The Crystal Structure of Succinylcholine Perchlorate

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Succinylcholine perchlorate crystallizes in space group $P2_1/c$ with a unit cell having dimensions a=6.537, b=13.67, c=12.69 Å, and $\beta=93.3^\circ$. Z=2. The structure was solved by the heavy-atom method and refined by full matrix least squares technique to an R index of 0.094, using 976 diffractometer-collected three-dimensional single crystal X-ray diffraction intensity data. The conformation of the succinylcholine ion seems to be essentially independent of the influence of the surrounding ions in this crystal structure, and the conformation of the system $O-C-C-N^+$ is gauche. Extreme "thermal" motion is shown by the perchlorate ions.

The crystal structure of succinylcholine perchlorate was determined as a part of an investigation^{1,2} of the influence of different surroundings on the conformation of the succinylcholine ion.

O
$$C-O-CH_{2}-CH_{2}-N(CH_{3})_{3}^{+}$$
 $H_{2}C$
 $H_{2}C$
 $C-O-CH_{2}-CH_{2}-N(CH_{3})_{3}^{+}$
O $C-O-CH_{3}-CH_{3}^{-}-N(CH_{3})_{3}^{+}$

EXPERIMENTAL

Succinylcholine perchlorate, $C_{14}H_{30}Cl_2O_{12}N_2$, was prepared by mixing a saturated aqueous solution of succinylcholine chloride with a 2 N aqueous solution of sodium perchlorate, and the resulting precipitate was purified by recrystallization from ethanol. The crystals show a pronounced tendency to twin-formation, and single crystals were obtained only from aqueous solutions containing 50 ± 5 % ethanol. M.p. $267 - 267.5^{\circ}C$. The crystals are monoclinic needles elongated in the a-direction. The unit cell parameters, obtained from precession photographs and from a series of diffractometer-measured θ values ($MoK\alpha$ radiation, $\lambda = 0.7107$ Å) and refined by the least squares method using the program CELSIUS, are: $a = 6.537 \pm 0.004$, $b = 13.67 \pm 0.01$, $c = 12.69 \pm 0.02$ Å, and $\beta = 93.3 \pm 0.1^{\circ}$. The space group is $P2_1/c$. With two formula units per unit cell the calcu-

lated density is 1.434 g/cm³, in good agreement with the density of 1.43 ± 0.01 g/cm³ measured by flotation in a mixture of tetrachloromethane and toluene. The linear ab-

sorption coefficient, $\mu(MoK\alpha)$, is 3.4 cm⁻¹.

Single crystal X-ray diffraction intensities were measured from a crystal of dimensions $0.38 \times 0.5 \times 0.8\,$ mm³ using quartz monochromatized Mo $K\alpha$ incident radiation and a NONIUS 3 circle automatic diffractometer. The ω -scanning mode was used with a scan speed of $0.6^{\circ}/\text{min}$, each reflection being scanned over a range of 1.2° .

Of the 1970 independent reflections within the range of $3^{\circ} \le \theta \le 25^{\circ}$, 976 had intensities greater than 2.5 times their corresponding estimated standard deviation and were considered as observed. Unobserved reflections were not included in any calculations.

The diffraction data were reduced to structure amplitudes by the ALGOL-program OUTDIFF-5, written by A. M. Sørensen of this laboratory. No absorption corrections were applied.

DETERMINATION AND REFINEMENT OF THE STRUCTURE

The structure was solved by the heavy-atom method. The coordinates of the chlorine atom were obtained from the three-dimensional Patterson map, and the positions of six further atoms, C(1), C(2), O(3), O(4), N(7) and C(10) (Fig. 1), were postulated from the three-dimensional Fourier synthesis calculated using phases from the contributions of the chlorine atoms to the structure factors. A second three-dimensional Fourier synthesis based upon the phases from the contributions of all these atoms gave the positions of the rest of the atoms in the succinylcholine ion. The coordinates of the oxygen atoms O(11) to O(14) of the perchlorate ion were postulated at the positions of shoulders which could be seen on the electron density peak corresponding to the chlorine atom.

