Supplementary Information Submitted to *Materials Advances*

Microwave-Assisted Intercalation: Exploring Electronic and Structural Features of Metastable MMo_6S_8 (M = Ag, Sn)

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XAS experiments and data analysis

Sample preparation

Prior to acquiring data all sample powders were ground as fine as possible using a mortar and pestle and then to obtain the smallest particles a suspension was made with acetone. This suspension was then added drop wise to a glass slide and set to dry. The dried powder was carefully scraped and placed onto Kapton tape in the XAS sample holder.

XANES analysis

XANES data was averaged in *Athena*[1] version 0.0.26. Processing of data was also performed in *Athena* including beam energy shift and the normalization of the pre and post edge regions. To analyze both the Mo L_3-edge and S K-edge spectra, data was truncated ~ 50 eV after the S K-edge to separate overlapping edges and allow for separate analysis. Normalized spectra can be found in Figure 3 and the first derivatives of the Mo L_3-edge can be found in Figure S6.

EXAFS analysis

Mo K-edge EXAFS data was processed similarly to XANES with an additional step to remove the background for the Mo K-edge spectra. Once processed the data was imported into *Artemis* version 0.9.26. In the software data is fit with theoretical models from a .cif file from the Inorganic Crystal Structure Database (ICSD) using an IFEFFIT model to perform calculations.[2]

For the fit, amplitude reduction factors (S_0^2) accounts for the multiple-electron excitations of the absorbing atom and was treated as set parameters and based on the appropriate metal references.[3] Debye-Waller factors (σ^2) which correlate to the thermal motion of a system were defined as being the same for any pathways with similar bonding environments and left as a floating parameter. ΔE_0 accounts for the relative difference between the edge position of the elements and the edge position from the FEFF calculation and was left as a floating parameter. Experimental E_0 can be seen as the first derivative of the Mo K-edge plot shown in Figure S9. All parameter details extracted from the fit shown in Figure 4 are in Table S3 and Table S4. The normalized first derivative for the Mo K-edge can be found in Figure S10. The data and fit is also represented in k-space in Figure S10. Extracted Mo-Mo_{intra} path lengths were used to calculate % anisotropy and the associated error according to equation 1 and equation 2.[4]

Computational details from collaborators

Bader charges of $AgMo_6S_8$, $SnMo_6S_8$, $CuMo_6S_8$, and $Cu_2Mo_6S_8$ were calculated using the Bader Charge Analysis Code.[5–8] The charge calculated for each intercalated cation is the difference between the valence charge in the pseudopotential for each element and their Bader valence charge.

MBXAS spectra were calculated according to the method outlined in.[9] In short, for a given elemental X-ray absorption edge (S in this case), we use density functional theory (DFT) to calculate the set of ground state and core-excited state Kohn-Sham (KS) orbitals – these are the outputs of two separate self-consistent field DFT calculations: one regular DFT calculation and the other employing a modified pseudopotential to introduce the core-excitation on a specific (S) atom. This process is repeated for each potentially excited atom within a supercell model of the condensed phase system under periodic boundary conditions – the supercell must be sufficiently large (>=1nm in linear dimension) to reduce the periodic interactions between the core-excited atoms. With these two sets of KS orbitals, we model the many-electron states as single Slater determinants – the ground state constructed from the occupied electronic orbitals and the core-excited states constructed from various configurations of that set of orbitals, typically including single electron-hole pair excitations involving the core-hole. X-ray absorption transition probabilities are calculated using the electric field dipole operator between the ground and core-excited states. Specifically, within the MBXAS formalism, there are contributions to the excitation intensity that can be viewed as originating from the polarization response of the occupied valence electrons to the core excitation, as outlined in more recent work on the MBXAS method defined within the core-excited orbital basis.[10] Simulated spectra have a final rigid shift applied to their excitation energies to match with experimental measurements – the pseudopotential model for the core-excited atoms does not accurately capture the core-excitation energy. However, this alignment is only performed once for all excited atoms of the same element and relative excitation energies between symmetry-distinct atoms (so-called chemical shifts) are captured within the method at the accuracy of DFT formation energy differences.

Table S1. Lattice parameters from Rietveld Refinement.

Parameter	$AgMo_6S_8$	$SnMo_6S_8$
R_{wp} (%)	14.596	11.074
MMo_6S_8 R_f (%)	4.385	5.284
Mo_6S_8 R_f (%)	4.809	4.907
A (Å)	9.272	9.304
C (Å)	11.181	10.839
Vol. ($Å^3$)	832.528	812.619

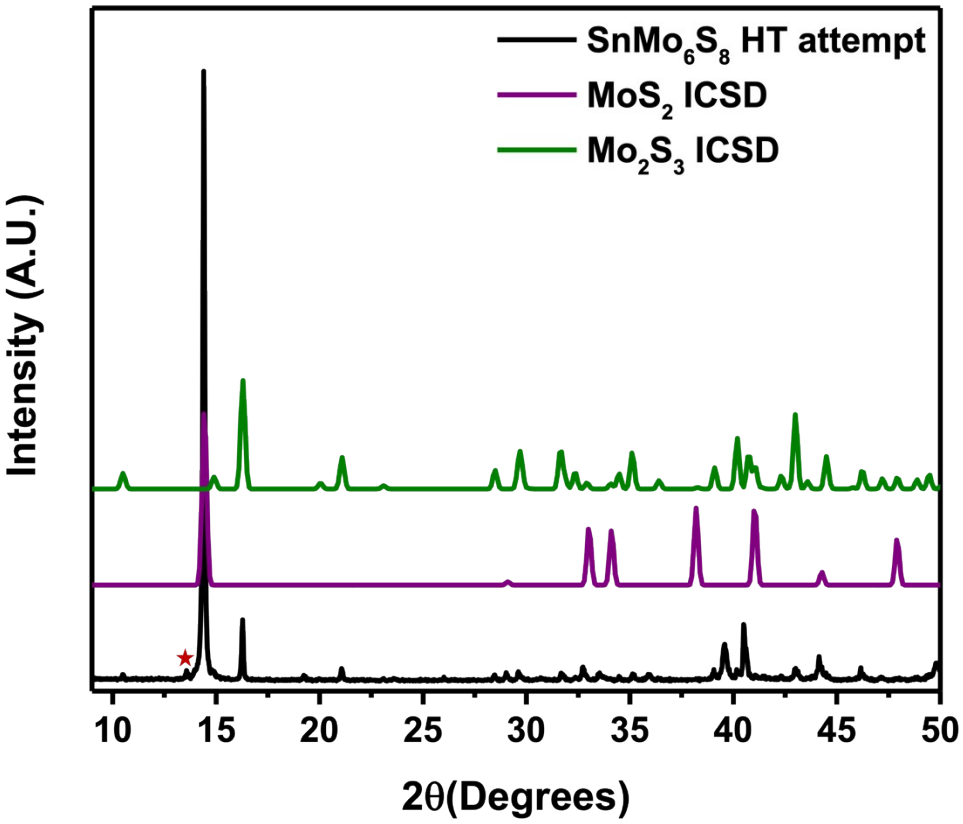

Figure S1. PXRD pattern of a high temperature microwave-assisted solid-state synthesis attempt showing major phases as MoS_2 and Mo_2S_3. The small star indicates the (101) peak associated with $SnMo_6S_8$.

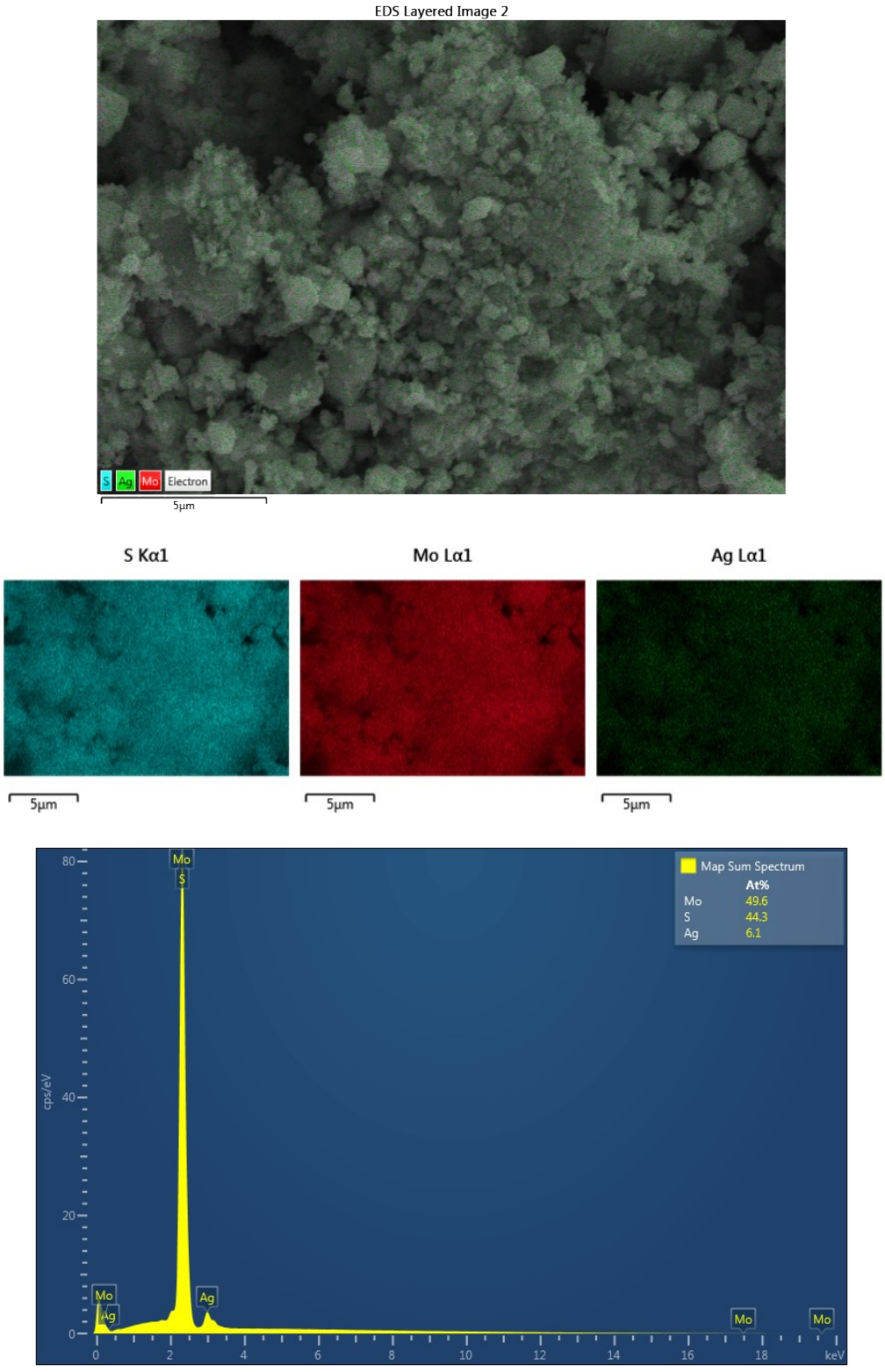

Figure S2. EDS Map sum spectra of $AgMo_6S_8$ shows homogeneous distribution of Ag throughout CP particles

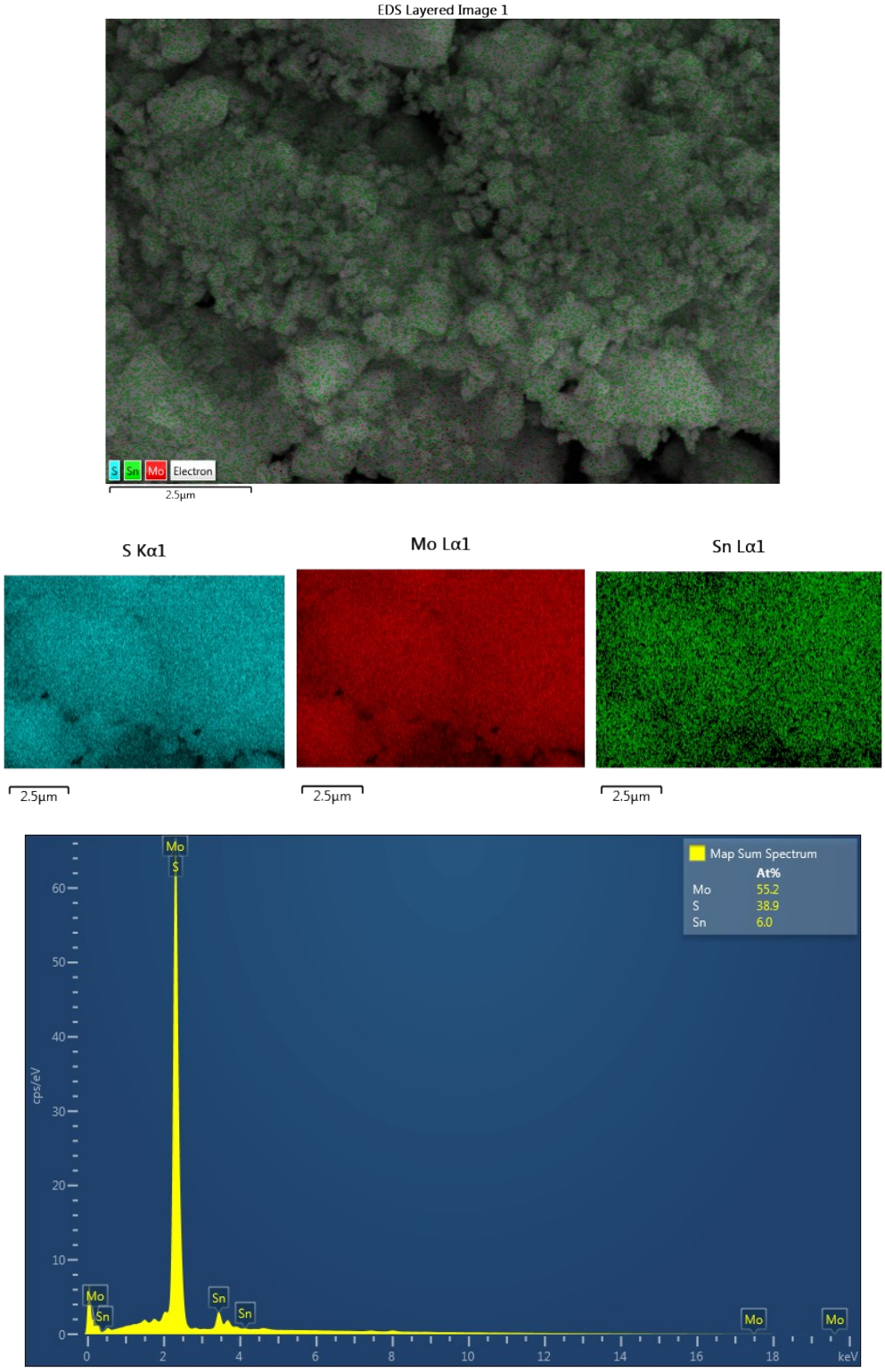

Figure S3. EDS map sum spectra of $SnMo_6S_8$ shows homogeneous distribution of Sn throughout CP particles.

