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Crystal structure of ilmenite ($FeTiO_3$) at high temperature and at high pressure

Barry A. Wechsler[1] and Charles T. Prewitt

Department of Earth and Space Sciences
State University of New York
Stony Brook, New York 11794

Abstract

The structures of two single crystals of synthetic ilmenite were refined using X-ray intensity data collected at 24, 400, 600, 800, and 1050°C (1 atm) and 0.001, 25.4, 34.6, and 46.1 kbar (room temperature). Thermal expansion of the unit cell was nearly isotropic, whereas compression was relatively anisotropic, with c/a decreasing linearly with increasing pressure. The isothermal bulk modulus and its pressure derivative determined from cell volume data are K_0 = 1.70(7) Mbar, K_0' = 8(4), or K_0 = 1.77(3) if K_0' is assumed to be 4(1). Mean Fe–O and Ti–O distances increased linearly with temperature and decreased linearly with pressure, ⟨Fe–O⟩ being about twice as expandable and compressible as ⟨Ti–O⟩. The responses of the two octahedral sites to temperature and pressure were quite different from one another, however. The longer of the two independent Fe–O bonds was more expandable and less compressible than the shorter one, whereas the opposite was true for the Ti site. The Ti atom was displaced toward the centroid of its coordination polyhedron at high temperature, but the Fe atom moved further away from its centroid position. Cation shifts were much smaller with pressure than with temperature. These results indicate that the reponses of the ilmenite structure to temperature and pressure are not inverse in character. The cation sites remained fully ordered at all temperatures and pressures studied.

Introduction

Ilmenite ($FeTiO_3$) occurs as an accessory mineral in a wide variety of igneous and metamorphic rocks (Haggerty, 1976; El Goresy, 1976a,b; Rumble, 1976). One of its most valuable characteristics for petrogenetic studies has been the use of compositions of coexisting hematite–ilmenite and magnetite–ulvöspinel solid solutions as an indicator of temperature and oxygen fugacity at the time of last equilibration (Lindsley, 1963; Buddington and Lindsley, 1964). More recently, other geothermometers have been based upon coexisting ilmenite and olivine or pyroxene (Andersen and Lindsley, 1979; Bishop, 1980) and have utilized solution models to extend the experimental calibrations. The ilmenite structure may also be an important one for metasilicates undergoing high-pressure transformations in the Earth's mantle (*e.g.*, Ringwood, 1969; Liu, 1977a). In order to improve thermochemical models, understand crystal-chemical partitioning behavior, and characterize the pressure–temperature systematics of compounds with the ilmenite structure, it would be useful to determine the effects of elevated temperature and pressure upon the crystal structure of ilmenite.

The ilmenite structure was determined by Barth and Posnjak (1934). Shirane *et al.* (1959) determined the magnetic structure at low temperature using neutron diffraction, and the structure of lunar ilmenite was studied by Raymond and Wenk (1971). Numerous other investigations have elucidated the magnetic properties of ilmenites and hematite–ilmenite solutions (*e.g.*, Ishikawa, 1958, 1962; Shirane and Ruby, 1962; Shirane *et al.*, 1962; Thorpe *et al.*, 1977) and have suggested the possibility of an order–disorder transformation at high temperatures as is observed for intermediate compositions. Burton (1980) studied such a transformation in an intermediate hematite–ilmenite by single-crystal X-ray diffraction.

Recently, high-pressure structure refinements have been reported for several materials with the closely related corundum structure (Finger and Hazen, 1980). Compression of ilmenite has also previously been studied by X-ray diffraction (Liu *et al.*, 1974) and Mössbauer spectroscopy (Vaughan and Drickamer, 1967) on polycrystalline specimens. A number of other studies have considered the elasticity, crystal-chemical systematics, and high-pressure phase transformations in other compounds possessing the ilmenite structure (Liebermann,

[1] Present address: Hughes Research Laboratories, 3011 Malibu Canyon Road, Malibu, California 90265.

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Ilmenite at 24°C.

L	OBS	CALC
-8 4 L		
0	6000	6009
-7 1 L		
4	6496	6572
-7 2 L		
0	7165	7156
6	5421	5417
-7 3 L		
2	3747	3770
-7 4 L		
1	513	362
-7 5 L		
0	6832	6805
6	5671	5725
-7 6 L		
5	653	558
-7 7 L		
1	433*	100
-6 -1 L		
1	447*	286
4	4401	4372
-6 0 L		
3	576	522
-6 1 L		
2	1356	1321
-6 2 L		
13	562	126
-6 3 L		
15	1129	1115
-6 5 L		
1	1372	1444
13	548	622
-6 7 L		
2	1379	1388
5	1068	994
-5 -3 L		
1	1795	1677
-5 -2 L		
3	1308	1267
-5 -1 L		
2	1969	1994
-5 1 L		
3	2806	2897
6	7574	7625
12	644	587
15	833	832
-5 2 L		
2	1791	1821
8	3875	3902
14	8198	8264
-5 4 L		
12	552	352
-5 5 L		
8	3292	3219
-5 6 L		
10	5985	5920
13	766	747
-4 -4 L		
3	559	422
-4 -3 L		
11	652	793
-4 -2 L		
1	1335	1308
4	8803	8666
-4 -1 L		
3	1222	1162
6	8096	8089
15	1415	1495
-4 0 L		
2	4705	4660
17	411	313
-4 1 L		
1	843	821
10	9042	9160
-4 2 L		
0	11524	11502
3	2010	1964
6	10367	10578
12	2195	2187
-4 4 L		
10	9787	9888
-4 5 L		
12	1723	1714
-4 6 L		
8	5111	4997
-3 -4 L		
4	4827	4814
10	7888	7815
-3 -3 L		
6	4424	4412
-3 -2 L		
2	1742	1703
5	403	265
11	1036	1092
17	547	245
-3 -1 L		
13	466	288
16	2562	2485
-3 0 L		
3	1162	1146
6	5431	5462
12	2332	2293
-3 1 L		
8	6121	6206
11	2474	2518
-3 3 L		
12	2281	2263
15	2007	2003
18	6935	6870
-3 4 L		
8	5896	5933
-3 5 L		
4	9998	9854
10	8258	8210
13	1374	1387
16	3293	3258
-3 6 L		
12	966	1056
-3 7 L		
2	2301	2300
5	631	281
-2 -5 L		
6	5038	4981
9	1294	1300
-2 -3 L		
7	846	860
-2 -2 L		
3	4972	4914
9	2971	2993
18	5224	5230
-2 -1 L		
5	2133	2125
-2 0 L		
4	14852	15221
13	1202	1127
-2 2 L		
8	6506	6531
17	700	613
-2 3 L		
4	14331	14234
7	2670	2761
10	10108	10083
-2 4 L		
12	671	574
15	1281	1237
-2 5 L		
8	4128	4082
-2 6 L		
10	6248	6136
13	1025	1106
-1 -5 L		
4	8287	8209
7	1462	1434
-1 -4 L		
6	8367	8317
9	1013	1034
-1 -3 L		
2	3399	3340
5	964	1058
-1 -2 L		
1	609	537
-1 0 L		
5	339	434
-1 1 L		
1	870	848
10	13666	13476
13	331*	130
19	508	530
-1 2 L		
3	5262	5057
15	2709	2659
21	471*	291
-1 3 L		
8	7047	7088
17	1015	952
-1 4 L		
4	8983	8864
10	11005	11029
19	570	258
-1 5 L		
12	1609	1546
0 -6 L		
9	521	390
0 -5 L		
5	1580	1512
11	559	214
0 -4 L		
4	8733	8667
7	1816	1834
13	556	663
0 -2 L		
2	3276	3355
14	10263	10313
20	5336	5374
0 -1 L		
7	2894	2794
16	4240	4217
22	1918	1903
0 0 L		
0	0	100
3	1048	1040
6	4754	5233
9	1834	1704
12	3690	3768
15	2636	2683
18	8223	8295
21	648	752
0 1 L		
11	1905	1881
17	601	507
20	6375	6395
0 2 L		
1	3173	3030
10	11534	11533
19	1314	1309
0 3 L		
15	1953	1916
0 4 L		
8	6632	6634
0 5 L		
10	7012	7072
13	1206	1169
1 -6 L		
4	7142	7198
7	644	492
10	7118	7103
1 -5 L		
9	2158	2111
1 -4 L		
5	954	1008
11	624	492
14	6926	7001
1 -3 L		
7	646	608
13	851	836
16	3438	3420
19	1068	1051
1 -2 L		
6	13177	13284
9	4906	4983
12	940	933
18	5916	5960
1 -1 L		
2	7001	6995
8	9325	9252
14	9960	9952
1 0 L		
4	15014	14921
1 1 L		
0	14143	14040
3	9406	9253
15	1767	1819
21	2454	2405
1 2 L		
17	598	508
1 3 L		
16	3905	4012

L	OBS	CALC
	1 4 L	
0	9157	9106
	1 6 L	
1	968	1000
	2 -7 L	
3	469*	590
9	553	371
	2 -6 L	
5	1515	1485
8	3821	3728
11	2250	2139
	2 -5 L	
1	683	774
4	10070	10244
7	747	750
13	488	306
	2 -4 L	
9	1926	1929
18	3585	3597
	2 -3 L	
2	2859	2963
5	1036	1041
14	9324	9316
20	5492	5548
	2 -2 L	
7	893	665
16	4411	4404

