The effect of pressure on the elastic properties and seismic anisotropy of diopside and jadeite from atomic scale simulation. Supplementary Information.

A. M. Walker[1,*]

[1] Department of Earth Sciences,
University of Bristol,
Wills Memorial Building,
Queen's Road,
Bristol, BS8 1RJ, UK

[*] andrew.walker@bris.ac.uk

1 Convergence tests

Table 1 shows the results of convergence tests for k-point sampling and plane-wave cutoff. The energy, force on one atom in one direction, and one element of the stress tensor are calculated for one particular geometry, without geometry optimisation. Only the energy derivatives strictly need to be converged and these converge much more rapidly then the total energy. By 700 eV and a 2×2×3 grid all three measures are well converged. Details of the convergence tests carried out for diopside can be found in [1].

2 Structure and athermal equation of state of jadeite

Table 2 shows the evolution of the lattice vectors and unit cell volume with pressure. Experimental cell parameters at 1.5K are $a = 9.41582(9)$, $b = 8.55515(4)$, $c = 5.22071(21)$ Å and $\beta = 107.5634(7)^\circ$ [2]. This gives a volume of 400.95 Å^3.

Assuming a PBE error of 4.3 GPa and interpolating gives V = 401 Å^3 and results in a P–V curve in agreement with the experimental data (Figure 3). This offset is similar to that found for diopside (4.6 GPa, [1]). Once the offset is taken into account, the calculated crystal structure (Table 3) agrees with experimental data for all sites to better than 0.002 fractional units (∼0.02 Å).

Fitting a third-order Birch-Murgahan equation of state to the calculated volumes gives parameters $V_0 = 415.1$ Å^3, $K_0 = 116.6$ GPa and $K_0' = 3.9$. Fitting following the pressure offset gives $V_0 = 401.3$ Å^3, $K_0 = 128.8$ GPa and $K_0' = 3.8$, while constraining K_0' to 5.0 gives $V_0 = 400.6$ Å^3 and $K_0 = 137.7$ GPa (experiments at ambient temperature give $V_0 = 402.26 \pm 0.02$ Å^3, $K_0 = 134.0 \pm 0.7$ GPa and $K_0' = 4.4 \pm 0.1$ [3] and $K_0 = 124.5 \pm 4.0$ assuming K_0' of 5.0 [4]).

The parameters given in Tables 2 and 3 have been used to extract bond lengths and measures of structural and polyhedral regularity for jadeite using the same approach as that previously used for diopside [1]. These results are given in Tables 4, 5, 6 and 7 and Figures 2, 3 and 4. All three polyhedra become more ideal with increasing pressure but the detail of the variation in bond lengths is rather different to those found for diopside [1]. Table 8 contrasts the polyhedral volumes fitted to the third-order Birch-Murgahan equation of state for diopside and jadeite. In both minerals the M2 sire is more compressible than the M1 site which is more compressible than the Si site and the compressibility scales with the site volume.

3 Elastic constants

The evolution of the calculated elastic constants of diopside and jadeite with pressure are reported in tabular form in Table 9 and 10. These tables also contain the upper Voigt (K^v and G^v) and lower Reuss (K^r and G^r) bound of the bulk and shear moduli of isotropic polycrystalline samples of diopside and jadeite along with the arithmetic mean (the Voigt-Reuss-Hill average K^{vrh} and G^{vrh}). In addition, the general anisotropy index ($\mathrm{A}^\star = V^2_{s(max)}/V^2_{s(min)}$, where the maximum and minimum phase velocities are found from a search over all propagation directions, [5]) and the universal anisotropy index (A^U, derived from the Voigt and Reuss estimates of the isotropic average bulk and shear moduli, [6]) are given as a function of pressure.

References

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Plane-wave cutoff (eV)	k-point grid	Total energy (eV)	Stress (GPa)	Force (eV/Å)
600.0000	1x1x1	-16838.78747346	6.913870	-2.31715
600.0000	1x1x2	-16840.83010537	6.269173	-2.34727
600.0000	2x2x2	-16840.86712288	6.234072	-2.35151
600.0000	2x2x3	-16840.81463594	6.265156	-2.34977
600.0000	3x3x3	-16840.81398394	6.263807	-2.34969
600.0000	3x3x4	-16840.81486317	6.263370	-2.34979
600.0000	4x4x4	-16840.81612706	6.261636	-2.34977
400.0000	2x2x2	-16839.16846679	5.962158	-2.36963
450.0000	2x2x2	-16839.27319045	6.211402	-2.36321
500.0000	2x2x2	-16839.72774798	6.314173	-2.35384
550.0000	2x2x2	-16840.35969584	6.259969	-2.35354
600.0000	2x2x2	-16840.86712288	6.234067	-2.35151
650.0000	2x2x2	-16841.16789494	6.247952	-2.34671
700.0000	2x2x2	-16841.28791297	6.293571	-2.34776
750.0000	2x2x2	-16841.30849070	6.323769	-2.34415
800.0000	2x2x2	-16841.31961932	6.351028	-2.34297
850.0000	2x2x2	-16841.37787710	6.330706	-2.34443
900.0000	2x2x2	-16841.47777662	6.328530	-2.34306
950.0000	2x2x2	-16841.61340398	6.322510	-2.34240
1000.000	2x2x2	-16841.75950744	6.306950	-2.34337

