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The x-ray crystal and molecular structure of an organic mineral: simonellite, $C_{19}H_{24}$

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Mineralogia. — *The x-ray crystal and molecular structure of an organic mineral: simonellite,* $C_{19}H_{24}$ [(*)]. Nota di ELISABETTA FORESTI e LODOVICO RIVA DI SANSEVERINO [(**)], presentata [(***)] dal Socio P. GALLITELLI.

RIASSUNTO. — Si descrive uno studio cristallografico della simonellite, chimicamente 1,1-dimetil-7-isopropil-1 , 2 , 3 , 4-tetraidrofenantrene. I dati cristallografici sono $a = 9.231$ Å, $b = 9.134$ Å, $c = 36.01$ Å, *Pnaa*, $Z = 8$.

Mentre ogni tentativo di risolvere la struttura per mezzo di un calcolo tridimensionale Patterson risultava inutile, l'impiego dei metodi diretti attraverso la formula « sigma 2 » di Karle e Karle (1966) ha rivelato subito 18 dei 19 atomi di carbonio della simonellite.

Il raffinamento con il metodo dei minimi quadrati con fattori di temperatura isotropi ha dato un R finale di 12%, su 2432 riflessi misurati.

Si discute la stereochimica intramolecolare e si prospetta una possibilità di biogenesi per questo minerale organico, trovato come incrostazioni biancastre in una miniera di lignite di Fognano, Siena.

INTRODUCTION.

Simonellite had been studied in this Institute by Boeris (1919) about fifty years ago; it appears as white-yellowish crusts in the lignite mine, at Fognano, Siena (Italy).

Optical, morphological and crystal data were then collected by Emiliani and Pellizzer (1952, 1953) and *x*-ray crystal structure analysis began during the fall 1964. Ghigi and Fabbri (1965) studied simonellite by chemical and spectroscopic means and then synthetized the mineral (Ghigi *et al.*, 1968). This is a report of the crystal structure analysis.

EXPERIMENTAL.

Simonellite, $C_{19}H_{24}$, M.W. 252, M.P. 59°–60° C; samples selected in the Museum of this Institute and recrystallized from benzene. Orthorhombic, *Pnaa* [(1)] from systematic absences; cell dimensions measured by Emiliani and Pellizzer (1953) have been confirmed, $a = 9.231 \pm 0.003$ Å, $b = 9.134 \pm 0.003$ Å, $c = 36.01 \pm 0.01$ Å. They have been calculated by a least squares refinement on 84 reflection angles ϑ, obtained from $o\,k\,l$ and $h\,o\,l$ Weissenberg photographs, calibrated with Al (Van den Berg, 1964), $V = 3037$ Å^3, $Dm = 1.08$,

(*) Istituto di Mineralogia e Petrografia dell'Università di Bologna.

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(***) Nella seduta del 12 giugno 1969.

(1) This space group has been preferred to the conventional *Pccn*, to respect a tendency to tetragonal symmetry pointed out by Emiliani and Pellizzer (1953).

$Dx = 1.10$, $Z = 8$. Crystal dimensions $0.5 \times 0.5 \times 0.6$ mm., radiation used CuK ($\lambda = 1.5418$ Å).

Of the 2432 densitometrically measured reflections, 899 have been classified as " unobserved ", giving them 1/2 of the minimum observed intensity. Data have been recorded with the Weissenberg multiple film equinclination technique along the *a* axis (*o k l* till *7 k l*) and corrected for spot deformation (Riva di Sanseverino, 1967) but not for absorption. Scaling was assured through cross layer correlation calculations.

Atomic scattering factors have been taken from the International Tables for Crystallography, vol. III. During the first steps computer programs written by Albano *et al.* (1963) have been used, but more recently the Stewart " X Ray 63 " system (1964) has been adopted.

The first trial for structure solution.

As the simonellite structure (fig. 1) was suspected to be similar to retene (Ghigi and Fabbri, 1965), it was then supposed that the stereographic projection of the Patterson function could reveal the molecular plane. This method,

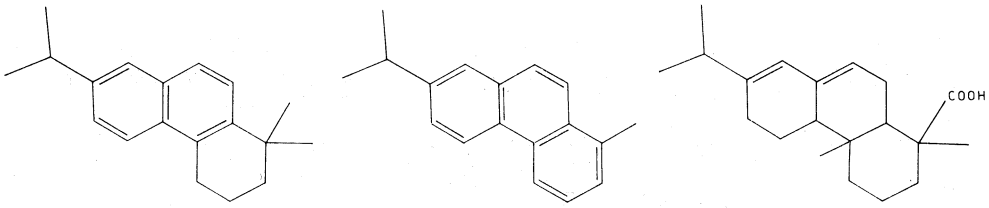


Fig. 1. – Simonellite (*a*) and the two related structures, retene (*b*) and abietic acid (*c*).

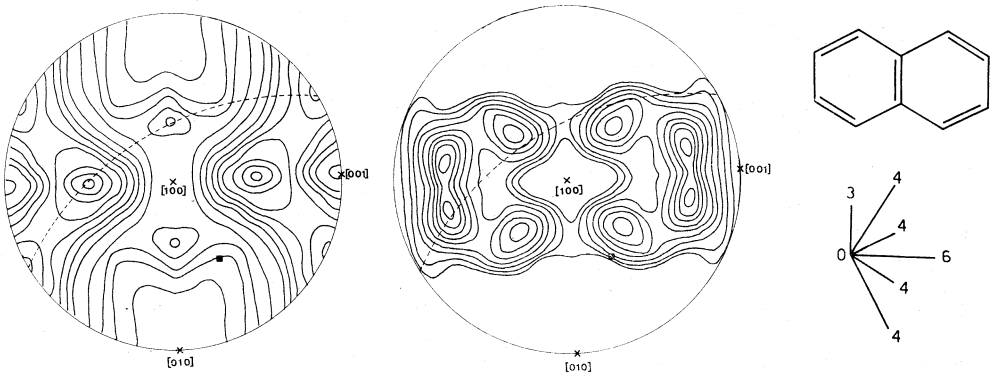
developed by the MacGillavry school in Amsterdam (Stam and Riva di Sanseverino, 1966; Bart and MacGillavry, 1968), consists in building spheres of a chosen radius around the origin of the Patterson function and then in plotting a stereographic projection of the maxima lying on the sphere.

In the case of planar hydrocarbon molecules, containing chains or rings, typical sequencies of 3 peaks will be aligned along the same major circle in the stereographic projection of the 1.4 and the 2.4 Å spheres. Alternatively three 1.4 Å peaks will be disposed at 60° interval, as well as the three 2.4 Å peaks, as shown by the scheme in fig. 2 *c*. Peak heights will be proportional to the vector multeplicity in the internal geometry of the molecule.

Fig. 2 *a* more than fig. 2 *b* shows these features. The direction cosines of the normal (full square in fig. 2) to the supposed molecular plane in the x, y, z coordinates system are respectively $\cos \varphi = 0.54$, $\cos \chi = 0.78$, $\cos \psi = 0.36$.

Although these values were later confirmed (Table V) no trial succeeded in the positioning of the molecule. A noteworthy influence on these negative

approaches could possibly be caused by the high symmetry of the orthorhombic system and/or by the not perfect planarity of the molecule and/or by the exaggerate grid of the Patterson function, forcedly imposed by the contrasting conditions of large cell dimensions and of the relatively small IBM 1620 computer.



(*a*) (*b*) (*c*)

Fig. 2. – Stereographic projection of spherical sections around the origin of the Patterson function for simonellite with radii 1.4 A (*a*) and 2.4 A (*b*). The dashed lines indicate the probable plane of two of the eight molecules in the unit cell and the full square the emergence of the normal to the plane. As an example, naphtalene and its Patterson vectors pattern are reported in (*c*): numbers indicate peak multiplicity.

THE APPLICATION OF Σ_2.

More recently a bigger computer (IBM 7094) and the development of direct methods (see Karle and Karle, 1966) encouraged a new attack to the structure solution from a different point.

