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THE CRYSTAL STRUCTURES OF COSTIBITE (CoSbS) AND PARACOSTIBITE (CoSbS)*

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Abstract

The crystal structures of natural costibite and synthetic paracostibite, two forms of CoSbS, have been refined by three-dimensional *x*-ray diffraction techniques to *R*-values of 0.046 and 0.053, respectively. Costibite is orthorhombic, with $a = 4.873(2)$, $b = 5.852(3)$, $c = 3.608(1)$Å, $Z = 2$, and space group $Pn2_1m$. Paracostibite is orthorhombic, with $a = 5.842(3)$, $b = 5.951(3)$, $c = 11.666(4)$Å, $Z = 8$, and space group $Pbca$. The structures are similar to those of rammelsbergite and pararammelsbergite, respectively, and the paracostibite structure can be described as consisting of portions of the costibite structure combined in two orientations.

Introduction

Until recently no minerals of the composition CoSbS were known, with the possible exception of the hypothetical end-member of the willyamite series, which has the composition (Co,Ni) SbS with Co > Ni (Cabri *et al.* 1970). Two minerals, costibite and paracostibite, have been found in samples from Broken Hill, N.S.W., Australia, and Red Lake, Ontario, Canada, respectively, by Cabri, Harris & Stewart (1970a, 1970b). The microprobe analysis reported for costibite is included in Table 1. The name of costibite was given because of its composition, and that of paracostibite because of its analogous relationship to the rammelsbergite-pararammelsbergite series. Attempts to synthesize CoSbS at these laboratories have always resulted in a structure corresponding to paracostibite. The powder diffraction pattern is essentially the same as that for natural material.

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Experimental

Suitable crystals of natural costibite from Broken Hill were available, but the paracostibite crystals from Red Lake were too fine-grained, and crystals of synthetic material were used. A preliminary survey using precession camera techniques confirmed that the orthorhombic cells used to index the powder diffraction patterns were correct.

The crystal fragments of both materials were irregular in shape and approximately 0.05 mm in dimension. The orientation matrices were determined and the cell dimensions were calculated on a Picker 4-circle diffractometer using an automatic alignment process (Busing 1970). For costibite the 2θ, χ and ω angles were obtained from 42 reflections, with 2θ between 64° and 70°, consisting of the equivalents of 623,

TABLE 1. CRYSTAL DATA

	Costibite	Paracostibite
Source	Consols Lode, Broken Hill, N.S.W., Australia (Smithsonian Institution, Washington, D.C., U.S.A. National Museum No. R849)	Synthesized in Mineralogy Section, Mineral Sciences Division, Mines Branch, Ottawa, Ontario, Canada
Microprobe Analysis (wt %)	(averages for 3 grains) Co 26.7 ± 0.5 Fe 0.6 ± 0.05 Ni 0.2 ± 0.05 Sb 57.0 ± 0.5 As 0.3 ± 0.1 S 13.1 ± 0.5 Total =99.9%	(starting composition, one phase only detected by microscopic and microprobe analysis) Co 27.70 Sb 57.23 S 15.07 Total = 100.00%
Chemical Composition	$(Co_{0.96}Fe_{0.02}Ni_{0.01})(Sb_{1.00}As_{0.01})S_{1.00}$	$Co_{1.00}Sb_{1.00}S_{1.00}$
System	Orthorhombic	Orthorhombic

	Costibite	Paracostibite
Space Group	$Pn2_1m$ (No. 31)	$Pbca$ (No. 61)
Cell Dimensions	a = 4.873(2) b = 5.852(3) c = 3.608(1) Å	a = 5.842(3) b = 5.951(3) c = 11.666(4) Å
Cell Content	$Co_2Sb_2S_2$ (Z=2)	$Co_8Sb_8S_8$ (Z=8)
Density	6.9 g/cm^3 (meas.) 6.87 g/cm^3 (calc.)	6.9 g/cm^3 (meas.) 6.97 g/cm^3 (calc.)
Absorption	μ = 220 cm^{-1}	μ = 220 cm^{-1}
Reflections	894 (measured 3 times)	3085 (measured 1 time)
Significant Intensities	843 (>10% level)	1886 (>10% level)

TABLE 2. STRUCTURE DATA

	Atom	Site	Atomic Coordinates x	y	z	Temperature Factors* (x 100) U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Costibite	Co	$2a$	0.2806(3)	0	0	0.69(3)	0.54(3)	0.45(3)	-0.03(3)	0	0
	Sb	$2a$	0.0412(1)	0.3740(3)	0	0.68(2)	0.54(1)	0.45(1)	-0.05(2)	0	0
	S	$2a$	0.4540(5)	0.6337(5)	0	0.68(6)	0.49(6)	0.35(4)	-0.03(6)	0	0
Paracostibite	Co	$8c$	0.0136(2)	0.1657(2)	0.3841(1)	0.35(2)	0.41(2)	0.28(2)	0.00(2)	-0.03(2)	0.01(2)
	Sb	$8c$	0.1180(1)	0.0500(1)	0.1800(1)	0.39(1)	0.40(1)	0.32(1)	-0.02(1)	0.03(1)	-0.02(1)
	S	$8c$	-0.1333(3)	0.3095(3)	0.0659(2)	0.45(4)	0.48(4)	0.23(4)	-0.07(4)	0.01(4)	0.01(3)

*The anisotropic temperature factors are expressed in the form $T=\exp[-2\pi^2(U_{11}a^{*2}h^2 + 2U_{12}a^*b^*hk\ldots)]$.

661, 273, 164, 505, 084, and 006. For paracostibite 52 reflections, with 2θ between 53° and 58°, consisting of the equivalents of 2.1.15, 276, 467, 539, 638, 3.4.11, 0.0.16 and 800 were used. The refined unit-cell dimensions are given in Table 1, with $\alpha = \beta = \gamma = 90.00(1)°$ for each material.

The intensity data were collected using graphite-monochromated Mo$K\alpha$ radiation. The $\theta/2\theta$ scan width, 2.4 to 3.5° for costibite and 2.0 to 3.1° for paracostibite, was adjusted automatically for $\alpha_1 - \alpha_2$ dispersion. The background counts were measured on each side of the peak for 45 seconds, and the 2θ scan rate was 2° per minute. The intensities of three reference reflections were recorded after every 50 measurements in order to monitor the crystal alignment and instrument stability. No significant variations were noted during data collection.

The initial data collection for both materials was done with a 2θ limit of 60° (Gabe *et al.* 1970). The occurrence of negative temperature factors in the subsequent refinement was attributed to both insufficient intensity data and lack of absorption corrections, and data collection was repeated for both materials with a 2θ limit of 120°.

For costibite the hkl segment was collected twice and the $hk\bar{l}$ segment once, and for paracostibite the hkl segment was collected once. These data yielded 894 reflections of which 843 were considered to have net intensities above the 10% significance level [*i.e.*, $I_{\text{net}} > 1.65\sigma(I)$] for costibite, and 3085 reflections with 1886 significant for paracostibite. These intensities were adjusted for absorption effects using a generalized Gaussian procedure (Gabe & O'Byrne 1970).

Structure Solution and Refinement

All calculations in these investigations were done on a CDC 6400 computer with the X-RAY system of crystallographic programs (Stewart *et al.* 1972). Lorentz and polarization factors were applied to the intensity data, and structure factors were calculated for both materials using the scattering factors of Doyle & Turner (1968) for neutral atoms. The structures were solved using Patterson and heavy atom techniques. The atomic sites were readily established in each case, and their identification as cobalt, antimony or sulphur was made from electron-density considerations. The atoms occupy the special positions $2a$ $(x,y,0)$ of $Pn2_1m$ for costibite, and the general positions $8c$ (x,y,z) of $Pbca$ for paracostibite.

Refinement was done by difference-Fourier and full-matrix least-squares methods. During refinement, the y parameter of the cobalt atom

TABLE 3. DISTANCES AND ANGLES

	Costibite		Paracostibite	
Cobalt Octahedron				
Distances:	Co-Sb	2.480(2)	Co-Sb	2.551(1)
	Co-Sb(a)	2.502(2)	Co-Sb(1)	2.521(1)
	Co-Sb(b)	2.502(2)	Co-Sb(2)	2.525(1)
	Co-S (c)	2.303(3)	Co-S (3)	2.291(2)
	Co-S (d)	2.354(2)	Co-S (4)	2.306(2)
	Co-S (e)	2.354(2)	Co-S (5)	2.306(2)
Angles:	Sb-Co-Sb(a)	87.99 (5)	Sb-Co-Sb(1)	82.48 (3)
	Sb-Co-Sb(b)	87.99 (5)	Sb-Co-Sb(2)	92.36 (3)
	Sb(a)-Co-Sb(b)	92.32 (6)	Sb(1)-Co-Sb(2)	83.18 (3)
	S(c)-Co-S (d)	96.18 (8)	S(3)-Co-S (4)	86.47 (6)
	S(c)-Co-S (e)	96.18 (8)	S(3)-Co-S (5)	94.36 (6)
	S(d)-Co-S (e)	100.10 (8)	S(4)-Co-S (5)	90.35 (6)
	Sb(b)-Co-S (e)	83.65 (6)	Sb(2)-Co-S (5)	90.61 (5)
	Sb(a)-Co-S (d)	83.65 (6)	Sb(1)-Co-S (4)	95.82 (5)
	Sb(a)-Co-S (c)	87.48 (5)	Sb(1)-Co-S (3)	87.08 (5)
	Sb(b)-Co-S (c)	87.48 (5)	Sb(2)-Co-S (3)	95.81 (5)
	Sb-Co-S (d)	88.01 (7)	Sb-Co-S (4)	85.18 (5)
	Sb-Co-S (e)	88.01 (7)	Sb-Co-S (5)	97.04 (5)
	Sb-Co-S (c)	173.45 (8)	Sb-Co-S (3)	165.89 (5)
	Sb(a)-Co-S (e)	174.42 (7)	Sb(1)-Co-S (5)	173.74 (5)
	Sb(b)-Co-S (d)	174.42 (7)	Sb(2)-Co-S (4)	177.45 (5)
Antimony Tetrahedron				
Distances:	Sb-Co	2.480(2)	Sb-Co	2.551(1)
	Sb-Co(f)	2.502(2)	Sb-Co(4)	2.525(1)
	Sb-Co(g)	2.502(2)	Sb-Co(5)	2.521(1)
	Sb-S	2.521(3)	Sb-S	2.510(2)
Angles:	Co(f)-Sb-Co(g)	92.32 (5)	Co(4)-Sb-Co(5)	115.98 (3)
	Co-Sb-Co(f)	123.71 (4)	Co-Sb-Co(4)	116.57 (3)
	Co-Sb-Co(g)	123.71 (4)	Co-Sb-Co(5)	114.91 (3)
	Co-Sb-S	98.98 (7)	Co-Sb-S	100.89 (5)
	Co(f)-Sb-S	108.83 (6)	Co(4)-Sb-S	102.86 (5)
	Co(g)-Sb-S	108.83 (6)	Co(5)-Sb-S	102.13 (5)
Sulphur Tetrahedron				
Distances:	S-Co(h)	2.303(3)	S-Co(6)	2.290(2)
	S-Co(i)	2.354(2)	S-Co(1)	2.306(2)
	S-Co(j)	2.354(2)	S-Co(2)	2.306(2)
	S-Sb	2.521(3)	S-Sb	2.510(2)
Angles:	Co(i)-S-Co(j)	100.10(10)	Co(1)-S-Co(2)	123.18 (7)
	Co(h)-S-Co(i)	120.71 (7)	Co(6)-S-Co(1)	126.32 (7)
	Co(h)-S-Co(j)	120.71 (7)	Co(6)-S-Co(2)	93.53 (6)
	Co(h)-S-Sb	105.53(10)	Co(6)-S-Sb	108.15 (7)
	Co(i)-S-Sb	103.78 (8)	Co(1)-S-Sb	99.20 (6)
	Co(j)-S-Sb	103.78 (8)	Co(2)-S-Sb	104.71 (6)

Distances and angles are listed to show comparative values for costibite and paracostibite with atoms in similar orientation.