Table 1: Convergence with key numerical parameters for jadeite.

P	a	b	c	β	V
-5.0	9.752	8.792	5.359	108.75	435.1
-4.0	9.700	8.758	5.342	108.51	430.3
-3.0	9.656	8.730	5.326	108.33	426.2
-2.0	9.616	8.702	5.311	108.18	422.3
-1.0	9.580	8.677	5.294	108.04	418.5
-0.0	9.545	8.653	5.279	107.91	414.9
1.0	9.509	8.633	5.266	107.83	411.5
2.0	9.479	8.610	5.251	107.72	408.2
3.0	9.450	8.588	5.237	107.61	405.1
4.0	9.423	8.567	5.224	107.51	402.2
5.0	9.397	8.546	5.211	107.41	399.3
6.0	9.374	8.525	5.197	107.32	396.5
7.0	9.350	8.505	5.184	107.22	393.8
8.0	9.328	8.486	5.171	107.13	391.2
9.0	9.305	8.465	5.159	107.00	388.6
10.0	9.284	8.446	5.147	106.93	386.2
11.0	9.264	8.428	5.136	106.86	383.8
12.0	9.245	8.411	5.124	106.79	381.5
13.0	9.227	8.393	5.113	106.72	379.2
14.0	9.208	8.375	5.100	106.59	376.9
15.0	9.191	8.357	5.088	106.50	374.7
16.0	9.174	8.339	5.077	106.42	372.6
17.0	9.158	8.322	5.066	106.33	370.5
18.0	9.142	8.305	5.055	106.25	368.5
19.0	9.128	8.288	5.045	106.17	366.5
20.0	9.113	8.272	5.034	106.10	364.6
21.0	9.099	8.255	5.024	106.03	362.7
22.0	9.085	8.239	5.015	105.96	360.9
23.0	9.072	8.223	5.005	105.89	359.1
24.0	9.059	8.208	4.996	105.82	357.4
25.0	9.046	8.192	4.987	105.76	355.6

Table 2: Calculated cell parameters for jadeite

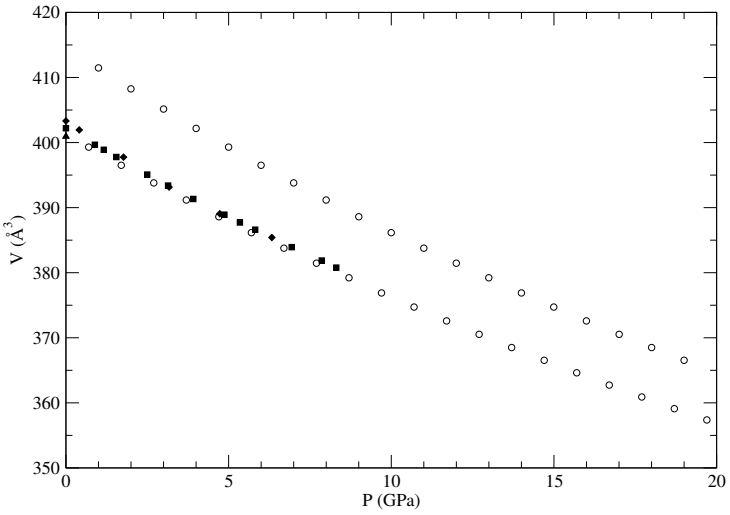

Figure 1: Unit cell volume as a function of pressure from the present calculations (open circles) and experiments (filled symbols: triangle [2], diamonds [4], squares [3]). Both the unshifted and corrected DFT results are shown (points plotting near the experimental data are shifted by 4.3 GPa to correct for the under-binding of the GGA)

