

MS19-2-3 Selenium in Charge Density Investigations

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R. Herbst-Irmer¹

¹Georg-August-Universität - Göttingen (Germany)

Abstract

Selenium compounds pose a challenge for X-ray structure analysis and especially for charge density studies because, on the one hand, selenium has a relatively high absorption coefficient at the Mo wavelength ($\lambda = 0.71073 \text{ \AA}$) and, on the other hand, shows X-ray fluorescence.

In spite of these problems, we were interested in the investigation of non-covalent interactions in the compounds dibenzyl diselenide BnSeSeBn (**1**) [1] and 1-mesitylselanyl-8-(dimethylsilyl)naphthalene (**2**) [2]. In **1** very short intermolecular Se \cdots Se distances of 3.44 Å were observed, while in **2** the Si–H \cdots Se contact caught our attention.

Several datasets for **1** were collected at different in-house diffractometers with various X-ray wavelengths, intensities and detectors at 100 K. Unfortunately, all multipole refinements ended up with two relatively high residual density peaks in the proximity of selenium at similar positions for all datasets. At the end, these peaks could be explained as disorder with radiation-induced radical species BnSeSe•/•Bn. This made a charge density investigation impossible, but extended DFT methods and solid state EPR showed that not only organo-selenide radicals like RSe• may occur, but also organo diselenide BnSeSe• radicals and organic radicals R•, which is particularly important to know in structural biology.

Also, the investigation on **2** was challenging. Resolution dependent errors need to be cured to model the Se atom properly and to characterize the Si–H \cdots Se contact as chalcogen–hydride bond.

References

[1] Schürmann, C. J., Teuteberg, T. T., Stückl, A. C., Ruth, P. N., Hecker, F., Herbst-Irmer, R., Mata, R. A. & Stalke, D. (2022). *Angew. Chem. Int. Ed.*, e202203665.

[2] Keil, H., Herbst-Irmer, R., Rathjen, S., Girschik, C., Müller, T. & Stalke, D. (2022). *Inorg. Chem.* **61**, 6319–6325.