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MARDER

685-690

Crystal Structure Determination of 3'-methoxy- 2-N-methyl stilbazolium triflate, **2**

A suitable crystal for X-ray diffraction was obtained by vapor diffusion of ether into a nearly saturated solution of **2** in acetone. A nearly colorless crystal was mounted with epoxy cement on a glass fiber and was centered on the diffractometer. Unit cell dimensions were obtained from the setting angles of 25 reflections with $27^o < 2\theta < 39^o$. Two equivalent data sets were collected; the data were corrected for a slight (<1%) decay, Lorentz and polarization factors were applied and the data were merged to give the final set. No absorption correction was made because μr_{max} was so small. The structure was solved with some difficulty by MULTAN. The computer solution revealed most of the cation, but the triflate anion was not recognizable in the E-map. Even in a subsequent Fourier map phased on the atoms of the cation, the sulfur peak was only 3.5 $eÅ^{-3}$, no larger than the oxygen atom. Packing considerations led us to introduce the sulfur atom at this site; the remaining atoms appeared in the subsequent Fourier map and refinement proceeded smoothly from then on. Hydrogen atoms were introduced at calculated positions (or, for the two methyl groups, at positions based on maps calculated in their expected planes) and both their positional and thermal parameters were included in the final single full matrix refinement. The final R-index for reflections with $F_o^2 > 3\sigma(F_o^2)$ is 0.0397; the final difference map had peaks of +0.33 $eÅ^{-3}$ (near the triflate oxygen atoms) and -0.20 $eÅ^{-3}$ (near nothing).

Calculations were done with programs of the CRYM Crystallographic Computing System and ORTEP. Scattering factors and correction for anomalous scattering were taken from a standard reference[1]. $R = \Sigma \mid F_o - |F_c| \mid / \Sigma F_o$, for $F_o^2>0$, and goodness of fit = $([\Sigma w (F_o^2 - F_c^2)^2 / (n - p)]^{1/2}$, where n is the number of data and p is the number of parameters refined. The function minimized in least squares was $\Sigma w (F_o^2 - F_c^2)^2$ where $w = 1/\sigma^2(F_o^2)$. Variances of the individual reflections were assigned based on counting statistics plus an additional term, $0.0141I^2$. Variances of the merged reflections were determined by standard propagation of error plus another additional term, $0.0014\langle I\rangle^2$. The secondary extinction parameter[2] refined to $0.19(11) \times 10^{-6}$.

Crystallographic data for 3'-methoxy-2-N-methyl stilbazolium triflate, **2**

Formula	$C_{15}H_{16}NO{\cdot}CF_3SO_3$
Formula wt.	397.37
Space group	Cc(No. 9)
a	18.126(4)Å
b	7.040(1)Å
c	13.315(2)Å
β	93.46(1)°
volume	1696.0(5)(11)Å^3
Z; ρ_{calc}	4; 1.470 g cm^{-3}
No. reflections; GOF	1493; 3.87
No., $F^2_o > .0$; R_F	1464; 0.041
No., $F^2_o > 3\sigma(F^2_o)$; R_F	1414; 0.040
T	22°C
λ	0.71073 Å
μ	2.5cm^{-1}

(1) *International Tables for X-ray Crystallography*, Kynoch Press, Birmingham, 1974, Vol. IV, p 71. p 149;