After four cycles of Fourier refinement, in which an overall temperature factor of 3.0 was used, and in which the R-value was lowered from 0.45 to 0.39, the structural parameters were further improved using the full matrix least squares method, firstly in three cycles, varying an overall scale factor and positional coordinates and individual isotropic temperature factors for all atoms which reduced the R-value to 0.26, and then with four further cycles with individual temperature factors for all atoms changed to anisotropic form, after which the R-value was 0.11. A difference Fourier synthesis was then calculated, and from this all the fifteen hydrogen atoms in the asymmetric unit could be located at stereochemically reasonable positions. The conformation about all three $N-C(H_3)$ bonds was staggered as expected. The heights of the peaks on the difference map corresponding to hydrogen atoms were 0.2-0.5 e ${\rm \AA}^{-3}$.

In three subsequent cycles of full matrix least squares refinement the contributions of the hydrogen atoms were included, but their parameters were kept constant. Their thermal parameters were assumed to be the same as those of the atoms to which they are bonded. The form factors for all atoms were taken from *International Tables for X-Ray Crystallography*. Unit weight was given to each observed reflection except for very weak and very strong amplitudes, which were given weights less than 1.0. The final *R*-value is 0.094. The observed structure amplitudes and the final calculated structure factors are given in Table 7. Nearly all calculations have been performed on the IBM 7094 computer at the NEUCC installation in Copenhagen using the integrated program system *X-RAY* 63.5

Table 1. Final atomic positional parameters, and their e.s.d. ($\times 10^4$) in parentheses.

		A CONTRACT OF A	
	x/a	y/b	z/c
Cl(1)	0.0776(4)	0.1363(2)	0.3297(3)
O(11)	0.0585(23)	0.2270(13)	0.3212(29)
O(12)	0.2905(14)	0.1251(13)	0.3579(10)
O(13)	-0.0431(27)	0.0924(15)	0.3947(15)
O(14)	0.0545(25)	0.1070(26)	0.2369(13)
C(1)	0.0577(14)	0.5463(8)	0.5087(9)
C(2)	0.2490(14)	0.5500(8)	0.4445(8)
O(3)	0.3155(10)	0.4825(6)	0.3987(7)
O(4)	0.3224(9)	0.6403(5)	0.4435(6)
C(5)	0.4957(15)	0.6519(8)	0.3738(11)
C(6)	0.5920(14)	0.7464(9)	0.3946(10)
N(7)	0.4805(11)	0.8372(6)	0.3526(7)
C(8)	0.3016(20)	0.8580(10)	0.4200(14)
C(9)	0.4208(21)	0.8293(11)	0.2389(11)
C(10)	0.6312(20)	0.9212(20)	0.3670(12)
$\mathbf{H}(11)$	-0.042(-)	0.608(-)	0.486(-)
$\mathbf{H}(12)$	0.100(-)	0.554(-)	0.592(-)
$\mathbf{H}(51)$	0.603(-)	0.592(-)	0.385(-)
$\mathbf{H}(52)$	0.437(-)	0.650(-)	0.291(-)
H(61)	0.611(-)	0.753(-)	0.481(-)
$\mathbf{H}(62)$	0.743(-)	0.745()	0.365(-)
$\mathbf{H}(81)$	0.350(-)	0.865(-)	0.500(-)
$\mathbf{H}(82)$	0.225(-)	0.805(-)	0.438(-)
$\mathbf{H}(83)$	0.200(-)	0.915(-)	0.390()
H(91)	0.525(-)	0.805(-)	0.172(-)
$\mathbf{H}(92)$	0.350(-)	0.755(-)	0.250(-)
$\mathbf{H}(93)$	0.350(-)	0.880(-)	0.188(-)
H(101)	0.600(-)	1.000(-)	0.360(-)
H(102)	0.740(-)	0.950(-)	0.430(-)
H(103)	0.740(-)	0.915(-)	0.290(-)