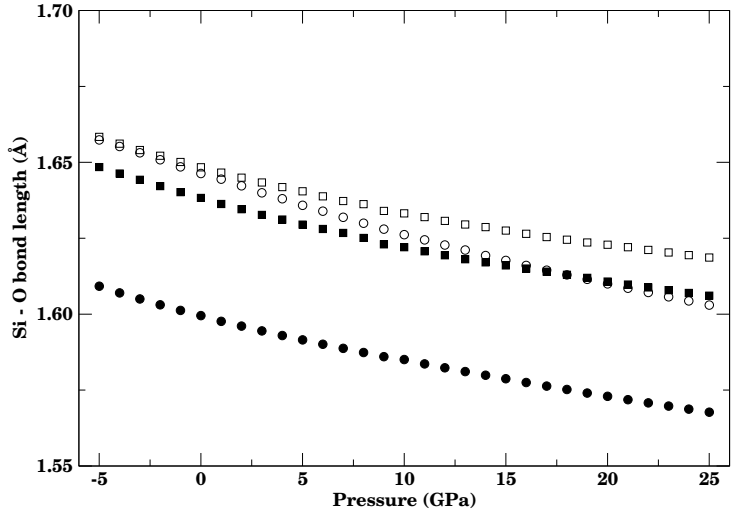

Figure 2: Bond lengths in the Si tetrahedron as a function of pressure. Closed circles Si–O1, open circles Si–O2, open squares Si–O3a, closed squares Si–O3b.

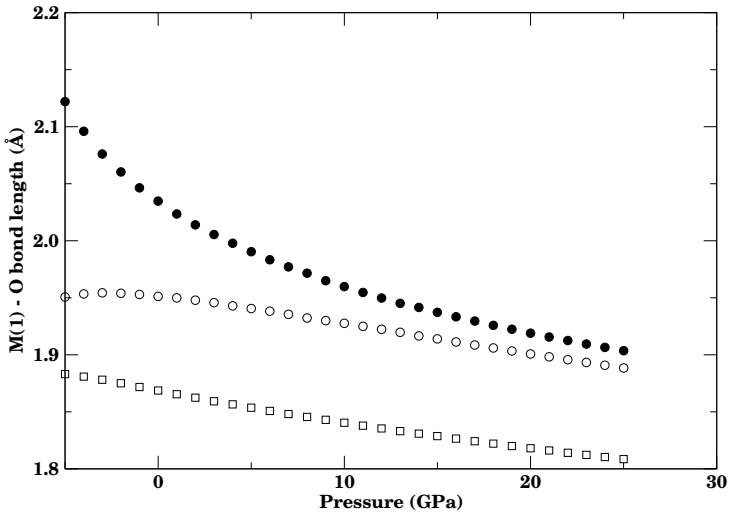

Figure 3: Bond lengths in the M1 octahedron as a function of pressure. Closed circles Al–O1a, open circles Al–O1b, open squares Al–O2.

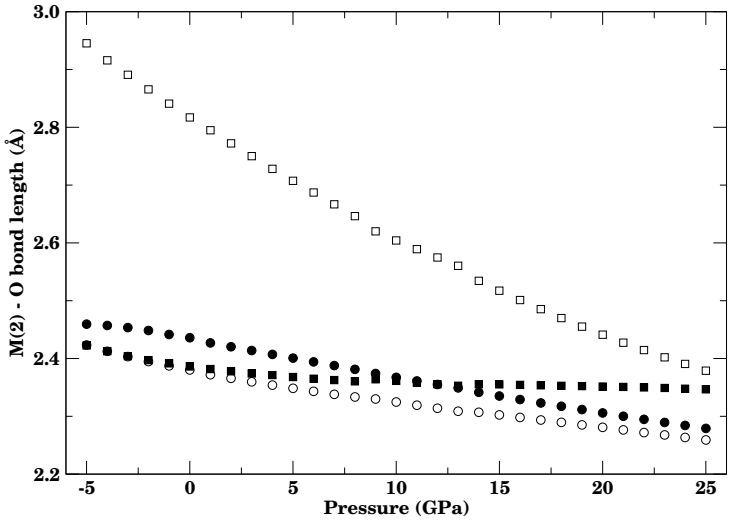

Figure 4: Bond lengths in the M2 polyhedron as a function of pressure. Closed circles Na–O1, open circles Na–O2, open squares Na–O3a, closed squares Na–O3b

