Electronic Supplementary Information

Redetermination of crystal structure of Ag(II)SO_4 and its high pressure behavior up to 30 GPa

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Contents.

S1. Remark on structure refinements.

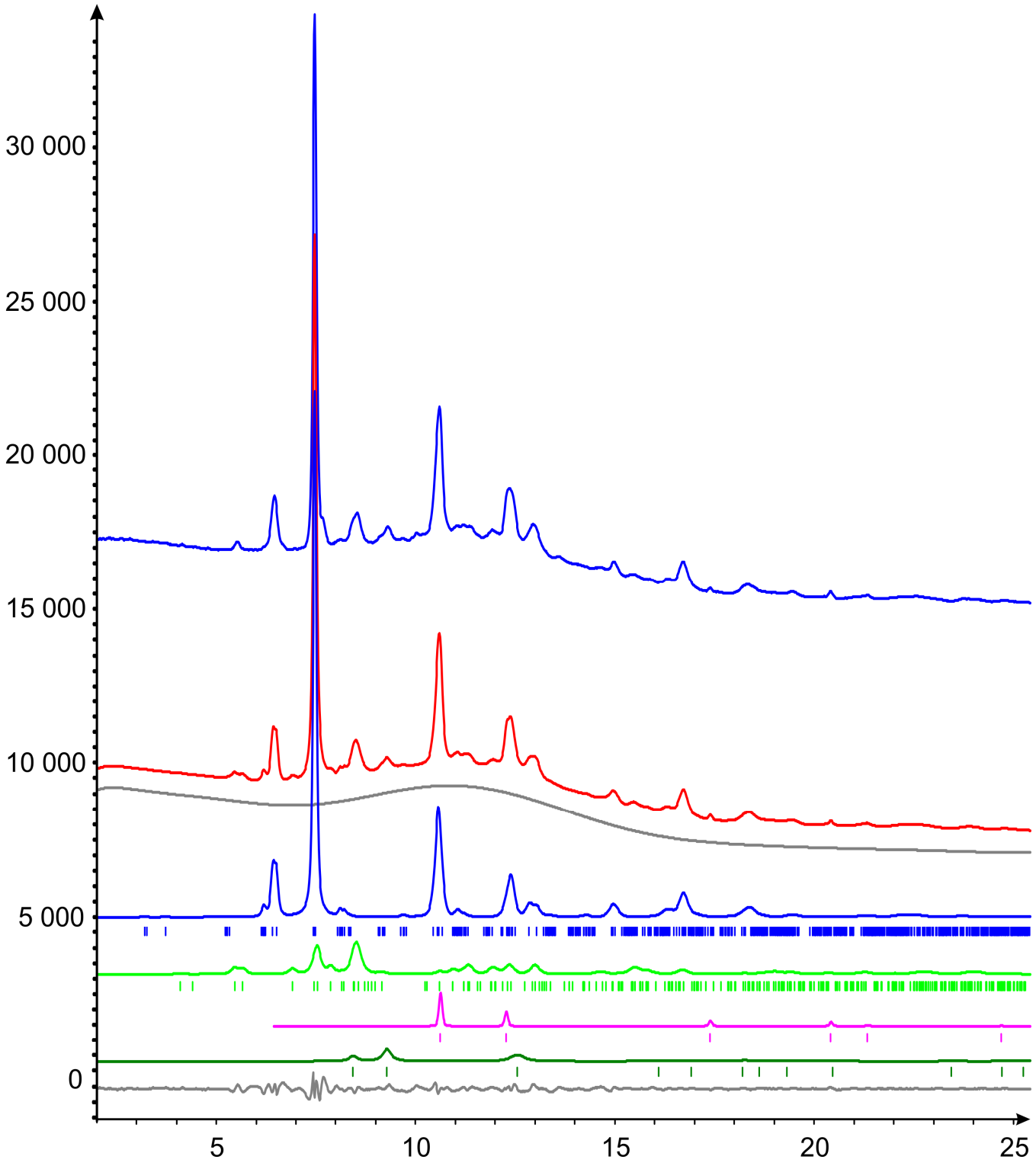
In all fits $AgSO_4$ (C2/c) has been fitted as an actual crystal structure, with fractional atomic positions frozen at their 1 atm values, and with a preferred orientation of crystallites, while HP-$Ag_2S_2O_7$ phase (also C2/c) has been represented by empty unit cell in the Lebail type fit. Only after confirming the identity of the HP-$Ag_2S_2O_7$ phase we have noticed presence of its small amounts also at the early stages of compression (from 14 GPa upwards), so this phase was included in all fits. Regretfully, the quality of the diffraction data did not permit us to refine atomic positions of $AgSO_4$.

Note: 13 very small reflexes have been detected which are independent on pressure, hence they do not originate from compressed sample inside DAC. They have been indexed in hexagonal cell, with lattice constants resembling very much those of WC. We anticipate that a very small thread coming from carbide seat might been present outside DAC on the way of the x-ray beam. Presence of WC has been taken into account in all refinements, together with small amount of Pt metal (pressure standard).

S2. Transformation matrixes (between P–1, C2/c, and NaCl-type cells).

