

Table 4. Observed and calculated structure factors.

Natural Beryl - Gatta et al. 2005 - Am. Mineralogists

Unique observed reflections after correcting

for dispersion and merging Friedel opposites

#

data_new

_shelx_title ' DMACA bei RT'

_shelx_refln_list_code 3

_shelx_F_calc_maximum 231.16

_exptl_crystal_F_000 0.00

_reflns_d_resolution_high 0.8056

loop_

_symmetry_equiv_pos_as_xyz

'x, y, z'

'x-y, x, z'

'-y, x-y, z'

'-x, -y, z'

'-x+y, -x, z'

'y, -x+y, z'

'x-y, -y, -z+1/2'

'-x, -x+y, -z+1/2'

'y, x, -z+1/2'

'-y, -x, -z+1/2'

'-x+y, y, -z+1/2'

'x, x-y, -z+1/2'

'-x, -y, -z'

'-x+y, -x, -z'

'y, -x+y, -z'

'x, y, -z'

'x-y, x, -z'

'-y, x-y, -z'

'-x+y, y, z-1/2'

'x, x-y, z-1/2'

'-y, -x, z-1/2'

'y, x, z-1/2'

'x-y, -y, z-1/2'

'-x, -x+y, z-1/2'

_cell_length_a 9.2099

_cell_length_b 9.2099

_cell_length_c 9.1894

_cell_angle_alpha 90.000

_cell_angle_beta 90.000

_cell_angle_gamma 120.000

loop_

_refln_index_h

_refln_index_k

_refln_index_l

_refln_F_meas

_refln_F_sigma

_refln_A_calc				_refln_B_calc			
0	1	0	57.4644	0.2180	-57.5209	0.0000	
-1	2	0	34.1499	0.2826	-34.5791	0.0000	
0	2	0	23.8854	0.3618	23.9855	0.0000	
-1	3	0	8.3455	2.2821	1.5807	0.0000	
0	3	0	22.1799	0.4216	-21.6650	0.0000	
-2	4	0	11.4772	0.7915	11.5333	0.0000	
-1	4	0	34.7569	0.2362	35.1627	0.0000	
0	4	0	11.4907	2.6770	5.8312	0.0000	
-2	5	0	32.0869	0.4486	-30.9857	0.0000	
-1	5	0	40.9980	0.4797	41.6958	0.0000	
0	5	0	100.9557	0.5307	-101.7861	0.0000	
-3	6	0	72.4872	0.4728	-71.4608	0.0000	
-2	6	0	44.2581	0.4131	45.1042	0.0000	
-1	6	0	42.2375	0.5735	-41.7334	0.0000	
0	6	0	113.8209	0.5929	115.6767	0.0000	
-3	7	0	12.7983	2.9964	6.4303	0.0000	
-2	7	0	60.4155	0.3859	62.4764	0.0000	
-1	7	0	49.0971	0.6253	-48.4545	0.0000	
0	7	0	69.8632	0.5230	-67.8104	0.0000	
-4	8	0	26.2667	1.0824	-25.6051	0.0000	
-3	8	0	31.8172	0.6088	-30.6276	0.0000	
-2	8	0	94.8590	0.3481	95.5301	0.0000	
-1	8	0	21.9128	0.9663	-20.4872	0.0000	
0	8	0	134.1991	0.8723	130.5117	0.0000	
-3	9	0	26.4754	2.7486	-25.9936	0.0000	
-2	9	0	20.0377	3.6077	-17.9239	0.0000	
-1	3	1	49.2689	0.1404	49.4000	0.0000	
-1	4	1	69.1230	0.1434	-69.8175	0.0000	
-1	5	1	24.1121	0.4953	-24.2195	0.0000	
-2	6	1	26.0985	0.4259	25.9097	0.0000	
-1	6	1	14.7593	2.6206	-8.6899	0.0000	
-3	7	1	15.9875	0.7028	-15.8422	0.0000	
-2	7	1	76.1101	0.2682	76.7593	0.0000	
-1	7	1	16.8431	1.0930	-17.6931	0.0000	
-2	8	1	25.2164	0.5313	-25.8113	0.0000	
-1	8	1	29.1929	0.5018	-29.0392	0.0000	
-4	9	1	29.2829	1.7930	-31.4707	0.0000	
-3	9	1	33.2120	2.3083	-33.1193	0.0000	
-2	9	1	38.5338	2.0528	-37.2980	0.0000	
-3	10	1	78.6369	1.6275	76.5586	0.0000	
0	0	2	22.9953	0.6144	22.2332	0.0000	
0	1	2	45.3365	0.1841	44.1442	0.0000	
-1	2	2	46.9803	0.1923	-45.2532	0.0000	
0	2	2	85.4976	0.1843	-83.0792	0.0000	
-1	3	2	28.6685	0.1783	27.9646	0.0000	
0	3	2	35.7956	0.2417	35.2121	0.0000	
-2	4	2	31.0993	0.4767	-31.0608	0.0000	
-1	4	2	29.8166	0.4346	29.4296	0.0000	
0	4	2	32.7031	0.5511	-33.0895	0.0000	
-2	5	2	12.1250	2.5813	-6.0959	0.0000	
-1	5	2	12.7819	1.0151	-10.5712	0.0000	
-3	6	2	29.5110	0.6046	-30.5098	0.0000	