L	OBS	CALC
	2 -1 L	
6	14984	14905
9	3354	3430
12	3305	3323
18	3859	3851
	2 0 L	
5	1859	1830
11	1076	1085
	2 1 L	
1	2938	2884
4	12093	12423
10	11648	11672
	2 2 L	
15	1915	1943
	3 -7 L	
7	980	992
10	6373	6448
	3 -6 L	
3	544	554
9	466*	176
12	1153	1100
	3 -5 L	
5	2111	2051
11	472	350
17	936	809
	3 -4 L	
4	10960	11129
7	2547	2662
13	930	849
19	559	73

L	OBS	CALC
	3 -3 L	
9	849	815
18	6935	6900
	3 -2 L	
2	4970	4874
11	423	444
14	9074	9041
20	5580	5550
	3 -1 L	
13	441*	325
16	4773	4719
19	467	473
	3 0 L	
0	18126	17977
3	943	950
6	5458	5484
9	970	951
	3 1 L	
2	5603	5644
8	7338	7404
17	959	784
	3 2 L	
10	7484	7659
16	3899	3853
	3 3 L	
0	10725	10823
6	4369	4385
	3 5 L	
1	721	686

L	OBS	CALC
	4 -8 L	
3	886	806
	4 -7 L	
5	423	481
8	5072	5216
11	496*	155
	4 -6 L	
1	851	925
4	6435	6534
7	489	391
10	8130	8221
	4 -5 L	
9	2029	2025
	4 -4 L	
5	411*	174
11	759	960
14	6774	6723
	4 -3 L	
1	1131	1129
7	1414	1465
	4 -2 L	
6	9679	9523
	4 -1 L	
11	2072	2151
14	7819	7809
17	485	565

L	OBS	CALC
	4 0 L	
1	525	261
16	2817	2796
	4 1 L	
0	9420	9384
3	2976	3043
6	7299	7354
15	829	869
	4 2 L	
2	1507	1469
14	6508	6552
	4 3 L	
4	6255	6325
	5 -7 L	
3	817	814
9	757	618
	5 -6 L	
5	1081	1022
8	3434	3429
11	1693	1712
	5 -5 L	
1	1928	1989
4	9017	8952
7	828	786
	5 -4 L	
9	1219	1220

L	OBS	CALC
	5 -3 L	
14	7838	7931
	5 -2 L	
1	2643	2668
	5 -1 L	
3	994	978
15	1342	1332
	5 0 L	
2	1141	1266
14	7632	7721
	6 -7 L	
7	1296	1283
	6 -6 L	
6	4017	3991
9	542*	130
	6 -5 L	
5	1299	1261
8	3761	3647
11	536	311
	6 -4 L	
7	1986	2006
	6 -3 L	
3	470	338
9	558	374
15	1300	1269

L	OBS	CALC
	6 -2 L	
2	3345	3363
5	888	922
11	488*	173
14	5913	5874
	6 -1 L	
1	841	836
	6 0 L	
0	8974	8984
3	436*	180
6	4104	4069
	6 1 L	
2	3363	3445
	7 -6 L	
7	719	483
	7 -5 L	
6	5448	5344
9	1037	1190
	7 -4 L	
8	4049	4023
	7 -3 L	
1	353	230
7	795	731
	7 -2 L	
3	1483	1444

Ilmenite at 400°C.

L	OBS	CALC
-8 4 L		
0	4457	4421
3	647	330
-7 0 L		
2	1538	1937
-7 1 L		
4	4991	5023
-7 2 L		
0	5758	5665
6	4073	4118
-7 3 L		
2	2987	2994
8	3993	4020
-7 4 L		
1	618*	403
7	574*	530
-7 5 L		
3	913	696
9	660	7
-7 6 L		
5	573*	454
-7 7 L		
1	606*	124
-6 0 L		
6	3095	3087
-6 1 L		
2	1160	1084
8	2771	2765
-6 2 L		
4	5360	5406
10	6414	6548
-6 4 L		
5	1245	1177
11	1739	1607

L	OBS	CALC
-6 5 L		
1	1138	1016
7	589*	584
13	452*	109
-6 6 L		
3	705	398
9	674*	139
-6 7 L		
2	1554	1007
5	817*	716
8	2408	2290
-5 0 L		
4	7655	7661
10	5530	5649
-5 1 L		
0	8166	8010
6	6348	6518
12	507*	492
-5 2 L		
2	1604	1579
8	3345	3369
14	6438	6533
-5 3 L		
1	734	634
7	404*	400
13	543*	104
-5 4 L		
3	2442	2436
9	2025	2075
15	677	547
-5 5 L		
5	1416	1430
11	542*	275
-5 6 L		
1	1034	810
4	6885	6739
7	924	901
10	4674	4549
13	1059	866
-5 7 L		
3	699*	907
6	3748	3726

L	OBS	CALC
-5 7 L		
9	1624	1242
-5 8 L		
2	560*	804
-4 0 L		
2	4145	4169
8	5836	5822
14	5401	5412
-4 1 L		
4	10196	10359
10	7846	7907
16	3080	3110
-4 2 L		
0	10943	10827
3	2045	2021
6	9414	9671
9	1214	1311
12	1995	1995
15	1782	1703
18	2807	2705
-4 3 L		
5	1032	1045
11	588	438
17	724	269
-4 4 L		
1	348*	159
7	1435	1438
13	840	945
-4 5 L		
3	1034	1055
6	7288	7197
9	471*	514
12	1303	1511
15	1233	1081
-4 6 L		
2	2727	2835
5	964	787
8	4285	4095
11	777*	140
14	4326	4332
-4 7 L		
1	465*	76
4	3772	3761
7	769*	342

L	OBS	CALC
-4 7 L		
10	5977	5862
-4 8 L		
3	811*	541
-3 0 L		
6	4958	4987
12	1843	1863
18	5325	5356
-3 1 L		
2	2699	2762
8	5707	5802
14	7920	7961
20	4045	4068
-3 2 L		
1	2748	2705
7	409	429
13	591*	311
19	1257	1172
-3 3 L		
3	630	641
9	441*	560
15	1961	1940
-3 4 L		
2	2983	2971
5	632	816
8	5243	5268
11	1902	1836
14	6528	6453
17	1115	748
-3 5 L		
1	2226	2301
4	8835	8760
7	1116	977
10	6846	6851
13	905	779
16	2549	2393
-3 6 L		
3	629*	132
6	3582	3604
9	685*	110
12	522*	761
15	1112	1118

L	OBS	CALC
-3 7 L		
2	1616	1748
5	522*	134
8	3035	3024
11	818*	439
-3 8 L		
1	963	1120
-2 0 L		
4	14791	15054
10	10683	10628
16	3650	3566
-2 2 L		
5	2101	2095
11	1131	1012
17	607*	222
-2 3 L		
1	599	565
4	13695	13793
7	2341	2447
10	8969	9073
13	876	701
16	3779	3787
19	730	713
-2 4 L		
3	4300	4363
6	8638	8594
9	2998	3032
12	855	505
15	612	842
18	4024	4063
-2 5 L		
2	1621	1521
5	443*	401
8	3661	3580
11	675	807
14	6214	6216
17	756	424
-2 6 L		
1	1180	1258
4	7345	7295
7	1467	1447
10	4891	4781
13	1093	1213
-2 7 L		
3	983	747
6	4002	4055

L	OBS	CALC
-2 7 L		
9	942	1144
-1 0 L		
2	6957	6931
8	9170	9033
14	8880	8839
20	5087	4881
-1 1 L		
1	874	859
7	2754	2650
13	507	463
19	876	813
-1 2 L		
3	5237	5087
6	14365	14626
9	2578	2714
12	3134	3204
15	2502	2498
18	3028	3065
21	790*	293
-1 3 L		
2	4751	4664
5	2182	2187
8	6506	6672
11	497*	466
14	7683	7690
17	510*	419
-1 4 L		
1	922	938
4	8295	8102
7	1036	1146
10	9606	9689
13	1091	628
16	1852	1811
19	799*	494
-1 5 L		
3	1319	1245
6	7032	6962
9	753	694
12	1232	1348
15	1298	1226
-1 6 L		
2	1721	1622
5	1246	1041
8	2786	2903
11	692*	267

L	OBS	CALC
-1 7 L		
1	598*	85
4	3281	3260
7	480*	136
0 0 L		
0	0	100
3	830	849
6	4542	5013
9	1300	1214
12	3259	3284
15	2720	2727
18	6706	6854
21	771*	761
0 1 L		
5	689	737
11	1792	1867
17	610	133
0 2 L		
1	3228	3034
7	786	464
13	799	595
19	1206	1439
0 3 L		
3	909	856
9	419	414
15	1825	1854
0 4 L		
5	322*	307
11	644	758
17	733*	122
0 5 L		
1	1673	1647
7	883	927
13	591	610
0 6 L		
3	410*	190
9	600*	320
1 0 L		
4	15283	15032
10	13015	12768
16	3453	3435
22	1332	1440