As only the listing of E's and the relative statistics were available, a program for the application of the Σ_2

$$sE_{\boldsymbol{h}} \cong s \sum_{\boldsymbol{k}} E_{\boldsymbol{k}} E_{\boldsymbol{h}-\boldsymbol{k}}$$

was prepared (Foresti and Guerrieri, 1969). While the statistics (Table I) confirmed the centrosymmetric space group, the criteria for the choice of the origin (Stout and Jensen, 1968) were applied, giving positive signs to reflections 4, 5, 16; 1, 1, 31; and 4, 4, 25.

These assignments were sufficient to attribute signs to 134 of the 153 chosen E's with $E > 1.85$, probably owing to the large number of internal relations among orthorhombic structure factors. When the refinement was terminated, it was found that only three signs were inverted.

The 134 signs produced the first E map, which showed all atoms but one (C16); this last was revealed by a successive three-dimensional F_o fourier, including all the observed structure factors.

A full matrix least squares refinement cycle with isotropic temperature factors lowered R from 28 % to 18.8 %. The successive difference fourier gave significant positive electron density at 20 sites which were correspondent to good positions for hydrogen atoms. The remaining 4 were assigned theoretical positions and the structure factor calculation gave R = 16.7 %.

TABLE I.

Normalized structure factors.

Values	Experimental for Simonellite	Theoretical for	
		Centrosymmetric	Non-centrosymmetric
$<\|E\|>$	0.745	0.798	0.886
$<\|E^2-1\|>$ . . .	1.083	0.968	0.736
$<\|E\|^2>$	1.000	1.000	1.000
$E>1$	30.5%	32.0%	36.8%
$E>2$	5.0%	5.0%	1.8%
$E>3$	0.9%	0.3%	0.01%

Two further refinement cycles as before, with hydrogen coordinates held constant (B = 6 Å^2), brought R [2] to 12.0 % and refinement was terminated, as standard deviations and stereochemical results seemed satisfactory.

Final parameters are listed in Table II, observed and calculated structure factors in Table III [3], bond distances in fig. 3 and angles in Table IV. Standard deviations for distances, obtained from the final least squares refinement cycle are $\bar{\sigma}$ = 0.008 Å for C—H (sp^2) with a maximum of 0.009 Å for C9—C10 and $\bar{\sigma}$ = 0.009 Å for C—H (sp^3) with a maximum of 0.01 Å for C17—C18.

DISCUSSION.

It is encouraging to notice from Table II that the refined temperature factors are highest for the atoms departing from the phenanthrene nucleus, as expected. Furthermore, while atom C16 could not be found, atoms C15, C17, C18 and C19 appeared well as peaks in the E map, but with a height about 30 % lower than the average peak height.

(2) The last cycle was run with weights, following the expression recommended by Cruickshank *et al.* (1961) for photographic data.

(3) Reflections 004, 006, 008, 019 and 0, 2, 10 were discarded as they were too strong to be measurable.

TABLE II

Fractional positional parameters with s.d. and temperature factors.

ATOM	x	y	z	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	B (Å^2)
C1	0.09458	0.58012	0.18070	0.00066	0.00059	0.00015	3.45
C2	0.11495	0.47394	0.21374	0.00071	0.00063	0.00015	4.07
C3	0.26874	0.46425	0.22579	0.00072	0.00065	0.00016	3.83
C4	0.36318	0.40037	0.19476	0.00067	0.00060	0.00015	3.47
C5	0.56490	0.37095	0.13186	0.00067	0.00061	0.00014	3.46
C6	0.66610	0.35811	0.10416	0.00070	0.00064	0.00016	4.06
C7	0.64867	0.43797	0.07029	0.00064	0.00058	0.00014	3.31
C8	0.53031	0.52239	0.06625	0.00067	0.00060	0.00015	3.39
C9	0.29930	0.62198	0.08954	0.00073	0.00067	0.00016	3.97
C10	0.19724	0.63518	0.11755	0.00069	0.00063	0.00015	3.55
C11	0.21548	0.56019	0.15204	0.00063	0.00057	0.00014	2.92
C12	0.33539	0.47711	0.15772	0.00060	0.00054	0.00013	2.74
C13	0.44191	0.45964	0.12869	0.00059	0.00052	0.00013	2.60
C14	0.42167	0.53550	0.09458	0.00062	0.00055	0.00013	2.98
C15	0.09385	0.74048	0.19488	0.00076	0.00074	0.00016	4.73
C16	—0.05379	0.54551	0.16356	0.00081	0.00077	0.00019	5.07
C17	0.76321	0.42646	0.03970	0.00071	0.00067	0.00016	4.34
C18	0.91250	0.46952	0.05351	0.00090	0.00085	0.00020	5.95
C19	0.76532	0.27374	0.02213	0.00083	0.00084	0.00019	5.71

The average distances C—C (sp^2) = 1.401 Å and C—C (sp^3) = 1.539 Å agree extremely well with those published by Sutton (1965). The observed trend in simonellite follows a certain regularity and corresponds with features found in phenanthrene (Trotter, 1963). Trotter compares theoretical and observed values for each bond length and concludes that for *f* bond and *g* bond (see fig. 3) there is no agreement. This is repeated in the simonellite structure: again, bond *f* in noteworthy longer and bond *g* somewhat shorter than foreseen. The first seems to show a smaller, and the second a larger aromatic character than it might be deduced by the resonance structures or by LCAO bond orders (Dictionary of values of molecular constants, 1955).

A fair analogy with these findings has been also found in different aromatic compounds, with a similar disposition of fused rings (Ferrier and Iball, 1963 a, b).

Regarding bond angles (Table IV), simonellite shows a remarkable planarity at junctions, while angles at C5 and C8 are slightly greater than expected; tetrahedral angles do not reveal any particular strain. The average standard deviation for angles is 0.5°.

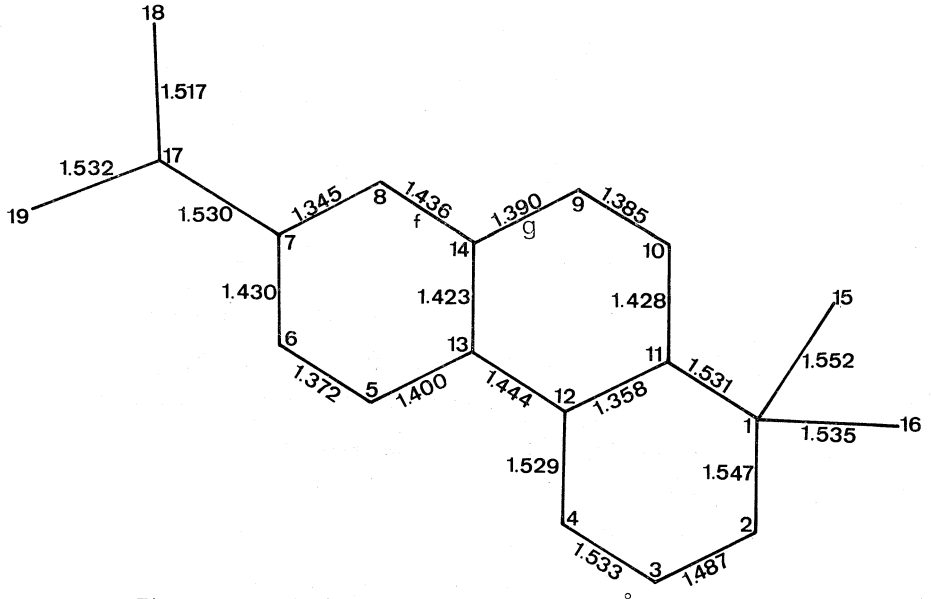


Fig. 3. – Numbering and bond distances in Å for simonellite.

The planarity of the aromatic part of the molecule is calculated through the equations (1 D and 1 A) listed in Table V, together with atomic distances in Angstrom from the least square plane. Two further equations (2 D and 2 A) are quoted for a comparison, calculated for the least square plane through the whole molecule. The equations have been listed both for fractional coordinates (direct space) and for actual position in the crystal cell (Angstrom space).

As already noticed, these equations (specially 1 A) correspond almost perfectly with that resulting from the stereographic projection of the Patterson function (fig. 2), regardless of the distance from the origin, obviously indeterminated in the three-dimensional synthesis.

