

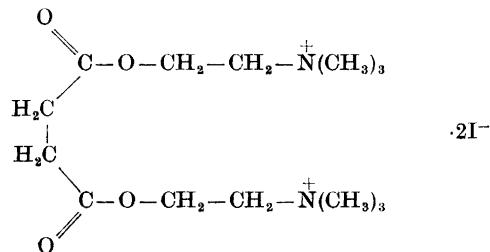
## The Crystal Structure of Succinylcholine Iodide

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Succinylcholine iodide crystallizes in space group  $P2_1$ , with a unit cell having dimensions:  $a=12.90$ ,  $b=8.221$ ,  $c=9.676 \text{ \AA}$ ,  $\beta=98.2^\circ$ .  $Z=2$ . The structure determination was based upon visually estimated three-dimensional X-ray data. The final  $R$ -value is 0.098. The conformation of the succinylcholine ions is far from centrosymmetric, but the two chemically identical but crystallographically independent choline moieties of each ion have the same nearly *gauche* conformation. Ionic forces seem to be the dominant feature in the structural packing.

The investigation of the crystal structure of succinylcholine iodide



was undertaken as a part of a study of compounds acting as neuromuscular blocking agents. The conformation of the succinylcholine ion is of interest, as a connection may exist between this and its biological action. Since, however, the conformation in solution may be different from that found in a crystal, a series<sup>1</sup> of succinylcholine salts forming non-isostuctural crystals is being investigated to examine the variation in conformation arising from different surroundings of the succinylcholine ion.

### EXPERIMENTAL

Succinylcholine iodide,  $\text{C}_{14}\text{H}_{30}\text{O}_4\text{N}_2\text{I}_2$ , was prepared by mixing saturated aqueous solutions of succinylcholine chloride and potassium iodide. The resulting precipitate was purified by recrystallization from 95% ethanol, and single crystals were grown

by slow evaporation of a 50 % ethanol solution. M.p. 250–255° (decomp., determined on a Leitz melting point microscope). The crystals are monoclinic needles elongated in the *b*-direction. The unit cell dimensions measured from precession films are  $a=12.90 \pm 0.02$ ,  $b=8.221 \pm 0.010$ ,  $c=9.676 \pm 0.014$  Å,  $\beta=98.2^\circ \pm 0.2^\circ$ . Systematic extinction of  $0kl$  diffracted spectra when  $k$  was odd indicated the space group  $P2_1$  or  $P2_1/m$ ; the structure solution showed the former to be correct. The calculated density for two formula units per unit cell is 1.78 g/cm<sup>3</sup> and the density measured by flotation in a mixture of C<sub>2</sub>H<sub>5</sub>I and CCl<sub>4</sub> is 1.76 g/cm<sup>3</sup>. The linear absorption coefficient,  $\mu$  (MoK $\alpha$ ), is 31.5 cm<sup>-1</sup>.

All X-ray data were measured from a needle with the dimensions 0.16 × 0.28 × 0.40 mm<sup>3</sup>, using MoK $\alpha$  radiation,  $\lambda=0.7107$  Å. The reflections  $hkl$ ,  $K=0-5$ , were recorded by equi-inclination Weissenberg multiple film techniques. The reflections  $hk0$  and  $0kl$  were recorded by the precession method and used to correlate the levels  $hkl$ . All intensities were estimated visually, corrected for Lorentz and polarization factors and for variations in spot shape<sup>2</sup> and finally scaled together to form a set of 1145 independent non-zero reflections. No corrections for extinction or absorption were applied.

#### DETERMINATION AND REFINEMENT OF THE STRUCTURE

The structure was solved by the heavy atom method. The co-ordinates of the iodine atoms were obtained from the three-dimensional Patterson synthesis, and the positions of the other twenty non-hydrogen atoms were postulated from a three-dimensional Fourier synthesis calculated using the phases from the contributions of the iodine atoms.

The refinement started with three cycles of Fourier refinement and was continued and completed using the full matrix least squares method, with

*Table 1.* Final positional parameters and  $10^4 \times$  their e.s.d. in parentheses.