Co, Sb and S are at x, y, z. Sites of equivalent atoms are as listed below.

Costibite				Paracostibite			
(a)	-x,	-½+y,	-½-z	(1)	-½+x,	y,	½-z
(b)	-x,	-½+y,	½-z	(2)	-x,	½+y,	½-z
(c)	x,	-1+y,	z	(3)	x,	½-y,	½+z
(d)	1-x,	-½+y,	-½-z	(4)	-x,	-½+y,	½-z
(e)	1-x,	-½+y,	½-z	(5)	½+x,	y,	½-z
(f)	-x,	½+y,	½-z	(6)	x,	½-y,	-½+z
(g)	-x,	½+y,	-½-z				
(h)	x,	1+y,	z				
(i)	1-x,	½+y,	½-z				
(j)	1-x,	½+y,	-½-z				

in costibite was fixed because of the polar space group. Anomalous dispersion corrections (Cromer & Liberman 1970) were introduced for both structures, and in the case of costibite which is non-centric, the absolute configuration was established by least-squares refinement of both enantiomorphs. The final atomic and thermal parameters are listed in Table 2, and the calculated bond lengths and angles are listed in Table 3. The final R values ($\Sigma|\Delta F|/\Sigma|F_o|$) are 0.046 and 0.053, "less thans" omitted, for costibite and paracostibite, respectively. The observed and calculated structure factors are listed in Tables 6 and 7.

TABLE 4

Costibite ($Pn2_1m$) This study a=4.873, b=5.852, c=3.608Å					Rammelsbergite ($Pnnm$)† a=4.88, b=5.90, c=3.60Å				
		x	y	z			x	y	z
Co	2a	0.28	0	0	Ni	2a	½	½	½
		0.72	½	½			0	0	0
Sb	2a	0.04	0.37	0	As	4g	0.28	0.87	½
		0.96	0.87	½			0.22	0.37	0
S	2a	0.45	0.63	0			0.72	0.13	½
		0.55	0.13	½			0.78	0.63	0

†Kaiman (1947). Rammelsbergite data reoriented to conventional marcasite setting, kX units converted to Å.

Discussion of the Structures

Costibite (CoSbS) has a marcasite-type structure, which is similar to that of rammelsbergite

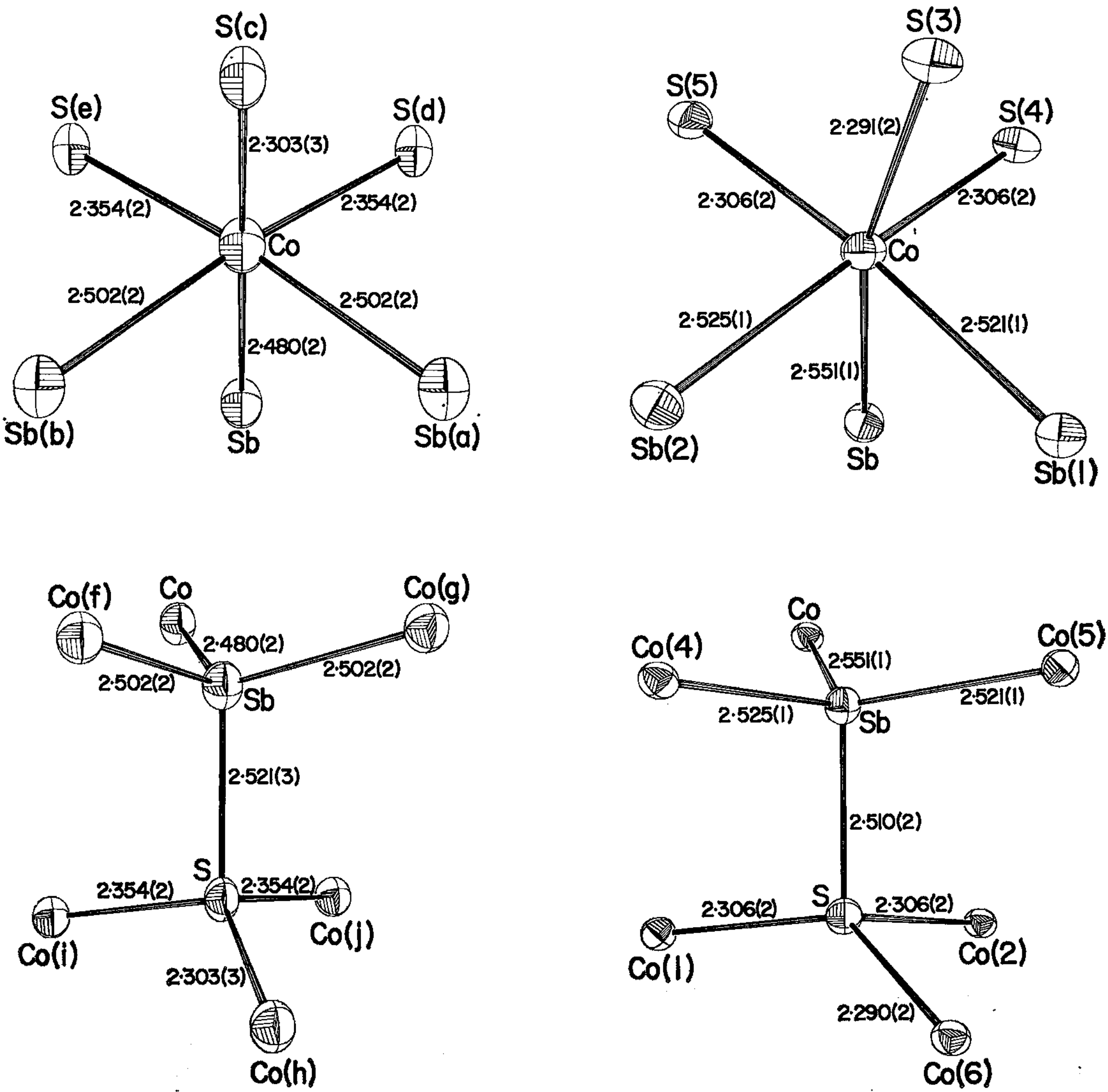

FIG. 1. The coordination of each atom type in costibite (left), and paracostibite (right), showing the interatomic distances (in Å). The estimated standard deviations are given in parentheses. The atoms are shown as thermal ellipsoids, plotted at the 99% probability limit (Johnson 1965).

(β-$NiAs_2$) reported by Kaiman (1947). The sites occupied by antimony and sulphur in costibite are equivalent to the sites occupied by arsenic in rammelsbergite. One of the glide planes of the rammelsbergite space group, *Pnnm* (No. 58), is absent in costibite and this results in the space group $Pn2_1m$ (No. 31).

The non-standard setting of this space group, which was chosen during interpretation of the Patterson map, facilitates the comparison of these structures. As shown in Table 4, an origin shift of ¼, ½, ½ results in costibite parameters that compare closely with those for rammelsbergite.

Similarly, the structure of paracostibite (CoSbS) is directly comparable to that of pararammelsbergite (α-$NiAs_2$) reported by Stassen & Heyding (1968). The space group is *Pbca* for both structures, and the atomic parameters reported for pararammelsbergite can be compared directly with those for paracostibite by an origin shift of $z = ½$, as shown in Table 5.

The coordination around each atom type is similar in the two structures. Cobalt is octahedrally-coordinated to three antimony plus three sulphur (Fig. 1a, b), and sulphur and antimony are tetrahedrally coordinated to three cobalt plus one antimony and three cobalt plus one sulphur, respectively (Fig. 1c, d). The tetrahedra are interpenetrating with the Sb-S bond shared, and with angles ranging between 92° and 126°. It should be noted that the angular distortion of the Sb tetrahedron in costibite agrees more closely with that of the S rather than the Sb tetrahedron in paracostibite, and vice versa. As expected, the Co-Sb bonds are longer than the Co-S bonds. In cobaltite (CoAsS), which has the pyrite-type structure, Co-S bonds of 2.26, 2.29 and 2.36Å were reported by Giese & Kerr (1965). Wyckoff (1960) includes Co-S and Co-Sb bonds of 2.33 and 2.58Å, respectively, for CoS and CoSb, both of which have the hexagonal NiAs-type structure.

Costibite has the marcasite-type structure composed of staggered layers of Co octahedra, with the Sb and S atoms occupying layers at $x \simeq 0$ and $x \simeq ½$, respectively, as shown in Figure 2. Each octahedron shares an edge with two other octahedra in the same layer, and the six corners are shared with corners of four octahedra above and four below the layer.

The paracostibite structure consists of layers of atoms perpendicular to the *c*-axis, with the

TABLE 5

Paracostibite (*Pbca*) This study a=5.842, b=5.951, c=11.666Å					Pararammelsbergite (*Pbca*) Stassen & Heyding (1968) a=5.77, b=5.84, c=11.42Å					
		x	y	z				x	y	z
Co	8c	0.01	0.17	0.38	Ni	8c	($-x, -y, -z$)	-0.02	0.18	0.87
Sb	8c	0.12	0.05	0.18	AsII	8c	($x, \frac{1}{2}-y, \frac{1}{2}+z$)	0.12	0.05	0.68
S	8c	-0.13	0.31	0.07	AsI	8c	($x, \frac{1}{2}-y, \frac{1}{2}+z$)	-0.14	0.31	0.57

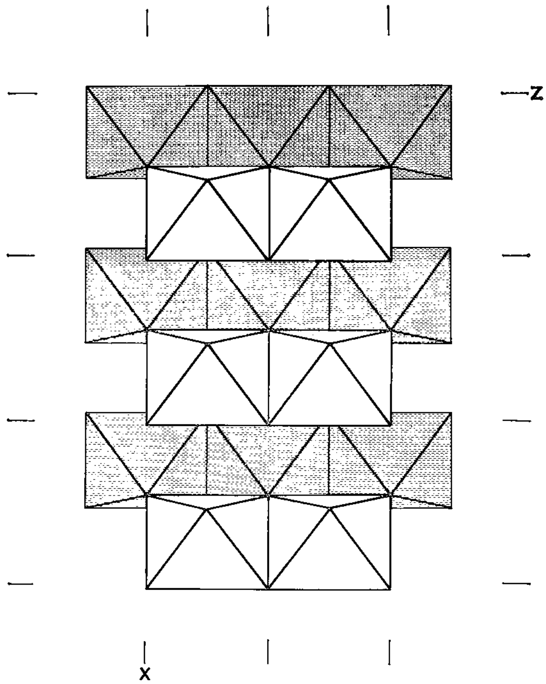

FIG. 2. The costibite structure in terms of the Co octahedra. The edges of the octahedra are joins between Sb and S atoms.

face-centered Co layers alternately stacked as pyrite-type (100) planes and marcasite-type (101) planes. In the paracostibite structure, these alternating layers have every second marcasite-type layer in reverse orientation. This arrangement has been described for the structure of pararammelsbergite by Stassen & Heyding (1968). They reported that the metal atoms of the pyrite-type and marcasite-type layers are separated by 2.63 and 3.08Å, respectively. In paracostibite, the corresponding values for the separation of Co layers are 3.16 and 2.72Å, respectively. With the pyrite-type layers containing Sb atoms and the marcasite-type layers containing S atoms, the reversal of separation distances is consistent with the larger ionic radius of the Sb atom.

