

Törnebohmitite, $\text{RE}_2\text{Al}(\text{OH})[\text{SiO}_4]_2$: crystal structure and genealogy of $\text{RE}(\text{III})\text{Si}(\text{IV}) \rightleftharpoons \text{Ca}(\text{II})\text{P}(\text{V})$ isomorphisms

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Abstract

Törnebohmitite, $\text{RE}_2\text{Al}(\text{OH})[\text{SiO}_4]_2$, monoclinic, $a = 7.383(3)$, $b = 5.673(3)$, $c = 16.937(6)\text{Å}$, $\beta = 112.04(2)^\circ$, $Z = 4$, space group $P2_1/c$, is structurally allied to the brackebuschite and pyrobelonite groups of minerals. It is isostructural with fornacite. $R = 0.033$ for 2586 independent reflections.

The basis of the structure consists of linear $\frac{1}{2}[\text{Al}(\text{OH})(\text{O}_7)_3]$ octahedral chains which run parallel to $[010]$. Insular $[\text{SiO}_4]$ which corner-link to the octahedral chains are arranged in *trans* configuration to these chains. These admit the large RE (rare earth) cations which form a serrated wall of linked $\text{RE}\phi_{10}$ polyhedra which is oriented parallel to the $\{001\}$ plane. Average distances are $^{10}\text{RE}(1)-\text{O} = 2.64$, $^{10}\text{RE}(2)-\text{O} = 2.68$, $^{16}\text{Al}-\text{O}$, $\text{OH} = 1.90$, $^{14}\text{Si}(1)-\text{O} = 1.62$ and $^{14}\text{Si}(2)-\text{O} = 1.63\text{Å}$.

Törnebohmitite is yet another example where isomorphisms of the type $\text{RE}^3\text{Si}^{4+} \rightleftharpoons \text{Ca}^{2+}\text{P}^{5+}$ can be found.

Introduction

Törnebohmitite is a hydrous rare earth silicate, consisting principally of the rare earth elements (= RE) lanthanum, cerium and neodymium. It was first discovered as a minor constituent of the cerite ores from the Bastnäs Mine, Riddarhyttan, Parish of Skinnskatteberg, Province of Västmanland, central Sweden. Geijer (1921) first announced the new species, and Geijer and Carlborg (1923) offered a comprehensive document from a geological and historical standpoint of this remarkable region, which is rich in mining history and has been a site of extensive mineralogical-chemical investigations. Jorpes (1966), for example, documents the journeys of Jöns Jacob Berzelius, in search of minerals which provided him with several new rare earth elements. Of the rare earth silicate species, cerite appeared to be the most predominant, along with allanite. Geijer discerned törnebohmitite in thin sections, where it occurs as green, pleochroic grains embedded in the

cerite ore and recognized its distinction from cerite. He named it after Alfred Elis Törnebohm (1838-1911), former Director of the Geological Survey of Sweden.

The chemical composition of törnebohmitite was obtained by Mauzelius and reported by Geijer. It is listed in Table 1 along with a calculated composition derived from our structure analytical study. Agreement between the chemical analysis of Mauzelius and the theoretical end member formula $\text{Ce}_2\text{Al}(\text{OH})[\text{SiO}_4]_2$ is good, bearing in mind that reported FeO could be Fe_2O_3 and that minor CaO probably substitutes for RE. Water was not reported; the low F content is not sufficient to warrant predominant $\text{F}^- - \text{OH}^-$ substitution. The hydroxyl anion is so tightly bound that it may be included with "ignition". The ignition content (1.70%) and theoretical water content (1.77%) make this proposition appealing.

Despite subsequent attempts to rationalize törnebohmitite's crystal chemistry, the literature is fraught

Table 4. Tornebohmitte $|F_o| - |F_c|$ table.
Shen and Moore.

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITTE CRYSTAL STRUCTURE										PAGE 1				
H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	0	0	125	123	3	3	0	45	40	8	6	0	164	157
2	0	0	271	-306	4	3	0	120	-117	1	7	0	87	91
3	0	0	453	-481	5	3	0	276	-279	2	7	0	72	74
4	0	0	424	440	6	3	0	36	33	3	7	0	85	-84
5	0	0	299	311	7	3	0	155	155	4	7	0	122	-118
6	0	0	155	165	8	3	0	148	149	5	7	0	95	-94
7	0	0	325	-341	9	3	0	107	-105	6	7	0	78	76
8	0	0	132	-138	10	3	0	108	-103	7	7	0	60	59
9	0	0	36	33	10	3	0	772	770	8	7	0	199	201
10	0	0	149	144	1	4	0	21	19	9	8	0	31	-24
11	0	0	26	-6	2	4	0	151	-145	1	8	0	38	30
1	1	0	75	71	3	4	0	342	-339	2	8	0	115	-116
2	1	0	64	-63	4	4	0	234	232	3	8	0	44	44
3	1	0	139	-139	5	4	0	163	162	4	8	0	26	-7
4	1	0	104	102	6	4	0	144	142	5	8	0	98	-99
5	1	0	336	349	7	4	0	218	215	1	9	0	61	-59
6	1	0	15	-16	8	4	0	114	-108	2	9	0	25	20
7	1	0	185	-192	1	5	0	49	-48	3	9	0	34	34
8	1	0	187	-193	2	5	0	71	-66	4	1	1	41	-45
9	1	0	111	114	3	5	0	52	50	5	1	1	20	-19
10	1	0	137	135	4	5	0	142	141	6	1	1	15	5
0	2	0	806	-795	5	5	0	191	191	7	1	1	88	89
1	2	0	238	-227	6	5	0	48	-42	8	1	1	17	-31
2	2	0	710	694	7	5	0	100	-94	9	1	1	27	-32
3	2	0	307	313	8	5	0	74	-69	10	1	1	81	-83
4	2	0	69	-68	9	5	0	103	98	1	1	1	51	53
5	2	0	352	-359	0	6	0	234	-236	2	1	1	76	74
6	2	0	32	32	1	6	0	95	-90	3	1	1	28	-28
7	2	0	-35	238	2	6	0	211	210	4	1	1	63	-64
8	2	0	241	247	3	6	0	129	130	5	1	1	63	-64
9	2	0	66	-66	4	6	0	27	21	6	1	1	58	59
10	2	0	69	-64	5	6	0	132	-132	7	1	1	13	-9
1	3	0	15	-13	6	6	0	25	-19	8	1	1	30	-34
2	3	0	75	69	7	6	0	73	70	9	1	1	48	50