-2	6	2	14.5284	1.0985	-12.0255	0.0000
-1	6	2	38.2291	0.4363	37.7020	0.0000
0	6	2	133.8629	0.4253	-134.8740	0.0000
-2	7	2	47.9734	0.3593	47.0717	0.0000
-1	7	2	27.1423	0.6470	25.8791	0.0000
0	7	2	20.8362	0.8712	19.8412	0.0000
-4	8	2	75.6864	0.4219	-76.7854	0.0000
-3	8	2	33.2900	0.4501	33.0515	0.0000
-2	8	2	30.5974	0.4640	-30.9042	0.0000
-1	8	2	14.9641	2.0833	8.5487	0.0000
-1	3	3	59.1036	0.1426	-58.3914	0.0000
-1	4	3	36.1698	0.3618	36.3484	0.0000
-2	5	3	55.7008	0.2476	-55.6103	0.0000
-1	5	3	71.9711	0.2897	-72.0492	0.0000
-2	6	3	22.4108	0.5215	21.6338	0.0000
-1	6	3	39.0826	0.4115	38.9477	0.0000
-3	7	3	111.8404	0.2722	112.3811	0.0000
-2	7	3	14.7026	3.4486	5.1301	0.0000
-1	7	3	14.4772	2.3584	9.7915	0.0000
-3	8	3	42.9071	0.3842	-42.8989	0.0000
-2	8	3	31.4631	0.5077	-31.2278	0.0000
-1	8	3	53.7217	0.9486	-52.0834	0.0000
-4	9	3	17.8259	4.0116	-15.8686	0.0000
-2	9	3	60.1429	1.6718	54.4891	0.0000
-3	10	3	39.9175	2.6140	-40.3298	0.0000
0	0	4	62.4099	0.5076	61.0625	0.0000
0	1	4	33.8719	0.2400	34.0319	0.0000
-1	2	4	44.0837	0.9630	-48.9085	0.0000
0	2	4	12.7999	1.7899	-11.3475	0.0000
-1	3	4	16.6359	0.7864	-17.4136	0.0000
0	3	4	66.2621	0.3831	65.0005	0.0000
-2	4	4	132.3802	0.4190	129.3638	0.0000
-1	4	4	33.8335	0.3863	-34.1764	0.0000
0	4	4	68.4145	0.4156	67.5412	0.0000
-2	5	4	50.0803	0.3211	-50.9566	0.0000
-1	5	4	31.1895	0.4765	-32.0528	0.0000
0	5	4	16.1027	1.1964	-15.4754	0.0000
-3	6	4	13.4388	1.2963	-10.1794	0.0000
-2	6	4	76.7497	0.2909	76.7035	0.0000
-1	6	4	19.5864	0.9107	17.1020	0.0000
0	6	4	82.2628	0.3598	-81.5372	0.0000
-3	7	4	63.5201	0.2894	-64.0387	0.0000
-2	7	4	40.8354	0.3660	40.3808	0.0000
-4	8	4	70.7510	0.4673	69.5871	0.0000
-1	8	4	21.0570	3.6830	20.5799	0.0000
-4	9	4	59.2850	1.1564	-58.6847	0.0000
-3	9	4	31.2581	2.8794	27.4226	0.0000
-4	10	4	61.7920	1.6119	66.4601	0.0000
-3	10	4	64.8752	1.8582	-63.1795	0.0000
-1	4	5	15.9433	0.9864	-14.5831	0.0000
-2	5	5	30.0953	0.4428	-30.0874	0.0000
-1	5	5	47.1228	0.3998	-47.2154	0.0000
-2	6	5	24.9287	0.6366	25.0647	0.0000
-1	6	5	15.9625	1.0561	14.8476	0.0000