The inverse and probably significant displacement of C4 and C5 needs one more comment; the same behaviour is shown by the equivalent atoms in the 1,2-*cyclo*-penteno-phenanthrene molecule studied by Entwistle and Iball (1961). In the simonellite molecule a noticeable agreement is found with the considerations made by Trotter (1963) who attributed the effect to « slight intermolecular overcrowding involving the hydrogen atoms bonded to C4 and C5 ».

TABLE III.

Structure factors for simonellite: columns are l, 10 F_o and 10 F_c. Unobserved reflections are marked with L.

	0,0,L	28	131 -123	6	29L 49		1,3,L	17	152 123	9	37L -47		2,1,L	18	103 73
		30	34L 39	8	89 -106			18	154 -149	10	198 -164			19	84 63
10	165 221	32	134 147	10	28L 37	1	117 82	19	35L -17	11	109 -136	0	343 392	20	26L -9
12	537 -482	34	64 -77	12	27L 17	2	239 223	20	36L 61	12	37L 71	1	96 95	21	102 -87
14	199 113	36	30L -52	14	26L -37	3	223 215	21	84 -75	13	129 148	2	512 -573	22	59 63
16	222 -243	38	27L 27			4	619 -639	22	147 -129	14	37L -70	3	206 -208	23	28L 6
18	106 10	40	24L 26		0,11,L	5	488 -495	23	37L -25	15	37L -78	4	407 431	24	82 -59
20	100 -5					6	233 -162	24	37L 4	16	37L 44	5	593 686	25	89 -100
22	171 -181		0,5,L	1	88 -127	7	74 -57	25	83 -55	17	37L -17	6	696 764	26	181 157
24	195 -140			3	89 158	8	22L -3	26	37L -24	18	36L -23	7	719 768	27	70 -73
26	129 112	1	103 78	5	138 175	9	23L -6	27	72 62	19	36L -40	8	539 -530	28	69 -57
28	313 -291	3	137 -96	7	57 -93	10	446 440	28	37L -11	20	35L -25	9	15L 4	29	115 76
30	169 142	5	516 -583	9	63 -86	11	126 131	29	37L 14	21	119 -119	10	201 195	30	181 -177
32	421 398	7	26L 67	11	19L -22	12	242 -241	30	66 61	22	103 110	11	275 212	31	211 203
34	245 -235	9	411 -394	13	17L 54	13	166 152	31	36L 10	23	33L 66	12	391 -299	32	30L 27
36	207 -197	11	170 -205	15	15L -22	14	585 526	32	172 151	24	32L 54	13	444 418	33	155 124
38	88 -32	13	355 379			15	209 155	33	123 108	25	31L -6	14	276 -195	34	60 79
40	64 30	15	64 -60		1,1,L	16	28L 5	34	83 69	26	73 -95	15	40 13	35	29L 9
42	57 -34	19	320 -317			17	78 79	35	60 -45	27	29L 29	16	473 440	36	28L -17
44	119 110	21	221 239	1	661 683	18	279 -262	36	59 -74	28	27L -17	17	115 -98	37	62 50
		23	239 212	2	936 933	19	163 -163	37	79 -93			18	151 -145	38	25L 38
	0,1,L	25	71 -69	6	364 -397	20	128 109	38	26L -13		1,9,L	19	23L 13	39	24L -19
		27	113 -142	7	74 -110	21	123 -93	39	24L 30			20	53 67	40	44 40
3	450 -403	29	34L -73	8	822 -757	22	63 66	40	55 43	1	37L -0	21	88 92	41	49 -57
5	806 -810	31	87 91	9	554 524	23	183 -144	41	18L -41	2	37L 33	22	87 -89	42	80 -102
7	208 -261	33	31L 30	10	314 292	24	109 105			3	37L -52	23	61 55		
11	480 -402	35	29L 15	11	139 71	25	35L 40		1,6,L	4	66 65	24	62 -61		2,4,L
13	213 214			12	121 -80	26	141 -133			5	84 70	25	175 -173		
15	193 -169		0,6,L	13	133 99	27	36L 35	1	71 51	6	95 75	26	300 255	0	443 426
17	152 -149			14	597 542	28	37L -43	2	93 81	7	36L 39	27	101 -104	1	155 134
19	67 -86	0	257 -250	15	562 524	29	37L 0	3	311 -337	8	112 -95	28	127 -136	2	183 187
21	26L 19	2	90 72	16	106 75	30	101 -76	4	269 253	9	103 -83	29	60 -10	3	618 640
23	28L -39	4	229 -203	17	200 -147	31	157 154	5	200 -190	10	125 -120	30	101 -97	4	403 -410
25	30L 8	6	335 -354	18	289 -245	32	93 93	6	78 104	11	35L 8	31	92 97	5	420 -416
27	224 216	8	350 336	19	430 -368	33	76 81	7	33L -13	12	35L 58	32	31L 23	6	531 -520
29	101 88	10	30L -58	20	61 -34	34	36L 62	8	233 -249			33	31L 36	7	287 -299
31	210 -203	12	31L 0	21	117 101	35	36L -51	9	318 358		1,10,L	34	56 46	8	233 -229
33	129 -121	14	126 146	22	70 54	36	161 -156	10	93 115			35	112 -87	9	535 527
35	217 195	16	130 -128	23	144 -126	37	165 -163	11	83 -91	1	33L 7	36	65 55	10	251 215
37	143 145	18	353 338	24	32L 28	38	90 -80	12	71 71	2	32L 13	37	28L -19	11	135 -110
39	30L -33	20	34L -10	25	61 2	39	30L -18	13	35L 61	3	74 -78	38	61 -63	12	23L 28
41	73 -71	22	70 -74	26	115 116	40	134 133	14	105 -152	4	94 94	39	26L -36	13	176 155
43	23L 15	24	34L 48	27	185 -166	41	26L 20	15	138 -124	5	121 140	40	25L 29	14	158 -145
45	59 64	26	169 -156	28	286 269	42	24L 29	16	36L 2	6	129 152			15	182 -185
		28	33L -17	29	137 114	43	52 42	17	130 126	7	32L -7		2,2,L	16	152 134
	0,2,L	30	31L 19	30	429 -374	44	50 -58	18	63 -74	8	95 -94			17	285 -244
				31	462 434			19	37L 48	9	141 -133	0	548 520	18	84 68
2	341 -333		0,7,L	32	192 -195		1,4,L	20	37L -4	10	123 -141	1	642 684	19	203 213
4	730 -693			33	93 -83			21	113 -132	11	105 -104	2	744 784	20	165 158
6	529 -529	1	176 -189	34	101 100	1	173 -179	22	106 120	12	29L 2	3	363 427	21	53 -50
8	779 -790	3	130 117	35	150 -149	2	238 -230	23	198 189	13	100 113	4	282 -307	22	29L -41
12	322 306	5	32L -38	36	95 78	3	266 -291	24	138 138	14	28L 44	5	539 -508	23	29L 53
