CCl_4) agreed with the spectrum of the isomeric mixture obtained in the nitration of thiophene with the exceptions noted above. (Found: C 36.83; H 2.06; N 10.87; S 24.50. Calc. for $C_4H_3NO_2S$: C 37.20; H 2.35; N 10.85; S 24.83).

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On the Crystal Structure of Nitritopentamminechromium (III) Chloride

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In connection with studies of nitro and nitrito compounds of transition metals, the crystal structure of $[Cr(ONO)(NH_3)_5]Cl_2$ has been investigated and a preliminary report is given in this note.

Starting with $KCr(SO_4)_2 \cdot 12H_2O$ $[Cr(ONO)(NH_3)_5]Cl_2$ was prepared through a series of syntheses.[1-3] The analyses of $[Cr(ONO)(NH_3)_5]Cl_2$ gave 32.6 % N, 27.4 % Cl, and 21.0 % Cr. The theoretical values are 33.1 % N, 27.9 % Cl, and 20.5 % Cr.

Integrated Weissenberg photographs corresponding to the reflections $hk0-hk4$ have been recorded, using Cu$K\alpha$ radiation. The crystals are of orthorhombic symmetry and from the systematically absent reflections the space group was determined to be either No. 62 — *Pnma* or No. 33 — $Pn2_1a$.[4] The cell dimensions, as calculated from the Weissenberg data, are $a=13.3$ Å, $b=10.6$ Å, and $c=7.0$ Å. The volume of the unit cell is thus approximately 990 Å^3. Assuming a cell content of four formula units, a calculated density of 1.71 g/cm^3 is obtained. From three-dimensional Patterson calculations, based on the $hk0-hk4$ intensities, the chromium atoms were found to occupy the four-fold position 4(*c*) in *Pnma* (No. 62) with $x=0.12$, $y=1/4$, $z=0.19$, and the chloride ions were found to occupy the eight-fold position 8(*d*) with $x=0.37$, $y=0.00$, and $z=0.19$. The positions of the nitrogen atoms and one oxygen atom were then deduced from successive electron density calculations. The position of one oxygen atom has not yet been completely determined. A preliminary three-dimensional least squares refinement of the structure was performed giving a *R*-value of 0.12 and the resulting parameters are listed in Table 1. The chromium atom is octahedrally coordinated by five NH_3-groups and one NO_2-group. A complete three-dimensional refinement is in progress, and a detailed presentation of the structure of $[Cr(ONO)(NH_3)_5]Cl_2$ will soon be published in *Acta Chem. Scand.*

Table 1.

Atom	Position	*x*	*y*	*z*
Cr	4(*c*)	0.107	1/4	0.175
Cl	8(*d*)	0.358	0.999	0.172
N1	8(*d*)	0.108	0.047	0.220
N2	4(*c*)	0.195	1/4	0.947
N3	4(*c*)	0.226	1/4	0.362
N4	4(*c*)	0.021	1/4	0.379
N5	4(*c*)	0.399	1/4	0.663
O1	4(*c*)	0.482	1/4	0.526
O2	4(*c*)	(0.32	1/4	0.66)

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