	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>
I(1)	0.2348 (3)	0.5303 (8)	0.5847 (3)
I(2)	0.1221 (2)	1.0 (—)	0.1405 (3)
C(1)	0.4437 (42)	0.8977 (96)	0.4652 (58)
C(2)	0.4159 (36)	0.9551 (74)	0.6058 (48)
O(3)	0.4645 (30)	0.8913 (62)	0.7189 (40)
O(4)	0.3302 (22)	1.0129 (76)	0.5899 (28)
C(5)	0.2866 (39)	1.0725 (77)	0.7251 (50)
C(6)	0.2042 (31)	0.9845 (88)	0.7534 (40)
N(7)	0.0988 (25)	1.0144(102)	0.6783 (33)
C(8)	0.1002 (30)	1.0137(120)	0.5218 (41)
C(9)	0.0329 (70)	0.8640(161)	0.7146 (96)
C(10)	0.0488 (66)	1.1572(146)	0.7156 (86)
C(1')	0.4165 (32)	1.0097(119)	0.3502 (42)
C(2')	0.4305 (41)	0.9135(100)	0.2128 (54)
O(3')	0.4348 (28)	1.0067 (92)	0.1084 (38)
O(4')	0.4249 (26)	0.7700 (58)	0.2032 (34)
C(5')	0.4246 (37)	0.6966 (78)	0.0678 (49)
C(6')	0.3215 (53)	0.6600 (96)	0.0104 (67)
N(7')	0.2643 (24)	0.5189 (98)	0.0531 (31)
C(8')	0.2613 (33)	0.5348(122)	0.2143 (42)
C(9')	0.3112 (71)	0.3471(128)	0.0137 (87)
C(10')	0.1520 (30)	0.4973 (99)	-0.0113 (39)

individual isotropic temperature factors for all atoms for three cycles and then with anisotropic temperature factors for the iodine atoms and individual isotropic temperature parameters for all other atoms for further two

Table 2. Final thermal parameters and their e.s.d. The anisotropic temperature factor are defined by the equation  
 $T.F. = \exp[-1/4(h^2a^{*2}B_{11} + k^2b^{*2}B_{22} + l^2c^{*2}B_{33} + 2hka^*b^*B_{12} + 2hla^*c^*B_{13} + 2klb^*c^*B_{23})]$ .

Atom	$B_{11}$	$B_{22}$	$B_{33}$	$B_{12}$	$B_{13}$	$B_{23}$
I(1)	5.24(.17)	3.36(.96)	2.81(.12)	0.22(.23)	1.52(.11)	0.18(.18)
I(2)	3.06(.11)	4.71(.99)	2.44(.11)	0.13(.21)	0.88(.09)	0.00(.18)
	Atom	$B$	Atom	$B$	Atom	$B$
C(1)	4.0(1.2)	C(8)	2.8(0.8)	C(5')	2.6(1.0)	
C(2)	3.0(1.0)	C(9)	6.0(1.9)	C(6')	2.5(1.2)	
O(3)	4.7(0.9)	C(10)	4.6(1.2)	N(7')	2.4(0.6)	
O(4)	3.4(0.6)	C(1')	3.3(0.9)	C(8')	2.9(0.9)	
C(5)	3.6(1.1)	C(2')	3.5(1.1)	C(9')	4.2(1.7)	
C(6)	2.6(0.9)	O(3')	5.8(0.9)	C(10')	2.9(0.8)	
N(7)	2.7(0.7)	O(4')	3.2(0.7)			

Table 3. Bond lengths and their e.s.d.  $\times 10^2$  in parentheses.

	$\text{\AA}$
C(1)–C(1')	1.45 (9)
C(1)–C(2)	1.53 (8)
C(1')–C(2')	1.58 (9)
C(2)–O(3)	1.29 (6)
C(2')–O(3')	1.27 (9)
C(2)–O(4)	1.19 (6)
C(2')–O(4')	1.19 (9)
O(4)–C(5)	1.57 (6)
O(4')–C(5')	1.44 (6)
C(5)–C(6)	1.35 (8)
C(5')–C(6')	1.40 (8)
C(6)–N(7)	1.47 (5)
C(6')–N(7')	1.47 (10)
N(7)–C(8)	1.51 (5)
N(7')–C(8')	1.57 (5)
N(7')–C(9)	1.57 (14)
N(7')–C(9')	1.60 (13)
N(7')–C(10)	1.41 (13)
N(7')–C(10')	1.51 (5)

Table 4. Bond angles and their e.s.d. in parentheses.