(2) Larson, E. C. *Acta Cryst.* **1967**, *23*, 664, eqn. 3

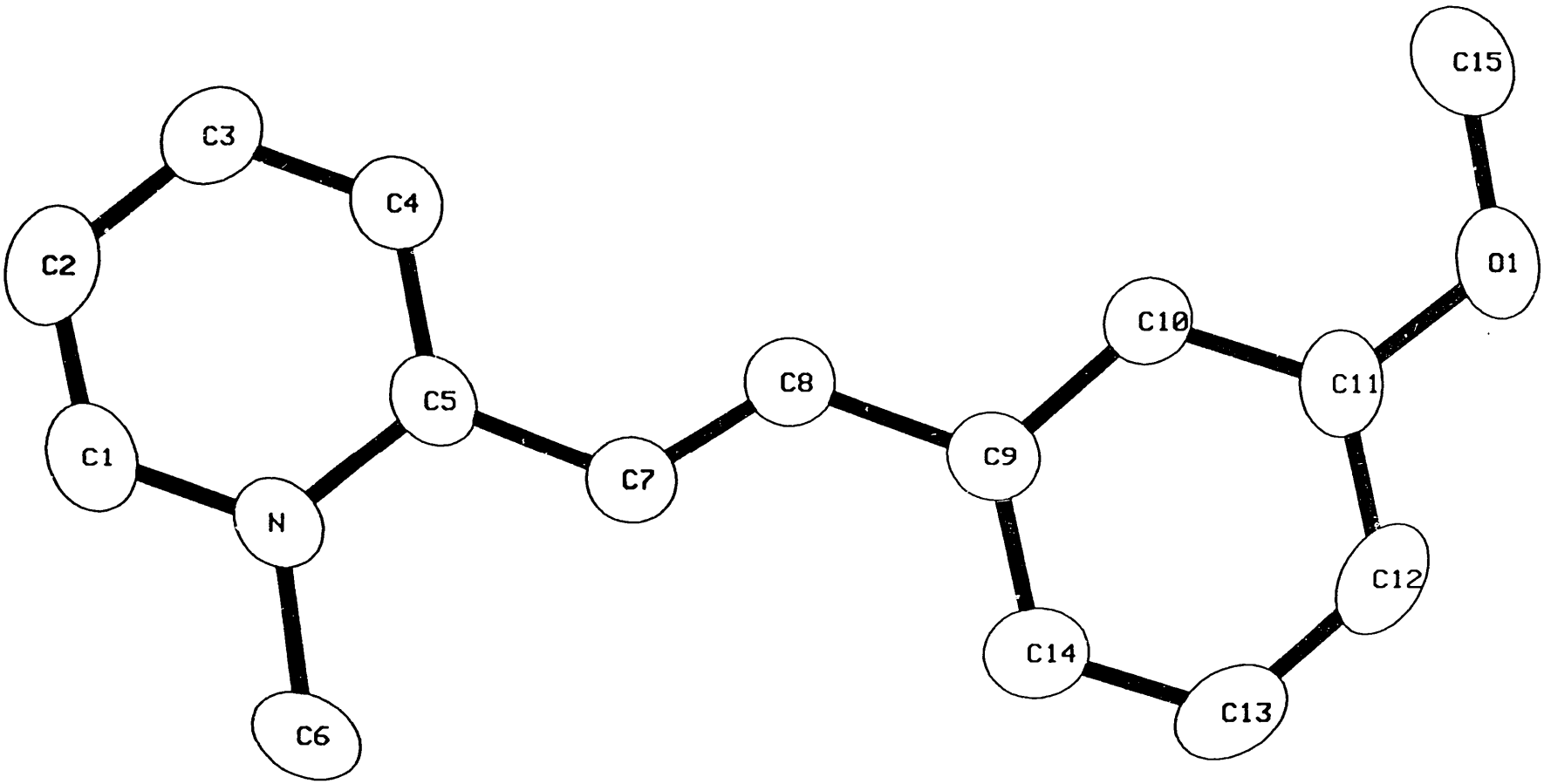

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Table S I. Final Heavy Atom Parameters for 3′-Methoxy-2-N-Methyl Stilbazolium Triflate.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq}
N	5260(2)	2106(5)	4323(3)	410(8)
C1	5040(3)	2120(6)	3329(4)	508(11)
C2	4317(3)	2322(7)	3016(4)	560(13)
C3	3791(3)	2498(6)	3733(4)	496(10)
C4	4017(3)	2441(6)	4729(3)	448(10)
C5	4760(2)	2264(5)	5045(3)	386(9)
C6	6061(3)	1983(8)	4591(5)	553(12)
C7	5029(2)	2242(6)	6103(3)	459(10)
C8	4628(3)	2719(6)	6849(3)	442(10)
C9	4876(2)	2713(5)	7922(3)	391(9)
C10	4333(3)	2758(6)	8626(3)	405(9)
C11	4537(3)	2768(6)	9648(3)	453(10)
C12	5283(3)	2776(6)	9971(4)	521(11)
C13	5812(3)	2772(7)	9274(4)	558(12)
C14	5621(3)	2727(6)	8253(4)	476(10)
O1	4051(2)	2770(5)	10385(3)	615(9)
C15	3284(3)	2626(9)	10092(5)	641(14)
S	7199	1490(2)	1789	519(3)
O2	6436(2)	1104(6)	1911(3)	812(10)
O3	7718(3)	615(6)	2463(4)	1109(14)
O4	7374(2)	1511(6)	742(3)	900(12)
C16	7273(2)	3938(8)	2073(3)	596(13)
F1	7966(2)	4630(5)	2001(3)	928(10)
F2	7138(2)	4347(5)	3038(3)	1043(10)
F3	6832(2)	5056(5)	1517(3)	1048(10)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table S II. Hydrogen Atom Parameters for 3′-Methoxy-2-N-Methyl Stilbazolium Triflate.

x, y and $z \times 10^4$

Atom	x	y	z	B
H1	5432(29)	1901(69)	2924(38)	4.8(11)
H2	4181(28)	2216(63)	2370(44)	4.6(11)
H3	3248(27)	2543(57)	3500(34)	4.1(10)
H4	3598(27)	2539(58)	5289(39)	4.3(10)
H7	5501(27)	1551(58)	6301(33)	4.1(9)
H8	4133(38)	2920(79)	6735(47)	7.0(15)
H10	3875(26)	2772(55)	8407(34)	3.5(9)
H12	5424(25)	2748(57)	10766(38)	4.2(10)
H13	6342(27)	2756(61)	9496(37)	4.1(10)
