Hanson, H. P., Herman, F., Lea, J. D. & Skillman, S. (1964). *Acta Cryst.* **17**, 1040.
Heavens, O. S. & Cheesman, G. H. (1950). *Acta Cryst.* **3**, 197.
Ibers, J. A. & Hamilton, W. C. (1964). *Acta Cryst.* **17**, 781.
*International Tables for X-ray Crystallography* (1962). Vol. III, Table 3.3.2C. Birmingham: The Kynoch Press.
Meerum-Terwogt, P. C. E. (1905). *Z. anorg. Chem.* **47**, 201.
Rundle, R. E. (1962). *Record Chem. Progr.* **23**, 195.
Swink, L. N. & Carpenter, G. B. (1967). *Acta Cryst.* **22**, 602.
Swink, L. N. (1968). Thesis: to be submitted to Brown University.
Vonnegut, B. & Warren, B. E. (1936). *J. Amer. Chem Soc.* **58**, 2459.
Zachariasen, W. H. (1963). *Acta Cryst.* **16**, 1139.

*Acta Cryst.* (1968). B **24**, 433

# A Case of 'Pseudo-Homometric' Structure in the Complex Nickel(II) Bis-(*N*,*N*-di-n-propyldithiocarbamate)*

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A case of 'pseudo-homometric' structure, observed in the complex nickel(II) bis-(*N*,*N*-di-n-propyldithiocarbamate), is described. The 'false' molecule $(\frac{1}{2}, \frac{1}{2}, 0)$ can be roughly obtained by shifting the molecule $(\frac{1}{3}, \frac{1}{6}, \frac{2}{3})$ or by a rotation of the true molecule $(\frac{1}{2}, \frac{1}{2}, 0)$.

Isovectorial structures which are different but have the same interatomic distances and, furthermore, the same structure factor values, have been defined as *homometric* (Patterson, 1944; Garrido, 1951): their solution will not be unique. Structure solutions characterized by almost identical Patterson functions have been called 'pseudo-homometric' (Luzzati, 1953; Hemily, 1957). When the chemical and geometric conditions do not allow us to discard the false solution easily, the right one may be found by using all the reflexions in a three-dimensional Patterson synthesis.

In some structures the correct solution can be obtained from the false one through crystallographic operations. In the case of *p*-nitroaniline the false structure (Abrahams & Robertson, 1948) has been corrected by shifting the origin (Donohue & Trueblood, 1956), and likewise for calcium ferrite (Decker & Kasper, 1957). The true structure of triphenylene was obtained (Pinnock, Taylor & Lipson, 1956) by simply correcting the position of the molecule which had been already correctly orientated (Klug, 1950). In other cases the true solution was reached by some rearrangement of the atoms, as in the case of DL-9,10-methyleneoctadecanoic acid (Brotherton, Craven & Jeffrey, 1958), of monoterpene isoiridomyrmecin $C_{10}H_{16}O_2$ (Schoenborn & McConnell, 1962), and of $Na_2O.GeO_2.6H_2O$ (Jamieson & Glasser, 1967).

In the course of the determination of the crystal structure of nickel(II) bis-(*N*,*N*-di-n-propyldithiocarbamate), $Ni[(C_3H_7)_2NCS_2]_2$, rhombohedral, space group $R\bar{3}$, $a=25{\cdot}20$, $c=8{\cdot}30$ Å (Peyronel & Pignedoli, 1967) we obtained a false structure by starting with a two-dimensional Patterson synthesis and by a trial-and-error method. The molecule was correctly located in the centre of symmetry. The refinement by means of three-dimensional Fourier sections gave a rather good representation of the molecule in the $XY$ projection [Fig. 1(*a*)] but it was impossible to reduce $R$ below 0·55. Also the interatomic distances and angles were not correct. Fig. 2 shows a combination of three-dimensional $YZ$ sections in the $YZ$ plane, which is arbitrarily schematic in order to avoid the atoms being superimposed as they would be in a correct projection.