L	OBS	CALC
1 1 L		
0	14040	14099
3	9141	9017
6	12778	12835
9	5134	5147
12	866	911
15	1362	1310
18	4833	4891
21	1942	1670
1 2 L		
5	813	765
11	2231	2279
17	733*	712
1 3 L		
1	846	869
7	2222	2256
13	1229	1146
19	695*	319

L	OBS	CALC
1 4 L		
3	2271	2284
9	1933	1986
15	923	508
1 5 L		
5	606	756
11	1160	1215
1 6 L		
1	759	927
7	949	738
2 0 L		
2	3178	3228
8	6314	6270
14	9033	8978
20	4120	4022

L	OBS	CALC
2 1 L		
4	11622	11947
10	10608	10618
16	2623	2646
2 3 L		
5	1946	1938
11	608	344
17	438*	304
2 4 L		
1	579	610
7	422*	151
13	555	424
2 5 L		
3	990	899
9	621*	219

L	OBS	CALC
3 0 L		
0	17594	17505
6	4995	5009
12	1861	1834
18	5320	5330
3 1 L		
2	5146	5242
8	6696	6705
14	5563	5684
3 2 L		
4	8898	9099
10	6222	6371
16	2914	2872
3 3 L		
0	9307	9242
3	544	236

L	OBS	CALC
3 3 L		
6	3451	3596
9	561*	100
12	609	775
15	960	961
3 4 L		
5	674	438
11	559	189
3 5 L		
1	500*	396
4 0 L		
4	7941	7847
10	8402	8435
16	1918	2086

L	OBS	CALC
4 1 L		
0	8389	8301
6	6242	6240
12	622*	270
4 2 L		
2	990	1176
8	3069	3004
14	4906	4901
4 3 L		
4	5005	5034
10	4662	4752
5 0 L		
2	1117	1060
8	2748	2689
14	5932	5856

L	OBS	CALC
5 1 L		
4	5937	5881
10	5490	5526
5 2 L		
0	5362	5338
6	4395	4399
5 3 L		
2	789	473
6 0 L		
0	7320	7224
6	3115	3155
6 1 L		
2	2515	2660
8	3703	3568

Ilmenite at 600°C.

L	OBS	CALC
-8 4 L		
0	3785	3764
3	820	228
-7 0 L		
2	1486	1645
-7 1 L		
4	4305	4355
-7 2 L		
0	5018	4997
6	3582	3593
-7 3 L		
2	2547	2638
8	3527	3496
-7 4 L		
1	485*	416
7	590*	422
-7 5 L		
3	728	711
9	587*	79
-7 6 L		
5	703	436
-7 7 L		
1	737*	122
-6 0 L		
6	2609	2686
-6 1 L		
2	982	981
8	2493	2454
-6 2 L		
4	4777	4889
10	5701	5794
-6 4 L		
5	1034	1009
11	1293	1363

L	OBS	CALC
-6 5 L		
1	917	891
7	666*	580
13	573*	96
-6 6 L		
3	608	402
9	792	24
-6 7 L		
2	678*	879
5	827*	617
8	1852	1967
-5 0 L		
4	7087	7099
10	4832	4961
-5 1 L		
0	7673	7517
6	5830	5975
12	566	436
-5 2 L		
2	1471	1484
8	3119	3151
14	5659	5676
-5 3 L		
1	507	614
7	558*	268
13	517*	279
-5 4 L		
3	2185	2221
9	2062	2069
15	702	451
-5 5 L		
5	1493	1377
11	521*	289
-5 6 L		
1	904	740
4	6201	6064
7	1091	720
10	4160	3971
13	970	911
-5 7 L		
3	464*	760
6	2826	3222

L	OBS	CALC
-5 7 L		
9	1136	1201
-5 8 L		
2	861	638
-4 0 L		
2	3923	3907
8	5435	5424
14	4672	4754
-4 1 L		
4	9813	9963
10	7255	7293
16	2695	2660
-4 2 L		
0	10723	10506
3	2090	2049
6	9013	9219
9	1063	1028
12	1987	1903
15	1609	1565
18	2398	2256
-4 3 L		
5	1194	1080
11	590*	391
17	547*	68
-4 4 L		
1	509	138
7	1220	1245
13	953	1060
-4 5 L		
3	1123	1085
6	6682	6661
9	737	322
12	1278	1413
15	1052	971
-4 6 L		
2	2729	2611
5	858	790
8	3723	3699
11	779*	158
14	3810	3645
-4 7 L		
1	943	64
4	3391	3334
7	564*	201

L	OBS	CALC
-4 7 L		
10	5275	5009
-4 8 L		
3	1007	518
-3 0 L		
6	4706	4706
12	1714	1665
18	4540	4592
-3 1 L		
2	2548	2678
8	5527	5582
14	7260	7246
20	3330	3351
-3 2 L		
1	2624	2630
7	469	337
13	459*	46
19	1196	1187
-3 3 L		
3	665	541
9	353*	322
15	1952	1830
-3 4 L		
2	2905	2819
5	799	699
8	4901	4964
11	1703	1667
14	5723	5745
17	502*	896
-3 5 L		
1	2182	2120
4	8348	8255
7	1127	955
10	6131	6163
13	710*	454
16	2210	2037
-3 6 L		
3	647*	185
6	3226	3213
9	681*	18
12	1281	645
15	1242	1029

L	OBS	CALC
-3 7 L		
2	1464	1548
5	730*	110
8	2863	2649
11	676*	354
-3 8 L		
1	886	931
-2 0 L		
4	14862	15063
10	10147	10101
16	3203	3146
-2 2 L		
5	2236	2229
11	645	904
17	617*	122
-2 3 L		
1	614	506
4	13421	13583
7	2205	2248
10	8371	8559
13	1008	946
16	3321	3285
19	1143	777
-2 4 L		
3	4086	4158
6	8108	8137
9	3043	3075
12	942	486
15	696*	709
18	3509	3468
-2 5 L		
2	1459	1392
5	385*	478
8	3376	3294
11	514*	672
14	5337	5440
17	866	559
-2 6 L		
1	1267	1178
4	6714	6635
7	1212	1244
10	4281	4208
13	1077	1253
-2 7 L		
3	960	632
6	3411	3472

L	OBS	CALC
-2 7 L		
9	799*	1114
-1 0 L		
2	6903	6882
8	9041	8903
14	8278	8180
20	4200	4128
-1 1 L		
1	839	889
7	2698	2482
13	720	777
19	757	925
-1 2 L		
3	5279	5136
6	14151	14481
9	2304	2329
12	3089	3119
15	2523	2368
18	2679	2638
21	836	431
-1 3 L		
2	4635	4579
5	2173	2238
8	6365	6481
11	471	408
14	6974	6940
17	664*	111
20	3808	3419
-1 4 L		
1	983	911
4	7918	7782
7	1174	954
10	8890	8966
13	559	779
16	1735	1510
19	467*	597
-1 5 L		
3	995	1235
6	6429	6464
9	1002	455
12	1363	1277
15	1357	1071
-1 6 L		
2	1560	1478
5	1159	987
8	2614	2599
11	667*	279

L	OBS	CALC
-1 7 L		
1	687*	68
4	2870	2803
7	665*	73
0 0 L		
0	0	100
3	607	751
6	4456	4849
9	1127	855
12	3033	3034
15	2497	2623
18	5921	6066
21	1028	863
0 1 L		
5	926	905
11	1858	1774
17	751	279
0 2 L		
1	3213	3012
7	835	369
13	695	225
19	1519	1439
0 3 L		
3	818	719
9	280*	202
15	1778	1761
0 4 L		
5	371	348
11	524	685
17	683	333
0 5 L		
1	1395	1507
7	859	928
13	566*	352
0 6 L		
3	480*	90
9	583*	333
1 0 L		
4	15428	15253
10	12601	12334
16	3055	3024
22	706	1171

