Solving these equations for a monoclinic system and putting $\mathbf{j}\,.\,\mathbf{k}=\cos\alpha$ (say) we get,

$$\begin{aligned} a_1 &= \cos\theta_1 \\ a_2 &= (\cos\theta_2 - \cos\alpha\cos\theta_3)/\sin^2\alpha \\ a_3 &= (\cos\theta_3 - \cos\alpha\cos\theta_2)/\sin^2\alpha\,. \end{aligned}$$

Substituting these values in the last equation we get

$$\sin^2\theta_1 = \operatorname{cosec}^2\alpha\,(\cos^2\theta_2+\cos^2\theta_3) - 2\operatorname{cosec}\alpha\cot\alpha\cos\theta_2\cos\theta_3.$$

If, however, the angles θ_2 and θ_3 are defined as above and an average value of the angles is taken,

$$\overline{\sin^2}\,\theta_1 = \operatorname{cosec}^2\alpha\,(\overline{\sin^2}\,\theta_2 + \overline{\sin^2}\,\theta_3)\,.$$

Finally the angle between face normals in a crystallographic system is given by

$$\cos^{-1} T(x, y)/[T(x, x)T(y, y)]^{\frac{1}{2}}\,,$$

where $T(x, y)$ is

$$\begin{aligned} &(\sin^2\alpha/x_1y_1) + (\sin^2\beta/x_2y_2) + (\sin^2\gamma/x_3y_3) \\ &\quad + (\cos\gamma\cos\beta - \cos\alpha)\{(1/x_3y_2) + (1/x_2y_3)\} \\ &\quad + (\cos\gamma\cos\alpha - \cos\beta)\{(1/x_3y_1) + (1/x_1y_3)\} \\ &\quad + (\cos\alpha\cos\beta - \cos\gamma)\{(1/x_1y_2) + (1/x_2y_1)\}\,, \end{aligned}$$

where x_1, x_2, x_3 and y_1, y_2, y_3 are intercepts along the three axes and α, β, γ are the axial angles. For a monoclinic system the angle between two paratropic planes in terms of Miller Indices and axial lengths is given by

$$\cos^{-1}\frac{h_1h_2(bc/a) + l_1l_2ab/c - b\cos\beta(l_1h_2 + h_1l_2)}{[(h_1{}^2/a_2 + l_1{}^2/c_2 - 2l_1h_1/ac\cos\beta)\,(h_2{}^2/a^2 + l_2{}^2/c_2 - 2l_2h_2/ac\cos\beta)]^{\frac{1}{2}}}\,.$$

Here β is the monoclinic angle. Thus the orientation factor can be completely evaluated.

Reference

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Space groups of some coordination compounds of cobalt.

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(*Received* 3 *May* 1961)

This is a preliminary report on the unit cell dimensions and space groups of some coordination compounds of cobalt. The cell dimensions were measured from rotation photographs and the space-group absences were determined from the zero- and first-layer Weissenberg photographs taken about the principal axes using Fe $K\alpha$ radiation.

(1) *Sodium salt of cobalt*(III) *ethylene diammine tetra-acetate tetrahydrate*: Na[CoEDTA], 4 H_2O

This crystallizes in long plates and belongs to the orthorhombic system. The axial lengths are

$$a=6{\cdot}45\pm0{\cdot}02,\ b=19{\cdot}28\pm0{\cdot}06,\ c=13{\cdot}70\pm0{\cdot}04\ \text{Å};$$
$$d_o=1{\cdot}760\ \text{g.cm.}^{-3},\ d_c=1{\cdot}733\ \text{g.cm.}^{-3};\ Z=4\,.$$

Systematic absences were found for $h0l$ reflections with h odd and $0kl$ with $k+l$ odd. The space group is therefore $Pna2_1$. The other possible space group $Pnam$ has three sets of four-fold positions (a), (b) and (c). Since there are four formula units of the compound in the unit cell, the cobalt atoms have to occur at one of these positions. The point symmetry at (a) and (b) is a symmetry centre and at (c) a mirror plane of symmetry. The cobalt coordination complex is not likely to have these symmetry elements* and therefore this space group is ruled out.

(2) *Cobalt*(III) *tris glycinate dihydrate* $Co(C_2NO_2H_4)_3$, $2H_2O$

This crystallizes in flat plates which belong to the monoclinic system. The cell dimensions are:

$$a=13{\cdot}50\pm0{\cdot}03,\ b=12{\cdot}87\pm0{\cdot}03,\ c=12{\cdot}71\pm0{\cdot}03\ \text{Å};$$
$$\beta=98°;\ d_o=1{\cdot}754\ \text{g.cm.}^{-3},\ d_c=1{\cdot}730\ \text{g.cm.}^{-3};\ Z=8\,.$$

The systematically absent reflection are $h0l$ with l odd and $0k0$ with k odd. This establishes the space group unequivocally as $P2_1/c$–C_{2h}^5.

(3) *Cobalt*(III) *bis dimethyl glyoximino diammine thiocyanate*

This coordination compound was prepared by treating its chloride salt with potassium thiocyanate and was purified by recrystallization from water.

The unit cell of this compound is orthorhombic having

$$a=23{\cdot}20\pm0{\cdot}06,\ b=7{\cdot}05\pm0{\cdot}03,\ c=10{\cdot}44\pm0{\cdot}03\ \text{Å};$$
$$d_o=1{\cdot}54\ \text{g.cm.}^{-3},\ d_c=1{\cdot}45\ \text{g.cm.}^{-3};\ Z=4\,.$$

The systematic absences of the X-ray reflections are $hk0$ for h odd and $0kl$ for $k+l$ odd. This is consistent with the space groups $Pnma$ and $Pn2_1a$.

(4) *Cobalt*(III) *bis dimethyl glyoximino diammine perchlorate*

This compound was prepared by treating the chloride salt of the corresponding complex compound with perchloric acid and was purified by recrystallization through water. It crystallizes in needles which belong to the monoclinic system. The cell dimensions are

$$a=19{\cdot}90\pm0{\cdot}06,\ b=6{\cdot}32\pm0{\cdot}03,\ c=12{\cdot}46\pm0{\cdot}04\ \text{Å};$$
$$\beta=103°;\ d_o=1{\cdot}83\ \text{g.cm.}^{-3},\ d_c=1{\cdot}84\ \text{g.cm.}^{-3};\ Z=4\,.$$

The systematically absent reflections are hkl with $h+k+l$ odd and $h0l$ with l odd. These correspond to the space groups Ic and $I2/c$.

The authors wish to thank Dr Jagdish Shankar for his interest and encouragement.

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* See Martell & Calvin (1956). *Chemistry of Metal Chelate Compounds*, Prentice Hall, Inc.