

## **A pseudo cubic structure with weak extra reflections: the structures of $[M\{N(CH_2CH_2P(i\text{-pr})_2)_3\}CO](BPh_4)$ M=Rh, Ir**

**A. C. Willis, A. D. Rae**

*Research School of Chemistry, Australian National University, Canberra, ACT, Australia*

The isomorphous crystals of  $[M\{N(CH_2CH_2P(i\text{-pr})_2)_3\}CO](BPh_4)$ , M=Rh, Ir, show  $I23$  diffraction symmetry with  $a = 33.6881 \text{ \AA}$  and  $33.6821 \text{ \AA}$  for Rh and Ir respectively. Only the even-even-even reflections are strong.

An initial structure solution could be found ignoring the extra reflections and reindexing the remaining reflections for the primitive cell ( $a_P = b_P = c_P = 16.84 \text{ \AA}$ ). A  $Z = 4$  solution in space group  $P2_13$  was obtained ( $h00$ :  $h = 4n$  only for the  $I$  centred lattice). Each cation and each anion lies on a three-fold axis.

The true structure can not be cubic, the  $I23$  diffraction symmetry being imposed by either a three-fold twinning of a monoclinic  $B.2_1$  structure ( $a = 2a_P$ ,  $b = b_P$ ,  $c = 2c_P$ ), or a four-fold twinning of a rhombohedral  $R3$  structure

Attempts to determine the true structure using RAELS2006 software will be presented.

We thank Professor Les Field and Dr Khuong Vuong of the University of New South Wales for supplying the crystals.