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITE CRYSTAL STRUCTURE

OBSERVED										CALCULATED									
H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-4	5	1	164	-163	-3	7	1	159	159	-3	0	2	20	6	9	1	2	37	33
-3	5	1	188	-184	-2	7	1	50	-46	-2	0	2	247	-252	10	1	2	37	33
-2	5	1	90	91	-1	7	1	169	-171	-1	0	2	22	11	-11	2	2	24	-15
-1	5	1	189	191	1	7	1	126	129	0	0	2	216	220	-10	2	2	53	-53
0	5	1	28	-28	2	7	1	36	32	0	0	2	253	264	-9	2	2	111	105
1	5	1	155	-157	3	7	1	58	-59	1	0	2	292	-295	-8	2	2	135	137
2	5	1	53	-47	4	7	1	65	-65	2	0	2	487	-510	-7	2	2	35	-30
3	5	1	101	104	5	7	1	32	31	3	0	2	135	-139	-6	2	2	79	-77
4	5	1	38	40	6	7	1	22	-17	4	0	2	376	391	-5	2	2	30	-20
5	5	1	38	-34	7	7	1	26	-25	5	0	2	191	200	-4	2	2	45	-44
6	5	1	31	-28	-5	8	1	44	-45	6	0	2	169	-170	-4	2	2	111	-116
7	5	1	81	74	-4	8	1	77	76	7	0	2	217	-221	-3	2	2	201	192
8	5	1	20	-5	-3	8	1	128	131	8	0	2	16	20	-2	2	2	100	101
9	5	1	41	-34	-2	8	1	51	-51	9	0	2	203	198	-1	2	2	192	173
-8	6	1	53	-44	-1	8	1	174	-178	10	0	2	76	72	0	2	2	329	-318
-6	6	1	99	95	0	8	1	62	-60	-11	1	2	178	-177	1	2	2	29	3
-5	6	1	99	98	1	8	1	182	182	-10	1	2	68	72	2	2	2	109	110
-4	6	1	85	-80	2	8	1	188	190	-9	1	2	283	-292	3	2	2	592	605
-3	6	1	162	-166	3	8	1	73	-77	-8	1	2	68	72	4	2	2	28	-22
-2	6	1	35	32	4	8	1	209	-207	-7	1	2	294	305	5	2	2	228	-233
-1	6	1	217	219	5	8	1	45	-42	-6	1	2	157	157	6	2	2	266	-273
0	6	1	82	84	-2	9	1	24	18	-5	1	2	478	-503	7	2	2	231	234
1	6	1	213	-215	1	9	1	116	120	-4	1	2	393	-409	8	2	2	131	127
2	6	1	251	-254	0	9	1	33	30	-3	1	2	233	238	9	2	2	26	26
3	6	1	77	79	1	9	1	75	-77	-2	1	2	815	829	10	2	2	239	-229
4	6	1	250	247	2	9	1	51	-52	-1	1	2	183	176	9	2	2	159	153
5	6	1	46	44	-11	0	2	102	104	0	1	2	394	-407	-9	2	2	239	234
6	6	1	190	-183	-10	0	2	136	-134	-8	1	2	438	-452	-8	2	2	63	-62
7	6	1	131	-124	-9	0	2	71	-71	-7	1	2	352	356	-7	2	2	241	-243
8	6	1	97	94	-8	0	2	19	20	-6	1	2	74	79	-6	2	2	111	-111
-7	7	1	65	-66	0	0	2	185	195	5	1	2	228	-240	-5	2	2	381	385
-6	7	1	177	-170	-7	0	2	44	-48	-4	1	2	167	-173	-4	2	2	325	319
-5	7	1	58	-57	-5	0	2	183	194	-3	1	2	40	41	-3	2	2	148	-144
-4	7	1	173	171	-4	0	2	68	62	-2	1	2	60	54	-2	2	2	584	-573
																		127	-124

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITE CRYSTAL STRUCTURE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-5	5	2	224	-223	-4	7	2	81	83	0	1	3	100	99	-7	3	3	86	85	9	4	3	76	-70
-4	5	2	137	-133	-2	7	2	168	-170	1	1	3	34	-37	-6	3	3	89	-86	-8	5	3	143	-132
-3	5	2	8	77	-1	7	2	65	-66	2	1	3	88	-90	-5	3	3	150	-152	-7	5	3	111	-109
-2	5	2	416	416	0	7	2	53	54	4	1	3	101	105	-4	3	3	24	26	-5	5	3	101	96
-1	5	2	116	115	1	7	2	151	150	5	1	3	40	40	-3	3	3	243	241	-5	5	3	171	171
0	5	2	95	-91	2	7	2	34	32	6	1	3	26	-26	-2	3	3	88	89	-4	5	3	63	-61
1	5	2	224	-225	3	7	2	63	-63	7	1	3	32	-36	-1	3	3	291	-283	-3	5	3	289	-289
2	5	2	110	112	4	7	2	56	-53	8	1	3	26	23	0	3	3	250	-246	-2	5	3	105	-106
3	5	2	165	167	5	7	2	63	66	9	1	3	34	23	1	3	3	88	87	-1	5	3	291	293
4	5	2	100	98	6	7	2	141	134	10	1	3	20	16	2	3	3	225	224	0	5	3	250	253
5	5	2	122	-119	-5	8	2	131	128	-11	2	3	56	-48	4	3	3	218	-219	1	5	3	114	-115
6	5	2	133	-128	-4	8	2	56	-54	-10	2	3	56	-49	5	3	3	99	-96	2	5	3	271	-272
7	5	2	28	-26	-3	8	2	82	-82	-9	2	3	36	31	6	3	3	114	111	3	5	3	24	-17
8	5	2	36	33	-1	8	2	145	148	-8	2	3	81	84	7	3	3	94	91	4	5	3	260	257
-8	6	2	51	45	0	8	2	47	47	-7	2	3	19	14	8	3	3	21	-13	5	5	3	115	-110
-7	6	2	39	-32	1	8	2	39	-36	-6	2	3	88	-91	9	3	3	76	-68	6	5	3	125	-121
-6	6	2	101	-95	2	8	2	107	-105	-5	2	3	46	-45	9	4	3	94	88	7	5	3	136	-129
-5	6	2	82	-79	3	8	2	69	-67	-4	2	3	96	100	-9	4	3	51	-51	8	5	3	33	28
-4	6	2	30	-25	4	8	2	39	33	-3	2	3	82	81	-8	4	3	133	-129	-8	6	3	158	148
-3	6	2	151	151	5	8	2	86	83	-2	2	3	16	-18	-7	4	3	27	-28	-7	6	3	34	32
-2	6	2	31	-25	-2	9	2	100	105	-1	2	3	63	-62	-6	4	3	151	149	-6	6	3	144	-142
-1	6	2	51	-47	-1	9	2	55	56	0	2	3	61	63	-5	4	3	78	77	-5	6	3	107	-103
0	6	2	172	-174	0	9	2	72	72	1	2	3	121	121	-4	4	3	113	-115	-4	6	3	88	89
1	6	2	81	79	1	9	2	62	-64	2	2	3	30	-29	-3	4	3	107	-105	-3	6	3	86	84
2	6	2	62	63	-10	1	3	18	6	3	2	3	49	-52	-2	4	3	45	48	-2	6	3	40	-42
3	6	2	247	249	-9	1	3	19	-9	4	2	3	43	43	-1	4	3	93	95	-1	6	3	96	-98
4	6	2	81	-83	-8	1	3	53	-55	5	2	3	70	74	0	4	3	58	-58	0	6	3	24	27
5	6	2	87	-87	-7	1	3	17	-10	6	2	3	22	-7	1	4	3	125	-125	1	6	3	74	80
6	6	2	104	-100	-6	1	3	36	34	7	2	3	70	-70	2	4	3	41	42	2	6	3	45	-43
7	6	2	145	142	-5	1	3	36	34	8	2	3	39	-27	3	4	3	69	74	3	6	3	44	-48
8	6	2	37	32	-4	1	3	34	-34	9	2	3	47	46	4	4	3	70	-69	4	6	3	73	73
-7	7	2	63	-64	-3	1	3	131	-136	10	2	3	35	25	5	4	3	103	-103	5	6	3	107	108
-6	7	2	23	-17	-2	1	3	73	-68	-10	2	3	57	-51	7	4	3	121	117	6	6	3	118	-23
-5	7	2	116	115	-1	1	3	117	111	-8	3	3	96	94	8	4	3	44	35	7	6	3	115	-106

