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Revealing Anion Order in Holmium Hydride Oxide HoHO by Neutron Diffraction

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Heteroanionic hydrides are an emerging class of compounds with representatives showing ionic conductivity [1] or catalytic activity [2]. For holmium hydride oxide HoHO, the disordered CaF₂ type structure was assigned and confirmed by powder neutron diffraction [2]. However, the analysis showed a deviation from the 1:1:1 composition: REH₂+xO_{1-x}. This demands the occupation of either octahedral interstices (H-rich) or the formation of defects (O-rich compound) and the differentiation and quantification of these species (H, O, voids) requests the combination of different methods. As the anionic ordering influences the ionic conductivity substantially [3], we conducted neutron diffraction measurements on both HoHO and the deuteride HoDO.

In contrast to the previous reports, both compounds crystallize in an ordered CaF₂ substructure with space group F-43m (Heusler-LiAlSi type; $a(\text{HoHO}) = 5.27550(13) \text{ \AA}$, $a(\text{HoDO}) = 5.27394(8) \text{ \AA}$) with no significant underoccupation, mixing of sites, or occupation of the octahedral interstice. They are the first ionic substances to crystallize in this structure type, which is usually observed for metallic half-Heusler phases. Furthermore, HoHO shows an unusual resistivity towards air, as it decomposes only above 600 K, independent of O₂ in the atmosphere.

1 K. Fukui et al., Nat. Commun. 2019, 10, 2578.

2 H. Yamashita et al., J. Am. Chem. Soc. 2018, 140, 11170.

3 H. Ubukata et al., Chem. Mat. 2019, 31, 7360.

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