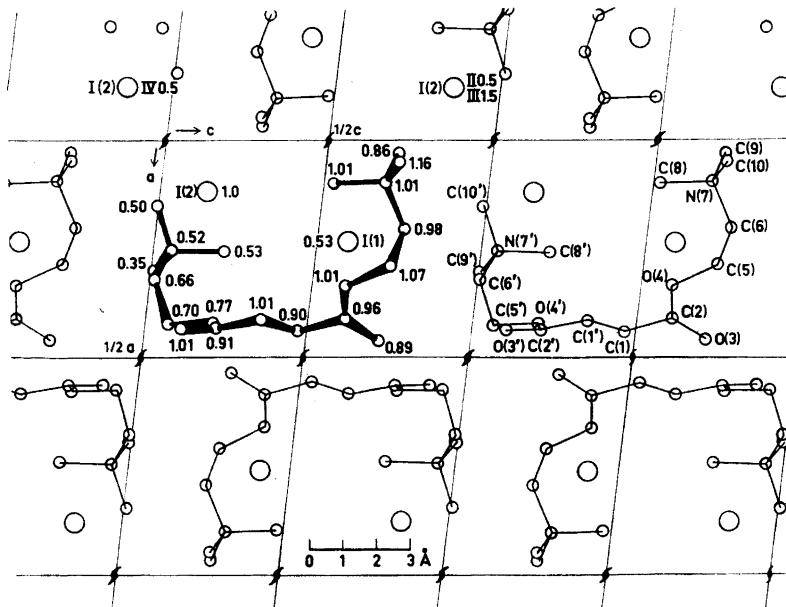
C(1')–C(1)–C(2)	115° (6°)
C(1)–C(1')–C(2')	106° (7°)
C(1)–C(2)–O(3)	119° (5°)
C(1')–C(2')–O(3')	113° (7°)
C(1)–C(2)–O(4)	110° (4°)
C(1')–C(2')–O(4')	124° (6°)
O(3)–C(2)–O(4)	127° (5°)
O(3')–C(2')–O(4')	123° (6°)
C(2)–O(4)–C(5)	117° (3°)
C(2')–O(4')–C(5')	119° (5°)
O(4)–C(5)–C(6)	113° (5°)
O(4')–C(5')–C(6')	109° (5°)
C(5)–C(6)–N(7)	121° (5°)
C(5')–C(6')–N(7')	123° (6°)
C(6)–N(7)–C(8)	111° (3°)
C(6')–N(7')–C(8')	107° (6°)
C(6)–N(7)–C(9)	104° (6°)
C(6')–N(7')–C(9')	114° (5°)
C(6)–N(7)–C(10)	116° (6°)
C(6')–N(7')–C(10')	118° (5°)
C(8)–N(7)–C(9)	108° (6°)
C(8')–N(7')–C(9')	112° (6°)
C(8)–N(7)–C(10)	109° (6°)
C(8')–N(7')–C(10')	105° (3°)
C(9)–N(7)–C(10)	109° (6°)
C(9')–N(7')–C(10')	100° (6°)

cycles. The form-factors for all atoms were taken from *International Tables for X-ray Crystallography*.<sup>3</sup> Unit weight was given to each observed reflection, and no unobserved reflections were included in the refinement. The final reliability index  $R$  is 0.098. The observed structure amplitudes and calculated structure factors are given in Table 6. Nearly all calculations have been performed on the IBM 7094 computer at the NEUCC installation in Copenhagen with the use of the integrated program system *X-RAY 63*.<sup>4</sup>

Attempts to determine the absolute chirality of the succinylcholine ion have not been made, as it is of no significance in relation to the present problem and crystals of each chirality may exist in any batch.

## DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The final positional and thermal parameters together with their estimated standard deviations are given in Tables 1 and 2, and in Tables 3 and 4 the inter-atomic distances and angles are shown. A detailed discussion of these results seems of little value since the influence of the iodine atoms gives rise to very high standard deviations (0.05–0.14 Å on inter-atomic distances and 3°–7° on angles).



*Fig. 1.* The structure viewed along the *b*-axis. The numbers show the *y* co-ordinates (*y/b*) of the atoms. The use of roman numerals is as in Table 5. The atomic numbering used in this paper is shown.

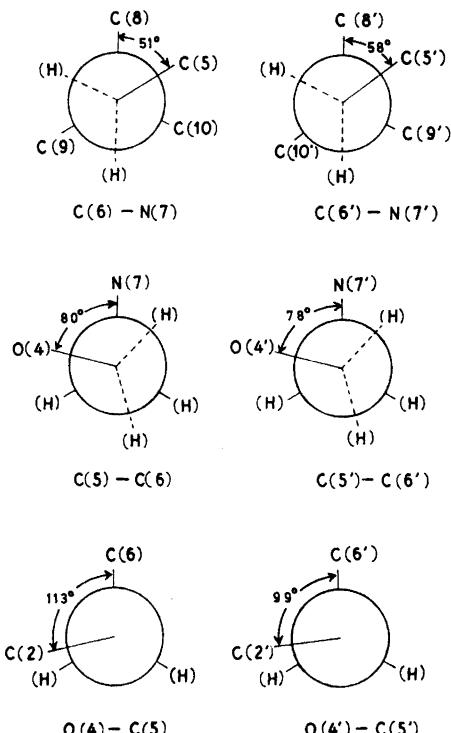


Fig. 2. The conformation of the choline moieties as viewed down the bond indicated below each figure. The dihedral angles are given.