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITE CRYSTAL STRUCTURE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-7	7	7	78	76	-5	0	4	136	-143	7	1	4	23	-20	-3	3	4	13	3	-8	5	4	54	55
-6	7	3	124	-116	-4	0	4	557	-683	8	1	4	302	302	-2	3	4	346	-334	-7	5	4	113	111
-5	7	3	165	-164	-3	0	4	77	-76	9	1	4	151	143	-1	3	4	128	-123	-6	5	4	67	65
-4	7	3	54	52	-2	0	4	316	318	10	1	4	98	-94	0	3	4	210	202	-5	5	4	80	-77
-3	7	3	244	248	-1	0	4	229	220	-11	2	4	198	-192	1	3	4	573	568	-4	5	4	94	-91
-2	7	3	67	69	0	0	4	203	-199	-10	2	4	71	72	2	3	4	27	26	-3	5	4	64	63
-1	7	3	254	-257	0	0	4	374	-375	-9	2	4	189	193	3	3	4	252	-250	-2	5	4	250	251
0	7	3	220	-223	2	0	4	228	-220	-8	2	4	115	115	4	3	4	246	-248	-1	5	4	69	68
1	7	3	102	105	3	0	4	197	206	-7	2	4	363	-372	5	3	4	219	218	0	5	4	131	-130
2	7	3	251	252	3	0	4	147	151	-6	2	4	284	-291	6	3	4	252	250	1	5	4	303	-305
3	7	3	31	28	4	0	4	85	-91	-5	2	4	57	58	7	3	4	27	17	2	5	4	33	33
4	7	3	216	-214	5	0	4	30	30	-4	2	4	543	551	8	3	4	258	-251	3	5	4	178	177
5	7	3	109	-104	6	0	4	44	-41	-3	2	4	22	15	9	3	4	129	-121	4	5	4	165	165
6	7	3	127	122	7	0	4	34	-35	-2	2	4	372	-356	-10	4	4	45	-40	5	5	4	133	-132
-5	8	3	101	99	8	0	4	91	-93	-2	2	4	292	-283	-9	4	4	162	-158	6	5	4	147	-144
-4	8	3	37	-34	9	0	4	64	63	-1	2	4	18	23	-8	4	4	88	-85	7	5	4	17	-3
-3	8	3	67	-68	10	0	4	33	-25	0	2	4	207	212	-7	4	4	223	222	8	5	4	178	170
-2	8	3	18	19	-11	1	4	31	-25	2	2	4	98	95	-6	4	4	211	209	-8	6	4	76	73
-1	8	3	63	67	-9	1	4	27	18	3	2	4	275	-280	-5	4	4	93	-85	-7	6	4	158	-150
0	8	3	21	8	-8	1	4	23	17	4	2	4	190	-196	-4	4	4	424	-422	-6	6	4	119	-118
1	8	3	25	-26	-7	1	4	137	144	5	2	4	41	-33	-3	4	4	127	-125	-5	6	4	21	-13
2	8	3	35	30	-6	1	4	203	211	6	2	4	52	-46	-2	4	4	121	114	-4	6	4	255	256
3	8	3	19	18	-5	1	4	50	-49	7	2	4	29	-28	-1	4	4	124	121	-3	6	4	65	64
4	8	3	73	73	-4	1	4	255	-259	8	2	4	27	24	0	4	4	81	-84	-2	6	4	23	-16
-2	9	3	43	-44	-3	1	4	24	16	9	2	4	29	23	1	4	4	241	-241	-1	6	4	141	-144
-1	9	3	188	193	-2	1	4	462	447	10	2	4	76	-71	2	4	4	149	-151	1	6	4	82	84
0	9	3	160	162	-1	1	4	246	241	-11	3	4	43	40	3	4	4	77	81	2	6	4	134	135
1	9	3	72	-78	0	1	4	242	-239	-10	3	4	56	50	4	4	4	160	155	3	6	4	72	-74
-10	0	4	188	185	1	1	4	743	-763	-9	3	4	19	-4	5	4	4	14	-10	4	6	4	148	-143
-11	0	4	65	-65	2	1	4	69	-72	-8	3	4	31	-20	5	4	4	29	26	5	6	4	92	-86
-9	0	4	253	-257	3	1	4	325	334	-7	3	4	114	-113	7	4	4	61	-59	6	6	4	20	-14
-8	0	4	107	-110	4	1	4	296	309	-6	3	4	127	-128	8	4	4	25	-23	7	6	4	35	30
-7	0	4	341	363	5	1	4	253	-263	-5	3	4	91	88	9	4	4	45	-39	-7	7	4	74	-69
-6	0	4	311	322	6	1	4	318	-327	-4	3	4	206	203	-9	5	4	27	15	-6	7	4	30	14

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHRITE CRYSTAL STRUCTURE

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC		
-5	7	7	44	112	109	0	1	1	5	48	46	-2	3	5	134	132	-4	5	5	97	101	-1	7	5	22	-23
-4	7	7	44	113	45	2	1	1	5	52	-53	-1	3	5	21	17	-3	5	5	23	23	0	7	5	115	-117
-3	7	7	44	56	-53	3	1	1	5	71	-76	0	3	5	106	-107	-2	5	5	122	-126	1	7	5	26	-25
-2	7	7	44	131	-135	4	1	1	5	20	17	1	3	5	32	-34	-1	5	5	19	-3	2	7	5	140	139
-1	7	7	44	47	43	5	1	1	5	38	36	2	3	5	142	145	0	5	5	133	132	3	7	5	123	120
0	7	7	44	107	108	7	1	1	5	45	-45	3	3	5	146	149	1	5	5	38	39	4	7	5	71	-71
1	7	7	44	169	171	-10	2	2	5	73	-69	4	3	5	27	-29	2	5	5	152	-151	5	7	5	145	-141
2	7	7	44	10	-42	-9	2	2	5	49	-48	5	3	5	121	-118	3	5	5	163	-163	-5	8	5	211	211
3	7	7	44	57	-59	-8	2	2	5	61	63	7	3	5	103	98	4	5	5	61	61	-4	8	5	27	23
4	7	7	44	76	-73	-7	2	2	5	95	95	8	3	5	63	60	5	5	5	148	143	-3	8	5	227	-230
5	7	7	44	91	90	-6	2	2	5	68	-70	9	3	5	59	-58	7	5	5	140	-132	-2	8	5	180	-184
6	7	7	44	58	58	-5	2	2	5	193	-199	9	3	5	116	110	8	5	5	79	-69	-1	8	5	98	98
-5	8	8	44	23	15	-4	2	2	5	45	-45	-9	4	5	66	61	-8	5	5	124	119	0	8	5	189	192
-4	8	8	44	117	-119	-3	2	2	5	149	147	-8	4	5	116	-114	-7	5	5	165	159	1	8	5	16	-15
-3	8	8	44	88	-86	-2	2	2	5	111	107	-7	4	5	172	-170	-6	5	5	103	-101	2	8	5	176	-174
-2	8	8	44	39	-36	-1	2	2	5	155	-151	-6	4	5	91	92	-5	5	5	284	-282	3	8	5	83	-83
-1	8	8	44	56	58	0	2	2	5	209	-206	-5	4	5	270	269	-4	5	5	44	-46	4	8	5	85	83
0	8	8	44	51	51	1	2	2	5	32	31	-4	4	5	42	42	-3	5	5	259	257	-1	9	5	48	44
1	8	8	44	66	-69	2	2	2	5	131	134	-3	4	5	261	-258	-2	5	5	196	199	0	9	5	86	85
2	8	8	44	121	-120	3	2	2	5	34	36	-2	4	5	196	-193	-1	5	5	152	-153	-1	9	5	84	83
3	8	8	44	30	-22	4	2	2	5	70	-72	-1	4	5	168	169	0	5	5	250	-253	-9	9	5	164	-170
4	8	8	44	124	122	5	2	2	5	61	-61	0	4	5	265	262	1	5	5	31	31	-8	9	5	237	-247
-2	9	9	44	83	85	6	2	2	5	27	29	1	4	5	46	-46	2	5	5	209	210	-7	9	5	109	112
-1	9	9	44	52	-49	7	2	2	5	45	47	2	4	5	210	-210	3	5	5	82	81	-6	9	5	132	129
0	9	9	44	58	-60	9	2	2	5	22	-14	3	4	5	65	-65	4	5	5	115	-112	-5	9	5	78	75
-1	9	9	44	24	-21	-11	3	3	5	33	31	4	4	5	113	114	5	5	5	125	-118	-4	9	5	592	-598
-10	1	1	55	26	-28	-10	3	3	5	61	60	4	4	5	109	108	6	5	5	20	20	-3	9	5	541	-517
-8	1	1	55	29	28	-9	3	3	5	41	-31	5	4	5	35	-32	7	5	5	72	66	-2	9	5	882	830
-7	1	1	55	12	2	-7	3	3	5	89	-88	6	4	5	71	65	7	5	5	31	-31	0	9	5	82	-65
-6	1	1	55	32	-29	-8	3	3	5	23	-22	-9	5	5	18	11	-6	5	5	34	36	0	9	5	608	-604
-4	1	1	55	36	38	-6	3	3	5	48	45	-8	5	5	89	88	-5	5	5	18	12	1	9	5	433	-441
-3	1	1	55	13	15	-5	3	3	5	18	1	-7	5	5	24	19	-4	5	5	62	-65	0	9	5	396	404
-2	1	1	55	81	-78	-4	3	3	5	113	-117	-6	5	5	58	-60	-3	5	5	17	-11	3	9	5	396	404
-1	1	1	55	20	-11	-3	3	3	5	34	-27	-5	5	5	16	-11	-2	5	5	80	80	4	9	5	306	317

