

**AN607****Atomic coordinate tables**

**Table 1.** Atom Coordinates and Isotropic Displacement Coefficients of  $(\text{NH}_4)\text{Fe}(\text{CO}_3)(\text{OH})_2$ . Space Group  $Cmcm$ ,  $a = 6.6154(6)$ ,  $b = 12.0639(10)$ ,  $c = 6.0263(5)$  Å. Upper values from the Rietveld refinement, lower from CASTEP optimization

Atom	$x$	$y$	$z$	$U_{iso}$ , Å $^2$
Fe1	0	0	0	0.0248(8)
	0	0	0	
N2	0	0.3465(6) 0.35200	1/4 1/4	0.029(3)
	0			
C3	0	0.7874(5) 0.79174	1/4 1/4	0.029(2)
	0			
O4	0	0.6805(4) 0.68579	1/4 1/4	0.029
	0			
O5	0	0.8395(2) 0.84295	0.0638(5) 0.05993	0.029
	0			
O6	0.1906(4) 0.18056	0.0163(4) 0.01948	1/4 1/4	0.012(2)
H7	0.19152 0.26415	0.09751 0.08744	1/4 1/4	0.04
H8	0	0.30273 0.30187	0.38241 0.39052	0.04
	0			
H9	0.13213 0.12728	0.38488 0.40326	1/4 1/4	0.04

**Table 5.** Refined and optimized atom coordinates in  $\text{Al}_4\text{H}_2(\text{SO}_4)_7(\text{H}_2\text{O})_{24}$ . Space group  $P\bar{1}$ ,  $a = 12.5881(5)$ ,  $b = 13.0726(5)$ ,  $c = 7.3354(2)$  Å,  $\alpha = 108.162(2)$ ,  $\beta = 70.536(2)$ ,  $\gamma = 112.658(2)^\circ$ .

Atom	$x$		$y$		$z$		$U_{iso}$ , Å <sup>2</sup>
	GSAS	CASTEP	GSAS	CASTEP	GSAS	CASTEP	
Al1	0.0754(10)	0.07016	0.8519(9)	0.85041	0.0657(15)	0.07100	0.0036(25)
Al2	0.5019(9)	0.50772	0.7189(9)	0.72117	0.3563(18)	0.35606	0.0036
S3	0.7758(8)	0.77230	0.4493(7)	0.44476	0.0146(13)	0.01044	0.028(2)
S4	0.2344(9)	0.23825	0.2955(8)	0.30147	0.3209(12)	0.32079	0.028
S5	0.8273(8)	0.82464	0.0948(8)	0.09301	0.3590(14)	0.35650	0.028
S6*	½	½	0	0	0	0	0.037(7)
O7*	0.3942(29)	0.39316	0.0278(39)	0.01545	0.1408(51)	0.14678	0.037(10)
O8*	0.5680(34)	0.55187	0.0889(28)	0.09550	-0.1177(51)	-0.11821	0.037
O9*	0.5670(31)	0.58953	-0.0056(38)	-0.00453	0.1111(57)	0.06780	0.037
O10*	0.4618(42)	0.45959	-0.1111(19)	-0.10919	-0.1342(53)	-0.15224	0.037
O11	0.6750(12)	0.67504	0.4894(14)	0.49229	0.0565(29)	0.05372	0.032(3)
O12	0.8768(13)	0.87787	0.5433(11)	0.53760	0.0757(27)	0.07019	0.032
O13	0.7390(16)	0.73325	0.3619(12)	0.35611	0.1291(25)	0.12507	0.032
O14	0.8135(18)	0.80804	0.4029(17)	0.39792	-0.1974(16)	-0.20464	0.032
O15	0.2296(17)	0.23308	0.2147(14)	0.21169	0.1311(18)	0.13502	0.032
O16	0.3578(11)	0.36192	0.3694(13)	0.37725	0.3106(26)	0.31170	0.032
O17	0.1567(16)	0.15844	0.3624(16)	0.36528	0.3548(29)	0.34448	0.032
O18	0.1965(16)	0.19975	0.2356(15)	0.24410	0.4821(22)	0.48947	0.032
O19	0.8790(14)	0.87423	0.0756(13)	0.07722	0.1454(15)	0.13773	0.032
O20	0.6993(10)	0.69547	0.0671(17)	0.07121	0.3834(29)	0.40380	0.032
O21	0.8745(16)	0.84964	0.0147(14)	0.00889	0.4397(26)	0.41866	0.032
O22	0.8824(16)	0.88359	0.2103(10)	0.21019	0.4579(27)	0.45103	0.032
O23	0.2199(14)	0.21581	0.8313(18)	0.83571	0.0153(29)	0.03616	0.046(3)
O24	-0.0809(13)	-0.08227	0.8544(19)	0.85759	0.1171(28)	0.12182	0.046
O25	-0.0222(24)	0.02390	0.2894(14)	0.70967	0.1067(28)	-0.09699	0.046
O26	0.5534(17)	0.55411	0.7765(16)	0.77932	0.1203(22)	0.12794	0.046

