Magnesium(I) Reduction of Benzophenone and Anthracene: First Structural Characterisation of a Magnesium Ketyl

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SUPPLEMENTARY INFORMATION

X-Ray Crystallography

Crystals of both compounds suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were made using an Nonius Kappa CCD diffractometer. The structures were solved by direct methods and refined on F^2 by full matrix least squares (SHELX97[1]) using all unique data. Hydrogen atoms were refined in calculated positions (riding model). Two crystallographically independent molecules were refined in the asymmetric unit of **2**. There are no significant geometric differences between them. The relatively high r-factors for the crystal structures of both complexes resulted from weak diffraction data collected above a theta angle of *ca.* 22° in each case. Despite this, the gross molecular connectivity determined for the compounds is unambiguous.

EPR Spectroscopy

The continuous wave EPR spectrum (298 K) of **1** was recorded on an X-band Bruker EMX spectrometer operating at 100kHz field modulation in an ER 4119HS cavity. The spectrum was calibrated with DPPH and the g-values were determined by simulation using the commercial Bruker SIMFONIA software

1. G.M. Sheldrick, *SHELX-97*, University of Göttingen, 1997.