H14	6031(33)	2679(76)	7782(51)	7.0(14)
H6 A	6314(31)	1607(82)	4033(50)	6.7(14)
H6 B	6183(25)	999(80)	5022(38)	4.7(11)
H6 C	6198(24)	3151(69)	4837(35)	3.8(10)
H15A	3090(53)	2396(114)	10921(73)	11.4(24)
H15B	3184(27)	1304(84)	9684(40)	5.8(12)
H15C	3105(26)	3511(74)	9747(39)	4.4(12)

Table S III. Anisotropic Displacement Parameters for 3′-Methoxy-2-N-Methyl Stilbazolium Triflate.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N	397(18)	418(19)	424(19)	−16(14)	97(15)	−16(15)
C1	603(29)	524(25)	410(25)	−52(20)	130(22)	−20(19)
C2	715(34)	560(28)	400(28)	−53(21)	−18(23)	−22(21)
C3	496(25)	484(24)	498(27)	−2(19)	−50(21)	7(19)
C4	437(23)	478(23)	434(26)	−14(16)	65(19)	−20(17)
C5	409(22)	371(20)	386(23)	−5(15)	101(17)	20(16)
C6	373(23)	687(33)	614(31)	−37(22)	143(21)	−77(29)
C7	387(21)	590(26)	400(23)	51(19)	29(18)	11(18)
C8	384(22)	544(24)	397(23)	−9(18)	24(18)	28(18)
C9	403(22)	354(19)	418(23)	6(15)	43(17)	−6(16)
C10	376(22)	463(22)	373(23)	36(18)	−4(17)	−19(17)
C11	582(27)	435(23)	345(23)	61(18)	44(19)	−6(16)
C12	628(28)	520(25)	394(26)	52(20)	−132(21)	−19(19)
C13	458(26)	612(28)	583(29)	14(20)	−130(21)	−42(21)
C14	397(23)	493(25)	534(27)	−15(17)	7(20)	9(18)
O1	627(21)	857(22)	368(16)	66(17)	97(14)	−28(15)
C15	602(32)	770(37)	566(32)	107(26)	157(25)	47(28)
S	336(5)	645(7)	570(6)	19(5)	−21(4)	−69(6)
O2	463(18)	1108(30)	869(25)	−218(19)	77(17)	−1(22)
O3	1066(31)	685(26)	1475(39)	30(21)	−769(29)	161(24)
O4	806(26)	1234(34)	686(24)	62(24)	254(20)	−258(23)
C16	425(28)	775(31)	595(34)	109(24)	77(26)	158(23)
F1	743(19)	783(22)	1251(28)	−218(17)	4(18)	43(19)
F2	1396(30)	1007(24)	739(21)	−6(22)	176(20)	−246(19)
F3	1115(25)	841(22)	1154(28)	326(22)	−205(21)	129(20)