O27	0.4411(17)	0.44576	0.5715(12)	0.57556	0.2180(27)	0.21366	0.046
O28	0.1254(19)	0.11723	-0.0101(13)	-0.00641	0.2237(26)	0.23781	0.046
O29	0.6537(13)	0.65249	0.6951(18)	0.69250	0.2851(27)	0.28502	0.046
O30	0.0156(18)	0.01279	0.7751(17)	0.78291	0.2810(26)	0.28746	0.046
O31	0.9551(21)	0.96049	0.5301(22)	0.53963	0.3417(33)	0.34242	0.046
O32	0.4640(20)	0.46604	0.6649(17)	0.66275	0.5853(24)	0.58544	0.046
O33	0.3558(14)	0.35872	0.7415(17)	0.74012	0.4281(33)	0.42488	0.046
O34	0.5712(17)	0.56911	0.8664(14)	0.86563	0.4917(26)	0.49716	0.046
H35	0.27991	0.29000	0.89894	0.90133	0.05858	0.03567	0.055
H36	0.23859	0.23695	0.76040	0.76454	-0.03822	-0.02508	0.055
H37	-0.13146	-0.13146	0.83067	0.82766	0.02650	0.02484	0.055
H38	-0.10690	-0.10999	0.91037	0.91682	0.22810	0.23328	0.055
H39	-0.03531	-0.03824	0.65142	0.64221	-0.03693	-0.04731	0.055
H40	0.04872	0.03130	0.73943	0.70668	-0.22554	-0.23601	0.055
H41	0.50958	0.53281	0.82182	0.84292	0.11678	0.12029	0.055
H42	0.62982	0.63059	0.77800	0.77816	0.02783	0.02967	0.055
H43	0.39752	0.40720	0.54784	0.55786	0.11870	0.10315	0.055
H44	0.40956	0.41388	0.49899	0.50507	0.25744	0.26749	0.055
H45	0.15913	0.16141	1.06598	1.06596	0.19749	0.19353	0.055
H46	0.13458	0.13347	0.98933	0.99849	0.34899	0.36483	0.055
H47	0.66149	0.65066	0.62209	0.61876	0.20930	0.19918	0.055
H48	0.70723	0.70954	0.71896	0.72308	0.37281	0.37200	0.055
H49	-0.06309	-0.07094	0.77048	0.77322	0.36833	0.37031	0.055
H50	0.05069	0.06168	0.78091	0.78577	0.38466	0.37334	0.055
H51	0.92283	0.92636	0.53441	0.53398	0.25133	0.22723	0.076
H52	1.04650	1.05073	0.55764	0.57165	0.28692	0.30580	0.076
H53	0.01325	0.91611	0.56800	0.58176	0.45466	0.47210	0.076
H54	0.39116	0.39106	0.65006	0.65836	0.68703	0.69192	0.055
H55	0.52330	0.52520	0.64874	0.65006	0.61958	0.63432	0.055
H56	0.29856	0.29621	0.69504	0.69034	0.35025	0.35365	0.055