1 1 L

L	OBS	CALC
0	14225	14231
3	9046	8921
6	12494	12642
9	5159	5266
12	913	930
15	1124	1121
18	4218	4275
21	1229	1215

1 2 L

L	OBS	CALC
5	421	560
11	2038	2073
17	902	881

1 3 L

L	OBS	CALC
1	736	869
7	2024	2069
13	1157	1311
19	703*	399

1 4 L

L	OBS	CALC
3	2048	2093
9	2038	1986
15	706	409

1 5 L

L	OBS	CALC
5	663	612
11	1026	1003

1 6 L

L	OBS	CALC
	993	874
7	823	606

2 0 L

L	OBS	CALC
2	3104	3168
8	6192	6140
14	8214	8223
20	3473	3365

2 1 L

L	OBS	CALC
4	11399	11735
10	9979	10026
16	2348	2284

2 3 L

L	OBS	CALC
5	1873	1871
11	577*	350
17	641*	71

2 4 L

L	OBS	CALC
1	529	561
7	472*	112
13	498	530

2 5 L

L	OBS	CALC
3	875	864
9	555*	72

3 0 L

L	OBS	CALC
0	17516	17397
6	4709	4718
12	1720	1649
18	4559	4578

3 1 L

L	OBS	CALC
2	4892	5001
8	6353	6334
14	4959	5029

3 2 L

L	OBS	CALC
4	8398	8584
10	5542	5738
16	2488	2426

3 3 L

L	OBS	CALC
0	8674	8553
3	522*	161

3 3 L

L	OBS	CALC
6	3124	3205
9	343*	206
12	694	657
15	1015	873

3 4 L

L	OBS	CALC
5	546	427
11	527	185

3 5 L

L	OBS	CALC
1	511*	325

4 0 L

L	OBS	CALC
4	7556	7489
10	7698	7694
16	1580	1762

4 1 L

L	OBS	CALC
0	7878	7756
6	5688	5754
12	582	268

4 2 L

L	OBS	CALC
2	1068	1073
8	2823	2692
14	4197	4164

4 3 L

L	OBS	CALC
4	4441	4460
10	3996	4038

5 0 L

L	OBS	CALC
2	1162	941
8	2480	2433
14	4934	5014

5 1 L

L	OBS	CALC
4	5277	5292
10	4814	4815

5 2 L

L	OBS	CALC
0	4724	4739
6	3706	3821

5 3 L

L	OBS	CALC
2	788	388

6 0 L

L	OBS	CALC
0	6647	6485
6	2918	2724

6 1 L

L	OBS	CALC
2	2338	2325
8	3129	3060

L	OBS	CALC
1 1 L		
0	13991	14122
3	8882	8699
6	12262	12393
9	5158	5297
12	814	952
15	826	891
18	3618	3701
21	934	782
1 2 L		
5	326	413
11	1773	1869
17	604*	1021
1 3 L		
1	921	867
7	1819	1818
13	1369	1414
19	761*	505
1 4 L		
3	1734	1811
9	1809	1927
15	623*	304
1 5 L		
5	540	482
11	642	761
1 6 L		
1	676	803
7	585*	413
2 0 L		
2	3010	3099
8	6010	5958
14	7580	7549
20	2939	2910
2 1 L		
4	11122	11413
10	9404	9459
16	2019	2035
2 3 L		
5	1714	1768
11	494*	322
17	962	219
2 4 L		
1	475*	435
7	494*	141
13	552*	648
2 5 L		
3	747	886
9	536*	23
3 0 L		
0	16984	16969
6	4426	4504
12	1458	1480
18	3952	3913
3 1 L		
2	4680	4792
8	5968	5942
14	4418	4496
3 2 L		
4	7867	7978
10	4932	5208
16	2139	2066
3 3 L		
0	7916	7813
3	513*	107
3 3 L		
6	2750	2868
9	484	388
12	685	584
15	706	688
3 4 L		
5	752	421
11	786	227
3 5 L		
1	495	233
4 0 L		
4	7121	7098
10	6986	6997
16	1507	1557
4 1 L		
0	7328	7229
6	5136	5305
12	481	284
4 2 L		
2	655	973
8	2393	2414
14	3449	3499
4 3 L		
4	3878	3934
10	3327	3426
5 0 L		
2	660	851
8	2345	2183
14	4220	4281
5 1 L		
4	4674	4747
10	4103	4163
5 2 L		
0	4198	4154
6	3295	3267
5 3 L		
2	674*	326
6 0 L		
0	5866	5744
6	2305	2378
6 1 L		
2	1964	2007
8	2806	2575

Ilmenite at 800°C.

L	OBS	CALC
-8 4 L		
0	3323	3157
3	524*	95
-7 0 L		
2	1354	1343
-7 1 L		
4	3729	3738
-7 2 L		
0	4398	4407
6	3027	3060
-7 3 L		
2	2273	2299
8	3024	2978
-7 4 L		
1	600	381
7	528*	235
-7 5 L		
3	937	732
9	670*	142
-7 6 L		
5	688*	405
-7 7 L		
1	622*	114
-6 0 L		
6	2254	2317
-6 1 L		
2	795	924
8	2304	2212
-6 2 L		
4	4368	4416
10	5018	5067
-6 4 L		
5	816	871
11	1055	1112

L	OBS	CALC
-6 5 L		
1	1037	697
7	539*	578
13	694*	279
-6 6 L		
3	534	454
9	589*	118
-6 7 L		
2	1061	750
5	829*	507
8	1492	1649
-5 0 L		
4	6516	6484
10	4348	4404
-5 1 L		
0	7092	6976
6	5405	5540
12	485	454
-5 2 L		
2	1120	1366
8	2844	2883
14	4865	4950
-5 3 L		
1	443*	573
7	503*	140
13	623*	462
-5 4 L		
3	1934	1938
9	1986	1991
15	656*	323
-5 5 L		
5	1318	1317
11	506*	311
-5 6 L		
1	872	693
4	5453	5397
7	459*	513
10	3592	3462
13	1110	928
-5 7 L		
3	1241	579
6	2765	2768

L	OBS	CALC
-5 7 L		
9	1304	1113
-5 8 L		
2	1243	557
-4 0 L		
2	3592	3636
8	5030	4975
14	4102	4246
-4 1 L		
4	9391	9553
10	6650	6690
16	2471	2342
-4 2 L		
0	10235	10135
3	2155	2089
6	8497	8673
9	820	785
12	1781	1677
15	1539	1462
18	1972	1966
-4 3 L		
5	1129	1127
11	487*	287
17	519*	272
-4 4 L		
1	465*	124
7	1158	1031
13	1114	1177
-4 5 L		
3	1328	1095
6	6097	6096
9	675*	134
12	1043	1206
15	824*	873
-4 6 L		
2	2037	2377
5	698*	721
8	3488	3302
11	765*	160
14	3188	3073
-4 7 L		
1	718*	59
4	3051	2934
7	771*	87

L	OBS	CALC
-4 7 L		
10	4400	4238
-4 8 L		
3	823*	520
-3 0 L		
6	4476	4479
12	1511	1509
18	3841	3935
-3 1 L		
2	2404	2613
8	5291	5398
14	6585	6550
20	3105	2884
-3 2 L		
1	2489	2509
7	413	252
13	463	343
19	918	1168
-3 3 L		
3	722	435
9	453*	28
15	1639	1629
-3 4 L		
2	2621	2633
5	296*	581
8	4469	4629
11	1285	1463
14	5111	5131
17	913	999
-3 5 L		
1	1879	1936
4	7798	7704
7	1000	987
10	5573	5584
13	575*	162
16	1958	1734
-3 6 L		
3	629*	272
6	2933	2885
9	697*	141
12	847	560
15	1009	849

L	OBS	CALC
-3 7 L		
2	1131	1313
5	722*	50
8	2367	2222
11	953	224
-3 8 L		
1	510*	735
-2 0 L		
4	14683	14829
10	9656	9635
16	2883	2806
-2 2 L		
5	2354	2356
11	874	811
17	667*	392
-2 3 L		
1	282*	499
4	13172	13257
7	2066	2014
10	7960	8041
13	890	1139
16	3122	2929
19	806*	860
-2 4 L		
3	3811	3864
6	7716	7713
9	2885	3038
12	682	490
15	403*	541
18	2892	2902
-2 5 L		
2	1418	1343
5	478	553
8	3202	3074
11	729	500
14	4787	4707
17	792	649
-2 6 L		
1	1098	1121
4	5999	6010
7	718	992
10	3662	3677
13	1394	1233
-2 7 L		
3	715	466
6	3154	3015

L	OBS	CALC
-2 7 L		
9	1030	1055
-1 0 L		
2	6865	6815
8	8849	8715
14	7681	7605
20	3728	3572
-1 1 L		
1	942	900
7	2578	2329
13	1145	1093
19	919	1010
-1 2 L		
3	5304	5177
6	14013	14123
9	1955	1963
12	2823	2892
15	2329	2246
18	2346	2366
21	807*	563
-1 3 L		
2	4471	4469
5	2253	2240
8	6120	6223
11	320*	374
14	6234	6305
17	724*	233
20	2977	2920
-1 4 L		
1	729	831
4	7518	7398
7	577	809
10	8199	8271
13	1116	983
16	1511	1349
19	480*	633
-1 5 L		
3	1232	1261
6	5923	5903
9	548*	285
12	1236	1089
15	760*	982
-1 6 L		
2	1351	1317
5	849	844
8	2398	2292
11	830	229

L	OBS	CALC
-1 7 L		
1	695	43
4	2489	2401
7	672*	117
0 0 L		
0	0	100
3	581	695
6	4263	4747
9	704	426
12	2887	2811
15	2424	2445
18	5256	5347
21	1271	880
0 1 L		
5	1114	1095
11	1732	1641
17	720	548
0 2 L		
1	3159	3031
7	747	233
13	623	112
19	1387	1427
0 3 L		
3	639	629
9	446*	106
15	1486	1565
0 4 L		
5	497	441
11	785	529
17	588	492
0 5 L		
1	1287	1364
7	826	960
13	735	101
0 6 L		
3	447*	71
9	565	446
1 0 L		
4	15536	15183
10	12150	11855
16	2752	2756
22	1227	941

