

MS19-P4 SACADA-the database of three periodic carbon allotropesAndrey A. Golov^{1,2}, Artem A. Kabanov¹, Davide M. Proserpio^{1,3}, Vladislav A. Blatov^{1,2}

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Nowadays the modeling of new carbon allotropes is very popular. There are more than 400 articles on the topic of hypothetical carbon allotropes by the data of Scopus database [1]. Mistakes in classification and naming of carbon allotropes are almost inevitable due to vast amount of unsystematized data. For example, the (RL3)2 structure was described for the first time in 1997 [2] and then rediscovered in 2013 [3] under the name of oC32. Another example of typical mistake is an assigning the same name to several different structures. For instance, Y-carbon corresponds to different structures in articles [4, 5]. The main purpose of the work is accumulation and systematization of the data on all three periodic carbon allotropes. We have extracted the data of crystal structures and physical properties for 260 unique carbon allotropes (corresponding to 236 topological types) from 195 articles. The topological characteristics of the structures were calculated by ADS program implemented in ToposPro [6]. The maximal symmetry embeddings of the nets corresponding to 236 topological types were obtained by Systre program [7]. The all results of the study are presented in Samara Carbon Allotrope Database (Fig.1) [8].

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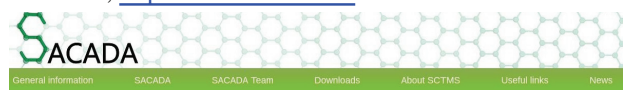


Figure 1. Image of SACADA.

Keywords: New carbon allotropes, topology of crystal structure, SACADA database.

MS19-P5 Syntheses and crystal structures of novel Zr(SeO₃)(SeO₄) and Zr(SeO₄)₂·H₂OGerald Giester¹, Manfred Wildner¹

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Two new compounds, a) Zr(SeO₃)(SeO₄) and b) Zr(SeO₄)₂·H₂O, were obtained in the course of a long-term project focusing on the crystal chemistry of Se⁴⁺, 6+ - M⁴⁺ oxysalts with M⁴⁺ = Ti, Zr, Hf, as well as Mn, Ge, Sn and Pb [1,2].

Both phases were synthesized at low-hydrothermal conditions (Teflon-lined steel vessels, 220°C) from mixtures of Zr₂O₂(CO₃)(OH)₂, H₂SeO₄ and minor contents of water. Colorless single crystals up to 0.2 mm in length were obtained within a period of one week and were studied by single crystal X-ray techniques (Bruker APEXII diffractometer, MoK α Incoatec Microfocus Source, 293 K). The crystal structures were solved and refined by a package of SHELX programs [3]. Zr(SeO₃)(SeO₄) crystallizes in the orthorhombic space group *Pbca* (No. 61), with $a = 8.295(2)$, $b = 9.476(2)$, $c = 15.370(3)$ Å, $V = 1208.1(5)$ Å³, $Z = 8$, $R_1 = 0.0316$; Zr(SeO₄)₂·H₂O is monoclinic, space group *P2₁n* (No. 14), with $a = 5.332(1)$, $b = 7.962(2)$, $c = 16.256(3)$ Å, $\beta = 92.19(1)^\circ$, $V = 689.6(3)$ Å³, $Z = 4$, $R_1 = 0.0195$.

Zr(SeO₃)(SeO₄) and Zr(SeO₄)₂·H₂O represent new structure types built from isolated a) ZrO₆ octahedra or b) ZrO₇ pentagonal dipyramids, further cornerlinked via a) SeO₄ tetrahedra and trigonal SeO₃ pyramids or b) only SeO₄ groups to three-dimensional frameworks. Mean cation-oxygen bond lengths, a) Zr⁶⁺: 2.063 Å, Se⁴⁺: 1.679 Å, Se⁶⁺: 1.623 Å and b) Zr⁷⁺: 2.137 Å, Se⁶⁺: 1.631 Å, Se²⁶⁺: 1.635 Å, are in accordance with literature. In case of b) one H₂O group is ligand of the ZrO₇ coordination forming hydrogen bonds with 2.65 and 2.76 Å donor-acceptor distances.

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Keywords: Zr(SeO₃)(SeO₄), Zr(SeO₄)₂·H₂O, crystal structure