14	677 655	7	32L 48	37	137 -119	4	637 612	25	37L 24	15	27L -13	6	209 -156	24	86 88
16	413 -355	9	33L -38	38	34L -27	5	196 211	26	110 -101			7	83 133	25	102 89
18	581 521	11	33L -63	39	33L 1	6	134 155	27	36L -39		1,11,L	8	88 -34	26	30L 8
20	109 -78	13	194 202	40	31L 37	7	102 89	28	96 -86			9	139 122	27	31L -32
22	115 91	15	34L 5	41	29L 16	8	426 -384	29	35L -58	1	51 -62	10	197 214	28	31L -5
24	105 90	17	69 87	42	27L 11	9	648 664	30	34L 34	2	25L -32	11	106 100	29	31L -44
26	31L -3	19	135 -137	43	25L -16	10	209 197	31	68 56	3	24L 30	12	19L 4	30	30L 35
28	33L -11	21	109 140	44	22L -34	11	27L -0	32	32L -31	4	24L -3	13	230 225	31	30L -18
30	90 76	23	33L 26	45	79 101	12	28L 26	33	31L -4	5	85 101	14	137 -160	32	86 63
32	324 332	25	82 -60	46	13L 68	13	28L -53	34	29L 8	6	24L 45	15	239 -204	33	29L 41
34	131 -104	27	113 -90			14	29L -19	35	27L 12	7	23L -32	16	405 369	34	87 66
36	238 -259	29	65 -66		1,2,L	15	30L -5	36	25L 36			17	240 -206	35	27L 5
38	30L 12	31	71 85			16	30L -30	37	23L 55		2,0,L	18	23L -38	36	26L -27
40	28L -1	33	23L 1	1	1419 1532	17	120 97	38	51 25			19	342 -346	37	140 -150
42	73 -50	35	20L 22	2	1020 1094	18	323 -282	39	17L -7	4	615 -631	20	198 -191	38	108 -114
44	76 87			3	78 -14	19	33L 16	40	9L -56	5	152 54	21	152 127	39	47 51
			0,8,L	4	903 965	20	33L 29			6	189 165	22	163 -128	40	66 -51
	0,3,L			5	1230 1302	21	237 -204		1,7,L	7	192 256	23	116 89	41	74 84
		0	34 59	6	583 585	22	159 156			8	732 -708	24	28L 17	42	49 68
1	554 -573	2	34L -20	7	162 -170	23	67 -42	1	137 121	9	381 341	25	165 127	43	10L -64
3	479 408	4	42 -74	8	352 -326	24	129 133	2	35L 30	10	197 -166	26	413 -406		
5	542 -539	6	55 -101	9	152 -138	25	70 -26	3	155 -156	11	559 -474	27	377 360		2,5,L
7	90 -83	8	111 114	10	122 -70	26	37L -57	4	245 253	12	81 -22	28	30L -41		
9	217 132	10	234 254	11	211 -170	27	186 -146	5	36L -0	13	409 435	29	340 -362	0	460 426
11	508 -482	12	106 -110	12	190 -176	28	37L -61	6	115 128	14	389 416	30	132 101	1	344 386
13	1248 1176	14	64 -28	13	155 210	29	108 -107	7	112 111	15	162 224	31	31L -19	2	132 -92
15	345 350	16	33L 67	14	414 363	30	37L 28	8	36L 14	16	923 894	32	31L 32	3	218 169
17	298 -238	18	33L -46	15	370 357	31	104 105	9	91 -91	17	391 -344	33	72 91	4	215 -187
19	154 152	20	32L 40	16	65 -27	32	82 -73	10	80 82	18	76 -52	34	54 25	5	294 284
21	49 52	22	31L -19	17	27L -15	33	127 -125	11	82 70	19	544 -483	35	130 -126	6	281 313
23	177 123	24	29L 13	18	416 -375	34	35L -12	12	37L -6	20	117 -110	36	29L -25	7	109 91
25	32L 59	26	53 -64	19	29L 3	35	72 74	13	37L 3	21	24L -22	37	28L 45	8	46 54
27	107 -107	28	93 -109	20	87 69	36	68 74	14	57 53	22	137 137	38	27L 34	9	137 -132
29	117 114	30	22L 18	21	71 -37	37	113 142	15	37L -63	23	158 115	39	25L 7	10	119 -131
31	353 -335	32	19L -3	22	31L 38	38	30L 50	16	37L 4	24	185 171	40	24L -34	11	88 41
33	275 -260			23	32L -22	39	28L -11	17	37L 13	25	296 295	41	70 58	12	163 -156
35	241 257		0,9,L	24	138 107	40	58 -76	18	37L 22	26	453 -473	42	89 80	13	170 148
37	30L -5			25	34L 23	41	23L -5	19	37L -21	27	439 427			14	83 -100
39	28L -12	1	94 -117	26	59 -4	42	20L -11	20	37L 64	28	29L -14		2,3,L	15	27L 45
41	78 -67	3	112 135	27	81 -105			21	66 60	29	431 -418			16	93 130
43	20L -30	5	187 174	28	36L 2		1,5,L	22	157 -185	30	307 299	0	163 -131	17	46 -32
		7	33L -2	29	37L -39			23	36L 2	31	148 -139	1	100 -91	18	104 -102
	0,4,L	9	205 -202	30	37L 25	1	55 24	24	63 -76	32	59 58	2	216 -184	19	139 143
		11	32L 4	31	129 119	2	28L -55	25	64 -61	33	31L 29	3	194 -229	20	164 135
0	451 507	13	65 85	32	177 -158	3	28L -7	26	77 78	34	63 -92	4	17L 67	21	168 -148
2	83 -78	15	31L -53	33	145 -142	4	28L 10	27	34L -14	35	97 -80	5	464 474	22	130 142
4	750 711	17	100 85	34	37L 2	5	179 -154	28	33L 23	36	29L -15	6	541 558	23	55 -52
6	298 287	19	95 -104	35	67 51	6	29L -29			37	119 99	7	230 229	24	84 -98
8	411 -429	21	54 66	36	111 118	7	126 138		1,8,L	38	113 99	8	19L -19	25	31L -26
10	385 -382	23	25L -66	37	137 115	8	29L 9			39	26L -1	9	289 -310	26	49 24
12	119 147	25	23L -63	38	33L 35	9	223 -187	1	63 62	40	57 -43	10	371 -391	27	31L 37
14	468 465	27	20L 45	39	32L -8	10	149 161	2	37L 34	41	24L 13	11	353 -367	28	126 -124
16	295 -272			40	87 -83	11	124 102	3	37L -36	42	36 29	12	153 -205	29	100 -91
18	238 239		0,10,L	41	28L 26	12	336 -306	4	37L 52	43	20L -1	13	137 133	30	29L 21
20	77 -36			42	26L -26	13	166 153	5	193 209	44	46 -38	14	241 -249	31	29L 25
22	273 -247	0	212 -237	43	24L -35	14	32L 46	6	260 287	45	14L 21	15	205 -207	32	28L 28
24	135 -114	2	30L -19	44	55 60	15	130 -136	7	37L 24	46	6L 9	16	271 260		
26	60 -73	4	133 153	45	17L -42	16	111 -116	8	172 -174			17	388 -373		