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITE CRYSTAL STRUCTURE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-5	3	3	209	199	-9	5	8	79	76	-5	7	8	27	21	-11	2	9	47	-44	-9	4	9	144	-141
-4	3	3	182	-177	-8	5	8	118	115	-4	7	8	47	-48	-10	2	9	46	45	-3	4	9	19	15
-3	3	3	505	-587	-7	5	8	32	-27	-3	7	8	200	-202	-9	2	9	87	89	-7	4	9	171	171
-2	3	3	24	-23	-6	5	8	279	-277	-2	7	8	32	-32	-8	2	9	20	-15	-6	4	9	89	87
-1	3	3	352	341	-5	5	8	142	-139	-1	7	8	36	27	-7	2	9	101	-105	-5	4	9	86	-86
0	3	3	221	217	-4	5	8	90	87	0	7	8	81	80	-6	2	9	54	-55	-4	4	9	113	-114
1	3	3	334	-338	-3	5	8	331	329	1	7	8	106	-110	-5	2	9	61	59	-3	4	9	95	95
2	3	3	314	-317	-2	5	8	14	9	2	7	8	123	-124	-4	2	9	70	73	-2	4	9	170	172
3	3	3	32	-32	-1	5	8	206	-205	3	7	8	88	-86	-3	2	9	64	-66	-1	4	9	15	15
4	3	3	248	248	0	5	8	162	-163	4	7	8	60	61	-2	2	9	125	-121	0	4	9	76	-78
5	3	3	123	121	1	5	8	166	169	5	7	8	80	73	0	2	9	57	60	1	4	9	13	-8
6	3	3	51	-54	2	5	8	201	201	-5	8	8	107	-109	1	2	9	15	13	2	4	9	57	58
7	3	3	80	-75	3	5	8	30	28	-4	8	8	53	-53	4	2	9	33	63	3	4	9	24	-7
8	3	3	23	-14	4	5	8	162	-161	-2	8	8	20	16	6	2	9	33	-34	4	4	9	85	-67
9	3	3	93	-91	5	5	8	135	-128	-3	8	8	168	171	8	2	9	39	39	5	4	9	21	-8
-10	4	4	41	-36	6	5	8	19	7	-1	8	8	16	7	-11	3	9	61	-59	6	4	9	55	53
-9	4	4	180	178	7	5	8	48	42	0	8	8	60	-57	-10	3	9	22	18	7	4	9	26	6
-8	4	4	23	-18	-8	6	8	56	-56	1	8	8	107	-111	-9	3	9	45	46	-10	5	9	30	31
-7	4	4	57	50	-7	6	8	96	-94	3	8	8	51	11	-8	3	9	80	80	-9	5	9	91	-89
-6	4	4	106	-102	-6	6	8	21	13	-11	1	9	16	11	-6	3	9	82	-81	-8	5	9	29	-22
-5	4	4	58	55	-5	6	8	27	23	-10	1	9	42	43	-5	3	9	80	-80	-7	5	9	77	75
-4	4	4	39	-31	-4	6	8	122	126	-9	1	9	33	-33	-4	3	9	54	51	-6	5	9	165	165
-3	4	4	197	197	-3	6	8	102	-102	-8	1	9	29	27	-4	3	9	239	238	-5	5	9	96	-93
-2	4	4	25	24	-2	6	8	65	-64	-7	1	9	20	13	-3	3	9	39	37	-4	5	9	39	-209
-1	4	4	64	65	-1	6	8	122	-120	-6	1	9	100	99	-2	3	9	145	-142	-3	5	9	39	-209
0	4	4	168	-167	0	6	8	138	139	-5	1	9	75	-35	-1	3	9	143	-142	-2	5	9	234	236
1	4	4	171	-170	1	6	8	55	51	-4	1	9	33	-34	0	3	9	126	131	-1	5	9	180	183
2	4	4	24	21	2	6	8	184	184	-3	1	9	27	-24	1	3	9	239	240	0	5	9	134	-134
3	4	4	204	207	3	6	8	115	-116	-2	1	9	102	97	3	3	9	160	-161	1	5	9	244	-244
4	4	4	20	21	4	6	8	42	-38	-1	1	9	63	65	4	3	9	72	-75	2	5	9	18	16
5	4	4	144	-138	5	6	8	37	-36	0	1	9	32	-44	5	3	9	133	131	3	5	9	240	238
6	4	4	102	-95	6	6	8	169	164	1	1	9	74	-83	6	3	9	90	85	4	5	9	76	70
7	4	4	80	72	7	7	8	28	18	3	1	9	80	87	8	3	9	98	-87	5	5	9	130	-125
8	4	4	113	-104	-6	7	8	135	135	6	1	9	58	-60	-10	4	9	75	-74	6	5	9	155	-147