P GPa	M1 y	M2 y	Si x	Si y	Si z	O1 x	O1 y	O1 z	O2 x	O2 y	O2 z	O3 x	O3 y	O3 z
-4.9995	0.899023	0.296287	0.288775	0.091496	0.224815	0.110007	0.075392	0.122291	0.363248	0.256651	0.285870	0.347274	0.000535	0.009546
-3.9955	0.900630	0.296967	0.289033	0.091830	0.225337	0.109811	0.075330	0.123831	0.362807	0.257786	0.286556	0.348214	0.001295	0.009275
-3.0021	0.901801	0.297535	0.289289	0.092069	0.225799	0.109682	0.075364	0.124954	0.362519	0.258659	0.287257	0.349054	0.001967	0.009080
-2.0017	0.902691	0.298102	0.289494	0.092324	0.226121	0.109564	0.075504	0.125815	0.362219	0.259492	0.288167	0.349830	0.002781	0.008604
-1.0032	0.903483	0.298728	0.289671	0.092688	0.226504	0.109461	0.075726	0.126654	0.361995	0.260329	0.289308	0.350508	0.003686	0.008100
-0.0003	0.904121	0.299298	0.289852	0.092915	0.226788	0.109351	0.075984	0.127226	0.361729	0.261048	0.290334	0.351185	0.004571	0.007530
0.9995	0.904806	0.299352	0.290522	0.093076	0.227427	0.109596	0.076028	0.127882	0.361669	0.261754	0.291611	0.352327	0.005491	0.007321
1.9979	0.905305	0.299924	0.290655	0.093301	0.227673	0.109505	0.076290	0.128356	0.361466	0.262391	0.292773	0.352898	0.006424	0.006654
2.9999	0.905755	0.300501	0.290760	0.093532	0.227883	0.109392	0.076567	0.128736	0.361285	0.263001	0.293922	0.353429	0.007335	0.005947
4.0026	0.906123	0.301077	0.290859	0.093721	0.228030	0.109307	0.076880	0.129029	0.361111	0.263526	0.295122	0.353921	0.008303	0.005147
5.0003	0.906501	0.301652	0.290953	0.093938	0.228259	0.109215	0.077162	0.129352	0.360944	0.264087	0.296293	0.354379	0.009180	0.004461
5.9984	0.906858	0.302226	0.291010	0.094173	0.228408	0.109133	0.077453	0.129683	0.360795	0.264633	0.297475	0.354796	0.010074	0.003744
6.9991	0.907145	0.302787	0.291092	0.094370	0.228564	0.109054	0.077759	0.129883	0.360644	0.265112	0.298674	0.355226	0.011003	0.002972
7.9985	0.907423	0.303427	0.291141	0.094586	0.228640	0.108956	0.078099	0.130007	0.360510	0.265584	0.299898	0.355580	0.011927	0.002047
9.0016	0.907568	0.303940	0.291225	0.094577	0.228265	0.108960	0.078139	0.130105	0.360462	0.265834	0.301345	0.356007	0.013387	0.000132
9.9985	0.907818	0.304316	0.291320	0.094766	0.228622	0.108903	0.078430	0.130334	0.360329	0.266300	0.302457	0.356390	0.014078	0.999791
11.0004	0.908061	0.304684	0.291393	0.094945	0.228947	0.108848	0.078723	0.130550	0.360203	0.266760	0.303527	0.356753	0.014759	0.999420
11.9982	0.908290	0.305026	0.291466	0.095119	0.229253	0.108791	0.079000	0.130729	0.360076	0.267197	0.304572	0.357097	0.015411	0.999053
12.9982	0.908503	0.305378	0.291525	0.095288	0.229509	0.108737	0.079268	0.130890	0.359957	0.267615	0.305609	0.357419	0.016057	0.998640
14.0006	0.908571	0.306265	0.291540	0.095465	0.229377	0.108683	0.079593	0.130789	0.359965	0.267853	0.307316	0.357656	0.017500	0.996836
14.9945	0.908756	0.306711	0.291575	0.095660	0.229472	0.108644	0.079882	0.130911	0.359899	0.268217	0.308552	0.357895	0.018389	0.995965
15.9984	0.908919	0.307166	0.291608	0.095825	0.229615	0.108590	0.080181	0.130981	0.359830	0.268569	0.309726	0.358138	0.019218	0.995204
17.0035	0.909065	0.307588	0.291636	0.095988	0.229754	0.108538	0.080478	0.131039	0.359769	0.268894	0.310853	0.358371	0.020021	0.994434
18.0015	0.909214	0.308043	0.291650	0.096154	0.229894	0.108493	0.080770	0.131094	0.359701	0.269240	0.312025	0.358588	0.020813	0.993683
18.9998	0.909345	0.308441	0.291669	0.096312	0.230011	0.108449	0.081056	0.131124	0.359645	0.269550	0.313126	0.358795	0.021594	0.992933
20.0012	0.909486	0.308820	0.291690	0.096474	0.230194	0.108404	0.081340	0.131170	0.359580	0.269883	0.314258	0.358973	0.022322	0.992245
21.0014	0.909617	0.309185	0.291703	0.096628	0.230360	0.108359	0.081626	0.131211	0.359518	0.270197	0.315380	0.359159	0.023055	0.991572
22.0022	0.909728	0.309498	0.291717	0.096762	0.230540	0.108323	0.081903	0.131237	0.359456	0.270501	0.316414	0.359357	0.023730	0.991010
23.0017	0.909843	0.309846	0.291729	0.096913	0.230762	0.108281	0.082175	0.131256	0.359389	0.270810	0.317504	0.359527	0.024404	0.990456
23.9931	0.909943	0.310140	0.291743	0.097042	0.231011	0.108244	0.082435	0.131279	0.359321	0.271109	0.318508	0.359709	0.025002	0.990028
25.0008	0.910040	0.310432	0.291756	0.097175	0.231239	0.108209	0.082698	0.131286	0.359249	0.271410	0.319535	0.359887	0.025631	0.989545