The paracostibite structure can also be described in terms of a marcasite-type structure alone. The relationship of the costibite and paracostibite structures can be seen in Figure 3. Figure 3 (a) shows alternate segments of costibite oriented with the (101) and ($\bar{1}$01) planes parallel to the (001) plane of paracostibite. The similarity of this arrangement to the actual structure of paracostibite, shown in Figure 3(b), is apparent. Small shifts will permit the S and Sb atoms at $y \simeq ⅜$ and $y \simeq ⅝$ in the costibite segments to coalesce, and a rearrangement of

TABLE 6. OBSERVED AND CALCULATED STRUCTURE FACTORS FOR COSTIBITE*

	0,0,L	
2	1288	1254
4	797	767
6	510	492
8	275	325
	0,1,L	
1	529	510
3	350	342
5	232	224
7	145	152
	0,2,L	
0	636	718
2	586	564
4	355	348
6	235	234
8	155	164
	0,3,L	
1	1056	1063
3	762	746
5	477	491
7	320	332
	0,4,L	
0	446	462
2	415	404
4	301	302
6	197	209
8	124	134
	0,5,L	
1	704	716
3	531	549
5	377	390
7	258	275
	0,6,L	
0	428	443
2	375	390
4	283	296
6	209	219
	0,7,L	
1	304	306
3	249	260
5	188	199
7	130	140
	0,8,L	
0	595	585
2	521	537
4	421	433
6	308	323
	0,9,L	
1	165	163
3	142	145
5	114	118
	0,10,L	
0	226	218
2	204	207
4	170	177
6	138	139
	0,11,L	
1	377	357
3	316	318
5	251	257
	0,12,L	
0	134	147
2	146	139
4	117	115
	0,13,L	
1	214	213
3	193	193
	0,14,L	
0	160	166
	1,0,L	
0	482	527
1	803	716
2	441	416
3	482	444
4	270	260
5	283	271
6	177	177
7	166	179
8	104	124
	1,1,L	
0	291	278
1	958	867
2	220	204
3	603	573
4	118	110
5	384	371
6	78	67
7	236	249
8	52	48
	1,2,L	
0	991	978
1	410	397
2	811	764
3	271	256
4	534	508
5	162	156
6	350	337
7	104	107
8	192	221
	1,3,L	
0	542	538
1	586	592
2	450	432
3	453	428
4	294	280
5	307	290
6	183	186
7	194	198
8	111	127
	1,4,L	
0	447	500
1	101	98
2	414	419
3	66	59
4	297	292
5	47	34
6	197	209
7	48*	26
8	147	147
	1,5,L	
0	373	371
1	526	525
2	319	317
3	420	416
4	226	226
5	296	300
6	155	160
7	202	208
8	118	112
	1,6,L	
0	552	551
1	228	232
2	487	493
3	182	183
4	369	378
5	130	134
6	259	271
7	91	97
	1,7,L	
0	105	98
1	337	352
2	89	87
3	285	296
4	65	68
5	219	228
6	47*	53
7	161	165
	1,8,L	
0	237	226
1	257	256
2	205	210
3	214	218
4	171	175
5	162	170
6	137	135
7	123	125
	1,9,L	
0	71	79
1	340	344
2	68	73
3	298	300
4	68	62
5	231	237
6	43	50
	1,10,L	
0	312	304
1	107	112
2	283	285
3	111	100
4	236	238
5	90	83
6	177	180
	1,11,L	
0	167	162
1	186	176
2	149	153
3	164	158
4	133	131
5	132	128
	1,12,L	
0	179	182
1	69*	28
2	181	173
3	54*	26
4	155	148
	1,13,L	
0	105	110
1	179	187
2	108	105
3	172	168
	1,14,L	
0	154	166
1	77	81
	2,0,L	
0	468	474
1	101	109
2	392	381
3	88	81
4	274	274
5	51	57
6	173	187
7	48*	43
8	106	119
	2,1,L	
0	481	492
1	850	941
2	433	392
3	709	642
4	277	257
5	430	415
6	165	173
7	264	280
8	99	117
	2,2,L	
0	581	591
1	412	442
2	524	478
3	354	318
4	336	310
5	227	213
6	222	212
7	131	142
8	127	148
	2,3,L	
0	279	271
1	357	356
2	248	229
3	293	275
4	174	162
5	212	197
6	113	111
7	134	136
8	81	74
	2,4,L	
0	893	869
1	292	292
2	764	744
3	220	218
4	563	532
5	162	154
6	376	370
7	111	111
8	227	251
	2,5,L	
0	248	244
1	228	233
2	223	216
3	188	188
4	174	163
5	142	141
6	123	116
7	105	101
8	69	77
	2,6,L	
0	307	311
1	280	279
2	274	278
3	234	230
4	219	218
5	168	171
6	164	165
7	115	120
	2,7,L	
0	174	206
1	505	503
2	182	188
3	417	423
4	150	151
5	317	323
6	108	114
7	224	232
	2,8,L	
0	195	213
1	68	67
2	192	198
3	62	60
4	161	161
5	57	49
6	117	117
7	48*	35
	2,9,L	
0	192	197
1	311	318
2	181	184
3	271	280
4	147	153
5	219	225
6	116	116
	2,10,L	
0	222	229
1	162	154
2	215	216
3	134	136
4	180	183
5	106	108
6	137	142
	2,11,L	
0	101	80
1	164	156
2	79	75
3	140	138
4	69	64
5	114	110
	2,12,L	
0	267	277
1	112	111
2	272	263
3	107	100
4	230	225
	2,13,L	
0	85	87
1	65	82
2	96	82
3	80	74
	2,14,L	
0	108	114
	3,0,L	
0	511	541
1	282	292
2	440	444
3	235	233
4	279	295
5	155	167
6	187	205
7	100	111
8	136	144
	3,1,L	
0	696	712
1	375	397
2	610	588
3	294	297
4	396	399
5	199	205
6	263	272
7	124	139
8	165	185
	3,2,L	
0	564	562
1	360	393
2	497	478
3	297	284
4	362	340
5	203	194
6	234	234
7	125	139
8	137	156
	3,3,L	
0	252	252
1	420	465
2	242	222
3	385	352
4	180	168
5	273	247
6	132	121
7	163	175
8	74	81
	3,4,L	
0	143	143
1	587	632
2	136	127
3	532	496
4	106	99
5	381	355
6	88	76
7	244	247
8	49	53
	3,5,L	
0	162	160
1	379	411
2	154	143
3	348	334
4	126	113
5	264	248
6	96	85
7	174	177
	3,6,L	
0	364	356
1	212	225
2	332	323
3	194	188
4	268	254
5	153	148
6	187	186
7	118	110
	3,7,L	
0	415	402
1	171	185
2	381	368
3	162	159
4	297	296
5	118	124
6	219	221
7	82	89
	3,8,L	
0	254	250
1	157	154
2	234	233
3	131	134
4	192	195
5	105	102
6	154	151
	3,9,L	
0	238	260
1	188	195
2	237	243
3	168	171
4	205	205
5	136	135
6	160	159
	3,10,L	
0	176	213
1	177	174
2	197	200
3	155	155
4	170	168
5	123	127
	3,11,L	
0	106	119
1	165	166
2	119	112
3	147	150
4	96	94
5	123	123
	3,12,L	
0	61	73
1	227	222
2	76	69
3	212	199
4	64	59
	3,13,L	
0	67	57
1	151	157
2	56	54
	4,0,L	
0	511	529
1	456	500
2	445	453
3	361	375
4	308	325
5	245	266
6	205	227
7	168	193
8	135	155
	4,1,L	
0	415	429
1	139	148
2	371	374
3	113	115
4	271	276
5	77	84
6	189	194
7	48*	60
8	116	129
	4,2,L	
0	258	266
1	543	572
2	223	228
3	470	453
4	166	166
5	321	325
6	116	121
7	211	224
8	75	85
	4,3,L	
0	487	497
1	373	396
2	416	435
3	327	313
4	340	325
5	232	226
6	236	236
7	145	160
8	147	164
	4,4,L	
0	120	120
1	111	125
2	107	111
3	124	106
4	102	89
5	109	85
6	81	63
7	66	64
	4,5,L	
0	452	459
1	284	297
2	403	416
3	278	246
4	359	328
5	200	187
6	258	242
7	134	136
	4,6,L	
0	196	201
1	368	387
2	186	184
3	362	328
4	160	148
5	276	251
6	113	113
7	172	179
	4,7,L	
0	219	215
1	103	109
2	197	199
3	107	95
4	177	163
5	70	75
6	120	123
7	64	53
	4,8,L	
0	264	260
1	262	268
2	229	243
3	251	238
4	206	202
5	197	194
6	161	154
	4,9,L	
0	239	223
1	78	71
2	199	209
3	65	64
4	177	174
5	66	52
6	136	131
	4,10,L	
0	120	109
1	239	246
2	102	104
3	221	219
4	103	89
5	174	175
	4,11,L	
0	185	189
1	142	170
2	177	180
3	151	153
4	147	155
	4,12,L	
0	48	43
1	68	74
2	55*	40
3	66	66
	4,13,L	
0	164	185
1	95	107
2	168	175
	5,0,L	
0	68	69
1	611	651
2	54	58
3	532	526
4	43*	39
5	363	386
6	44*	27
7	247	270
	5,1,L	
0	311	327
1	244	258
2	278	293
3	210	205
4	228	227
5	148	151
6	167	166
7	106	109
	5,2,L	
0	204	212
1	277	300
2	177	187
3	250	246
4	148	142
5	192	189
6	100	103
7	137	140
	5,3,L	
0	501	520
1	112	114
2	429	469
3	92	92
4	375	365
5	76	69
6	261	267
7	48*	50
	5,4,L	
0	230	232
1	337	351
2	185	209
3	316	297
4	176	165
5	240	225
6	123	125
7	147	156
	5,5,L	
0	383	391
1	105	108
2	330	359
3	102	91
4	319	290
5	61	70
6	228	219
7	57	51
	5,6,L	
0	147	146
1	233	246
2	131	135
3	224	215
4	127	111
5	187	172
6	86	84
7	126	128
	5,7,L	
0	254	256
1	154	161
2	234	239
3	147	141
4	221	198
5	122	114
6	150	148
	5,8,L	
0	50	34
1	362	362
2	53*	32
3	324	319
4	58*	27
5	265	254
6	51*	22
	5,9,L	
0	157	148
1	142	132
2	139	140
3	112	118
4	127	120
5	96	96
	5,10,L	
0	107	101
1	167	159
2	88	96
3	125	144
4	77	83
5	129	118
	5,11,L	
0	274	243
1	56*	40
2	200	231
3	51*	37
4	191	197
	5,12,L	
0	111	101
1	135	137
2	84	97
3	94	122
	6,0,L	
0	72	78
1	95	110
2	69	70
3	105	97
4	71	55
5	77	81
6	47	40
7	55	60
	6,1,L	
0	461	486
1	67	63
2	413	442
3	64	52
4	347	353
5	46*	40
6	247	264
7	44*	30
	6,2,L	
0	68	70
1	431	458
2	65	63
3	397	386
4	60	50
5	293	294
6	47*	38
7	200	209
	6,3,L	
0	279	287
1	77	66
2	245	264
3	61	56
4	216	213
5	49*	43
6	165	158
7	44*	31
	6,4,L	
0	53	52
1	345	362
2	37	48
3	310	314
4	49*	39
5	268	251
6	49*	31
7	183	187
	6,5,L	
0	285	290
1	68	62
2	253	269
3	54	54
4	242	220
5	57*	42
6	166	163
	6,6,L	
0	53	49
1	353	358
2	49*	46
3	317	313
4	53	38
5	273	247
6	51*	29
	6,7,L	
0	295	296
1	44*	44
2	271	279
3	55*	39
4	256	237
5	57*	33
6	195	184
	6,8,L	
0	51	46
1	83	93
2	57	44
3	85	84
4	56*	37
5	83	68
	6,9,L	
0	306	292
1	50*	36
2	285	276
3	54*	32
4	231	235
5	57*	27
	6,10,L	
0	50*	39
1	238	224
2	53*	38
3	185	201
4	50*	33
	6,11,L	
0	137	115
1	53*	28
2	101	109
3	47*	25
	6,12,L	
0	50*	28
1	181	183
	7,0,L	
0	103	98
1	311	335
2	86	90
3	306	289
4	79	71
5	220	224
6	52	54
7	151	159
	7,1,L	
0	302	323
1	165	178
2	286	299
3	157	154
4	249	246
5	115	122
6	183	186
7	87	91
	7,2,L	
0	158	160
1	198	218
2	148	148
3	189	192
4	121	121
5	159	155
6	100	92
7	117	115
	7,3,L	
0	270	280
1	120	125
2	241	260
3	113	108
4	227	215
5	84	85
6	169	162
	7,4,L	
0	149	153
1	334	347
2	129	143
3	305	303
4	130	121
5	248	239
6	101	96
	7,5,L	
0	210	211
1	101	99
2	188	199
3	73	86
4	182	167
5	81	69
6	132	128
	7,6,L	
0	145	143
1	175	182
2	132	135
3	161	164
4	128	114
5	148	134
6	93	88
	7,7,L	
0	265	258
1	122	115
2	245	243
3	109	104
4	227	205
5	97	86
	7,8,L	
0	65	58
1	220	209
2	65	55
3	199	184
4	61*	47
5	167	149
	7,9,L	
0	182	174
1	126	117
2	175	166
3	109	106
4	143	142
	7,10,L	
0	84	78
1	147	137
2	81	74
3	109	123
	7,11,L	
0	174	152
1	75	65
2	128	144
	8,0,L	
0	158	164
1	267	287
2	143	153
3	269	255
4	125	126
5	204	208
6	91	94
	8,1,L	
0	185	197
1	119	127
2	178	184
3	110	111
4	164	152
5	89	89
6	108	115
	8,2,L	
0	78	77
1	273	287
2	70	73
3	260	253
4	77	63
5	209	201
6	55	50
	8,3,L	
0	267	279
1	122	126
2	252	263
3	112	111
4	242	223
5	92	88
6	185	173
	8,4,L	
0	152	152
1	62	62
2	139	142
3	65	56
4	118	118
5	48*	45
6	96	90
	8,5,L	
0	267	277
1	95	96
2	248	261
3	92	85
4	245	222
5	82	69
	8,6,L	
0	58	70
1	226	225
2	70	67
3	200	201
4	71	58
5	179	162
	8,7,L	
0	132	122
1	107	105
2	120	116
3	91	94
4	104	98
	8,8,L	
0	114	106
1	211	206
2	101	100
3	200	186
4	99	85
	8,9,L	
0	141	131
1	81	71
2	130	124
3	60	64
	8,10,L	
0	49	50
1	171	157
2	51*	48
	9,0,L	
0	186	198
1	159	165
2	192	188
3	161	147
4	168	162
5	118	117
	9,1,L	
0	163	167
1	127	135
2	161	157
3	126	120
4	147	134
5	103	95
	9,2,L	
0	200	213
1	122	128
2	192	201
3	118	115
4	179	169
5	99	94
	9,3,L	
0	142	145
1	176	192
2	133	137
3	179	172
4	130	116
5	150	141
	9,4,L	
0	43*	14
1	175	176
2	45*	13
3	170	157
4	48*	11
5	143	127
	9,5,L	
0	121	119
1	191	197
2	111	113
3	179	177
4	111	96
	9,6,L	
0	168	162
1	115	105
2	160	153
3	99	95
4	140	131
	9,7,L	
0	143	140
1	94	93
2	132	133
3	86	83
	9,8,L	
0	155	146
1	113	110
2	153	140
	9,9,L	
0	111	96
1	94	86
	10,0,L	
0	149	163
1	40*	9
2	157	154
3	46*	8
4	136	130
	10,1,L	
0	150	154
1	171	174
2	149	147
3	178	156
4	132	126
	10,2,L	
0	119	117
1	121	123
2	113	111
3	129	111
4	111	96
	10,3,L	
0	72	68
1	122	133
2	63	64
3	128	119
4	64	55
	10,4,L	
0	191	198
1	147	145
2	186	187
3	138	132
4	183	160
	10,5,L	
0	77	71
1	101	104
2	66	67
3	97	94
	10,6,L	
0	104	96
1	116	102
2	99	91
3	99	92
	10,7,L	
0	132	117
1	155	147
2	120	112
	11,0,L	
0	50	53
1	78	76
2	62	50
3	85	69
	11,1,L	
0	45*	32
1	178	183
2	45*	31
3	185	165
	11,2,L	
0	174	174
1	47*	53
2	179	165
3	60	48
	11,3,L	
0	74	70
1	117	110
2	74	66
	11,4,L	
0	150	155
1	43*	8
2	161	148
	11,5,L	
0	63	60
1	114	111

