# Electronic supplementary information

# MODERN CRITERIA OF AROMATICITY FOR ORGANOMETALLIC COMPOUNDS

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## Computation and visualization details for the NICS-scan, ACID, GIMIC, and EDDB results

To compute the NICS dependence on the distance $R$, the virtual Bq atoms were placed under the ring center with 0.1 Å separation for $R = 0 \div 2$ Å and 0.25 Å for $R = 2 \div 5$ Å. The geometry optimization and subsequent calculation of the magnetic shielding constants ($\sigma$) for a set of the Bq atoms were performed at the recommended [S1] GIAO-B3LYP level of theory with the Def2-TZVP [S2] basis set using the Gaussian program [S3]. The NICS-scan curves for benzene, cyclobutadiene, and cyclohexa-1,3-diene (Fig. 4 in the main text) were plotted using OriginPro [S4], where $NICS_{iso} = -\sigma_{iso}$, $NICS_{in-plane} = -\frac{1}{3}(\sigma_{xx} + \sigma_{yy})$, and $NICS_{zz} = NICS_{out-of-plane} = -\frac{1}{3}\sigma_{zz}$. The correlation $NICS_{in-plane}$ and $NICS_{out-of-plane}$ components named $NICS_{in-out}$ (Figs. 4 and 17) were plotted for each Bq atom in the series using OriginPro.

The results of the ACID and GIMIC methods (Figs. 11–13) were performed at the recommended [S5] GIAO-B3LYP/Def2-TZVP level of theory using Gaussian. Since the magnetic current distribution depends on the direction of the external magnetic field, the latter is accepted to choose as a normal to the ring plane ($Z$ axis). NoSymm and Int(NoBasisTransform) commands were used to avoid the possible molecule reorientation and the basis set transformation, respectively. The basis set and magnetic shielding matrix were extracted from the FormCHK output file of Gaussian and converted using Gaussian2gimic.py script [S6] to the format (MOL and XDENS files) suitable for the GIMIC calculation. The ACID function and IC distribution were calculated using the GIMIC 2.0 program [S5]. The isosurfaces of the ACID (Fig. 11) and the signed-modulus of the ICs (Jmod) (Fig. 12) being in the VTK format (acid.vti and jmod.vti files) were visualized using Paraview (version 5.6) [S7]. The IC distribution presented as vector map and streamlines (Fig. 13) were obtained using the Glyph and Streamline modules implemented in Paraview, the parameters were adopted for the best view.

The geometry optimization and subsequent EDDB analysis were performed for benzene and germylene **1Ge** [S8] at the PBE0/Def2-TZVP level using Gaussian. The additional commands Pop(NBORead) and Density=Current for Gaussian and also the command set $NBO SKIPBO FILE=molecule_name DMNAO=W49 AONAO=W49 $END for built-in NBO v3.1 module were used. The application of the new NBO program version [S9] is not needed. The EDDB analysis was performed using the RunEDDB script [S10]. The visualization of the NODB orbitals for benzene (Fig. 5) was done using the Avogadro program [S11] with default settings. For plotting the EDDB(**r**) isosurface with a set of

isovalues using Paraview, the RunEDDB FCHK output files were recalculated to the Cub-format using the standard Cubgene utility and converted to the VTK-format using MultiWFN [S12].

**References**

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