



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

Volume 56 (2023)

Supporting information for article:

***CrysFieldExplorer*: software for rapid optimization of the crystal field Hamiltonian**

Qianli Ma, Xiaojian Bai, Erxi Feng, Guannan Zhang and Huibo Cao

Section S1. Complete results of $\text{Er}_3\text{Mg}_2\text{Sb}_3\text{O}_{14}$ CEF parameters from *CrysFieldExplorer*

We provide the complete 150 solutions produced by *CrysFieldExplorer* plotted versus the custom-defined χ^2 as mentioned in the main paper. Panel (b) of Fig. S1 shows the rotational angle α instead of B_2^1 . It follows from the calculations by Rudowicz (1985, 1986). Under this transformation rule, all B_2^1 become 0. No obvious segregation is observed for solutions with $\chi^2 < 1$, suggesting there exist multiple solutions that fit the given observables (neutron scattering, susceptibility, magnetizations) almost equally well.

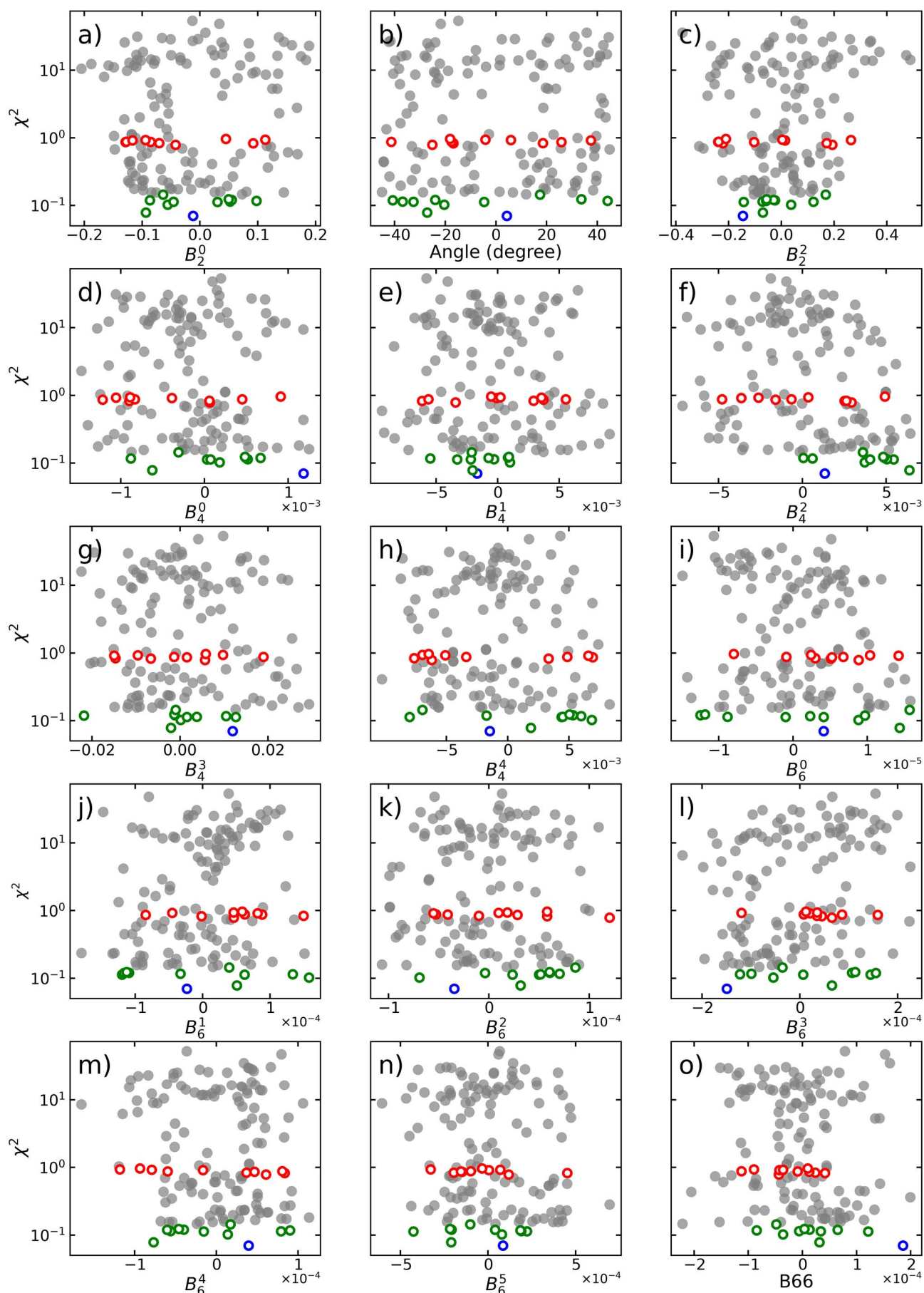


Fig. S1 A complete list of all 15 CEF parameters of EMSO. They are plotted against the custom-defined χ^2 on a log plot. The open green circles indicate the top ten solutions and the open red circles indicate the last ten solutions from CrysFieldExplorer with $\chi^2 < 1$.

References

Rudowicz, C. (1985). *J. Magn. Reson.* **63**, 95-106.

Rudowicz, C. (1986). *J. Chem. Phys.* **84**, 5045-5058.