H57	0.33626	0.34307	0.81042	0.81437	0.49139	0.49263	0.055
H58	0.53468	0.55189	0.87924	0.88867	0.63274	0.64284	0.055
H59	0.61614	0.61248	0.93854	0.93577	0.45288	0.44463	0.055

$*frac = 1/2$

**Table 6.** Optimized atom coordinates in alunogen,  $\text{Al}_2(\text{SO}_4)(\text{H}_2\text{O})_{17}$ . Space group  $P1$ ,  $a = 7.420$ ,  $b = 26.970$ ,  $c = 6.062 \text{ \AA}$ ,  $\alpha = 89.57^\circ$ ,  $\beta = 97.34^\circ$ ,  $\gamma = 91.53^\circ$ ,  $Z = 2$ .

Atom	$x$	$y$	$z$	$U_{iso}, \text{ \AA}^2$
S1	0.23108	0.93819	0.47867	0.01
S2	0.23699	0.56262	0.47969	0.01
S3	0.64495	0.74712	0.48528	0.01
Al4	0.27862	0.09817	0.00283	0.01
Al5	0.73214	0.59825	-0.00003	0.01
O6	0.37391	0.90222	0.45009	0.02
O7	0.69971	0.02544	0.34653	0.02
O8	0.93158	0.08847	0.45471	0.02
O9	0.17934	0.96408	0.26332	0.02
O10	0.68666	0.47337	0.35025	0.02
O11	0.37617	0.60178	0.44712	0.02
O12	0.92583	0.41359	0.45228	0.02
O13	0.18082	0.53665	0.26501	0.02
O14	0.21478	0.28348	0.38728	0.02
O15	0.59964	0.72848	0.25473	0.02
O16	0.71333	0.79937	0.47629	0.02
O17	0.52360	0.25348	0.40529	0.02
O18	0.81448	0.84235	0.11227	0.02
O19	0.33869	0.12467	0.28494	0.02
O20	0.37348	0.03782	0.11463	0.02
O21	0.76856	0.93014	0.27973	0.02
O22	0.48588	0.88253	0.05563	0.02
O23	0.04773	0.07785	0.06494	0.02
O24	0.81661	0.66023	0.11398	0.02

O25	0.31538	0.37363	0.28358	0.02
O26	0.03462	0.41827	0.05314	0.02
O27	0.77338	0.56865	0.28158	0.02
O28	0.50004	0.61291	0.05349	0.02
O29	0.35871	0.46318	0.11626	0.02
O30	0.70860	0.32572	0.15631	0.02
O31	0.60376	0.21053	0.03169	0.02
O32	-0.00746	0.20977	0.11732	0.02
O33	0.13619	0.69665	0.24374	0.02
O34	0.14507	0.78583	0.41340	0.02
H35	0.77631	0.82490	0.24436	0.04
H36	0.89763	0.82103	0.03470	0.04
H37	0.44811	0.11212	0.38192	0.04
H38	0.30552	0.15642	0.35293	0.04
H39	0.29646	0.01077	0.17211	0.04
H40	0.50002	0.03490	0.19191	0.04
H41	0.74425	0.96580	0.30529	0.04
H42	0.87893	0.92059	0.38354	0.04
H43	0.44215	0.89169	0.19858	0.04
H44	0.44566	0.84697	0.01865	0.04
H45	-0.00052	0.08106	0.21097	0.04
H46	-0.04518	0.06292	-0.05111	0.04
H47	0.73117	0.68450	0.16372	0.04
H48	0.94595	0.67299	0.16357	0.04
H49	0.42386	0.38426	0.38771	0.04
H50	0.27516	0.33882	0.32056	0.04
H51	-0.01421	0.41451	0.19951	0.04

