High-pressure behaviour and elastic constants of 1M and 2M1 polytypes of phlogopite $KMg_3Si_3AlO_{10}(OH)_2$

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Supplementary Materials

Table S1. Crystal structure parameters of Phlogopite-1*M* as a function of pressure, obtained from DFT/B3LYP-D* simulations.

	Pressure (GPa)										
	17.36	13.05	9.51	6.59	4.20	2.24	0.63	0.05	-0.68	-1.76	-2.65
a (Å)	5.1354	5.1645	5.1927	5.2198	5.2453	5.2688	5.2902	5.2984	5.3094	5.3270	5.3430
b (Å)	8.8992	8.9542	9.0065	9.0557	9.1013	9.1428	9.1801	9.1944	9.2134	9.2441	9.2728
c (Å)	9.3775	9.4901	9.6061	9.7284	9.8579	9.9960	10.1438	10.2081	10.3010	10.4689	10.6562
β (°)	100.91	100.81	100.69	100.58	100.48	100.38	100.27	100.24	100.20	100.26	100.70
V (Å^3)	420.811	431.073	441.460	452.032	462.754	473.654	484.733	489.380	495.944	507.271	518.779
T_{thick} (Å)	2.2068	2.2151	2.2222	2.2294	2.2363	2.2424	2.2484	2.2506	2.2537	2.2584	2.2631
M_{thick} (Å)	2.1326	2.1427	2.1515	2.1590	2.1655	2.1717	2.1762	2.1786	2.1804	2.1839	2.1856
I_{thick} (Å)	2.6787	2.7522	2.8343	2.9247	3.0254	3.1378	3.2625	3.3175	3.3986	3.5434	3.6978
ψ (°)	58.08	58.13	58.19	58.25	58.30	58.35	58.40	58.41	58.44	58.48	58.54
α_r (°)	14.58	14.11	13.53	12.90	12.26	11.62	11.03	10.78	10.45	9.80	8.98
Δz (Å)	0.0063	0.0081	0.0094	0.0102	0.0102	0.0105	0.0106	0.0107	0.0105	0.0105	0.0106
TQE											
T1	1.0016	1.0015	1.0014	1.0014	1.0014	1.0014	1.0015	1.0015	1.0016	1.0017	1.0019
T2	1.0025	1.0023	1.0021	1.0020	1.0019	1.0018	1.0016	1.0016	1.0015	1.0014	1.0014
T3	1.0032	1.0029	1.0027	1.0024	1.0022	1.0021	1.0019	1.0019	1.0018	1.0017	1.0015
T4	1.0020	1.0018	1.0017	1.0016	1.0014	1.0014	1.0013	1.0013	1.0013	1.0014	1.0017
mean	1.0023	1.0021	1.0020	1.0019	1.0017	1.0017	1.0016	1.0016	1.0016	1.0016	1.0016
V_T (Å^3)											
T1	2.1664	2.1834	2.1991	2.2122	2.2252	2.2355	2.2461	2.2494	2.2536	2.2599	2.2655
T2	2.1456	2.1679	2.1860	2.2044	2.2211	2.2347	2.2470	2.2524	2.2591	2.2683	2.2731
T3	2.1530	2.1762	2.1971	2.2158	2.2328	2.2470	2.2620	2.2670	2.2739	2.2838	2.2903
T4	2.6166	2.6466	2.6712	2.6948	2.7145	2.7351	2.7508	2.7563	2.7649	2.7764	2.7861
mean	2.2704	2.2935	2.3134	2.3318	2.3484	2.3631	2.3765	2.3813	2.3879	2.3971	2.4038
TAV											
T1	6.6733	6.2242	5.8474	5.6930	5.6465	5.6884	5.8077	5.9691	6.1760	6.8520	7.7975
T2	10.9318	9.8765	9.2129	8.6174	8.0949	7.6844	7.0516	6.8177	6.5159	6.0623	5.7233
T3	13.8184	12.3888	11.4494	10.4006	9.5281	8.9059	8.1187	7.9092	7.5711	6.8496	6.3742
T4	7.0267	6.5342	6.1014	5.6988	5.2548	5.0137	4.9102	4.9493	5.0012	5.6500	6.8758
mean	9.6126	8.7559	8.1528	7.6025	7.1311	6.8231	6.4721	6.4113	6.3161	6.3535	6.6927
OQE											
M1	1.0064	1.0064	1.0065	1.0067	1.0069	1.0072	1.0074	1.0075	1.0077	1.0079	1.0081
M2	1.0076	1.0080	1.0084	1.0088	1.0092	1.0096	1.0099	1.0100	1.0101	1.0102	1.0103
M3	1.0075	1.0071	1.0070	1.0069	1.0069	1.0069	1.0070	1.0070	1.0071	1.0073	1.0076
M4	1.0102	1.0104	1.0107	1.0110	1.0114	1.0117	1.0122	1.0122	1.0125	1.0127	1.0131
M5	1.0084	1.0080	1.0079	1.0079	1.0080	1.0082	1.0083	1.0084	1.0086	1.0089	1.0093