Formally the succinylcholine ion is centrosymmetric, and the molecular symmetry  $\bar{1}$  is found in the crystal structures of succinylcholine perchlorate and succinylcholine picrate.<sup>1</sup> But in this structure the conformation of the succinylcholine ions is far from this (*cf.* Fig. 1). Nevertheless the two choline moieties in each ion show approximately the same nearly *gauche* conformation (Fig. 2). This or the enantiomeric conformation of the system  $O-C-C-N^+$  is found in a great number of crystal structures.<sup>5</sup> Recently Chothia and Pauling<sup>6</sup> reported two conformations of acetyl- $\alpha$ -methylcholine in a single crystal, one nearly *gauche* and one midway between *eclipsed* and *trans*. The intramolecular  $N^+\cdots O$  and  $C\cdots O$  distances in succinylcholine iodide are:  $N(7)\cdots O(4)$  3.22 Å,  $N(7')\cdots O(4')$  3.14 Å,  $(C8)\cdots O(4)$  2.95 Å and  $C(8')\cdots O(4')$  2.88 Å.

The atomic arrangement in the ester groups deviates somewhat from planarity, and the conformation about the two independent groups of each ion differs in the same way from the most common<sup>7</sup> ester conformation. The alcohol moieties are situated *s-cis* to the  $C=O$  groups, but the  $\beta$ -carbon atoms in the acid moieties are *s-trans* to the carbonyl groups. As illustrated in Fig. 3 the twists of the ions arise through deviations (up to about 45°) from the expected *trans* conformation in the succinyl backbone.

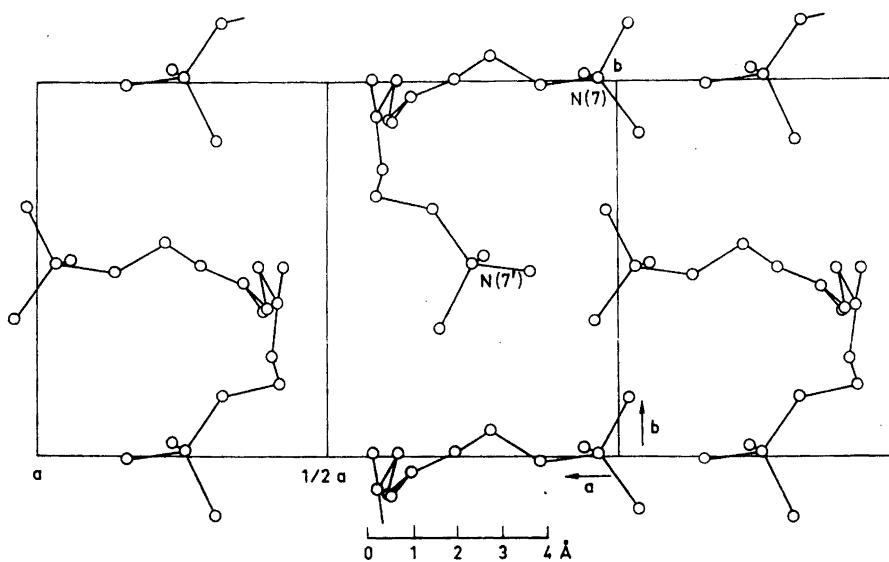


Fig. 3. Succinylecholine ions viewed along the  $c^*$ -axis.

The molecular packing is rather compact, and many intermolecular distances corresponding to van der Waals contacts are observed. But the ionic forces seem to be the dominant feature in the structure. Table 5 lists a series of close contacts to  $\text{I}^-$ . Since the bonds  $\text{N}(7) - \text{C}(8)$ ,  $\text{N}(7) - \text{C}(9)$ , and  $\text{N}(7) - \text{C}(10)$  are directed towards an  $\text{I}^-$  and since this is also the case for the bonds  $\text{N}(7') - \text{C}(8')$  and  $\text{N}(7') - \text{C}(10')$ , the positive charge of the nitrogen atoms seems to be delocalized to the whole quaternary ammonium group. In addition four  $\text{I}^-$  ions are nested between the carbon atoms around  $\text{N}(7)$  and three are situated in the same way around  $\text{N}(7')$ . Many of the distances from these iodide ions to the methyl carbon atoms are equal to or somewhat less than the sum of the respective van der Waals radii,  $4.2 \text{ \AA}$  ( $= 2.0 + 2.2$ ).<sup>8</sup>

Table 5. Close contacts between  $\text{CH}_3$ -groups and iodide ions, together with the  $\text{N}-\text{C}\cdots\text{I}$  angles. The positions of the ions are: I ( $x, y, z$ ); II ( $-x, y + \frac{1}{2}, 1-z$ ); III ( $-x, y - \frac{1}{2}, 1-z$ ); IV ( $-x, y - \frac{1}{2}, -z$ ).