L	OBS	CALC
1 1 L		
0	13871	13637
3	8583	8387
6	11588	11786
9	5238	5348
12	960	830
15	1050	776
18	3012	3058
21	978	522
1 2 L		
5	370	272
11	1522	1618
17	708	1074
1 3 L		
1	805	952
7	1613	1586
13	1286	1575
19	637	419
1 4 L		
3	1393	1447
9	1883	1858
15	591*	248
1 5 L		
5	511*	423
11	700	546
1 6 L		
1	814	786
7	576*	212
2 0 L		
2	2932	3007
8	5744	5701
14	6678	6589
20	2336	2309
2 1 L		
4	10604	10883
10	8550	8667
16	1855	1669
2 3 L		
5	1660	1668
11	742	408
17	576*	324
2 4 L		
1	422*	315
7	585	353
2 4 L		
13	738	665
2 5 L		
3	841	878
9	518*	171
3 0 L		
0	16504	16094
6	4131	4188
12	1401	1332
18	3069	3121
3 1 L		
2	4414	4503
8	5472	5423
14	3682	3746
3 2 L		
4	7235	7329
10	4289	4417
16	1719	1747
3 3 L		
0	6929	6908
3	553*	184
6	2478	2519
3 3 L		
9	435	411
12	513*	458
15	516*	601
3 4 L		
5	502*	367
11	688	283
3 5 L		
1	567*	80
4 0 L		
4	6572	6498
10	6162	6185
16	1183	1248
4 1 L		
0	6703	6563
6	4605	4678
12	667*	155
4 2 L		
2	829	854
8	2058	2014
14	2834	2805
4 3 L		
4	3296	3277
10	2669	2760
5 0 L		
2	840	749
8	1980	1902
14	3313	3400
5 1 L		
4	3984	4073
10	3475	3477
5 2 L		
0	3524	3511
6	2715	2708
5 3 L		
2	750	259
6 0 L		
0	4991	4876
6	2020	1997
12	711	269
6 1 L		
2	1635	1660
8	2109	2053

Ilmenite at 1050°C.

L	OBS	CALC
-8 4 L		
0	2648	2567
3	532	114
-7 0 L		
2	945	1107
-7 1 L		
4	3064	3043
-7 2 L		
0	3813	3701
6	2407	2550
-7 3 L		
2	1919	1960
8	2487	2448
-7 4 L		
1	624	460
7	627*	82
-7 5 L		
3	708	766
9	687*	274
-7 6 L		
5	657	323
-7 7 L		
1	626	194
-6 0 L		
6	1922	1966
12	690*	314
-6 1 L		
2	630	794
8	1819	1846
-6 2 L		
4	3744	3822
10	4242	4298
-6 4 L		
5	723	735
11	902	818

L	OBS	CALC
-6 5 L		
1	634	533
7	899	719
13	711*	367
-6 6 L		
3	497	570
9	711*	173
-6 7 L		
2	809*	626
5	807*	403
8	1537	1286
-5 0 L		
4	5773	5802
10	3558	3636
16	1417	1378
-5 1 L		
0	6499	6362
6	4745	4861
12	508*	283
-5 2 L		
2	1096	1237
8	2484	2555
14	3934	4063
-5 3 L		
1	418	403
7	396	160
13	495*	579
-5 4 L		
3	1505	1553
9	1908	1921
15	622	276
-5 5 L		
5	1224	1203
11	564*	401
-5 6 L		
1	705*	733
4	4823	4675
7	490*	261
10	2668	2816
13	772	922

L	OBS	CALC
-5 7 L		
3	596*	301
6	2071	2262
9	746*	1035
-5 8 L		
2	861*	437
-4 0 L		
2	3374	3396
8	4479	4482
14	3516	3510
-4 1 L		
4	8781	8862
10	5926	5980
16	1930	1930
-4 2 L		
0	9760	9565
3	2201	2136
6	7876	8073
9	569	452
12	1515	1535
15	1109	1210
18	1534	1463
-4 3 L		
5	970	1092
11	503*	219
17	595	469
-4 4 L		
1	483*	98
7	792	782
13	1137	1286
-4 5 L		
3	1107	1184
6	5516	5470
9	679	80
12	1174	1070
15	832*	679
-4 6 L		
2	2193	2090
5	620	649
8	2841	2795
11	816*	199
14	2607	2418

L	OBS	CALC
-4 7 L		
1	732*	128
4	2375	2442
7	759*	143
10	3569	3441
-4 8 L		
3	758	564
-3 0 L		
6	4127	4176
12	1440	1347
18	3087	3132
-3 1 L		
2	2318	2495
8	4967	5024
14	5659	5699
20	2357	2225
-3 2 L		
1	2425	2432
7	508	176
13	631	507
19	942	1107
-3 3 L		
3	492	220
9	444*	134
15	1753	1509
-3 4 L		
2	2520	2483
5	506*	456
8	4131	4177
11	1293	1186
14	4219	4370
17	1181	1013
-3 5 L		
1	1712	1685
4	7000	7036
7	1161	1105
10	4790	4803
13	770	42
16	1707	1425
-3 6 L		
3	755	453
6	2686	2500
9	696*	198
12	642*	485
15	858*	740

L	OBS	CALC
-3 7 L		
2	1324	1141
5	776	32
8	2040	1823
11	830*	55
-3 8 L		
1	541*	494
-2 0 L		
4	13861	14303
10	8838	8800
16	2599	2456
-2 2 L		
5	2435	2452
11	624	654
17	767	524
-2 3 L		
1	395*	572
4	12364	12642
7	1824	1799
10	7202	7301
13	771	1342
16	2528	2508
19	961	784
-2 4 L		
3	3447	3475
6	7075	7083
9	2964	3022
12	1044	358
15	455*	481
18	2738	2325
-2 5 L		
2	1208	1199
5	619	532
8	2946	2733
11	520*	330
14	3829	3841
17	834*	692
-2 6 L		
1	1154	1121
4	5253	5237
7	1130	718
10	3111	3067
13	1214	1250
-2 7 L		
3	535*	211
6	2319	2443

L	OBS	CALC
-2 7 L		
9	788	979
-1 0 L		
2	6680	6681
8	8445	8355
14	6783	6754
20	3066	2853
-1 1 L		
1	928	916
7	2411	2150
13	1221	1329
19	840	967
-1 2 L		
3	5344	5195
6	13026	13533
9	1463	1559
12	2716	2754
15	2001	2023
18	1960	1827
21	678*	558
-1 3 L		
2	4335	4298
5	2241	2256
8	5773	5835
11	307*	293
14	5498	5435
17	619	430
20	2693	2294
-1 4 L		
1	541	730
4	6976	6866
7	638	487
10	7331	7433
13	900	1046
16	1270	1040
19	746	620
-1 5 L		
3	1153	1310
6	5352	5310
9	549*	45
12	1139	969
15	1256	753
-1 6 L		
2	1013	1130
5	518*	764
8	2022	1884
11	745	294

L	OBS	CALC
-1 7 L		
1	634*	101
4	2073	1944
7	665*	280
0 0 L		
0	0	100
3	370	547
6	4127	4526
9	819	173
12	2622	2625
15	2364	2329
18	4415	4470
21	1335	887
0 1 L		
5	1304	1263
11	1550	1520
17	630*	724
0 2 L		
1	3145	2933
7	695	172
13	488	364
19	1199	1331
0 3 L		
3	475	367
9	553	237
15	1476	1455
0 4 L		
5	547	463
11	418*	362
17	930	588
0 5 L		
1	1194	1103
7	1039	1041
13	664*	77
0 6 L		
3	417*	254
9	660	421
1 0 L		
4	14566	14603
10	11187	11108
16	2547	2342
22	755*	649

L	OBS	CALC
	1 3 L	
1	728	817
7	2660	2731
13	875	881
19	604*	75
	1 4 L	
3	2848	2926
9	2018	2039
15	585*	787
	1 5 L	
5	940	1009
11	1689	1764
	1 6 L	
1	1023	982
7	1452	1350
	2 0 L	
2	3210	3373
8	6592	6621
14	10585	10511
20	5482	5421

L	OBS	CALC
	2 1 L	
4	12588	12947
10	12030	12043
16	3396	3386
	2 3 L	
5	1973	2058
11	518*	287
17	953	811
	2 4 L	
1	880	955
7	523*	413
13	635	110
	2 5 L	
3	766	767
9	719	599
	3 0 L	
0	20181	19555
6	5511	5541
12	2284	2250
18	6973	6910

L	OBS	CALC
	3 1 L	
2	5592	5691
8	7423	7478
14	7014	7082
	3 2 L	
4	10249	10480
10	7605	7702
16	3959	3911
	3 3 L	
0	11099	11039
3	481	579
6	4286	4425
9	536	182
12	1013	1077
15	1175	1176
	3 4 L	
5	336*	517
11	571*	155
	3 5 L	
1	647	719

L	OBS	CALC
	4 0 L	
4	8835	8810
10	10036	10058
16	2814	2818
	4 1 L	
0	9691	9552
6	7372	7416
12	537*	325
	4 2 L	
2	1506	1476
8	3802	3758
14	6531	6591
	4 3 L	
4	6372	6373
10	6412	6500
	5 0 L	
2	1461	1268
8	3248	3240
14	7858	7790

L	OBS	CALC
	5 1 L	
4	7263	7245
10	7194	7220
	5 2 L	
0	6864	6877
6	5805	5753
	6 0 L	
0	9186	9100
6	4058	4105
	6 1 L	
2	3384	3457

L	OBS	CALC	L	OBS	CALC

1973) A Meagher, E. P. and Lager, G. A. (1979) Polyhedral thermal expansion in the TiO_2 polymorphs: refinement of the crystal

Ilmenite at room temperature after heating.