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table S IV. Complete Distances and Angles for 3′-Methoxy-2-N-Methyl Stilbazolium Triflate.

Distance(Å)		Angle(°)		Angle(°)	
N –C1	1.359(6)	C5 –N –C1	121.1(4)	H12 –C12 –C13	122.1(24)
N –C5	1.365(5)	C6 –N –C1	117.5(4)	C14 –C13 –C12	121.3(5)
N –C6	1.476(7)	C6 –N –C5	121.3(4)	H13 –C13 –C12	120.2(28)
C1 –C2	1.358(7)	C2 –C1 –N	121.4(4)	H13 –C13 –C14	118.5(28)
C1 –H1	0.93(5)	H1 –C1 –N	111.9(31)	C13 –C14 –C9	119.4(4)
C2 –C3	1.396(7)	H1 –C1 –C2	126.6(31)	H14 –C14 –C9	122.9(35)
C2 –H2	0.88(5)	C3 –C2 –C1	119.1(5)	H14 –C14 –C13	117.6(35)
C3 –C4	1.364(6)	H2 –C2 –C1	119.9(33)	C15 –O1 –C11	117.9(4)
C3 –H3	1.01(5)	H2 –C2 –C3	120.7(33)	H15A–C15 –O1	95.4(44)
C4 –C5	1.392(6)	C4 –C3 –C2	119.0(4)	H15B–C15 –O1	109.2(29)
C4 –H4	1.10(5)	H3 –C3 –C2	118.9(26)	H15C–C15 –O1	116.1(35)
C5 –C7	1.462(6)	H3 –C3 –C4	121.8(26)	H15B–C15 –H15A	107.3(52)
C6 –H6 A	0.93(6)	C5 –C4 –C3	121.7(4)	H15C–C15 –H15A	119.3(56)
C6 –H6 B	0.92(5)	H4 –C4 –C3	118.6(25)	H15C–C15 –H15B	108.6(45)
C6 –H6 C	0.91(5)	H4 –C4 –C5	119.7(25)	O3 –S –O2	117.4(3)
C7 –C8	1.310(6)	C4 –C5 –N	117.7(4)	O4 –S –O2	112.4(2)
C7 –H7	1.01(5)	C7 –C5 –N	118.7(4)	C16 –S –O2	102.8(2)
C8 –C9	1.472(6)	C7 –C5 –C4	123.6(4)	O4 –S –O3	116.3(3)
C8 –H8	0.91(6)	H6 A–C6 –N	110.3(37)	C16 –S –O3	104.6(3)
C9 –C10	1.399(6)	H6 B–C6 –N	113.1(32)	C16 –S –O4	100.2(2)
C9 –C14	1.394(6)	H6 C–C6 –N	106.1(29)	F1 –C16 –S	113.2(3)
C10 –C11	1.389(6)	H6 B–C6 –H6 A	99.8(48)	F2 –C16 –S	113.3(3)
C10 –H10	0.86(4)	H6 C–C6 –H6 A	113.7(47)	F3 –C16 –S	115.3(4)
C11 –C12	1.394(7)	H6 C–C6 –H6 B	113.9(43)	F2 –C16 –F1	102.3(4)
C11 –O1	1.359(6)	C8 –C7 –C5	124.0(4)	F3 –C16 –F1	106.2(4)
C12 –C13	1.375(7)	H7 –C7 –C5	119.1(26)	F3 –C16 –F2	105.6(4)
C12 –H12	1.07(5)	H7 –C7 –C8	115.3(26)		
C13 –C14	1.383(7)	C9 –C8 –C7	125.8(4)		
C13 –H13	0.99(5)	H8 –C8 –C7	119.9(39)		
C14 –H14	1.00(6)	H8 –C8 –C9	113.7(39)		
O1 –C15	1.424(7)	C10 –C9 –C8	117.7(4)		
C15 –H15A	1.19(9)	C14 –C9 –C8	122.6(4)		
C15 –H15B	1.09(5)	C14 –C9 –C10	119.7(4)		
C15 –H15C	0.83(5)	C11 –C10 –C9	120.0(4)		
S –O2	1.429(4)	H10 –C10 –C9	118.4(30)		
S –O3	1.403(5)	H10 –C10 –C11	121.6(30)		
S –O4	1.448(4)	C12 –C11 –C10	119.9(4)		
S –C16	1.768(5)	O1 –C11 –C10	124.2(4)		
C16 –F1	1.357(6)	O1 –C11 –C12	115.9(4)		
C16 –F2	1.354(6)	C13 –C12 –C11	119.7(4)		
C16 –F3	1.317(6)	H12 –C12 –C11	118.2(24)		