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

Atom	B ₁₁	B_{22}	B_{33}	B ₁₈	B ₁₃	B ₂₃
Cl(1)	2.79(.10)	5.46(.15)	5.39(.14)	-0.11(.12)	0.65(.09)	0.43(.14)
O(11)	7.3(0.8)	9.5(1.0)	$62.8(\hat{5.0})^{'}$	$3.5(0.8)^{'}$	5.8(1.6)	7.8(1.8)
O(12)	4.5(0.5)	22.4(1.5)	13.1(0.9)	3.0(0.7)	-0.5(0.5)	4.7(1.0)
O(13)	17.3(1.3)	23.1(1.7)	21.0(1.5)	-5.2(1.3)	15.1(1.3)	2.8(1.3)
O(14)	12.2(1.1)	53.8(4.0)	9.8(0.9)	-14.2(1.7)	2.5(0.7)	-13.7(1.7)
C(1)	2.9(0.4)	4.6(0.5)	5.6(0.6)	-0.9(0.4)	1.7(0.4)	-0.9(0.5)
C(2)	2.7(0.4)	3.4(0.5)	4.6(0.5)	-0.0(0.4)	0.5(0.4)	0.6(0.4)
O(3)	3.8(0.3)	4.6(0.4)	8.0(0.5)	0.0(0.3)	2.5(0.3)	-0.9(0.4)
O(4)	2.6(0.3)	4.3(0.4)	6.8(0.4)	0.3(0.3)	1.8(0.3)	1.1(0.3)
C(5)	3.1(0.5)	4.7(0.6)	9.9(0.8)	0.3(0.4)	3.8(0.5)	1.2(0.6)
C(6)	2.4(0.4)	5.2(0.6)	7.8(0.7)	0.2(0.4)	1.0(0.4)	1.0(0.6)
N(7)	2.9(0.3)	3.7(0.4)	5.4(0.5)	-0.5(0.3)	1.0(0.3)	0.5(0.3)
C(8)	6.3(0.7)	5.2(0.7)	14.3(1.2)	2.1(0.6)	6.6(0.8)	1.4(0.8)
C(9)	6.9(0.7)	8.9(1.0)	6.0(0.7)	-2.1(0.7)	-1.7(0.6)	1.6)0.7)
C(10)	6.2(0.7)	5.0(0.7)	8.6(0.8)	-3.4(0.6)	0.3(0.6)	-0.3(0.6)

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The final structural parameters, together with their estimated standard deviations, are given in Tables 1 and 2, and the interatomic distances and angles are shown in Tables 3 and 4.

Table 3. Bond lengths, and their e.s.d. ($\times 10^2$) in parentheses. Cl-O distances calculated assuming riding motion of the oxygen atoms on Cl(1) are also given.

× /	Å	Corrected value Å
C(1') - C(1)	1.48(1)	
$egin{array}{c} { m C(1)} - { m C(2)} \\ { m C(2)} - { m O(3)} \end{array}$	$1.53(1) \\ 1.19(1)$	
C(2) - O(4)	1.32(1)	
O(4) - C(5) C(5) - C(6)	$1.49(1) \\ 1.45(2)$	
C(6) - C(0)	1.52(1)	
$egin{array}{c} {\bf N}(7) - {f C}(8) \ {f N}(7) - {f C}(9) \end{array}$	$1.52(2) \\ 1.48(2)$	•
N(7) - C(9) N(7) - C(10)	1.52(1)	
Cl(1) - O(11)	1.25(2)	1.57
Cl(1) - O(12) Cl(1) - O(13)	$1.43(1) \\ 1.32(2)$	$\begin{array}{c} 1.55 \\ 1.54 \end{array}$
Cl(1) - O(13)	1.32(2) $1.25(2)$	1.56

Table 4. Bond angles, (°), and their e.s.d. in parentheses.