TABLE III (*continued*).

	2,5,L		24	65 -49	29	52 56	11	339 -308	35	123 -146	7	23L -14	3	507 432	23	187 156							
			25	69 -78	30	132 108	12	244 -244	36	50 31	8	23L 31	4	17L 10	24	258 -214							
33	76 54		26	24L 62	31	165 -139	13	67 -38	37	57 77	9	22L -4	5	238 -243	25	387 347							
34	61 -60		27	52 6	32	30L -25	14	118 89	38	11L -40	10	22L -3	6	44 -13	26	34L 5							
35	25L 4		28	44 70	33	180 183	15	165 168			11	64 72	7	54 19	27	34L -35							
36	24L 15		29	20L 60	34	189 176	16	214 196		3,7,L	12	21L -4	8	131 132	28	34L 28							
37	87 105		30	39 34	35	28L -5	17	250 -210			13	21L -7	9	21L 45	29	144 -126							
38	89 118		31	17L -38	36	65 -59	18	88 75	1	29L -5	14	69 8	10	191 -188	30	106 84							
39	56 -49		32	15L 0	37	71 -75	19	137 130	2	181 -193	15	59 47	11	63 85	31	32L -15							
40	39 47				38	25L -28	20	69 52	3	29L 51	16	18L -75	12	56 -43	32	31L -40							
				2,9,L	39	24L -3	21	64 -73	4	29L -76	17	63 57	13	24L 10									
	2,6,L						22	143 135	5	29L -16	18	17L -17	14	25L -6		4,5,L							
			1	30L 25		3,2,L	23	29L -1	6	49 -65	19	15L -38	15	26L -9									
0	176 164		2	30L 63			24	208 -193	7	148 -137			16	67 70	1	58 -51							
1	102 89		3	101 -69	1	307 252	25	325 300	8	29L -34		4,0,L	17	137 132	2	51 42							
2	218 246		4	30L 8	2	547 549	26	146 -127	9	29L 1			18	28L 15	3	28L 44							
3	27L 44		5	30L 46	3	14L -20	27	30L -1	10	90 -89	2	468 596	19	195 -165	4	29L -24							
4	63 80		6	29L 23	4	41 -47	28	52 69	11	81 -66	3	667 792	20	30L 40	5	53 -44							
5	106 -102		7	100 11	5	66 40	29	65 35	12	198 -188	4	295 323	21	31L 4	6	29L -19							
6	83 -62		8	29L 21	6	15L -20	30	80 -51	13	30L -21	5	315 -274	22	117 99	7	118 83							
7	189 207		9	114 -87	7	107 114	31	72 73	14	169 173	6	158 -100	23	56 37	8	30L 22							
8	27L -62		10	170 -184	8	121 -125	32	50 41	15	240 234	7	571 -509	24	75 -57	9	30L -7							
9	28L -52		11	128 -125	9	17L 17	33	27L -24	16	30L 39	8	714 671	25	173 169	10	63 -69							
10	190 -191		12	28L -19	10	132 -130	34	62 58	17	155 144	9	249 237	26	242 205	11	417 -379							
11	229 -253		13	65 67	11	82 -80	35	80 -99	18	119 -144	10	697 -673	27	34L 49	12	447 -438							
12	28L -28		14	86 83	12	173 132	36	24L 25	19	106 -112	11	48 -5	28	34L -19	13	277 -243							
13	51 76		15	127 139	13	113 -88	37	42 38	20	131 149	12	59 -72	29	197 -174	14	157 112							
14	92 91		16	91 89	14	194 -185	38	51 -67	21	144 -147	13	22L 6	30	159 113	15	194 157							
15	29L -6		17	81 -96	15	106 -118	39	19L -28	22	74 59	14	50 -44	31	34L -21	16	748 692							
16	101 -42		18	44 54	16	125 -101	40	17L -27	23	28L -4	15	71 -147	32	33L -17	17	33L 21							
17	30L 53		19	25L 28	17	275 -281			24	54 -70	16	417 -366	33	33L 20	18	126 -112							
18	78 -87		20	57 -39	18	96 85		3,5,L	25	27L 20	17	312 -293	34	32L -10	19	131 107							
19	30L 24		21	41 126	19	220 214			26	26L -15	18	75 58	35	31L -25	20	342 -306							
20	51 18		22	114 -129	20	261 257	1	125 130	27	25L 13	19	211 123	36	30L 31	21	207 205							
21	31L -26		23	108 47	21	102 -108	2	125 110	28	24L 25	20	320 -262	37	28L -30	22	34L 10							
22	79 -31		24	41 17	22	262 258	3	117 106	29	42 50	21	357 250	38	119 -111	23	158 -144							
23	31L 35		25	19L-103	23	141 -122	4	69 71	30	22L 10	22	30L 38	39	46 -60	24	73 65							
24	59 -8		26	86 110	24	365 -341	5	108 -43	31	21L 10	23	120 -89	40	23L 22	25	34L -19							
25	30L -49		27	81 -21	25	306 308	6	354 -362			24	32L 21	41	51 26	26	34L -30							
26	30L -1				26	232 -218	7	356 -393		3,8,L	25	74 45	42	78 -75									
27	55 29			2,10,L	27	29L 26	8	178 -148			26	72 72	43	12L 78		4,6,L							
28	29L 35				28	144 126	9	122 72	1	30L -46	27	34L -10											
29	45 20		1	65 60	29	108 -97	10	256 244	2	82 88	28	34L -32		4,3,L		1 32L 49							
30	67 30		2	26L -3	30	30L 33	11	166 166	3	165 -177	29	34L 14				2 129 -119							
31	27L -48		3	26L 0	31	30L -9	12	26L 32	4	116 137	30	34L -22	0	158 -164	3	32L -7							
32	38 27		4	26L 23	32	93 69	13	26L -35	5	30L 25	31	34L 5	1	321 320	4	32L -5							
33	24L 21		5	26L 4	33	29L 44	14	145 140	6	62 -72	32	34L -17	2	384 376	5	32L 37							
34	49 -0		6	57 -20	34	29L 3	15	197 196	7	78 94	33	33L -25	3	229 206	6	32L -27							
35	42 52		7	25L 25	35	28L 21	16	261 230	8	29L 18	34	106 96	4	178 155	7	32L 8							
36	44 -60		8	71 3	36	27L 1	17	55 -46	9	29L -62	35	32L 45	5	91 -54	8	208 -213							
			9	54 -70	37	26L -28	18	84 -66	10	29L -30	36	31L -17	6	390 -352	9	120 -119							
	2,7,L		10	24L -25	38	59 -58	19	103 -89	11	29L 4	37	54 -65	7	114 142	10	173 160							
			11	24L 32	39	104 -99	20	29L 34	12	77 -63	38	135 -107	8	204 -163	11	259 268							
1	103 125		12	23L 13	40	22L -39	21	29L 36	13	29L -16	39	77 -86	9	235 -218	12	33L 61							
2	139 170		13	23L -23	41	20L 30	22	29L -60	14	138 133	40	24L 5	10	134 91	13	118 124							