$\text{C}(8)\cdots\text{I}(2)_\text{I}$	$3.73 \text{ \AA}$	$\angle \text{N}(7)-\text{C}(8)\cdots\text{I}(2)_\text{I}$	$176^\circ$
$\text{C}(9)\cdots\text{I}(2)_{\text{II}}$	$3.97 \text{ \AA}$	$\angle \text{N}(7)-\text{C}(9)\cdots\text{I}(2)_{\text{II}}$	$172^\circ$
$\text{C}(10)\cdots\text{I}(2)_{\text{III}}$	$3.95 \text{ \AA}$	$\angle \text{N}(7)-\text{C}(10)\cdots\text{I}(2)_{\text{III}}$	$168^\circ$
$\text{C}(8')\cdots\text{I}(1)_\text{I}$	$3.64 \text{ \AA}$	$\angle \text{N}(7')-\text{C}(8')\cdots\text{I}(1)_\text{I}$	$173^\circ$
$\text{C}(10')\cdots\text{I}(2)_{\text{IV}}$	$3.58 \text{ \AA}$	$\angle \text{N}(7')-\text{C}(10')\cdots\text{I}(2)_{\text{VI}}$	$172^\circ$

The shorter  $\text{N}^+\cdots\text{I}^-$  distances are about  $4.5 \text{ \AA}$ ; obviously the steric influence from the carbon atoms in the quaternary ammonium groups prevents the existence of close direct  $\text{N}^+\cdots\text{I}^-$  contacts.

Table 6. Observed and calculated structure factors for succinylcholine iodide. The column headings are the index  $h$ ,  $|F_o|$  and  $|F_c|$ .