C(1') - C(1) - C(2)	112(1)
C(1)' - C(2)' - O(3)	125(1)
C(1) - C(2) - O(4)	110(1)
O(3) - C(2) - O(4)	125(1)
C(2) - O(4) - C(5)	113(1)
O(4) - C(5) - C(6)	109(1)
C(5) - C(6) - N(7)	118(1)
C(6) - N(7) - C(8)	109(1)
C(6) - N(7) - C(9)	112(1)
C(6) - N(7) - C(10)	106(1)
C(8) - N(7) - C(9)	113(1)
C(8) - N(7) - C(10)	108(1)
C(9) - N(7) - C(10)	109(1)
O(11) - Cl(1) - O(12)	103(1)
O(11) - Cl(1) - O(13)	117(2)
O(11) - Cl(1) - O(14)	103(2)
O(12) - Cl(1) - O(13) O(12) - Cl(1) - O(14)	114(1)
	105(1)
O(13) - Cl(1) - O(14)	114(1)

In the perchlorate ions the oxygen atoms have very high thermal parameters (cf. Table 2 and Fig. 1), and the bond lengths and angles deviate somewhat (cf. Table 3) from those of the regular tetrahedron with ideal Cl-O distances of 1.46 Å.8 If interatomic distances are not corrected for thermal motion,

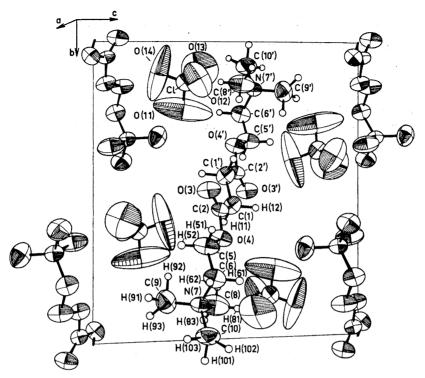


Fig. 1. The structure of succinylcholine perchlorate viewed in perspective along the a-axis. The 50 % probability thermal ellipsoids calculated from the final thermal parameters of the least squares refinement are drawn for the non hydrogen atoms, while spheres of an arbitrary size are drawn for the hydrogen atoms. The atomic numbering used in this paper is shown. The drawing was produced by ORTEP.¹¹

the observed mean separation is generally shorter than the real mean distance between the atoms. 9,10 Hence, when approximate corrections for the "thermal motion" were calculated assuming "riding motion" of the oxygen atoms on the chlorine atoms, calculated Cl-O bond lengths of about 1.55 Å (Table 3) were obtained. These are greater than any reported Cl-O distances in perchlorate ions and may indicate that the ellipsoidal representation of the oxygen atoms assumed in the refinement is unsatisfactory. Some refinements using fractional perchlorate oxygen atoms in multiple sites were performed, but these gave results which clearly had no physical meaning. The thermal ellipsoids of two of the oxygen atoms, O(11) and O(14), indicate large vibrational amplitudes of these atoms in preferred directions. This may have physical meaning, suggesting oscillation of each perchlorate ion with the oscillation axis centered in Cl(1) and perpendicular to the plane O(11)-Cl(1)-O(14).

In this structure each succinylcholine ion has a rather extended conformation. The backbone is not completely planar but has a shallow twist (cf. Table 5 which lists the deviations of the backbone atoms from the plane through the

Table 5. Deviations	of atoms from	n the p	olane t	through	the c	entral	atoms	in t	the	succiny	1-
	backbone,	C(1),	C(2),	C(1'),	and	C(2')	•			·	

Atom	Deviation (Å)	
O(3)	-0.18	
O(4)	$-0.18 \\ 0.29$	
C(5)	0.45	
C(6)	$\begin{array}{c} \textbf{0.45} \\ \textbf{0.48} \end{array}$	
N(7)	1.76	

central atoms C(1), C(2), C(1'), and C(2')). The atomic arrangement in the ester group is planar within the experimental limits, and C(5) and the β -carbon atom in the acid moiety, C(1'), are s-cis to the carbonyl group. This is the most common ester conformation ⁶ but in the related structure of succinylcholine iodide ² a more unusual conformation was found about the ester groups.