Crystal Structure Determination of 2'-methoxy- 2-N-methyl stilbazolium triflate, **4**

In an opaque test tube crystals of **4** were grown by vapor diffusion of ether into a nearly saturated acetone solution. A small chunk was cut from a needle with a razor blade and glued to a glass fiber with epoxy cement. The crystal was coated with epoxy to prevent damage and then painted with India ink to protect it from light. A preliminary oscillation photograph about the **b** axis appeared normal; the crystal was moved to the diffractometer and preliminary cell dimensions plus an orientation matrix were calculated from the setting angles of 18 reflections with $12^o < 2\theta < 17^o$. Final cell dimensions came from 25 reflection with $30^o < 2\theta < 33^o$. The cell chosen had a **c** axis 42Å long; data were collected in this cell. Subsequent events indicated the presence of a twin, about 16% as large as the parent crystal. The twin plane was (001), and two of the indexing reflections were from the twin, giving a cell four times larger than the correct one. Thus roughly three-quarters of the data collected were worthless and were discarded later. The reflections belonging to the small cell all had h -l = 4n; this relationship implies that the correct cell dimensions are obtained with the matrix 1, 0, 0; 0, 1, 0; -1/4, 0, 1/4. The data were reduced to structure factors, corrected for a slight decay and placed on an approximately absolute scale by Wilson's method. The structure was solved by MULTAN and refined by full matrix least squares. Reflections of the type 5, k, l were closely superimposed on 5,k, l+3 from the twin and 7, k, l on 7, k, l+4; the 0kl's were also composite. We eventually corrected the 0 k l's by dividing F_o and σF_o by 1.08 but were unable to make systematic corrections to the 5 k l's and the 7 k l's so we deleted those for which F_c for the twin components was greater than about 0.4 times the measured value for the composite reflection. With the smaller data set we had only 935 data and the structure required 227 parameters, a data : parameter ratio of only 4.1, but it was not feasible to collect additional data. The final least squares cycles varied positional and anisotropic thermal parameters for the 25 heavy atoms, a scale factor and a secondary extinction parameter. Hydrogen atoms were included as fixed contributions to the structure factors at calculated positions or, for the methyl groups, at idealized positions based on

difference maps calculated in the expected plane. They were assigned arbitrary isotropic thermal parameters. The final R- index for the 868 reflections with $F_0^2 > 0$ is 0.029, with a goodness of fit for all 935 reflections of 2.15. The R-index for the 798 reflections with $F_0^2 > 3\sigma(F_0^2)$ is 0.025. The final difference map was featureless, with maximum excursions of +0.14 and -0.10eÅ^{-3}.

