1 **American Mineralogist July 2014 AM-14-703, Moon et al.**

2

3 **SUPPLEMENTARY TABLE 1.** Selected geometric parameters (Å, °).

	$C_4AC̈H_{11}$							$C_4AC̈H_8$					
	Exp.	LDA			GGA			LDA			GGA		
P (GPa)	0.0	0.0	2.0	5.0	0.0	2.0	5.0	0.0	2.0	5.0	0.0	2.0	5.0
Ca1-O10	2.350 (3)	2.549	2.538	2.527	2.353	2.334	2.312	2.669	2.634	2.622	2.337	2.314	2.327
Ca1-O5	2.351 (3)	2.543	2.530	2.520	2.362	2.339	2.311	2.575	2.893	2.837	2.351	2.311	2.332
Ca1-O3^{i}	2.359 (3)	2.563	2.545	2.528	2.369	2.345	2.314	2.939	2.594	2.589	2.398	2.316	2.369
Ca1-O4^{ii}	2.445 (3)	2.590	2.577	2.570	2.459	2.440	2.410	2.690	2.581	2.562	2.463	2.374	2.365
Ca1-O10	2.455 (2)	2.627	2.614	2.602	2.480	2.467	2.454	2.512	2.806	2.775	2.489	2.324	2.435
Ca1-O12	2.457 (2)	2.654	2.608	2.580	2.500	2.469	2.430	3.216	2.752	2.731	2.510	2.452	2.493
Ca1-O13^{i}	2.546 (3)	2.672	2.638	2.616	2.590	2.603	2.573	2.602	2.631	2.607	2.591	4.593	2.416
Ca2-O9	2.349 (3)	2.556	2.541	2.528	2.356	2.338	2.317	2.572	2.578	2.593	2.350	2.310	2.282
Ca2-O4^{iii}	2.360 (2)	2.548	2.532	2.514	2.367	2.344	2.315	2.666	2.636	2.628	2.330	2.305	2.293
Ca2-O6	2.366 (3)	2.553	2.539	2.523	2.373	2.352	2.326	2.518	3.221	3.097	2.334	2.374	2.279
Ca2-O3^{iv}	2.447 (3)	2.608	2.586	2.566	2.477	2.463	2.422	3.312	2.950	2.916	2.453	2.419	2.469
Ca2-O11	2.457 (2)	2.618	2.578	2.554	2.485	2.449	2.414	3.209	2.614	2.588	2.398	2.345	2.388
Ca2-O2	2.472 (2)	2.614	2.599	2.581	2.497	2.475	2.455	2.675	3.456	3.369	2.414	2.383	2.387
Ca2-O14^{iii}	2.518 (3)	2.691	2.650	2.622	2.575	2.563	2.524	-	-	-	-	-	-
Ca3-O2^{v}	2.346 (3)	2.549	2.536	2.518	2.349	2.343	2.331	2.606	2.692	2.660	2.368	2.360	2.300
Ca3-O11	2.355 (3)	2.527	2.516	2.506	2.351	2.337	2.319	2.596	2.768	2.733	2.364	2.322	2.299
Ca3-O7^{v}	2.365 (2)	2.559	2.555	2.559	2.362	2.348	2.323	2.523	2.583	2.564	2.354	2.327	2.339
Ca3-O9	2.446 (2)	2.599	2.565	2.550	2.459	2.423	2.380	2.495	2.631	2.620	2.484	2.370	2.405
Ca3-O8	2.447 (3)	2.591	2.560	2.538	2.452	2.420	2.384	2.549	3.259	3.161	2.485	2.470	2.412
Ca3-O6^{v}	2.508 (3)	2.585	2.560	2.535	2.499	2.466	2.433	2.676	2.944	2.882	2.596	2.750	2.467
Ca3-O19	2.515 (3)	2.763	2.694	2.649	2.697	2.648	2.593	2.863	2.627	2.593	2.446	2.386	2.476
Ca4-O8^{vi}	2.348 (2)	2.547	2.533	2.524	2.358	2.339	2.311	2.584	2.705	2.671	2.367	2.314	2.337
Ca4-O1^{iv}	2.354 (3)	2.546	2.528	2.518	2.352	2.341	2.321	2.634	2.668	2.654	2.370	2.300	2.339
Ca4-O12	2.358 (3)	2.540	2.529	2.517	2.358	2.348	2.329	2.645	2.716	2.701	2.362	2.340	2.349
Ca4-O7	2.389 (2)	2.567	2.547	2.536	2.428	2.388	2.355	2.496	2.560	2.523	2.421	2.299	2.354
Ca4-O10	2.449 (3)	2.618	2.589	2.571	2.484	2.451	2.419	2.631	2.641	2.614	2.503	2.436	2.456
Ca4-O5^{vi}	2.464 (2)	2.589	2.570	2.546	2.473	2.460	2.440	2.572	2.516	2.494	2.551	2.387	2.445
Ca4-O15	2.553 (3)	2.683	2.637	2.616	2.614	2.573	2.537	2.619	2.545	2.513	2.493	4.443	2.392
Al1-O10^{vii}	1.897 (3)	1.854	1.840	1.826	1.929	1.913	1.896	1.855	1.831	1.821	1.938	2.064	1.922
Al1-O3^{viii}	1.901 (3)	1.861	1.851	1.849	1.921	1.919	1.908	1.966	1.854	1.850	1.952	1.926	1.925
Al1-O4^{v}	1.907 (3)	1.876	1.871	1.869	1.934	1.932	1.923	1.838	1.836	1.824	1.924	1.910	1.905
Al1-O2^{ix}	1.916 (3)	1.869	1.864	1.856	1.942	1.932	1.921	1.861	1.871	1.857	1.924	1.925	1.880