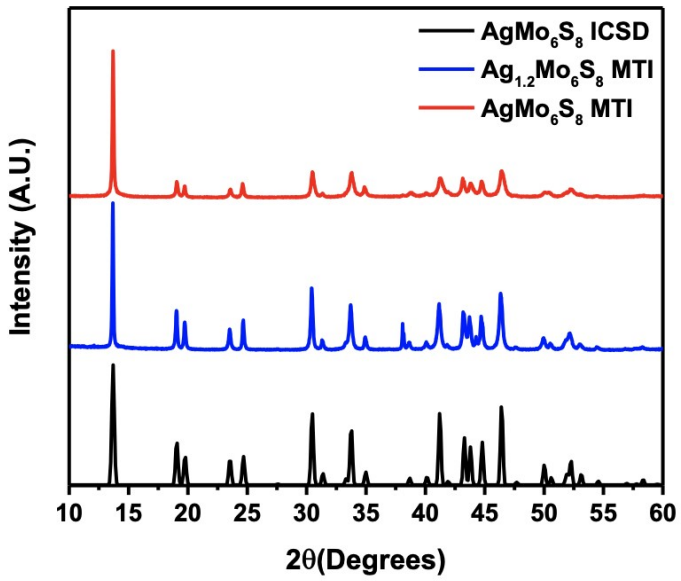

Figure S4. PXRD of $AgMo_6S_8$ with varying amounts of Ag content.

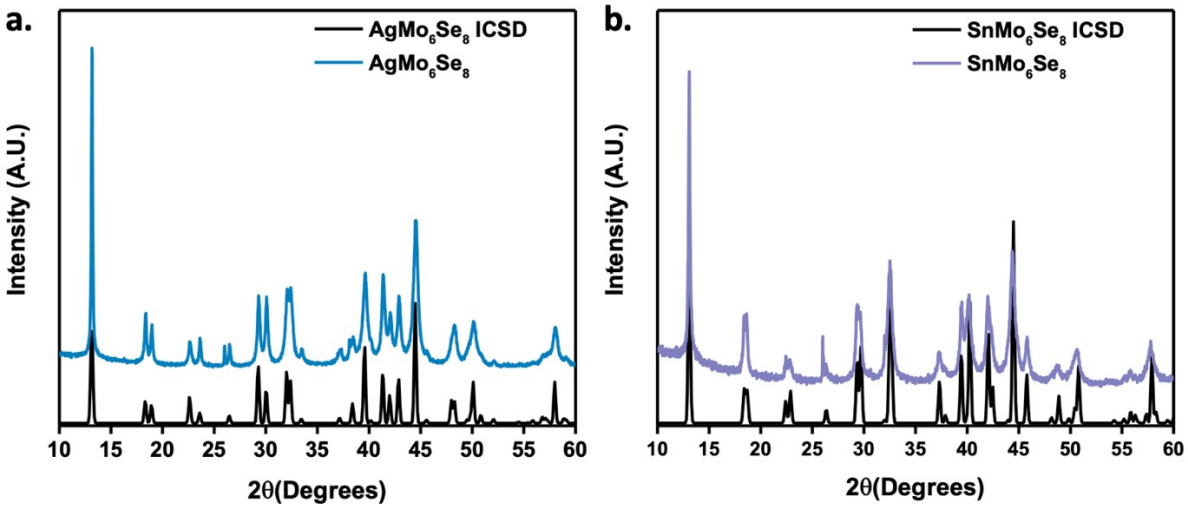

Figure S5. PXRD of a.) $AgMo_6Se_8$ and b.) $SnMo_6Se_8$.

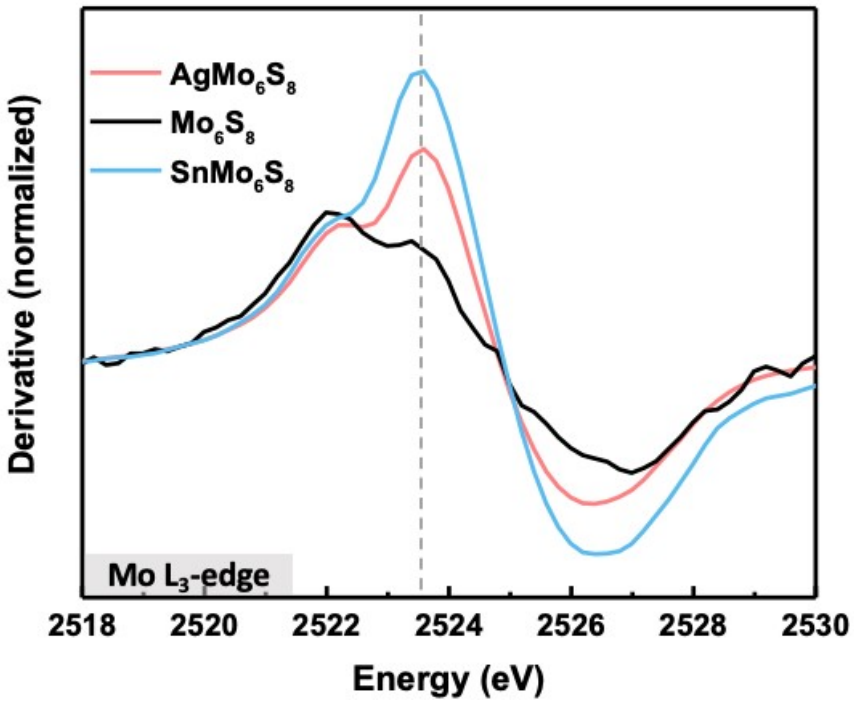

Figure S6. Mo L_3-edge plotted as normalized first derivative with dashed lines indicating peak maxima.

Table S2. Calculated Bader charges on intercalated metal cation in $AgMo_6S_8$, $SnMo_6S_8$, $CuMo_6S_8$, and $Cu_2Mo_6S_8$. For Ag and Cu about half an electron is donated per metal intercalant is donated to the Mo_6S_8 cluster resulting in assigned oxidation state +1. Sn donates more electrons to the Mo_6S_8 cluster resulting in assigned oxidation state +2.

Chevrel Phase	Bader Charge	Oxidation State
$AgMo_6S_8$ (Ag)	+0.49	+1
$SnMo_6S_8$ (Sn)	+0.93	+2
$CuMo_6S_8$ (Cu)	+0.60	+1
$Cu_2Mo_6S_8$ (Cu)	+0.57	+1

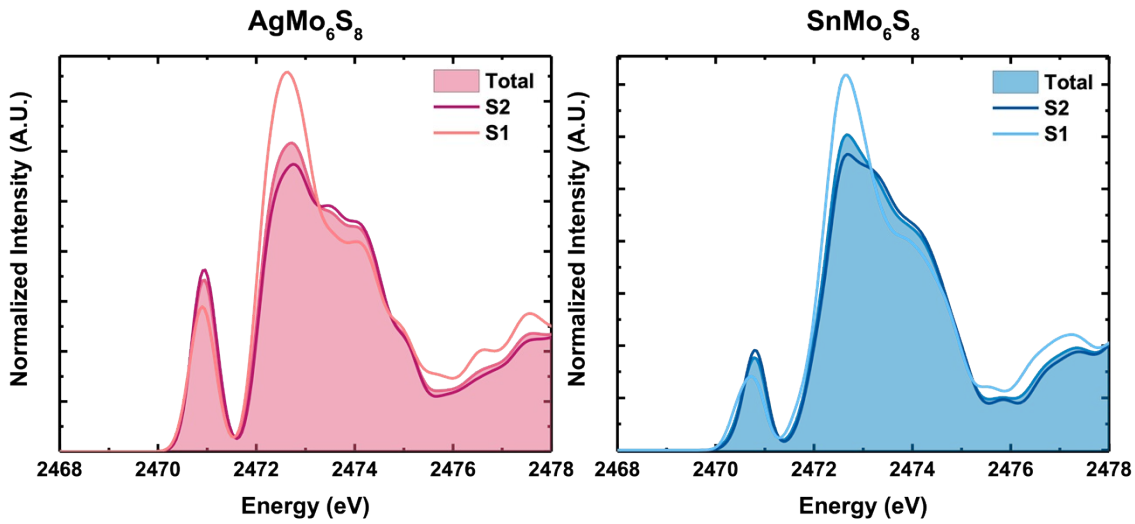

Figure S7. Calculated sulfur K-edge spectra of $AgMo_6S_8$ and $SnMo_6S_8$ for S1, S2, and total contribution.

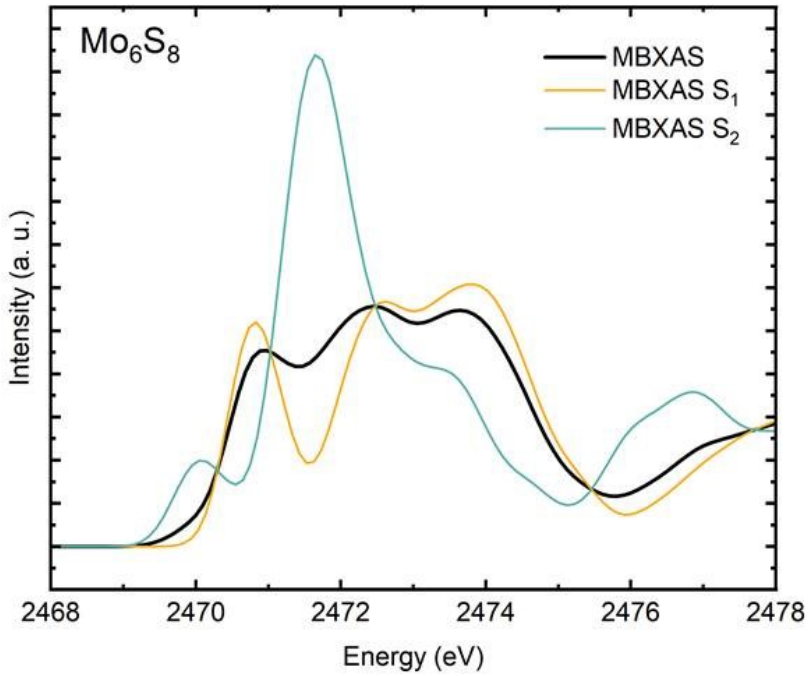

Figure S8. Calculated sulfur K-edge spectra of Mo_6S_8 for S1, S2, and total sulfur contribution reproduced from Hyler et. al with permission.[11]

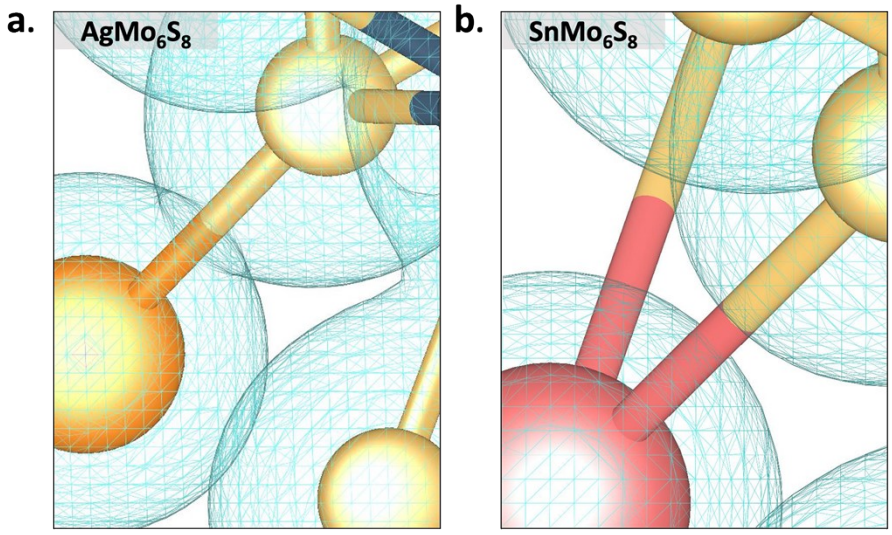

Figure S9. Close up visual representations of electron density for specific isosurface values surrounding a.) Ag in $AgMo_6S_8$ and b.) Sn in $SnMo_6S_8$.

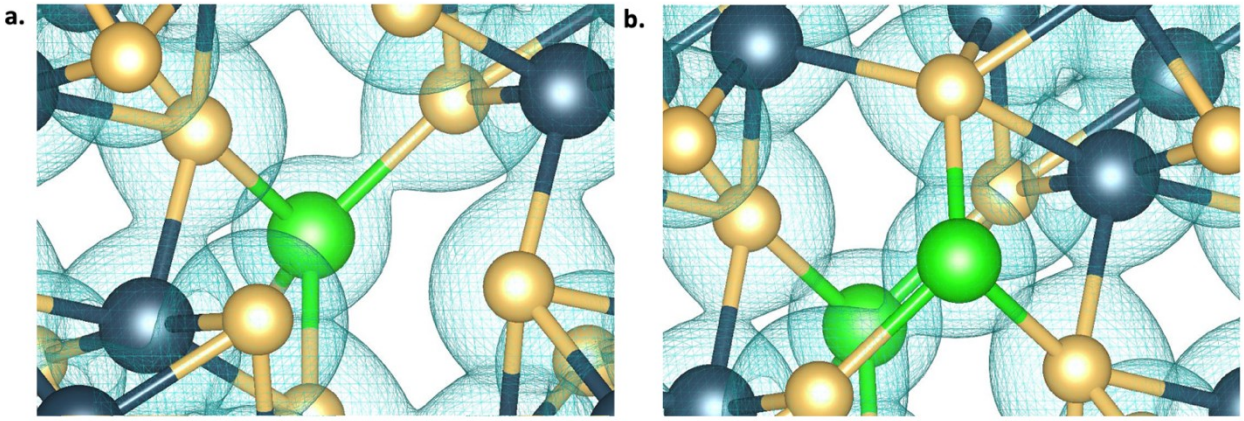

Figure S10. Visual representation of isosurface values for a.) $CuMo_6S_8$ and b.) $Cu_2Mo_6S_8$.