From three-dimensional Patterson syntheses it was possible to obtain the correct orientation of the molecule as shown in the final composite $XY$ projection of three-dimensional Fourier sections [Fig. 1(*b*)]. This structure refined satisfactorily to $R=0{\cdot}075$ (Peyronel & Pignedoli, 1967).

The false molecule appears in the $XY$ projection [Fig. 1(*c*)] as having been rotated about 42–50° anticlockwise from the true position. This false orientation may also be roughly obtained by shifting the molecule ($B$) located in the $(\frac{1}{3}, \frac{1}{6}, \frac{2}{3})$ position into the $(\frac{1}{2}, \frac{1}{2}, 0)$ position. This molecule has in the $XY$ projection an orientation of 60° with respect to the real molecule ($A$) located in the $(\frac{1}{2}, \frac{1}{2}, 0)$ position [Fig. 1(*c*)]. Therefore the false structure may be considered very roughly as 'pseudo-homometric' to the true one.

Other conditions may contribute to the rather good representation of the molecule in the false position: nickel, being in the right place, gives an important and correct contribution to the calculated structure factors of the false solution; some atomic positions in the false structure are very near to those of other atomic posi-

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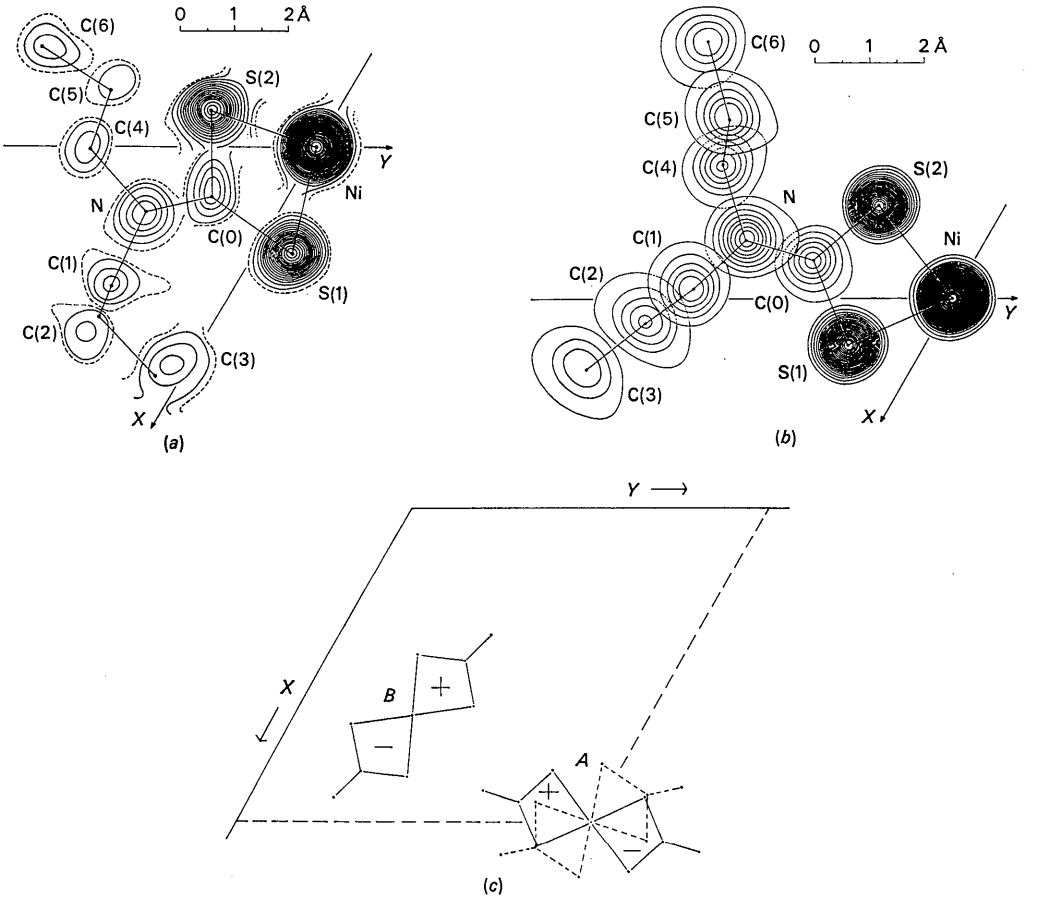

