Table 2.

Cu $K\alpha = 1{\cdot}5418$ Å

	CoMoO$_4$			NiMoO$_4$		
	$A \neq B \neq D$	$A = B \neq D$	$A = B = D$	$A \neq B \neq D$	$A = B \neq D$	$A = B = D$
A	0·007570	0·007581	0·007581	0·007767	0·007771	0·007771
B	0·007586			0·007775		
D	0·007589	0·007593		0·007770	0·007773	
C	0·011784	0·011782	0·011775	0·011988	0·011987	0·011986
a	9·675 Å	9·668 Å	9·666 Å	9·555 Å	9·555 Å	9·555 Å
$a \sin \beta$	8·860	8·854	8·854	8·747	8·745	8·745
b	8·851	8·854	8·854	8·743	8·745	8·745
$c \sin \beta$	7·102	7·102	7·104	7·041	7·041	7·042
c	7·755	7·755	7·755	7·691	7·693	7·694
β	113° 41′	113° 41′	113° 39′	113° 44′	113° 45′	113° 45′

4 hr. heating at 750 °C. or 2 hr. at 800–820 °C. was found to be necessary. The powder pattern was almost identical with that of cobalt molybdate apart from a slight increase in θ values. The same least-squares analysis of the $\sin^2 \theta$ values again indicated that the constants A, B and D were equal. The data are tabulated in Tables 1 and 2. The calculated and measured densities of nickel molybdate are 4·94 g.cm.$^{-3}$ and 4·91 g.cm.$^{-3}$ respectively.

These two molybdates have a different crystal structure from the tungstate analogues, which belong to an isomorphous series RWO$_4$, where R = Co, Fe, Mg, Ni and Zn. Until the iron, magnesium and zinc molybdates have been formed it is not possible to conclude whether a similar isomorphous molybdate series does exist. (The data are being sent to Prof. A. J. C. Wilson (Cardiff) for inclusion in the X-ray Powder Data File).

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Crystallographic data for *N*-Benzyldithiocyanopyrrole.

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Preliminary X-ray crystallographic data were gathered for *N*-Benzyldithiocyanopyrrole during the search for a dithiocyanated pyrrole whose unit cell dimensions and symmetry would allow a rapid determination by two-dimensional Patterson and Fourier methods of the substitution position of the thiocyanate groups on the pyrrole ring. Chemical proof of structure (Matteson & Snyder, 1957) has indicated the substitution to be β, that is two carbons removed from the nitrogen, whereas *NMR* spectra (Gronowitz, Hörnfeldt, Gestblom & Hoffman, 1961) point strongly to α substitution.

Crystals were grown by slow cooling of a saturated 95% ethanol solution. They appeared as transparent light brown colored orthorhombic prisms, elongated in the direction subsequently designated as the b axis. Rotation, Weissenberg and precession photographs (Cu $K\alpha$ radiation) showed the crystals to be orthorhombic and having the following cell dimensions:

$$a_0 = 17{\cdot}26 \pm 0{\cdot}01,\ b_0 = 10{\cdot}22 \pm 0{\cdot}01,\ c_0 = 14{\cdot}54 \pm 0{\cdot}01 \text{ Å}\,.$$

The space group was unambiguously determined to be $Pbca\text{–}D_{2h}^{15}$ by noting the systematic absences of reflection on Weissenberg and precession photographs. The density was experimentally determined by flotation to be 1·396 g.cm.$^{-3}$ which agrees closely with a calculated density of 1·405 g.cm.$^{-3}$ for a unit cell containing 8 molecules. The molecules are thus in general positions.

During the course of the X-ray investigation, it was observed that all photographs exhibited a very sharp fall-off in the diffracted intensities, with virtually no recorded diffraction occurring at interplanar spacings shorter than 1·2 Å. It was thought that this was indicative of rather large temperature motions, however intensity measurements made at −140 °C. using the General Electric Single Crystal Orienter (Cu $K\alpha$ radiation) and Precession Photographs (Mo $K\alpha$ radiation) showed only a small amount of sharpening, thus ruling out the possibility of large thermal motions. On the basis of the low temperature data, it must be concluded that the observed sharp fall-off in intensities is not due to excessive thermal motions but rather very likely due to stacking disorders.

No further work on this compound is contemplated at this time.

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