

Adventures in Symmetry with GSAS-II

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To honor the memory of the first recipient of the Trueblood Award, Dick Marsh, who spent much of his career in pursuit of correct crystallographic symmetry [1, 2], I would like to present some of my thoughts on space group treatment. How do we know when we have the optimal space group to describe a structure? What does optimal mean anyway?

The key concept for this talk will be that of subgroup and supergroup relationships, which create family trees for space groups and a “relatively” convenient way to consider the idea of extra and missing symmetry [3, 4]. Fortunately for us, crystallographers in Bilbao, Spain have provided a web site that facilitates finding these interrelationships between space groups [5]. In our work on GSAS-II [6], we want to provide tools to encourage examination of symmetry choices for structures. I will talk about what has been done and where we plan to go with this.

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References

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