

taken from Cromer & Waber (1974) without correction for anomalous scattering. The view of the molecule was produced by *ORTEPII* (Johnson, 1976) (Fig. 1). The atomic coordinates and thermal parameters are listed in Table 1; the important bond lengths and bond angles are given in Table 2.*

Related literature. The synthesis and characterization of the novel cubane-like clusters $[M_2Cu_2S_4(PPH_3)_2-(SCH_2CH_2S)_2]$ ($M = Mo, W$) have been described by Zhu, Zheng & Wu (1990) who also reported briefly on the structure of the Mo cluster.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53864 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of a Platinum(II) Complex with a Ligand Containing Thiazole and Benzimidazole

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Abstract. Dibromo[2-(4-thiazolyl)benzimidazole]platinum(II), $[PtBr_2(C_{10}H_7N_3S)]$, $M_r = 556.16$, monoclinic, $P2_1/n$, $a = 10.090$ (3), $b = 7.578$ (6), $c = 16.454$ (5) Å, $\beta = 103.92$ (1)°, $V = 1221$ (1) Å³, $Z = 4$, $D_x = 3.028$ g cm⁻³, $\lambda(Mo K\alpha) = 0.71073$ Å, $\mu = 182.59$ cm⁻¹, $F(000) = 1008$, $T = 296$ K, final $R = 0.048$ for 1790 unique observed reflections. The complex is essentially planar, with all non-H atoms located within 0.095 (2) Å of the plane of the molecule. The ligand coordinates to Pt through two N atoms, one from the thiazole ring and one from the imidazole ring. The average Pt—Br and Pt—N bond lengths are 2.408 (4) and 2.025 (8) Å, respectively. The small C—S—C angle [91.1 (8)°] compared with the average C—N—C angle [110 (2)°] suggests that the S atom might be using unhybridized p orbitals for bonding.

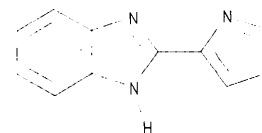
Experimental. To 0.200 g (0.177 mmol) $[NEt_4]_2[Pt_2Br_6]$ in 50 ml of methanol were added 0.080 g (0.38 mmol) of 2-(4-thiazolyl)benzimidazole (tzbm)

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in 20 ml of methanol. The reaction mixture was stirred and heated for 1 h, then left until crystals formed. Analysis for $C_{10}H_7Br_2N_3PtS$: Calc. C 21.60, H 1.27%; found C 21.71, H 1.33%. There are several possible ways for tzbm to coordinate to the metal: through N or S atoms of the thiazole ring, through one N atom of the benzimidazole ring or through one atom from each ring to form a chelate. Therefore, the structure of the complex was determined by X-ray diffraction to establish unequivocally through which atom(s) the ligand coordinates to the Pt atom.



Yellow rectangular crystal, $D_m > 1.99$ g cm⁻³ [crystal sinks rapidly in concentrated $Hg(NO_3)_2$ solution], $0.4 \times 0.2 \times 0.2$ mm. Enraf–Nonius CAD-4 diffractometer, monochromated $Mo K\alpha$, ω - 2θ scan,

Table 1. Atomic coordinates and equivalent isotropic temperature factors (\AA^2) for $\text{Pt}(\text{tzim})\text{Br}_2$

$$B_{\text{eq}} = (4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)].$$

	x	y	z	B_{eq} (\AA^2)
Pt	0.09479 (5)	0.71983 (7)	0.06492 (3)	2.085 (9)
Br1	0.3386 (2)	0.7518 (2)	0.1109 (1)	3.79 (4)
Br2	0.0927 (2)	0.5909 (2)	0.19866 (9)	3.76 (4)
S	-0.3651 (4)	0.6769 (6)	-0.0034 (3)	3.80 (9)
N1	-0.110 (1)	0.704 (2)	0.0247 (7)	2.6 (2)
N2	0.072 (1)	0.815 (1)	-0.0535 (7)	2.4 (2)
N3	-0.068 (1)	0.886 (1)	-0.1730 (7)	2.4 (2)
C1	-0.205 (1)	0.658 (2)	0.061 (1)	3.3 (3)
C2	-0.300 (2)	0.755 (2)	-0.082 (1)	3.3 (3)
C3	-0.162 (1)	0.762 (2)	-0.0575 (7)	2.0 (2)
C4	-0.059 (1)	0.820 (2)	-0.0970 (8)	2.1 (3)
C5	0.059 (1)	0.925 (2)	-0.1825 (8)	2.3 (3)
C6	0.149 (1)	0.876 (2)	-0.1056 (8)	2.4 (3)
C7	0.291 (1)	0.902 (2)	-0.0940 (8)	2.6 (3)
C8	0.335 (1)	0.976 (2)	-0.1581 (9)	3.4 (3)
C9	0.245 (1)	1.026 (2)	-0.2334 (9)	3.6 (4)
C10	0.106 (2)	1.002 (2)	-0.2461 (9)	3.3 (3)