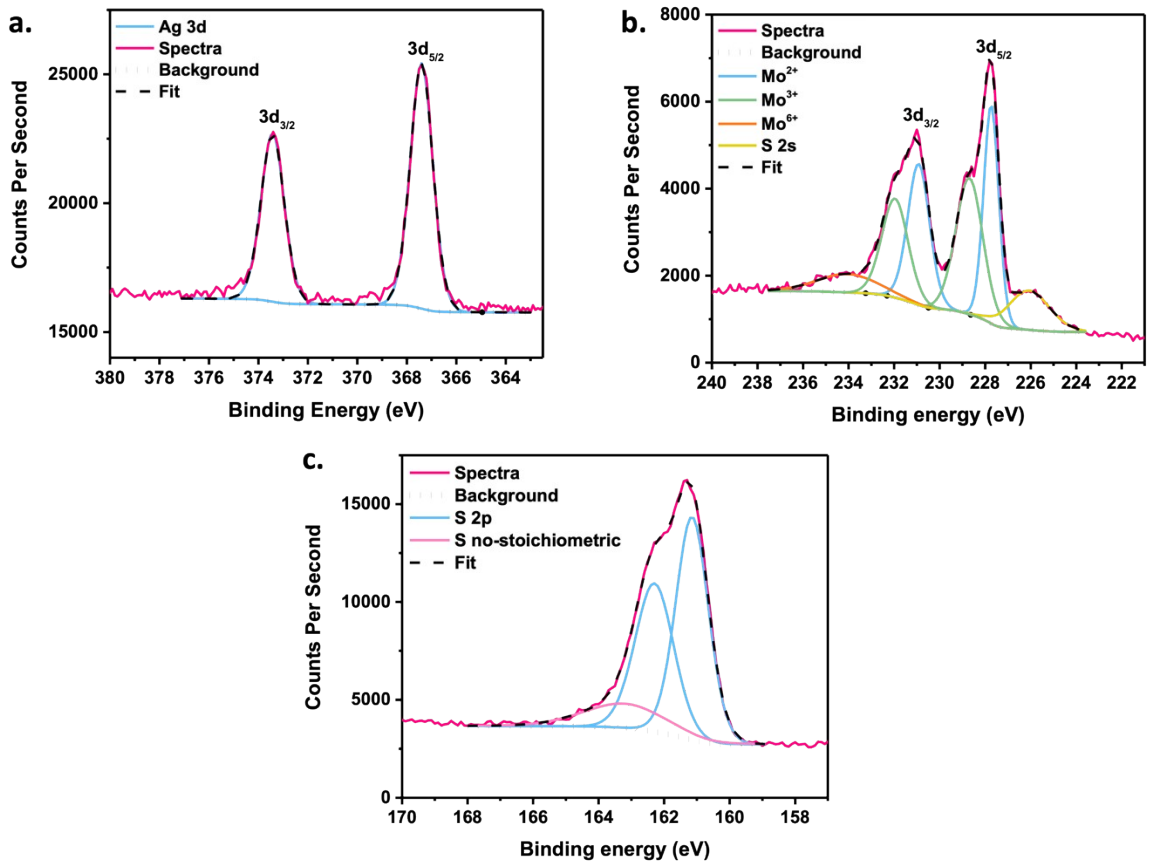

Figure S11. XPS for $AgMo_6S_8$ with a.) Ag 3d spectra, b.) Mo 3d spectra and c.) S 2p spectra/ Mo 3d and S 2p spectra are in good agreement with previously published CP XPS data. Mo^{6+} is a result of a native oxide layer consistently seen in CPs.

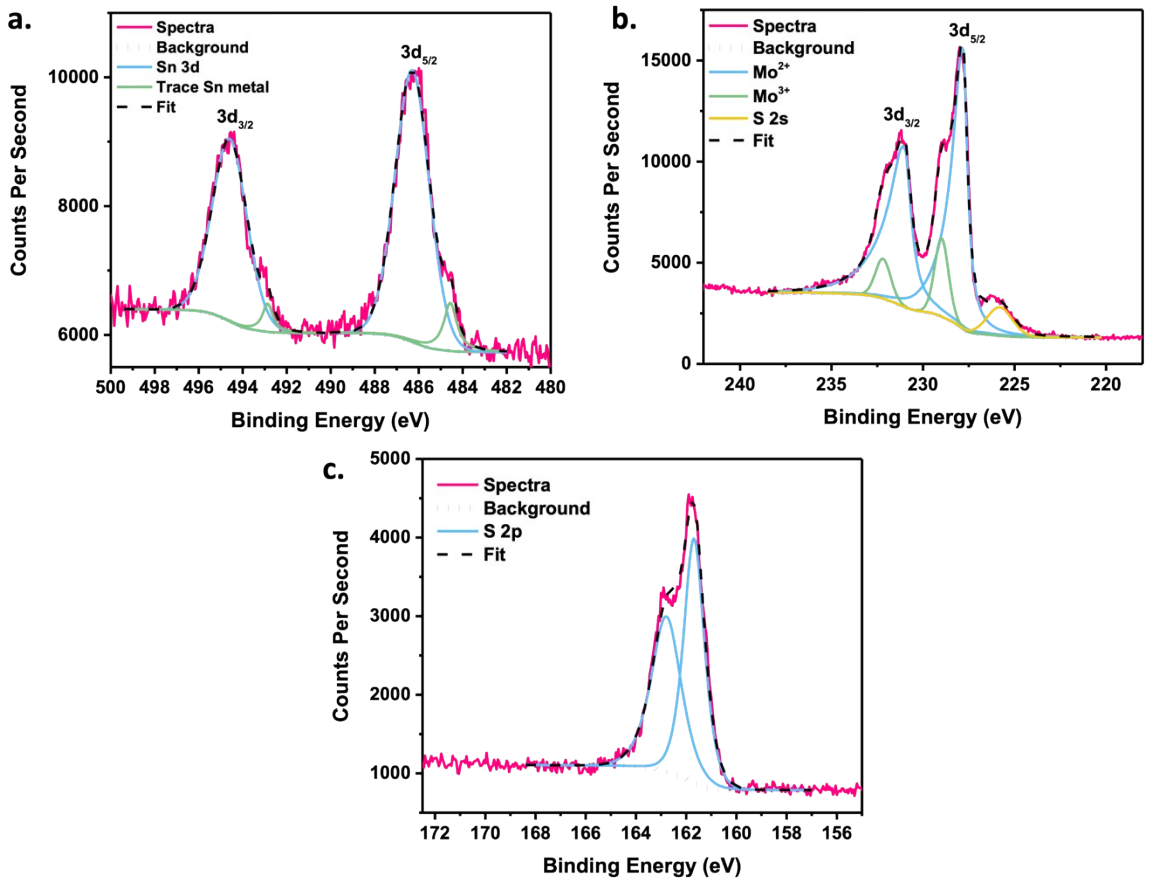

Figure S12. XPS for $SnMo_6S_8$ with a.) Sn 3d spectra, b.) Mo 3d spectra, and c.) S 2p spectra. Mo 3d and S 2p spectra are in good agreement with previously published CP XPS data. No Mo^{6+} is seen as etching prior to data collection was performed at a higher voltage.

Table S3. Fitting parameters for the Mo K-edge of SnMo6S_8. S_0^2 is the amplitude factor, ΔE_0 is the energy offset of the white line between the E_0 from table SX and that calculated by FEFF, σ^2 is the Debye-Waller Factor, N is the scattering pathway degeneracy. The distances obtained by the EXAFS analysis are listed as absorber-scatterer pairs.

Chevrel-phase	Parameter	Value		R-factor
$SnMo_6S_8$	S_0^2	.85	set	0.0162765
	ΔE_0	0.53	+/- 0.651	
	σ^2_{Mo}	0.005	+/- 0.0004	
	σ^2_S	0.003	+/- 0.001	
	Mo-S1	2.39 Å	+/- 0.003	
	Mo-S2	2.45 Å	+/- 0.003	
	Mo-Mo1	2.67 Å	+/- 0.004	
	Mo-Mo2	2.72 Å	+/- 0.004	
	Mo-Mo3	3.17 Å	+/- 0.07	
	N (Mo-S1)	1	set	
	N (Mo-S2)	2.92	+/- 0.291	
	N (Mo-Mo1)	2	set	
	N (Mo-Mo2)	2	set	
	N (Mo-Mo3)	1	set	
	R-range	1.25 – 4 Å	set	
	k-range	3 – 13.9 Å	set	

Table S4. Fitting parameters for the Mo K-edge of $AgMo_6S_8$.

Chevrel-phase	Parameter	Value		R-factor
$AgMo_6S_8$	S_0^2	.85	set	0.0189861
	ΔE_0	2.11	+/- 0.633	
	σ^2_{Mo}	0.007	+/- 0.001	
	σ^2_S	0.002	+/- 0.001	
	Mo-S1	2.42 Å	+/- 0.007	
	Mo-S2	2.48 Å	+/- 0.007	
	Mo-Mo1	2.70 Å	+/- 0.002	
	Mo-Mo2	2.79 Å	+/- 0.002	
	Mo-Mo3	3.15 Å	+/- 0.002	
	N (Mo-S1)	3.4	+/- 0.318	
	N (Mo-S2)	1	set	
	N (Mo-Mo1)	2	set	
	N (Mo-Mo2)	2	set	
	N (Mo-Mo3)	1	set	
	R-range	1.25 – 4 Å	set	
	k-range	3 – 13.9 Å	set	

Error of cluster anisotropy equation

Anisotropy of the Mo_6 cluster was calculated according to equations previously detailed by Levi and Aurbach[4] using the difference between R_{long} and R_{short}.

Equation 1:

$$\% \text{ Anisotropy} = ((R_{long} - R_{short})/R_{long}) * 100$$

Equation 2:

$$\Delta\text{Anisotropy} = \sqrt{(((R_{short}/R_{long}) * 100 * \Delta R_{long})^2 + ((-100/R_{long}) * \Delta R_{short})^2)}$$

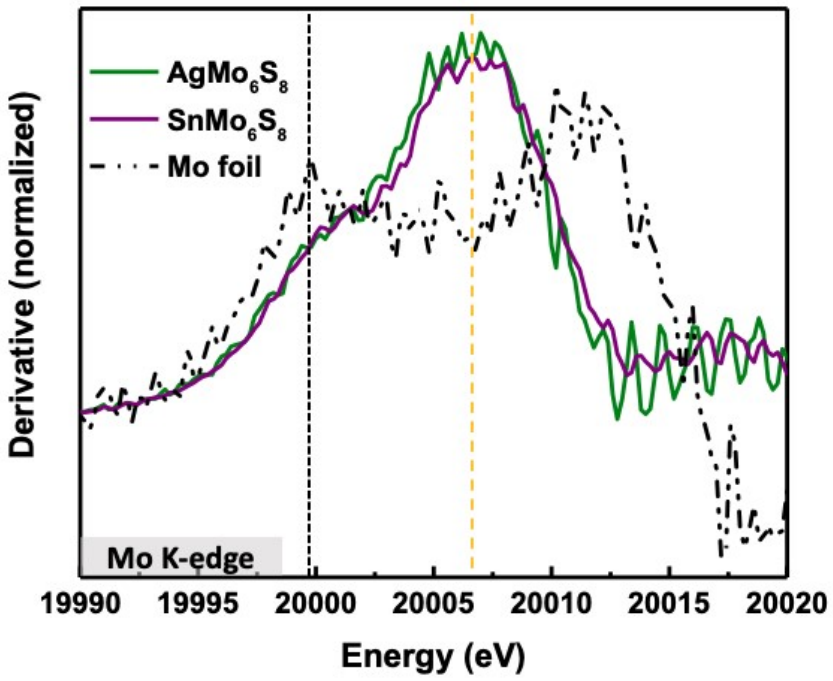

Figure S13. Mo K-edge plotted as the normalized first derivative with dashed lines indicating peak maxima.

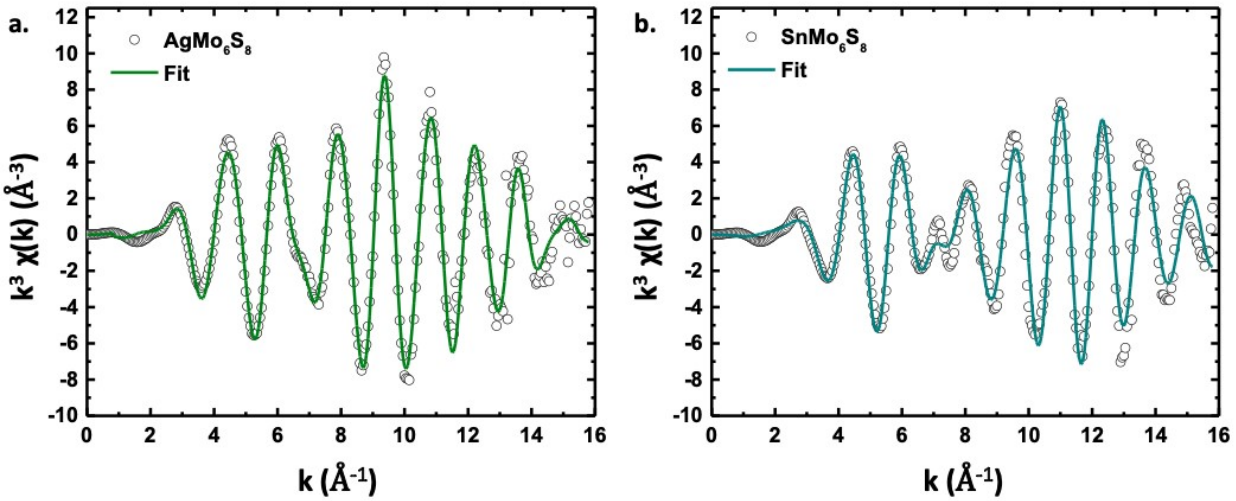

Figure S14. Mo K-edge data and fits in k-space for a.) $AgMo_6S_8$ and b.) $SnMo_6S_8$

Atomic structures used for FEFF calculations and Rietveld Refinement

$AgMo_6S_8$

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Chalcogen ordering on special-positions sites in ternary molybdenum

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6 'x, y, z'

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Sn2+ 2

S2- -2

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S1 S2- 6 c 0 0 0.241 . 1.

