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Criteria for hydrogen bonding. II. A hydrogen bond in the edge of a coordination polyhedron around a cation.

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The bond length Cs-O(4) given in Table 1 in *Acta Cryst.* (1973), **B29**, 139 should be 3.515 Å.

Because of a misprint the value of the bond length Cs-O(4) in Table 1 (Baur, 1973) reads as 3.315 Å. The correct value of Cs-O(4) is 3.515 Å. Therefore the statement (Baur, 1973) 'that the distance Cs-O(4) to the acceptor atom of the hydrogen bond is the largest of the distances considered to belong to the coordination polyhedron around the Cs-atom' is correct after all, even though it is not apparent from Table 1 as

it was printed. Since atom O(4) is the acceptor atom of the hydrogen bond located in the edge of the coordination polyhedron around the Cs atom it is significant that Cs-O(4) is a long bond.

Reference

BAUR, W. H. (1973). *Acta Cryst.* **B29**, 139-140.

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Orientation relation in the transformation of the NaCl-related to the CsCl-related structure in rubidium nitrate.

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The structure transformation RbNO_3 I (NaCl-like) \rightarrow II \rightarrow III (CsCl-like) proceeds topotaxically, with an orientation relation in which $[100]_{\text{I}} \parallel [100]_{\text{III}}$. Despite the presence of the complex ion the relation is similar to one of the relations observed in the transformations NaCl-type \rightleftharpoons CsCl-type in NH_4Br .

It has already been shown that the forward and reverse transformations CsCl-type (simple cubic) \rightleftharpoons NaCl-type (f.c.c.) are topotaxial in that definite orientation relations result, and there is evidence that at least on supercooling the mechanism is martensitic (Fraser & Kennedy, 1972; Kennedy, Patterson, Chaplin & Mackay, 1973). It has not been known how far crystal-chemical relations can result in topotaxy when in addition to a large lattice deformation, the planar complex ions such as NO_3^- , CO_3^{2-} , must tilt during the transformation. Rubidium nitrate affords a test of this. In rubidium nitrate an NaCl-like f.c.c. phase (I) (having randomized orientations of anions) (Kennedy, 1970a; Strømme, 1971) is linked to a CsCl-like cubic phase III (Korhonen, 1951) through a phase II which is stable between 219 and 284°C. Phase II is commonly considered to be rhombohedral, calcite-like (*e.g.* Salhotra, Subbarao & Venkateswarlu, 1968) but tetragonal symmetry has also been suggested (Brown & McClaren, 1962). The primitive cubic cell of phase III is a sub-cell, the plane of the anion being differently oriented in neighbouring sub-cells. The volume change III \rightarrow I of 16% is the same as in CsCl and NH_4Br , but $\Delta V_{\text{III} \rightarrow \text{II}}/V_{\text{III}} = 0.1$ and $\Delta V_{\text{II} \rightleftharpoons \text{I}}$ is small, the remainder being accounted for by thermal expansion of II (Salhotra, Subbarao & Venkateswarlu, 1968). Because of the disruption previously observed at the transformation III \rightarrow II in needle-like crystals it has been considered that in practice the large structure and volume-change do not permit topotaxy (Brown & McClaren, 1962). Topotaxy in the transformation II \rightarrow I (Kennedy, 1966), and in I \rightarrow II with fine twinning (Kennedy, 1970a) has already been reported. The present work shows that a definite orientation

relation is also maintained between the NaCl-like phase I and the CsCl-like phase III during the transformations I \rightarrow II \rightarrow III.

Single crystals of RbNO_3 I were grown from the melt at 310°C on glass cover-slips on a flat heater carried on the goniometer head of an X-ray camera, which itself carried a detachable polarising microscope. Form I was oriented, and the orientation of III determined, by precession and front-reflexion Laue photographs, the X-rays being transmitted through the glass.

The resulting finely twinned specimens of phase II detwinned after 15 min, giving up to six reproducible orientations. When such detwinned specimens were maintained slightly below 219°C fine platelets of phase III appeared in three orientations within each single block of phase II (Kennedy, 1970b). The traces of the platelets were parallel to the traces of the twin-plane of the calcite-like structure. The platelets grew first into blocks and then into an irregular shape. Fine remnants of phase II trapped between adjacent regions of phase III could be supercooled to 164°C. Only one type of orientation was found both in individual specimens, and in repeated experiments:

$$\begin{aligned} (001)_{\text{I}} \parallel (011)_{\text{III}} \\ [100]_{\text{I}} \parallel [100]_{\text{III}} \end{aligned}$$

This however is a mean orientation. The reflexions were split into several components which corresponded to individual orientations differing from this mean by up to 5°. The splitting of the reflexions is probably due to variants of an irrational relation. This result is the converse of relation C of Kennedy, Patterson, Chaplin & Mackay (1973)