X-Ray Structure of a Novel Bidentate Polypyrazolylborate Complex: Carbonyl[hydridotris(pyrazol-1-yl)borato]methylplatinum

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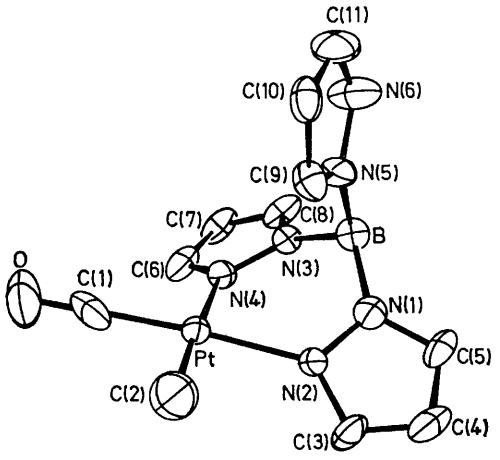
Summary The crystal structure of a bidentate hydridotris(pyrazol-1-yl)borate complex with platinum(II) is reported.

SYNTHESES of a wide variety of complexes with hydridotris(pyrazol-1-yl)boratomethylplatinum(II) have recently been reported.[1,2] The ^1H n.m.r. spectrum of the carbonyl complex indicates a stereochemically non-rigid, five-co-ordinate geometry about platinum.

Crystals of the carbonyl complex, $C_{11}H_{13}BN_6OPt$, kindly supplied by Clark and Manzer, were grown from hexane solution and are monoclinic, $P2_1/c$ with $a = 14{\cdot}416(1)$, $b = 7{\cdot}951(1)$, $c = 12{\cdot}990(1)$ Å, $\beta = 104{\cdot}35(1)°$ and $Z = 4$. A total of 2738 (2124 observed) independent reflections were measured on a Diano XRD-700 diffractometer using Cu-K_α radiation with a balanced nickel-cobalt filter pair. The structure was solved by the heavy atom method and has been refined by full-matrix least-squares procedures to a final conventional R of 0·039 (0·033 for weighted R), including the 13 hydrogen atoms. A perspective drawing of the molecule is shown in the Figure from which the hydrogen atoms have been omitted for clarity.

The co-ordination about platinum is a slightly distorted square-planar arrangement of C(1), C(2), N(2), and N(4). The six-membered PtN_4B ring is in the boat conformation with Pt and B being 0·709 and 0·529 Å above the plane defined by the four nitrogen atoms. As one might expect, the non-bonded Pt–B distance (3·36 Å) observed in this molecule is significantly longer than the value (3·20 Å) found in the five-co-ordinate Pt^{II} complex containing a tridentate hydridotris(pyrazol-1-yl)borate ligand.[3] Each pyrazolyl ring is planar.

The Pt–N(2), Pt–N(4), Pt–C(1), and Pt–C(2) distances are 2·038(7), 2·068(7), 1·814(13) and 2·028(13) Å, respectively. The average values for the bond lengths in the pyrazolyl rings are: N–N 1·357(9), C–C 1·361(17), and C–N 1·355 (15) Å. Pertinent bond angles are < N–Pt–N = 87·2(3)°,



FIGURE

C–Pt–C = 85·3(6)°, N–Pt–C(Me) = 90·6(5)°, N–Pt–C,-(CO) = 96·9(4)°, N–B–N (average) = 109·7(9)°, and N–B–H (average) = 109(7)°. These values are representative of those observed in similar compounds.[3,4]

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