*The structure factors are listed in blocks of constant *hk* in columns of *l*, $[F_o] \times 10$, and $[F_c] \times 10$.

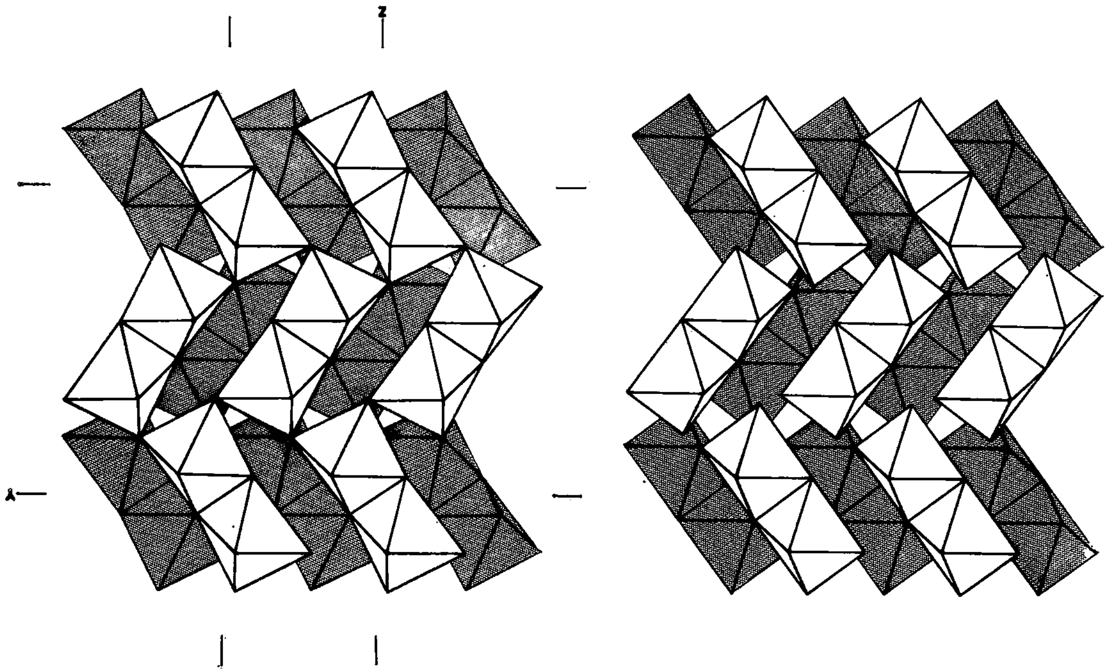

FIG. 3. The relationship of the costibite and paracostibite structures in terms of the Co octahedra. Left side shows a structural model constructed from alternate segments of costibite oriented with the (101) and ($\bar{1}$01) planes parallel. Right side shows the paracostibite structure.

sulphur and antimony will give the paracostibite distribution. In paracostibite, each Co octahedron has one shared edge, and all corners are shared with two other octahedra.

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TABLE 7. pt. 1. OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PARACOSTIBITE*