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITTE CRYSTAL STRUCTURE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC					
7	5	9	57	50	2	8	9	21	12	5	1	10	224	-226	0	3	10	325	325	-1	5	10	158	-158
-9	6	9	184	169	-11	0	10	101	-103	6	1	10	48	41	1	3	10	75	-72	0	5	10	204	-204
-8	6	9	24	3	-10	0	10	240	-249	7	1	10	261	256	2	3	10	204	-202	1	5	10	59	60
-7	6	9	160	-157	-8	0	10	364	377	8	1	10	90	85	3	3	10	123	-123	2	5	10	121	123
-6	6	9	91	-87	-7	0	10	337	345	-11	2	10	147	148	4	3	10	265	269	3	5	10	52	53
-5	6	9	109	107	-6	0	10	291	-296	-10	2	10	181	183	5	3	10	187	181	4	5	10	192	-188
-4	6	9	134	136	-5	0	10	479	-467	-9	2	10	73	74	6	3	10	30	-29	5	5	10	117	-110
-3	6	9	50	-52	-4	0	10	30	29	-8	2	10	390	-399	7	3	10	224	-212	6	5	10	31	29
-2	6	9	144	-148	-3	0	10	520	476	-7	2	10	178	-180	8	3	10	75	-68	-9	6	10	34	34
-1	6	9	20	-7	-2	0	10	147	135	-6	2	10	170	173	-10	4	10	156	-154	-8	6	10	202	-192
0	6	9	73	72	-1	0	10	177	-174	-5	2	10	609	608	-9	4	10	20	22	-7	6	10	76	-74
1	6	9	24	26	0	0	10	426	-416	-4	2	10	117	-114	-8	4	10	258	256	-6	6	10	21	9
2	6	9	42	-42	1	0	10	98	94	-3	2	10	170	-157	-7	4	10	244	243	-5	6	10	263	264
3	6	9	21	17	2	0	10	205	209	-2	2	10	242	-233	-6	4	10	153	-152	-4	6	10	44	-39
4	6	9	70	69	3	0	10	283	291	-1	2	10	438	434	-5	4	10	284	-282	-3	6	10	43	-30
6	6	9	69	-62	4	0	10	103	-105	0	2	10	268	272	-3	4	10	298	290	-2	6	10	149	-151
-7	7	9	100	-97	5	0	10	43	47	1	2	10	189	193	-2	4	10	105	107	-1	6	10	140	143
-6	7	9	93	-92	7	0	10	108	105	2	2	10	259	-265	-1	4	10	87	-80	0	6	10	105	108
-5	7	9	82	80	-11	1	10	17	-12	3	2	10	70	-70	0	4	10	281	-281	1	6	10	172	172
-4	7	9	222	220	-10	1	10	67	67	4	2	10	25	28	2	4	10	110	109	2	6	10	110	-111
-2	7	9	201	-204	-9	1	10	40	-39	5	2	10	109	105	3	4	10	227	225	3	6	10	78	-71
-1	7	9	161	-165	-8	1	10	32	31	6	2	10	41	-39	4	4	10	62	-63	4	6	10	35	-28
0	7	9	121	122	-7	1	10	78	76	7	2	10	25	4	5	4	10	25	21	5	6	10	83	79
1	7	9	217	219	-6	1	10	49	-49	8	2	10	34	-30	6	4	10	38	-39	-7	7	10	30	28
2	7	9	32	-34	-5	1	10	92	-84	-11	3	10	31	20	7	4	10	78	69	-6	7	10	76	77
3	7	9	213	-208	-4	1	10	70	65	-10	3	10	70	-67	7	5	10	64	59	-5	7	10	31	-30
4	7	9	102	-96	-3	1	10	395	375	-8	3	10	42	-38	-9	5	10	34	34	-4	7	10	111	-111
-5	8	9	64	-67	-2	1	10	137	131	-7	3	10	54	-51	-8	5	10	46	43	-4	7	10	120	-120
-4	8	9	115	-117	-1	1	10	237	-226	-6	3	10	62	59	-7	5	10	19	-10	-2	7	10	82	80
-3	8	9	28	26	0	1	10	385	-387	-5	3	10	47	44	-6	5	10	74	-70	-1	7	10	89	92
-2	8	9	114	114	1	1	10	81	78	-4	3	10	79	-77	-5	5	10	27	-23	0	7	10	105	107
-1	8	9	39	41	2	1	10	279	281	-3	3	10	311	-299	-4	5	10	103	103	1	7	10	72	-69
0	8	9	34	-36	3	1	10	171	175	-2	3	10	53	-48	-3	5	10	184	179	2	7	10	41	-39
1	8	9	19	-22	4	1	10	302	-306	-1	3	10	196	187	-2	5	10	27	-24	4	7	10	129	129

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITTE CRYSTAL STRUCTURE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-5	8	10	70	-68	6	2	11	32	34	5	4	11	32	-37	-5	7	11	49	-49	-8	1	12	106	-109
-4	8	10	45	-44	8	2	11	37	-34	6	4	11	67	-64	-4	7	11	65	-63	-7	1	12	358	-357
-3	8	10	54	55	-11	3	11	91	88	-9	5	11	115	111	-3	7	11	22	23	-6	1	12	19	11
-2	8	10	45	42	-9	3	11	75	-73	-8	5	11	28	25	-2	7	11	15	9	-5	1	12	311	300
-1	8	10	43	41	-8	3	11	31	-32	-7	5	11	101	-100	-1	7	11	62	-62	-4	1	12	136	131
0	8	10	99	-105	-7	3	11	104	104	-6	5	11	63	-63	0	7	11	30	-24	-3	1	12	300	-292
1	8	10	66	-65	-6	3	11	20	20	-5	5	11	94	93	1	7	11	92	94	-2	1	12	275	-269
-11	1	11	23	-23	-5	3	11	82	-84	-4	5	11	57	57	2	7	11	67	66	-1	1	12	72	-73
-10	1	11	18	-6	-4	3	11	83	-82	-3	5	11	33	-34	3	7	11	65	-62	0	1	12	109	110
-9	1	11	37	40	-3	3	11	36	33	-2	5	11	38	-41	-4	8	11	200	-195	1	1	12	85	84
-7	1	11	33	-31	-2	3	11	22	13	0	5	11	85	89	-3	8	11	114	-115	2	1	12	51	-45
-6	1	11	30	-31	-1	3	11	97	-98	0	5	11	53	55	-2	8	11	156	159	3	1	12	54	52
-5	1	11	45	45	0	3	11	82	-86	1	5	11	101	-100	-1	8	11	178	181	5	1	12	23	7
-2	1	11	30	-30	1	3	11	59	61	2	5	11	83	-83	0	8	11	39	-39	6	1	12	111	113
-1	1	11	34	36	2	3	11	66	68	3	5	11	48	48	1	8	11	193	-195	7	1	12	104	108
1	1	11	35	-38	2	3	11	54	-57	4	5	11	109	105	-10	0	12	65	-68	-10	2	12	104	108
4	1	11	23	40	4	3	11	81	-81	5	5	11	21	-19	-9	0	12	73	-74	-9	2	12	53	48
6	1	11	26	-23	6	3	11	102	96	6	5	11	113	-104	-8	0	12	137	138	-8	2	12	76	-75
8	1	11	30	30	7	3	11	26	22	8	6	11	139	133	-7	0	12	151	151	-7	2	12	140	-136
-11	2	11	47	-48	-10	4	11	55	51	-7	6	11	103	-102	-5	0	12	399	-379	-6	2	12	87	84
-10	2	11	25	-19	-9	4	11	113	-114	-6	6	11	211	-208	-4	0	12	130	-121	-5	2	12	339	332
-9	2	11	76	77	-8	4	11	107	-110	-5	6	11	22	-14	-3	0	12	218	196	-4	2	12	198	186
-8	2	11	90	90	-7	4	11	91	90	-4	6	11	278	277	-2	0	12	653	619	-3	2	12	209	-196
-7	2	11	45	-43	-6	4	11	220	217	-3	6	11	156	159	-1	0	12	120	-108	-2	2	12	462	-454
-6	2	11	112	-113	-5	4	11	27	22	-2	6	11	170	-170	0	0	12	381	-372	-1	2	12	77	75
-5	2	11	15	-4	-4	4	11	255	-252	-1	6	11	199	-201	1	0	12	409	-417	0	2	12	400	401
-4	2	11	194	190	-4	4	11	151	-152	0	6	11	70	69	1	0	12	182	-183	1	2	12	109	111
-3	2	11	116	114	-2	4	11	192	190	1	6	11	240	241	2	0	12	258	262	2	2	12	305	-311
-2	2	11	111	-110	-1	4	11	204	204	2	6	11	73	72	4	0	12	19	-8	3	2	12	284	-285
-1	2	11	120	-123	0	4	11	55	-57	3	6	11	147	-140	5	0	12	342	-346	4	2	12	53	53
0	2	11	26	47	1	4	11	216	-219	4	6	11	116	-109	6	0	12	97	-96	5	2	12	270	264
1	2	11	141	144	2	4	11	50	-50	5	6	11	47	42	7	0	12	125	118	6	2	12	130	125
3	2	11	84	-99	3	4	11	154	153	7	7	11	90	87	7	0	12	302	310	7	2	12	150	-144
4	2	11	62	-65	4	4	11	106	102	-6	7	11	48	48	-10	1	12	176	181	-10	3	12	251	-249