Calculations were done with programs of the CRYM Crystallographic Computing System and ORTEP. Scattering factors and corrections for anomalous scattering were taken from a standard reference[1]. $R = \Sigma \mid F_o - \mid F_c \mid \mid / \Sigma F_o$, for only $F_o^2 > 0$, and goodness of fit $[\Sigma w (F_o^2 - F_c^2)^2 / (n - p)]^{1/2}$, where n is the number of data, and p is the number of parameters refined. The function minimized in least squares was $\Sigma w (F_o^2 - F_c^2)^2$ where $1/\sigma^2(F_o^2)$. Variances of the individual reflection were assigned based on counting statistics plus an additional term, $0.0141I^2$. Variances of the merged reflection were determined by standard propagation of error plus another additional term, $0.0014\langle I\rangle^2$. The secondary extinction parameter[2] refined to $0.34(10) \times 10^{-6}$.

Crystallographic data for 2'-methoxy-2-N-methyl stilbazolium triflate, **4**.

Formula	$C_{15}H_{16}NO{\cdot}CF_3SO_3$
Formula wt.	397.37
Space group	$P2_1/n$,(No. 14)
a	11.999(2)Å
b	13.458(2)Å
c	11.043(2)Å
β	108.47(1)°
volume	1691.4(6)Å^3
Z; ρ_{calc}	4; 1.474 g cm^{-3}
No. reflections; GOF	935; 2.15
No., $F^2_o > .0$; R_F	868; 0.029
No., $F^2_o > 3\sigma(F^2_o)$; R_F	798; 0.025
T	23°C
λ	0.71073 Å
μ	2.5cm^{-1}

(1) *International Tables for X-ray Crystallography*, Kynoch Press, Birmingham, 1974, Vol. IV, p 71. p 149;