O (4)

$$\begin{array}{c}
N(7) \\
H \\
H
\end{array}$$
 $\begin{array}{c}
C(5) \rightarrow C(6)
\end{array}$

Fig. 2. The conformation of the system $O-C-C-N^+$, as viewed down the bond C(5)-C(6). The dihedral angle is given.

The system $O-C-C-N^+$ has the usual gauche conformation,⁷ the dihedral angle O(4)-C(5)-C(6)-N(7) being 75° (Fig. 2) and the intramolecular distances $N(7)\cdots O(4)$, $C(8)\cdots O(4)$, and $H(82)\cdots O(4)$ being 3.13, 2.99, and 2.34 Å, respectively.

Table 6. Distances (Å) between atoms that are less than the sum of the respective van der Waals radii, excluding those within a single chain.

$C(1)_{(x,y,x)} \cdots O(14)_{(-x,\frac{1}{2}+y,\frac{1}{2}-x)}$	3.27
$U(0)_{(x,y,z)} \cdots U(12)_{(1-x,\frac{1}{2}+y,\frac{1}{2}-z)}$	3.28
$U(2)(x,y,z) \cdots U(14)(-x,1+y,1-z)$	3.05
$C(8)_{(x,y,z)} \cdots C(13)_{(-x,1-y,1-z)}$	3.05
$U(10)_{(x,y,z)} \cdots U(13)_{(1+x,1+y,z)}$	3.17
$O(3)_{(x,y,z)} \cdots C(9)_{(1-x,y-\frac{1}{2},\frac{1}{2}-z)}$	3.28

The molecular packing is not very compact, and the few close intermolecular contacts (\leq the sum of the respective van der Waals radii) are listed in Table 6. Four out of the six are of interionic character: the negative charge of the perchlorate ion and the positive charge of the quaternary ammonium group are delocalized from the chlorine and nitrogen atom, respectively, and the carbonyl carbon atom C(2) has a fractional positive charge. Nevertheless

Table 7. Observed structure amplitudes and calculated structure factors for succinylcholine perchlorate. The column headings are the index $l,\ |F_{\rm o}|\ (\times\,10)$ and $|F_{\rm c}|\ (\times\,10)$.