P–1 → C2/c	**C2/c → NaCl**	**P–1 → NaCl**
1 -1 1	0 1 0	3 1 -1
3 1 -1	1 0 -2	-1 -3 -1
1 1 1	-1 0 0	-1 1 -1
C2/c → P–1	**NaCl → C2/c**	**NaCl → P–1**
0.25 0.25 0	0 0 -1	0.25 0 -0.25
-0.5 0 0.5	1 0 0	0 -0.25 0.25
0.25 -0.25 0.5	0 -0.5 -0.5	-0.25 -0.25 -0.5

S3. Fit to the powder x-ray diffraction pattern for p= 14 GPa (1st point on compression) (2θ *vs.* intensity).



From top to bottom: blue – experimental profile, red – fitted profile, gray – backgroud with amorphous hump, blue – $AgSO_4$, light green – HP-form of $Ag_2S_2O_7$, pink – platinum pressure standard, dark green – tungsten carbide, gray – differential profile.

Rexp : 2.29 Rwp : 3.29 Rp : 2.19 GOF : 1.44
Rexp`: 6.65 Rwp`: 9.56 Rp` : 9.36 DW : 0.14

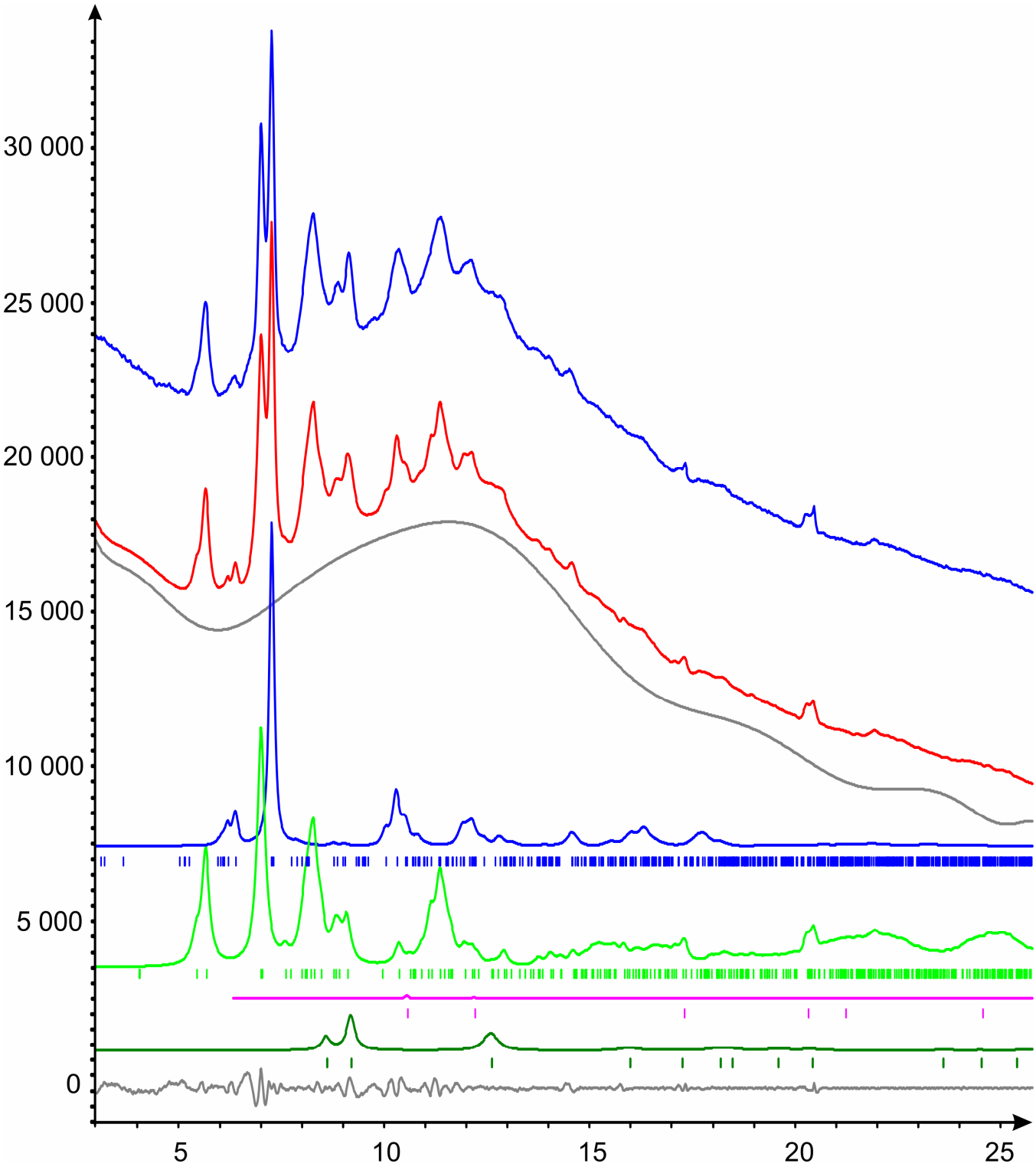
Quantitative Analysis - Rietveld

Phase 1 : AgSO4-C2c	94(31) %
Phase 2 : WC	3(19) %
Phase 3 : Pt	2(12) %
Phase 4 : Ag2S2O7	0.000 %*)

*) empty cell

Zero error	0.0146(68)

S4. Fit to the powder x-ray diffraction pattern for p= 7 GPa (last point on decompression) (2θ *vs.* intensity).



From top to bottom: blue – experimental profile, red – fitted profile, gray – backgroud with amorphous hump, blue – $AgSO_4$, light green – HP-form of $Ag_2S_2O_7$, pink – platinum pressure standard, dark green – tungsten carbide, gray – differential profile.

