Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information for

All-Metal Aromatic Clusters M_4^{2-} (M = B, Al, and Ga). Are π-Electrons Distortive or Not?

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Table S1. Bond-energy decomposition (in kcal/mol) of all-metal clusters B_4^{2-}, Al_4^{2-} and Ga_4^{2-} and the organic systems C_4H_4, $C_4H_4^{2+}$ and $C_4H_4^{2-}$ constructed from two equivalent rigid fragments as defined in Figure 1, computed at BP86/TZ2P.

	B_4^{2-}	Al_4^{2-}	Ga_4^{2-}	C_4H_4	$C_4H_4^{2+}$	$C_4H_4^{2-}$
$\Delta E_{oi}(\sigma)$	-710.03	-180.11	-153.34	-747.36	-827.42	-707.02
$\Delta E_{oi}(\pi)$	-65.47	-26.83	-24.64	-108.53	-121.41	-325.22
ΔE_{oi}	-775.51	-206.96	-177.98	-855.87	-948.83	-1032.25
ΔE_{Pauli}	784.44	245.15	250.45	665.37	684.66	549.92
ΔV_{elstat}	-211.43	-110.38	-128.62	-438.33	-257.36	-286.90
ΔE_{int}	-202.49	-72.18	-56.15	-628.83	-521.53	-769.23
R(X-X)	1.657	2.603	2.641	1.582 1.338	1.452	1.478
θ	90.0	90.0	90.0	99.5	90.0	90.0

Table S2. Cartesian coordinates (in Å) of all stationary points occurring in this study, computed at BP86/TZ2P.

B_4^{2-}

B	1.171683	0.000000	0.000000
B	0.000000	1.171683	0.000000
B	-1.171683	0.000000	0.000000
B	0.000000	-1.171683	0.000000

Al_4^{2-}

Al	1.840918	0.000000	0.000000
Al	0.000000	1.840918	0.000000
Al	-1.840918	0.000000	0.000000
Al	0.000000	-1.840918	0.000000

Ga_4^{2-}

Ga	1.321174	1.321174	0.000000
Ga	1.321174	-1.321174	0.000000
Ga	-1.321174	-1.321174	0.000000
Ga	-1.321174	1.321174	0.000000

C_4H_4

C	0.000000	-1.021364	0.000000
C	1.021364	0.000000	0.000000
C	0.000000	1.021364	0.000000
C	-1.021364	0.000000	0.000000
H	-2.106958	0.000000	0.000000
H	0.000000	2.106958	0.000000
H	2.106958	0.000000	0.000000
H	0.000000	-2.106958	0.000000

$C_4H_4^{2-}$

C	0.739130	0.739130	0.000000
H	1.519701	1.519701	0.000000
C	0.739130	-0.739130	0.000000
H	1.519701	-1.519701	0.000000
C	-0.739130	-0.739130	0.000000
H	-1.519701	-1.519701	0.000000
C	-0.739130	0.739130	0.000000
H	-1.519701	1.519701	0.000000

$C_4H_4^{2+}$

C	1.026470	0.000000	0.000000
H	2.128695	0.000000	0.000000
C	0.000000	1.026470	0.000000
H	0.000000	2.128695	0.000000
C	-1.026470	0.000000	0.000000
H	-2.128695	0.000000	0.000000
C	0.000000	-1.026470	0.000000
H	0.000000	-2.128695	0.000000