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Supporting information for article:

Crystal structures and spectroscopic characterization of *M*Br2(CNXyl)*n* (*M* = Fe and Co, *n* = 4; *M* = Ni, *n* = 2; Xyl = 2,6-dimethylphenyl), and of formally zero-valent iron as a cocrystal of Fe(CNXyl)5 and Fe2(CNXyl)9

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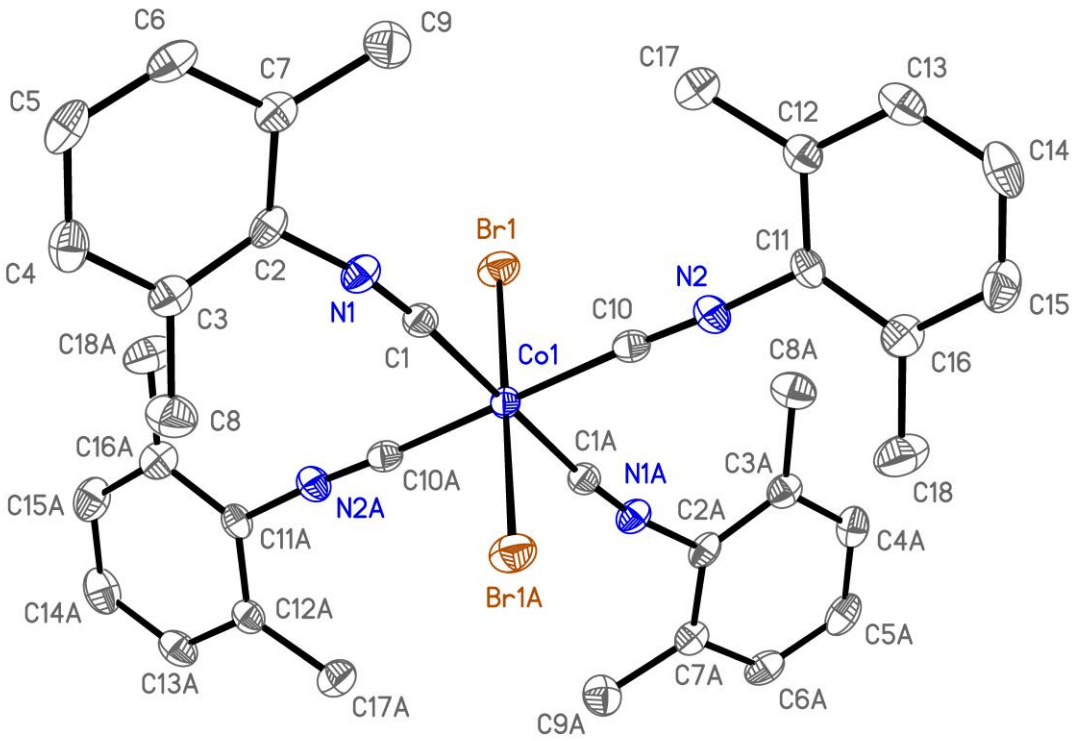

Fig. S1 Anisotropic displacement ellipsoid plot of **4**, drawn at the 50% probability level and with H atoms omitted. The symmetry-equivalent portion is generated by the inversion operation (-x, -y + 1, -z + 1) (symmetry code A).