Chemistry. — *On the crystal structure of strychnine sulfate and selenate.* II. [010] *projection and structure formula.* By C. BOKHOVEN, J. C. SCHOONE and J. M. BIJVOET.

(Communicated at the meeting of September 25, 1948.)

Fig. 1 gives the Fourier synthesis of the electron distribution in the [010] projection of strychnine sulfate [1]).

The Fourier coefficients were deduced from the photometrically measured intensities of Weissenberg diagrams. Their signs were derived from the comparison of the structure factors of the isomorphous sulfate and selenate. Full data will be published in due time in the Acta Crystallographica.

The atomic configuration revealed by the Fourier map affords good agreement between calculated and observed intensities, which was still improved by small adjustments of the atomic parameters in a somewhat systematic way.

With this projection and the known interatomic distances only one model is compatible; its bonds are designed in fig. 1 [2]).

This conclusion was made easier by reference to a rough [001] projection. The structure of the strychnine molecule is seen in fig. 2 and again in fig. 3 in a projection suitable to act as an ordinary structure formula. It would not be easy to differentiate in this frame between *C*, *N* and *O* atoms by means of X-rays.

We think our deduction of the strychnine structure convincing already at this stage of the analysis. The definite proof however has to be supplied by a further study of the — non symmetrical — [001] projection, which is in progress now.

The above result was reached before we were aware of the fact that quite recently organic chemistry itself succeeded in making the right choice between the models in question [3]).

So our X-ray result constitutes an independent confirmation of this choice.

Van 't Hoff Laboratorium
der Rijksuniversiteit, Utrecht.

---

[1]) C. BOKHOVEN, J. C. SCHOONE and J. M. BIJVOET, These Proceedings, L, 825 (1947).

[2]) Our hearty thanks are due to Mr D. M. W. DEN BOER for cooperation in this part of the investigation.

[3]) R. ROBINSON, Nature **162**, 177 (1948).

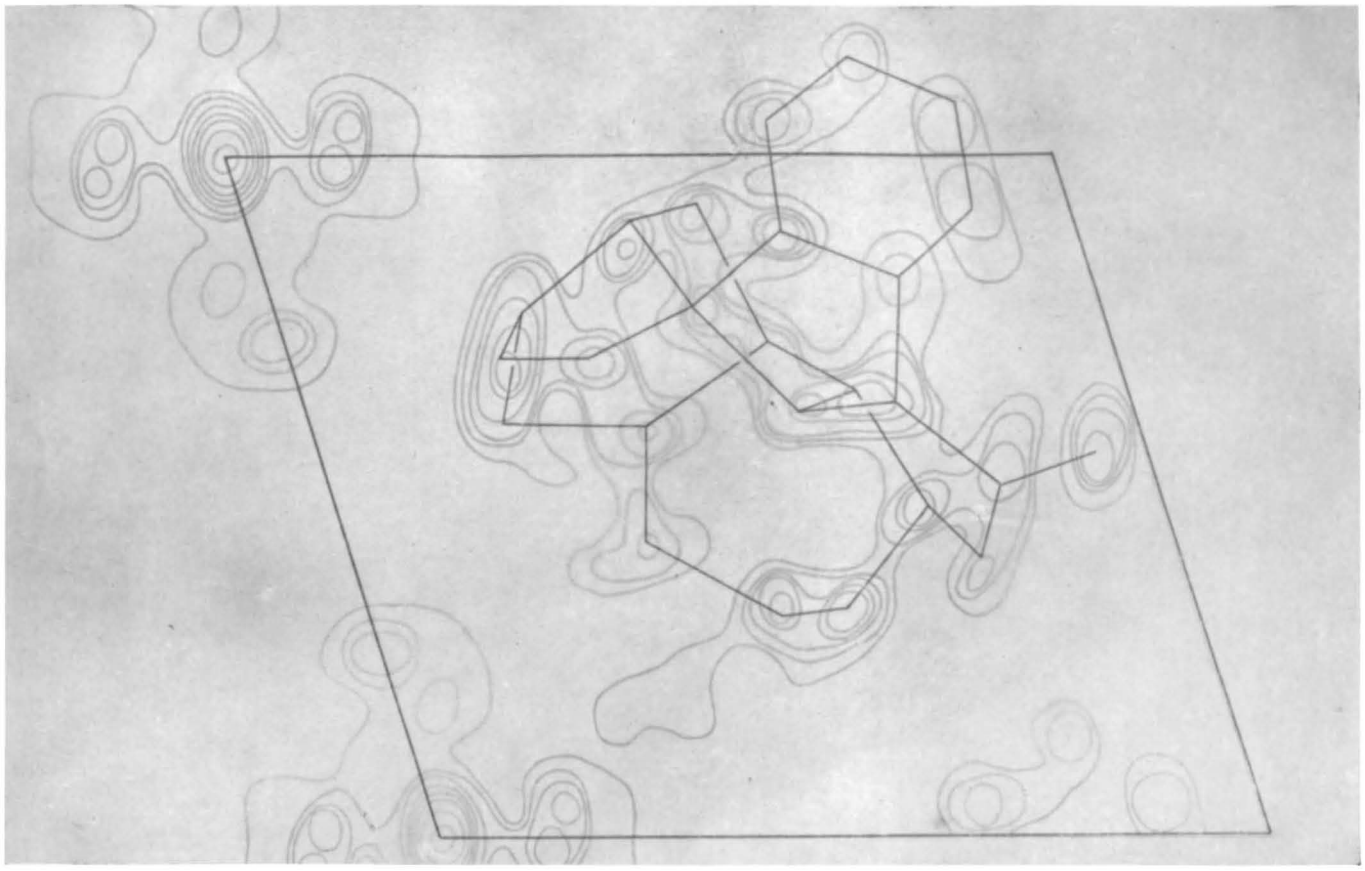

Fig. 1. Electron-density map of strychnine sulfate $(C_{21}H_{22}N_2O_2)_2 \cdot H_2SO_4 5\,aq$ in [010] propection. In the corners of the cell SO_4 groups with the water-molecules around it *). In the middle the strychnine molecule. This projection may be compared with the model of fig. 2 or with the projections of the latter in a slightly different orientation, fig. 3.