3	95 86		14	22L 15	42	54 44	23	46 -41	15	150 148	41	55 37	11	25L -5	14	34L 32							
4	140 -133		15	56 -7	43	15L -19	24	72 43	16	70 -76	42	78 -69	12	66 80	15	240 -215							
5	97 89		16	39 -35	44	11L 8	25	93 -86	17	96 93	43	111 138	13	146 -127	16	389 316							
6	30L -4		17	50 43			26	50 88	18	27L -36			14	27L -9	17	34L 30							
7	115 -139		18	19L 50		3,3,L	27	29L -37	19	27L -25		4,1,L	15	232 187	18	98 -79							
8	230 229		19	18L -32			28	112 -92	20	101 106			16	256 248	19	90 -77							
9	175 -138		20	17L 7	1	173 156	29	77 75	21	124 -141	0	18 -2	17	239 233	20	121 -89							
10	354 -358		21	64 84	2	290 243	30	55 -64	22	56 43	1	28 46	18	80 -39	21	128 -80							
11	164 -153		22	14L -37	3	81 109	31	53 50	23	24L 23	2	32 70	19	31L -13	22	34L 2							
12	30L -0		23	11L -24	4	17L 43	32	74 -45	24	70 -68	3	69 118	20	249 -217	23	101 94							
13	65 71				5	217 -202	33	25L -26	25	23L 33	4	42 54	21	413 385	24	125 -102							
14	113 90			2,11,L	6	584 -630	34	24L 30	26	42 -54	5	77 -136	22	122 104	25	32L 40							
15	116 118				7	482 -478	35	23L 18	27	21L 23	6	178 -327	23	135 -125	26	32L 37							
16	31L 5		1	19L 25	8	312 -288	36	54 -45	28	19L 17	7	160 -290	24	33L -62	27	31L -2							
17	117 -133		2	38 41	9	175 195	37	20L -17	29	31 48	8	237 -392	25	153 -158	28	30L -4							
18	83 82		3	19L -20	10	336 340	38	18L -1	30	16L -12	9	138 -217	26	181 -183	29	29L 14							
19	65 84		4	36 -13	11	213 199	39	51 -68	31	14L -37	10	239 291	27	71 51	30	77 64							
20	73 -66		5	18L -23	12	244 256	40	12L -10			11	150 -195	28	144 132	31	26L 6							
21	30L -25		6	18L -7	13	167 -140				3,9,L	12	181 185	29	137 -117	32	25L -6							
22	30L 29		7	18L 6	14	92 -100		3,6,L			13	136 -169	30	34L -7	33	41 -53							
23	29L 18		8	17L -21	15	120 124			1	28L 4	14	90 -113	31	33L -37	34	21L -7							
24	67 41		9	17L 7	16	140 131	1	52 44	2	28L -13	15	71 54	32	33L -41									
25	28L -20		10	47 -75	17	100 -110	2	71 55	3	95 81	16	59 40	33	32L 26		4,7,L							
26	28L -17		11	51 -81	18	93 -73	3	119 -119	4	100 -111	17	58 -62	34	55 40									
27	27L -1				19	46 20	4	110 121	5	28L -33	18	43 -45	35	84 -76	0	90 -86							
28	64 -60			3,1,L	20	242 -222	5	109 77	6	91 108	19	28L 20	36	28L -51	1	34L 48							
29	47 -62				21	214 167	6	99 73	7	76 -59	20	62 94	37	27L -0	2	112 148							
30	24L -9		1	94 -69	22	248 -241	7	401 426	8	27L 59	21	156 144	38	43 53	3	34L 67							
31	23L 14		2	251 -299	23	28L 24	8	91 78	9	27L -5	22	112 93	39	23L -29	4	34L 8							
			3	194 247	24	213 218	9	118 -127	10	27L -40	23	31L -38	40	20L 11	5	34L 2							
	2,8,L		4	277 -308	25	220 -210	10	275 -283	11	27L -16	24	131 -95			6	34L -56							
			5	66 -73	26	135 151	11	278 -267	12	26L -31	25	33L -9		4,4,L	7	171 166							
1	31L -37		6	230 236	27	29L -26	12	302 -298	13	26L 25	26	82 -35			8	108 110							
2	31L -4		7	181 191	28	137 -114	13	28L 29	14	62 69	27	34L 11	1	24L -16	9	34L 29							
3	31L 0		8	348 -323	29	128 137	14	213 216	15	25L 29	28	48 56	2	63 42	10	105 -107							
4	31L 78		9	188 154	30	30L 14	15	173 171	16	25L 26	29	34L 9	3	194 156	11	127 -127							
5	31L 60		10	303 261	31	29L -0	16	135 147	17	65 86	30	34L 40	4	71 69	12	272 -287							
6	31L 40		11	552 -532	32	29L -30	17	29L -38	18	23L -32	31	34L 15	5	64 -44	13	34L -67							
7	116 124		12	1062 992	33	28L 27	18	29L -9	19	23L -21	32	34L -20	6	26L 15	14	91 71							
8	31L -70		13	415 -344	34	181 153	19	88 -67	20	90 84	33	75 38	7	26L -40	15	34L 39							
9	31L -96		14	273 -250	35	27L -19	20	30L -34	21	72 -94	34	32L -11	8	26L 30	16	359 360							
10	191 -177		15	404 383	36	26L -40	21	213 -220	22	70 79	35	32L 11	9	27L 19	17	34L -2							
11	221 -211		16	120 67			22	60 38	23	19L -13	36	30L 0	10	27L 20	18	63 -36							
12	30L -71		17	173 155		3,4,L	23	29L 44	24	85 -106	37	29L 4	11	59 -64	19	80 72							
13	94 74		18	162 -146			24	29L -29	25	43 -38	38	28L 5	12	89 32	20	145 -162							
14	141 130		19	71 -109	1	89 73	25	29L 40	26	15L -44	39	26L 12	13	29L -15	21	109 113							
15	98 99		20	394 -356	2	263 218	26	28L -41			40	24L 9	14	29L -32	22	32L -21							
16	30L 10		21	99 -99	3	255 -267	27	49 -49		3,10,L	41	22L -1	15	30L 34	23	102 -91							
17	30L 13		22	162 -152	4	48 41	28	27L 14			42	19L -15	16	169 125	24	30L 23							
18	29L -39		23	237 203	5	80 81	29	88 103	1	24L -0			17	170 139	25	29L -13							
19	29L -7		24	177 204	6	203 199	30	80 -60	2	24L 17		4,2,L	18	89 -32	26	62 -49							
20	28L 38		25	136 -124	7	316 312	31	24L 10	3	24L -17			19	236 -225	27	81 -71							
21	28L 20		26	41 32	8	132 113	32	23L 21	4	24L -1	0	107 -120	20	188 -146	28	67 49							
22	27L -1		27	29L 12	9	166 -177	33	22L -5	5	23L 19	1	269 248	21	312 -324	29	62 59							
23	26L 2		28	96 -106	10	335 -320	34	84 81	6	23L -14	2	40 -73	22	34L -27									

