

Inorganic Chemistr

Page 7622. Two crystal structure solutions were treated by the following method. Substantial numbers of reflections, at various angles, were deleted primarily because of their large deviation between F_{obs} and F_{calc} as shown by the SHELXL-97 refinement program (in the relevant *.LST file). We did this because the large scattering of the heavy-metal centers in these polyoxometalate compounds (such as W and Mo) can, in our view, lead to unreliable reflections during collection of the crystal data. Reviewers have pointed out that this is not an appropriate method of crystal structure refinement and that it is not appropriate to delete reflections primarily because their F_{obs} deviates from that in the preferred structure solution. The two compounds are $K_4Na_{10}[\alpha_1-CuP_2W_{17}O_{60} (OH)_2 \sim 58H_2O$ (1), for which 129 reflections were deleted, and $Na_3[H_2hn]_{2.5}[\alpha_1-P_2W_{17}O_{60}Cu(OH)_2] \cdot \sim 14H_2O$ (3), for which 54 reflections were deleted. In both cases, the deletion of reflections did not affect the completeness of the data and did not materially change the structural results. A revised CIF for each structure is given as Supporting Information.

Supporting Information Available: Crystallographic data in CIF format. This material is available free of charge via the Internet at http://pubs.acs.org.

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