Structure of Bis-(2-aminoethylsalicylideneiminato)chromium(III) Iodide

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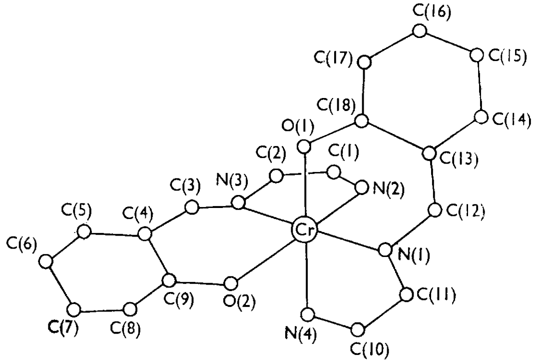
THE structure of this compound was determined as the result of a suggestion that it might be ethylenediamine-*NN'*-ethylenebis(salicylideneiminato)-chromium(III) iodide.[1] The structure postulated was that of a planar quadridentate ligand surrounding chromium, with the additional ethylenediamine molecule acting as a bridging group between chromium atoms. I.r. spectral measurements indicated the presence of a co-ordinated ethylenediamine molecule.[1] It was subsequently realised that the complex could consist of two tridentate ligands about the central chromium atom, and this was confirmed by the structure analysis.

The magnetic and spectral data have been given elsewhere together with the preparative details.[2] The crystals used in this study were provided by Dr. M. J. O'Connor.

The crystals of bis-(2-aminoethylsalicylideneiminato)chromium(III) iodide are dark red triclinic prisms, space group $P1$ or $P\bar{1}$, with $a = 9{\cdot}92$, $b = 9{\cdot}93$, $c = 10{\cdot}45$ Å, $\alpha = 93{\cdot}8°$, $\beta = 92{\cdot}7°$, $\gamma = 93{\cdot}8°$, $D_m = 1{\cdot}69$ g.cm.$^{-3}$, $Z = 2$, $D_c = 1{\cdot}64$ g.cm.$^{-3}$. The intensities of 1481 independent non-zero reflections were measured using the integrating multiple-film Weissenberg technique with Cu-K_α radiation. The *h*0–5*l*, 0*kl*, and *hk*0 levels were photographed, together with precession photographs which were used to confirm the angles obtained. Since $Z = 2$, space group $P\bar{1}$ was assumed and was justified by the subsequent smooth refinement. The co-ordinates of the iodine and chromium atoms were obtained from a three-dimensional Patterson synthesis and the carbon, nitrogen, and oxygen atoms were then located by three-dimensional Fourier synthesis. No attempt has been made to locate hydrogen atoms. Anisotropic temperature factors were refined for the chromium and iodine atoms, and individual isotropic temperature factors for the other atoms. Using least-squares refinement and suitable weighting factors the final R value was 0·114. So far no allowance has been made for anomalous dispersion. Since the chromium and iodide ions account for 90% of the X-ray scattering, standard deviations of bond lengths for the six bonds involving chromium were *ca.* 0·03 Å and for the remaining bonds *ca.* 0·06 Å. The results confirm octahedral co-ordination around the chromium atom by the two tridentate ligands (see Figure). The octahedron is slightly distorted, probably owing to the effects of hydrogen-bonding between the terminal ethylenediamine nitrogen atoms and the iodide ion, and also from the small 'bite' of the ethylenediamine molecule. Each tridentate ligand is reasonably planar, with the two planes approximately at right angles.



FIGURE

	C–C (benzene)	1·42 Å
	C–C (ethyl)	1·55
	C(3)–C(4) andC(12)–C(13)	1·46
	C=N	1·31
	C–N	1·52
	C–O	1·36
	Cr–N	2·10
	Cr–O	1·92
	Cr–I	4·19
Chelate 'bites'	N(3) ··· N(2), N(1) ··· N(4)	2·71
	O(1) ··· N(1), O(2) ··· N(3)	2·83

Average bond lengths in the molecule are listed in the Table and agree with those reported elsewhere for similar situations. The structure will be discussed in detail at a later date.

This work forms part of a project supported by a grant from the Australian Research Grants Committee.

(*Received, April* 16*th*; *Com.* 469.)

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[1] M. J. O'Connor, Ph.D. Thesis, Monash University, 1966.

[2] M. J. O'Connor and B. O. West, *Austral. J. Chem.*, 1968, **21**, 369.