Rexp : 1.81 Rwp : 1.50 Rp : 1.02 GOF : 0.83
Rexp`: 5.11 Rwp`: 4.22 Rp` : 5.23 DW : 0.19

Quantitative Analysis - Rietveld

Phase 1 : AgSO4-C2c	90(160) %
Phase 2 : Pt	0.2(34) %
Phase 3 : WC	8(150) %
Phase 4 : Ag2S2O7	0.000 %

*) empty cell

Zero error	-0.014(10)

S5. The refined lattice vectors of $AgSO_4$ (C2/c).

p [GPa]	a [Å]	b [Å]	c [Å]	beta [deg]
14.0	12.701	12.709	9.039	44.42
15.3	12.692	12.692	9.030	44.40
16.5	12.563	12.582	8.998	44.64
18.6	12.500	12.512	8.945	44.68
23.4	12.373	12.464	8.871	44.61
29.5	12.394	12.264	8.745	45.09
29.5	12.359	12.255	8.812	44.61
23.0	12.522	12.477	8.953	44.44
7.0	12.974	12.901	9.349	44.32

Numbers are rounded to the third (lattice constants) or second (angle) decimal place.

S6. The refined lattice vectors of HP-$Ag_2S_2O_7$ (C2/c).

p [GPa]	a [Å]	b [Å]	c [Å]	beta [deg]
29.5	11.215	6.522	5.906	95.65
23.0	11.270	6.558	6.017	95.62
7.0	11.759	6.726	6.245	94.84

Numbers are rounded to the third (lattice constants) or second (angle) decimal place.

S7. Equation of state of $AgSO_4$ – experimental and theoretical (p,V) values.

Experiment		Theory	
p /GPa	2 V_{FU} /Å^3	p /GPa	2 V_{FU} /Å^3
0	151.76	0	155.89
14	128.10	5	141.24
15.3	126.96	10	132.97
16.5	124.91	15	126.84
18.6	122.54	20	122.35
23.4	120.66	25	119.17
29.5	117.17	30	114.71
29.5	116.92		
23	122.82		
7	138.40		

S8. Equation of state of HP-$Ag_2S_2O_7$ – experimental and theoretical (p,V) values.

Experiment		Theory	
p /GPa	V_{FU} /Å^3	p /GPa	V_{FU} /Å^3
29.5	107.48	29.5	105.84
23	110.63	23	109.76
7	123.04	7	124.92
0	---	0	138.93

S9. Magnetic models yielding minimum energy at 0 GPa and at 30 GPa (DFT results). CIF file

Model P-1 @ 0GPa: a = 12.955, b = 13.787, c = 9.480, α = 90.09, β = 48.07 , γ = 90.01

atom	x	y	z	atom	x	y	z	atom	x	y	z
Ag(up)1	0.25000	0.25000	0.50000	O1	0.90444	0.19680	0.21742	O33	0.34621	0.45904	0.98868
Ag(up)2	0.75000	0.75000	0.50000	O2	0.09556	0.80320	0.78258	O34	0.65379	0.54096	0.01132
Ag(up)3	0	0.50000	0.50000	O3	0.09545	0.19687	0.28281	O35	0.65491	0.45908	0.50873
Ag(up)4	0	0.50000	0	O4	0.90455	0.80313	0.71719	O36	0.34509	0.54092	0.49127
Ag(up)5	0.50000	0	0.50000	O5	0.40444	0.69680	0.21742	O37	0.84621	0.95904	0.98868
Ag(up)6	0.50000	0	0	O6	0.59556	0.30320	0.78258	O38	0.15379	0.04096	0.01132
Ag(up)7	0.25000	0.25000	0	O7	0.59545	0.69687	0.28281	O39	0.15491	0.95908	0.50873
Ag(up)8	0.75000	0.75000	0	O8	0.40455	0.30313	0.71719	O40	0.84509	0.04092	0.49127
Ag(down)1	0.75000	0.25000	0	O9	0.91822	0.36402	0.14143	O41	0.20026	0.60329	0.10175
Ag(down)2	0.25000	0.75000	0	O10	0.08178	0.63598	0.85857	O42	0.79974	0.39671	0.89825
Ag(down)3	0	0	0	O11	0.08184	0.36397	0.35919	O43	0.79970	0.60363	0.39844
Ag(down)4	0	0	0.50000	O12	0.91816	0.63603	0.64081	O44	0.20030	0.39637	0.60156
Ag(down)5	0.50000	0.50000	0	O13	0.41822	0.86402	0.14143	O45	0.70026	0.10329	0.10175
Ag(down)6	0.50000	0.50000	0.50000	O14	0.58178	0.13598	0.85857	O46	0.29974	0.89671	0.89825
Ag(down)7	0.75000	0.25000	0.50000	O15	0.58184	0.86397	0.35919	O47	0.29970	0.10363	0.39844
Ag(down)8	0.25000	0.75000	0.50000	O16	0.41816	0.13603	0.64081	O48	0.70030	0.89637	0.60156
S1	0.97135	0.26575	0.05706	O17	0.94027	0.23948	0.93758	O49	0.17032	0.46161	0.97796
S2	0.02865	0.73425	0.94294	O18	0.05973	0.76052	0.06242	O50	0.82968	0.53839	0.02204
S3	0.02835	0.26574	0.44370	O19	0.05963	0.23959	0.56283	O51	0.83168	0.46151	0.51801
S4	0.97165	0.73426	0.55630	O20	0.94037	0.76041	0.43717	O52	0.16832	0.53849	0.48199
S5	0.47135	0.76575	0.05706	O21	0.44027	0.73948	0.93758	O53	0.67032	0.96161	0.97796
S6	0.52865	0.23425	0.94294	O22	0.55973	0.26052	0.06242	O54	0.32968	0.03839	0.02204
S7	0.52835	0.76574	0.44370	O23	0.55963	0.73959	0.56283	O55	0.33168	0.96151	0.51801
S8	0.47165	0.23426	0.55630	O24	0.44037	0.26041	0.43717	O56	0.66832	0.03849	0.48199
S9	0.27255	0.52444	0.95711	O25	0.12400	0.25826	0.92899	O57	0.36902	0.57201	0.76877
S10	0.72745	0.47556	0.04289	O26	0.87600	0.74174	0.07101	O58	0.63098	0.42799	0.23123
S11	0.72814	0.52429	0.54149	O27	0.87576	0.25852	0.57171	O59	0.63168	0.57075	0.73064
S12	0.27186	0.47571	0.45851	O28	0.12424	0.74148	0.42829	O60	0.36832	0.42925	0.26936
S13	0.77255	0.02444	0.95711	O29	0.62400	0.75826	0.92899	O61	0.86902	0.07201	0.76877
S14	0.22745	0.97556	0.04289	O30	0.37600	0.24174	0.07101	O62	0.13098	0.92799	0.23123
S15	0.22814	0.02429	0.54149	O31	0.37576	0.75852	0.57171	O63	0.13168	0.07075	0.73064
S16	0.77186	0.97571	0.45851	O32	0.62424	0.24148	0.42829	O64	0.86832	0.92925	0.26936