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CIF file used for $AgMo_6S_8$ MBXAS spectra generation

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Mo19	1.0	0.241479	0.606516	0.427177	Uiso	?	Mo
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Mo22	1.0	0.629067	0.382743	0.577327	Uiso	?	Mo
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Mo24	1.0	0.435273	0.494629	0.727477	Uiso	?	Mo
Mo25	1.0	0.564727	0.505371	0.373423	Uiso	?	Mo
Mo26	1.0	0.564727	0.281597	0.523574	Uiso	?	Mo
Mo27	1.0	0.370933	0.617257	0.523574	Uiso	?	Mo
Mo28	1.0	0.370933	0.393484	0.673724	Uiso	?	Mo
Mo29	1.0	0.758521	0.617257	0.523574	Uiso	?	Mo

Mo30	1.0	0.758521	0.393484	0.673724	Uiso	?	Mo
Mo31	1.0	0.564727	0.729144	0.673724	Uiso	?	Mo
Mo32	1.0	0.564727	0.505371	0.823874	Uiso	?	Mo
Mo33	1.0	0.537015	0.446630	0.277027	Uiso	?	Mo
Mo34	1.0	0.537015	0.222856	0.427177	Uiso	?	Mo
Mo35	1.0	0.343221	0.558517	0.427177	Uiso	?	Mo
Mo36	1.0	0.343221	0.334743	0.577327	Uiso	?	Mo
Mo37	1.0	0.730808	0.558517	0.427177	Uiso	?	Mo
Mo38	1.0	0.730808	0.334743	0.577327	Uiso	?	Mo
Mo39	1.0	0.537015	0.670404	0.577327	Uiso	?	Mo
Mo40	1.0	0.537015	0.446630	0.727477	Uiso	?	Mo
Mo41	1.0	0.462985	0.553370	0.373423	Uiso	?	Mo
Mo42	1.0	0.462985	0.329596	0.523574	Uiso	?	Mo
Mo43	1.0	0.269192	0.665257	0.523574	Uiso	?	Mo
Mo44	1.0	0.269192	0.441483	0.673724	Uiso	?	Mo
Mo45	1.0	0.656779	0.665257	0.523574	Uiso	?	Mo
Mo46	1.0	0.656779	0.441483	0.673724	Uiso	?	Mo
Mo47	1.0	0.462985	0.777144	0.673724	Uiso	?	Mo
Mo48	1.0	0.462985	0.553370	0.823874	Uiso	?	Mo
Ag1	1.0	0.500000	0.500000	0.100000	Uiso	?	Ag
Ag2	1.0	0.500000	0.276226	0.250150	Uiso	?	Ag
Ag3	1.0	0.306206	0.611887	0.250150	Uiso	?	Ag
Ag4	1.0	0.306206	0.388113	0.400300	Uiso	?	Ag
Ag5	1.0	0.693794	0.611887	0.250150	Uiso	?	Ag
Ag6	1.0	0.693794	0.388113	0.400300	Uiso	?	Ag
Ag7	1.0	0.500000	0.723774	0.400300	Uiso	?	Ag
Ag8	1.0	0.500000	0.500000	0.550450	Uiso	?	Ag
S1	1.0	0.500000	0.500000	0.200901	Uiso	?	S
S2	1.0	0.500000	0.276226	0.351051	Uiso	?	S
S3	1.0	0.306206	0.611887	0.351051	Uiso	?	S

S4	1.0	0.306206	0.388113	0.501201	Uiso	?	S
S5	1.0	0.693794	0.611887	0.351051	Uiso	?	S
S6	1.0	0.693794	0.388113	0.501201	Uiso	?	S
S7	1.0	0.500000	0.723774	0.501201	Uiso	?	S
S8	1.0	0.500000	0.500000	0.651351	Uiso	?	S
S9	1.0	0.500000	0.500000	0.449550	Uiso	?	S
S10	1.0	0.500000	0.276226	0.599700	Uiso	?	S
S11	1.0	0.306206	0.611887	0.599700	Uiso	?	S
S12	1.0	0.306206	0.388113	0.749850	Uiso	?	S
S13	1.0	0.693794	0.611887	0.599700	Uiso	?	S
S14	1.0	0.693794	0.388113	0.749850	Uiso	?	S
S15	1.0	0.500000	0.723774	0.749850	Uiso	?	S
S16	1.0	0.500000	0.500000	0.900000	Uiso	?	S
S17	1.0	0.450970	0.393372	0.287087	Uiso	?	S
S18	1.0	0.450970	0.169598	0.437237	Uiso	?	S
S19	1.0	0.257177	0.505259	0.437237	Uiso	?	S
S20	1.0	0.257177	0.281485	0.587387	Uiso	?	S
S21	1.0	0.644764	0.505259	0.437237	Uiso	?	S
S22	1.0	0.644764	0.281485	0.587387	Uiso	?	S
S23	1.0	0.450970	0.617145	0.587387	Uiso	?	S
S24	1.0	0.450970	0.393372	0.737538	Uiso	?	S
S25	1.0	0.549030	0.606628	0.363363	Uiso	?	S
S26	1.0	0.549030	0.382855	0.513514	Uiso	?	S
S27	1.0	0.355236	0.718515	0.513514	Uiso	?	S
S28	1.0	0.355236	0.494741	0.663664	Uiso	?	S
S29	1.0	0.742823	0.718515	0.513514	Uiso	?	S
S30	1.0	0.742823	0.494741	0.663664	Uiso	?	S
S31	1.0	0.549030	0.830402	0.663664	Uiso	?	S
S32	1.0	0.549030	0.606628	0.813814	Uiso	?	S
S33	1.0	0.616858	0.510853	0.287087	Uiso	?	S

S34	1.0	0.616858	0.287079	0.437237	Uiso	?	S
S35	1.0	0.423064	0.622740	0.437237	Uiso	?	S
S36	1.0	0.423064	0.398966	0.587387	Uiso	?	S
S37	1.0	0.810651	0.622740	0.437237	Uiso	?	S
S38	1.0	0.810651	0.398966	0.587387	Uiso	?	S
S39	1.0	0.616858	0.734627	0.587387	Uiso	?	S
S40	1.0	0.616858	0.510853	0.737538	Uiso	?	S
S41	1.0	0.383142	0.489147	0.363363	Uiso	?	S
S42	1.0	0.383142	0.265373	0.513514	Uiso	?	S
S43	1.0	0.189349	0.601034	0.513514	Uiso	?	S
S44	1.0	0.189349	0.377260	0.663664	Uiso	?	S
S45	1.0	0.576936	0.601034	0.513514	Uiso	?	S
S46	1.0	0.576936	0.377260	0.663664	Uiso	?	S
S47	1.0	0.383142	0.712921	0.663664	Uiso	?	S
S48	1.0	0.383142	0.489147	0.813814	Uiso	?	S
S49	1.0	0.432172	0.595775	0.287087	Uiso	?	S
S50	1.0	0.432172	0.372002	0.437237	Uiso	?	S
S51	1.0	0.238379	0.707662	0.437237	Uiso	?	S
S52	1.0	0.238379	0.483888	0.587387	Uiso	?	S
S53	1.0	0.625966	0.707662	0.437237	Uiso	?	S
S54	1.0	0.625966	0.483888	0.587387	Uiso	?	S
S55	1.0	0.432172	0.819549	0.587387	Uiso	?	S
S56	1.0	0.432172	0.595775	0.737538	Uiso	?	S
S57	1.0	0.567828	0.404225	0.363363	Uiso	?	S
S58	1.0	0.567828	0.180451	0.513514	Uiso	?	S
S59	1.0	0.374034	0.516112	0.513514	Uiso	?	S
S60	1.0	0.374034	0.292338	0.663664	Uiso	?	S
S61	1.0	0.761621	0.516112	0.513514	Uiso	?	S
S62	1.0	0.761621	0.292338	0.663664	Uiso	?	S
S63	1.0	0.567828	0.627998	0.663664	Uiso	?	S

S64 1.0 0.567828 0.404225 0.813814 Uiso ? S

Charge cube CIF for $AgMo_6S_8$ used for isosurface visualization

```
#======================================================================
==
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                ' Cubefile created from PWScf calculati'
_cell_length_a                       12.946022
_cell_length_b                       12.946022
_cell_length_c                       12.946083
_cell_angle_alpha                    91.966988
_cell_angle_beta                     91.966988
_cell_angle_gamma                    91.966812
_cell_volume                         2165.831489
_space_group_name_H-M_alt            'P 1'
_space_group_IT_number               1

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
```

```
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol

#======================================================================
==
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_2

_chemical_name_common                  ' Cubefile created from PWScf calculati'
_cell_length_a                         1.000000
_cell_length_b                         1.000000
_cell_length_c                         1.000000
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           1.000000
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
```

_atom_site_fract_y

_atom_site_fract_z

_atom_site_adp_type

_atom_site_U_iso_or_equiv

_atom_site_type_symbol

Mo1	1.0	0.665665	1.321386	4.492704	Uiso	? Mo
Mo2	1.0	0.665665	-4.053745	8.099370	Uiso	? Mo
Mo3	1.0	-3.989336	4.008951	8.099370	Uiso	? Mo
Mo4	1.0	-3.989335	-1.366180	11.706037	Uiso	? Mo
Mo5	1.0	5.320664	4.008951	8.099370	Uiso	? Mo
Mo6	1.0	5.320665	-1.366180	11.706037	Uiso	? Mo
Mo7	1.0	0.665664	6.696516	11.706037	Uiso	? Mo
Mo8	1.0	0.665665	1.321386	15.312703	Uiso	? Mo
Mo9	1.0	-0.665665	-1.500558	6.808184	Uiso	? Mo
Mo10	1.0	-0.665664	-6.875689	10.414850	Uiso	? Mo
Mo11	1.0	-5.320665	1.187007	10.414850	Uiso	? Mo
Mo12	1.0	-5.320664	-4.188123	14.021517	Uiso	? Mo
Mo13	1.0	3.989335	1.187007	10.414850	Uiso	? Mo
Mo14	1.0	3.989336	-4.188123	14.021517	Uiso	? Mo
Mo15	1.0	-0.665665	3.874572	14.021517	Uiso	? Mo
Mo16	1.0	-0.665665	-1.500558	17.628183	Uiso	? Mo
Mo17	1.0	-1.554770	-0.218589	4.492704	Uiso	? Mo
Mo18	1.0	-1.554769	-5.593719	8.099370	Uiso	? Mo
Mo19	1.0	-6.209770	2.468976	8.099370	Uiso	? Mo
Mo20	1.0	-6.209769	-2.906155	11.706037	Uiso	? Mo
Mo21	1.0	3.100230	2.468976	8.099370	Uiso	? Mo
Mo22	1.0	3.100230	-2.906155	11.706037	Uiso	? Mo
Mo23	1.0	-1.554771	5.156541	11.706037	Uiso	? Mo
Mo24	1.0	-1.554770	-0.218589	15.312703	Uiso	? Mo
Mo25	1.0	1.554770	0.039417	6.808184	Uiso	? Mo

Mo26	1.0	1.554771	-5.335713	10.414850	Uiso ? Mo
Mo27	1.0	-3.100230	2.726982	10.414850	Uiso ? Mo
Mo28	1.0	-3.100230	-2.648148	14.021517	Uiso ? Mo
Mo29	1.0	6.209769	2.726982	10.414850	Uiso ? Mo
Mo30	1.0	6.209770	-2.648148	14.021517	Uiso ? Mo
Mo31	1.0	1.554769	5.414548	14.021517	Uiso ? Mo
Mo32	1.0	1.554770	0.039417	17.628183	Uiso ? Mo
Mo33	1.0	0.889105	-1.371555	4.492704	Uiso ? Mo
Mo34	1.0	0.889105	-6.746685	8.099370	Uiso ? Mo
Mo35	1.0	-3.765895	1.316011	8.099370	Uiso ? Mo
Mo36	1.0	-3.765895	-4.059120	11.706037	Uiso ? Mo
Mo37	1.0	5.544105	1.316011	8.099370	Uiso ? Mo
Mo38	1.0	5.544105	-4.059120	11.706037	Uiso ? Mo
Mo39	1.0	0.889104	4.003576	11.706037	Uiso ? Mo
Mo40	1.0	0.889105	-1.371555	15.312703	Uiso ? Mo
Mo41	1.0	-0.889105	1.192382	6.808184	Uiso ? Mo
Mo42	1.0	-0.889104	-4.182748	10.414850	Uiso ? Mo
Mo43	1.0	-5.544105	3.879948	10.414850	Uiso ? Mo
Mo44	1.0	-5.544105	-1.495183	14.021517	Uiso ? Mo
Mo45	1.0	3.765895	3.879948	10.414850	Uiso ? Mo
Mo46	1.0	3.765895	-1.495183	14.021517	Uiso ? Mo
Mo47	1.0	-0.889105	6.567513	14.021517	Uiso ? Mo
Mo48	1.0	-0.889105	1.192383	17.628183	Uiso ? Mo
Ag1	1.0	0.000000	-0.089586	0.240444	Uiso ? Ag
Ag2	1.0	0.000001	-5.464717	3.847111	Uiso ? Ag
Ag3	1.0	-4.655000	2.597979	3.847111	Uiso ? Ag
Ag4	1.0	-4.655000	-2.777152	7.453777	Uiso ? Ag
Ag5	1.0	4.655000	2.597979	3.847111	Uiso ? Ag
Ag6	1.0	4.655000	-2.777152	7.453777	Uiso ? Ag
Ag7	1.0	-0.000001	5.285544	7.453777	Uiso ? Ag

