

AM-87-343

Neutron-diffraction structures of a low-water grossular at 20K

Lager, et al.

American Mineralogist, 72,7-8, 766-768

Table 4. Comparison of observed and calculated structural amplitudes for Ramona grossular.

Low-Water Grossular 20K Ia3d (No. 230) FOBS & FCALC in cm * 10**--11 & WAVL in Angstroms * 10**--3 PAGE 1

K	L	FOBS	FCAL	WAVL	K	L	FOBS	FCAL	WAVL	K	L	FOBS	FCAL	WAVL	K	L	FOBS	FCAL	WAVL						
*****	H = -20	*****	*****	*****	*****	H = -13	*****	*****	*****	*****	H = -15	*****	*****	*****	*****	H = -14	*****	*****	*****	*****					
-16	6	92	90	727	-15	-2	76	77	762	-18	-5	118	117	769	-15	-7	28	36	791	-14	-5	34	34	925	
					-15	14	37	43	740	-18	3	39	34	842	-15	-5	34	38	888	-14	-3	52	52	1027	
					-14	-7	38	43	785	-16	-5	46	45	834	-15	7	30	36	813	-14	-1	21	22	794	
					-14	11	27	23	820	-16	5	49	45	763	-15	13	40	51	739	-14	9	40	33	847	
					-13	-6	50	48	810	-16	11	48	52	743	-14	-8	76	74	752	-13	17	49	53	729	
					-12	-7	41	36	823	-15	-8	106	101	730	-14	-6	123	122	860	-13	-8	34	32	775	
-13	-8	43	42	754	-12	-7	37	36	836	-15	-6	43	48	823	-14	2	36	34	845	-13	-6	26	30	901	
-12	-5	26	32	833	-12	-7	37	34	939	-15	-6	40	43	785	-14	8	71	74	875	-13	-4	67	65	1027	
					-12	-1	35	34	939	-15	2	40	43	785	-14	8	71	74	875	-13	4	63	65	941	
					-11	-8	75	77	857	-15	6	47	48	821	-14	10	77	74	837	-13	6	29	30	941	
					-11	-2	41	40	997	-15	8	101	101	810	-14	16	39	45	751	-13	8	32	32	925	
					-9	-8	40	43	808	-15	10	35	28	799	-13	18	50	47	717	-13	10	26	22	885	
					-9	-8	41	43	951	-15	12	51	51	762	-13	16	47	49	835	-13	16	47	52	784	
					-9	-6	21	15	1026	-14	-3	20	14	991	-13	-7	47	49	835	-13	18	60	55	750	
					-12	-10	53	55	739	-14	-1	30	28	819	-13	-5	36	34	954	-13	20	49	50	718	
					-12	-8	66	66	729	-14	-1	30	28	819	-13	3	54	58	944	-12	-7	33	29	810	
					-11	-9	38	39	799	-14	9	24	14	858	-13	7	45	49	939	-12	-7	28	29	871	
					-11	-7	25	29	863	-14	13	39	36	784	-13	9	53	52	911	-12	-5	29	19	881	
					-11	-7	34	29	784	-13	-6	47	44	885	-13	17	42	40	768	-12	-5	23	19	1010	
					*****	H = -14	*****	*****	*****	-13	10	20	14	899	-13	19	55	47	734	-12	-1	32	31	952	
					-18	-4	75	76	796	-12	-9	49	52	771	-12	-8	49	47	797	-12	3	25	25	1012	
					-17	-5	55	60	795	-12	-7	48	49	863	-12	8	48	47	1000	-12	5	19	19	1027	