TABLE III (*continued*).

	4,7,L	32	32L -17	21	279 -272	16	134 -121	18	147 130	10	329 -311	10	63 43	15	29L -14
		33	31L 14	22	113 -99	17	110 -164	19	99 93	11	314 308	11	77 90	16	30L -44
30	65 54	34	30L 15	23	34L 18	18	128 -115	20	97 -102	12	94 97	12	74 -85	17	30L 21
31	21L -27	35	29L -0	24	34L -5	19	120 117	21	127 -152	13	159 -143	13	141 -152	18	158 152
32	33 -45	36	47 41	25	33L -55	20	31L -51	22	145 -151	14	146 126	14	131 144	19	31L -45
33	16L 15	37	88 75	26	33L -34	21	30L 28	23	88 -64	15	69 -62	15	124 -122	20	31L 54
34	11L -32	38	170 -151	27	75 -55	22	29L 34	24	33L -27	16	32L 53	16	81 65	21	31L 13
		39	23L 9	28	32L -28	23	60 -57	25	139 121	17	32L 52	17	104 91	22	144 -120
	4,8,L	40	20L 17	29	32L 60	24	27L 21	26	69 47	18	33L 1	18	47 -75	23	31L 36
		41	71 -74	30	103 98	25	26L 2	27	33L -0	19	83 62	19	28L 59	24	31L 43
1	156 -156			31	82 84			28	110 78	20	76 -82	20	28L -38		
2	34L 87		5,2,L	32	29L 34		5,8,L	29	32L -12	21	33L -27	21	44 -48		7,3,L
3	101 -102			33	93 -75			30	62 -67	22	33L -28	22	44 38		
4	34L -9	1	79 -60	34	26L -8	1	105 101	31	31L -41	23	100 -60	23	58 45	1	24L 26
5	81 81	2	46 25	35	24L -8	2	197 -178	32	30L -3	24	91 81	24	24L -22	2	25L -19
6	114 -115	3	18L 83			4	101 78			25	32L 18	25	22L -29	3	25L 11
7	34L -34	4	18L -23		5,5,L	3	33L -23		6,2,L	26	31L 30			4	25L -41
8	34L -40	5	281 -278			5	32L 38			27	62 66		6,8,L	5	25L 14
9	33L -14	6	221 218	1	59 61	6	82 -83	0	181 -170	28	101 71			6	152 -148
10	33L 37	7	136 -140	2	29L -24	7	32L -43	1	174 170	29	29L -39	0	83 87	7	111 88
11	138 138	8	81 75	3	74 -82	8	64 74	2	43 23	30	28L -2	1	31L -49	8	174 172
12	72 87	9	132 105	4	81 -80	9	32L 43	3	101 -93	31	27L -2	2	30L -4	9	358 -331
13	81 71	10	263 -237	5	96 92	10	32L -19	4	20L 27	32	25L 19	3	63 -63	10	62 3
14	32L 25	11	74 79	6	30L -16	11	31L -43	5	51 -23	33	24L 22	4	30L -55	11	28L -40
15	152 -161	12	124 141	7	30L -30	12	86 -89	6	171 192	34	22L -9	5	30L -5	12	29L 55
16	94 106	13	216 194	8	79 -88	13	80 -91	7	157 -141	35	19L -83	6	30L 25	13	211 185
17	90 -85	14	42 -38	9	31L -15	14	30L -43	8	102 -122	36	61 -58	7	30L 13	14	60 -54
18	30L 2	15	83 -61	10	188 168	15	79 69	9	24L 35	37	25 -7	8	30L 16	15	54 47
19	81 71	16	141 136	11	283 -252	16	29L 53	10	62 -47			9	29L -24	16	70 -44
20	110 -124	17	224 229	12	129 113	17	28L 83	11	110 115		6,5,L	10	29L -4	17	80 -35
21	28L 1	18	159 148	13	32L -6	18	62 81	12	142 131			11	29L -30	18	68 -76
22	27L -12	19	102 74	14	211 -174	19	95 -109	13	68 -68	0	271 296	12	28L 29	19	31L 37
23	26L 15	20	349 -319	15	169 151	20	26L 6	14	117 129	1	128 -128	13	73 72	20	83 -73
24	25L -18	21	244 -211	16	33L -2	21	25L -26	15	59 12	2	31L 45	14	107 -97	21	31L -13
25	24L -43	22	81 -76	17	33L 33			16	95 96	3	31L -42	15	116 119	22	83 79
26	79 -65	23	51 -58	18	33L 0		5,9,L	17	114 -133	4	31L -14	16	65 -84	23	31L -35
27	21L -25	24	156 138	19	159 124			18	420 -131	5	238 237	17	59 -78	24	31L -20
28	19L 40	25	69 -75	20	272 -252	1	29L 56	19	175 115	6	102 -97	18	60 63	25	48 54
29	85 109	26	34L 36	21	101 -89	2	193 -147	20	32L 5	7	69 -53	19	100 -114	26	74 73
30	13L 7	27	34L 46	22	33L -20	3	29L -38	21	237 -233	8	32L 28			27	29L 1
		28	88 -86	23	114 -106	4	29L -7	22	352 -341	9	161 165		6,9,L		
	4,9,L	29	100 98	24	33L 77	5	28L -47	23	64 -51	10	151 -122				7,4,L
		30	33L -2	25	93 96	6	28L 17	24	88 -69	11	174 151	0	72 82		
0	94 -63	31	32L -1	26	80 88	7	28L 0	25	203 180	12	79 -66	1	48 30	1	164 176
1	31L 41			27	31L 49	8	28L 27	26	169 145	13	133 -108	2	25L -51	2	28L 16
2	99 81		5,3,L	28	30L 10	9	27L -32	27	33L -28	14	262 258	3	25L -35	3	83 -83
3	31L 78			29	29L -21	10	27L -18	28	32L -21	15	68 -60	4	25L 15	4	201 -227
4	76 56	1	95 95	30	28L -24	11	26L 18	29	32L 8	16	57 -51	5	25L 22	5	29L -97
5	31L 5	2	22L 12	31	27L 43	12	26L 41	30	31L 38	17	101 -97	6	25L -24	6	109 -109
6	31L -70	3	68 -48	32	86 77	13	25L 61	31	30L 30	18	81 -88	7	24L 3	7	124 108
7	31L 53	4	22L -28	33	55 -39	14	25L 28	32	29L -16	19	81 73	8	24L 3	8	139 126
8	30L -52	5	244 231	34	50 -52	15	24L -18	33	81 53	20	85 -72	9	84 16	9	207 -181
9	30L 20	6	153 -147	35	20L -15	16	61 -87	34	64 -48	21	32L -41	10	122 43	10	137 132
10	30L 2	7	64 -70	36	17L 30	17	54 -76	35	25L -26	22	62 40	11	22L 10	11	30L 18
11	29L -32	8	128 -145			18	68 -65	36	23L 33	23	32L 48	12	69 -80	12	80 -78
12	29L -55	9	81 -56		5,6,L	19	47 36			24	56 -25	13	125 -122	13	67 -66
13	28L -6	10	307 281			20	19L 3		6,3,L	25	30L 7	14	20L 22	14	109 74
14	28L 21	11	350 -330	1	32L 38	21	17L 37			26	29L -37	15	19L -54	15	75 -58
15	27L -32	12	27L 15	2	109 -120			0	139 141	27	80 -56			16	31L -29
16	67 68	13	27L -10	3	72 -112		6,0,L	1	63 -38	28	63 27		7,1,L	17	74 76
17	82 -71	14	147 -123	4	55 51			2	39 32	29	26L 39			18	31L 34
18	48 -50	15	154 160	5	33L -20	4	90 -168	3	71 -64	30	25L 35	1	141 179	19	31L 21
19	65 43	16	175 167	6	33L -53	5	220 246	4	54 -36	31	47 46	2	64 -74	20	31L 36
20	50 46	17	268 235	7	33L -34	6	176 -193	5	143 134	32	83 74	3	90 -70	21	47 24
21	22L 16	18	264 234	8	66 69	7	34 -11	6	133 -112	33	49 -40	4	118 136	22	31L -40
22	20L -3	19	72 41	9	33L -10	8	38 -10	7	25L -67	34	16L -44	5	160 199	23	53 31
		20	329 -292	10	33L 54	9	152 -102	8	114 98	35	11L -53	6	148 -198	24	43 45
	4,10,L	21	267 -248	11	187 -151	10	86 53	9	237 182			7	20L 22	25	45 31
		22	99 -85	12	149 134	11	22L 103	10	208 -201		6,6,L	8	237 258	26	63 -25
1	91 -117	23	33L -25	13	34L 45	12	283 290	11	168 147			9	454 -477	27	27L -17
2	26L 74	24	165 136	14	233 -201	13	181 191	12	182 -152	0	158 163	10	156 126	28	26L 35
3	91 -129	25	34L 18	15	266 288	14	124 124	13	363 -326	1	33L 8	11	61 52	29	45 19
4	25L -10	26	65 40	16	83 -67	15	214 201	14	216 189	2	33L -20	12	25L 23	30	23L -21
5	72 73	27	33L 53	17	183 185	16	28L 22	15	141 -123	3	120 -139	13	26L 9	31	62 33
6	25L -79	28	33L -16	18	222 221	17	184 -145	16	64 20	4	33L -47	14	52 -47	32	42 -59
7	24L 41	29	33L -35	19	234 -244	18	156 149	17	31L 17	5	88 -90	15	46 18	33	37 34
		30	78 -77	20	88 86	19	53 52	18	151 119	6	147 156	16	49 -26	34	12L 4
	5,1,L	31	53 -24	21	80 -104	20	110 109	19	32L -44	7	33L -21	17	72 63		
		32	31L 32	22	32L -44	21	292 -290	20	32L -48	8	64 -38	18	82 -98		7,5,L
1	125 120	33	29L -5	23	97 88	22	410 -407	21	152 -136	9	33L 10	19	232 181		
2	101 -111	34	46 -26	24	160 -139	23	32L 12	22	141 -111	10	33L -20	20	111 -89	1	31L -32
3	27 -38	35	27L 2	25	30L 16	24	33L -65	23	33L -25	11	61 45	21	76 -86	2	31L 13
4	189 194	36	39 30	26	29L -49	25	237 224	24	33L -13	12	33L 18	22	31L -26	3	80 89
5	310 317	37	60 45	27	28L -42	26	220 194	25	100 100	13	33L -26	23	355 -346	4	100 -110
6	319 -352	38	66 -66	28	27L -4	27	92 -85	26	91 118	14	136 -138	24	90 -75	5	64 -68
7	548 -566	39	18L -18	29	63 49	28	101 100	27	101 95	15	98 82	25	156 153	6	61 -69
8	578 -567	40	15L -12	30	95 93	29	68 -30	28	125 113	16	32L -34	26	232 215	7	83 85
9	185 -145			31	123 130	30	32L 25	29	31L -28	17	81 -61	27	180 209	8	125 144
10	167 148		5,4,L	32	21L 22	31	31L 13	30	47 -28	18	32L 9	28	93 77	9	31L -43
11	74 61			33	77 -95			31	29L 43	19	85 -89	29	29L -14	10	85 -43
12	91 34	1	26L 27	34	45 -44		6,1,L	32	28L 39	20	31L 30	30	65 -59	11	31L -35
13	169 174	2	77 -70	35	10L -10			33	26L 4	21	52 44	31	71 -74	12	65 62
14	90 105	3	26L 17			0	34 29	34	25L -1	22	30L -20	32	54 -37	13	78 85
15	26L -32	4	26L 30		5,7,L	1	91 -124	35	23L -37	23	49 26			14	31L 14
16	26L 7	5	87 -90			2	93 126	36	21L-100	24	48 -23		7,2,L	15	31L -18
17	195 162	6	27L 6	1	79 76	3	56 94	37	96 74	25	27L 10				
18	194 185	7	27L -32	2	103 -102	4	38 45	38	61 -16	26	26L 52	1	20L -3		7,6,L
19	99 67	8	80 30	3	64 61	5	120 139					2	44 37		
20	198 -140	9	89 25	4	70 26	6	51 -30		6,4,L		6,7,L	3	77 51	1	211 237
21	97 -86	10	60 -112	5	34L -26	7	59 -60					4	229 -253	2	31L 9
22	31L 12	11	117 -95	6	65 72	8	135 156	0	233 -250	0	270 265	5	193 185	3	31L -91
23	94 86	12	132 191	7	34L -33	9	367 370	1	225 232	1	33L 30	6	246 -264	4	190 -169
24	186 164	13	192 195	8	34L -11	10	148 -142	2	27L -17	2	95 -83	7	97 70	5	177 -146
25	179 -185	14	176 -194	9	34L -55	11	56 52	3	112 -122	3	135 -138	8	231 210	6	31L 36
26	144 -144	15	252 210	10	109 87	12	124 -89	4	28L -35	4	33L -30	9	282 -290	7	102 94
27	34L 25	16	99 -84	11	33L -42	13	173 -135	5	182 -182	5	89 83	10	247 227	8	31L -26
28	34L -5	17	250 221	12	207 217	14	26L 36	6	209 194	6	33L -56	11	26L -16	9	44 -63
29	34L 23	18	300 254	13	138 154	15	101 72	7	29L -24	7	33L 56	12	181 -174	10	31L 7
30	33L 15	19	224 -223	14	68 41	16	28L -31	8	29L -7	8	50 -49	13	28L -4	11	31L 45
31	59 -50	20	138 -93	15	67 -62	17	29L 14	9	152 139	9	60 -42	14	80 -85		

TABLE III (*continued*).