L	OBS	CALC
-8 4 L		
0	6102	6060
3	898	830
-7 1 L		
4	6543	6626
-7 2 L		
0	7290	7231
6	5393	5452
-7 3 L		
2	3757	3780
8	5161	5236
-7 4 L		
1	603*	350
7	1023	1075
-7 5 L		
3	836	545
9	584*	347
-7 6 L		
5	731	574
-7 7 L		
1	497*	111
-6 0 L		
6	4008	4016
-6 1 L		
2	1226	1334
8	3520	3480
-6 2 L		
4	6393	6571
10	8229	8355
-6 4 L		
5	1626	1469
11	2042	2188
-6 5 L		
1	1492	1475
7	822	475
13	561	660
-6 6 L		
3	652	168
9	466*	393
-6 7 L		
2	1367	1389
5	901	975
-5 0 L		
4	8999	9097
10	7092	7127
-5 1 L		
0	9400	9269
6	7614	7693
12	444	560
-5 2 L		
2	1818	1820
8	3871	3905
14	8298	8377
-5 3 L		
1	648	802
7	738	764
13	419*	352
-5 4 L		
3	3023	3067
9	1914	2116
15	735	814
-5 5 L		
5	1541	1532
11	429*	191
-5 6 L		
1	823	809
4	8436	8326
7	1597	1457
10	5919	5927
13	796	694
-5 7 L		
3	1634	1473
6	4841	5002
9	1123	1302
-4 0 L		
2	4711	4682
8	6687	6677
14	6758	6812
-4 1 L		
4	11253	11450
10	9257	9294
16	3999	4050
-4 2 L		
0	12101	11899
3	1968	1934
6	10640	10849
9	1837	1886
12	2281	2212
15	1915	1961
18	3640	3597
-4 3 L		
5	1003	1037
11	515*	532
17	865	822
-4 4 L		
1	621	269
7	1968	1913
13	908	711
-4 5 L		
3	925	943
6	8530	8432
9	1063	1006
12	1764	1732
15	1248	1356
-4 6 L		
2	3389	3376
5	1028	928
8	5071	5020
11	657	163
14	5951	5922
-4 7 L		
1	542*	252
4	4824	4843
7	731	800
10	8052	7899
-4 8 L		
3	392*	382
-3 0 L		
6	5513	5515
12	2320	2284
18	6973	6944
-3 1 L		
2	2782	2980
8	6174	6293
14	9469	9439
20	5688	5609
-3 2 L		
1	2961	2916
7	632	616
13	734	852
19	960	1096
-3 3 L		
3	1075	949
9	798	969
15	2210	2098
-3 4 L		
2	3360	3349
5	1076	1027
8	5864	5973
11	2153	2181
14	7845	7911
17	540	514
-3 5 L		
1	2682	2699
4	10177	10028
7	683	847
10	8384	8343
13	1458	1423
16	3319	3227
-3 6 L		
3	677	358
6	4444	4438
9	303*	388
12	1271	1055
15	1402	1344
-3 7 L		
2	2170	2302
5	746	251
8	4174	4022
11	755	814
-3 8 L		
1	1779	1709
-2 0 L		
4	16174	16421
10	11978	11886
16	4481	4426
-2 2 L		
5	1901	1854
11	1201	1142
17	518	637
-2 3 L		
1	692	523
4	14893	15047
7	2624	2787
10	10155	10274
13	524	310
16	4763	4778
19	520	532
-2 4 L		
3	4945	4964
6	9742	9685
9	3065	3028
12	557	537
15	1038	1199
18	5442	5303
-2 5 L		
2	1709	1712
5	676	286
8	4149	4132
11	1013	1134
14	8019	7978
17	512	207
-2 6 L		
1	1140	1288
4	8861	8795
7	2150	2050
10	6263	6162
13	988	1089
-2 7 L		
3	1240	1304
6	5366	5367
9	1326	1205
-1 0 L		
2	7261	7253
8	9582	9512
14	10235	10160
20	6537	6434
-1 1 L		
1	861	847
7	3028	2844
13	392*	126
19	642	555
-1 2 L		
3	5235	5091
6	15588	16011
9	3346	3375
12	3326	3375
15	2732	2677
18	3897	3836
21	561*	223
-1 3 L		
2	4938	4912
5	2198	2137
8	6993	7165
11	495	515
14	9133	9192
17	925	953
20	5689	5579
-1 4 L		
1	990	1146
4	9119	9011
7	1481	1511
10	11193	11301
13	484	302
16	2447	2473
19	726	266
-1 5 L		
3	1096	1127
6	8230	8206
9	1296	1195
12	1491	1572
15	1505	1523
-1 6 L		
2	1818	1996
5	1284	1261
8	3689	3644
11	618*	239
-1 7 L		
1	557*	313
4	4487	4390
7	599*	528
0 0 L		
0	0	100
3	1055	988
6	4865	5318
9	1895	1745
12	3640	3766
15	2834	2807
18	8281	8373
21	902	752
0 1 L		
5	428	476
11	2028	1920
17	726	543
0 2 L		
1	3255	3066
7	1128	663
13	1329	1153
19	1196	1377
0 3 L		
3	1244	1140
9	757	836
15	2008	2014
0 4 L		
5	459*	216
11	933	972
17	418	380
0 5 L		
1	2021	2021
7	948	766
13	1259	1211
0 6 L		
3	402	546
9	546*	116
1 0 L		
4	16268	16506
10	14190	14134
16	4219	4237
22	1890	1914
1 1 L		
0	15725	15409
3	9775	9611
6	13829	13995
9	5043	5064
12	908	877
15	1749	1778
18	6044	6057
21	2495	2469
1 2 L		
5	999	1015
11	2495	2563
17	495*	469

L	OBS	CALC
1 -1 L		
20	6190	6038
1 1 L		
3	9198	8729
9	4829	4859
15	1706	1723
21	2411	2275
1 2 L		
5	1052	1047
11	2442	2489
17	454	458
1 3 L		
1	829	829
7	2589	2651
13	841	834
19	177*	66
1 4 L		
3	2831	2869
9	1989	1987
15	772	781
1 5 L		
5	1033	1035
11	1732	1696
1 6 L		
1	1008	998
7	1261	1263
2 -7 L		
0	6693	6663
6	5495	5601
2 -6 L		
2	1452	1429
8	3599	3657
14	6168	6307
2 -5 L		
4	9765	9953
10	7346	7388
16	3699	3725
2 -4 L		
0	10803	11003
6	10050	10146
12	2138	2149
18	3416	3482
2 -3 L		
2	2895	2920
8	6055	6076
14	8693	8888
20	5370	5261
2 -2 L		
4	14076	13956
10	10954	10851
16	4219	4229
2 -1 L		
6	13769	13487
12	3178	3258
18	3744	3741
2 3 L		
5	2061	2056
11	368	335
17	810	781
2 4 L		
1	934	918
7	309	375
13	154*	112
2 5 L		
3	778	793
9	591	588
3 -8 L		
2	685	657
3 -7 L		
4	6066	6188
10	6191	6263
3 -6 L		
0	10229	10477
6	4221	4321
12	1063	1038
3 -5 L		
2	1843	1800
8	3790	3835
14	7612	7936
3 -4 L		
4	10814	10718
10	8801	8824
3 -4 L		
16	3812	3852
19	252	66
3 -3 L		
0	16973	16791
6	5404	5363
12	2208	2211
18	6568	6560
3 -2 L		
2	4908	4801
8	6855	6883
14	8514	8659
20	5430	5241
3 3 L		
3	497	524
9	158*	182
15	1048	1084
3 4 L		
5	504	472
11	149*	154
3 5 L		
1	727	689
4 -8 L		
0	5829	5916
4 -7 L		
2	3777	3752
8	5092	5127
4 -6 L		
4	6350	6404
10	8001	7967
4 -5 L		
0	8990	8923
6	7427	7441
12	625	584
4 -4 L		
2	4676	4642
8	6517	6505
14	6353	6486
4 -3 L		
4	8786	8614
10	10567	10528
16	2368	2386
19	288	236
5 -8 L		
4	5859	5879
5 -7 L		
0	6995	7008
6	5278	5305
5 -6 L		
2	1321	1271
8	3350	3366
14	5957	6171
5 -5 L		
4	8820	8745
10	6875	6867
16	3151	3121
5 -4 L		
6	7972	7877
12	1479	1512
5 -3 L		
2	1717	1671
8	4079	4028
14	7517	7592
5 0 L		
11	162*	211
6 -7 L		
4	6495	6450
6 -6 L		
6	3881	3920
12	779	791
6 -5 L		
2	1962	1972
8	3615	3575
14	6244	6318
6 -4 L		
4	8561	8489
10	5978	5937
6 -3 L		
6	4314	4330
12	995	1020
6 0 L		
3	138*	180
7 -7 L		
2	2696	2683
7 -6 L		
4	4356	4277
7 -5 L		
6	5291	5254
7 -4 L		
2	2295	2278
8	3961	3940
7 -3 L		
1	259	204
8 -5 L		
4	6168	6068

Ilmenite at room temperature and pressure.