					-17	-3	32	31	857	-12	-5	30	34	970	-12	16	43	44	819	-12	7	28	29	1009	
					-16	10	65	58	750	-12	3	60	58	937	-11	-7	37	29	887	-12	17	38	37	807	
					-16	12	41	45	727	-12	5	35	34	1009	-11	-5	21	19	1029	-12	19	33	37	770	
					-15	7	42	43	825	-12	7	48	49	995	-11	-5	28	19	964	-11	-10	47	48	748	
					-15	9	32	38	811	-12	9	49	52	966	-11	-3	26	25	1015	-11	-6	55	53	987	
					-14	-8	60	62	758	-12	11	23	23	920	-11	-1	31	31	1044	-11	-6	52	53	923	
					-14	4	27	27	869	-11	-8	29	32	858	-11	5	20	19	1092	-11	-2	28	25	1034	
					-14	8	62	62	860	-11	-8	31	32	810	-11	7	31	29	1074	-11	6	53	53	1104	
					-13	7	23	2	925	-11	-6	31	30	941	-10	-8	54	52	834	-11	10	47	48	1010	
					-13	13	33	36	834	-11	-6	33	30	928	-10	-8	52	52	910	-10	-9	49	50	861	
					-12	-10	76	74	740	-11	-2	43	43	1027	-10	-2	91	89	1124	-10	-5	20	21	1043	
					-12	-8	76	74	786	-11	4	67	65	1074	-9	-7	31	31	1026	-10	-5	18	21	1092	
					-12	-6	126	122	897	-10	-5	30	28	1041	-9	-7	31	31	1026	-10	-5	20	21	1043	
					-11	-9	38	33	821	-10	-1	26	28	1121	-9	-3	16	18	1263	-10	-3	38	36	1203	
					-11	-9	37	33	741	-9	-8	29	31	970	-9	-3	18	18	1195	-10	5	21	21	1217	
					-11	-5	38	34	954	-9	-4	18	18	1141	-9	-1	35	36	1235	-10	9	51	50	1105	
					-11	-3	53	52	998	-9	-2	18	17	1193	-8	-8	95	94	858	-9	-6	80	79	1079	
					-11	-1	23	22	1025	-8	-9	32	31	772	-8	-6	83	83	1041	-9	-4	44	43	1177	
					-10	-6	31	34	943	-8	-7	59	60	1086	-8	-6	83	83	1156	-9	-4	43	43	1227	
					-10	-6	31	34	983	-8	-7	59	60	940	-8	-6	83	83	1156	-9	-2	16	16	1244	
					-10	-4	18	23	1045	-8	-7	59	60	940	-8	-4	59	59	1250	-9	-2	16	16	1244	
					-10	-2	18	10	1087	-8	-5	100	100	1090	-8	-7	29	28	1105	-8	-7	29	28	1105	
					-9	-9	66	68	760	*****	H = -12	*****	*****	*****	*****	*****	H = -11	*****	*****	*****	*****	*****	*****	*****	*****
					-9	-7	60	57	1009	-19	3	35	29	807	-18	-5	64	62	772	-8	-5	59	59	1229	
					-9	-7	59	57	896	-19	3	35	29	807	-18	-5	64	62	772	-8	-5	58	59	1173	
					-9	-5	27	23	1089	-17	-6	81	82	762	-17	-6	81	82	762	-8	-3	44	44	1363	
					-9	-5	22	23	1028	-18	-6	59	64	735	-17	-4	34	33	924	-8	-3	45	44	1325	
					-8	-6	26	25	1109	-17	3	49	51	896	-16	-7	76	76	750	-7	-6	52	53	1381	
					-8	-6	26	25	1109	-16	-6	47	61	797	-15	-8	77	77	728	-6	-5	23	24	1251	
					-9	-7	25	24	978	-16	12	48	44	717	-14	-7	28	23	809	-6	-5	12	9	1425	

