MS14-P01 | Reassessing Pauling's Rules

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Pauling's rules play an essential role for solid state chemistry [1,2]. In the first publication of the rules, Pauling has already mentioned several of their drawbacks [2]. For instance, they are expected to only work for very ionic compounds such as oxides [2]. Surprisingly, there is no statistical sound answer on how well *all* Pauling's rules perform for oxides up to today. We will provide such an answer in this contribution. To do so, all five Pauling rules are checked on around 6000 oxides from the Materials Project [3] that originally stem from the experimental database ICSD. We will start from a very recent analysis of the statistics of the coordination environments of oxides [4]. Structural exceptions from the rules and trends within the exceptions will be discussed.

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