Model P21/c @ 30 GPa: a = 12.329, b = 12.204, c = 8.533, α = 90, β = 45.41 , γ = 90

atom	x	y	z	atom	x	y	z	atom	x	y	z
Ag(up)1	0.74928	0.24981	0.00065	O1	0.92557	0.16346	0.20355	O33	0.31250	0.45026	0.06129
Ag(up)2	0.25072	0.75019	-0.00065	O2	0.07443	0.83654	0.79645	O34	0.68750	0.54974	0.93871
Ag(up)3	0.24928	0.25019	0.50065	O3	0.07260	0.16336	0.29684	O35	0.68707	0.44967	0.43935
Ag(up)4	0.75072	0.74981	0.49935	O4	0.92740	0.83664	0.70316	O36	0.31293	0.55033	0.56065
Ag(up)5	0	0.50000	0	O5	0.42740	0.66336	0.20316	O37	0.81293	0.94967	0.06065
Ag(up)6	0.50000	0	0.50000	O6	0.57260	0.33664	0.79684	O38	0.18707	0.05033	0.93935
Ag(up)7	0	0	0	O7	0.57443	0.66346	0.29645	O39	0.18750	0.95026	0.43871
Ag(up)8	0.50000	0.50000	0.50000	O8	0.42557	0.33654	0.70355	O40	0.81250	0.04974	0.56129
Ag(up)9	0.24965	0.25020	0.00039	O9	0.93213	0.35288	0.16738	O41	0.14329	0.59805	0.16581
Ag(up)10	0.75035	0.74980	-0.00039	O10	0.06787	0.64712	0.83262	O42	0.85671	0.40195	0.83419
Ag(up)11	0.74965	0.24980	0.50039	O11	0.06705	0.35277	0.33322	O43	0.85645	0.59746	0.33474
Ag(up)12	0.25035	0.75020	0.49961	O12	0.93295	0.64723	0.66678	O44	0.14355	0.40254	0.66526
Ag(down)1	0	0.50000	0.50000	O13	0.43295	0.85277	0.16678	O45	0.64355	0.09746	0.16526
Ag(down)2	0.50000	0	0	O14	0.56705	0.14723	0.83322	O46	0.35645	0.90254	0.83474
Ag(down)3	0	0	0.50000	O15	0.56787	0.85288	0.33262	O47	0.35671	0.09805	0.33419
Ag(down)4	0.50000	0.50000	0	O16	0.43213	0.14712	0.66738	O48	0.64329	0.90195	0.66581
S1	0.99012	0.25092	0.04004	O17	0.94400	0.23689	0.92715	O49	0.18138	0.44540	0.95377
S2	0.00988	0.74908	0.95996	O18	0.05600	0.76311	0.07285	O50	0.81862	0.55460	0.04623
S3	0.00876	0.25070	0.46054	O19	0.05539	0.23630	0.57264	O51	0.81759	0.44501	0.54795
S4	0.99124	0.74930	0.53946	O20	0.94461	0.76370	0.42736	O52	0.18241	0.55498	0.45205
S5	0.49124	0.75070	0.03946	O21	0.44461	0.73630	0.92736	O53	0.68241	0.94502	0.95205
S6	0.50876	0.24930	0.96054	O22	0.55539	0.26370	0.07264	O54	0.31759	0.05499	0.04795
S7	0.50988	0.75092	0.45996	O23	0.55600	0.73689	0.57285	O55	0.31862	0.94540	0.54623
S8	0.49012	0.24908	0.54004	O24	0.44400	0.26311	0.42715	O56	0.68138	0.05460	0.45377
S9	0.25396	0.51755	-0.00677	O25	0.15664	0.24644	0.87023	O57	0.37699	0.58063	0.79618
S10	0.74604	0.48245	0.00677	O26	0.84336	0.75356	0.12977	O58	0.62301	0.41937	0.20382
S11	0.74554	0.51696	0.50749	O27	0.84221	0.24605	0.63106	O59	0.62247	0.58029	0.70409
S12	0.25446	0.48304	0.49251	O28	0.15779	0.75395	0.36894	O60	0.37753	0.41971	0.29591
S13	0.75446	0.01696	-0.00749	O29	0.65779	0.74605	0.86894	O61	0.87753	0.08029	0.79591
S14	0.24554	0.98304	0.00749	O30	0.34221	0.25395	0.13106	O62	0.12247	0.91971	0.20409
S15	0.24604	0.01755	0.50677	O31	0.34336	0.74644	0.62977	O63	0.12301	0.08063	0.70382
S16	0.75396	0.98245	0.49323	O32	0.65664	0.25356	0.37023	O64	0.87699	0.91937	0.29618

