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# Is bis (thiourea) strontium chloride a potential optoelectronic material?

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## Abstract

The authors of a recent paper (Optik 127 (2016) 3582–3589) report to have grown a so called bis (thiourea) strontium chloride (BTSC) and claim it to be a potential optoelectronic material. In this comment it is shown that this claim is dubious and BTSC reported once earlier by Hajiyani et al (Modern Phys. Lett. B, 21 (2010) 735–747) is actually thiourea.

**Keywords**: bis (thiourea) strontium chloride; optoelectronic; dubious crystal; thiourea

## Comment

During a literature survey of metal-thiourea compounds, a claim of Rajagopalan and Krishnamoorthy [1] reporting on the growth of a so called bis (thiourea) strontium chloride (BTSC) **1** attracted my attention because the oxophilic alkaline-earth metal strontium is not known to bind to a S-donor ligand like thiourea. Hence, the paper was taken up for scrutiny to verify the claim. A perusal of the paper revealed that crystals of **1** previously reported by Hajiyani et al [2] were grown by the slow evaporation of an aqueous solution containing strontium chloride and thiourea in 1:2 mole ratio. The authors of [1] claim to have characterized **1** with the aid of single crystal X-ray diffraction and reported, "*The structure has been solved and refined by the full-matrix least-square method using SHELXL program*". However, only the unit cell parameters and the space group ($Pna2_1$) but no CIF file was reported. Hence, the single crystal work cannot be considered as reliable. Without providing CIF data, the authors declared that the Sr(II) in **1** is four coordinated and bonded to two S atoms from two thiourea ligands and two chlorine atoms and also provided an ellipsoidal figure and claimed "*This creates a three-dimensional bonding network, due to which its thermo mechanical properties may be improved*". This claim can be termed absurd because the proposed structure

without any bridging ligands shows discrete units. The dubious nature of the X-ray work is revealed by the thermal study and IR spectrum, which contradict the single crystal findings. Although it was reported that the elemental analysis for **1** is in agreement for the formula $Sr[CS(NH_2)_2]_2Cl_2$ ($CS(NH_2)_2$ = thiourea), it is observed that the TG curve (referred to as TG spectrum by authors) does not show any residue indicating that **1** does not contain any Sr but is an organic compound. The reported IR spectrum of **1** is in accordance with the thermal study as it perfectly matches with the spectrum of thiourea proving that **1** is actually thiourea [3]. The IR spectral result can be better explained due to no chemical reaction between the oxophilic Sr(II) and thiourea and the fractional crystallization of the less soluble thiourea. Similar cases of fractional crystallization of thiourea have been demonstrated recently [3, 4]. Since thiourea is a centrosymmetric solid, the observation of SHG signal (1.54 times of KDP) for **1** appears to be another dubious claim. In view of the above mentioned discussion, one wonders if any single crystal measurement or elemental analysis was really performed.

In summary, a so called bis (thiourea) strontium chloride reported in [1] and earlier by Hajiyani et al [2] is not a potential optoelectronic material but a dubious crystal.

Footnotes

Compound is identified by number **1** to avoid use of non-standard code.

## References

[1] N.R. Rajagopalan, P. Krishnamoorthy, Contemporary studies on growth and characterization of bis (thiourea) strontium chloride—A potential optoelectronic NLO material, Optik 127 (2016) 3582–3589.

[2] R.R. Hajiyani, D.J. Deve, C.K. Chauhan, P.M. Vyas, M.J. Joshi, Growth and charcaterization of bis-thiourea strontium chloride single crystals, Modern Phys. Lett. B, 21 (2010) 735–747.

[3] B.R. Srinivasan, On the existence of 'thiourea urea magnesium chloride' and 'urea thiourea sodium chloride' J. Therm. Anal. Calor. **119** 985-988 (2015).

[4] B.R. Srinivasan, Z. Tylczyński, On the crystal growth of ‘tris thiourea chromium(III) sulphate’, ‘potassium thiourea thiocyanide’ and ‘bis thiourea iron(II) sulphate’ J. Therm. Anal. Calor. **121** 1183-1184 **(**2015).