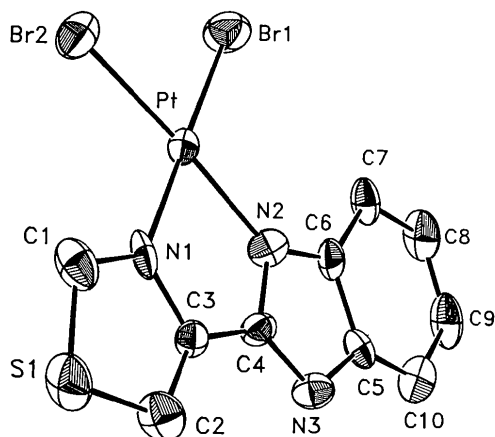
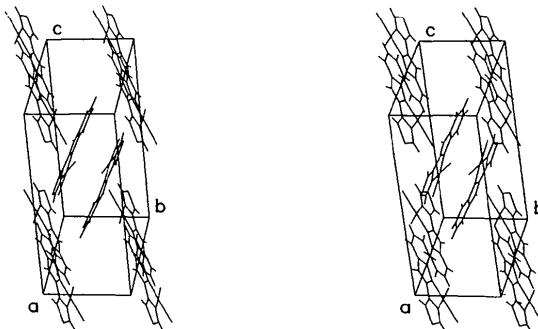
Table 2. Bond distances (\AA) and angles ($^\circ$) for $\text{Pt}(\text{tzim})\text{Br}_2$ with e.s.d.'s in parentheses

Pt	Br1	2.404 (2)	N3	C4	1.33 (2)		
Pt	Br2	2.413 (2)	N3	C5	1.36 (2)		
Pt	N1	2.01 (1)	C2	C3	1.35 (2)		
Pt	N2	2.04 (1)	C3	C4	1.42 (2)		
S	C1	1.71 (1)	C5	C6	1.41 (2)		
S	C2	1.70 (2)	C5	C10	1.38 (2)		
N1	C1	1.29 (2)	C6	C7	1.42 (2)		
N1	C3	1.40 (2)	C7	C8	1.36 (2)		
N2	C4	1.35 (2)	C8	C9	1.40 (2)		
N2	C6	1.36 (2)	C9	C10	1.37 (2)		
Br1	Pt	Br2	89.22 (6)	N1	C3	C2	114. (1)
Br1	Pt	N1	177.6 (3)	N1	C3	C4	113. (1)
Br1	Pt	N2	97.7 (3)	C2	C3	C4	133. (1)
Br2	Pt	N1	92.4 (4)	N2	C4	N3	110. (1)
Br2	Pt	N2	172.7 (3)	N2	C4	C3	119. (1)
N1	Pt	N2	80.7 (5)	N3	C4	C3	131. (1)
C1	S	C2	91.1 (8)	N3	C5	C6	105. (1)
Pt	N1	C1	133. (1)	N3	C5	C10	133. (1)
Pt	N1	C3	115. (1)	C6	C5	C10	122. (1)
C1	N1	C3	112. (1)	N2	C6	C5	108. (1)
Pt	N2	C4	113. (1)	N2	C6	C7	132. (1)
Pt	N2	C6	140.6 (9)	C5	C6	C7	120. (1)
C4	N2	C6	107. (1)	C6	C7	C8	118. (1)
C4	N3	C5	110. (1)	C7	C8	C9	122. (1)
S	C1	N1	113. (1)	C8	C9	C10	121. (1)
S	C2	C3	110. (1)	C5	C10	C9	118. (1)