S10. Database of structural phase transitions for metal sulfates.

Table. The pressure- and temperature-driven 1st order crystallographic phase transitions in anhydrous metal sulfates.

Formula	p	T /K	Transition	Comment	Ref.
Li_2SO_4	1 atm	713	*R*–3 → ?	This phase transition has not been confirmed by others researches eg. [5, 2].	1
Li_2SO_4	1 atm	848 ↑ 859 ↑	$P2_1/c$ (II beta)→ *Fm*–3*m* (I alpha)	Structure of *Fm*3*m* has been determined from powder neutron experiment at 908 K [4]. Beta phase (II) is above 90 K [2] and its structure has been determined in $P2_1/c$ by [7].	3, 4, 5, 6, 7, 8
Li_2SO_4	0.5 GPa	863 ↑	$P2_1/c$ (II beta)→ *Fm*–3*m* (I alpha)		4, 5, 7
Li_2SO_4	1.3 GPa	873↑	*Fm*–3*m* (I alpha) → (III)		4, 5
Li_2SO_4	1.6 GPa	833 ↑	$P2_1/c$ (II beta) → (IV)	Phase (IV) by [5] is probably the same as phase *delta* by [9].	5, 7
Li_2SO_4	2.0 GPa	703 ↑	$P2_1/c$ (II beta) → (IV)		5, 7
Li_2SO_4	3 GPa ↑	475	(VI gamma) → (delta)		9
Li_2SO_4	1.3 GPa ↑	293	$P2_1/c$ (II beta) → (gamma)		2, 5, 7, 9
Li_2SO_4	3.5 GPa ↑	293	(VI gamma)→ (delta)		2, 9
Li_2SO_4	7 GPa ↑	475	(delta) → (epsilon) *Cmcm* (VII)	Structure *Cmcm* at 6.7 GPa/723 K & 7.2GPa/700K [9] is isostrucutral with Na_2SO_4 (III) [10].	9
Li_2SO_4	1.5 GPa	923 ↑	(III) → *Fm*–3*m* (I alpha)		4, 5
Li_2SO_4	1.7 GPa	903 ↑	(IV) → (III)		5
Li_2SO_4	2.3 GPa	1023 ↑	(V) → *Fm*–3*m* (I) *alpha*		4, 5
Li_2SO_4	2.5 GPa	970 ↑	(IV) → (V)	Pistorius [8] observed some phase transition at 2.5 GPa/ 1021 K ↑.	5
Na_2SO_4	1 atm	443 [3, 11] 453 [10] 480 [6]	*Fddd* (V) → (IV)	Some have observed only phase transition (V) → (I) during heating at about 508/514 K, which is said to be unusual [12] and very sluggish [13, 14], however some authors indicate that new phases sometimes appear during heating between phases (V) and (I) [3, 15, 16, 25], eg.: (V) → (III) at 450 or 473 K [15, 17, 25]. The DSC analysis show transition range between 516 and 526 K [13, 14]. Phase (IV) is probably monoclinic [18].	13, 19
Na_2SO_4	1 atm	458 [3, 11] 473 [10]	(IV) → *Cmcm* (III)	Dasgupta suggested space group *I*-42*d* [20] for phase (III) without showing the structure. Authors of [10], conclude that the correct structure is in *Cmcm* space group instead of *Pbnn* [18, 21]. Phase (III) is probably metastable at RT [14, 22].	10, 13, 22, 23
Na_2SO_4	1 atm	501 [10] 503 [17]	*Cmcm* (III) → *Pbnm* (II)	Some authors suggest that there is no evidence of phase transition (III)	10, 13, 22, 23

