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Ruthenium biimidazole complexes as anion receptors

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X-ray crystallographic studies of the adducts [RuCl(cym)(H_2biim)]$^+\cdot Cl^-$ and [RuCl(cym)(H_2biim)]$^+\cdot NO_3^-$

Crystals of the adducts [RuCl(cym)(H_2biim)]$^+\cdot Cl^-$ and [RuCl(cym)(H_2biim)]$^+\cdot NO_3^-$ were mounted directly from solution under argon using an inert oil which protects them from atmospheric oxygen and moisture. X-ray intensity data were collected using a Nonius Kappa CCD diffractometer. The structures were solved by direct methods and refined by full-matrix least squares on F^2.[1] The structure of adduct [RuCl(cym)(H_2biim)]$^+\cdot Cl^-$ contains two molecules per asymmetric unit. One of the chloride anions [Cl(2)] exhibited disorder and was resolved into two components of *ca*. 75:25 occupancy. Within the lattice of [RuCl(cym)(H_2biim)]$^+\cdot Cl^-$ there are also two half molecules of dichloromethane and a total of two molecules of water per equivalent position. In addition there is residual electron density of *ca*. three electrons in a chemically unreasonable position possibly due to a small amount of a cocrystalised contaminant. All the hydrogen atoms of the adducts [RuCl(cym)(H_2biim)]$^+\cdot Cl^-$ and [RuCl(cym)(H_2biim)]$^+\cdot NO_3^-$ were included in idealised positions.

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

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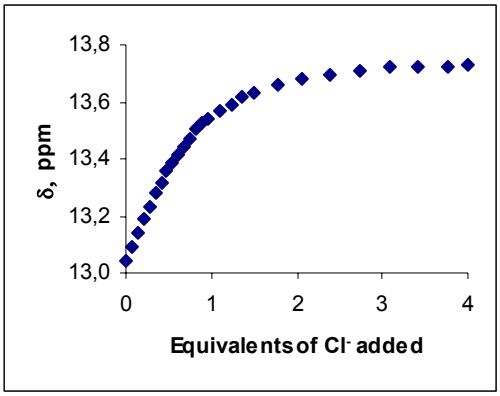
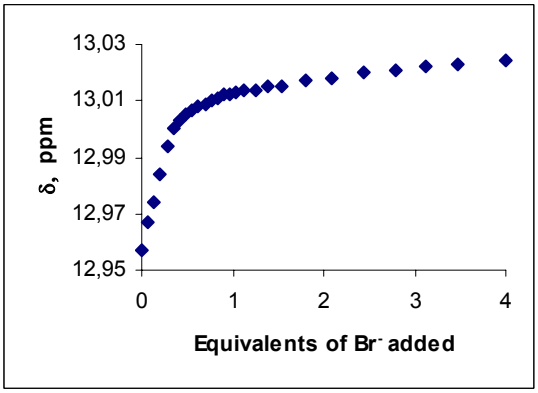
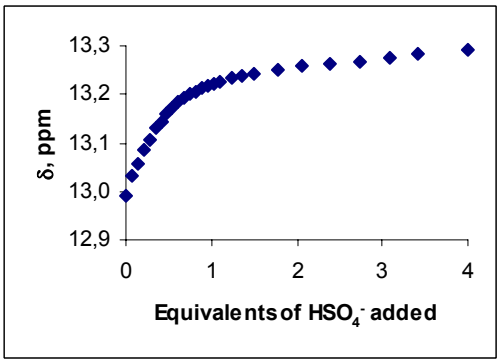
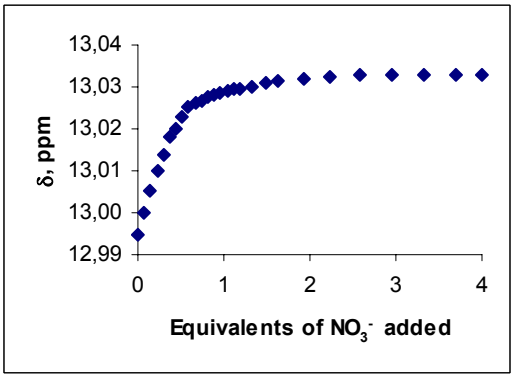
^{1}H NMR titration profiles of 1 in DMSO-d_6.









^{1}H NMR titration profiles of 1 in CD_3CN.