L	OBS	CALC
-8 4 L		
3	800	785
-7 4 L		
1	360	383
7	1036	1009
-7 5 L		
3	566	566
9	346	337
-7 6 L		
5	576	533
-7 7 L		
1	150*	95
-6 2 L		
13	228	112
-6 4 L		
5	1424	1481
11	2072	2101
-6 5 L		
1	1478	1469
7	631	529
13	645	643
-6 6 L		
3	302	180
9	472	371
-6 7 L		
5	967	981
-5 3 L		
1	768	757
7	694	741
13	339	317
-5 4 L		
3	2994	3010
9	2068	2065
15	785	808
-5 5 L		
5	1498	1510
11	284	211
-5 6 L		
1	895	851
7	1422	1411
13	692	700
-5 7 L		
3	1463	1403
9	1252	1259
-4 -3 L		
5	322	282
-4 2 L		
3	1880	1947
9	1828	1886
15	1832	1879
-4 3 L		
5	991	1000
11	535	496
17	788	770
-4 4 L		
1	261	234
7	1807	1861
13	714	684
-4 5 L		
3	1015	979
9	1021	1019
15	1303	1300
-4 6 L		
5	874	905
11	178*	161
-4 7 L		
1	199*	204
7	786	754
-4 8 L		
3	421	434
-3 -5 L		
2	1081	1050
-3 -4 L		
4	4734	4702
10	7591	7563
-3 -2 L		
17	297	218
-3 -1 L		
13	210*	290
-3 2 L		
1	2920	2901
7	638	581
13	799	846
19	1045	1014
-3 3 L		
3	995	944
9	882	935
15	1951	1946
-3 4 L		
5	1034	1042
11	2059	2104
17	514	503
-3 5 L		
1	2631	2687
7	893	887
13	1391	1382
-3 6 L		
3	411	353
9	353	340
15	1214	1209
-3 7 L		
5	180*	282
11	752	770
-3 8 L		
1	1677	1686
-2 -5 L		
6	4909	4896
-2 -4 L		
2	3351	3330
8	4931	4903
11	250	161
14	5661	5662
-2 -3 L		
4	9668	9561
10	7899	7966
-2 -3 L		
16	3124	3090
-2 -2 L		
6	9238	9176
12	687	588
18	5041	4999
-2 2 L		
5	1839	1816
11	1140	1096
17	653	609
-2 3 L		
1	565	553
7	2639	2738
13	303	297
19	406	472
-2 4 L		
3	4728	4840
9	2902	2937
15	1170	1169
-2 5 L		
5	283	251
11	1070	1086
17	118*	218
-2 6 L		
1	1323	1314
7	2013	1978
13	1045	1059
-2 7 L		
3	1254	1229
9	1138	1158
-1 -6 L		
2	1362	1343
8	3122	3075
-1 -5 L		
4	8064	8076
10	5722	5706
-1 -4 L		
6	8114	8096
12	1670	1670
-1 -3 L		
2	3374	3316
8	5770	5821
14	7476	7507
-1 -2 L		
4	13298	13328
10	9703	9602
16	4568	4549
-1 -1 L		
21	154*	238
-1 1 L		
1	821	839
7	2800	2786
13	144*	129
19	494	504
-1 2 L		
3	5163	4947
9	3270	3358
15	2580	2579
21	328	238
-1 3 L		
5	2166	2124
11	423	461
17	944	923
-1 4 L		
1	1110	1109
7	1384	1472
13	293	290
19	148*	236
-1 5 L		
3	1186	1166
9	1233	1207
15	1405	1461
-1 6 L		
5	1280	1270
11	303	299
-1 7 L		
1	306	260
7	541	490
0 -7 L		
4	4449	4426
0 -6 L		
0	8752	8773
6	4024	4006
12	642	644
0 -5 L		
2	1269	1256
8	3200	3183
14	7320	7392
0 -4 L		
4	8517	8440
10	9562	9526
16	2710	2683
0 -3 L		
6	5375	5390
12	2191	2178
18	6602	6529
0 -2 L		
2	3228	3318
8	6315	6374
14	9667	9774
20	5251	5105
0 -1 L		
4	13197	13246
10	12577	12370
16	4065	4055
22	1869	1826
0 0 L		
0	0	100
3	955	1031
6	4537	5068
9	1721	1689
12	3634	3626
15	2601	2619
18	7989	7855
21	644	662
0 1 L		
5	431	445
11	1838	1862
17	566	525
0 2 L		
1	3200	3018
7	648	658
13	1052	1123
19	1277	1259
0 3 L		
3	1118	1138
9	864	802
15	1838	1865
0 4 L		
5	132*	176
11	907	936
17	370	336
0 5 L		
1	1970	1986
7	809	790
13	1158	1151
0 6 L		
3	550	515
9	187*	138
1 -7 L		
2	3432	3415
8	4658	4691
1 -6 L		
4	7014	7037
10	6946	6925
1 -5 L		
0	9247	9183
6	7112	7178
12	397	353
1 -4 L		
2	5585	5580
8	7094	7222
14	6633	6758
1 -3 L		
4	11624	11713
10	11069	11067
16	3276	3267
1 -2 L		
0	12500	12811
6	12371	12197
12	907	927
18	5706	5716
1 -1 L		
2	6869	6676
8	8783	8765
14	9343	9457

Ilmenite at 25.4 kbar.

L	OBS	CALC
-6 3 L		
18	4744	4812
-6 4 L		
14	6483	6152
17	1246	1308
-5 -1 L		
14	6389	6179
17	852	533
-5 2 L		
11	692	393
-5 3 L		
10	7378	7220
-5 5 L		
1[illegible]	797	217
17	619*	401
-4 7 L		
7	775	688
-3 -1 L		
13	361*	392
-3 6 L		
0	10453	10212
-2 -6 L		
10	4668	4641
-2 -5 L		
6	4860	4753
-2 5 L		
-4	10029	9808
-2 6 L		
-2	1303	1365
-2 7 L		
-3	711	559
-2 8 L		
-1	341*	322
-1 -4 L		
0	8906	8742
-1 5 L		
-6	7168	7036
-3	2802	2880
-1 6 L		
-7	527*	625
-4	6852	6891
-1	1465	1479
-1 7 L		
-5	634	528
-2	3352	3288
-1 8 L		
-3	505*	573
0 -7 L		
7	661*	451
0 -6 L		
3	620	186
0 -5 L		
-1	1834	1911
0 -3 L		
-3	1115	1135
0 0 L		
0	0	100
0 1 L		
-4	13261	13614
-1	868	863
0 3 L		
-3	859	943
0	16469	16477
0 4 L		
-7	1759	1787
0 5 L		
-5	1497	1493
-2	1232	1197
0 6 L		
-9	225*	243
-6	3761	3875
-3	578*	186
0	8376	8455
0 7 L		
-7	820	451
-4	4291	4160
-1	368*	98
1 -8 L		
0	5616	5487
1 -7 L		
-1	311*	219
5	530*	528
1 -6 L		
-5	1344	1336
-2	1914	1870
1 -5 L		
-6	7518	7629
-3	1272	1189
0	8999	9010
1 -3 L		
-5	2289	2238
1 -2 L		
0	12892	12945
1 0 L		
-2	6667	6701
1 3 L		
-11	1876	2105
1 4 L		
-9	1022	980
-3	1007	1003
1 5 L		
-7	1438	1399
-4	8017	7898
-1	704	915
1 6 L		
-8	3005	2993
-5	1007	934
1 7 L		
-9	504*	217
2 -8 L		
-2	1033	1032
2 -7 L		
-6	5030	5105
-3	1244	1082
0	6574	6418
3	385*	559
2 -6 L		
-7	1895	1903
-4	8260	8298
-1	1370	1324
2 -5 L		
-5	229*	215
2 -3 L		
-4	13424	13283
2 -2 L		
-8	6263	6370
2 0 L		
-13	941	997
-10	10949	10892
-7	643	641
2 1 L		
-14	8373	8650
-2	4669	4693
2 2 L		
-15	1136	1155
-12	845	764
-9	2902	2966
2 3 L		
-13	1281	1323
-7	873	964
2 4 L		
-11	378*	194
-5	909	949
2 5 L		
-9	1276	1215
3 -9 L		
-3	255*	133
3 -8 L		
-7	1366	1424
-4	5698	5826
-1	1600	1624
3 -7 L		
-8	3958	3899
-5	211*	271
-2	2257	2249
3 -6 L		
-9	292*	172
-6	4213	4208
-3	329*	358
3 -5 L		
-10	7863	7798
-4	9528	9426
3 -4 L		
-14	7132	7367
3 -3 L		
-15	1942	1909
-12	2194	2143
3 -2 L		
-13	782	762
-4	11588	11719
3 -1 L		
-14	8730	8862
-5	1053	1061
3 0 L		
-15	1827	1827
-12	2098	2181
3 1 L		
-16	2192	2247
-13	594	392
-10	10770	10464
3 2 L		
-14	7543	7542
-11	1064	1110
-8	3932	3937
3 3 L		
-15	1296	1108
-12	1203	966
3 4 L		
-13	754	804
4 -8 L		
-9	426*	126
-6	4555	4564
4 -7 L		
-10	7489	7382
-7	447*	688
-4	4419	4491
4 -6 L		
-14	5473	5517
-8	4911	4807
4 -5 L		
-15	1232	1392
-12	1597	1645
-6	7892	7849
4 -4 L		
-16	2376	2493
-13	708	776
-10	9513	9445
4 -3 L		
-17	795	722
-14	6567	6636
-11	443*	437
4 -2 L		
-15	1828	2000
-12	2113	2179
-9	1838	1843
4 -1 L		
-16	3728	3710
-13	1154	917
-10	8941	8738
4 0 L		
-17	371*	247
-14	6551	6307
-11	953	913
-8	6565	6536
4 1 L		
-18	3236	3246
-15	1572	1562
-12	1252	1492
-9	1189	1172
4 2 L		
-16	3626	3695
-13	1039	1143
-10	5649	5743
4 3 L		
-14	4793	4922
5 -8 L		
-11	416*	120
5 -7 L		
-12	473*	143
5 -6 L		
-16	3581	3499
-13	804	842
-10	5544	5482
5 -5 L		
-17	665	401
-14	7228	7299
-11	577*	217
-8	3083	3102
5 -4 L		
-18	4321	4340
-15	717	792
-12	456*	481
-9	2011	2081
5 -3 L		
-16	3629	3613
-13	367*	166

