Electronic supplementary materials *Mendeleev Commun.*, 2011, **21**, 82–83

Convenient synthesis of the ruthenium complexes CpRu(diene)X (X = Cl, Br, I) by naphthalene substitution in $[CpRu(C_{10}H_8)]^+$

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Details of X-ray diffraction data collection.

Single-crystal of **2b** was grown by slow evaporation of its solution in CH_2Cl_2:hexane mixture. X-ray diffraction data were collected using a Bruker APEX2 CCD diffractometer [λ(MoKα) = 0.71073 Å, graphite monochromator]. The obtained images were integrated[i]. The precise unit cell dimensions and errors were determined. The absorption correction was applied semiempirically using the SADABS program[ii]. Crystals of **2b** ($C_{12}H_{13}BrRu$, M = 338.20) are tetragonal, space group P–421c, at 100(2) K: a = 12.248(9), c = 13.892(9) Å, V = 2084(2) Å^3, Z = 8, d_{calc} = 2.156 g·cm^{-3}, μ(MoKα) = 5.292 cm^{-1}, F(000) = 1312. Intensities of 8097 reflections were measured and 2764 independent reflections [R_{int} = 0.0522] were used in further refinement. Initially spherical atom refinements were undertaken with SHELXTL PLUS 5.0[iii] using the full-matrix least-squares method. All non-hydrogen atoms were allowed to have an anisotropic thermal motion. The refinement converged to wR2 = 0.0645 and GOF = 0.916 for all independent reflections (R1 = 0.0322 was calculated against F for 2479 observed reflections with $I > 2\sigma(I)$). Atomic coordinates, bond lengths, angles, and thermal parameters have been deposited at the Cambridge Crystallographic Data Center (CCDC) with number 800299.

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[i]. Bruker (2001) *SAINT-Plus* Bruker AXS Inc., Madison, Wisconsin, USA.
[ii]. G.M. Sheldrick, *SADABS*, Bruker AXS Inc., Madison,WI-53719, 1997.
[iii]. G.M. Sheldrick, *Acta Crystallogr.*, 2008, **A64**, 112.