	7,6,L		16	30L	14	22	26L	14	28	50	45	2	30L	29	8	29L	19	14	27L	13	20	23L	-3
			17	57	18	23	51	-46	29	13L	-20	3	30L	44	9	101	92	15	62	-44	21	43	-28
12	31L	-27	18	59	-31	24	24L	-8				4	104	-109	10	107	-92	16	26L	-14	22	20L	0
13	70	-57	19	28L	9	25	43	45		7,7,L		5	85	-54	11	29L	1	17	78	72	23	19L	-3
14	30L	32	20	50	-21	26	21L	3				6	30L	-32	12	28L	17	18	42	35			
15	30L	-6	21	27L	3	27	59	-70	1	100	-99	7	30L	16	13	58	-55	19	64	66			

TABLE IV.

Interatomic angles.

apex	end	end		apex	end	end	
			sp^3 atoms				
C1	C2	C11	110°.81	C2	C1	C3	112°.20
C1	C2	C15	109°.86	C3	C2	C4	110°.67
C1	C2	C16	106°.77	C4	C3	C12	111°.47
C1	C11	C15	109°.71	C17	C7	C18	111°.95
C1	C11	C16	110°.78	C17	C7	C19	111°.63
C1	C15	C16	108°.84	C17	C18	C19	111°.10
			sp^2 atoms				
C5	C6	C13	122°.87	C11	C10	C12	119°.69
C6	C5	C7	119°.99	C12	C4	C11	121°.64
C7	C6	C8	118°.43	C12	C4	C13	117°.82
C7	C6	C17	120°.06	C12	C11	C13	120°.52
C7	C8	C17	121°.51	C13	C5	C12	123°.87
C8	C7	C14	122°.57	C13	C5	C14	117°.33
C9	C10	C14	120°.46	C13	C12	C14	118°.80
C10	C9	C11	120°.74	C14	C8	C9	121°.48
C11	C1	C10	116°.31	C14	C8	C13	118°.76
C11	C1	C12	124°.01	C14	C9	C13	119°.75

TABLE V.

PLANE FORMED BY	EQUATIONS FOR	
	Direct space	Angstrom space
13 sp^2 bonded atoms . . .	(1D) $4.537x+7.222y+13.168z=7.029$	(1A) $0.491x+0.790y+0.366z=7.029$
all C atoms .	(2D) $4.298x+7.575y+11.147z=6.867$	(2A) $0.465x+0.829y+0.310z=6.867$

DISTANCES IN ANGSTROM FROM THE PLANE (1 A)

C1	0.031	C10	—0.001
C4	—0.074	C11	0.004
C5	0.051	C12	—0.015
C6	0.049	C13	0.010
C7	—0.002	C14	0.003
C8	—0.022	C17	—0.036
C9	0.000	σ	0,033

TABLE VI.

Intermolecular distances smaller than 4 Å

Atom 1	Atom 2	Symmetry operation on atom 2	Distances in Å
C6	C16	$1+x \quad y \quad z$	3.78
C18	C10	$1+x \quad y \quad z$	3.81
C17	C19	$3/2-x \quad 1/2-y \quad z$	3.88
C15	C15	$x \quad 3/2-y \quad 1/2-z$	3.97
C4	C15	$1/2+x \quad 3/2-y \quad z$	3.91
C8	C10	$1/2+x \quad 3/2-y \quad z$	3.95
C12	C15	$1/2+x \quad 3/2-y \quad z$	3.76
C13	C15	$1/2+x \quad 3/2-y \quad z$	3.89
C15	C16	$1/2+x \quad 3/2-y \quad z$	3.95
C3	C2	$1/2+x \quad y \quad 1/2-z$	3.87
C6	C12	$1/2+x \quad 1/2-y \quad z$	3.94
C6	C13	$1/2+x \quad 1/2-y \quad z$	3.96
C19	C8	$1/2+x \quad 1/2-y \quad z$	3.98

The large angle at C13 (ends C5 and C12) and perhaps also the long distance C12—C13 are probably caused by interactions of this kind. The effect is less comprehensible here, as C4 is a tetrahedrally bonded atom, and its two hydrogens (instead of a single one) ought to be symmetrically disposed in respect of the least square plane 1A and then of H5. The observed distances between the hydrogens attached to C4 and H5 are in fact 2.1 Å.

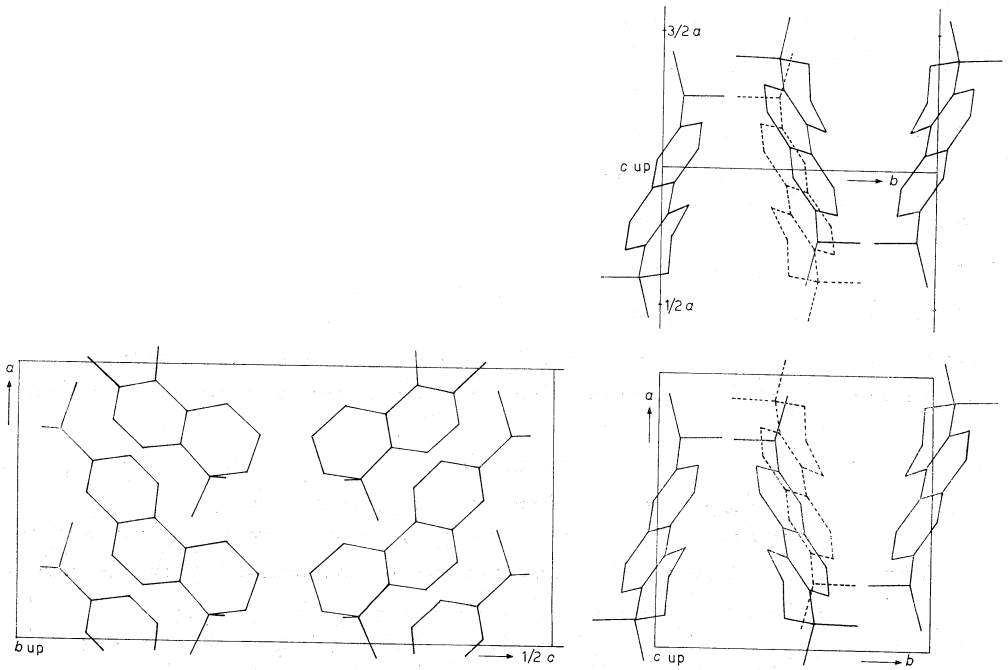


Fig. 4. – Projections of the simonellite structure along [010] (*a*, half cell) and [001] (*b*); the second projection is divided into two parts, to overcome exaggerated superposition.

The molecular packing is shown in fig. 4: fig. 4 *b* has been split owing to the overlapping of the molecules along the *c* axis. Few intermolecular contacts smaller than 4 Å are shown in Table VI.

It is interesting to notice how the molecules lie almost linearly along *a*, in agreement with high refraction index in this direction, called *b* by Emiliani and Pellizzer (1952).

The possible biogenetical provenience of simonellite could be a double-step action on abietic acid (fig. 1 *c*): hydrogenation of the carboxyl group and contemporary loss of the methyl group at C12, followed by an incomplete aromatization.

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