Fig. 1. (*a*). *XY* projection of three-dimensional sections of the 'false' asymmetric unit $(\frac{1}{2}, \frac{1}{2}, 0)$. (*b*) *XY* projection of three-dimensional sections of the true asymmetric unit $(\frac{1}{2}, \frac{1}{2}, 0)$. (*c*) *XY* projection of the central part of the true $(\frac{1}{2}, \frac{1}{2}, 0)$ and $(\frac{1}{3}, \frac{1}{6}, \frac{2}{3})$ molecules and of the 'false' molecule $(\frac{1}{2}, \frac{1}{2}, 0)$ (dashed lines).

tions of the true molecule; the large dimensions of the *ab* plane reduce the influence of the rotation of the molecule on the *XY* parameters of some atoms.

It may be noted that the atoms of the central part of the true molecule (*A*) have low *Z* parameter values. The rotated molecule (*A*) should have an inclination on the *XY* plane opposite to that of the molecule (*B*) transferred into the $(\frac{1}{2},\frac{1}{2},0)$ position [Fig. 1(*c*)]. The false molecule (*A*) has for all those central atoms, from nickel to nitrogen, a *Z* parameter equal to zero. Also the strange elongated shape of the atoms in the false *YZ* sections, inclined on the *XY* plane, is worthy of note.

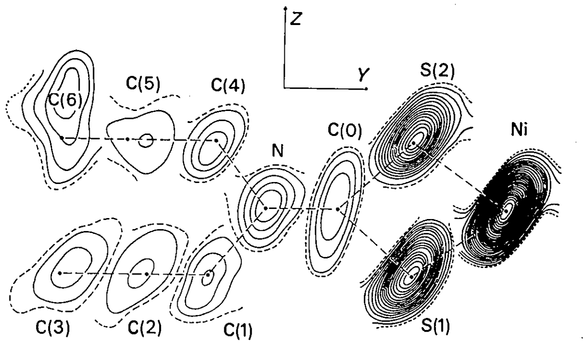

Fig. 2. *YZ* projection of three-dimensional sections of the 'false' asymmetric unit $(\frac{1}{2}, \frac{1}{2}, 0)$ in an arbitrarily schematic combination of the atoms.

## References

Abrahams, S. C. & Robertson, J. M. (1948). *Acta Cryst.* **1**, 252.

Brotherton, T., Craven, B. & Jeffrey, G. A. (1958). *Acta Cryst.* **11**, 546.

Decker, B. F. & Kasper, J. S. (1957). *Acta Cryst.* **10**, 332.

Donohue, J. & Trueblood, K. N. (1956). *Acta Cryst.* **9**, 960.

Garrido, J. (1951). *Bull. Soc. franç. Minér. Crist.* **74**, 397.

Hemily, P. W. (1957). *Acta Cryst.* **10**, 45.

Jamieson, P. B. & Glasser, L. S. (1957). *Acta Cryst.* **22**, 507.

Klug, A. (1950). *Acta Cryst.* **3**, 165.

Luzzati, V. (1953). *Acta Cryst.* **6**, 152.

Patterson, A. L. (1944). *Phys. Rev.* **65**, 195.

Peyronel, G. & Pignedoli, A. (1967). Acta Cryst. **23**, 398.

Pinnock, P. R., Taylor, C. A. & Lipson, H. (1956). *Acta Cryst.* **9**, 173.

Schoenborn, B. P. & McConnell, J. F. (1962). *Acta Cryst.* **15**, 779.