-3	7	5	45.8312	0.3535	45.5486	0.0000
-2	7	5	37.5430	0.4228	37.0110	0.0000
-3	8	5	17.7779	4.0332	-17.8408	0.0000
-1	8	5	42.4779	1.5773	-40.0975	0.0000
-4	9	5	21.4022	3.0227	-21.8535	0.0000
-4	10	5	24.1255	4.1986	16.3173	0.0000
-1	2	6	38.4076	1.1480	-37.3932	0.0000
0	2	6	60.6617	0.6856	-62.4521	0.0000
-1	3	6	35.9832	0.5006	36.6646	0.0000
0	3	6	11.9451	3.1572	-9.4636	0.0000
-2	4	6	87.9056	0.4266	-88.4177	0.0000
-1	4	6	57.7781	0.3621	58.3960	0.0000
0	4	6	64.0386	0.5134	-63.1500	0.0000
-2	5	6	12.6154	3.4387	5.0223	0.0000
-1	5	6	28.4644	0.4395	28.6985	0.0000
0	5	6	46.5576	0.4611	-46.5732	0.0000
-3	6	6	59.8018	0.3896	-58.7600	0.0000
-2	6	6	26.4856	0.5191	-26.3261	0.0000
-1	6	6	14.6501	3.6576	8.4446	0.0000
0	6	6	33.5676	1.2823	-32.3145	0.0000
-3	7	6	31.3683	1.2349	33.1131	0.0000
-2	7	6	50.2604	0.8877	51.7662	0.0000
-4	8	6	121.3965	0.5315	-117.6610	0.0000
-4	9	6	30.6310	3.1882	30.8398	0.0000
-3	9	6	21.1448	4.7123	-15.8567	0.0000
-1	3	7	72.8263	0.4290	73.6941	0.0001
-1	4	7	87.9712	0.2434	-87.1849	-0.0001
-2	5	7	15.6419	2.3054	10.1364	0.0000
-1	5	7	15.8556	1.3752	-10.4858	0.0000
-2	6	7	24.9450	1.7616	23.7340	0.0000
-1	6	7	21.9668	2.3649	-20.7005	0.0000
-3	7	7	47.1050	1.1709	-46.6219	-0.0001
-2	7	7	89.2273	0.4852	87.7308	0.0000
-1	7	7	23.9499	3.8068	-22.4456	0.0000
-3	8	7	24.5536	3.7530	18.9921	0.0000
0	0	8	229.6064	0.7309	231.1649	0.0000
0	1	8	30.9315	0.4983	-30.7091	0.0000
-1	2	8	30.1672	0.5222	-30.3433	0.0000
0	2	8	19.1842	0.7874	16.9878	0.0000
-2	4	8	37.9854	0.5542	37.9953	0.0000
-1	4	8	19.1526	1.2894	16.5048	0.0000
0	4	8	18.8386	3.9235	18.1257	0.0000
-2	5	8	30.9036	1.4648	-33.7824	0.0000
-1	5	8	17.4326	3.1538	18.6859	0.0000
0	5	8	73.4716	1.4957	-70.3532	0.0000
-3	6	8	50.4432	1.9361	-49.2983	0.0000
-2	6	8	51.2838	1.3391	48.5180	0.0000
0	6	8	60.8949	1.3086	60.5718	0.0000
-2	7	8	49.3773	1.2933	50.3934	0.0000
-1	7	8	40.6542	1.8520	-37.2841	0.0000
0	7	8	44.1308	2.6547	-44.9167	0.0000
-1	5	9	46.4759	1.6042	-47.4236	0.0000
-1	6	9	19.2386	5.1076	16.9555	0.0000
-3	7	9	59.4335	1.5172	58.2343	0.0000