K	L	FOBS	FCAL	WAVL	K	L	FOBS	FCAL	WAVL	K	L	FOBS	FCAL	WAVL
*****	H	--10	*****											
-16	-4	28	29	899	-6	-4	34	36	1539	-10	-5	23	18	1128
-16	2	72	72	950	*****	H	--9	*****		-10	-3	18	17	1325
-16	10	130	128	718	*****	H	--9	*****		-10	-3	15	17	1092
-15	-7	33	23	774	-22	9	65	66	738	-10	5	20	18	1227
-15	-3	21	16	979	-21	6	51	46	763	-10	7	17	16	1109
-15	1	36	35	978	-20	8	51	70	773	-9	-2	31	31	1253
-14	-6	31	34	870	-20	-1	74	77	856	-9	2	31	31	1341
-14	-4	23	23	883	-20	7	34	26	822	-12	4	58	59	997
-14	-2	17	10	1089	-18	5	35	32	896	-12	6	82	83	996
-14	16	62	58	741	-17	-6	25	18	750	-12	8	93	94	966
-14	18	50	49	716	-16	-5	23	23	847	-12	12	42	47	901
-13	-5	23	28	973	-16	3	45	46	980	-12	14	73	74	859
-13	-1	25	28	845	-15	-4	35	34	936	-12	16	49	46	822
-13	1	30	28	880	-15	4	36	34	1071	-12	18	66	66	788
-13	11	24	22	858	-15	8	50	43	772	-11	-7	29	28	883
-13	15	34	28	796	-14	-7	59	57	796	-11	-5	59	59	1076
-12	-8	54	52	796	-14	-5	18	23	926	-11	-3	44	44	1267
-12	-6	121	124	825	-14	-3	20	17	1044	-11	1	51	53	1038
-12	2	87	89	995	-14	1	23	19	1055	-11	3	44	44	1091
-12	8	54	52	990	-14	3	18	17	1120	-11	5	59	59	1105
-12	10	53	71	942	-14	7	53	57	846	-11	7	30	28	1073
-12	14	73	74	876	-14	9	68	68	821	-11	13	31	32	938
-12	18	61	55	786	-14	11	33	33	786	-11	15	77	77	996
-11	-5	21	21	1073	-14	15	41	38	751	-11	19	36	29	796
-11	-5	21	21	940	-13	-8	33	31	761	-10	-6	25	26	1026
-11	-3	35	36	1229	-13	-4	17	18	1045	-10	-4	89	91	1026
-11	-3	36	36	1009	-13	-2	20	17	1171	-10	-2	12	5	1090
-11	-1	14	8	1042	-13	6	18	11	925	-10	6	27	26	1206
-11	3	35	36	1109	-13	8	33	31	905	-10	12	53	52	1028
-11	5	22	21	1120	-12	-7	29	31	873	-10	16	27	20	919
-11	9	51	50	1041	-12	-5	18	13	1026	-10	20	51	48	803
-10	-8	60	62	842	-12	-3	20	18	1178	-9	-5	43	42	1092
-10	-4	90	92	1076	-12	-1	37	36	909	-9	-3	28	29	1448
-10	8	65	62	1151	-12	1	37	36	950	-9	-3	31	29	1207
-9	-7	19	16	1013	-12	5	19	13	1013	-9	-1	50	52	1265
-9	-7	16	16	953	-12	7	31	31	998	-9	1	52	52	1305
-9	-5	16	18	1160	-12	13	48	52	883	-9	5	43	42	1349
-9	-5	20	18	1117	-12	21	35	21	731	-9	13	31	31	1073
-9	-3	19	17	1226	-11	-6	80	79	874	-9	15	42	43	997
-9	-3	19	17	1363	-11	-6	79	79	984	-8	-4	38	40	1392
-9	3	15	17	1339	-11	-4	42	43	1180	-8	4	40	40	1289
-9	5	20	18	1324	-11	-2	15	16	1326	-8	4	42	40	1520
-9	7	16	16	1288	-11	-2	16	16	1006	-7	-5	42	41	1304
-8	-6	26	26	1090	-11	4	44	43	1121	-7	-5	41	41	1360
-8	-6	26	16	1172	-11	4	44	43	1121	-7	-5	41	41	1360
-7	-7	15	16	994	-11	6	80	79	1108	-6	-2	38	39	1791
-7	-5	17	17	1347	-11	14	32	33	920	-6	-2	38	39	1791
-7	-5	22	17	1242	-11	18	39	39	823	-6	-2	38	39	1791
-7	-1	33	32	1558	-11	22	74	69	728	-6	-2	38	39	1791
-6	-4	35	36	1404	-10	-7	16	16	929	-6	-2	38	39	1791