(2) Larson, E. C. *Acta Cryst.* **1967**, *23*, 664, eqn. 3

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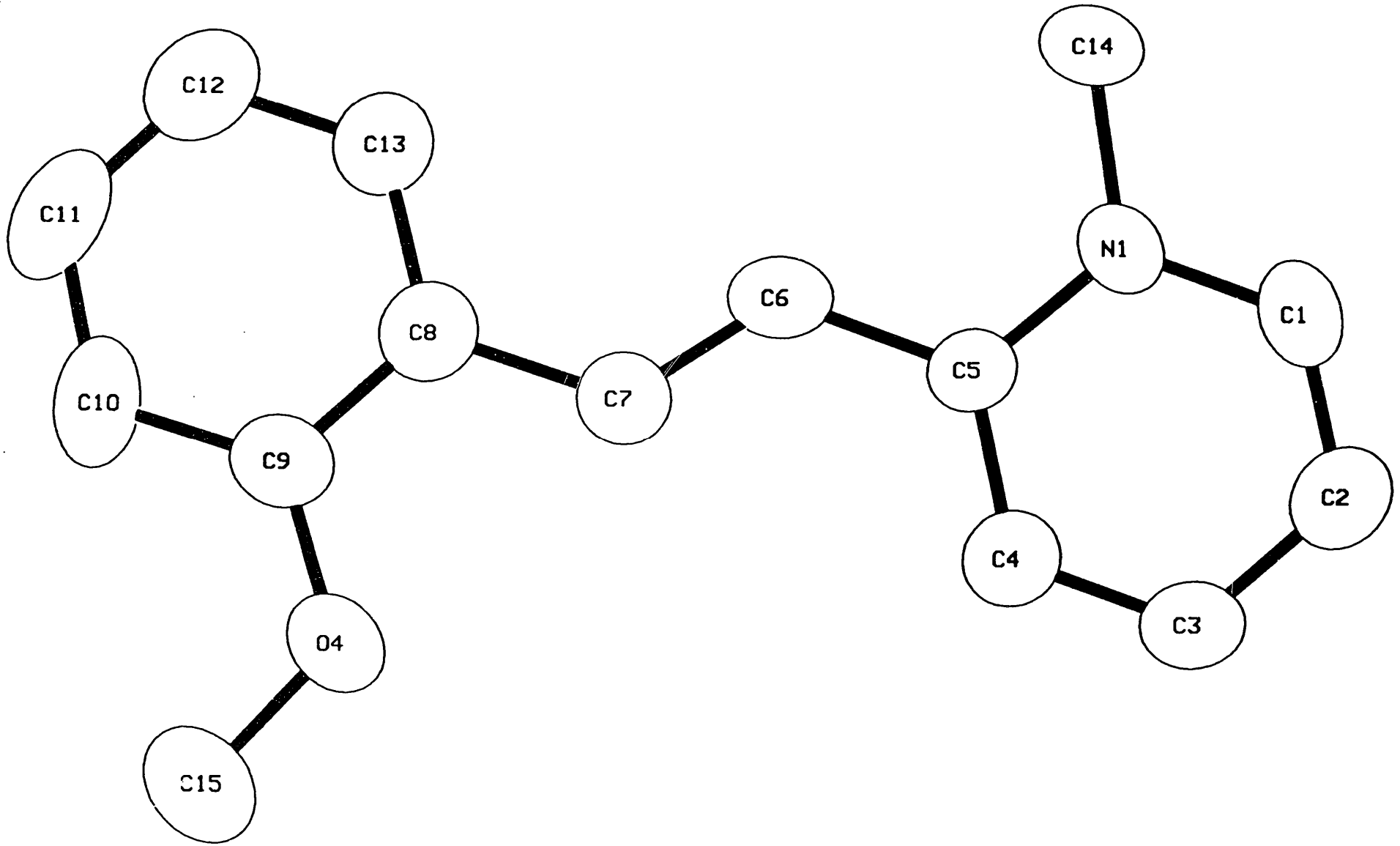

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Table S VI. Final Heavy Atom Parameters for 2′-Methoxy-2-N-Methyl Stilbazolium Triflate.

x, y, z and U_{eq}[a] $\times 10^4$

Atom	x	y	z	U_{eq}
N1	4114(4)	1441(2)	2613(4)	439(12)
C1	2970(5)	1540(3)	1910(4)	508(13)
C2	2101(4)	1570(3)	2451(5)	547(14)
C3	2398(4)	1493(3)	3761(5)	518(13)
C4	3552(5)	1405(3)	4469(4)	512(13)
C5	4436(4)	1379(2)	3910(5)	433(14)
C6	5673(5)	1288(3)	4645(5)	569(14)
C7	6085(4)	1097(3)	5885(4)	486(13)
C8	7318(4)	997(3)	6665(5)	487(15)
C9	7592(5)	930(3)	7998(5)	526(15)
C10	8760(5)	889(3)	8773(4)	673(16)
C11	9641(4)	887(3)	8222(6)	777(20)
C12	9389(5)	925(3)	6914(6)	762(18)
C13	8233(5)	985(3)	6154(4)	625(14)
C14	4996(4)	1396(3)	1938(4)	639(13)
O4	6652(3)	918(2)	8430(3)	667(10)
C15	6838(4)	878(3)	9757(4)	801(15)
S	2949(1)	1701(1)	7829(1)	628(4)
O1	2100(3)	1827(2)	6597(2)	771(10)
O2	2492(3)	1769(2)	8875(2)	897(10)
O3	3777(3)	925(2)	7906(3)	1134(13)
C	3825(5)	2811(4)	8014(5)	671(15)
F1	4341(2)	2893(2)	7115(2)	960(8)
F2	4667(2)	2859(2)	9134(3)	1049(10)
F3	3183(3)	3634(2)	7925(2)	977(9)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table S VII. Assigned Hydrogen Parameters for 2′-Methoxy-2-N-Methyl Stilbazolium Triflate.