H52	-0.05299	0.43545	-0.05991	0.04
H53	0.74438	0.53270	0.30306	0.04
H54	0.88410	0.57785	0.38826	0.04
H55	0.45640	0.60678	0.20009	0.04
H56	0.41781	0.63773	-0.03782	0.04
H57	0.48564	0.46664	0.19255	0.04
H58	0.28455	0.48942	0.17433	0.04
H59	0.64451	0.30092	0.23937	0.04
H60	0.76230	0.30919	0.03704	0.04
H61	0.53691	0.23170	-0.08503	0.04
H62	0.55921	0.22122	0.17119	0.04
H63	0.04848	0.24035	0.18533	0.04
H64	-0.13851	0.21399	0.07095	0.04
H65	0.20222	0.67532	0.35539	0.04
H66	0.12881	0.73037	0.31372	0.04
H67	0.27052	0.78489	0.48655	0.04
H68	0.07180	0.79985	0.51914	0.04

**Table 9.** Refined and optimized atom coordinates of  $\text{MgCl}_2(\text{H}_2\text{O})_4$ . Space group  $P2_1/c$ ,  $a = 5.9001(9)$ ,  $b = 7.2709(7)$ ,  $c = 8.4199(7)$  Å,  $\beta = 111.007(15)^\circ$ .

Atom	$x$		$y$		$z$		$U_{iso}$ , Å <sup>2</sup>
	GSAS	CASTEP	GSAS	CASTEP	GSAS	CASTEP	
Mg1	0	0	0	0	0	0	0.006(3)
Cl2	0.3089(16)	0.30875	0.2557(16)	0.26543	0.0787(28)	0.07772	0.006
O3	-0.0006(27)	0.00614	-0.0003(43)	-0.00836	0.2406(18)	0.24957	0.006
O4	0.2792(33)	0.27477	-0.2138(30)	-0.20082	0.0834(40)	0.06661	0.006
H5	0.0871	0.10911	0.0597	0.06774	0.3251	0.34503	0.02
H6	-0.0897	-0.10262	-0.0656	-0.07803	0.2852	0.29311	0.02
H7	0.3919	0.38450	-0.2161	-0.21125	0.1608	0.18620	0.02
H8	0.3791	0.38061	-0.2150	-0.21917	0.0208	0.00026	0.02

**Table 10.** Refined and optimized atom coordinates for  $\text{MgCl}_2(\text{H}_2\text{O})_2$ . Space group  $C2/m$ ,  $a = 7.3886(29)$ ,  $b = 8.5498(24)$ ,  $c = 3.6488(17)$  Å,  $\beta = 98.96(3)^\circ$ .

Atom	$x$		$y$		$z$		$U_{iso}$ , Å <sup>2</sup>
	GSAS	CASTEP	GSAS	CASTEP	GSAS	CASTEP	
Mg1	0	0	0	0	0	0	0.002
Cl2	0.2441(9)	0.24368	0	0	0.5703(15)	0.57759	0.002
O3	0	0	0.2363(12)	0.23971	0	0	0.002
H4	0.0710	0.08700	0.3013	0.30812	0.1304	0.15690	0.02

**Table 11.** Refined and optimized atom coordinates for MgCl<sub>2</sub>(H<sub>2</sub>O). Space group *Pnma*,  $a = 8.899(7)$ ,  $b = 3.6339(20)$ ,  $c = 11.398(8)$  Å.

Atom	<i>x</i>		<i>y</i>		<i>z</i>		$U_{iso}$ , Å <sup>2</sup>
	GSAS	CASTEP	GSAS	CASTEP	GSAS	CASTEP	
Mg1	0.1782(14)	0.19181	1/4	1/4	0.0192(11)	0.03324	0.003
Cl2	0.3139(12)	0.31826	-1/4	-1/4	-0.0847(9)	-0.06072	0.003
Cl3	0.0332(11)	0.01965	3/4	3/4	0.1227(8)	0.13009	0.003
O4	0.3224(25)	0.33439	1/4	1/4	0.1558(17)	0.17530	0.003
H5		0.38365		0.46043		0.21207	