***** H = -7 *****

***** H = -7 *****

K	L	FOBS	FCAL	WAVL	K	L	FOBS	FCAL	WAVL	K	L	FOBS	FCAL	WAVL
*****	H = -7	*****												
-11	14	28	23	911	-20	-2	92	92	849	-11	11	51	53	955
-11	16	31	76	860	-20	0	39	36	910	-11	13	28	30	924
-11	18	37	76	812	-20	6	73	70	776	-11	17	83	82	823
-11	20	55	57	763	-20	8	88	85	798	-11	19	58	55	775
-11	22	31	28	721	-19	-3	43	39	749	-17	-6	68	67	727
-10	-5	17	17	1128	-19	-1	101	101	923	-17	4	45	42	894
-10	1	32	32	1135	-18	-10	31	23	727	-16	-9	22	23	818
-10	5	15	17	1219	-18	-4	64	64	821	-16	-3	35	34	965
-10	7	19	16	1157	-18	-2	25	25	923	-16	3	29	34	939
-10	15	23	23	939	-18	2	31	25	814	-16	7	57	56	995
-10	21	43	38	776	-18	4	62	64	861	-16	7	57	56	995
-9	-6	76	77	1056	-17	-7	30	29	896	-15	-2	20	23	1089
-9	-4	32	34	1329	-17	-5	68	67	795	-15	2	20	23	981
-9	-4	33	34	1106	-17	-3	39	39	913	-15	4	22	19	1042
-9	-2	13	13	1205	-17	-1	66	67	1022	-14	-9	20	23	832
-9	-2	12	13	1595	-17	1	66	67	823	-14	-7	17	15	993
-9	2	12	13	1343	-17	3	36	39	890	-14	-5	18	20	890
-9	4	34	34	1365	-17	5	67	67	927	-14	-3	28	26	1071
-9	10	17	16	1173	-17	7	26	29	946	-14	-1	39	40	1227
-9	12	29	31	1107	-16	-10	27	20	739	-14	1	40	40	1013
-9	14	58	57	1047	-16	-4	72	70	895	-14	3	26	26	1106
-9	16	25	24	961	-16	-2	35	34	1025	-14	5	23	20	1142
-9	18	38	37	894	-16	2	30	34	926	-14	7	13	15	1149
-9	20	28	26	830	-16	4	68	70	983	-13	-8	102	100	922
-8	-5	41	41	1249	-15	-1	28	29	1140	-13	-4	48	47	1024
-8	-5	41	41	1175	-15	-1	28	29	854	-13	2	87	86	1163
-8	-3	69	72	1327	-15	1	33	29	955	-13	4	48	47	1231
-8	-1	10	10	1422	-15	7	70	66	1086	-13	6	50	50	1246
-8	1	12	10	1486	-14	-10	29	34	749	-13	12	34	34	777
-8	5	44	41	1499	-14	-2	14	13	1139	-12	-1	19	16	1056
-8	13	60	60	1140	-14	0	64	63	982	-12	1	21	16	1214
-7	-2	51	50	1590	-14	4	35	34	1146	-12	3	48	46	1324
-6	-5	47	46	1491	-14	12	124	122	737	-12	9	16	13	856
-6	-5	47	46	1362	-13	-1	46	44	994	-12	13	35	34	834
-6	3	8	2	1983	-13	1	45	44	1131	-12	15	38	38	799
*****	H = -6	*****			*****	H = -5	*****			*****	H = -4	*****		
-23	-7	43	41	762	-12	0	55	54	1170	-11	2	43	45	1414
-22	-8	33	27	750	-12	4	17	13	1361	-11	4	12	10	1489
-22	0	47	51	837	-12	6	67	67	923	-11	8	65	62	785
-21	-9	49	46	729	-12	8	82	83	895	-11	14	39	34	882
-21	-7	85	90	807	-12	16	61	61	799	-11	18	65	62	785
-21	-3	34	30	764	-12	18	65	64	759	-10	-10	19	18	1280
-21	-1	51	49	834	-12	20	38	40	719	-10	7	18	17	1072
-21	7	90	90	740	-11	-1	21	20	1169	-10	9	18	18	1056
-21	9	41	46	749	-11	1	19	20	1363	-10	11	21	21	1026
-20	-8	82	85	798	-11	7	23	24	1010	-10	13	25	28	970
-20	-6	70	70	868	-11	9	80	79	974	-9	2	19	18	1761

