

MS29-1-6 Fractal transitions of selenourea

#MS29-1-6

K. Roszak¹, A. Katrusiak¹

¹Faculty of Chemistry, Adam Mickiewicz University - Poznan (Poland)

Abstract

Fractal phase transitions have been found in the crystal lattices of selenourea, $\text{SeC}(\text{NH}_2)_2$. At room temperature, selenourea crystallizes in phase α , of the enantiomorphic space-group type $P3_1$ and the unit cell containing nine symmetry-independent molecules, i.e. the Z' number equal to 9 [1-3]. The lattice of phase α is similarity-related to that of a 3-fold smaller unit-cell ($Z'=3$), which in turn is likewise related to another 3-fold smaller unit-cell ($Z'=1$), all of the same space-group type. Indeed, at 374 K, phase α transforms to phase γ , for which the space-group type $P3_1$ is retained, and the Z' number is reduced to 3. The same similarity fractal rule relating phases α and γ , also applies to the lattice of a hypothetical phase δ ($Z'=1$). Analogous fractal rules like this between the α - γ - δ phases of selenourea have been identified also for other compounds described in the literature. The unit-cell dimensions in crystals naturally limit the down-scaling of all natural fractals. The temperature-induced fractal transitions described for selenourea α - γ - δ phases, contrast with the high-pressure transition at 0.21 GPa to phase β , which is centrosymmetric and for which the aggregation of molecules is significantly different [1]. Relations between crystallographic macroscopic and microscopic fractals will be discussed.

References

- [1]. Roszak K, Katrusiak A. High-pressure and environment effects in selenourea and its labile crystal field around molecules. *Acta Crystallogr Sect B* 2021, 77, 449–455. DOI: DOI: 10.1107/S205252062100398X
- [2]. Luo Z, Dauter Z. Embarras de richesses—It is not good to be too anomalous: Accurate structure of selenourea, a chiral crystal of planar molecules. *PLoS One*. 2017, 12, e0171740(1–13). DOI:10.1371/journal.pone.0171740
- [3]. Rutherford JS, Calvo C. The crystal structure of selenourea. *Z. Kristallogr.* 1969, 128, 229–258. DOI: 10.1524/zkri.1969.128.3-6.229