0,0,L		
2	1409	1385
4	2425	2455
6	1544	1425
8	1935	1841
10	982	948
12	480	445
14	1861	1822
16	1919	1886
18	741	749
20	1283	1320
22	282	322
24	473	508
26	185*	16
28	803	845
0,2,L		
0	1145	1127
1	2416	2563
2	2193	2219
3	241	182
4	355	351
5	2074	2060
6	2542	2543
7	348	325
8	1906	1864
9	407	409
10	508	471
11	1059	1028
12	1052	1038
13	1124	1084
14	1368	1326
15	1427	1447
16	406	376
17	180*	20
18	216	277
19	617	605
20	535	567
21	565	590
22	1164	1222
23	195*	114
24	211	228
25	190*	104
26	404	459
27	181*	9
28	462	521
0,4,L		
0	165	153
1	1708	1709
2	542	535
3	892	848
4	504	474
5	298	288
6	789	751
7	2826	2968
8	1129	1080
9	1780	1738
10	155*	85
11	1393	1368
12	607	585
13	970	942
14	183*	169
15	782	746
16	228*	134
17	745	751
18	245	218
19	340	397
20	196*	169
21	1005	972
22	448	505
23	910	987
24	226	181
25	185*	69
26	307	301
27	911	944
0,6,L		
0	675	649
1	1458	1462
2	742	692
3	865	843
4	777	767
5	1313	1320
6	993	985
7	1537	1542
8	873	879
9	878	845
10	170*	102
11	175*	106
12	680	678
13	1332	1297
14	186*	165
15	1066	1076
16	236	242
17	267	246
18	416	451
19	226	268
20	186*	11
21	984	999
22	755	781
23	675	655
24	182*	80
25	177*	110
0,8,L		
0	1830	1888
1	1221	1202
2	481	459
3	277	322
4	539	542
5	717	706
6	595	604
7	231	300
8	1097	1081
9	430	410
10	319	273
11	314	348
12	434	405
13	505	506
14	824	817
15	1070	1017
16	946	942
17	196*	173
18	323	312
19	659	633
20	725	726
21	292	323
22	335	303
23	173*	65
0,10,L		
0	1226	1218
1	258	226
2	881	864
3	194*	205
4	505	469
5	376	339
6	1081	1058
7	457	408
8	512	555
9	256	183
10	583	555
11	541	482
12	382	291
13	207*	86
14	1243	1222
15	372	325
16	596	619
17	194*	136
18	263	177
19	260	216
20	602	630
0,12,L		
0	371	383
1	636	594
2	476	494
3	195*	73
4	198*	256
5	197*	171
6	713	731
7	483	536
8	1079	1040
9	397	420
10	190*	12
11	192*	200
12	639	631
13	316	272
14	306	322
15	423	440
16	280	244
0,14,L		
0	410	433
1	448	379
2	186*	81
3	485	527
4	231*	179
5	389	359
6	177*	88
7	902	902
1,0,L		
2	1147	1119
4	2795	2847
6	798	703
8	820	750
10	1162	1111
12	1442	1408
14	165*	71
16	768	739
18	646	619
20	669	715
22	244	227
24	649	703
26	395	393
28	252	195
1,1,L		
1	122	107
2	553	516
3	1794	1809
4	537	492
5	2437	2467
6	1847	1771
7	188	205
8	702	617
9	1676	1614
10	1602	1539
11	1567	1493
12	500	445
13	331	306
14	269	288
15	434	423
16	335	311
17	539	523
18	285	232
19	862	842
20	354	403
21	477	425
22	201*	116
23	614	630
24	476	507
25	707	775
26	292	319
27	217	215
28	351	362
1,2,L		
1	906	865
2	1753	1743
3	1014	966
4	1177	1131
5	849	809
6	916	869
7	449	416
8	446	392
9	1011	964
10	1360	1290
11	793	731
12	627	596
13	251	152
14	247	247
15	179*	26
16	511	485
17	602	592
18	911	885
19	495	434
20	193*	208
21	191*	14
22	194*	106
23	199*	153
24	362	391
25	501	441
26	483	512
27	205	195
28	178*	47
1,3,L		
1	2013	2050
2	1136	1104
3	1824	1822
4	1758	1753
5	459	442
6	631	599
7	137*	24
8	552	522
9	147*	45
10	1025	989
11	603	598
12	1039	992
13	1012	971
14	172*	38
15	180*	14
16	619	601
17	1290	1269
18	679	649
19	368	293
20	496	471
21	464	477
22	209	178
23	193*	90
24	590	538
25	191*	119
26	287	392
27	478	487
1,4,L		
1	321	312
2	450	425
3	1695	1703
4	548	503
5	1343	1316
6	188	157
7	348	349
8	161	137
9	546	505
10	356	299
11	1154	1131
12	372	332
13	773	772
14	179*	55
15	551	558
16	191*	213
17	637	616
18	196*	248
19	633	630
20	198*	131
21	224	225
22	190*	56
23	476	528
24	187*	154
25	459	436
26	226*	141
27	314	303
1,5,L		
1	745	718
2	2040	2071
3	187	171
4	1396	1401
5	543	569
6	141*	154
7	165	153
8	157*	177
9	167*	112
10	521	513
11	172*	95
12	1391	1393
13	181*	151
14	482	469
15	283*	193
16	1050	1049
17	355	397
18	1016	1026
19	184*	70
20	191*	111
21	327	312
22	245	314
23	293	220
24	206	244
25	177*	77
26	414	449
1,6,L		
1	809	789
2	553	551
3	1051	1059
4	145*	129
5	793	786
6	259	238
7	291	323
8	162*	68
9	949	932
10	410	408
11	901	884
12	181*	108
13	390	334
14	188*	135
15	186*	62
16	190*	164
17	795	790
18	313	357
19	544	583
20	208*	17
21	193*	22
22	194*	37
23	212	243
24	182*	87
25	515	549
1,7,L		
1	469	477
2	337	302
3	993	968
4	825	829
5	282	279
6	1177	1146
7	175*	238
8	532	528
9	176*	17
10	1634	1385
11	555	535
12	190*	151
13	673	641
14	190*	142
15	293	276
16	191*	68
17	627	620
18	585	525
19	302	294
20	518	542
21	194*	92
22	187*	11
23	236	189
24	627	669
1,8,L		
1	174*	170
2	363	378
3	478	537
4	1057	1042
5	533	512
6	186	220
7	177*	18
8	306	319
9	407	379
10	479	471
11	503	487
12	735	729
13	194*	227
14	196*	35
15	192*	149
16	407	428
17	280	309
18	375	363
19	306	323
20	456	409
21	245*	111
22	181*	146
23	236	214
1,9,L		
1	183*	86
2	182*	33
3	586	558
4	522	496
5	1230	1217
6	186*	43
7	231	210
8	190*	137
9	1067	1056
10	196*	115
11	868	848
12	406	349
13	192*	59
14	212*	53
15	215	218
16	229	166
17	198*	168
18	190*	72
19	606	623
20	198	228
21	424	436
22	200*	54
1,10,L		
1	187*	81
2	716	702
3	181*	58
4	605	592
5	185*	25
6	482	479
7	190*	112
8	266	249
9	192*	121
10	802	795
11	198*	11
12	396	413
13	191*	90
14	199*	118
15	187*	71
16	325	345
17	185*	30
18	655	617
19	177*	1
20	296	224
1,11,L		
1	565	577
2	244	288
3	815	769
4	434	409
5	391	339
6	409	427
7	191*	86
8	253	271
9	399	397
10	500	454
11	588	582
12	189*	14
13	473	431
14	315	254
15	163*	100
16	183*	103
17	648	699
18	174*	43
1,12,L		
1	195*	26
2	426	399
3	434	397
4	494	512
5	323	354
6	202*	186
7	197*	109
8	247*	162
9	196*	147
10	428	379
11	349	338
12	326	410
13	195*	223
14	176*	67
15	183*	197
1,13,L		
1	224	208
2	670	670
3	474	494
4	462	421
5	190*	150
6	187*	62
7	189*	150
8	185*	48
9	187*	35
10	198	178
11	275	292
12	518	535
1,14,L		
1	270	298
2	181*	67
3	423	435
4	186*	199
5	310	305
6	179*	55
7	202*	96
2,0,L		
0	1843	1956
2	113*	48
4	1565	1563
6	268	195
8	1005	939
10	658	628
12	580	593
14	727	719
16	440	448
18	517	500
20	205*	293
22	336	340
24	196*	79
26	353	360
28	179*	66
2,1,L		
0	410	411
1	2567	2977
2	1172	1130
3	340	319
4	340	329
5	1436	1375
6	1209	1150
7	2325	2304
8	144*	56
9	1561	1509
10	603	550
11	372	345
12	159*	86
13	1263	1226
14	962	932
15	1445	1435
16	185*	43
17	580	550
18	191*	25
19	702	722
20	285*	215
21	902	943
22	437	465
23	690	678
24	201*	70
25	219*	72