C, at. 4 680 747 8 08 69 10 100 107 12 8 89 71110 3 654 014 5 51 51 7 207 207 17 1/2 110 17 3/2 110 17 3/3 44	3 50 51 1;74;L 1 70 84 -1 60 53 1;12;L -6 102 101 1 14 142 1;32;L 7, 67 56 6 67 63	1,4,L 12 57 60 11 62 66 7 76 13 13 6 4 15 13 6 4 15 13 6 1 7 12 13 6 1 7 12 13 6 2 94 121 1 246 221 2 410 414 	-5 73 88 -6 270 281 -3 192 211 -2 476 429 -1 367 302 -1 267 302 -1 267 408 2 144 408 2 144 408 3 197 226 6 132 77 7 95 106 8 45 64	8 128 125 2 mm 92 1 189 197 -1 86 65 -6 217 216 -6 217 19 -1 140 135 2,10;L -8 81 81 -6 12 159 -5 56 57	7 134 112 8 84 43 319 128 84 43 319 128 319 128 319 129 129 129 129 129 129 129 129 129 1	a 181 100-3 101 107 2 229 220 1 54 56 0 26 247 1 177 185 2 19 77 6 2 2 19 77 6 2 2 19 77 6 2 19 77 8 2 11 5 6 5 3	,
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# 246 203 5	11 60 63 8 73 79 7 126 101 5 137 111 4 69 62 3 136 166 2 336 346 10 262 244 -1 126 152 -2 377 360 -3 252 208 -4 77 67 -5 101 124 -6 162 158 -7 210 176 -8 61 67	-6 334 360 -4 554 544 -2 615 711 0 633 518 2 267 396 4 378 368 6 163 205 8 167 165 10 53 67 12 64 65 2,1,1 12 51 45 6 140 112 5 147 136	7 67 48 9 77 86 10 100 88 11 53 89 247+1 9 115 93 7 165 168 6 53 7 165 168 104 101 1 156 163 -2 179 172 -3 145 139 -5 164 151	-A 112 103 3,9,4 -5 119 130 -4 109 103 0 172 179 2 122 123 6 133 124 6 82 75 3,0,4 11 59 42 10 59 56 5 78 80 4 154 156 2 143 133	1 196 206 2 170 184 3 148 162 5 68 94 6 197 222 7 161 182 8 192 161 11 00 58 19 112 114 6 120 61 4 398 427 2 99 70 0 719 656	4.7.L 7 72 h3 6 118 110 5 171 157 2 115 110 1 126 110 -1 70 43 -2 1.95 117 -3 143 134 -4 124 143 -5 137 129 -6 115 110 -7 101 126 -4 184 L	
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0,14,L C 92 H7 1 80 75 4 57 45 1,15,L -5£250	1 87 134 2 335 401 4 168 215 6 242 231 8 216 211 9 119 117 10 58 95 12 49 27	-10 210 210 -12 79 71 2,2,4, -13 71 77 -12 71 52 -11 143 129 -9 198 193	173 160 5 92 75 6 56 46 7 73 76 2,9,L 9 52 43	-6 122 123 -5 225 23 -2 194 201 -1 284 257 0 160 186 1 73 .74 2 97 91 5 127 114	4,1,L 10 66 63 7 109 113 6 173 158 5 148 139	-7 54 61 4,10,L -5 52 92 -3 63 59	÷