Table 3: Atomic positions in the calculated structure of jadeite.

P GPa	O3O3O3	Δ_{Si} Å	υ_{Si} (%)	Δ_{Al} Å	Σ_{Al}	υ_{Al} (%)	Δ_{Na} Å	Σ_{Na}	υ_{Na} (%)
-5.0	179.54	0.0343	0.9616	0.1691	0.9852	1.7767	0.2009	0.9228	2.5715
-4.0	178.96	0.0343	0.9108	0.1528	0.9896	1.7257	0.1906	0.9256	2.6070
-3.0	178.47	0.0342	0.8699	0.1408	0.9928	1.6916	0.1821	0.9279	2.6489
-2.0	177.87	0.0342	0.8285	0.1321	0.9952	1.6609	0.1741	0.9304	2.6722
-1.0	177.17	0.0339	0.7910	0.1248	0.9972	1.6246	0.1664	0.9330	2.6814
-0.0	176.53	0.0338	0.7525	0.1189	0.9987	1.6035	0.1589	0.9355	2.6972
1.0	175.88	0.0338	0.7097	0.1133	0.9997	1.5683	0.1536	0.9378	2.7547
2.0	175.18	0.0336	0.6798	0.1088	0.9985	1.5488	0.1471	0.9404	2.7607
3.0	174.49	0.0334	0.6517	0.1051	0.9975	1.5303	0.1408	0.9429	2.7645
4.0	173.76	0.0333	0.6272	0.1016	0.9968	1.5188	0.1348	0.9456	2.7686
5.0	173.10	0.0332	0.6058	0.0984	0.9960	1.5059	0.1292	0.9480	2.7677
6.0	172.44	0.0330	0.5883	0.0954	0.9952	1.4939	0.1239	0.9504	2.7624
7.0	171.75	0.0328	0.5702	0.0929	0.9947	1.4856	0.1187	0.9530	2.7611
8.0	171.05	0.0328	0.5548	0.0907	0.9944	1.4796	0.1133	0.9556	2.7543
9.0	169.96	0.0323	0.5445	0.0880	0.9938	1.4694	0.1073	0.9600	2.7699
10.0	169.44	0.0321	0.5306	0.0860	0.9933	1.4651	0.1043	0.9617	2.7635
11.0	168.93	0.0321	0.5182	0.0842	0.9930	1.4632	0.1016	0.9634	2.7588
12.0	168.44	0.0321	0.5077	0.0823	0.9926	1.4629	0.0991	0.9650	2.7549
13.0	167.96	0.0320	0.4994	0.0806	0.9923	1.4643	0.0966	0.9667	2.7505
14.0	166.88	0.0321	0.4939	0.0797	0.9924	1.4540	0.0903	0.9709	2.7389
15.0	166.22	0.0320	0.4894	0.0781	0.9921	1.4522	0.0877	0.9734	2.7267
16.0	165.61	0.0321	0.4841	0.0768	0.9920	1.4532	0.0850	0.9756	2.7151
17.0	165.02	0.0321	0.4798	0.0757	0.9918	1.4548	0.0827	0.9778	2.7061
18.0	164.43	0.0321	0.4767	0.0745	0.9917	1.4587	0.0803	0.9800	2.6929
19.0	163.85	0.0322	0.4740	0.0735	0.9916	1.4626	0.0783	0.9821	2.6805
20.0	163.31	0.0323	0.4715	0.0725	0.9915	1.4691	0.0767	0.9840	2.6674
21.0	162.76	0.0324	0.4699	0.0714	0.9914	1.4765	0.0753	0.9860	2.6547
22.0	162.27	0.0325	0.4688	0.0706	0.9913	1.4847	0.0742	0.9877	2.6406
23.0	161.78	0.0326	0.4683	0.0697	0.9913	1.4949	0.0730	0.9894	2.6267
24.0	161.34	0.0326	0.4687	0.0689	0.9913	1.5059	0.0720	0.9909	2.6134
25.0	160.88	0.0327	0.4687	0.0682	0.9912	1.5183	0.0712	0.9924	2.6002