L	OBS	CALC
5 -2 L		
-17	868	728
-14	7718	7870
-11	462*	393
5 -1 L		
-18	4217	4165
-15	443*	774
-12	794	715
5 0 L		
-19	1565	1569
-16	3054	2976
-13	1085	1037
5 1 L		
-17	359*	533
6 -6 L		
-15	963	1022
6 -5 L		
-16	2254	2287
-13	842	615
6 -3 L		
-15	1045	1037
6 -2 L		
-19	368*	522
-16	[illegible]	[illegible]

Ilmenite at 34.6 kbar.

K	OBS	CALC
	-8 K -1	
2	1385	1372
5	1592	1608
	-8 K 2	
5	876	683
	-7 K -3	
2	1393	1309
5	1184	1152
	-7 K -1	
0	381*	98
3	850	190
6	378*	240
	-7 K 1	
4	800	376
	-6 K -3	
0	514*	163
3	383*	389
6	672	498
	-6 K -1	
-2	391*	276
1	880	849
4	1320	1262
7	914	937

K	OBS	CALC
	-5 K -3	
-2	455*	546
1	1008	978
4	1144	1153
7	781	758
	-5 K -1	
-1	1548	1473
5	1886	1907
8	515*	631
	-4 K -3	
-1	2909	2939
5	2726	2811
	-4 K -1	
-3	433*	376
6	913	916
9	288*	327
	-3 K -3	
-3	361*	499
0	1000	972
3	1119	1152
	-2 K -3	
-5	488*	758
	-1 K -4	
6	7014	7006

K	OBS	CALC
	-1 K -1	
0	839	856
	0 K -5	
5	1357	1445
	0 K 0	
0	0	100
	0 K 3	
-6	613	163
6	529*	498
	1 K -4	
213783		13983
5	8111	8048
	1 K -2	
0	6819	6997
	2 K -5	
-5	376*	203
4	965	928
	2 K -4	
310042		9624
	2 K -2	
1	4970	4801

K	OBS	CALC
	2 K 0	
-114168		13936
	2 K 3	
-7	637	546
	3 K -4	
-211941		12222
4	4640	4659
	3 K -2	
-1	2966	2948
	3 K -1	
4	407*	190
	3 K 0	
-317711		17735
6	5771	5562
	3 K 3	
3	651	499
	3 K 4	
210179		10060
	4 K -4	
2	8449	8461

K	OBS	CALC
	4 K -3	
4	392*	440
	4 K -2	
-6	3281	3265
3	2306	2294
	4 K -1	
5	1146	1185
	5 K -5	
-2	2143	2032
1	1378	1297
	5 K -4	
0	8814	8712
	5 K -2	
-8	877	1037
-5	1206	1269
1	1875	1953
4	1611	1552
	5 K 0	
-4	9315	9240
-1	8987	8991
	6 K -5	
-4	1409	1440
-1	1044	1026

K	OBS	CALC
	6 K -4	
-2	6402	6411
1	4348	4265
	6 K -2	
-7	1289	1355
-4	1533	1443
-1	1223	1249
2	1124	1082
	6 K 0	
-310473		10555
0	8763	8706
	6 K 2	
-8	597*	823
	7 K -4	
-4	6032	6087
-1	6464	6346
	7 K -2	
-6	3208	3316
-3	3703	3690
0	2674	2659
	7 K -1	
2	1064	1107

K	OBS	CALC
	7 K 0	
-5	6566	6598
-2	7012	6919
	8 K -3	
-4	747	751
	8 K -2	
-5	427*	683
-2	875	823
	8 K -1	
-3	804	631
0	985	1068
	8 K 0	
-7	5466	5632
-4	5878	5892
-1	5033	5057
	9 K -2	
-4	476*	707
	9 K -1	
-2	381*	89
	9 K 0	
-6	5792	5565

"Values given are 100 times the observed and calculated structure factor amplitudes. Those marked with an asterisk are considered below the minimum observable and were excluded from structure refinements."

Ilmenite at 46.1 kbar.

OBS	CALC
H -9 2	
552*	689
H -9 3	
712	159
H -8 0	
5979	5853
5031	5025
H -8 1	
549*	615
H -8 2	
818	681
H -8 4	
145	5617
H -7 -2	
250	2289
287	1360
H -7 0	
553	6542
374	6839
550	5557
1 -7 1	
722	95
I -7 5	
599	562
I -6 -2	
139	1905
114	3168
98	3217

H	OBS	CALC
H -6 -1		
2	612*	1180
H -6 0		
0	8671	8716
	310479	10566
9	5560	5569
H -6 4		
-2	894*	5564
H -6 5		
-1	646*	837
H -5 -4		
6	6877	7020
H -5 -3		
7	323*	565
H -5 -2		
-1	1266	1218
5	1237	1257
8	517*	681
H -5 -1		
9	389*	395
H -5 0		
1	9096	9192
4	8856	8961
H -5 5		
-3	583*	571
H -4 -4		
7	6040	6044

H	OBS	CALC
H -4 -2		
6	1542	1436
H -3 -4		
	510065	10065
H -3 -2		
1	4805	4692
7	3642	3606
H -3 -1		
-4	540*	338
H -3 0		
	317600	17756
H -2 -4		
6	6448	6465
H -2 -2		
-1	2927	2925
8	926	810
H -2 0		
	114129	13936
H -1 -4		
7	6309	6285
H 0 -4		
5	8737	8712
H 0 -2		
1	6754	6907
7	2548	2630
H 0 0		
0	0	100

H	OBS	CALC
H 1 -6		
4	7864	7788
H 1 -5		
2	2124	2253
H 1 -4		
	-314175	13972
6	4351	4317
H 1 -3		
7	401*	538
H 1 -1		
0	957	929
H 2 -4		
4	8451	8412
H 2 -2		
6	1193	1030
H 3 -6		
3	4118	4210
H 3 -5		
-5	342*	260
-2	888	896
4	378*	227
H 3 -4		
	-112176	12300
2	9675	9648
5	6080	5930
H 3 -3		
-3	1136	1150
0	985	984
3	323*	416
6	340*	178

H	OBS	CALC
H 3 -2		
-8	1109	1002
H 3 -1		
-7	737	222
H 4 -6		
1	7890	7980
H 4 -5		
2	951	997
H 4 -4		
3	4668	4699
H 4 -3		
-5	1180	1180
1	968	1020
4	782	465
H 4 -2		
5	1561	1506
H 4 -1		
-6	1236	1180
3	319*	222
H 5 -6		
-4	7570	7400
-1	6965	7169
2	4887	4888
H 5 -5		
-6	1358	1363
-3	2140	2069
0	1299	1457
3	721	571
H 5 -4		
1	8021	8030

H	OBS	CALC
H 5 -3		
-7	1262	1208
-4	2815	2850
-1	2940	2969
2	1281	1355
H 5 -1		
-8	1654	1585
-5	1857	1858
1	870	804
H 6 -6		
-3	4113	4195
0	3719	3871
H 6 -5		
-5	912	939
-2	1373	1309
1	773	837
H 6 -3		
-6	470*	497
-3	302*	499
0	522*	153
3	527*	264
H 6 -1		
-7	346*	283
-4	887	968
-1	1513	1507
2	1505	1387
H 6 3		
-6	752	153
H 7 -6		
-2	5547	5474
H 7 -5		
-4	449*	493
-1	402*	562

H	OBS	CALC
H 7 -4		
0	4152	4308
H 7 -3		
-5	779	759
-2	819	565
1	341*	205
H 7 -1		
-6	817	869
-3	794	338
0	395*	95
H 8 -5		
-3	1368	1458
H 8 -4		
-5	5837	5777
H 8 -3		
-7	401*	429
-4	908	823
-1	797	689
H 8 -1		
-8	1036	1050
-5	789	615
-2	415*	265
H 9 -3		
-3	417*	159
H 9 -2		
-5	890	689