Al1-O9[i]	1.918 (3)	1.872	1.857	1.848	1.935	1.923	1.910	1.794	1.785	1.780	1.935	1.826	1.917
Al1-O1[iv]	1.923 (3)	1.879	1.876	1.867	1.951	1.940	1.931	1.886	1.921	1.914	1.945	1.942	1.921
Al2-O8	1.898 (3)	1.842	1.828	1.822	1.918	1.905	1.888	1.820	1.856	1.857	1.936	1.926	1.909
Al2-O7	1.899 (3)	1.856	1.849	1.847	1.924	1.914	1.901	1.829	1.854	1.840	1.903	1.903	1.888
Al2-O11	1.909 (3)	1.894	1.885	1.876	1.943	1.938	1.927	1.947	1.870	1.850	1.938	1.933	1.913
Al2-O12	1.917 (3)	1.875	1.866	1.853	1.931	1.920	1.907	1.937	1.887	1.887	1.938	1.904	1.925
Al2-O6	1.918 (3)	1.875	1.864	1.851	1.948	1.940	1.929	1.857	1.815	1.808	1.946	1.973	1.900
Al2-O5	1.925 (3)	1.880	1.873	1.863	1.947	1.942	1.933	1.896	1.821	1.807	1.948	1.954	1.941
O18-C1	1.283 (3)	1.293	1.291	1.289	1.304	1.302	1.299	1.305	1.323	1.324	1.379	1.303	1.369
O19-C1[v]	1.299 (4)	1.299	1.296	1.295	1.308	1.305	1.302	1.283	1.286	1.283	1.276	1.298	1.274
O20-C1	1.284 (3)	1.271	1.270	1.268	1.295	1.291	1.289	1.288	1.274	1.272	1.267	1.305	1.271
H13A-O13-H13B	98 (2)	109.7	109.9	109.5	106.4	106.5	106.2	107.2	94.5	94.0	103.7	132.1	101.2
O18-C1-O20	120.2 (2)	121.1	121.4	121.7	120.6	120.7	120.7	118.9	118.2	118.1	115.9	120.7	115.5
O18-C1-O19[vi]	120.2 (2)	118.7	118.4	118.2	119.6	119.4	119.3	118.7	119.0	118.6	117.4	119.44	118.0
O20-C1-O19[vi]	119.6 (3)	120.2	120.2	120.0	119.7	119.9	120.0	122.3	122.4	122.7	126.8	119.8	126.5

Note: Experimental data is from (François et al., 1998). Symmetry codes: (i) x,y-1,z; (ii) x,y,1+z; (iii) x,1+y,z; (iv) x,y,z-1; (v) x-1,y,z; (vi) 1+x,y,z; (vii) x-1,y,z-1; (viii) x,y-1,z-1; (ix) x-1,y-1,z.

