of Sc the same is true and the main contribution orginates from $3d\ 4s^2$. In order to discriminate between $3d$ and $4s^2$ we have also computed a of Ca $4s^2$. Table 1 shows that a of Ca and Sc both are much larger than a of Ca^{2+}.

An extension of the present investigation to include atoms with several d-electrons outside the closed shell is going on. It would be of special interest to look at Ni, for which an experimental value of a is available [3].

We are indebted to Dr. P. Spiegelberg, Stockholm, who has drawn our attention to this problem. The present investigation has been supported by *Statens Naturvetenskapliga Forskningsråd (The Swedish Natural Science Research Council)*. Full details of the work will be published by one of us (M.S.).

1. Spiegelberg, P. *Private communication.*
2. Sternheimer, R. M. *Phys. Rev.* **96** (1954) 951.
3. Liepack, H. and Drechsler, M. *Naturwiss.* **43** (1956) 52.
4. Drechsler, M. and Müller, E. W. *Z. Physik* **132** (1952) 195.

Received July 31, 1957.

Note on the Crystal Structures of Hexagonal HgO and Hg_2O_2NaI

KARIN AURIVILLIUS and
INGA-BRITT CARLSSON

Institute of Inorganic and Physical Chemistry, University of Stockholm, Stockholm, Sweden

The hexagonal modification of mercury (II)oxide and the compound Hg_2O_2NaI have been prepared according to Laruelle [1] and studied by X-ray diffraction methods.

HgO. Hexagonal form. Space group $P3_121$ No. 152. Unit cell dimensions $a = 3.577$ Å, $c = 8.681$ Å in agreement with the values given by Laruelle. The cell content is 3 formula units of HgO. The positions of the mercury atoms have been derived by means of trial methods from powder data registered with a Geiger-Mueller diffractometer using Cu$K\alpha$ radiation. A probable arrangement of the oxygen atoms has been obtained from space considerations. The point positions are:

3Hg in $3(a)$:$x0\frac{1}{3}$, $0x\frac{2}{3}$, $\bar{x}\bar{x}0$ with $x = 0.745$
3O in $3(b)$:$x0\frac{5}{6}$, $0x\frac{1}{6}$, $\bar{x}\bar{x}\frac{1}{2}$ with $x = 0.46$

This structure is built up of infinite spiral chains -O-Hg-O- running parallel to the c axis of the hexagonal unit cell. The distances and angles within the chains are:

Hg-O 2.03 Å The angle Hg-O-Hg 109°
Hg-Hg 3.30 Å The angle O-Hg-O 180°

This atomic arrangement is isostructural with the hexagonal modification of mercury(II)sulphide (cinnabar)[2]. The Hg-O distance and the bond angles are identical with those found in the planar zigzag chains -O-Hg-O- in orthorhombic mercury(II)oxide [3].

This investigation is to be continued by means of neutron diffraction methods in order to investigate the proposed oxygen arrangement. Studies on the stability relations between the modifications of mercury(II)oxide are in progress.

Hg_2O_2NaI. Space group $P6_222$ No. 180. Unit cell dimensions $a = 6.667$ Å, $c = 10.054$ Å. Cell content 3 formula units of Hg_2O_2NaI.

The positions of the mercury and iodine atoms have been derived on the basis of single crystal data.

6 Hg in $6(f)$:$\frac{1}{2}0z\frac{2}{3}, 0\frac{1}{2}\frac{2}{3}+z, \frac{1}{2}\frac{1}{2}\frac{1}{3}+z$
$\frac{1}{2}0\bar{z}, 0\frac{1}{2}\frac{2}{3}-z, \frac{1}{2}\frac{1}{2}\frac{1}{3}-z$ with $z=\frac{1}{3}$
3 I in $3(c)$:$\frac{1}{2}00, 0\frac{1}{2}\frac{2}{3}, \quad \frac{1}{2}\frac{1}{2}\frac{1}{3}$

This investigation is being continued in order to find the positions of the sodium and oxygen atoms.

These studies form part of a research program financially supported by the *Swedish Natural Science Research Council.*

1. Laruelle, M. P. *Compt. rend.* **241** (1955) 802.
2. Aurivillius, K. *Acta Chem. Scand.* **4** (1950) 1413.
3. Aurivillius, K. *Acta Chem. Scand.* **10** (1956) 852.

Received July 11, 1957.