				→ (II). X-ray, DSC and electrical conductivity measurements show that phase (III) (obtained e.g. by cooling) was always converted to phase (I) between at 514 and 522 K [3, 6, 11, 13, 14, 15, 18, 22, 24, 25].	
Na_2SO_4	1 atm	502 ↓ [14] near 439 ↓ [13]	*Pbnm* (II) → *Cmcm* (III)	Phase (II) appears on cooling [13].	10, 13, 22, 23
Na_2SO_4	1 atm	508 [10], 510 [17]	*Pbnm* (II) → $P6_3/mmc$ with disorder (I)	The m.p. is 1154–1156 K [6, 10, 25]. The database contains the *P*3*m* structure [26], but temperature is not speciied.	13, 17, 27, 28
Na_2SO_4	1 atm	506-509↓	$P6_3/mmc$ with disorder (I) → (II) *Pbnm*	Phase (II) appears only on cooling [13].	3, 10, 11, 13, 14, 17, 27, 28,
Na_2SO_4	~1.3 GPa	~373	*Fddd* (V) → *Cmcm* (III)		18,12
Na_2SO_4	~2.8 GPa	~373	*Cmcm* (III) → (VI)		18,12
Na_2SO_4	~2.0 GPa	~653	$P6_3/mmc$ (I) → (VII)		18
Na_2SO_4	~2.3 GPa	~690	$P6_3/mmc$ (I) → (VIII)		18
Na_2SO_4	~0.5 GPa	~548	$P6_3/mmc$ (I) → *Cmcm* (III)		18
Na_2SO_4	~2.0 GPa	~568	*Cmcm* (III) → (VII)		18
Na_2SO_4	~3.5 GPa	~533	(VI) → (VII)		18
K_2SO_4	1 atm	860 [29] 844 ↑ [30, 31]	*Pmcn* (II) → $P6_3/mmc$ (I)	$P6_3/mmc$ @ 1073K [29]. There is also one known structure in space group *P*-3*m* [26].	26, 27, 29, 31, 32, 33 30, 34, 35
K_2SO_4	1 atm	839↓	$P6_3/mmc$ (I) → *Pmcn* (II)	Structure in *Pmcn* of (II) appears between 15K and 832K [30].	26, 27, 29, 30, 31, 32, 33, 34, 35
K_2SO_4	1 atm	143	*Pmcn* (II) → $Pna2_1$	Single crystal structure at 15K is *Pmcn* (*Pnma*) [30]. However, [36] mentions the $Pna2_1$ structure.	37, 38, 30
K_2SO_4	1 atm	56	? → ?	Calorimetric method	38, 39
K_2SO_4	1.2 GPa ↑	1073 ↑	*Pmcn* (II) → $P6_3/mmc$ (I)		30, 34, 40
K_2SO_4	3.1 GPa ↑	1373 ↑	*Pmcn* (II) → (III)		30, 34, 40
K_2SO_4	~4 GPa	~1500 ↑	*Pmcn* (II) → (III)		30, 34, 40
Rb_2SO_4	1 atm	930	*Pmcn* (II) → $P6_3/mmc$ or *P*-3*m* (I)		3, 27, 34, 41, 42,
Cs_2SO_4	1 atm	940	$P6_3/mmc$ (I) → *Pmcn* (II)		3, 42, 43
Cs_2SO_4	--	295		No phase transitions < 16.4 GPa.	44
$(NH_4)_2SO_4$	1 atm	223	(II) $Pna2_1$ or *Pmcn* disordered → (I)	@ RT *Pnma* (*Pmcn*) [45, p.26].	3, 45
$LiNaSO_4$	1 atm	788 791 794	$P3_1c$ → *Im*-3*m*		46, 47
$LiNaSO_4$	0.5 GPa	851	$P3_1c$ → *Im*-3*m*		46
$LiNaSO_4$	1 GPa	914	$P3_1c$ → *Im*-3*m*		46
$LiNaSO_4$	2 GPa	1037	$P3_1c$ → *Im*-3*m*		46
$LiNaSO_4$	2.2 or 2.39 GPa	295	$P3_1c$ → *Im*-3*m*		46, 48
$LiKSO_4$	1 atm	941/943	$P2_1cn$ or *Pmcn* disordered or *Cmmm* (α 0 0) with modulation (II) → $P6_3/mc$ or $P6_3/mmc$ (I)	Phase (I) exist up to 1005 K [49]	49, 50, 51, 52, 53, 54
$LiKSO_4$	1 atm	708	$P2_1cn$ or *Pmcn* disordered or *Cmmm* (α 0 0) with		49, 50, 51, 52, 53, 54