	M6	1.0080	1.0085	1.0090	1.0096	1.0102	1.0108	1.0114	1.0116	1.0118	1.0122	1.0124
	mean	1.0080	1.0081	1.0083	1.0085	1.0088	1.0091	1.0094	1.0095	1.0096	1.0099	1.0101
V_O (Å^3)												
	M1	10.7509	10.9359	11.1129	11.2778	11.4246	11.5666	11.6952	11.7421	11.8035	11.9045	11.9997
	M2	10.9900	11.1461	11.3042	11.4473	11.5924	11.7219	11.8339	11.8795	11.9433	12.0380	12.1191
	M3	10.7533	10.9516	11.1337	11.3044	11.4574	11.6025	11.7246	11.7787	11.8314	11.9325	12.0095
	M4	10.8552	11.0367	11.2085	11.3717	11.5251	11.6603	11.7833	11.8353	11.9006	11.9984	12.0834
	M5	10.7069	10.9026	11.0826	11.2519	11.4020	11.5451	11.6623	11.7085	11.7628	11.8586	11.9329
	M6	10.9158	11.0835	11.2357	11.3767	11.5123	11.6385	11.7513	11.8011	11.8573	11.9551	12.0390
	mean	10.8287	11.0094	11.1796	11.3383	11.4856	11.6225	11.7418	11.7909	11.8498	11.9479	12.0306
OAV												
	M1	21.7980	21.6368	21.8126	22.3380	22.9983	23.6038	24.1663	24.3780	24.7741	25.3148	25.9644
	M2	21.1952	22.4931	24.0685	25.6111	27.1508	28.4713	29.7099	29.9842	30.4588	31.0207	31.4415
	M3	24.8686	23.6203	22.8323	22.4067	22.2294	22.1414	22.3105	22.4842	22.7713	23.3354	24.4020
	M4	33.5517	34.1569	35.1030	36.0813	37.0088	37.8034	38.9527	39.6922	40.2746	41.4229	39.0787
	M5	27.8809	26.6329	26.0204	25.9347	26.1626	26.4992	27.0459	27.1920	27.8677	28.8367	30.1875
	M6	26.1541	27.9356	29.6783	31.5629	33.4526	35.2194	36.8132	37.2858	37.9419	38.8434	39.2735
	mean	25.9081	26.0793	26.5859	27.3225	28.1671	28.9564	29.8331	30.1694	30.6814	31.4623	31.7246