26	194*	16
27	580	619
28	183*	142
2,2,L		
0	521	494
1	1076	1063
2	193	175
3	1074	1064
4	641	627
5	631	599
6	360	325
7	845	821
8	710	672
9	185	146
10	227	237
11	740	710
12	410	393
13	167*	20
14	179*	171
15	696	661
16	181*	96
17	207*	57
18	279	216
19	506	506
20	193*	26
21	194*	127
22	204*	268
23	208*	302
24	194*	76
25	234*	219
26	192*	224
27	216	191
2,3,L		
0	2340	2474
1	1044	1007
2	1143	1152
3	1135	1127
4	427	410
5	1254	1220
6	1429	1421
7	1341	1326
8	1774	1798
9	592	576
10	337	341
11	162*	164
12	822	780
13	1164	1101
14	1089	1047
15	685	656
16	972	940
17	189*	87
18	196*	126
19	196*	28
20	802	780
21	812	789
22	699	684
23	485	516
24	371	379
25	194*	170
26.	273	302
27	208	251
2,4,L		
0	579	561
1	522	518
2	133*	107
3	936	899
4	571	550
5	300	272
6	263	224
7	932	917
8	505	471
9	257	269
10	210	216
11	643	624
12	311	315
13	220	168
14	226	204
15	483	417
16	193*	164
17	190*	95
18	265	231
19	416	387
20	198*	83
21	271	260
22	287	242
23	338	369
24	197*	51
25	195*	222
26	188*	203
27	208	258
2,5,L		
0	1993	2090
1	260	265
2	1190	1218
3	551	550
4	242	244
5	395	404
6	1567	1564
7	148*	47
8	1847	1858
9	166*	227
10	370	360
11	371	329
12	917	895
13	267	292
14	1225	1174
15	187*	72
16	939	922
17	194*	195
18	194*	46
19	207	274
20	777	824
21	219*	159
22	910	900
23	194*	41
24	363	413
25	187*	155
26	388	391
2,6,L		
0	789	772
1	150*	130
2	152*	107
3	145*	26
4	777	784
5	154*	40
6	259	278
7	165*	167
8	733	718
9	176*	108
10	370	362
11	177*	71
12	487	501
13	182*	76
14	354	383
15	192*	74
16	240	272
17	192*	43
18	410	393
19	202*	47
20	196*	151
21	196*	71
22	365	397
23	195*	61
24	187*	92
25	179*	4
2,7,L		
0	1035	1032
1	988	896
2	1098	1060
3	215*	80
4	291	304
5	294	320
6	1297	1296
7	978	958
8	637	661
9	668	666
10	550	545
11	357	324
12	443	406
13	480	489
14	1197	1200
15	624	584
16	497	471
17	308	302
18	196*	24
19	434	350
20	539	550
21	421	457
22	726	741
23	351	371
24	183*	133
2,8,L		
0	345	357
1	444	440
2	178*	58
3	501	439
4	235	293
5	341	301
6	180*	24
7	441	418
8	209	180
9	187*	94
10	198	175
11	528	451
12	191*	137
13	188*	27
14	196*	259
15	467	456
16	199*	150
17	193*	56
18	200*	166
19	334	366
20	188*	118
21	186*	94
22	182*	89
23	182*	243
2,9,L		
0	742	709
1	1161	1182
2	182*	40
3	189*	152
4	183*	98
5	567	673
6	186*	90
7	1053	1057
8	599	601
9	758	740
10	196*	26
11	195*	108
12	200*	220
13	746	774
14	195*	111
15	957	937
16	421	400
17	328	319
18	195*	76
19	469	482
20	244	254
21	625	658
22	198*	82
2,10,L		
0	433	396
1	316	289
2	191*	18
3	384	353
4	370	285
5	195*	180
6	186*	19
7	384	353
8	190*	127
9	193*	89
10	196*	146
11	393	340
12	197*	130
13	200*	21
14	234	224
15	349	331
16	197*	194
17	189*	50
18	191*	184
19	306	291
20	174*	139
2,11,L		
0	496	515
1	760	776
2	193*	105
3	438	440
4	232*	140
5	682	693
6	201*	151
7	848	897
8	375	326
9	523	522
10	186*	52
11	192*	19
12	200*	133
13	800	786
14	194*	210
15	656	676
16	351	279
17	187*	183
18	177*	101
2,12,L		
0	349	340
1	190*	58
2	200*	85
3	194*	7
4	362	372
5	194*	62
6	225	183
7	185*	18
8	378	391
9	190*	12
10	259	182
11	187*	34
12	289	302
13	181*	47
14	206	191
15	175*	61
2,13,L		
0	666	627
1	505	468
2	392	405
3	189*	10
4	193*	76
5	192*	118
6	552	554
7	533	514
8	644	630
9	416	388
10	183*	139
11	231	207
12	344	347
2,14,L		
0	240*	143
1	184*	136
2	179*	1
3	249	243
4	200*	134
5	185*	111
6	176*	26
3,0,L		
2	1069	1039
4	2403	2570
6	1015	996
8	888	827
10	1495	1422
12	1389	1305
14	206*	109
16	777	714
18	799	735
20	792	786
22	212*	218
24	776	833
26	428	501
3,1,L		
1	1044	1037
2	1950	2018
3	1930	1988
4	282	288
5	767	718
6	482	457
7	356	299
8	321	322
9	258	249
10	151*	27
11	1052	1004
12	385	359
13	1012	964
14	612	603
15	470	396
16	519	503
17	971	916
18	723	703
19	483	525
20	420	458
21	299*	42
22	204*	111
23	212*	308
24	261	271
25	309	308
26	204*	242
27	362	408
3,2,L		
1	583	557
2	1656	1686
3	921	907
4	1269	1252
5	1027	1020
6	755	731
7	401	376
8	418	402
9	1061	1060
10	1236	1234
11	869	821
12	797	768
13	187*	119
14	316	259
15	189*	57
16	636	607
17	544	534
18	997	948
19	493	503
20	235	247
21	199*	108
22	201*	156
23	313	251
24	448	435
25	502	521
26	491	534
27	226	179
3,3,L		
1	131*	105
2	784	773
3	133*	8
4	1300	1315
5	1369	1387
6	339	368
7	786	806
8	372	378
9	1633	1631
10	675	672
11	684	666
12	848	821
13	592	574
14	182*	36
15	207	167
16	540	489
17	219*	51
18	514	493
19	470	509
20	390	389
21	377	362
22	203*	146
23	238	268
24	404	419
25	649	689
26	330	295
27	178*	47
3,4,L		
1	563	573
2	535	525
3	1756	1803
4	467	497
5	1197	1199
6	145*	95
7	283	287
8	202*	117
9	574	559
10	240	274
11	1170	1198
12	409	388
13	855	859
14	185*	96
15	523	528
16	306	271
17	850	833
18	284	302
19	730	690
20	202*	107
21	204*	136
22	203*	78
23	494	519
24	190*	141
25	418	483
26	183*	155
3,5,L		
1	142*	48
2	149*	20
3	356	373
4	1377	1413
5	151*	164
6	1090	1126
7	508	485
8	675	678
9	622	609
10	1288	1311
11	177*	6
12	456	469
13	425	461
14	281	288
15	264	262
16	195*	153
17	197*	75
18	389	386
19	199*	63
20	729	767
21	198*	55
22	197*	38
23	200*	47
24	739	795
25	226	210
26	375	399
3,6,L		
1	739	763
2	664	657
3	1157	1176
4	248	203
5	902	890
6	164*	104
7	327	258
8	229*	47
9	953	953
10	345	310
11	989	990
12	251	244
13	392	416
14	202*	180
15	198*	143
16	259	267
17	831	851
18	370	400
19	642	651
20	200*	39
21	197*	47
22	197*	79
23	334	319
24	185*	62
25	576	599
3,7,L		
1	241	193
2	1360	1365
3	352	364
4	292	318
5	789	803
6	190*	18
7	179*	15
8	176*	22
9	559	534
10	389	403
11	569	508
12	634	584
13	197*	22
14	464	458
15	201*	210
16	592	601
17	200*	34
18	789	806
19	289	350
20	237*	166
21	318	297
22	194*	150
23	332.	336
24	173*	9
3,8,L		
1	180*	132
2	491	458
3	579	539
4	1048	1065
5	625	629
6	302	343
7	183*	56
8	319	361
9	507	499
10	616	639
11	584	553
12	705	718
13	201*	179
14	195*	34
15	200*	162
16	437	442
17	318	293
18	437	451
19	302	375
20	413	436
21	190*	164
22	183*	150
23	210	262
3,9,L		
1	663	646
2	179*	34
3	1015	1002
4	532	455
5	229*	132
6	186*	54
7	195*	195
8	186*	100
9	187*	37
10	189*	11
11	567	540
12	309	362
13	735	765
14	194*	30
15	315	233
16	289	179
17	840	819
18	201*	48
19	215	301
20	229	188
21	184*	210
3,10,L		
1	186*	6