American Mineralogist July 2014 AM-14-703, Moon et al.

SUPPLEMENTARY TABLE 2. Hydrogen-bonding geometry (Å, °).

	$C_4Al_2H_{11}$							$C_4Al_2H_8$					
	Exp	LDA			GGA			LDA			GGA		
P (GPa)	0.0	0.0	2.0	5.0	0.0	2.0	5.0	0.0	2.0	5.0	0.0	2.0	5.0
$O17^{i}$-$H17B^{i}$	0.82 (3)	1.03	1.04	1.04	1.01	1.01	1.02	-	-	-	-	-	-
$O15^{iv}$-$H15B^{iv}$	0.92 (2)	1.05	1.05	1.05	1.02	1.02	1.02	1.01	1.00	1.00	1.47	1.22	1.37
$O16^{iv}$-$H16A^{iv}$	0.97 (3)	1.00	1.00	1.00	0.99	0.99	0.99	-	-	-	-	-	-
$O16^{iv}$-$H16B^{iv}$	0.95 (3)	1.02	1.02	1.02	1.01	1.01	1.01	-	-	-	-	-	-
O14-H14A	0.92 (3)	1.02	1.02	1.02	1.00	1.01	1.01	-	-	-	-	-	-
O14-H14B	0.90 (4)	1.04	1.04	1.04	1.02	1.02	1.02	-	-	-	-	-	-
$H17B^{i}$-O14	1.85 (3)	1.55	1.51	1.48	1.67	1.62	1.57	7.82	7.54	7.46	8.28	8.00	7.69
$H15B^{iv}$-O18	1.71 (2)	1.47	1.47	1.46	1.59	1.58	1.56	1.73	1.82	1.79	1.07	5.85	1.10
$H16A^{iv}$-O18	1.79 (3)	1.73	1.70	1.68	1.78	1.74	1.71	12.75	14.04	13.85	13.29	13.78	12.73
$H16B^{iv}$-O19	1.75 (3)	1.57	1.56	1.54	1.64	1.61	1.59	12.12	12.73	12.59	12.91	13.40	12.25
H14A-O19	1.86 (3)	1.58	1.55	1.52	1.72	1.66	1.62	3.73	3.55	3.52	4.38	4.49	3.88
H14B-O20	1.74 (4)	1.52	1.49	1.46	1.61	1.59	1.56	5.90	6.80	6.70	6.68	6.79	6.05
$O17^{i}$-O14	2.746 (4)	2.580	2.547	2.521	2.675	2.631	2.586	7.820	7.541	7.458	8.284	8.002	7.692
$O15^{iv}$-O18	2.631 (4)	2.514	2.505	2.499	2.607	2.594	2.573	2.725	2.821	2.791	2.529	5.617	2.458
$O16^{iv}$-O18	2.750 (4)	2.727	2.700	2.679	2.771	2.724	2.690	12.745	14.043	13.848	13.293	13.779	12.729
$O16^{iv}$-O19	2.681 (4)	2.585	2.569	2.550	2.645	2.614	2.585	12.117	12.734	12.587	12.905	13.396	12.253
O14-O19	2.774 (4)	2.605	2.568	2.540	2.726	2.665	2.623	3.729	3.554	3.524	4.381	4.491	3.877
O14-O20	2.626 (4)	2.553	2.523	2.499	2.633	2.608	2.577	5.898	6.799	6.696	6.677	6.794	6.051
$O17^{i}$-$H17B^{i}$-O14	163 (3)	175	175	175	174	175	176	-	-	-	-	-	-
$O15^{iv}$-$H15B^{iv}$-O18	171 (3)	170	169	168	171	171	170	169	177	176	173	73	170
$O16^{iv}$-$H16A^{iv}$-O18	165 (5)	175	175	174	177	175	173	-	-	-	-	-	-
$O16^{iv}$-$H16B^{iv}$-O19	165 (4)	171	170	170	170	168	167	-	-	-	-	-	-
O14-H14A-O19	173 (3)	178	177	177	175	174	173	-	-	-	-	-	-
O14-H14B-O20	171 (4)	171	172	172	175	175	176	-	-	-	-	-	-

Note: Experimental data is from (François et al., 1998). Symmetry codes: (i) x,y-1,z; (iv) x,y,z-1.