

Synthesis and catalytic application of palladium imidazol(in)ium-2-dithiocarboxylate complexes

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The X-ray crystal structure of **2**

Both of the included dichloromethane solvent molecules in the structure of **2** were found to be disordered. For the C(70)-based molecule, two orientations of *ca.* 87 and 13% occupancy were identified, whilst for the C(80)-based molecule (which was found to be situated adjacent to a centre of symmetry) two unique orientations of *ca.* 38 and 12% occupancy were identified, with two further orientations of the same occupancies being generated by operation of the centre of symmetry. In each case the geometries of the two orientations were optimised and the thermal parameters of adjacent atoms were restrained to be similar. For the C(70)-based molecule the major occupancy non-hydrogen atoms were refined anisotropically and the minor occupancy ones were refined anisotropically, whilst for the C(80)-based molecule all of the atoms were refined isotropically.

The X-ray crystal structure of **5**

No significant disorder was found in this structure.