*) Four water molecules are located each on top of an O-atom of the SO_4 group. The vague maximum between the SO_4 group and the strychnine molecule corresponds in total density to about half a water molecule. It may possibly be attributed to the fifth molecule in statistical distribution over the twofold position about the axis of symmetry.

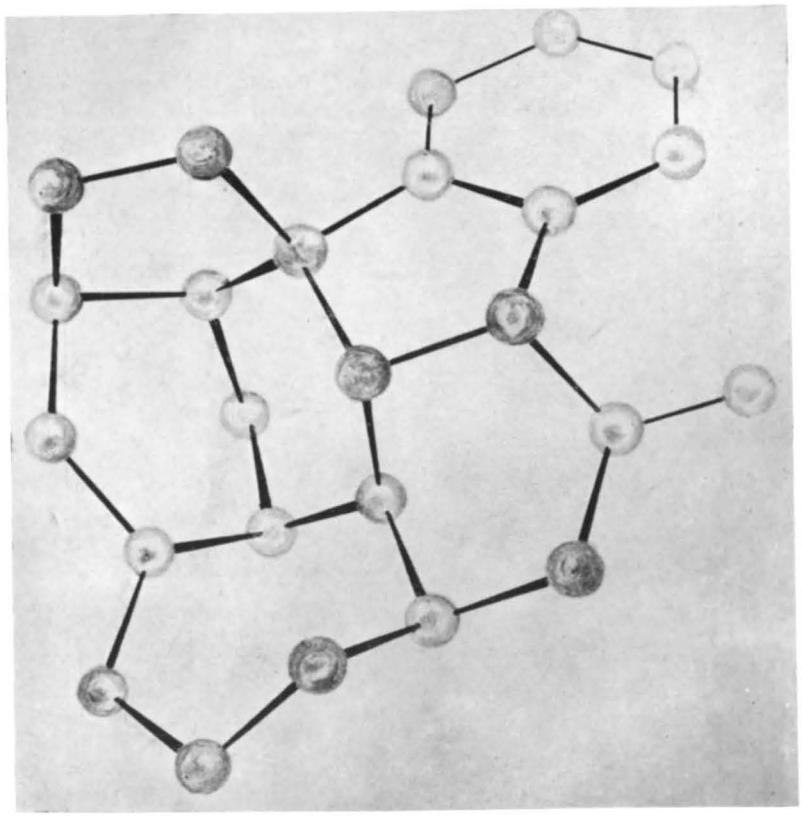

Fig. 2. Model of the strychnine molecule.

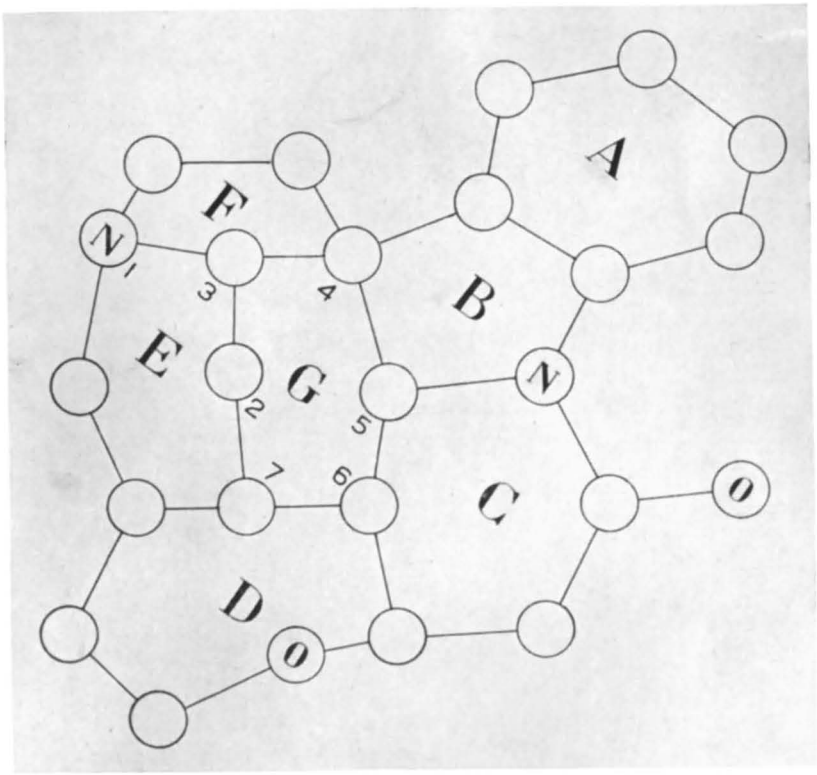

Fig. 3. Projection of the strychnine molecule in a direction slightly different from that of fig. 1 or 2.