ESI

Towards high-valent uranium compounds from metallacyclic uranium(IV) precursors

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Crystallography measurements details

Data were collected at 150(2) K on a Nonius Kappa-CCD area-detector diffractometer and processed with HKL2000.¹ Absorption effects were corrected with SCALEPACK.¹ The structures were solved by direct methods and refined by full-matrix least-squares on F^2 with SHELXTL.² All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were introduced at calculated positions. In **5b**·0.5*n*-pentane, the pentane solvent molecules have been given 0.5 occupancy factors in order to retain acceptable displacement parameters, and they were refined with restraints on bond lengths and angles. The absolute configuration in **5b**·0.5*n*-pentane was determined from the value of the Flack parameter [-0.008(6)]. The highest residual electron density peak in **6** is located near atom I(2).

1 Z. Otwinowski and W. Minor, *Methods Enzymol.*, 1997, 276, 307.

2 G. M. Sheldrick, *Acta Crystallogr.*, *Section A*, 2008, **64**, 112.