T_{thick}, M_{thick}, and I_{thick} are tetrahedral sheet thickness (calculated from the *z* coordinates of the basal and apical oxygen atoms), the octahedral sheet thickness (calculated from the *z* coordinates of the apical and hydroxyl O atoms) and interlayer thickness (calculated from the *z* coordinates of the basal oxygen atoms), respectively. ψ and α are the octahedral flattening angle and the tetrahedral rotation angle, respectively (Donnay et al., 1964a, b; Hazen and Burnham, 1973). Δz is the departure from coplanarity of the basal oxygen atoms O(b) (Güven, 1971). TQE and OQE are the tetrahedral and octahedral quadratic elongations, respectively, whereas TAV and OAV are the tetrahedral and octahedral bond angle variance, respectively (Robinson et al., 1971). V_T and V_O are the volumes of tetrahedra and octahedra, respectively. T and M represent the generic tetrahedral and octahedral sites, respectively.

Table S2. Crystal structure parameters of Phlogopite-2M_1 as a function of pressure, obtained from DFT/B3LYP-D* simulations.

	Pressure (GPa)										
	13.66	9.96	6.94	4.46	2.45	0.80	0.05	-0.54	-1.62	-2.52	-3.25
a (Å)	5.1631	5.1919	5.2186	5.2436	5.2667	5.2878	5.2984	5.3069	5.3244	5.3408	5.3552
b (Å)	8.9453	8.9962	9.0452	9.0911	9.1335	9.1719	9.1910	9.2065	9.2385	9.2682	9.2959
c (Å)	18.706	18.935	19.178	19.433	19.704	19.993	20.156	20.297	20.612	20.931	21.256
β (°)	94.90	94.87	94.85	94.82	94.79	94.75	94.72	94.69	94.55	94.11	93.29
V (Å^3)	860.778	881.229	902.014	923.107	944.528	966.294	978.198	988.361	1010.709	1033.407	1056.412
T_{thick} (Å)	2.2158	2.2230	2.2300	2.2369	2.2424	2.2484	2.2506	2.2530	2.2578	2.2629	2.2671
M_{thick} (Å)	2.1402	2.1502	2.1587	2.1650	2.1717	2.1757	2.1788	2.1800	2.1835	2.1858	2.1865
I_{thick} (Å)	2.7618	2.8401	2.9283	3.0269	3.1371	3.2590	3.3291	3.3916	3.5339	3.6828	3.8441
ψ (°)	57.30	57.22	57.13	57.08	57.00	56.98	56.93	56.92	56.85	56.82	56.76
α_r (°)	14.24	13.68	13.05	12.40	11.76	11.17	10.85	10.59	9.97	9.19	8.30
Δz (Å)	0.0025	0.0038	0.0048	0.0065	0.0098	0.0100	0.0097	0.0081	0.0075	0.0059	0.0007
TQE											
T1	1.0020	1.0018	1.0018	1.0018	1.0017	1.0016	1.0015	1.0015	1.0014	1.0014	1.0014
T2	1.0022	1.0020	1.0019	1.0018	1.0017	1.0015	1.0015	1.0015	1.0013	1.0012	1.0012