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITE CRYSTAL STRUCTURE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-9	3	12	149	-147	-7	5	12	203	-199	-4	8	12	43	41	-2	3	13	74	78	-7	6	13	49	46
-8	3	12	76	76	-6	5	12	29	-20	-3	8	12	35	38	-1	3	13	168	172	-5	6	13	69	-68
-7	3	12	308	307	-5	5	12	147	146	-2	8	12	92	96	1	3	13	94	-99	-4	6	13	45	41
-5	3	12	218	-214	-4	5	12	130	128	-1	8	12	80	-83	2	3	13	50	-52	-3	6	13	126	130
-4	3	12	130	-130	-3	5	12	75	-73	0	8	12	24	-18	4	3	13	52	48	-1	6	13	142	-142
-3	3	12	227	222	-2	5	12	144	-143	-10	1	13	45	-43	6	3	13	37	-34	0	6	13	92	-92
-2	3	12	224	220	-1	5	12	67	-68	-9	1	13	22	22	-10	4	13	40	34	0	6	13	99	98
-1	3	12	96	100	0	5	12	56	57	-8	1	13	43	43	-9	4	13	61	62	2	6	13	132	128
0	3	12	81	-80	1	5	12	138	139	-7	1	13	30	-28	-7	4	13	46	-46	3	6	13	48	-47
1	3	12	84	-79	2	5	12	46	40	-6	1	13	96	-97	-6	4	13	19	15	4	6	13	153	-144
2	3	12	21	15	3	5	12	35	28	-5	1	13	53	-52	-5	4	13	91	94	-7	7	13	21	14
3	3	12	24	-15	4	5	12	51	-50	-3	1	13	15	25	-4	4	13	25	-23	-6	7	13	198	194
4	3	12	41	40	5	5	12	33	28	-2	1	13	59	-65	-3	4	13	132	-132	-5	7	13	82	83
5	3	12	21	6	6	6	12	67	-65	-1	1	13	100	-101	-1	4	13	132	125	-4	7	13	155	-154
7	3	12	94	-90	-7	6	12	17	-7	-10	2	13	23	-24	0	4	13	88	91	-3	7	13	178	-182
-10	4	12	67	-64	-6	6	12	112	111	-9	2	13	38	-41	1	4	13	95	-96	-2	7	13	62	61
-9	4	12	37	-32	-5	6	12	157	157	-7	2	13	30	32	2	4	13	136	-135	-1	7	13	185	187
-8	4	12	117	114	-4	6	12	46	46	-5	2	13	68	-70	3	4	13	25	25	0	7	13	108	-106
-7	4	12	55	51	-3	6	12	100	-105	-3	2	13	89	87	4	4	13	130	125	1	7	13	108	-106
-6	4	12	48	-47	-2	6	12	159	-165	-1	2	13	83	-82	6	4	13	94	-86	2	7	13	84	-81
-5	4	12	283	-276	-1	6	12	67	65	0	2	13	55	-60	-9	5	13	111	110	-3	8	13	98	-98
-4	4	12	52	-54	0	6	12	138	142	1	2	13	52	59	6	5	13	192	193	-2	8	13	23	14
-3	4	12	129	124	2	6	12	147	-147	2	2	13	84	90	-7	5	13	37	-35	-1	8	13	119	121
-2	4	12	380	378	3	6	12	123	124	4	2	13	73	-74	-6	5	13	236	-232	-10	0	14	71	71
-1	4	12	112	-109	-7	7	12	138	137	6	2	13	57	54	-5	5	13	105	-104	-9	0	14	223	228
0	4	12	201	-202	-6	7	12	43	43	7	2	13	49	51	-4	5	13	105	104	-8	0	14	112	-113
1	4	12	104	-103	-5	7	12	31	-29	-10	3	13	59	60	-4	5	13	150	148	-8	0	14	163	-161
2	4	12	294	295	-4	7	12	94	-97	-9	3	13	103	-103	-2	5	13	105	-102	-6	0	14	109	-106
3	4	12	169	168	-3	7	12	40	34	-8	3	13	177	-178	-3	5	13	163	165	-7	0	14	124	115
4	4	12	22	19	-2	7	12	97	101	-7	3	13	18	11	0	5	13	42	-43	-5	0	14	139	136
5	4	12	231	-224	-1	7	12	124	126	-6	3	13	164	163	1	5	13	101	101	-2	0	14	22	-20
6	4	12	73	-67	1	7	12	93	-92	-5	3	13	61	60	2	5	13	70	69	-1	0	14	30	15
-9	5	12	118	117	2	7	12	54	-49	-4	3	13	145	-142	3	5	13	53	-52	0	0	14	60	-55
-8	5	12	31	-24	3	7	12	44	34	-3	3	13	153	-151	4	5	13	62	-60	1	0	14	176	-181

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITE CRYSTAL STRUCTURE

OBSERVED				CALCULATED				TORNEBOHMITE CRYSTAL STRUCTURE				PAGE 12												
H	K	L	FO	H	K	L	FO	H	K	L	FO	H	K	L	FO	H	K	L	FO	FC				
2	0	14	28	24	1	2	14	138	138	1	4	14	102	-105	-3	7	14	58	62	-1	3	15	93	95
3	0	14	119	120	2	2	14	91	-94	2	4	14	44	40	-2	7	14	88	94	0	3	15	105	112
5	0	14	220	-222	3	2	14	121	-121	3	4	14	63	62	-1	7	14	69	70	1	3	15	28	-36
6	0	14	98	-97	4	2	14	52	-46	4	4	14	44	-41	0	7	14	105	-109	2	3	15	156	-153
7	0	14	59	55	5	2	14	201	194	5	4	14	185	-177	1	7	14	75	-77	4	3	15	102	99
-10	1	14	140	142	6	2	14	46	39	-9	5	14	87	84	-10	1	15	32	-34	5	3	15	83	80
-9	1	14	175	181	-10	3	14	126	-128	-8	5	14	61	-63	1	15	14	14	6	6	3	15	29	-33
-8	1	14	48	-50	-9	3	14	131	-134	-7	5	14	218	-215	-7	1	15	24	29	-10	4	15	144	-142
-7	1	14	387	-385	-8	3	14	63	62	-6	5	14	66	-65	-6	1	15	32	-32	-9	4	15	19	14
-6	1	14	201	-188	-7	3	14	332	330	-5	5	14	120	116	-5	1	15	41	-41	-8	4	15	136	134
-5	1	14	252	245	-6	3	14	148	145	-4	5	14	240	240	-3	1	15	65	64	-7	4	15	39	38
-4	1	14	512	499	-5	3	14	175	-172	-3	5	14	65	-67	-2	1	15	28	36	-6	4	15	167	-167
-3	1	14	108	-103	-4	3	14	384	-376	-2	5	14	186	-190	2	1	15	55	59	-5	4	15	125	-124
-2	1	14	397	-389	-3	3	14	113	110	-1	5	14	96	-93	4	1	15	25	-37	-4	4	15	59	62
-1	1	14	165	-166	-2	3	14	320	320	0	5	14	233	235	-10	2	15	76	78	-3	4	15	134	131
0	1	14	462	469	-1	3	14	155	156	3	5	14	179	180	-9	2	15	23	-11	-2	4	15	17	15
1	1	14	312	345	0	3	14	351	-358	1	5	14	148	-145	-8	2	15	91	-91	0	4	15	99	-102
2	1	14	66	-67	1	3	14	262	-262	4	5	14	65	-64	-7	2	15	26	-25	1	4	15	37	-34
3	1	14	277	-279	2	3	14	39	48	5	5	14	65	64	-6	2	15	92	96	0	4	15	57	62
4	1	14	75	-72	3	3	14	238	234	5	6	14	48	-43	-5	2	15	69	68	2	4	15	22	28
5	1	14	139	134	4	3	14	76	75	-7	6	14	35	34	-4	2	15	53	-56	3	4	15	29	-33
6	1	14	95	89	5	3	14	105	-101	-6	6	14	65	64	-3	2	15	92	-92	4	4	15	18	-16
7	1	14	52	-50	5	3	14	87	-79	-5	6	14	19	8	-1	2	15	45	54	5	4	15	28	22
-10	2	14	88	-39	-10	4	14	31	28	-4	6	14	128	-133	1	2	15	37	-57	-9	5	15	41	-39
-9	2	14	190	-194	-9	4	14	177	175	-3	6	14	115	-116	2	2	15	23	-26	-8	5	15	64	62
-8	2	14	48	47	-8	4	14	30	-33	-2	6	14	43	-40	5	2	15	22	-22	-7	5	15	75	76
-7	2	14	155	152	-7	4	14	80	-76	-1	6	14	90	89	-10	3	15	23	25	-6	5	15	88	-86
-6	2	14	54	52	-6	4	14	100	-101	0	6	14	29	28	-9	3	15	40	41	-5	5	15	141	-142
-5	2	14	96	-93	-5	4	14	61	56	1	6	14	43	43	-8	3	15	76	-75	-4	5	15	16	-11
-4	2	14	194	-192	-4	4	14	117	116	2	6	14	89	-92	-7	3	15	66	-69	-3	5	15	186	184
-3	2	14	50	-50	-3	4	14	87	89	3	6	14	34	-30	-6	3	15	35	37	-2	5	15	97	101
-2	2	14	62	-52	-2	4	14	16	-7	-6	7	14	16	11	-5	3	15	111	110	-1	5	15	125	-125
-1	2	14	15	-13	-1	4	14	51	-51	-5	7	14	26	-32	-3	3	15	158	-156	0	5	15	147	-148
0	2	14	19	-8	0	4	14	67	-70	-4	7	14	101	-104	-2	3	15	99	-104	1	5	15	54	53