Ag8	1.0	-0.000000	-0.089586	11.060444	Uiso ? Ag
S1	1.0	0.000000	-0.089586	2.664124	Uiso ? S
S2	1.0	0.000001	-5.464717	6.270791	Uiso ? S
S3	1.0	-4.655000	2.597979	6.270791	Uiso ? S
S4	1.0	-4.655000	-2.777152	9.877457	Uiso ? S
S5	1.0	4.655000	2.597979	6.270791	Uiso ? S
S6	1.0	4.655000	-2.777152	9.877457	Uiso ? S
S7	1.0	-0.000001	5.285544	9.877457	Uiso ? S
S8	1.0	-0.000000	-0.089586	13.484124	Uiso ? S
S9	1.0	-0.000000	-0.089586	8.636764	Uiso ? S
S10	1.0	0.000001	-5.464717	12.243431	Uiso ? S
S11	1.0	-4.655000	2.597979	12.243431	Uiso ? S
S12	1.0	-4.655000	-2.777152	15.850098	Uiso ? S
S13	1.0	4.655000	2.597979	12.243431	Uiso ? S
S14	1.0	4.655000	-2.777152	15.850098	Uiso ? S
S15	1.0	-0.000001	5.285544	15.850098	Uiso ? S
S16	1.0	-0.000000	-0.089586	19.456764	Uiso ? S
S17	1.0	-1.177715	-2.650836	4.734351	Uiso ? S
S18	1.0	-1.177714	-8.025967	8.341018	Uiso ? S
S19	1.0	-5.832716	0.036730	8.341018	Uiso ? S
S20	1.0	-5.832714	-5.338401	11.947683	Uiso ? S
S21	1.0	3.477285	0.036730	8.341018	Uiso ? S
S22	1.0	3.477285	-5.338401	11.947683	Uiso ? S
S23	1.0	-1.177716	2.724295	11.947683	Uiso ? S
S24	1.0	-1.177715	-2.650836	15.554350	Uiso ? S
S25	1.0	1.177715	2.471663	6.566538	Uiso ? S
S26	1.0	1.177716	-2.903467	10.173203	Uiso ? S
S27	1.0	-3.477286	5.159229	10.173203	Uiso ? S
S28	1.0	-3.477285	-0.215902	13.779870	Uiso ? S
S29	1.0	5.832714	5.159229	10.173203	Uiso ? S

S30	1.0	5.832715	-0.215902	13.779870	Uiso	? S
S31	1.0	1.177714	7.846794	13.779870	Uiso	? S
S32	1.0	1.177715	2.471663	17.386536	Uiso	? S
S33	1.0	2.806965	0.171107	4.734351	Uiso	? S
S34	1.0	2.806965	-5.204023	8.341018	Uiso	? S
S35	1.0	-1.848035	2.858673	8.341018	Uiso	? S
S36	1.0	-1.848035	-2.516458	11.947683	Uiso	? S
S37	1.0	7.461965	2.858673	8.341018	Uiso	? S
S38	1.0	7.461965	-2.516458	11.947683	Uiso	? S
S39	1.0	2.806964	5.546238	11.947683	Uiso	? S
S40	1.0	2.806965	0.171107	15.554350	Uiso	? S
S41	1.0	-2.806965	-0.350280	6.566538	Uiso	? S
S42	1.0	-2.806964	-5.725410	10.173203	Uiso	? S
S43	1.0	-7.461965	2.337286	10.173203	Uiso	? S
S44	1.0	-7.461965	-3.037845	13.779870	Uiso	? S
S45	1.0	1.848035	2.337286	10.173203	Uiso	? S
S46	1.0	1.848035	-3.037845	13.779870	Uiso	? S
S47	1.0	-2.806965	5.024851	13.779870	Uiso	? S
S48	1.0	-2.806965	-0.350280	17.386536	Uiso	? S
S49	1.0	-1.629250	2.210970	4.734351	Uiso	? S
S50	1.0	-1.629249	-3.164161	8.341018	Uiso	? S
S51	1.0	-6.284251	4.898535	8.341018	Uiso	? S
S52	1.0	-6.284250	-0.476595	11.947683	Uiso	? S
S53	1.0	3.025749	4.898535	8.341018	Uiso	? S
S54	1.0	3.025750	-0.476595	11.947683	Uiso	? S
S55	1.0	-1.629251	7.586101	11.947683	Uiso	? S
S56	1.0	-1.629250	2.210970	15.554350	Uiso	? S
S57	1.0	1.629250	-2.390142	6.566538	Uiso	? S
S58	1.0	1.629251	-7.765273	10.173203	Uiso	? S
S59	1.0	-3.025751	0.297423	10.173203	Uiso	? S

S60	1.0	-3.025749	-5.077708	13.779870	Uiso	? S
S61	1.0	6.284250	0.297423	10.173203	Uiso	? S
S62	1.0	6.284251	-5.077708	13.779870	Uiso	? S
S63	1.0	1.629249	2.984988	13.779870	Uiso	? S
S64	1.0	1.629250	-2.390142	17.386536	Uiso	? S

CIF file used for $SnMo_6S_8$ MBXAS spectra generation

```
#======================================================================
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# CRYSTAL DATA
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data_VESTA_phase_1

_chemical_name_common                  'Mo6 S8 Sn 2 x 2 x 2 supercell'
_cell_length_a                         15.393229
_cell_length_b                         15.393229
_cell_length_c                         15.393229
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           1.000000
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'
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loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  Mo1    1.0    0.198027    0.340321    0.279990    Uiso  ? Mo
  Mo2    1.0    0.200982    0.343255    0.703208    Uiso  ? Mo
  Mo3    1.0    0.200982    0.763549    0.279990    Uiso  ? Mo
  Mo4    1.0    0.203936    0.766483    0.703208    Uiso  ? Mo
  Mo5    1.0    0.621265    0.340321    0.279990    Uiso  ? Mo
  Mo6    1.0    0.624220    0.343255    0.703208    Uiso  ? Mo
  Mo7    1.0    0.624220    0.763549    0.279990    Uiso  ? Mo
  Mo8    1.0    0.627174    0.766483    0.703208    Uiso  ? Mo
  Mo9    1.0    0.431121    0.289608    0.351768    Uiso  ? Mo
  Mo10   1.0    0.434075    0.292542    0.774986    Uiso  ? Mo
  Mo11   1.0    0.434075    0.712836    0.351768    Uiso  ? Mo
  Mo12   1.0    0.437030    0.715770    0.774986    Uiso  ? Mo
  Mo13   1.0    0.854359    0.289608    0.351768    Uiso  ? Mo
  Mo14   1.0    0.857313    0.292542    0.774986    Uiso  ? Mo
  Mo15   1.0    0.857313    0.712836    0.351768    Uiso  ? Mo
  Mo16   1.0    0.860268    0.715770    0.774986    Uiso  ? Mo
  Mo17   1.0    0.278049    0.198670    0.341484    Uiso  ? Mo
  Mo18   1.0    0.281004    0.201604    0.764701    Uiso  ? Mo
  Mo19   1.0    0.281004    0.621897    0.341484    Uiso  ? Mo
  Mo20   1.0    0.283958    0.624832    0.764701    Uiso  ? Mo
  Mo21   1.0    0.701287    0.198670    0.341484    Uiso  ? Mo
```

Mo22	1.0	0.704242	0.201604	0.764701	Uiso	?	Mo
Mo23	1.0	0.704242	0.621897	0.341484	Uiso	?	Mo
Mo24	1.0	0.707196	0.624832	0.764701	Uiso	?	Mo
Mo25	1.0	0.351099	0.431259	0.290275	Uiso	?	Mo
Mo26	1.0	0.354053	0.434193	0.713492	Uiso	?	Mo
Mo27	1.0	0.354053	0.854487	0.290275	Uiso	?	Mo
Mo28	1.0	0.357008	0.857421	0.713492	Uiso	?	Mo
Mo29	1.0	0.774337	0.431259	0.290275	Uiso	?	Mo
Mo30	1.0	0.777291	0.434193	0.713492	Uiso	?	Mo
Mo31	1.0	0.777291	0.854487	0.290275	Uiso	?	Mo
Mo32	1.0	0.780246	0.857421	0.713492	Uiso	?	Mo
Mo33	1.0	0.339116	0.278267	0.199410	Uiso	?	Mo
Mo34	1.0	0.342071	0.281201	0.622627	Uiso	?	Mo
Mo35	1.0	0.342071	0.701495	0.199410	Uiso	?	Mo
Mo36	1.0	0.345025	0.704429	0.622627	Uiso	?	Mo
Mo37	1.0	0.762354	0.278267	0.199410	Uiso	?	Mo
Mo38	1.0	0.765309	0.281201	0.622627	Uiso	?	Mo
Mo39	1.0	0.765309	0.701495	0.199410	Uiso	?	Mo
Mo40	1.0	0.768263	0.704429	0.622627	Uiso	?	Mo
Mo41	1.0	0.290032	0.351662	0.432349	Uiso	?	Mo
Mo42	1.0	0.292986	0.354596	0.855566	Uiso	?	Mo
Mo43	1.0	0.292986	0.774889	0.432349	Uiso	?	Mo
Mo44	1.0	0.295941	0.777824	0.855566	Uiso	?	Mo
Mo45	1.0	0.713270	0.351662	0.432349	Uiso	?	Mo
Mo46	1.0	0.716224	0.354596	0.855566	Uiso	?	Mo
Mo47	1.0	0.716224	0.774889	0.432349	Uiso	?	Mo
Mo48	1.0	0.719179	0.777824	0.855566	Uiso	?	Mo
S1	1.0	0.415929	0.157974	0.264881	Uiso	?	S
S2	1.0	0.418883	0.160908	0.688099	Uiso	?	S
S3	1.0	0.418883	0.581202	0.264881	Uiso	?	S

S4	1.0	0.421838	0.584136	0.688099	Uiso	?	S
S5	1.0	0.839167	0.157974	0.264881	Uiso	?	S
S6	1.0	0.842121	0.160908	0.688099	Uiso	?	S
S7	1.0	0.842121	0.581202	0.264881	Uiso	?	S
S8	1.0	0.845076	0.584136	0.688099	Uiso	?	S
S9	1.0	0.213219	0.471955	0.366877	Uiso	?	S
S10	1.0	0.216174	0.474889	0.790094	Uiso	?	S
S11	1.0	0.216174	0.895182	0.366877	Uiso	?	S
S12	1.0	0.219128	0.898116	0.790094	Uiso	?	S
S13	1.0	0.636457	0.471955	0.366877	Uiso	?	S
S14	1.0	0.639412	0.474889	0.790094	Uiso	?	S
S15	1.0	0.639412	0.895182	0.366877	Uiso	?	S
S16	1.0	0.642366	0.898116	0.790094	Uiso	?	S
S17	1.0	0.263198	0.416681	0.159246	Uiso	?	S
S18	1.0	0.266152	0.419615	0.582464	Uiso	?	S
S19	1.0	0.266152	0.839908	0.159246	Uiso	?	S
S20	1.0	0.269107	0.842842	0.582464	Uiso	?	S
S21	1.0	0.686436	0.416681	0.159246	Uiso	?	S
S22	1.0	0.689390	0.419615	0.582464	Uiso	?	S
S23	1.0	0.689390	0.839908	0.159246	Uiso	?	S
S24	1.0	0.692345	0.842842	0.582464	Uiso	?	S
S25	1.0	0.365950	0.213248	0.472512	Uiso	?	S
S26	1.0	0.368905	0.216183	0.895730	Uiso	?	S
S27	1.0	0.368905	0.636476	0.472512	Uiso	?	S
S28	1.0	0.371859	0.639410	0.895730	Uiso	?	S
S29	1.0	0.789188	0.213248	0.472512	Uiso	?	S
S30	1.0	0.792143	0.216183	0.895730	Uiso	?	S
S31	1.0	0.792143	0.636476	0.472512	Uiso	?	S
S32	1.0	0.795097	0.639410	0.895730	Uiso	?	S
S33	1.0	0.158295	0.264678	0.418679	Uiso	?	S

S34	1.0	0.161250	0.267612	0.841896	Uiso	?	S
S35	1.0	0.161250	0.687906	0.418679	Uiso	?	S
S36	1.0	0.164205	0.690840	0.841896	Uiso	?	S
S37	1.0	0.581533	0.264678	0.418679	Uiso	?	S
S38	1.0	0.584488	0.267612	0.841896	Uiso	?	S
S39	1.0	0.584488	0.687906	0.418679	Uiso	?	S
S40	1.0	0.587443	0.690840	0.841896	Uiso	?	S
S41	1.0	0.470852	0.365251	0.213080	Uiso	?	S
S42	1.0	0.473807	0.368185	0.636297	Uiso	?	S
S43	1.0	0.473807	0.788478	0.213080	Uiso	?	S
S44	1.0	0.476762	0.791413	0.636297	Uiso	?	S
S45	1.0	0.894091	0.365251	0.213080	Uiso	?	S
S46	1.0	0.897045	0.368185	0.636297	Uiso	?	S
S47	1.0	0.897045	0.788478	0.213080	Uiso	?	S
S48	1.0	0.900000	0.791413	0.636297	Uiso	?	S
S49	1.0	0.204025	0.205185	0.206858	Uiso	?	S
S50	1.0	0.206980	0.208119	0.630076	Uiso	?	S
S51	1.0	0.206980	0.628413	0.206858	Uiso	?	S
S52	1.0	0.209935	0.631347	0.630076	Uiso	?	S
S53	1.0	0.627263	0.205185	0.206858	Uiso	?	S
S54	1.0	0.630218	0.208119	0.630076	Uiso	?	S
S55	1.0	0.630218	0.628413	0.206858	Uiso	?	S
S56	1.0	0.633173	0.631347	0.630076	Uiso	?	S
S57	1.0	0.425122	0.424744	0.424900	Uiso	?	S
S58	1.0	0.428077	0.427678	0.848118	Uiso	?	S
S59	1.0	0.428077	0.847971	0.424900	Uiso	?	S
S60	1.0	0.431032	0.850906	0.848118	Uiso	?	S
S61	1.0	0.848360	0.424744	0.424900	Uiso	?	S
S62	1.0	0.851315	0.427678	0.848118	Uiso	?	S
S63	1.0	0.851315	0.847971	0.424900	Uiso	?	S