T3	1.0014	1.0014	1.0014	1.0014	1.0013	1.0014	1.0015	1.0015	1.0016	1.0018	1.0021
T4	1.0014	1.0013	1.0013	1.0013	1.0012	1.0012	1.0012	1.0012	1.0013	1.0015	1.0018
mean	1.0018	1.0016	1.0016	1.0016	1.0015	1.0014	1.0014	1.0014	1.0014	1.0015	1.0016
V_T (Å^3)											
T1	2.1653	2.1832	2.2014	2.2182	2.2329	2.2465	2.2519	2.2573	2.2667	2.2741	2.2791
T2	2.1712	2.1937	2.2132	2.2280	2.2446	2.2597	2.2663	2.2714	2.2832	2.2914	2.2941
T3	2.1846	2.2010	2.2137	2.2279	2.2362	2.2471	2.2499	2.2548	2.2607	2.2679	2.2723
T4	2.6456	2.6701	2.6939	2.7169	2.7338	2.7492	2.7574	2.7624	2.7748	2.7835	2.7950
mean	2.2917	2.3120	2.3306	2.3478	2.3619	2.3756	2.3814	2.3865	2.3964	2.4042	2.4101
TAV											
T1	8.7670	7.9201	7.7938	7.6536	7.2782	6.8914	6.4878	6.3898	5.8480	5.7742	5.6343
T2	9.3465	8.5208	7.9532	7.4991	7.0701	6.2889	6.1873	5.9200	5.2435	4.8459	4.6857
T3	5.6795	5.4856	5.4484	5.4292	5.1392	5.4588	5.6500	5.5244	6.2617	7.1022	8.4387
T4	5.3158	4.9999	4.9166	4.8963	4.6933	4.6968	4.6918	4.7290	4.9050	5.8909	7.2501
mean	7.2772	6.7316	6.5280	6.3696	6.0452	5.8340	5.7542	5.6408	5.5646	5.9033	6.5022
OQE											
M1	1.0076	1.0078	1.0080	1.0083	1.0086	1.0090	1.0091	1.0093	1.0096	1.0099	1.0102
M2	1.0068	1.0069	1.0071	1.0076	1.0079	1.0083	1.0084	1.0086	1.0089	1.0091	1.0095
M3	1.0089	1.0089	1.0090	1.0092	1.0094	1.0096	1.0097	1.0098	1.0101	1.0104	1.0107
mean	1.0078	1.0079	1.0080	1.0084	1.0086	1.0090	1.0091	1.0092	1.0095	1.0098	1.0101
V_O (Å^3)											
M1	10.9819	11.1613	11.3275	11.4712	11.6131	11.7332	11.7963	11.8434	11.9414	12.0272	12.0988
M2	11.0249	11.1943	11.3509	11.4878	11.6276	11.7373	11.8073	11.8504	11.9562	12.0489	12.1174
M3	10.9384	11.1177	11.2841	11.4389	11.5779	11.6996	11.7608	11.8076	11.9014	11.9876	12.0639
mean	10.9817	11.1578	11.3208	11.4660	11.6062	11.7234	11.7881	11.8338	11.9330	12.0212	12.0934
OAV											
M1	24.7226	25.1851	25.8170	26.7405	27.5401	28.5645	28.9297	29.4432	30.2918	31.1641	32.0950
M2	22.6128	23.1668	23.8637	25.2275	26.1522	27.4350	27.8962	28.4783	29.2945	30.0863	31.1538
M3	29.2789	29.2291	29.5374	29.9321	30.2862	30.8173	31.0595	31.3262	32.1278	32.9727	34.0748
mean	25.5381	25.8603	26.4060	27.3000	27.9928	28.9389	29.2951	29.7492	30.5714	31.4077	32.4412