Table 4: The effect of pressure on some measures of structural regularity

P GPa	Si–O1	Si–O2	Si–O3a	Si–O3b	$\overline{\mathrm{Si-O}}$	r_{Si}	V_{Si}
-5.0	1.657	1.609	1.658	1.648	1.643	1.643	2.252
-4.0	1.655	1.607	1.656	1.646	1.641	1.640	2.244
-3.0	1.653	1.605	1.654	1.644	1.639	1.638	2.237
-2.0	1.651	1.603	1.652	1.642	1.637	1.636	2.230
-1.0	1.648	1.601	1.650	1.640	1.635	1.634	2.222
-0.0	1.646	1.600	1.648	1.638	1.633	1.632	2.215
1.0	1.644	1.598	1.647	1.636	1.631	1.630	2.209
2.0	1.642	1.596	1.645	1.635	1.629	1.629	2.202
3.0	1.640	1.594	1.643	1.633	1.628	1.627	2.195
4.0	1.638	1.593	1.642	1.631	1.626	1.625	2.189
5.0	1.636	1.592	1.640	1.630	1.624	1.624	2.183
6.0	1.634	1.590	1.639	1.628	1.623	1.622	2.177
7.0	1.632	1.589	1.637	1.627	1.621	1.620	2.171
8.0	1.630	1.587	1.636	1.625	1.620	1.619	2.165
9.0	1.628	1.586	1.634	1.623	1.618	1.617	2.159
10.0	1.626	1.585	1.633	1.622	1.617	1.616	2.154
11.0	1.624	1.584	1.632	1.621	1.615	1.614	2.148
12.0	1.623	1.582	1.631	1.619	1.614	1.613	2.143
13.0	1.621	1.581	1.630	1.618	1.612	1.612	2.138
14.0	1.619	1.580	1.629	1.617	1.611	1.610	2.133
15.0	1.618	1.579	1.628	1.616	1.610	1.609	2.128
16.0	1.616	1.577	1.626	1.615	1.609	1.608	2.123
17.0	1.614	1.576	1.625	1.614	1.608	1.607	2.118
18.0	1.613	1.575	1.625	1.613	1.606	1.606	2.114
19.0	1.611	1.574	1.624	1.612	1.605	1.604	2.109
20.0	1.610	1.573	1.623	1.611	1.604	1.603	2.105
21.0	1.609	1.572	1.622	1.610	1.603	1.602	2.101
22.0	1.607	1.571	1.621	1.609	1.602	1.601	2.096
23.0	1.606	1.570	1.620	1.608	1.601	1.600	2.092
24.0	1.604	1.569	1.619	1.607	1.600	1.599	2.088
25.0	1.603	1.568	1.619	1.606	1.599	1.598	2.084

Table 5: Variation in bond lengths in the Si tetrahedera in jadeite with pressure

P GPa	Al–O1a	Al–O1b	Al–O2	$\overline{\mathrm{Al-O}}$	r_{Al}	V_{Al}
-5.0	1.951	2.122	1.883	1.985	1.980	10.164
-4.0	1.953	2.096	1.881	1.977	1.972	10.047
-3.0	1.954	2.076	1.878	1.969	1.965	9.946
-2.0	1.954	2.060	1.875	1.963	1.959	9.856
-1.0	1.953	2.046	1.872	1.957	1.953	9.771
-0.0	1.951	2.035	1.869	1.952	1.948	9.694
1.0	1.950	2.023	1.865	1.946	1.943	9.622
2.0	1.948	2.014	1.862	1.941	1.938	9.554
3.0	1.946	2.006	1.859	1.937	1.933	9.490
4.0	1.943	1.998	1.857	1.932	1.929	9.428
5.0	1.941	1.990	1.854	1.928	1.925	9.369
6.0	1.938	1.983	1.851	1.924	1.921	9.311
7.0	1.936	1.977	1.848	1.920	1.917	9.256
8.0	1.932	1.972	1.846	1.916	1.913	9.203
9.0	1.930	1.965	1.843	1.913	1.910	9.151
10.0	1.928	1.960	1.840	1.909	1.906	9.103
11.0	1.925	1.955	1.838	1.906	1.903	9.055
12.0	1.922	1.950	1.835	1.903	1.900	9.008
13.0	1.920	1.945	1.833	1.899	1.897	8.962
14.0	1.917	1.942	1.831	1.896	1.894	8.921
15.0	1.914	1.937	1.829	1.893	1.891	8.879
16.0	1.911	1.933	1.826	1.890	1.888	8.838
17.0	1.909	1.930	1.824	1.887	1.885	8.798
18.0	1.906	1.926	1.822	1.885	1.882	8.759
19.0	1.903	1.922	1.820	1.882	1.879	8.721
20.0	1.901	1.919	1.818	1.879	1.877	8.683
21.0	1.898	1.916	1.816	1.877	1.874	8.647
22.0	1.896	1.913	1.814	1.874	1.872	8.611
23.0	1.893	1.909	1.812	1.872	1.869	8.577
24.0	1.891	1.907	1.810	1.869	1.867	8.543
25.0	1.888	1.904	1.809	1.867	1.864	8.509