$h$	$ F_o $	$-g$	152 161	-1	6.7 325	-11	291 270	4	322 331	-6	225 306	3	320 361	
2	837 709	-10	579 681	1	366 981	-9	277 275	5	144 181	-2	425 354	4	261 254	
2	817 757	-11	467 527	2	549 600	-8	435 384	6	236 267	-2	325 314	5	315 357	
4	416 145	-12	525 376	3	137 255	-7	406 345	7	400 583	-1	164 134	6	233 243	
5	350 145	-13	252 335	4	9 798	-6	940 904	8	400 583	-2	165 137	7	232 252	
6	789 934	-14	180 160	5	101 163	-5	576 567	9	332 356	1	344 345	6	310 343	
7	428 405	-15	101 163	6	273 344	-4	476 431	10	307 588	2	175 143	10	229 213	
8	655 805	-16	101 163	7	204 204	-3	185 561	11	222 199	3	212 192	11	311 344	
9	769 810	12	225 111	8	192 204	-2	185 561	12	183 142	4	637 424			
11	429 425	11	225 157	9	701 787	-1	191 131			5	323 277	H <sub>3/4</sub>		
12	176 185	10	357 300	10	334 332	0	319 298			6	323 277			
13	342 185	9	357 300	11	231 156	1	231 156			7	323 277			
14	290 232	8	357 749	12	221 182	2	491 536	-12	323 134	-10	324 426	-12	231 152	
15	235 217	3	174 148	13	221 182	3	541 594	-11	482 441	-5	264 253	-11	344 354	
16	235 217	4	93 745	14	214 187	4	285 313	-10	202 164	-8	253 244	-10	287 263	
17	214 187	5	174 148	15	140 160	5	245 253	-9	202 164	-7	253 244	-9	287 263	
18	160 113	1	455 451	16	134 160	6	245 253	-8	229 218	-6	224 155	-7	407 324	
19	142 95	7	140 160	17	12 466 469	H <sub>1/4</sub>	7	174 141	-4	176 123	-7	242 267		
20	202 186	-10	214 187	18	12 466 469	-11	231 345	8	668 620	2	374 378	5	387 366	
21	745 165	-11	180 160	19	139 160	-10	180 160	9	540 487	-1	174 123	-4	424 316	
22	12591154	-3	425 368	20	510 455	-9	612 637	4	694 629	1	452 471	-4	340 282	
24	857 805	4	882 889	21	759 627	-7	272 274	3	1272 121	2	222 211	-3	12541167	
25	241 216	-7	174 148	22	1977172	-6	211 154	4	281 242	-2	566 554			
26	300 203	-7	174 148	23	1977172	-5	211 154	5	281 242	-1	323 221			
27	762 727	-6	225 265	24	134 120	-2	209 167	6	257 290	-12	222 231	C	469 464	
28	935 867	-12	216 214	25	15451441	-3	371 361	3	486 498	-6	322 342	1	498 486	
29	146 165	4	174 148	26	15451441	-2	366 600	4	386 479	-5	355 417	2	336 364	
30	12581233	H <sub>1/4</sub>	1	170 342	27	15451441	-1	366 600	5	386 479	-4	345 417	3	345 417
31	364 375	9	272 233	28	656 652	1	702 723	6	424 461	-1	275 241	4	251 217	
32	345 357	8	422 344	29	3 283 223	3	243 258	7	258 256	2	252 185	5	405 356	
33	745 165	7	140 160	30	416 455	4	260 260	8	258 256	3	252 220	6	435 725	
34	405 405	5	494 446	31	9581044	5	228 242	9	398 446	2	215 204	7	528 896	
35	197 171	2	212 188	32	6 346 354	6	223 240	10	214 241	3	211 211	8	371 456	
36	349 400	1	166 141	33	7 536 687	7	223 240	11	214 241	4	252 267	9	228 285	
37	202 242	C	8 194 216	34	13 245 243	-1	888 805	12	233 367					
38	202 242	-2	566 572	35	216 216	H <sub>1,9</sub>	-12	253 299	-14	233 219	-5	245 235	H <sub>3,5</sub>	
39	205 185	-2	695 737	36	258 271	-13	262 271	-12	232 242	-2	225 165	-13	255 267	
40	125 154	1	174 148	37	258 271	-14	262 271	-13	232 242	C	253 211			
41	222 292	-6	451 488	38	226 221	-5	218 177	-9	444 423	1	254 179	-6	178 147	
42	69 676	-5	467 529	39	242 253	-9	493 493	8	728 664	2	230 185	-6	530 466	
43	319 262	-11	244 462	40	689 690	-5	447 493	-7	377 311	3	245 245	-7	528 896	
44	965 522	-12	367 365	41	9581044	-7	398 446	4	398 446	2	215 204	8	371 456	
45	695 522	-7	566 510	42	1 221 216	-5	912 862	H <sub>2,12</sub>	-4	405 353				
46	494 427	-6	12711197	43	1 222 122	-4	416 392	-4	366 282	-3	394 366			
47	258 162	7	216 145	48	465 359	2	258 271	-3	342 312	-2	245 222			
48	189 193	5	213 198	49	465 359	4	258 271	-2	245 222	-1	315 317			