TABLE 7. pt. 2. OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PARACOSTIBITE*

3,10,L		
2	693	702
3	186*	79
4	715	734
5	192*	54
6	517	539
7	192*	105
8	342	311
9	200*	160
10	896	886
11	196*	9
12	545	489
13	198*	128
14	194*	83
15	187*	48
16	425	384
17	185*	31
18	658	648
19	178*	17
3,11,L		
1	206*	240
2	432	449
3	374	398
4	251	186
5	555	548
6	296	323
7	243	236
8	194*	77
9	705	657
10	216	207
11	546	504
12	344	414
13	192*	30
14	239	203
15	191*	19
16	366	362
17	341	315
3,12,L		
1	193*	79
2	529	514
3	462	433
4	529	554
5	432	382
6	201*	155
7	190*	73
8	198*	159
9	194*	215
10	401	384
11	430	380
12	456	486
13	258	222
14	179*	110
3,13,L		
1	233*	139
2	186*	5
3	200*	280
4	488	458
5	426	454
6	406	427
7	192*	28
8	277	257
9	208*	274
10	561	538
11	256	296
3,14,L		
1	342	344
2	182*	67
3	502	531
4	295	202
4,0,L		
0	1859	1903
2	1260	1266
4	620	613
6	1745	1790
8	2012	2176
10	167*	160
12	1626	1528
14	691	628
16	967	928
18	298	246
20	762	784
22	1141	1139
24	656	617
26	753	739
4,1,L		
0	646	627
1	488	492
2	137*	37
3	141*	28
4	372	368
5	362	359
6	150*	82
7	176	174
8	151*	53
9	163	138
10	182*	105
11	214*	121
12	176*	99
13	291	239
14	186*	148
15	323	319
16	216	222
17	195*	31
18	203*	163
19	190*	167
20	242*	138
21	200*	155
22	208*	113
23	201*	46
24	200*	18
25	196*	11
26	193*	79
27	173*	66
4,2,L		
0	1879	1993
1	466	416
2	1414	1416
3	1472	1477
4	832	797
5	673	648
6	1601	1607
7	1787	1808
8	681	663
9	745	728
10	838	818
11	463	458
12	321	331
13	1003	971
14	1625	1588
15	262	217
16	726	685
17	318	200
18	236	188
19	350	268
20	695	706
21	826	843
22	647	703
23	660	725
24	204*	139
25	212	295
26	185*	66
27	428	450
4,3,L		
0	271	273
1	154*	3
2	294	226
3	255	236
4	142*	63
5	149*	129
6	278	280
7	513	491
8	189	192
9	254	242
10	170*	85
11	368	350
12	182*	113
13	192*	84
14	263	226
15	195*	73
16	203*	99
17	196*	104
18	202*	17
19	195*	51
20	205*	121
21	204*	126
22	204*	142
23	205*	186
24	198*	26
25	192*	54
26	213*	53
4,4,L		
0	1075	1130
1	2235	2421
2	283	303
3	653	653
4	551	552
5	909	939
6	275	306
7	1125	1127
8	167*	162
9	1104	1111
10	299	326
11	176*	37
12	180*	14
13	747	787
14	588	582
15	1612	1602
16	449	458
17	516	505
18	269	233
19	1082	1096
20	374	347
21	605	598
22	200*	57
23	324	325
24	194*	86
25	228	305
26	184*	85
4,5,L		
0	165*	25
1	149*	45
2	276	248
3	153*	23
4	227	177
5	159*	134
6	339	357
7	163*	137
8	450	410
9	174*	79
10	176*	19
11	205	173
12	272	272
13	192*	39
14	192*	123
15	196*	77
16	209*	19
17	200*	48
18	205*	100
19	200*	22
20	201*	79
21	198*	4
22	276	272
23	192*	53
24	187*	63
25	161*	10
4,6,L		
0	903	942
1	1218	1253
2	374	408
3	662	662
4	776	739
5	1129	1138
6	371	378
7	1251	1277
8	278	377
9	721	725
10	562	547
11	190*	125
12	298	248
13	1118	1140
14	871	866
15	1032	1005
16	[illegible]	356
17	236	228
18	309	342
19	256	281
20	332	349
21	918	898
22	194*	16
23	496	574
24	186*	62
4,7,L		
0	442	461
1	169*	49
2	186*	56
3	183*	162
4	180*	223
5	178*	63
6	176*	56
7	261	238
8	185*	77
9	187*	104
10	189*	97
11	189*	93
12	195*	11
13	196*	132
14	247	203
15	194*	19
16	292	219
17	227*	28
18	201*	134
19	194*	34
20	220*	167
21	183*	123
22	189*	25
23	203*	115
4,8,L		
0	1113	1117
1	396	377
2	512	472
3	509	538
4	192*	21
5	201	155
6	735	712
7	1133	1138
8	1323	1370
9	641	609
10	190*	11
11	475	525
12	704	687
13	506	494
14	448	462
15	205*	170
16	598	620
17	301	288
18	192*	26
19	195*	60
20	509	524
21	491	544
22	586	575
4,9,L		
0	189*	8
1	275	289
2	188*	71
3	189*	76
4	185*	15
5	266	217
6	190*	85
7	192*	30
8	194*	12
9	190*	62
10	195*	43
11	234*	136
12	197*	7
13	199*	144
14	204*	82
15	308	277
16	206*	2
17	194*	14
18	198*	4
19	191*	180
20	174*	20
4,10,L		
0	652	602
1	329	301
2	774	829
3	387	423
4	188*	60
5	189*	57
6	1121	1110
7	322	298
8	926	935
9	193*	23
10	284	258
11	266	229
12	624	603
13	199*	98
14	804	814
15	323	309
16	423	320
17	195*	14
18	189*	153
19	334	317
4,11,L		
0	199*	171
1	198*	115
2	195*	37
3	214*	51
4	198*	135
5	236*	29
6	192*	27
7	218	212
8	189*	74
9	283*	129
10	194*	83
11	189*	110
12	194*	62
13	217*	93
14	186*	136
15	186*	64
16	182*	84
4,12,L		
0	1081	1090
1	473	499
2	366	367
3	191*	17
4	523	478
5	192*	135
6	436	426
7	543	534
8	297	322
9	417	396
10	367	357
11	197	225
12	182*	71
13	222	257
4,13,L		
0	190*	8
1	196*	8
2	187*	89
3	187*	98
4	183*	70
5	192*	34
6	191*	135
7	187*	119
8	261	171
9	179*	47
5,0,L		
2	978	967
4	1471	1475
6	205	140
8	276	267
10	185*	235
12	1249	1209
14	198*	141
16	813	727
18	523	505
20	358	357
22	219*	237
24	345	326
26	274	221
5,1,L		
1	1014	1008
2	1437	1448
3	1847	1932
4	158*	90
5	921	938
6	295	303
7	268*	158
8	174	159
9	553	576
10	180*	79
11	1202	1204
12	483	488
13	950	948
14	476	461
15	440	418
16	523	532
17	1149	1098
18	620	626
19	699	689
20	306	292
21	211*	28
22	213*	140
23	449	406
24	227*	148
25	486	486
26	200*	228
5,2,L		
1	851	846
2	708	735
3	712	715
4	533	552
5	221*	50
6	758	761
7	234	199
8	262	290
9	324	332
10	1080	1016
11	332	390
12	313	215
13	317	333
14	194*	99
15	200*	70
16	229	203
17	633	657
18	568	591
19	360	253
20	272	217
21	207*	187
22	210*	19
23	215*	12
24	317	348
25	199*	195
26	399	407
5,3,L		
1	150*	23
2	918	945
3	319	352
4	1322	1359
5	1284	1314
6	529	494
7	579	528
8	405	436
9	1391	1388
10	916	907
11	791	784
12	929	897
13	382	307
14	194*	69
15	201*	14
16	568	597
17	206*	155
18	695	694
19	621	580
20	445	430
21	479	379
22	240	186
23	368	381
24	515	527
25	667	701
5,4,L		
1	218	221
2	152*	28
3	833	828
4	400	353
5	1117	1134
6	239	280
7	186	206
8	242	163
9	498	495
10	298	334
11	764	797
12	263*	134
13	356	333
14	201*	62
15	375	431
16	202*	48
17	211*	175
18	205*	107
19	531	494
20	216*	198
21	378	369
22	200*	1
23	520	482
24	207*	203
25	415	410
5,5,L		
1	162*	48
2	452	411
3	250	248
4	1413	1508
5	175*	180
6	1079	1114
7	273	294
8	666	701
9	374	426
10	1440	1472
11	190*	16
12	669	647
13	331	335
14	270	204
15	221*	145
16	348	336
17	208*	107
18	626	630
19	205*	59
20	798	785
21	206*	86
22	197*	101
23	194*	14
24	838	886
5,6,L		
1	539	563
2	175*	65
3	629	638
4	176*	80
5	467	481
6	452	482
7	279	290
8	185*	156
9	680	678
10	561	544
11	556	594
12	189*	133
13	216	198
14	196*	59
15	196*	15
16	199*	77
17	572	572
18	213*	161
19	386	420
20	208*	138
21	192*	11
22	197*	51
23	198*	138
5,7,L		
1	185*	23
2	1267	1286
3	518	511
4	642	636
5	813	824
6	193*	86
7	188*	52
8	190*	100
9	625	634
10	477	522
11	602	617
12	777	769
13	196*	84
14	325	384
15	268	216
16	684	694
17	209*	194
18	846	846
19	319	428
20	203*	12
21	264	260
22	192*	193
5,8,L		
1	207	287
2	236	317
3	468	507
4	730	745
5	191*	158
6	187*	8
7	196*	78
8	210	176
9	189*	54
10	252	181
11	353	308
12	594	623
13	308	361
14	200*	28
15	203*	113
16	372	379
17	355	387
18	306	262
19	219	194
20	226	258
21	186*	53
5,9,L		
1	706	705
2	193*	146
3	1105	1133
4	441	398
5	344	327
6	224*	35
7	195*	133
8	196*	103
9	205	187
10	196*	126
11	700	715
12	268	317
13	791	775
14	195*	7
15	214*	268
16	232	183
17	912	931
18	194*	137
19	367	423
5,10,L		
1	216	218
2	570	639
3	196*	46
4	280	348
5	194*	193
6	304	253
7	201*	41
8	202*	116
9	188*	58
10	489	495
11	200*	48
12	356	327
13	194*	72
14	196*	178
15	189*	69
16	282	302
17	188*	169
18	498	514
5,11,L		
1	281	259
2	446	480
3	557	586
4	201*	222
5	675	684
6	260	233
7	193*	168
8	196*	39
9	688	696
10	194*	89
11	643	648
12	324	407
13	189*	146
14	210	190
15	219*	116
5,12,L		
1	187*	14
2	188*	104
3	317	294
4	359	412
5	264	253
6	290	297
7	190*	116
8	194*	187
9	186*	57
10	437	607
11	305	236
12	242	204
5,13,L		
1	182*	42
2	183*	136
3	286	265
4	565	550
5	465	466
6	443	459
7	179*	25
6,0,L		
0	456	464
2	513	502
4	656	656
6	755	754
8	851	845
10	211	159
12	558	607
14	206*	57
16	263*	159
18	314	361
20	211*	30
22	577	628
24	207*	88
6,1,L		
0	273	272
1	1443	1472
2	711	693
3	430	432
4	293	289
5	719	699
6	865	883
7	1691	1731
8	317	349
9	1069	1101
10	207	178
11	535	457
12	350	350
13	929	941
14	500	464
15	942	936
16	210*	136
17	366	462
18	300	242
19	419	425
20	217*	70
21	858	835
22	589	588
23	667	685
24	214*	13
25	197*	8
6,2,L		
0	823	856
1	174	143
2	167*	122
3	486	493
4	432	427
5	259	220
6	176*	116
7	767	805
8	190*	112
9	398	342
10	262	192
11	537	602
12	200*	20
13	205*	136
14	423	373
15	255	236
16	360	357
17	207*	164
18	266	229
19	287	199
20	407	271
21	277	248
22	206*	35
23	422	347
24	202*	57
25	198*	156
6,3,L		
0	1505	1531
1	967	988
2	748	718
3	262	292
4	252	253
5	1021	1054
6	947	945
7	502	463
8	1238	1259
9	234	289
10	199*	249
11	491	508
12	598	590
13	799	800
14	793	822
15	901	870
16	801	739
17	209*	43
18	212*	90
19	357	288
20	613	633
21	571	542
22	574	580
23	209*	205
24	305	316
25	193*	9
6,4,L		
0	471	462
1	661	681
2	166*	39
3	293	233
4	369	344
5	578	593
6	181*	5
7	219*	130
8	213	170
9	195*	40
10	225	179
11	461	479
12	197*	147
13	331	322
14	238	262
15	649	632
16	230	191
17	212*	41
18	221*	187
19	408	378
20	216*	137
21	243*	130
22	210*	110
23	196*	97
24	199*	12
6,5,L		
0	1724	1849
1	176*	42
2	804	807
3	245	210
4	528	551
5	385	380
6	1028	1016
7	251	213
8	1102	1056
9	201	213
10	440	457
11	367	400
12	438	451
13	266*	198
14	1087	1150
15	200*	92
16	939	917
17	215*	166
18	220*	240
19	212*	82
20	754	785
21	203*	76
22	528	552
23	191*	67
6,6,L		
0	772	745
1	289	350
2	181*	37
3	181*	13
4	498	548
5	189*	138
6	189*	127
7	278	312
8	291	273
9	298	228
10	232	247
11	196*	94
12	334	266
13	206*	185
14	422	346
15	225	249
16	370	337
17	236*	101
18	411	343
19	209*	171
20	309	218
21	207*	167
22	244	271
6,7,L		
0	495	491
1	701	810
2	802	830
3	194*	92
4	186*	66
5	390	350
6	1043	1087
7	574	573
8	832	808
9	446	470
10	351	281
11	207*	80
12	576	539
13	363	393
14	828	792
15	652	631
16	219*	262
17	310	225
18	211*	160
19	444	411
20	354	371
21	314	338
6,8,L		
0	186*	47
1	188*	119
2	256	240
3	338	368
4	192*	153
5	194*	87
6	275	345
7	488	507
8	361	307
9	226	194
10	199*	6
11	394	366
12	304	240
13	204*	132
14	210*	131
15	209*	196
16	202*	20
17	200*	92
18	195*	122
19	214	211
20	196*	63
6,9,L		
0	538	531
1	716	743
2	189*	52
3	375	380
4	191*	61
5	377	405
6	198*	99
7	1027	1127
8	481	486
9	719	684
10	199*	16
11	293	347
12	205*	190
13	610	661
14	200*	100
15	545	532
16	281	313
17	276	300
18	189*	49
6,10,L		
0	213*	90
1	280	179
2	202*	149
3	205	217
4	201*	145
5	202*	174
6	324	245
7	316	300
8	418	431
9	296*	104
10	222*	64
11	327	316
12	282	274
13	190*	6
14	191*	45
15	195*	244
16	191*	58
6,11,L		
0	194*	185
1	672	724
2	200*	116
3	227	258
4	197*	107
5	619	614
6	276	200
7	653	650
8	466	458
9	426	414
10	191*	64
11	195*	104
12	199*	268
13	642	641
14	180*	41
6,12,L		
0	475	466
1	191*	83
2	184*	65
3	189*	93
4	292	330
5	184*	106
6	188*	34
7	192*	134
8	204*	132
9	181*	61
10	206	196
6,13,L		
0	680	691
1	515	469
2	274	320
3	180*	87
4	231	229
7,0,L		
2	1416	1416
4	1487	1472
6	205*	164
8	307	348
10	746	730
12	1259	1276
14	313	276
16	911	927
18	961	947
20	323	331
22	291	304
24	462	449
7,1,L		
1	175*	73
2	181*	93
3	559	545
4	187*	30
5	907	886
6	869	790
7	205*	29
8	211*	228
9	545	593
10	784	805
11	628	626
12	452	378
13	224*	131
14	218*	122
15	310	214
16	303	256
17	224*	163
18	227*	157
19	408	434
20	225*	204
21	261	294
22	216*	106
23	349	349
24	215	289
7,2,L		
1	740	733
2	777	768
3	971	963
4	971	999
5	250	284
6	803	760
7	197*	17
8	421	434
9	384	315
10	1127	1137
11	608	599
12	580	556
13	499	544
14	225*	33
15	221*	127
16	409	404
17	842	782
18	692	703
19	394	373
20	458	422
21	223*	150
22	215*	103
23	207*	142
24	547	566
7,3,L		
1	878	923
2	284	302
3	614	620
4	693	695
5	255	316
6	258	179
7	196*	131
8	257	206
9	203*	26
10	325	348
11	214*	228
12	448	492
13	475	470
14	218*	8
15	218*	100
16	342	283
17	798	765
18	316	275
19	221*	120
20	222*	277
21	372	356
22	207*	88
23	215	164
24	325	275
7,4,L		
1	216*	140
2	182*	93
3	979	1033
4	441	433
5	1259	1277
6	289	338
7	195*	39
8	200*	205
9	907	941
10	454	442
11	1070	1067
12	215*	185
13	342	322
14	213*	72
15	438	377
16	221*	86
17	477	492
18	221*	173
19	731	709
20	335	251
21	313	340
22	203*	15
23	545	557
7,5,L		
1	460	457
2	806	849
3	185*	32
4	595	592
5	354	351
6	242	164
7	197*	185
8	197*	33
9	200*	19
10	201*	119
11	208*	75
12	726	740
13	212*	49
14	224*	279
15	354*	182
16	606	570
17	320	290
18	523	517
19	215*	54
20	214*	22