scan width $(0.9 + 0.34\tan\theta)^\circ$, $2\theta_{\text{max}} = 54^\circ$, lattice parameters from least-squares fit of 25 reflections in the range $7 < \theta < 11^\circ$. Systematic absences $h0l$ ($h + l = 2n + 1$), $0k0$ ($k = 2n + 1$); $+h, +k, \pm l$, $h \leq 13$, $k \leq 8$, $|l| \leq 19$; three standard reflections ($\bar{4}0\bar{4}$, $\bar{5}13$, $12\bar{9}$), total intensity loss 0.7% during 15.1 h exposure, total unique reflections measured 2647, 1790 with $F^2 > 3\sigma^2(F_o)$, $\sigma(F_o) = [\sigma^2(I_{\text{raw}}) + (0.04F_o^2)^2]^{1/2}/2F_o$. Structure was solved with the Enraf-Nonius *Structure Determination Package* (Frenz, 1985), heavy-atom and difference Fourier methods; isotropic, then anisotropic refinement of F of all non-H atoms, H atoms on the complex at calculated positions, riding model [C—H 0.95 \AA , $U(\text{H}) = 1.3U(\text{C})$]; 154 parameters refined, $R = 0.048$, $wR = 0.056$, $w = 1/[\sigma^2(F_o)]$, $S = 1.694$; difference syntheses showed no densities above 0.93 e \AA^{-3} (min. -3.672); max. $\Delta/\sigma = 0.01$. Neutral-atom scattering factors were used (*International Tables for X-ray Crystallography*, 1974, Vol. IV, Tables 2.2B and 2.3.1), and were corrected for anomalous dispersion (Cromer & Liberman, 1970). Empirical absorption correction: $T_{\text{max}} = 0.9929$, $T_{\text{min}} = 0.2346$. No correction for secondary extinction.

The atomic coordinates and equivalent isotropic temperature factors are listed in Table 1,* and selected bond lengths and angles in Table 2. An *ORTEP* (Johnson, 1976) plot of the complex with the atom numbering is shown in Fig. 1, and the packing of the molecules (Motherwell & Clegg, 1978) in Fig. 2.

* Lists of structure factors, anisotropic thermal parameters, least-squares planes and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53893 (34 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Fig. 1. Labeling of atoms in $[\text{Pt}(\text{tzim})\text{Br}_2]$ (50% probability ellipsoids).Fig. 2. Packing diagram of $[\text{Pt}(\text{tzim})\text{Br}_2]$ in the unit cell.

Related literature. Platinum(II) complexes with imidazole, thiazole and other N-donor heterocyclic ligands have shown significant biological activity (Dehand & Jordanov, 1976; Van Kralingen & Reedijk, 1978; Van Kralingen, Reedijk & De Ridder, 1979) and are of interest as potential antitumor agents (Hacker, Douple & Krakoff, 1984). Thiazole is a potentially ambidentate ligand with either the N or S atom available for coordination. Although coordination by the soft S might be predicted (Pearson, 1963), the thiazole ring in tzbim is coordinated through the N atom. This behavior has been observed in Pd^{II} and Rh^{III} benzothiazole complexes (Churchill, Wasserman & Young, 1980; Muir, Rong & Muir, 1989), and in several Pt^{II} styrylbenzothiazole complexes (Muir, Gómez, Muir, Cox & Cádiz, 1987; Gómez, Muir & Muir, 1988; Muir, Gómez, Muir, Cádiz, Cox & Barnes, 1988; Muir, Gómez, Muir & Cádiz, 1990). The average C—N, C—S and C—C distances and bond angles are similar to those found in the other complexes.

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Potassium 4-(4-Nitrophenyl)phenolate Monohydrate

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Abstract. K⁺.C₁₂H₈NO₃⁻.H₂O, *M_r* = 271.32, monoclinic, *P*2₁/*c*, *a* = 14.388 (2), *b* = 7.362 (1), *c* = 11.280 (2) Å, β = 107.79 (2)°, *V* = 1137.7 (3) Å³, *Z* = 4, *D_x* = 1.58 g cm⁻³, λ(Mo *K*α) = 0.71069 Å, μ = 4.66 cm⁻¹, *F*(000) = 560, *T* = 298 K, *R* = 0.0362 for 1710 unique reflections. The dihedral angle between the phenyl rings is 4° and the dihedral angle between one phenyl group and the adjacent NO₂ group is 4°. The anion shows a partial quinoid character and is stacked antiparallel. The potassium cation is eight-

fold coordinated through oxygen atoms in the range up to 3.1 Å. Hydrogen bridges between water and phenolate oxygens O—H···O with distances of 2.783 (3) and 2.784 (3) Å are indicated.

Experimental. 4-(4'-Nitrophenyl)phenol was prepared as described by Jones & Chapman (1952). The final product was obtained by reaction with potassium hydroxide dissolved in water. For recrystallization, water-containing ethanol was used. After evaporation blue-red plate-like crystals resulted. Size of the crystal 0.28 × 0.12 × 0.37 mm. Stoe Stadi-4 four-circle diffractometer, graphite-monochromated Mo *K*α radiation, lattice parameters from a least-

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