859	-2.708407	0.000000	
C	1.698938	-0.703723	0.000000	
H	2.708407	-1.121859	0.000000	
H	-2.708407	-1.121859	0.000000	
C	-0.703723	-1.698938	0.000000	
H	-1.121859	-2.708407	0.000000	

$C_{10}H_{10}$ (D_{10h})	–2804.10 kcal/mol		Nimag = 2 (*i*68 cm^{-1})
C	2.271236	0.000000	0.000000
C	0.701850	2.160074	0.000000
C	-1.837468	1.334999	0.000000
C	-1.837468	-1.334999	0.000000
C	0.701850	-2.160074	0.000000
C	1.837468	1.334999	0.000000
C	-0.701850	2.160074	0.000000
C	-2.271236	0.000000	0.000000
C	-0.701850	-2.160074	0.000000
C	1.837468	-1.334999	0.000000
H	3.365153	0.000000	0.000000
H	1.039889	3.200450	0.000000
H	-2.722466	1.977987	0.000000
H	-2.722466	-1.977987	0.000000
H	1.039889	-3.200450	0.000000
H	2.722466	1.977987	0.000000
H	-1.039889	3.200450	0.000000
H	-3.365153	0.000000	0.000000
H	-1.039889	-3.200450	0.000000
H	2.722466	-1.977987	0.000000

$C_{10}H_{10}$ (C_2)	–2807.48 kcal/mol		Nimag = 0
C	2.164694	0.041426	-0.283916
C	0.620966	2.019657	0.501235
C	-1.690331	1.254944	-0.526890
C	-1.767166	-1.226940	0.352331
C	0.670278	-2.086032	-0.042101
C	1.767166	1.226940	0.352331
C	-0.670278	2.086032	-0.042101
C	-2.164694	-0.041426	-0.283916
C	-0.620966	-2.019657	0.501235
C	1.690331	-1.254944	-0.526890
H	3.224215	0.103529	-0.556179
H	0.879510	2.968788	0.980456
H	-2.457977	1.850164	-1.030126
H	-2.648443	-1.782853	0.690118
H	0.998436	-3.131313	-0.082433
H	2.648443	1.782853	0.690118
H	-0.998436	3.131313	-0.082433
H	-3.224215	-0.103529	-0.556179
H	-0.879510	-2.968788	0.980456
H	2.457977	-1.850164	-1.030126