S64	1.0	0.854270	0.850906	0.848118	Uiso	? S
Sn65	1.0	0.100000	0.101884	0.104270	Uiso	? Sn
Sn66	1.0	0.102955	0.104818	0.527488	Uiso	? Sn
Sn67	1.0	0.102955	0.525111	0.104270	Uiso	? Sn
Sn68	1.0	0.105909	0.528045	0.527488	Uiso	? Sn
Sn69	1.0	0.523238	0.101884	0.104270	Uiso	? Sn
Sn70	1.0	0.526193	0.104818	0.527488	Uiso	? Sn
Sn71	1.0	0.526193	0.525111	0.104270	Uiso	? Sn
Sn72	1.0	0.529148	0.528045	0.527488	Uiso	? Sn

Charge cube CIF for $SnMo_6S_8$ used for isosurface visualization

```
#======================================================================
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# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                ' Cubefile created from PWScf calculati'
_cell_length_a                       13.030015
_cell_length_b                       13.030015
_cell_length_c                       13.030011
_cell_angle_alpha                    89.599869
_cell_angle_beta                     89.599861
_cell_angle_gamma                    89.599861
_cell_volume                         2212.091022
_space_group_name_H-M_alt            'P 1'
_space_group_IT_number               1

loop_
_space_group_symop_operation_xyz
```

'x, y, z'

loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_U_iso_or_equiv
_atom_site_type_symbol

#==========
==
CRYSTAL DATA
#----------
data_VESTA_phase_2

_chemical_name_common ' Cubefile created from PWScf calculati'
_cell_length_a 1.000000
_cell_length_b 1.000000
_cell_length_c 1.000000
_cell_angle_alpha 90.000000
_cell_angle_beta 90.000000
_cell_angle_gamma 90.000000
_cell_volume 1.000000
_space_group_name_H-M_alt 'P 1'
_space_group_IT_number 1

loop_

```
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   Mo1       1.0    1.620565    3.888989    2.922054    Uiso  ? Mo
   Mo2       1.0    1.666048    3.934155    9.436738    Uiso  ? Mo
   Mo3       1.0    1.666048   10.403831    2.922054    Uiso  ? Mo
   Mo4       1.0    1.711532   10.448997    9.436738    Uiso  ? Mo
   Mo5       1.0    8.135565    3.888989    2.922054    Uiso  ? Mo
   Mo6       1.0    8.181048    3.934155    9.436738    Uiso  ? Mo
   Mo7       1.0    8.181048   10.403831    2.922054    Uiso  ? Mo
   Mo8       1.0    8.226531   10.448997    9.436738    Uiso  ? Mo
   Mo9       1.0    5.208632    3.108353    4.026944    Uiso  ? Mo
   Mo10      1.0    5.254115    3.153520   10.541629    Uiso  ? Mo
   Mo11      1.0    5.254115    9.623194    4.026944    Uiso  ? Mo
   Mo12      1.0    5.299598    9.668360   10.541629    Uiso  ? Mo
   Mo13      1.0   11.723631    3.108353    4.026944    Uiso  ? Mo
   Mo14      1.0   11.769114    3.153520   10.541629    Uiso  ? Mo
   Mo15      1.0   11.769114    9.623194    4.026944    Uiso  ? Mo
   Mo16      1.0   11.814597    9.668360   10.541629    Uiso  ? Mo
   Mo17      1.0    2.852361    1.708520    3.868637    Uiso  ? Mo
   Mo18      1.0    2.897844    1.753686   10.383322    Uiso  ? Mo
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Mo19	1.0	2.897844	8.223360	3.868637	Uiso	? Mo
Mo20	1.0	2.943327	8.268527	10.383322	Uiso	? Mo
Mo21	1.0	9.367361	1.708520	3.868637	Uiso	? Mo
Mo22	1.0	9.412845	1.753686	10.383322	Uiso	? Mo
Mo23	1.0	9.412845	8.223360	3.868637	Uiso	? Mo
Mo24	1.0	9.458326	8.268527	10.383322	Uiso	? Mo
Mo25	1.0	3.976836	5.288823	3.080360	Uiso	? Mo
Mo26	1.0	4.022319	5.333989	9.595045	Uiso	? Mo
Mo27	1.0	4.022319	11.803664	3.080360	Uiso	? Mo
Mo28	1.0	4.067802	11.848830	9.595045	Uiso	? Mo
Mo29	1.0	10.491836	5.288823	3.080360	Uiso	? Mo
Mo30	1.0	10.537318	5.333989	9.595045	Uiso	? Mo
Mo31	1.0	10.537318	11.803664	3.080360	Uiso	? Mo
Mo32	1.0	10.582801	11.848830	9.595045	Uiso	? Mo
Mo33	1.0	3.792382	2.933783	1.681658	Uiso	? Mo
Mo34	1.0	3.837865	2.978949	8.196342	Uiso	? Mo
Mo35	1.0	3.837865	9.448623	1.681658	Uiso	? Mo
Mo36	1.0	3.883348	9.493791	8.196342	Uiso	? Mo
Mo37	1.0	10.307382	2.933783	1.681658	Uiso	? Mo
Mo38	1.0	10.352864	2.978949	8.196342	Uiso	? Mo
Mo39	1.0	10.352864	9.448623	1.681658	Uiso	? Mo
Mo40	1.0	10.398348	9.493791	8.196342	Uiso	? Mo
Mo41	1.0	3.036815	4.063560	5.267340	Uiso	? Mo
Mo42	1.0	3.082298	4.108726	11.782023	Uiso	? Mo
Mo43	1.0	3.082298	10.578401	5.267340	Uiso	? Mo
Mo44	1.0	3.127780	10.623567	11.782023	Uiso	? Mo
Mo45	1.0	9.551814	4.063560	5.267340	Uiso	? Mo
Mo46	1.0	9.597298	4.108726	11.782023	Uiso	? Mo
Mo47	1.0	9.597298	10.578401	5.267340	Uiso	? Mo
Mo48	1.0	9.642781	10.623567	11.782023	Uiso	? Mo

S1	1.0	4.974778	1.082086	2.689479	Uiso	? S
S2	1.0	5.020261	1.127252	9.204164	Uiso	? S
S3	1.0	5.020261	7.596926	2.689479	Uiso	? S
S4	1.0	5.065744	7.642094	9.204164	Uiso	? S
S5	1.0	11.489778	1.082086	2.689479	Uiso	? S
S6	1.0	11.535261	1.127252	9.204164	Uiso	? S
S7	1.0	11.535261	7.596926	2.689479	Uiso	? S
S8	1.0	11.580744	7.642094	9.204164	Uiso	? S
S9	1.0	1.854419	5.915257	4.259518	Uiso	? S
S10	1.0	1.899902	5.960423	10.774202	Uiso	? S
S11	1.0	1.899902	12.430097	4.259518	Uiso	? S
S12	1.0	1.945385	12.475264	10.774202	Uiso	? S
S13	1.0	8.369419	5.915257	4.259518	Uiso	? S
S14	1.0	8.414902	5.960423	10.774202	Uiso	? S
S15	1.0	8.414902	12.430097	4.259518	Uiso	? S
S16	1.0	8.460385	12.475264	10.774202	Uiso	? S
S17	1.0	2.623756	5.064410	1.063414	Uiso	? S
S18	1.0	2.669239	5.109576	7.578098	Uiso	? S
S19	1.0	2.669239	11.579250	1.063414	Uiso	? S
S20	1.0	2.714722	11.624417	7.578098	Uiso	? S
S21	1.0	9.138755	5.064410	1.063414	Uiso	? S
S22	1.0	9.184238	5.109576	7.578098	Uiso	? S
S23	1.0	9.184238	11.579250	1.063414	Uiso	? S
S24	1.0	9.229721	11.624417	7.578098	Uiso	? S
S25	1.0	4.205441	1.932932	5.885584	Uiso	? S
S26	1.0	4.250924	1.978099	12.400268	Uiso	? S
S27	1.0	4.250924	8.447773	5.885584	Uiso	? S
S28	1.0	4.296407	8.492940	12.400268	Uiso	? S
S29	1.0	10.720441	1.932932	5.885584	Uiso	? S
S30	1.0	10.765924	1.978099	12.400268	Uiso	? S

S31	1.0	10.765924	8.447773	5.885584	Uiso	?	S
S32	1.0	10.811407	8.492940	12.400268	Uiso	?	S
S33	1.0	1.008964	2.724604	5.056915	Uiso	?	S
S34	1.0	1.054447	2.769770	11.571600	Uiso	?	S
S35	1.0	1.054447	9.239445	5.056915	Uiso	?	S
S36	1.0	1.099930	9.284612	11.571600	Uiso	?	S
S37	1.0	7.523964	2.724604	5.056915	Uiso	?	S
S38	1.0	7.569447	2.769770	11.571600	Uiso	?	S
S39	1.0	7.569447	9.239445	5.056915	Uiso	?	S
S40	1.0	7.614930	9.284612	11.571600	Uiso	?	S
S41	1.0	5.820232	4.272738	1.892082	Uiso	?	S
S42	1.0	5.865716	4.317905	8.406766	Uiso	?	S
S43	1.0	5.865716	10.787579	1.892082	Uiso	?	S
S44	1.0	5.911200	10.832746	8.406766	Uiso	?	S
S45	1.0	12.335232	4.272738	1.892082	Uiso	?	S
S46	1.0	12.380716	4.317905	8.406766	Uiso	?	S
S47	1.0	12.380716	10.787579	1.892082	Uiso	?	S
S48	1.0	12.426199	10.832746	8.406766	Uiso	?	S
S49	1.0	1.712902	1.808813	1.796316	Uiso	?	S
S50	1.0	1.758385	1.853980	8.311000	Uiso	?	S
S51	1.0	1.758385	8.323654	1.796316	Uiso	?	S
S52	1.0	1.803868	8.368821	8.311000	Uiso	?	S
S53	1.0	8.227901	1.808813	1.796316	Uiso	?	S
S54	1.0	8.273384	1.853980	8.311000	Uiso	?	S
S55	1.0	8.273384	8.323654	1.796316	Uiso	?	S
S56	1.0	8.318868	8.368821	8.311000	Uiso	?	S
S57	1.0	5.116295	5.188529	5.152681	Uiso	?	S
S58	1.0	5.161778	5.233696	11.667365	Uiso	?	S
S59	1.0	5.161778	11.703370	5.152681	Uiso	?	S
S60	1.0	5.207261	11.748536	11.667365	Uiso	?	S

S61	1.0	11.631295	5.188529	5.152681	Uiso ? S	
S62	1.0	11.676778	5.233696	11.667365	Uiso ? S	
S63	1.0	11.676778	11.703370	5.152681	Uiso ? S	
S64	1.0	11.722260	11.748536	11.667365	Uiso ? S	
Sn65	1.0	0.111616	0.218667	0.217157	Uiso ? Sn	
Sn66	1.0	0.157098	0.263834	6.731841	Uiso ? Sn	
Sn67	1.0	0.157098	6.733509	0.217157	Uiso ? Sn	
Sn68	1.0	0.202582	6.778675	6.731841	Uiso ? Sn	
Sn69	1.0	6.626615	0.218667	0.217157	Uiso ? Sn	
Sn70	1.0	6.672099	0.263834	6.731841	Uiso ? Sn	
Sn71	1.0	6.672099	6.733509	0.217157	Uiso ? Sn	
Sn72	1.0	6.717581	6.778675	6.731841	Uiso ? Sn	

CIF file used for $SnMo_6S_8$ MBXAS spectra generation

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#======================================================================
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# CRYSTAL DATA
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data_VESTA_phase_1

_chemical_name_common                  'S Mo 2 x 2 x 2 supercell'
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_cell_length_b                         21.340961
_cell_length_c                         21.340961
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           1.000000
_space_group_name_H-M_alt              'P 1'
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_space_group_IT_number           1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   Mo1       1.0    0.531552    0.566650    0.186713    Uiso  ? Mo
   Mo2       1.0    0.531552    0.316085    0.357747    Uiso  ? Mo
   Mo3       1.0    0.314556    0.691933    0.357747    Uiso  ? Mo
   Mo4       1.0    0.314556    0.441367    0.528780    Uiso  ? Mo
   Mo5       1.0    0.748548    0.691933    0.357747    Uiso  ? Mo
   Mo6       1.0    0.748548    0.441367    0.528780    Uiso  ? Mo
   Mo7       1.0    0.531552    0.817216    0.528780    Uiso  ? Mo
   Mo8       1.0    0.531552    0.566650    0.699814    Uiso  ? Mo
   Mo9       1.0    0.426503    0.494000    0.186713    Uiso  ? Mo
   Mo10      1.0    0.426503    0.243434    0.357747    Uiso  ? Mo
   Mo11      1.0    0.209507    0.619283    0.357747    Uiso  ? Mo
   Mo12      1.0    0.209507    0.368717    0.528780    Uiso  ? Mo
   Mo13      1.0    0.643499    0.619283    0.357747    Uiso  ? Mo
   Mo14      1.0    0.643499    0.368717    0.528780    Uiso  ? Mo
   Mo15      1.0    0.426503    0.744565    0.528780    Uiso  ? Mo
```

