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MS43-O4

Assigning transition metal oxidation states to entries in the cambridge structural database

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In coordination chemistry the concept of formal oxidation states is essential to the understanding of metal centre geometries and in the interpretation of corresponding chemical and physical characteristics. The Cambridge Structural Database (CSD) currently contains over 400,000 transition metal-containing entries,[1] however only about half contain a specified oxidation state. Surveying and editing the remaining entries is far too resource and time intensive to be carried out manually. A system in which entries missing this information can be quickly analysed and rectified is particularly desirable. Procedures have already been explored that could potentially semi-automate oxidation state validation by using the Bond Valence Sum (BVS) Method.[2] This method proposes that the valence of an atom can be determined using only knowledge of its bond lengths, atomic neighbours, and some predetermined constants.[3]

Here we present the implementation of BVS to the CSD through CSD python API scripts, discussing the strengths and limitations of the method. Testing of the BVS method against entries containing named oxidation states has already proved applicable to over 80% of entries with a 94% success rate across over 40,000 structures. We also explore the use of complementary methods for improved assignment confidence and greater applicability, addressing potential issues with the BVS method. A process in which ligand fragment charges are automatically assigned from computational formation energy calculations is discussed, resulting in a combined methods assignment success for over 99% of transition metal environments.

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