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITE CRYSTAL STRUCTURE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC					
2	5	15	196	192	3	0	16	199	-202	5	2	16	60	-54	-3	5	16	62	-62	-1	2	17	48	55
3	5	15	55	61	4	0	16	67	-63	6	2	16	74	-65	-2	5	16	61	-66	0	2	17	125	129
4	5	15	134	-125	5	0	16	19	-3	-9	3	16	59	58	-1	5	16	89	-92	2	2	17	57	-72
-8	6	15	179	-175	6	0	16	93	88	-8	3	16	28	25	0	5	16	107	110	3	2	17	40	-38
-7	6	15	68	-66	-9	1	16	78	-81	-7	3	16	22	-16	1	5	16	68	60	4	2	17	32	43
-6	6	15	137	138	-8	1	16	23	-5	-6	3	16	16	-5	5	16	194	-189	5	2	17	50	51	
-4	6	15	117	118	-7	1	16	40	29	-5	3	16	99	-100	4	5	16	75	-68	5	3	17	21	-17
-5	6	15	81	-79	-6	1	16	30	-24	-4	3	16	165	-160	-7	6	16	46	44	-8	3	17	125	126
-3	6	15	157	-158	-5	1	16	67	63	-2	3	16	99	96	-6	6	16	184	188	-7	3	17	53	56
-2	6	15	44	-46	-4	1	16	196	190	-1	3	16	152	152	-5	6	16	98	-98	-5	3	17	78	-78
-1	6	15	81	84	-3	1	16	18	-10	0	3	16	110	-110	-4	6	16	97	-95	-4	3	17	71	75
0	6	15	33	36	-2	1	16	121	-116	1	3	16	147	-149	-3	6	16	104	-106	-3	3	17	65	68
1	6	15	60	-59	-1	1	16	231	-231	3	3	16	233	228	-2	6	16	137	142	-1	3	17	19	-24
2	6	15	34	-31	0	1	16	106	106	4	3	16	112	106	-1	6	16	90	92	0	3	17	32	37
3	6	15	20	17	1	1	16	173	174	5	3	16	73	-68	0	6	16	71	72	1	3	17	62	66
-6	7	15	81	84	2	1	16	33	27	-9	4	16	230	225	1	6	16	136	-141	3	3	17	36	-37
-5	7	15	137	138	3	1	16	282	-280	-8	4	16	123	123	5	7	16	75	-70	5	3	17	72	69
-3	7	15	161	-161	4	1	16	138	-137	-7	4	16	190	-189	-2	7	16	134	-135	-9	4	17	73	-73
-2	7	15	79	-79	5	1	16	71	68	-6	4	16	244	-238	-4	7	16	64	-66	-8	4	17	81	80
-1	7	15	130	131	6	1	16	195	185	-5	4	16	58	55	-3	7	16	63	64	-7	4	17	164	165
0	7	15	141	140	-9	2	16	388	-395	-4	4	16	266	266	-2	7	16	51	50	-5	4	17	190	-186
1	7	15	48	-49	-8	2	16	124	-125	-3	4	16	31	28	0	7	16	92	-95	-4	4	17	77	-80
-9	0	16	350	357	-7	2	16	151	150	-2	4	16	203	-202	-7	1	17	37	-36	-3	4	17	140	143
-8	0	16	194	198	-6	2	16	388	380	-1	4	16	246	-252	-6	1	17	56	57	-2	4	17	147	154
-7	0	16	280	-279	-5	2	16	220	-217	1	4	16	126	125	-5	1	17	22	25	-1	4	17	84	-87
-6	0	16	368	-353	-4	2	16	324	-318	2	4	16	105	104	-2	1	17	31	34	0	4	17	211	-208
-5	0	16	114	104	-3	2	16	163	-163	3	4	16	118	-119	5	1	17	20	-6	2	4	17	118	116
-4	0	16	457	429	-2	2	16	365	366	4	4	16	52	-46	-9	2	17	38	36	3	4	17	76	73
-3	0	16	29	20	-1	2	16	194	195	-9	5	16	38	-36	-8	2	17	58	-57	4	4	17	70	-70
-2	0	16	358	-353	0	2	16	26	33	-8	5	16	39	-42	-7	2	17	115	-115	-9	5	17	19	4
-1	0	16	364	-360	1	2	16	272	-275	-7	5	16	28	-24	-5	2	17	105	107	-8	5	17	89	-87
0	0	16	31	23	2	2	16	48	-55	-6	5	16	47	46	-4	2	17	35	44	-7	5	17	95	-92
1	0	16	177	178	3	2	16	94	91	-5	5	16	109	110	-3	2	17	90	-92	-6	5	17	90	88
2	0	16	85	87	4	2	16	90	85	-4	5	16	124	122	-2	2	17	94	-101	-5	5	17	98	97