Mo16	1.0	0.426503	0.494000	0.699814	Uiso	?	Mo
Mo17	1.0	0.458055	0.560650	0.300186	Uiso	?	Mo
Mo18	1.0	0.458055	0.310084	0.471220	Uiso	?	Mo
Mo19	1.0	0.241059	0.685933	0.471220	Uiso	?	Mo
Mo20	1.0	0.241059	0.435367	0.642253	Uiso	?	Mo
Mo21	1.0	0.675051	0.685933	0.471220	Uiso	?	Mo
Mo22	1.0	0.675051	0.435367	0.642253	Uiso	?	Mo
Mo23	1.0	0.458055	0.811215	0.642253	Uiso	?	Mo
Mo24	1.0	0.458055	0.560650	0.813287	Uiso	?	Mo
Mo25	1.0	0.541945	0.439350	0.186713	Uiso	?	Mo
Mo26	1.0	0.541945	0.188785	0.357747	Uiso	?	Mo
Mo27	1.0	0.324949	0.564633	0.357747	Uiso	?	Mo
Mo28	1.0	0.324949	0.314067	0.528780	Uiso	?	Mo
Mo29	1.0	0.758941	0.564633	0.357747	Uiso	?	Mo
Mo30	1.0	0.758941	0.314067	0.528780	Uiso	?	Mo
Mo31	1.0	0.541945	0.689916	0.528780	Uiso	?	Mo
Mo32	1.0	0.541945	0.439350	0.699814	Uiso	?	Mo
Mo33	1.0	0.573497	0.506000	0.300186	Uiso	?	Mo
Mo34	1.0	0.573497	0.255435	0.471220	Uiso	?	Mo
Mo35	1.0	0.356501	0.631283	0.471220	Uiso	?	Mo
Mo36	1.0	0.356501	0.380717	0.642253	Uiso	?	Mo
Mo37	1.0	0.790493	0.631283	0.471220	Uiso	?	Mo
Mo38	1.0	0.790493	0.380717	0.642253	Uiso	?	Mo
Mo39	1.0	0.573497	0.756566	0.642253	Uiso	?	Mo
Mo40	1.0	0.573497	0.506000	0.813287	Uiso	?	Mo
Mo41	1.0	0.468448	0.433350	0.300186	Uiso	?	Mo
Mo42	1.0	0.468448	0.182784	0.471220	Uiso	?	Mo
Mo43	1.0	0.251452	0.558633	0.471220	Uiso	?	Mo
Mo44	1.0	0.251452	0.308067	0.642253	Uiso	?	Mo
Mo45	1.0	0.685444	0.558633	0.471220	Uiso	?	Mo

Mo46	1.0	0.685444	0.308067	0.642253	Uiso	?	Mo
Mo47	1.0	0.468448	0.683915	0.642253	Uiso	?	Mo
Mo48	1.0	0.468448	0.433350	0.813287	Uiso	?	Mo
S1	1.0	0.424948	0.607433	0.201375	Uiso	?	S
S2	1.0	0.424948	0.356867	0.372408	Uiso	?	S
S3	1.0	0.207952	0.732716	0.372408	Uiso	?	S
S4	1.0	0.207952	0.482150	0.543442	Uiso	?	S
S5	1.0	0.641944	0.732716	0.372408	Uiso	?	S
S6	1.0	0.641944	0.482150	0.543442	Uiso	?	S
S7	1.0	0.424948	0.857998	0.543442	Uiso	?	S
S8	1.0	0.424948	0.607433	0.714475	Uiso	?	S
S9	1.0	0.500000	0.500000	0.100000	Uiso	?	S
S10	1.0	0.500000	0.249435	0.271033	Uiso	?	S
S11	1.0	0.283004	0.625283	0.271033	Uiso	?	S
S12	1.0	0.283004	0.374717	0.442067	Uiso	?	S
S13	1.0	0.716996	0.625283	0.271033	Uiso	?	S
S14	1.0	0.716996	0.374717	0.442067	Uiso	?	S
S15	1.0	0.500000	0.750566	0.442067	Uiso	?	S
S16	1.0	0.500000	0.500000	0.613101	Uiso	?	S
S17	1.0	0.555514	0.618714	0.285525	Uiso	?	S
S18	1.0	0.555514	0.368148	0.456558	Uiso	?	S
S19	1.0	0.338518	0.743996	0.456558	Uiso	?	S
S20	1.0	0.338518	0.493431	0.627592	Uiso	?	S
S21	1.0	0.772510	0.743996	0.456558	Uiso	?	S
S22	1.0	0.772510	0.493431	0.627592	Uiso	?	S
S23	1.0	0.555514	0.869279	0.627592	Uiso	?	S
S24	1.0	0.555514	0.618714	0.798625	Uiso	?	S
S25	1.0	0.630566	0.511281	0.201375	Uiso	?	S
S26	1.0	0.630566	0.260715	0.372408	Uiso	?	S
S27	1.0	0.413570	0.636563	0.372408	Uiso	?	S

S28	1.0	0.413570	0.385998	0.543442	Uiso	?	S
S29	1.0	0.847562	0.636563	0.372408	Uiso	?	S
S30	1.0	0.847562	0.385998	0.543442	Uiso	?	S
S31	1.0	0.630566	0.761846	0.543442	Uiso	?	S
S32	1.0	0.630566	0.511281	0.714475	Uiso	?	S
S33	1.0	0.369434	0.488719	0.285525	Uiso	?	S
S34	1.0	0.369434	0.238154	0.456558	Uiso	?	S
S35	1.0	0.152438	0.614002	0.456558	Uiso	?	S
S36	1.0	0.152438	0.363437	0.627592	Uiso	?	S
S37	1.0	0.586430	0.614002	0.456558	Uiso	?	S
S38	1.0	0.586430	0.363437	0.627592	Uiso	?	S
S39	1.0	0.369434	0.739285	0.627592	Uiso	?	S
S40	1.0	0.369434	0.488719	0.798625	Uiso	?	S
S41	1.0	0.444486	0.381286	0.201375	Uiso	?	S
S42	1.0	0.444486	0.130721	0.372408	Uiso	?	S
S43	1.0	0.227490	0.506569	0.372408	Uiso	?	S
S44	1.0	0.227490	0.256004	0.543442	Uiso	?	S
S45	1.0	0.661482	0.506569	0.372408	Uiso	?	S
S46	1.0	0.661482	0.256004	0.543442	Uiso	?	S
S47	1.0	0.444486	0.631852	0.543442	Uiso	?	S
S48	1.0	0.444486	0.381286	0.714475	Uiso	?	S
S49	1.0	0.500000	0.500000	0.386900	Uiso	?	S
S50	1.0	0.500000	0.249435	0.557933	Uiso	?	S
S51	1.0	0.283004	0.625283	0.557933	Uiso	?	S
S52	1.0	0.283004	0.374717	0.728966	Uiso	?	S
S53	1.0	0.716996	0.625283	0.557933	Uiso	?	S
S54	1.0	0.716996	0.374717	0.728966	Uiso	?	S
S55	1.0	0.500000	0.750566	0.728966	Uiso	?	S
S56	1.0	0.500000	0.500000	0.900000	Uiso	?	S
S57	1.0	0.575052	0.392567	0.285525	Uiso	?	S

S58	1.0	0.575052	0.142002	0.456558	Uiso	?	S
S59	1.0	0.358056	0.517850	0.456558	Uiso	?	S
S60	1.0	0.358056	0.267284	0.627592	Uiso	?	S
S61	1.0	0.792048	0.517850	0.456558	Uiso	?	S
S62	1.0	0.792048	0.267284	0.627592	Uiso	?	S
S63	1.0	0.575052	0.643133	0.627592	Uiso	?	S
S64	1.0	0.575052	0.392567	0.798625	Uiso	?	S

Charge cube CIF for $CuMo_6S_8$ used for isosurface visualization

```
#======================================================================
==
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  ' Cubefile created from PWScf calculati'
_cell_length_a                         12.879404
_cell_length_b                         12.795889
_cell_length_c                         12.891242
_cell_angle_alpha                      92.914185
_cell_angle_beta                       96.028168
_cell_angle_gamma                      93.576447
_cell_volume                           2105.130233
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
  'x, y, z'
```

```
loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol


#=============================================================================
==
# CRYSTAL DATA
#-----------------------------------------------------------------
data_VESTA_phase_2


_chemical_name_common                  ' Cubefile created from PWScf calculati'
_cell_length_a                         1.000000
_cell_length_b                         1.000000
_cell_length_c                         1.000000
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           1.000000
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
```

'x, y, z'

loop_

_atom_site_label

_atom_site_occupancy

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_adp_type

_atom_site_U_iso_or_equiv

_atom_site_type_symbol

Cu1	1.0	5.323076	-0.044567	5.681606	Uiso	? Cu
Cu2	1.0	4.658623	-0.586291	12.069981	Uiso	? Cu
Cu3	1.0	5.502198	6.346648	5.914006	Uiso	? Cu
Cu4	1.0	4.837744	5.804924	12.302381	Uiso	? Cu
Cu5	1.0	11.736313	-0.624100	5.617155	Uiso	? Cu
Cu6	1.0	11.071860	-1.165824	12.005528	Uiso	? Cu
Cu7	1.0	11.915436	5.767114	5.849555	Uiso	? Cu
Cu8	1.0	11.250982	5.225390	12.237929	Uiso	? Cu
Mo1	1.0	1.001386	3.273633	2.553805	Uiso	? Mo
Mo2	1.0	0.336933	2.731910	8.942180	Uiso	? Mo
Mo3	1.0	1.180508	9.664847	2.786206	Uiso	? Mo
Mo4	1.0	0.516055	9.123123	9.174580	Uiso	? Mo
Mo5	1.0	7.414623	2.694100	2.489354	Uiso	? Mo
Mo6	1.0	6.750170	2.152376	8.877728	Uiso	? Mo
Mo7	1.0	7.593745	9.085315	2.721755	Uiso	? Mo
Mo8	1.0	6.929293	8.543591	9.110128	Uiso	? Mo
Mo9	1.0	4.546056	2.248974	3.769591	Uiso	? Mo
Mo10	1.0	3.881603	1.707250	10.157965	Uiso	? Mo
Mo11	1.0	4.725178	8.640188	4.001991	Uiso	? Mo

Mo12	1.0	4.060725	8.098464	10.390366	Uiso	? Mo
Mo13	1.0	10.959294	1.669440	3.705139	Uiso	? Mo
Mo14	1.0	10.294841	1.127716	10.093513	Uiso	? Mo
Mo15	1.0	11.138415	8.060655	3.937540	Uiso	? Mo
Mo16	1.0	10.473963	7.518930	10.325913	Uiso	? Mo
Mo17	1.0	2.084497	0.951167	3.386804	Uiso	? Mo
Mo18	1.0	1.420044	0.409443	9.775178	Uiso	? Mo
Mo19	1.0	2.263619	7.342381	3.619204	Uiso	? Mo
Mo20	1.0	1.599167	6.800658	10.007579	Uiso	? Mo
Mo21	1.0	8.497736	0.371634	3.322352	Uiso	? Mo
Mo22	1.0	7.833282	-0.170090	9.710727	Uiso	? Mo
Mo23	1.0	8.676857	6.762848	3.554753	Uiso	? Mo
Mo24	1.0	8.012403	6.221124	9.943127	Uiso	? Mo
Mo25	1.0	3.448719	4.556499	2.945868	Uiso	? Mo
Mo26	1.0	2.784266	4.014775	9.334242	Uiso	? Mo
Mo27	1.0	3.627841	10.947714	3.178268	Uiso	? Mo
Mo28	1.0	2.963388	10.405990	9.566644	Uiso	? Mo
Mo29	1.0	9.861957	3.976966	2.881416	Uiso	? Mo
Mo30	1.0	9.197503	3.435241	9.269791	Uiso	? Mo
Mo31	1.0	10.041079	10.368180	3.113817	Uiso	? Mo
Mo32	1.0	9.376626	9.826456	9.502192	Uiso	? Mo
Mo33	1.0	3.192998	2.293554	1.310078	Uiso	? Mo
Mo34	1.0	2.528545	1.751831	7.698452	Uiso	? Mo
Mo35	1.0	3.372120	8.684769	1.542478	Uiso	? Mo
Mo36	1.0	2.707667	8.143045	7.930853	Uiso	? Mo
Mo37	1.0	9.606236	1.714021	1.245626	Uiso	? Mo
Mo38	1.0	8.941782	1.172297	7.634001	Uiso	? Mo
Mo39	1.0	9.785358	8.105236	1.478027	Uiso	? Mo
Mo40	1.0	9.120904	7.563511	7.866402	Uiso	? Mo
Mo41	1.0	2.330428	3.239700	5.040088	Uiso	? Mo

Mo42	1.0	1.665974	2.697976	11.428462	Uiso ? Mo
Mo43	1.0	2.509550	9.630915	5.272488	Uiso ? Mo
Mo44	1.0	1.845096	9.089190	11.660862	Uiso ? Mo
Mo45	1.0	8.743665	2.660167	4.975636	Uiso ? Mo
Mo46	1.0	8.079212	2.118443	11.364011	Uiso ? Mo
Mo47	1.0	8.922788	9.051381	5.208036	Uiso ? Mo
Mo48	1.0	8.258334	8.509657	11.596411	Uiso ? Mo
S1	1.0	0.304553	2.059187	4.607966	Uiso ? S
S2	1.0	-0.359900	1.517463	10.996341	Uiso ? S
S3	1.0	0.483675	8.450400	4.840367	Uiso ? S
S4	1.0	-0.180778	7.908677	11.228741	Uiso ? S
S5	1.0	6.717791	1.479653	4.543515	Uiso ? S
S6	1.0	6.053337	0.937930	10.931890	Uiso ? S
S7	1.0	6.896913	7.870868	4.775915	Uiso ? S
S8	1.0	6.232460	7.329144	11.164289	Uiso ? S
S9	1.0	5.239118	3.447085	1.736197	Uiso ? S
S10	1.0	4.574665	2.905361	8.124573	Uiso ? S
S11	1.0	5.418239	9.838300	1.968598	Uiso ? S
S12	1.0	4.753786	9.296576	8.356973	Uiso ? S
S13	1.0	11.652355	2.867552	1.671746	Uiso ? S
S14	1.0	10.987902	2.325828	8.060122	Uiso ? S
S15	1.0	11.831477	9.258766	1.904147	Uiso ? S
S16	1.0	11.167024	8.717042	8.292521	Uiso ? S
S17	1.0	4.220174	0.354930	2.335080	Uiso ? S
S18	1.0	3.555721	-0.186794	8.723454	Uiso ? S
S19	1.0	4.399296	6.746145	2.567480	Uiso ? S
S20	1.0	3.734843	6.204421	8.955855	Uiso ? S
S21	1.0	10.633411	-0.224603	2.270628	Uiso ? S
S22	1.0	9.968959	-0.766327	8.659003	Uiso ? S
S23	1.0	10.812533	6.166611	2.503029	Uiso ? S