Table 7. Continued

4 (1.5)	. 62 63	-5 54 37	2 45 35	+2 23 : 241	5 76 78	7,5,L
-2 h. 69	4 75 54	-4 233 223	1 258 248	107 133	6 75 76	~4 59 90
1 55 51		-3 7'1 81	-1 145 144			9 64 68
2 134 126	5.8.4	-2 154 158	-3 102, 93	6,1,4	6,5,L	
2 54 93	4 59 54	-1 82 70	-4 50 60	4 118 120	2 236 233	7.4.6
4 47 29	2 45 37	0 214 179	-6 245 229	3 91 112	04 67	4 AH A7
4	1 70 79	3 59 50	-7 79 66	2 100 109	-2 207 224	1 60 64
4 . 1 1 . L	0 145 147	4 138 115	-9 40 66	97 95	-3 79 82	0 102 119
5 42 46	-4 170 170	5 60 46	-1-1 5 : 44	-2 165 193	-5 64 78	-2 59 77
1 75 70	-4 175 175	6 90 82	-11 21 86	-3 142 148	-7 51 66	-6 90 130
-1 145 171	5,7,L	6 90 62	-11 91 66	-4 68 64	-, 31	
-2 56 62	-9 67 7C		5,1,L	-6 102 131	6,6,1	7.3.L
-5 6 59	-7 104 101	5,4,L 4 82 91	-9 (1) 77	-9 54 36	-7 71 78	~6 56 A1
-6 5: 49			-8 123 115	-9 54 36	+6 55 58	-5 52 64
-0 5. 49			-7 1. 96	5.2.6	-5 99 112	-7 60 50
		3 63 61 2 153 147	-6 53 63	-1 56 65	-2 79 83	5 72 A9
4,12,L	-3 75 61 -2 57 47	2 183 147	-6 53 63	-7 B1 79	-1 195 110	3 /2 /19
						7.2.L
-1 61 65	-1 115 55	-1 122 123				
1 57 71	144 152	-2 97 94	-2 120 134	-4 6 73	3 86 79 5 85 9∩	2 62 54
2 37 65	1 76 60	-3 149 154	-1 179 179	-1 87 96	5 85 90	
3 91 42	2 52 85	-4 319 308	0 114 127	3 147 155		
	3 113 156	-17 73 79	1 180 172	4 54 39	6,7,L	-3 53 65 -7 50 56
5,12,L	5 64 70		1 130 133	5 93 1/12	3 60 73	-7 5° 56
1 55 70		5,3,L	4 121 125	7 99 158	1 89 52	
	₹,6,6	-8 148 143	5 167 158		-1 137 143	7,1,L
5.11,L	7 78 95	-7 176 167	9 64 61	6,3,L	-3 68 79	-4 95 95
-3 69 76	4 72 71	-6 55 31		4 70 67		-3 98 116
-2 4E 39	2 61 77	-4 129 141	ちゃい。し	2 77 77	6,9,L	n .84 91
	1 64 65	-1 207 197	R 174 141	1 101 107	-6 79 91	3 64 Ail
5,10,L	.1 209 215	-2 112 112	6 174 156	-1 116 97	-4 80 93	
2 61 73	-1 227 224	-1 295 357	2 143 178	-3 96 114	-2 97 102	7.0.L
1 79 82	-2 71 56	1 75 47	11 375 418	-5 93 86	1 54 51	4 57 56
3 A6 82	-3 806 195	3 196 201	-2 143 135	-9 54 79	2 55 66	2 74 100
-2 55 46	-4 231 246	4 114 106	-4 446 423	-9 82 79		-1 130 148
-3 AS 46	-5 1(9 111	5 63 64	-6 135 105		6,9,L	
-4 56 59	-8 51 41		-9 64 73	6,4,L	-1 56 62	
		5 , 2 , 1.	-10 129 133	-6 104 112	-2 58 68	
£,9,L	5,5,L	7 88 84		-5 67 69		
-8 51 5)	-8 150 137	6 91 82	5	-2 156 150	7.5.6	
-2 91 96	-7 77 72	3 72 58	-6 210 207	2 91 94	1 79 92	

ionic forces seem to be much less dominant in the present structure than in the structure of succinylcholine iodide ² and the conformation of the succinylcholine ion in succinylcholine perchlorate is apparently essentially independent of the influence of the surrounding ions.

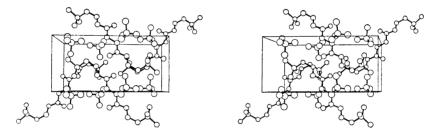


Fig. 3. Stereodiagrams of the succinylcholine perchlorate structure viewed along the c-axis. The atoms are represented by spheres of arbitrary sizes.

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REFERENCES

- 1. Jensen, B. Acta Chem. Scand. 22 (1968) 2035.
- 2. Jensen, B. Acta Chem. Scand. 24 (1970) 2517.
- 3. Liminga, R. Acta Chem. Scand. 19 (1965) 1631.
- International Tables for X-Ray Crystallography, Kynoch Press, Birmingham 1962, Vol. III.
- Stewart, J. M. X-RAY 63, Technical Report Tr 64-6, NSG-398, Computer Science Center of the University of Maryland, College Park 1964.

- Mathieson, A. McL. and Welsh, H. K. Acta Cryst. 18 (1965) 953.
 Sundaralingam, M. Nature 217 (1968) 35.
 Cruickshank, D. W. J. J. Chem. Soc. 1961 5486.
 Busing, W. R. and Levy, H. A. Acta Cryst. 17 (1964) 142.
 Johnson, C. K. In Crystallographic Computing, Munksgaard, Copenhagen 1970, p. 220.
 Johnson, C. K. ORTEP, A Fortran Thermal Ellipsoid Plot Program for Crystal Structures, U.S. Atomic Energy Commission Publication ORNL-3794, 1966.

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