49	146 165	6	174 148	50	177 199	5	234 208	-1	402 362	H <sub>3,4</sub>	C	462 371		
50	1417 423	4	564 542	51	191 156	-1	10041010	2	377 265	1	715 755			
51	190 135	1	494 479	52	191 156	H <sub>1,10</sub>	1	662 492	3	12321373	2	458 445		
52	173 172	1	466 410	53	1 231 128	-9	321 415	4	396 479	4	342 371			
53	173 172	-1	466 410	54	1 231 128	-7	259 280	3	788 682	5	164125	4	456 717	
54	184 95	-1	171 127	55	1 231 128	-6	294 354	6	490 539	6	638 824	5	196 156	
55	258 162	-5	215 215	56	1 231 128	-5	243 196	7	530 335	7	262 162	6	170 116	
56	259 392	-3	243 114	57	1 231 128	-4	239 196	8	530 335	8	262 162	6	170 116	
57	627 600	-4	155 233	58	466 474	0	373 380	9	730 253	9	242 266	9	282 263	
58	9421046	-5	524 920	59	6 169 179	1	209 164	9	354 393	10	241 312	H <sub>3,6</sub>		
59	566 596	-7	144 215	60	1 231 128	-7	231 201	11	211 202	12	217 202	-12	315 317	
60	156 115	-8	180 200	61	10 309 396	H <sub>1,11</sub>	-12	238 237	-12	244 314	-5	313 315		
61	175 115	-11	235 255	62	1 231 128	-5	238 237	-12	244 314	-7	356 316			
62	175 115	-11	235 255	63	1 231 128	-4	238 237	-12	244 314	-5	313 444			
63	175 115	-10	260 268	64	1 231 128	-3	238 237	-12	244 314	-7	356 316			
64	216 242	-14	245 233	65	1 231 128	-2	238 237	-12	244 314	-5	313 444			
65	1 231 128	-1	174 148	66	1 231 128	H <sub>1,4</sub>	-14	253 241	-12	244 314	-7	356 316		
66	324 303	2	317 310	67	411 459	-5	261 254	-7	174 157	-7	622 532	-1	933 874	
67	119 171	1	525 540	68	1 458 425	H <sub>1,12</sub>	-14	262 254	-10	202 254	-6	255 205		
68	254 425	-5	510 540	69	1 458 425	-5	261 254	-7	174 157	-7	622 532			
69	255 392	-6	510 540	70	1 458 425	-4	261 254	-7	174 157	-7	622 532			
70	516 472	7	354 446	71	229 214	H <sub>1,13</sub>	-4	849 612	-4	463 414	2	339 296		
71	720 703	-2	282 270	72	282 270	-5	246 242	-3	266 231	3	191 171			
72	715 726	-6	295 345	73	286 273	-6	249 90	-9	197 161	8	157 115	-11	244 237	
73	715 726	-7	295 345	74	91 975	-1	117 123	-1	117 123	9	544 532	-5	195 175	
74	346 364	-8	174 148	75	91 975	-1	117 123	-1	117 123	10	215 222	-3	219 311	
75	576 242	-6	224 258	76	626 611	-2	1242 114	-2	824 224	-4	1554133E			
76	3 12851292	-2	387 266	77	1 552 931	3	234 228	-2	715 668			H <sub>3,8</sub>		
77	545 495	H <sub>1,13</sub>	-5	556 532	78	809 413	4	642 704	-2	11315125	-11	265 305		
78	1 230 216	1	245 233	79	809 413	5	642 704	-2	11315125	-11	265 305			
79	751 726	1	245 233	80	1 23711197	2	371 385	10	226 216	C	364 445	-9	265 146	
80	121 151	-4	227 158	81	2 561 567	3	923 0111	11	212 123	-6	494 479			
81	327 154	-7	285 343	82	4 692 497	4	883 933	-2	233 361	-7	237 222			
82	327 154	-8	285 343	83	4 692 497	5	883 933	-3	237 222	-8	237 222			
83	605 883	H <sub>1,1</sub>	9	266 611	84	1 272 282	-4	127 282	-4	127 282	-5	287 264		
84	847 923	2	656 619	85	10 191 236	11	170 123	-9	554 562	12	201 156	-7	344 324	
85	340 343	3	207 2282	86	1 237 198	12	221 195	-7	167 130	8	221 221	-1	180 115	
86	417 455	4	685 873	87	217 198	13	221 195	-7	167 130	9	203 156	6	534 557	
87	147 247	5	685 873	88	217 198	14	221 195	-7	167 130	10	203 156	1	569 581	
88	207 221	6	686 1076	89	272 298	15	281 250	-4	324 301	12	201 156	1	569 581	
89	147 247	7	140 164	90	405 405	H <sub>2,2</sub>	-1	803 611	13	247 175	3	244 166		
90	236 185	8	140 164	91	405 405	-1	803 611	-1	803 611	14	247 175	3	244 166	
91	126 151	9	236 185	92	405 405	-2	803 611	-2	803 611	15	247 175	3	244 166	
92	591 693	7	140 164	93	405 405	-3	803 611	-3	803 611	16	247 175	3	244 166	
93	667 424	14	306 303	94	2 699 446	-2	538 536	5						

