Electronic Supplementary Information for Dalton Transactions
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Supramolecular structures from mono and dimetalated biscarbene ligands

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Supporting Information

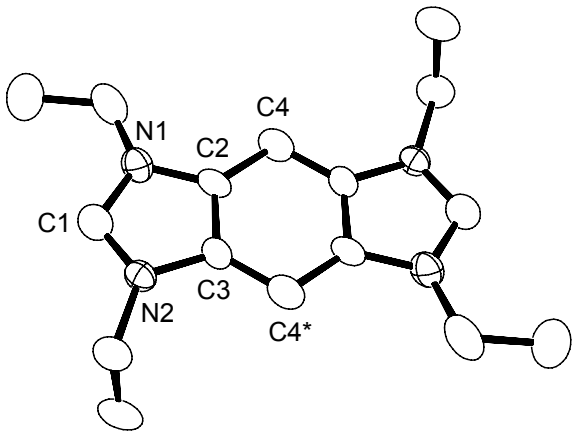

Fig. S1 Molecular structure of the benzobisimidazolium cation in **1b**. Anions and solvent molecules have been omited. The cation resides on crystallographic inversion center located in the center of the central phenyl ring. Selected bond lengths (Å) and bond angles (°): N1–C1 1.348(10), N2–C1 1.326(10), N1–C1–C2 111.0(9).

X- ray diffraction data were collected with a Bruker AXS APEX diffractometer equipped with a rotation anode at 153(2) K using graphite monochromated Cu-Kα radiation, λ = 1.54178 Å). Diffraction data were collected over the full sphere and were corrected for absorption.
Crystal data for 1b. Formula $C_{16}H_{24}N_4Br$, M = 432.21, colorless crystal, 0.12 × 0.06 × 0.03 mm, monoclinic, space group $P2_1/n$, a = 5.1257(7), b = 14.067(2), c = 12.839(2), β = 100.602(8), V = 909.6(2) Å^3, ρ_{calc} = 1.578 g cm^{-3}, μ = 5.661 mm^{-1}, ω- and ϕ-scans, 4364 measured intensities (9.4 ≤ 2θ ≤ 143.5°), semiempirical absorption correction (0.5499 ≤ T ≤ 0.8485), 1547 independent (R_{int} = 0.1170) and 733 observed ($I \geq 2\sigma(I)$) intensities, Z = 2, R = 0.0734, wR = 0.1506, refinement of 102 parameters against all $|F^2|$ with H atoms on calculated positions. The cation of **1b** resides on a crystallographic inversion center. The asymmetric asymmetric unit contains 0.5 of the one formula unit of **1b**.