Table 6: Variation in bond lengths in the M1 octahedron in jadeite with pressure

P GPa	Na–O1	Na–O2	Na–O3a	Na–O3b	$\overline{\mathrm{Na-O}}$	r_{Na}	V_{Na}
-5.0	2.423	2.459	2.945	2.423	2.563	2.550	27.753
-4.0	2.413	2.457	2.916	2.413	2.550	2.537	27.346
-3.0	2.403	2.453	2.891	2.404	2.538	2.526	26.981
-2.0	2.395	2.448	2.866	2.397	2.527	2.516	26.631
-1.0	2.387	2.442	2.841	2.392	2.515	2.505	26.296
-0.0	2.380	2.436	2.817	2.386	2.505	2.495	25.980
1.0	2.372	2.427	2.795	2.382	2.494	2.484	25.632
2.0	2.366	2.420	2.772	2.378	2.484	2.475	25.342
3.0	2.360	2.414	2.750	2.374	2.474	2.466	25.064
4.0	2.354	2.407	2.728	2.371	2.465	2.457	24.794
5.0	2.348	2.401	2.707	2.368	2.456	2.449	24.537
6.0	2.343	2.394	2.687	2.365	2.447	2.440	24.289
7.0	2.338	2.388	2.667	2.363	2.439	2.432	24.046
8.0	2.333	2.381	2.646	2.360	2.430	2.424	23.810
9.0	2.330	2.374	2.620	2.364	2.422	2.416	23.574
10.0	2.325	2.367	2.604	2.361	2.414	2.409	23.359
11.0	2.319	2.361	2.589	2.358	2.407	2.402	23.151
12.0	2.314	2.355	2.575	2.356	2.400	2.395	22.952
13.0	2.309	2.349	2.560	2.353	2.393	2.388	22.758
14.0	2.307	2.342	2.534	2.355	2.385	2.380	22.539
15.0	2.302	2.335	2.517	2.355	2.378	2.373	22.348
16.0	2.298	2.329	2.501	2.354	2.371	2.367	22.163
17.0	2.294	2.323	2.485	2.354	2.364	2.360	21.983
18.0	2.289	2.317	2.470	2.353	2.357	2.354	21.808
19.0	2.285	2.312	2.455	2.352	2.351	2.347	21.640
20.0	2.281	2.306	2.441	2.351	2.345	2.341	21.476
21.0	2.276	2.300	2.427	2.351	2.339	2.335	21.314
22.0	2.272	2.295	2.415	2.350	2.333	2.330	21.160
23.0	2.268	2.289	2.402	2.349	2.327	2.324	21.009
24.0	2.263	2.284	2.391	2.348	2.322	2.319	20.865
25.0	2.259	2.279	2.379	2.347	2.316	2.313	20.720

Table 7: Variation in bond lengths in the M2 polyhedron in jadeite with pressure

Site	V_0 Å^3	K_0 GPa	K_0'
Si (diopside)	2.26	334.4	6.4
Si (jadeite)	2.22	315.7	8.8
Mg (M1 diopside)	12.63	88.9	4.3
Al (M1 jadeite)	9.70	129.0	6.05
Ca (M2 diopside)	27.10	75.3	4.8
Na (M2 jadeite)	25.96	81.9	2.8

Table 8: EOS parameters for polyhedera in diopside and jadeite

Table 9: Elastic constants (in GPa) of diopside to elevated pressure.