			modulation (II) → $P6_3/mc$ or $P6_3/mmc$ (I)		
$LiKSO_4$	1 atm	248- 265 ↑	(III) $P6_3$, $P2_1$ →$Cmc2_1$ or Cc		50
$LiKSO_4$	1 atm	178-203 (32K of hysteresis) 205	$Cmc2_1$ or $P6_3$ or Cc or $P6_3mc$ → $Cmc2_1$ or Cc		49, 50
$LiKSO_4$	1 atm	200-210 ↓	$P6_3$, $P2_1$ → $Cmc2_1$ or Cc		50
$LiKSO_4$	1 atm	205	(V) → (IV)	Authors of [54] suggest the $P3_1c$ space group between 190K and 240 K.	53, 54
$LiKSO_4$	1 atm	190	Cc (VI) → (V)		53, 54
$LiKSO_4$	1 atm	135	(VII) → Cc (VI)		53, 54
$LiKSO_4$	1 atm	80	(VIII) → (VII)		53, 54
$LiKSO_4$	1 atm	60	(IX) → (VIII)		53, 54
$LiKSO_4$	1 atm	30	(X) → (IX)		53, 54
$LiKSO_4$	0.8 GPa	295	$P6_3mc$ (III-alpha) → $Cmc2_1$ or Cc (beta)		51
$LiKSO_4$	3.0 or 4.0 GPa	295	$Cmc2_1$ or Cc (beta) → $P2_1/m$ or $P2_1$(gamma)		51, 54
$LiKSO_4$	6.7 GPa	295	$P2_1/m$ or $P2_1$ (gamma) → 'highly disordered' (delta)		51
$LiK_{0.8}(NH_4)_{0.2}SO_4$	0.9 GPa	295		Analogue of 0.8 GPa transition for $LiKSO_4$.	55
$LiK_{0.8}(NH_4)_{0.2}SO_4$	2.5 GPa	295		Analogue of 3.0 GPa transition for $LiKSO_4$.	55
$Li(NH_4)SO_4$	1 atm	28	(IV) → (III) $P2_1/c$ ($P2_1/a$)		56, 57
$Li(NH_4)SO_4$	1 atm	283-284	(III) $P2_1/c$ ($P2_1/a$) → (II & II') $P2_1cn$ ($P2_1nb$),	There is one communicate about $P2_1$ [58].	6, 56, 58, 59
$Li(NH_4)SO_4$	1 atm	460-462	(II) $P2_1cn$ ($P2_1nb$) , $P2_1$ → (I) $Pmcn$ or $P2_1nb$	$P2_1nb$ is at 483 K /1atm and 523 K/ 1atm [60]. $Pmcn$ is at 478K / 1atm [61]. @ 950 MPa / RT is $P2_1$ (powder) [62].	6, 56, 58, 59, 60, 61, 62
$LiCsSO_4$	1 atm	203	$Pcmn$ → $P2_1/n$		63, 64
$LiCsSO_4$	2.0 GPa	295	$Pcmn$ → $P2_1/n$		65
$LiCsSO_4$	4.0 GPa	295	$P2_1/n$ → ?		65
$LiCsSO_4$	7.2 GPa	295	? → ?		65
$NaKSO_4$	1.2 GPa	295	$P3m$ or $P\text{-}3m$ → amorphous		66
Tl_2SO_4	1 atm	765-772	$Pmcn$ (II) → $P6_3/mmc$ (I)		6, 12, 27
Ag_2SO_4	1 atm	698- 701↑ 685-675↓ [67]	$Fddd$ (II beta) → $P6_3/mmc$ (I alpha)	Electrical conductivity measurements suggest that (II) → (I) is at 473-518 K [68]. Reports from impedance measurement show transition temp. 689K [69].	70
Ag_2SO_4	1 atm	701	$Fddd$ (II) → $P6_3/mmc$ (I)		71
Ag_2SO_4	~1 GPa	708	$Fddd$ (II) → $P6_3/mmc$ (I)		71
$BeSO_4$	1 atm	863-883	$I\text{–}4$ (III) → Orthorhombic (pseudo-tetragonal) (II)	@ 298 K $I\text{–}4$.	3
$BeSO_4$	1 atm	908-913	Orthorhombic (pseudo-tetragonal) (II) → cubic (I)		3
$CaSO_4$	1 atm	1453	$Cmcm$ (II) → cubic (I)		3
$CaSO_4$	1.8-3.4 GPa	273	$Cmcm$ anhydrite → $P2_1/n$ monazite		72, 73, 74
$CaSO_4$	11.8-21 GPa	Between 273 &	$P2_1/n$ monazite → $Pbnm$ barite	$Pbnm$ has been measured at 1450K and 21 GPa (powder data).	75

		1450 ↑			
$CaSO_4$	Between 21 & 19.9 GPa ↓	Between 1450 & 295	*Pbnm* barite at 1450K/21GPa→ $P2_1/n$ (metastable)	$P2_1/n$ $AgMnO_4$–type 295 K/19.9GPa (metastable).	75
$CaSO_4$	Below 19.9 GPa	295	$P2_1/n$ → *Cmcm*	*Cmcm* anhydrite at 295 K/1 atm.	75
$CaSO_4$	33.2 GPa	(laser heating) ↑	Pbnm barite → Weird, black;	The black phase exists up to 1800 K [74].	74
$SrSO_4$	1 atm	1425	*Pnma* (II) → *F*-43*m*(I)		3, 76
$BaSO_4$	1 atm	1363	*Pnma* (II) → *F*-43*m* (I)		3, 6, 76, 77 78
$BaSO_4$	---	295	*Pnma* (II)	Authors claim no phase transitions for p < 21.5 GPa.	79, 80, 81, 82 83
$BaSO_4$	10 GPa	295	*Pnma* (II)		84
$BaSO_4$	15–27 GPa	295	$P2_12_12_1$ (III)	Transition pressure depends crucially on the pressure-transmitting medium	85
$MnSO_4$	5.5 GPa	771	*Cmcm* (I) → (II)		3, 86
$MnSO_4$	7.4 GPa	771	(II) → (III)		3, 86
$MnSO_4$	9.7 GPa	771	(III) → (IV)		3, 86
$FeSO_4$	0.5 GPa	1073	*Cmcm* (I) → *Pbnm* (II)	Phase (I) exists at 1 atm.	86, 87
$CoSO_4$	0.6 GPa	773	*Cmcm* (I) → *Pbnm* (II)		3, 86, 88, 89, 90, 91
$CoSO_4$	2.5 GPa	773	*Cmcm* (I) → (III)		3, 86, 88, 89, 91
$CoSO_4$	3.1 GPa	623	*Cmcm* (I) → (IV)		3, 86, 88, 89, 91
$CoSO_4$	2.1 GPa	973	*Pbnm* (II) → (III)		3, 86, 89, 90, 91
$CoSO_4$	3.8 GPa	773	(III) → (IV)		3, 86, 91
$CoSO_4$	4.1 GPa	773	(IV) → (V)		3, 86, 91
$CoSO_4$	4.9 GPa	773	(V) → (VI)		3, 86, 91
$CoSO_4$	9.8 GPa	773	(VI) → (VII)		3, 86, 91
$NiSO_4$	1.9 GPa	773	*Cmcm* (I) → (II)		3, 86
$NiSO_4$	2.5 GPa	573	*Cmcm* (I) → (III)		3, 86
$NiSO_4$	2.9 GPa	773	(II) → (III)		3, 86
$NiSO_4$	4.2 GPa	773	(III) → (IV)		3, 86
$NiSO_4$	6.5 GPa	773	(IV) → (V)		3, 86
$NiSO_4$	9.4 GPa	773	(V) → (VI)		3, 86
$NiSO_4$	10.7 GPa	773	(VI) → (VII)		3, 86
$NiSO_4$	10.8 GPa	943	(VI) → (VIII)		3, 86
$NiSO_4$	11.2 GPa	773	(VII) → (VIII)		3, 86
$NiSO_4$	12.3 GPa	773	(VIII) → (IX)		3, 86
$CuSO_4$	5.0 GPa	523	*Pmnb* (I) → (II)		3, 86
$ZnSO_4$	1 atm	1013	(II) → (I)	@ RT *Pmna* [3, 92].	[45 p. 24, p.60] , 86
$ZnSO_4$	1 atm		@ 973K *F*23		86, 93
$ZnSO_4$	1 atm		@ 973K *F*-43*m*		86, 93
$ZnSO_4$	2.3 GPa	773	(I) → (II)		3, 86, 94
$ZnSO_4$	1.0 GPa	1053	(I) → (III)		3, 86
$ZnSO_4$	1.5 GPa	1063	(I) → (IV)		3, 86
$ZnSO_4$	2.8 GPa	773	(I) → (V)		3, 86
$ZnSO_4$	3.7 GPa	773	(II) → (VI)		3, 86
$ZnSO_4$	1.6 GPa	1123	(III) → (IV)		3, 86
$ZnSO_4$	5.0 GPa	773	(VI) → (VII)		3, 86
$ZnSO_4$	7.3 GPa	773	(VII) → (VIII)		3, 86