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITTE CRYSTAL STRUCTURE

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-1	5	17	22	-14	-7	1	18	157	150	-1	3	18	119	-121	-2	6	18	74	79	0	4	19	61	-61
-3	5	17	59	-60	-6	1	18	317	309	0	3	18	79	-77	-1	6	18	134	137	1	4	19	56	-57
-2	5	17	35	41	-5	1	18	105	105	1	3	18	64	61	0	6	18	41	-45	2	4	19	57	52
-1	5	17	42	44	-4	1	18	269	-268	2	3	18	47	49	1	6	18	110	-107	3	4	19	108	106
1	5	17	43	-44	-3	1	18	225	-227	4	3	18	72	-65	-5	1	19	92	95	-8	5	19	38	-39
2	5	17	21	23	-2	1	18	29	24	-9	4	18	108	109	-4	1	19	43	49	-7	5	19	153	-155
3	5	17	74	69	-1	1	18	143	146	-8	4	18	32	-34	-2	1	19	40	44	-6	5	19	54	-55
-7	6	17	190	-184	0	1	18	57	57	-7	4	18	45	-44	0	1	19	31	49	-5	5	19	213	211
-5	6	17	186	186	1	1	18	94	-94	-6	4	18	210	-208	3	1	19	24	49	-4	5	19	142	145
-4	6	17	66	68	2	1	18	63	-59	-5	4	18	36	30	-8	2	19	54	53	-3	5	19	81	-80
-3	6	17	167	-169	4	1	18	64	58	-4	4	18	61	63	-6	2	19	20	-27	-2	5	19	171	-174
-2	6	17	171	-177	5	1	18	19	12	-3	4	18	216	219	-4	2	19	46	47	0	5	19	138	135
-1	6	17	78	81	-9	2	18	45	-41	-2	4	18	197	-200	-2	2	19	51	-54	1	5	19	62	58
0	6	17	203	206	-8	2	18	73	-71	-1	4	18	106	-107	-1	2	19	37	-41	2	5	19	60	-60
1	6	17	39	37	-7	2	18	129	130	0	4	18	57	-60	0	2	19	37	40	-6	6	19	26	-22
2	6	17	147	-138	-6	2	18	171	165	1	4	18	286	285	1	2	19	36	39	-5	6	19	21	12
-3	7	17	35	35	-5	2	18	127	129	2	4	18	77	73	3	2	19	61	-61	-4	6	19	74	75
-2	7	17	20	-9	-4	2	18	220	-216	3	4	18	20	4	-7	3	19	162	163	-3	6	19	25	25
-1	7	17	19	-19	-3	2	18	177	-175	-8	5	18	182	-181	-6	3	19	25	32	-2	6	19	74	-77
-9	0	18	106	109	-2	2	18	106	105	-7	5	18	44	43	-5	3	19	129	-132	-1	6	19	38	-36
-7	0	18	37	-32	-1	2	18	286	290	-6	5	18	145	146	-4	3	19	116	-120	0	6	19	90	91
-6	0	18	311	-301	0	2	18	29	-25	-5	5	18	75	73	-3	3	19	88	95	-8	0	20	180	-179
-5	0	18	32	-27	1	2	18	248	-248	-4	5	18	152	-152	-2	3	19	135	136	-7	0	20	95	-95
-4	0	18	115	104	2	2	18	211	-212	-3	5	18	164	-166	0	3	19	90	-98	-6	0	20	235	227
-3	0	18	359	350	3	2	18	101	102	-2	5	18	59	-60	1	3	19	64	-38	-5	0	20	134	131
-2	0	18	242	-238	4	2	18	173	166	-1	5	18	59	57	2	3	19	64	67	-4	0	20	51	48
-1	0	18	175	-172	5	2	18	75	70	0	5	18	67	68	3	3	19	52	45	-3	0	20	101	-100
0	0	18	92	-91	-9	3	18	117	118	1	5	18	46	-42	-8	4	19	66	-63	-2	0	20	26	30
1	0	18	402	407	-8	3	18	243	243	2	5	18	70	-67	-7	4	19	23	-18	-1	0	20	49	48
2	0	18	150	151	-7	3	18	113	-112	-7	6	18	114	120	-6	4	19	47	50	2	0	20	72	74
3	0	18	19	-1	-6	3	18	250	-249	-6	6	18	60	61	-4	4	19	57	-60	3	0	20	43	-41
-4	0	18	245	-243	-5	3	18	97	-101	-5	6	18	18	13	-3	4	19	24	-24	4	0	20	108	-107
-9	1	18	157	-157	-4	3	18	215	213	-4	6	18	111	-113	-2	4	19	94	95	-8	1	20	290	-287
-8	1	18	290	-289	-3	3	18	191	193	-3	6	18	32	-34	-1	4	19	61	62	-7	1	20	63	-61

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TORNEBOHMITE CRYSTAL STRUCTURE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-6	1	20	156	154	-7	4	20	100	-101	-1	2	21	25	25	1	0	22	21	16
-5	1	20	252	248	-6	4	20	136	135	1	2	21	22	-18	2	0	22	172	169
-4	1	20	172	-172	-5	4	20	117	116	3	2	21	32	24	-7	1	22	67	61
-3	1	20	331	-335	-4	4	20	86	89	-7	3	21	35	34	-6	1	22	41	38
-2	1	20	78	-76	-3	4	20	63	-67	-6	3	21	91	95	-5	1	22	60	56
-1	1	20	356	370	-1	4	20	29	26	-4	3	21	84	-81	-4	1	22	21	11
0	1	20	205	206	0	4	20	42	43	-3	3	21	25	-31	-3	1	22	23	-16
1	1	20	92	-92	1	4	20	47	44	-2	3	21	76	78	-2	1	22	58	-55
2	1	20	230	-226	2	4	20	18	14	-1	3	21	66	70	-1	1	22	109	108
3	1	20	22	1	-7	5	20	86	86	0	3	21	43	-49	0	1	22	93	92
4	1	20	173	165	-6	5	20	138	138	1	3	21	114	-114	2	1	22	206	205
-8	2	20	220	220	-5	5	20	116	-115	-7	4	21	124	-126	-7	2	22	242	243
-7	2	20	55	61	-4	5	20	149	-154	-6	4	21	83	-85	-6	2	22	211	-211
-6	2	20	125	-124	-3	5	20	29	-34	-5	4	21	83	86	-5	2	22	270	-268
-5	2	20	170	-170	-2	5	20	213	218	-4	4	21	137	137	-4	2	22	40	-44
-1	2	20	36	32	0	5	20	105	106	-2	4	21	90	-93	-3	2	22	300	303
-3	2	20	47	46	1	5	20	32	-34	-1	4	21	29	-28	-2	2	22	173	177
-2	2	20	79	81	1	5	20	127	-128	0	4	21	48	53	-1	2	22	70	-69
-1	2	20	82	-84	-5	6	20	51	-49	1	4	21	47	44	0	2	22	201	-200
0	2	20	81	82	-4	6	20	23	11	-7	5	21	54	-54	2	2	22	155	148
1	2	20	58	-57	-3	6	20	94	96	-6	5	21	105	-108	-7	3	22	55	-58
2	2	20	28	22	-2	6	20	19	-21	-4	5	21	101	102	-6	3	22	42	-43
-8	3	20	224	224	-7	1	21	37	-40	-3	5	21	21	17	-5	3	22	43	-38
-7	3	20	35	32	-6	1	21	21	-12	-2	5	21	109	-108	-4	3	22	30	28
-6	3	20	142	-140	-5	1	21	27	26	-1	5	21	103	-106	-3	3	22	23	22
-5	3	20	205	-201	-4	1	21	29	-36	0	5	21	56	56	-2	3	22	32	38
-4	3	20	138	138	-2	1	21	27	31	-7	0	22	247	-245	-1	3	22	97	-100
-3	3	20	252	266	1	1	21	29	-31	-6	0	22	232	226	0	3	22	65	-60
-2	3	20	42	47	3	1	21	86	90	-5	0	22	339	329	1	3	22	17	21
-1	3	20	297	-303	-7	2	21	55	59	-4	0	22	49	44	-7	4	22	158	-158
0	3	20	178	-175	-6	2	21	23	-40	-3	0	22	301	-302	-6	4	22	152	154
1	3	20	71	75	-5	2	21	73	-73	-2	0	22	195	-194	-5	4	22	208	210
2	3	20	190	184	-4	2	21	67	70	-1	0	22	115	115	-4	4	22	22	28
-8	4	20	118	-118	-2	2	21	70	70	0	0	22	215	215	-3	4	22	208	-210

M/S	TYPE OF	NUMBER	UNIT	RATE OF	CHARGE
CODE	CHARGE	OF UNITS		CHARGE	
0054	JOB FEE	1	JOB	0.1284	= 0.13
0575	STEP FEE	1	STEP	0.0642	= 0.06
0075	I/O OPER	108	OPER	0.0001	= 0.01
0557	CPU TIME	0.0018	HR	660.0000	= 1.19
0563	CORE MEM	0.4994	PGHR	0.2500	= 0.12
1091	PAGES OUT	55	PAGE	0.0104	= 0.57
0258	LINES	2395	LINE	0.0003	= 0.72
2WD218.TQ				TOTAL =	\$2.80

JOB: TORNEB (5569) ON: TERM.RDR - 08-15-81/01:39:50
 FC: SHEN OFF: PRINTER3 - 08-15-81/02:38:06
 RUNS REMAINING = N/A ACCUMULATED = \$1,677.41