Nominal pressure Applied pressure	0 GPa 4.66 GPa	5 GPa 9.66 GPa	10 GPa 14.66 GPa	15 GPa 19.66 GPa	20 GPa 24.66 GPa
C_{11}	243.8±1.4	273.2±1.4	298.9±0.5	326.9±0.7	348.5±1.7
C_{12}	91.2±0.7	114.3±0.7	135.2±1.1	150.1±1.1	168.3±1.5
C_{13}	80.5±1.1	102.3±1.3	121.0±1.5	138.7±1.7	158.4±1.5
C_{15}	9.1±0.3	4.4±0.2	1.1±0.3	1.2±0.2	0.8±0.2
C_{22}	184.2±1.2	205.3±1.6	226.7±1.6	255.2±3.5	271.6±1.9
C_{23}	68.0±0.7	84.9±0.9	102.7±1.1	122.5±1.5	138.3±1.0
C_{25}	4.5±0.1	1.0±0.2	-1.2±0.3	-4.4±0.3	-3.1±0.5
C_{33}	251.0±1.9	277.9±2.4	305.4±2.7	330.9±2.8	351.9±2.8
C_{35}	50.9±0.1	45.8±0.2	42.4±0.3	37.5±0.2	35.3±0.2
C_{44}	76.9±0.4	81.1±1.2	83.2±1.1	88.4±1.0	80.1±1.0
C_{46}	3.9±0.2	-0.6±0.4	-4.8±0.4	-6.4±0.5	-5.7±0.7
C_{55}	69.3±0.1	77.4±0.1	84.0±0.2	89.5±0.1	91.8±0.1
C_{66}	80.6±0.7	92.2±0.8	102.2±0.9	109.1±1.1	115.0±1.3
K^v	128.7±0.4	151.1±0.4	172.1±0.5	192.9±0.6	211.3±0.6
K^r	119.8±0.8	144.2±1.1	166.3±1.7	188.4±2.2	206.3±2.4
K^{vrh}	124.3±0.6	147.6±0.7	169.2±1.1	190.6±1.4	208.8±1.5
G^v	74.6±0.3	80.5±0.4	85.3±0.4	90.8±0.5	91.2±0.4
G^r	68.8±0.2	75.1±0.3	79.8±0.3	86.0±0.3	86.2±0.3
G^{vrh}	71.7±0.2	77.8±0.3	82.6±0.3	88.4±0.4	88.7±0.4
A^U	0.495	0.404	0.383	0.303	0.312
$A^\star$	1.91	1.86	1.87	1.78	1.74

Table 10: Elastic constants (in GPa) of jadeite to elevated pressure.

Nominal pressure	0 GPa	5 GPa	10 GPa	15 GPa	20 GPa
Applied pressure	4.30 GPa	9.30 GPa	14.30 GPa	19.30 GPa	24.30 GPa
C_{11}	283.4±2.6	322.0±2.3	357.0±2.9	389.0±2.9	418.1±2.8
C_{12}	93.3±0.8	110.4±0.8	127.6±0.9	144.1±0.9	160.3±1.0
C_{13}	72.5±1.2	89.5±1.1	107.4±1.3	124.8±1.4	141.2±1.5
C_{15}	4.4±0.4	0.5±0.3	-1.5±0.3	-2.5±0.3	-2.8±0.2
C_{22}	252.6±1.7	275.1±1.5	292.0±1.2	306.8±1.2	322.6±1.5
C_{23}	81.8±0.9	91.8±0.6	100.8±0.6	113.6±0.9	128.3±1.1
C_{25}	14.0±0.1	14.6±0.1	15.0±0.1	15.7±0.2	16.0±0.2
C_{33}	281.8±3.0	297.6±2.1	315.6±2.7	337.4±3.2	362.1±3.8
C_{35}	41.5±0.6	45.9±0.5	47.8±0.3	47.5±0.2	46.0±0.1
C_{44}	86.7±0.2	93.0±0.1	96.5±0.1	100.2±0.1	102.6±0.1
C_{46}	11.9±0.2	10.3±0.1	9.5±0.1	9.0±0.2	9.1±0.2
C_{55}	71.4±0.2	76.2±0.2	81.0±0.1	85.7±0.1	90.6±0.0
C_{66}	96.6±1.4	107.7±1.1	117.2±1.0	125.2±1.1	132.3±1.0
K^v	145.9±0.6	164.2±0.5	181.8±0.5	199.8±0.6	218.1±0.6
K^r	139.7±0.9	157.0±0.8	173.4±0.9	190.7±1.1	209.0±1.4
K^{vrh}	142.8±0.7	160.6±0.6	177.6±0.7	195.3±0.8	213.5±1.0
G^v	88.9±0.4	95.6±0.3	100.8±0.4	105.6±0.4	110.0±0.4
G^r	84.1±0.3	89.8±0.2	94.5±0.2	99.3±0.2	103.9±0.2
G^{vrh}	86.5±0.3	92.7±0.3	97.7±0.3	102.4±0.3	106.9±0.3
A^U	0.334	0.369	0.382	0.365	0.334
$A^\star$	1.86	1.96	1.96	1.90	1.82