T_{thick}, M_{thick}, and I_{thick} are tetrahedral sheet thickness (calculated from the z coordinates of the basal and apical oxygen atoms), the octahedral sheet thickness (calculated from the z coordinates of the apical and hydroxyl O atoms) and interlayer thickness (calculated from the z coordinates of the basal oxygen atoms), respectively. ψ and α are the octahedral flattening angle and the tetrahedral rotation angle, respectively (Donnay et al., 1964a, b; Hazen and Burnham, 1973). Δz is the departure from coplanarity of the basal oxygen atoms O(b) (Güven, 1971). TQE and OQE are the tetrahedral and octahedral quadratic elongations, respectively, whereas TAV and OAV are the tetrahedral and octahedral bond angle variance, respectively (Robinson et al., 1971). V_T and V_O are the volumes of tetrahedra and octahedra, respectively. T and M represent the generic tetrahedral and octahedral sites, respectively.

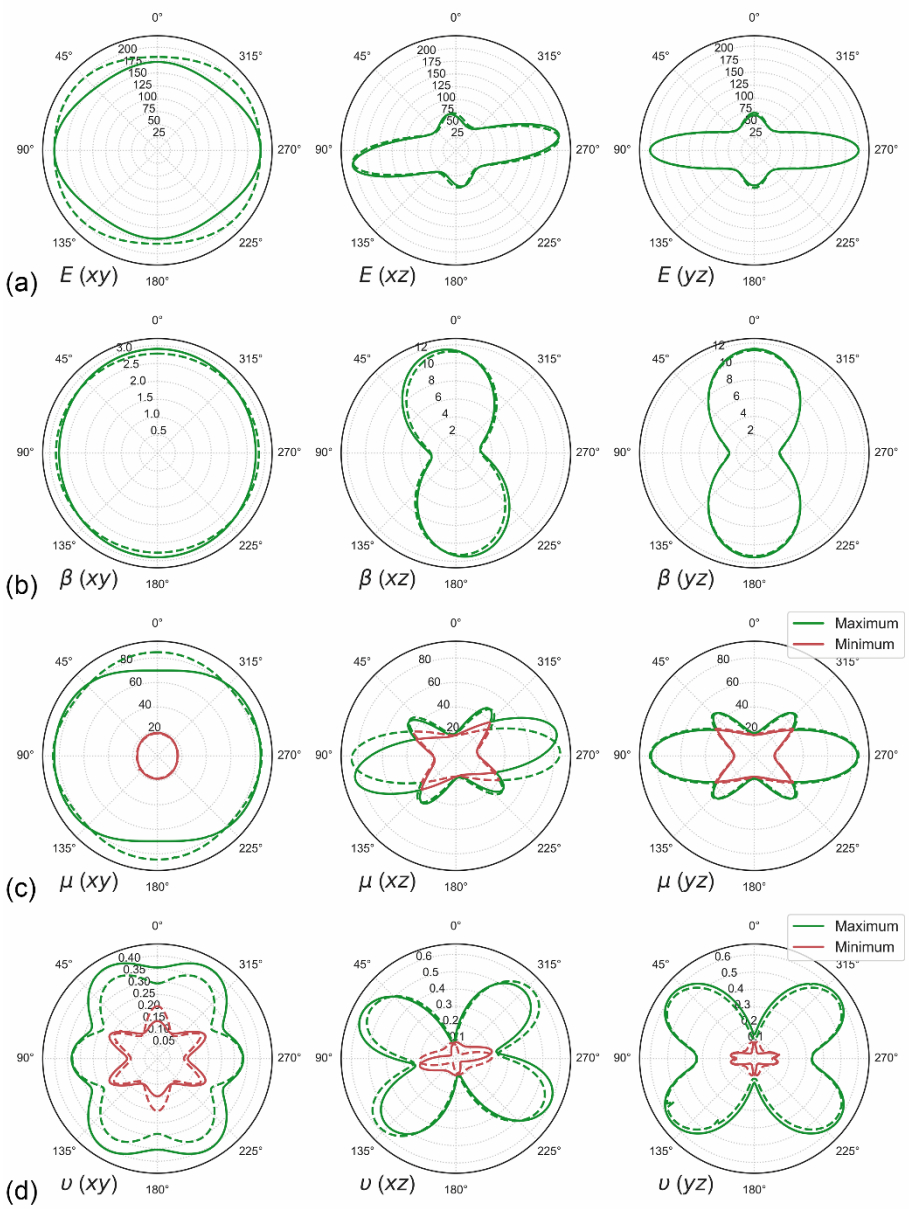

Figure S1. (a) Young's modulus (GPa), (b) linear compressibility (TPa^{-1}), (c) shear modulus (GPa) and (d) Poisson's ratio (dimensionless) of phlogopite-1*M* (solid lines) and phlogopite-2*M*1 (dashed lines), as obtained from DFT/B3LYP-D* calculations. Each panel reports the directional variation of the elastic property calculated on the *xy*, *xz* and *yz* Cartesian planes.