TABLE 7. pt. 3. OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PARA-COSTIBITE*

7,5,L		
21	300	243
22	272*	163
7,6,L		
1	498	543
2	191*	13
3	951	975
4	363	335
5	737	788
6	476	486
7	197*	157
8	206*	240
9	806	785
10	598	584
11	867	884
12	213*	24
13	311	392
14	214*	131
15	221*	185
16	210*	14
17	690	735
18	216*	153
19	590	600
20	238	272
21	201*	78
7,7,L		
1	201*	189
2	196*	142
3	481	467
4	303	289
5	192*	102
6	662	667
7	204*	174
8	281	260
9	236*	94
10	765	797
11	353	247
12	206*	50
13	368	389
14	211*	72
15	210*	167
16	206*	57
17	300	317
18	338	290
19	239*	129
20	280	295
7,8,L		
1	399	393
2	604	648
3	699	679
4	830	820
5	249	243
6	205*	183
7	205*	78
8	216	238
9	207*	137
10	468	496
11	460	443
12	661	691
13	427	460
14	209*	103
15	204*	157
16	519	505
17	542	542
18	525	534
19	278	281
7,9,L		
1	199*	136
2	201*	47
3	204*	218
4	303	339
5	571	676
6	208*	20
7	204*	118
8	205*	85
9	554	573
10	199*	11
11	430	428
12	257	250
13	203*	94
14	201*	56
15	198*	103
16	201*	104
17	193*	14
7,10,L		
1	205	179
2	808	792
3	203*	107
4	702	678
5	231*	175
6	340	291
7	194*	44
8	214	219
9	204*	134
10	655	635
11	200*	29
12	559	587
13	243*	144
14	194*	174
15	187*	7
7,11,L		
1	347	369
2	252	254
3	382	384
4	220	243
5	191*	113
6	244	255
7	194*	92
8	196*	167
9	243	207
10	233	245
11	249	282
12	186*	19
7,12,L		
1	183*	129
2	210	197
3	431	402
4	583	567
5	322	318
6	395	406
7	179*	38
8,0,L		
0	2136	2237
2	594	565
4	782	766
6	705	695
8	1057	1030
10	472	444
12	348	333
14	1137	1083
16	1127	1113
18	464	420
20	793	846
22	301	294
8,1,L		
0	203*	65
1	254	259
2	256*	42
3	267	333
4	282	299
5	233	222
6	223*	135
7	650	597
8	553	541
9	299	295
10	316	187
11	242*	192
12	270	325
13	351	362
14	247*	156
15	266*	163
16	239*	10
17	242*	94
18	266*	154
19	236*	3
20	226*	10
21	242*	330
22	312	214
23	254	277
8,2,L		
0	561	573
1	906	900
2	889	875
3	203*	53
4	207*	59
5	836	829
6	1127	1146
7	220*	291
8	834	879
9	227*	262
10	229*	283
11	415	453
12	560	564
13	642	632
14	834	819
15	847	846
16	306	306
17	240*	44
18	233*	155
19	321	384
20	432	408
21	423	398
22	787	806
23	208*	114
8,3,L		
0	343	318
1	536	556
2	255	278
3	399	374
4	201*	64
5	216	229
6	372	365
7	212*	56
8	302	275
9	214*	121
10	217*	110
11	222*	182
12	221*	174
13	228*	91
14	346	323
15	512	481
16	232*	149
17	227*	67
18	230*	20
19	474	407
20	222*	185
21	222*	29
22	287	227
8,4,L		
0	199*	166
1	865	909
2	258	251
3	310	319
4	203*	157
5	273	224
6	415	370
7	1413	1481
8	502	540
9	907	939
10	213*	19
11	658	685
12	346	319
13	645	617
14	228*	138
15	549	545
16	226*	114
17	461	476
18	226*	128
19	322	270
20	220*	129
21	645	679
22	321	334
8,5,L		
0	650	686
1	201*	167
2	282	261
3	328	239
4	393	375
5	202*	14
6	229	294
7	202*	107
8	208*	61
9	213*	19
10	226	261
11	213*	47
12	208*	10
13	215*	66
14	488	528
15	223*	140
16	330	331
17	218*	29
18	279	212
19	235	177
20	308	309
21	202*	69
8,6,L		
0	200*	227
1	816	840
2	354	361
3	472	456
4	385	334
5	772	748
6	531	526
7	901	934
8	542	481
9	537	548
10	206*	41
11	206*	41
12	373	387
13	837	825
14	292*	121
15	747	730
16	263*	104
17	218*	192
18	260	267
19	207*	202
20	201*	34
8,7,L		
0	200*	126
1	274	298
2	218	149
3	197*	40
4	217	181
5	254	248
6	248	259
7	205*	64
8	552	545
9	207*	71
10	209*	93
11	214*	140
12	357	334
13	221*	179
14	210*	26
15	278	293
16	208*	79
17	204*	11
18	204*	112
19	212	175
8,8,L		
0	1096	1115
1	655	721
2	325	326
3	234	147
4	320	309
5	441	427
6	447	434
7	295	254
8	669	695
9	293	292
10	256	194
11	267	191
12	217*	280
13	242	353
14	579	571
15	668	664
16	586	613
17	208*	125
8,9,L		
0	195*	7
1	199*	90
2	200*	104
3	279	307
4	204*	5
5	201*	78
6	286*	130
7	495	513
8	203*	19
9	318	239
10	213*	50
11	229	256
12	203*	34
13	242	253
14	209*	108
15	199*	6
8,10,L		
0	836	823
1	199*	128
2	616	570
3	195*	128
4	352	292
5	254	187
6	740	708
7	273	244
8	433	427
9	251*	106
10	371	363
11	344	283
12	231	221
13	188*	48
8,11,L		
0	196*	130
1	299	307
2	193*	99
3	191*	72
4	199*	175
5	187*	144
6	228	165
7	192*	157
8	285	229
9	223	149
8,12,L		
0	275	304
1	434	397
9,0,L		
2	285	258
4	851	860
6	386	419
8	339	358
10	501	487
12	311	372
14	281*	262
16	268*	61
18	256*	18
20	592	573
22	218*	7
9,1,L		
1	292	288
2	212*	12
3	974	966
4	355	340
5	1081	1069
6	536	542
7	228*	100
8	243*	262
9	912	894
10	616	633
11	998	975
12	249*	11
13	333	318
14	385*	131
15	392	280
16	298*	49
17	574	570
18	273*	170
19	586	675
20	293	301
21	243	244
9,2,L		
1	206*	51
2	655	649
3	210*	1
4	217*	121
5	416	416
6	226*	137
7	282	329
8	228*	12
9	601	619
10	375	328
11	359	261
12	246*	218
13	252*	244
14	250*	234
15	249*	93
16	252*	248
17	241*	22
18	505	451
19	317	225
20	231*	58
21	229*	174
9,3,L		
1	652	654
2	724	659
3	781	829
4	935	923
5	216*	138
6	399	393
7	226*	28
8	364	325
9	254	147
10	728	738
11	552	499
12	635	666
13	609	570
14	243*	58
15	242*	132
16	490	473
17	727	756
18	573	591
19	238*	287
20	360	351
21	217*	190
9,4,L		
1	209*	165
2	332	287
3	614	668
4	308*	117
5	231*	192
6	220*	113
7	362	319
8	218*	27
9	257	198
10	252*	37
11	412	348
12	281	219
13	620	578
14	236*	127
15	336	276
16	264	185
17	359	382
18	229*	165
19	228*	193
20	217*	46
9,5,L		
1	212*	206
2	1059	1094
3	206*	77
4	891	933
5	216*	181
6	212*	172
7	214*	12
8	222*	225
9	239*	86
10	634	620
11	224*	27
12	909	915
13	234*	104
14	288	264
15	227*	35
16	775	735
17	232*	169
18	833	816
19	216*	40
9,6,L		
1	325	334
2	531	518
3	216*	318
4	211*	103
5	213*	214
6	212*	163
7	218*	186
8	218*	116
9	360	364
10	219*	57
11	349	308
12	223*	148
13	278*	110
14	230	258
15	218*	47
16	249	225
17	350	342
18	365	291
9,7,L		
1	331	320
2	334	334
3	631	631
4	706	715
5	362	294
6	608	613
7	216*	74
8	287	360
9	260	180
10	872	866
11	397	450
12	371	330
13	422	398
14	229*	65
15	213*	184
16	256	196
17	493	481
9,8,L		
1	201*	123
2	204*	56
3	206*	66
4	419	472
5	420	404
6	210*	147
7	213*	92
8	214*	170
9	403	350
10	217*	203
11	215*	232
12	325	272
13	208*	104
14	207*	105
15	200*	50
9,9,L		
1	199	108
2	205*	124
3	599	558
4	271	283
5	845	826
6	204*	93
7	207*	135
8	202*	92
9	727	753
10	197*	172
11	673	684
12	274	206
13	191*	84
9,10,L		
1	192*	85
2	242	174
3	234	160
4	244	202
5	193*	128
6	275	336
7	191*	149
8	199*	131
9	296	240
10	415	443
9,11,L		
1	356	367
2	183*	74
3	646	642
4	312	280
10,0,L		
0	621	693
2	302	358
4	419	413
6	341	401
8	252*	9
10	399	348
12	273*	13
14	628	675
16	287*	318
18	272*	232
20	312	323
10,1,L		
0	445	432
1	1089	1054
2	329	315
3	229*	4
4	315	362
5	607	577
6	245	326
7	770	769
8	319	204
9	712	601
10	375	346
11	262*	8
12	268*	126
13	580	613
14	655	580
15	886	879
16	305	201
17	266*	278
18	261*	167
19	502	488
20	242*	218
10,2,L		
0	328	313
1	518	488
2	291	196
3	234*	258
4	222*	73
5	284	223
6	312	309
7	233*	31
8	448	543
9	254*	146
10	249*	33
11	285*	138
12	352	311
13	257*	145
14	259*	145
15	479	439
16	255*	179
17	249*	53
18	246*	48
19	375	351
10,3,L		
0	818	905
1	234	198
2	492	439
3	668	632
4	296*	161
5	300	322
6	579	593
7	820	829
8	771	769
9	372	367
10	244*	179
11	251*	223
12	457	374
13	491	538
14	538	572
15	283*	121
16	457	501
17	241*	121
18	237*	59
19	232*	187
10,4,L		
0	210*	38
1	244	159
2	222*	102
3	493	431
4	222*	132
5	230	229
6	226*	166
7	562	615
8	313	245
9	248	260
10	237*	49
11	277	203
12	242*	170
13	380	382
14	239*	6
15	237*	88
16	232*	10
17	228*	86
18	227*	96
10,5,L		
0	647	661
1	276	188
2	567	576
3	346	306
4	219*	122
5	222*	82
6	813	820
7	226*	98
8	1109	1092
9	229*	54
10	225*	86
11	225*	14
12	646	629
13	231*	121
14	533	515
15	230*	147
16	424	385
17	220*	68
10,6,L		
0	211*	79
1	386	367
2	203*	72
3	212*	28
4	285	240
5	222*	155
6	226*	161
7	397	386
8	486	419
9	317	269
10	225*	146
11	265*	127
12	299	274
13	242	232
14	220*	112
15	273	272
16	210*	21
10,7,L		
0	736	782
1	287	352
2	516	484
3	242	170
4	277	359
5	220*	119
6	543	574
7	585	613
8	218*	227
9	384	381
10	397	379
11	363	271
12	212*	88
13	352	291
14	773	773
10,8,L		
0	367	328
1	300	326
2	278	228
3	212*	134
4	206*	164
5	273	222
6	297	277
7	210*	17
8	210*	80
9	237*	64
10	204*	169
11	202*	178
12	201*	52
10,9,L		
0	297	365
1	804	790
2	200*	54
3	195*	77
4	201*	63
5	471	488
6	198*	84
7	343	395
8	345	296
9	379	357
10,10,L		
0	486	472
1	189*	153
2	189*	142
3	227	188
4	194*	181
5	242*	57
11,0,L		
2	374	341
4	1092	1071
6	724	761
8	567	499
10	1083	1086
12	598	530
14	282*	153
16	280*	298
18	593	501
11,1,L		
1	231*	150
2	445	458
3	459	381
4	240*	170
5	247*	150
6	245*	51
7	254*	93
8	257*	106
9	260*	2
10	265*	48
11	359	247
12	270*	47
13	374	301
14	276*	219
15	268*	120
16	265*	150
17	265*	254
11,2,L		
1	239*	29
2	812	801
3	400	346
4	706	669
5	685	703
6	317	211
7	250*	174
8	253*	190
9	677	687
10	520	545
11	584	533
12	643	621
13	256*	44
14	263*	192
15	254*	110
16	494	507
17	252*	154
11,3,L		
1	225*	53
2	226*	115
3	234*	42
4	315	312
5	288	284
6	241*	58
7	362	279
8	248*	82
9	487	489
10	249*	125
11	252*	160
12	285	246
13	257*	228
14	244*	11
15	243*	126
16	242*	132
17	234*	11
11,4,L		
1	645	550
2	388	384
3	1017	1011
4	252	236
5	490	438
6	231*	45
7	229*	103
8	235*	22
9	334	280
10	237*	85
11	770	705
12	252*	305
13	652	650
14	242*	135
15	241	260
16	258	257
11,5,L		
1	220*	72
2	219*	51
3	226*	133
4	375	368
5	224*	13
6	336	298
7	232*	199
8	234*	184
9	260	230
10	341	351
11	231*	20
12	229*	122
13	253	192
14	224*	98
15	252*	139
11,6,L		
1	430	373
2	459	530
3	750	744
4	221*	163
5	553	586
6	251*	168
7	263*	69
8	223*	39
9	583	539
10	219*	17
11	640	670
12	382	345
13	375	336
11,7,L		
1	210*	108
2	400	442
3	211*	82
4	210*	21
5	355	245
6	214*	13
7	214*	17
8	210*	42
9	213*	135
10	213*	127
11	212*	140
11,8,L		
1	201*	25
2	356	301
3	246	260
4	634	624
5	597	555
6	367	371
7	201*	107
8	264	266
9	495	498
11,9,L		
1	277	201
2	197*	21
3	253	307
4	194*	195
12,0,L		
0	721	726
2	435	422
4	249*	56
6	654	621
8	999	1009
10	269*	37
12	463	531
14	407	389
12,1,L		
0	550	557
1	483	495
2	232*	15
3	240*	8
4	376	335
5	429	376
6	250*	54
7	261*	241
8	257*	51
9	262*	193
10	268*	137
11	269*	131
12	264*	122
13	272*	330
14	318*	231
15	424	463
12,2,L		
0	626	620
1	240*	244
2	519	463
3	256	362
4	241*	205
5	249	259
6	631	575
7	523	574
8	402	356
9	355	279
10	282	287
11	259*	132
12	259*	189
13	276	379
14	663	644
12,3,L		
0	325	323
1	222*	37
2	296	253
3	292	250
4	227*	74
5	231*	98
6	254*	337
7	633	568
8	250*	264
9	291	291
10	240*	109
11	381	424
12	243*	164
13	245*	143
14	333	322
12,4,L		
0	310	352
1	820	801
2	225*	124
3	224*	101
4	233*	145
5	450	357
6	257*	145
7	519	531
8	237*	124
9	401	467
10	229*	117
11	231*	31
12	226*	33
13	418	400
12,5,L		
0	217*	88
1	222*	58
2	314	310
3	224*	44
4	222*	197
5	221*	141
6	445	464
7	227*	165
8	511	564
9	224*	89
10	221*	24
11	226*	213
12,6,L		
0	292	319
1	548	541
2	209*	153
3	218*	245
4	212*	214
5	495	448
6	218*	159
7	607	574
8	216*	50
9	386	353
12,7,L		
0	598	610
1	205*	84
2	202*	104
3	235	213
4	284	303
5	201*	86
6	207*	111
13,0,L		
2	300	352
4	245*	250
6	262*	317
8	262*	68
10	289	240
13,1,L		
1	393	378
2	305	345
3	784	768
4	249*	153
5	531	515
6	248*	11
7	250*	7
8	249*	18
9	411	421
10	252*	111
11	637	643
13,2,L		
1	413	356
2	235*	28
3	238*	226
4	234*	62
5	250*	222
6	247*	289
7	241*	8
8	248*	88
9	246*	126
10	396	327
13,3,L		
1	226*	78
2	395	467
3	325	329
4	527	603
5	530	487
6	243*	272
7	237*	92
8	240*	216
9	471	458
10	494	516
13,4,L		
1	352	273
2	223*	130
3	216*	32
4	227*	103
5	434	423
6	231*	177
7	225*	15
8	225*	86
13,5,L		
1	211*	38
2	385	408
3	212*	43
4	756	711
5	216*	58
6	473	449
14,0,L		
0	251	194
2	303	334
4	241*	47
14,1,L		
0	222*	191
1	382	406
2	232*	207
3	231*	236
4	283	241
14,2,L		
0	454	448
1	219*	169
2	226*	154
3	260*	98

*The structure factors are listed in blocks of constant *hk* in columns of *l*, $[F_o] \times 10$, and $[F_c] \times 10$.