Table 6. Continued.

1. 241.3	7. 512.651	-9. 297.300	0. 284.266	+5. 185.170	+5. 513.554	+2. 178.162
4. 380.364	6. 151.155	-7. 172.181	2. 689.703	-3. 181.192	-4. 513.681	-1. 418.364
5. 247.196	10. 155.162	-6. 552.505	4. 444.449	-2. 381.337	3. 258.255	1. 615.523
7. 219.142	10. 255.269	-5. 276.159	3. 256.266	-1. 313.370	2. 733.345	2. 615.377
7. 222.186		-4. 290.265	7. 186.162	1. 352.339	-1. 458.415	3. 245.277
H.3.1.		-3. 315.276	8. 172.113	2. 205.178	C. 445.445	4. 535.431
H.3.1.		-3. 162.138	10. 292.262	-1. 182.182	1. 144.166	5. 264.203
-1. 241.360	-1. 151.150	-9. 297.306	8. 199.56	2. 252.252		
-1. 314.346	-9. 352.342	-9. 814.805	H.4.7		2. 513.345	H.5.6
-7. 242.765	-8. 155.156	1. 559.508	-12. 222.219	F.4.10	4. 411.552	-5. 258.261
-7. 238.441	-7. 783.778	3. 32.272	-11. 236.307	6. 271.276	5. 452.282	-4. 276.284
-1. 314.267	-5. 352.326	5. 370.329	-8. 374.368	4. 255.255	4. 513.544	-3. 254.226
2. 362.372	-4. 374.263	9. 244.275	-5. 179.211	-1. 213.210		-1. 655.542
-1. 314.267	-3. 547.531	6. 149.109	-4. 241.309	1. 184.120	5. 297.285	1. 297.285
-1. 314.267	-3. 547.531	7. 149.109	-5. 211.210	3. 126.120	1. 297.285	1. 297.285
H.3.11		-1. 1255.104C	8. 195.193	-2. 310.334	5. 254.214	2. 222.293
-5. 272.307	C. 242.233	9. 344.346	-1. 457.447		-7. 226.274	3. 241.243
-2. 421.421	1. 408.944	11. 259.270	0. 427.472	F.4.11	4. 455.415	5. 273.251
-2. 258.335	1. 408.944	12. 218.167	1. 427.472	-9. 204.204	5. 455.415	7. 326.343
-2. 258.335	1. 408.944	12. 218.167	1. 427.472	2. 251.227	-8. 247.179	-4. 245.244
H.3.12		4. 425.300	3. 155.110	6. 231.250	-3. 171.156	H.5.7
-8. 271.440	6. 152.144	2. 8.226	1. 178.165	-5. 213.226	-2. 254.337	-6. 546.335
-5. 245.355	7. 415.369	3. 126.144	5. 213.226	-1. 251.226	4. 252.337	-5. 546.335
-5. 435.143	7. 415.369	-11. 710.262	6. 207.204	0. 349.330	5. 476.356	-4. 241.245
C. 461.469	8. 329.328	-1. 7. 516.587	8. 294.292		2. 244.365	-3. 293.293
C. 461.469	8. 329.328	-1. 7. 516.587	8. 294.292	-7. 44.12	3. 273.264	-2. 255.256
3. 588.581	-7. 199.167	H.4.8		2. 239.236	4. 273.264	-1. 201.201
4. 455.501	-6. 217.268	-13. 214.224	F.5.0	5. 273.264	5. 273.264	2. 277.241
5. 172.180	-1. 12. 315	4. 455.494	-1. 178.186	2. 245.255	7. 152.145	3. 367.349
5. 172.180	-1. 12. 315	4. 455.494	-1. 178.186	3. 262.205	8. 215.192	5. 259.211
7. 178.214	-1. 30.200	-10. 173.92	4. 214.206			
8. 545.401	-6. 310.359	-2. 774.763	-9. 190.181	5. 223.473	H.5.4	H.5.8
9. 342.422	6. 231.359	-1. 7. 214.224	6. 310.431	-7. 210.293	6. 310.431	-6. 310.311
10. 200.219	-1. 515.229	0. 348.374	2. 236.241	-6. 213.263	-7. 233.212	
-6. 443.352	1. 395.383	-6. 200.228		-5. 352.355	-4. 220.194	
-5. 336.344	2. 250.299	-5. 452.447	H.5.1	4. 216.237	2. 231.267	
-11. 244.282	3. 362.342	3. 44.242	-4. 231.267	-7. 231.267	-2. 231.267	
-11. 179.171	-3. 935.795	3. 362.308	-3. 345.334	-7. 259.416	2. 231.267	C. 377.386
-11. 179.171	-3. 212.205	5. 168.187	-2. 391.369	6. 173.266	-1. 224.224	1. 355.345
-11. 179.171	-3. 212.205	5. 168.187	-2. 391.369	6. 173.266	C. 452.422	
-11. 179.171	-3. 212.205	5. 168.187	-2. 391.369	6. 173.266	1. 344.344	H.5.8
-7. 372.410	9. 170.111	1. 287.270	-3. 242.334	3. 232.323	-5. 278.292	
-7. 372.410	9. 170.111	1. 287.270	-3. 242.334	3. 232.323	-5. 278.292	
-3. 70.351	2. 273.282	2. 174.172	-2. 248.427	3. 213.275	-4. 308.376	
5. 544.517	3. 380.367	H.4.9	3. 489.459	-1. 342.296	4. 252.273	-2. 284.246
5. 544.517	3. 380.367	H.4.9	3. 489.459	4. 252.273	-2. 284.246	
-3. 735.446	5. 710.711	-1. 0. 270.132	4. 233.355	0. 09.199	5. 245.273	
-2. 724.792	6. 343.310	-9. 167.171	5. 262.352	1. 602.615	6. 541.556	H.5.1C
-1. 368.298	7. 150.161	-7. 384.418	H.4.1	3. 492.482		
-1. 368.298	7. 150.161	-7. 384.418	H.4.1	3. 492.482		
1. 162.162	9. 183.177	-5. 143.102	-11. 298.119	4. 241.216		
2. 492.421	10. 155.131	-4. 665.623	-9. 235.302	5. 262.358	-8. 241.216	
3. 940.892	-3. 393.374	-8. 215.197	9. 246.384	-7. 188.163	-5. 242.455	
4. 872.906	H.4.4	-2. 314.334	-6. 244.346	-8. 241.216		
6. 447.416	-10. 176.186	-1. 144.29	-6. 166.154	-8. 241.216		

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