K	L	FOBS FCAL	WAVL	K	L	FOBS FCAL	WAVL	K	L	FOBS FCAL	WAVL	K	L	FOBS FCAL	WAVL									
****H = -4 ****																								
-17	-7	67	938	-10	14	29	23	916	-18	5	79	80	795	-9	-4	43	41	1658	-16	-2	46	44	998	
-17	-5	43	42	1055	-10	16	26	29	860	7	32	37	818	-9	-2	31	32	1653	-16	0	34	33	1120	
-17	-5	44	42	785	-10	20	33	28	751	13	35	34	810	-9	2	31	32	1710	-16	4	90	91	855	
-17	-3	39	34	912	-9	3	41	41	1811	15	86	88	804	-9	4	41	41	1783	-16	6	35	34	827	
-17	-1	49	51	1023	-9	7	34	34	1155	-17	-4	32	34	-9	8	31	29	1104	-16	12	74	70	902	
-17	1	49	51	771	-9	11	41	43	1090	-17	-2	37	36	-9	10	19	17	1073	-15	-9	39	40	858	
-17	3	36	34	843	-9	15	35	34	950	-17	2	38	36	-9	16	42	46	884	-15	-5	23	23	1175	
-17	5	39	42	884	-9	17	82	82	878	-17	4	34	34	-9	1	7	3	2041	-15	-3	79	78	980	
-17	7	66	67	908	-9	19	97	95	823	-17	6	38	39	-8	-1	29	29	1227	-15	-1	51	50	1127	
-16	-10	30	29	777	-8	21	39	43	764	-8	9	31	31	-8	9	28	29	1227	-15	3	49	50	1246	
-16	-8	63	63	897	-8	8	38	40	1305	-16	-9	46	46	-8	11	44	44	1145	-15	3	77	78	893	
-16	-6	71	70	1029	-8	12	59	59	1142	-16	-7	41	42	-8	13	54	56	1060	-15	5	24	23	950	
-16	-2	92	91	1027	-8	14	77	77	1065	-16	-5	33	34	-8	15	48	49	975	-15	11	41	40	968	
-16	0	42	41	1140	-8	16	63	63	966	-16	-5	37	34	-8	17	43	44	896	-14	-8	62	61	954	
-16	2	88	88	871	-8	18	80	80	884	-16	-1	48	49	-7	2	29	29	2302	-14	-6	14	13	1140	
-16	6	74	70	966	-8	20	99	99	1140	-16	1	48	49	-7	12	57	56	1195	-14	0	12	13	1278	
-15	-9	33	34	844	-7	3	30	30	1706	-16	5	36	34	-7	16	44	42	983	-14	12	31	34	1026	
-15	-5	17	19	846	-7	9	32	34	1413	-15	-8	48	49	-6	9	41	40	1521	-13	-7	58	58	1073	
-15	-5	22	19	1141	-7	10	36	36	1488	-15	-4	47	48	-6	13	16	14	1211	-13	-3	30	31	1092	
-15	-3	47	48	1012	-6	12	14	13	1324	-15	-2	77	78	-5	10	33	34	1578	-13	-1	20	20	1303	
-15	-1	21	19	1157	-6	14	35	34	1188	-15	2	78	78	-5	12	46	46	1381	-13	1	19	20	1450	
-15	3	51	48	983	-6	16	72	70	1066	-14	-5	26	26	-5	12	46				-13	7	58	58	1107
-15	5	15	19	1028	-5	13	48	47	1323	-14	-1	38	38	-5	12	46				-13	9	18	17	1124
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