$ZnSO_4$	8.7 GPa	773	(VIII) → (IX)		3, 86
$ZnSO_4$	9.7 GPa	773	(IX) → (X)		3, 86
$ZnSO_4$	10.3 GPa	773	(X) → (XI)		3, 86
$CdSO_4$	1 atm	773 ↑	*Pn*2$_1$*m* (III) → (II)	authors deduced the most probable space group@ 298K: *Pmmn* – there are only unit cell parameters (95), later authors solved and refined structure in *Pn*2$_1$*m* (97). Although a later paper (101) suggests another space group *P*2$_1$22$_1$, but *Pn*2$_1$*m* has been confirmed (98).	3, 95, 96, 97, 98
$CdSO_4$	1 atm	1073 ↑ [3] 1053 [104] >1083 ↑ [99] 1093 [100]	(II) → *Cmcm* (I)		101, 102, 104
$CdSO_4$	1 atm	1023-1116 ↑ [6] 1084 ↑ [104]	(III alpha) *Pn*2$_1$*m* => (I beta) *Cmcm*		104, 103
$CdSO_4$	1 atm	1085-1079 ↓	(I beta) *Cmcm* => (III alpha) *Pn*2$_1$*m*		104, 103
$CdSO_4$	1 atm	1103-1170 ↑ [104] 1130 ↑ [103]	(I beta) *Cmcm* => (gamma) *P*-3*m*1	Structure *P*-3*m* at 1123 K [104], however the temperature does not agree with other experimental phase transition data.	104, 103
$CdSO_4$	1 atm	1128-1115 ↓	(gamma) *P*-3*m*1 => (I beta) *Cmcm*		104, 103
$CdSO_4$	1 atm	1178-1309 ↑ [104] 1130 ↑ [103] 1283 ↑ [105]	(gamma) *P*-3*m*1 => synthesis of Cd_2OSO_4		104, 103
$SnSO_4$	Between 0.15-0.2 GPa	295	*Pnma* barite (I) → *P*2$_1$/*a* (II)	Second order phase transition	106, 107
$SnSO_4$	Between 4.4-5.1 GPa	295	*P*2$_1$/*a* (II) → *P*–1 (III)	Structure *P*2$_1$/*a* (II) has been measured at 0.2GPa. Structure *P*–1 (III) has been measured 13.5 GPa.	106
$SnSO_4$	Between 13.6 - 15.3 GPa	295	*P*–1 (III)→ *P*–1 (IV)	Structure *P*–1 (IV) has been measured 20.5 GPa.	106
$(NH_4)_2Eu(SO_4)_2$	~3.0 GPa	295	*P*2$_1$/*c* → ?		108, 109
$(NH_4)_2Eu(SO_4)_2$	~7.0 GPa	295	? → ?		108
$PbSO_4$	1atm	-	@ RT *Pnma*	Structure type of $BaSO_4$ [81]	(45 p. 24), 110, 81, 82, 83
H_2SO_4	1atm	-	@ 113 K *C*2/*c*		111, 112
Cu_2SO_4	1atm	-	@ RT *Fddd*		112
Hg_2SO_4	1atm	-	@ RT *P*2/*c*		113
$HgSO_4$	1atm	-	@ 298 K *Pmn*2$_1$	Previously as *Pn* [114].	97, 98, 115

Cu_2SO_4, $PbSO_4$, Hg_2SO_4, $HgSO_4$,-$AuSO_4$, $PdSO_4$, $TiSO_4$, and many other sulphates have never been studied under high pressure.

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