S24	1.0	10.148081	5.624887	8.891404	Uiso	? S
S25	1.0	1.306110	5.155812	3.999154	Uiso	? S
S26	1.0	0.641656	4.614088	10.387527	Uiso	? S
S27	1.0	1.485232	11.547027	4.231555	Uiso	? S
S28	1.0	0.820779	11.005302	10.619929	Uiso	? S
S29	1.0	7.719347	4.576278	3.934702	Uiso	? S
S30	1.0	7.054894	4.034555	10.323077	Uiso	? S
S31	1.0	7.898470	10.967493	4.167103	Uiso	? S
S32	1.0	7.234016	10.425769	10.555477	Uiso	? S
S33	1.0	2.246855	4.507870	0.864497	Uiso	? S
S34	1.0	1.582401	3.966146	7.252872	Uiso	? S
S35	1.0	2.425977	10.899084	1.096897	Uiso	? S
S36	1.0	1.761523	10.357360	7.485271	Uiso	? S
S37	1.0	8.660092	3.928336	0.800046	Uiso	? S
S38	1.0	7.995639	3.386612	7.188420	Uiso	? S
S39	1.0	8.839214	10.319551	1.032446	Uiso	? S
S40	1.0	8.174761	9.777826	7.420821	Uiso	? S
S41	1.0	3.242387	0.991796	5.486126	Uiso	? S
S42	1.0	2.577933	0.450072	11.874500	Uiso	? S
S43	1.0	3.421508	7.383010	5.718526	Uiso	? S
S44	1.0	2.757056	6.841286	12.106901	Uiso	? S
S45	1.0	9.655624	0.412262	5.421674	Uiso	? S
S46	1.0	8.991171	-0.129462	11.810049	Uiso	? S
S47	1.0	9.834746	6.803476	5.654075	Uiso	? S
S48	1.0	9.170294	6.261753	12.042450	Uiso	? S
S49	1.0	0.987509	1.243901	1.183596	Uiso	? S
S50	1.0	0.323056	0.702177	7.571970	Uiso	? S
S51	1.0	1.166631	7.635116	1.415997	Uiso	? S
S52	1.0	0.502178	7.093391	7.804371	Uiso	? S
S53	1.0	7.400747	0.664368	1.119145	Uiso	? S

S54	1.0	6.736293	0.122644	7.507519	Uiso	? S
S55	1.0	7.579869	7.055582	1.351545	Uiso	? S
S56	1.0	6.915416	6.513858	7.739920	Uiso	? S
S57	1.0	4.540906	4.323483	5.128391	Uiso	? S
S58	1.0	3.876453	3.781760	11.516766	Uiso	? S
S59	1.0	4.720028	10.714698	5.360792	Uiso	? S
S60	1.0	4.055575	10.172975	11.749166	Uiso	? S
S61	1.0	10.954144	3.743950	5.063940	Uiso	? S
S62	1.0	10.289691	3.202226	11.452314	Uiso	? S
S63	1.0	11.133265	10.135164	5.296340	Uiso	? S
S64	1.0	10.468813	9.593441	11.684714	Uiso	? S

Charge cube CIF for $Cu_2Mo_6S_8$ used for isosurface visualization

```
#======================================================================
==

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_chemical_name_common                  ' Cubefile created from PWScf calculati'
_cell_length_a                         13.102716
_cell_length_b                         12.851088
_cell_length_c                         13.097470
_cell_angle_alpha                      92.436745
_cell_angle_beta                       97.436829
_cell_angle_gamma                      96.757301
_cell_volume                           2167.926506
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1


loop_
```

```
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol

#==========================================================================
==
# CRYSTAL DATA
#--------------------------------------------------------------------------
data_VESTA_phase_2

_chemical_name_common                  ' Cubefile created from PWScf calculati'
_cell_length_a                         1.000000
_cell_length_b                         1.000000
_cell_length_c                         1.000000
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           1.000000
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1
```

```
loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  Cu1       1.0    5.386984    0.231946    5.790153    Uiso  ? Cu
  Cu2       1.0    4.630202   -0.338562   12.269945    Uiso  ? Cu
  Cu3       1.0    4.933930    6.637179    6.025062    Uiso  ? Cu
  Cu4       1.0    4.177149    6.066671   12.504853    Uiso  ? Cu
  Cu5       1.0   11.930067   -0.074159    5.670397    Uiso  ? Cu
  Cu6       1.0   11.173285   -0.644667   12.150188    Uiso  ? Cu
  Cu7       1.0   11.477013    6.331074    5.905306    Uiso  ? Cu
  Cu8       1.0   10.720232    5.760566   12.385098    Uiso  ? Cu
  Cu9       1.0   -0.053751    5.296657    0.804701    Uiso  ? Cu
  Cu10      1.0   -0.810533    4.726149    7.284492    Uiso  ? Cu
  Cu11      1.0   -0.506805   11.701889    1.039610    Uiso  ? Cu
  Cu12      1.0   -1.263587   11.131381    7.519402    Uiso  ? Cu
  Cu13      1.0    6.489331    4.990552    0.684945    Uiso  ? Cu
  Cu14      1.0    5.732549    4.420044    7.164737    Uiso  ? Cu
  Cu15      1.0    6.036278   11.395784    0.919854    Uiso  ? Cu
  Cu16      1.0    5.279495   10.825276    7.399645    Uiso  ? Cu
  Mo1       1.0    0.885141    3.193749    2.691926    Uiso  ? Mo
```

Mo2	1.0	0.128359	2.623242	9.171718	Uiso	? Mo
Mo3	1.0	0.432087	9.598982	2.926835	Uiso	? Mo
Mo4	1.0	-0.324695	9.028474	9.406627	Uiso	? Mo
Mo5	1.0	7.428224	2.887645	2.572170	Uiso	? Mo
Mo6	1.0	6.671442	2.317137	9.051961	Uiso	? Mo
Mo7	1.0	6.975170	9.292877	2.807079	Uiso	? Mo
Mo8	1.0	6.218388	8.722369	9.286871	Uiso	? Mo
Mo9	1.0	4.448131	2.334890	3.903071	Uiso	? Mo
Mo10	1.0	3.691349	1.764382	10.382863	Uiso	? Mo
Mo11	1.0	3.995077	8.740122	4.137980	Uiso	? Mo
Mo12	1.0	3.238295	8.169615	10.617772	Uiso	? Mo
Mo13	1.0	10.991214	2.028785	3.783315	Uiso	? Mo
Mo14	1.0	10.234431	1.458277	10.263107	Uiso	? Mo
Mo15	1.0	10.538159	8.434018	4.018225	Uiso	? Mo
Mo16	1.0	9.781378	7.863510	10.498015	Uiso	? Mo
Mo17	1.0	2.155896	1.013641	3.526927	Uiso	? Mo
Mo18	1.0	1.399115	0.443132	10.006720	Uiso	? Mo
Mo19	1.0	1.702842	7.418873	3.761836	Uiso	? Mo
Mo20	1.0	0.946061	6.848365	10.241628	Uiso	? Mo
Mo21	1.0	8.698978	0.707536	3.407171	Uiso	? Mo
Mo22	1.0	7.942197	0.137028	9.886963	Uiso	? Mo
Mo23	1.0	8.245926	7.112769	3.642080	Uiso	? Mo
Mo24	1.0	7.489143	6.542261	10.121871	Uiso	? Mo
Mo25	1.0	3.177462	4.514933	3.067975	Uiso	? Mo
Mo26	1.0	2.420681	3.944425	9.547767	Uiso	? Mo
Mo27	1.0	2.724408	10.920166	3.302884	Uiso	? Mo
Mo28	1.0	1.967627	10.349658	9.782677	Uiso	? Mo
Mo29	1.0	9.720546	4.208828	2.948219	Uiso	? Mo
Mo30	1.0	8.963763	3.638320	9.428012	Uiso	? Mo
Mo31	1.0	9.267491	10.614060	3.183128	Uiso	? Mo

Mo32	1.0	8.510710	10.043552	9.662920	Uiso	? Mo
Mo33	1.0	3.145613	2.313672	1.472751	Uiso	? Mo
Mo34	1.0	2.388831	1.743164	7.952542	Uiso	? Mo
Mo35	1.0	2.692559	8.718904	1.707660	Uiso	? Mo
Mo36	1.0	1.935777	8.148396	8.187451	Uiso	? Mo
Mo37	1.0	9.688696	2.007566	1.352995	Uiso	? Mo
Mo38	1.0	8.931914	1.437058	7.832787	Uiso	? Mo
Mo39	1.0	9.235641	8.412799	1.587904	Uiso	? Mo
Mo40	1.0	8.478859	7.842291	8.067696	Uiso	? Mo
Mo41	1.0	2.187652	3.214924	5.122167	Uiso	? Mo
Mo42	1.0	1.430870	2.644416	11.601958	Uiso	? Mo
Mo43	1.0	1.734598	9.620157	5.357076	Uiso	? Mo
Mo44	1.0	0.977816	9.049649	11.836867	Uiso	? Mo
Mo45	1.0	8.730734	2.908819	5.002411	Uiso	? Mo
Mo46	1.0	7.973953	2.338311	11.482203	Uiso	? Mo
Mo47	1.0	8.277681	9.314052	5.237320	Uiso	? Mo
Mo48	1.0	7.520898	8.743544	11.717113	Uiso	? Mo
S1	1.0	0.211213	1.926077	4.706327	Uiso	? S
S2	1.0	-0.545570	1.355569	11.186119	Uiso	? S
S3	1.0	-0.241841	8.331310	4.941236	Uiso	? S
S4	1.0	-0.998623	7.760802	11.421028	Uiso	? S
S5	1.0	6.754295	1.619972	4.586571	Uiso	? S
S6	1.0	5.997513	1.049464	11.066362	Uiso	? S
S7	1.0	6.301241	8.025205	4.821480	Uiso	? S
S8	1.0	5.544459	7.454697	11.301272	Uiso	? S
S9	1.0	5.121930	3.602616	1.888635	Uiso	? S
S10	1.0	4.365148	3.032109	8.368427	Uiso	? S
S11	1.0	4.668876	10.007849	2.123544	Uiso	? S
S12	1.0	3.912094	9.437341	8.603336	Uiso	? S
S13	1.0	11.665012	3.296511	1.768879	Uiso	? S

S14	1.0	10.908231	2.726003	8.248671	Uiso ? S
S15	1.0	11.211959	9.701744	2.003788	Uiso ? S
S16	1.0	10.455176	9.131235	8.483580	Uiso ? S
S17	1.0	4.326624	0.448386	2.435904	Uiso ? S
S18	1.0	3.569842	-0.122122	8.915696	Uiso ? S
S19	1.0	3.873570	6.853619	2.670813	Uiso ? S
S20	1.0	3.116788	6.283111	9.150604	Uiso ? S
S21	1.0	10.869707	0.142281	2.316148	Uiso ? S
S22	1.0	10.112925	-0.428227	8.795939	Uiso ? S
S23	1.0	10.416653	6.547513	2.551057	Uiso ? S
S24	1.0	9.659871	5.977005	9.030849	Uiso ? S
S25	1.0	1.006600	5.080233	4.159067	Uiso ? S
S26	1.0	0.249818	4.509725	10.638859	Uiso ? S
S27	1.0	0.553546	11.485466	4.393975	Uiso ? S
S28	1.0	-0.203236	10.914958	10.873768	Uiso ? S
S29	1.0	7.549683	4.774128	4.039311	Uiso ? S
S30	1.0	6.792901	4.203619	10.519102	Uiso ? S
S31	1.0	7.096629	11.179360	4.274220	Uiso ? S
S32	1.0	6.339847	10.608852	10.754012	Uiso ? S
S33	1.0	2.071905	4.488697	0.917428	Uiso ? S
S34	1.0	1.315123	3.918189	7.397220	Uiso ? S
S35	1.0	1.618851	10.893930	1.152337	Uiso ? S
S36	1.0	0.862069	10.323422	7.632129	Uiso ? S
S37	1.0	8.614987	4.182592	0.797672	Uiso ? S
S38	1.0	7.858206	3.612084	7.277463	Uiso ? S
S39	1.0	8.161934	10.587824	1.032581	Uiso ? S
S40	1.0	7.405151	10.017317	7.512373	Uiso ? S
S41	1.0	3.261354	1.039963	5.677551	Uiso ? S
S42	1.0	2.504572	0.469456	12.157343	Uiso ? S
S43	1.0	2.808300	7.445196	5.912459	Uiso ? S

S44	1.0	2.051518	6.874688	12.392251	Uiso ? S
S45	1.0	9.804438	0.733859	5.557794	Uiso ? S
S46	1.0	9.047655	0.163351	12.037586	Uiso ? S
S47	1.0	9.351383	7.139091	5.792703	Uiso ? S
S48	1.0	8.594602	6.568583	12.272494	Uiso ? S
S49	1.0	1.003274	1.139694	1.297557	Uiso ? S
S50	1.0	0.246492	0.569186	7.777349	Uiso ? S
S51	1.0	0.550220	7.544926	1.532466	Uiso ? S
S52	1.0	-0.206562	6.974418	8.012259	Uiso ? S
S53	1.0	7.546357	0.833588	1.177801	Uiso ? S
S54	1.0	6.789575	0.263080	7.657593	Uiso ? S
S55	1.0	7.093303	7.238822	1.412710	Uiso ? S
S56	1.0	6.336521	6.668314	7.892502	Uiso ? S
S57	1.0	4.329947	4.388886	5.297412	Uiso ? S
S58	1.0	3.573165	3.818379	11.777205	Uiso ? S
S59	1.0	3.876892	10.794119	5.532321	Uiso ? S
S60	1.0	3.120111	10.223611	12.012114	Uiso ? S
S61	1.0	10.873030	4.082781	5.177657	Uiso ? S
S62	1.0	10.116247	3.512274	11.657448	Uiso ? S
S63	1.0	10.419975	10.488014	5.412565	Uiso ? S
S64	1.0	9.663194	9.917506	11.892357	Uiso ? S

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