x, y and $z \times 10^4$

Atom	x	y	z	B
H1	2788	1584	994	6.0
H2	1287	1642	1892	6.0
H3	1786	1515	4164	6.0
H4	3751	1354	5397	6.0
H6	6252	1390	4215	6.0
H7	5492	993	6303	6.0
H10	8943	869	9712	6.0
H11	10441	865	8809	6.0
H12	10051	910	6572	6.0
H13	8054	992	5234	6.0
H14A	5538	1966	2176	7.0
H14B	4653	1407	1040	7.0
H14C	5491	810	2172	7.0
H15A	7198	1466	10196	7.0
H15B	7328	316	10157	7.0
H15C	6097	788	9953	7.0

Table S VIII. Anisotropic Displacement Parameters for 2′-Methoxy-2-N-Methyl Stilbazolium Triflate.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N1	477(35)	484(20)	347(29)	−2(18)	117(26)	45(16)
C1	537(36)	527(26)	385(28)	29(25)	38(37)	5(20)
C2	472(35)	532(27)	636(38)	20(25)	173(32)	−10(22)
C3	516(42)	555(26)	539(33)	15(24)	246(31)	−32(21)
C4	482(37)	549(26)	515(30)	11(24)	170(34)	−25(21)
C5	386(41)	488(25)	442(39)	−1(22)	155(35)	30(21)
C6	509(38)	766(30)	504(33)	−49(26)	262(33)	42(23)
C7	480(37)	502(24)	476(32)	13(23)	152(31)	48(21)
C8	509(42)	383(25)	565(42)	6(24)	166(36)	32(21)
C9	599(47)	490(26)	520(41)	−37(26)	222(39)	6(22)
C10	510(38)	651(30)	670(34)	−73(28)	−78(38)	14(24)
C11	407(39)	840(35)	982(47)	−5(30)	74(35)	92(31)
C12	567(47)	857(34)	877(42)	−26(30)	251(36)	135(30)
C13	525(36)	735(31)	606(33)	−36(28)	168(36)	129(24)
C14	578(31)	953(34)	466(26)	90(25)	278(26)	102(22)
O4	632(24)	948(22)	416(21)	57(18)	157(18)	20(15)
C15	876(37)	973(34)	540(32)	51(29)	206(29)	70(25)
S	474(9)	869(10)	547(10)	26(8)	171(8)	82(7)
O1	621(20)	1181(24)	433(18)	−149(18)	58(19)	−22(16)
O2	819(23)	1486(28)	495(17)	−193(20)	365(19)	85(17)
O3	796(28)	852(23)	1736(35)	317(24)	374(24)	151(22)
C	557(32)	974(41)	494(33)	31(34)	184(32)	2(30)
F1	819(20)	1343(22)	880(18)	−276(18)	500(18)	−66(16)
F2	738(19)	1543(24)	691(18)	−269(20)	−20(18)	−67(17)
F3	1077(27)	856(19)	1001(21)	74(19)	333(20)	−35(15)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table S IX. Complete Distances and Angles for 2′-Methoxy-2-N-Methyl Stilbazolium Triflate.

	Distance(Å)		Distance(Å)
N1 –C1	1.353(6)	C –F3	1.334(6)
N1 –C5	1.363(6)		
N1 –C14	1.476(5)		
C1 –C2	1.356(7)		
C1 –H1	0.967		
C2 –C3	1.379(7)		
C2 –H2	0.981		
C3 –C4	1.362(6)		
C3 –H3	0.973		
C4 –C5	1.386(6)		
C4 –H4	0.978		
C5 –C6	1.454(7)		
C6 –C7	1.325(6)		
C6 –H6	0.968		
C7 –C8	1.464(6)		
C7 –H7	0.974		
C8 –C9	1.406(7)		
C8 –C13	1.384(7)		
C9 –C10	1.393(7)		
C9 –O4	1.357(6)		
C10 –C11	1.377(7)		
C10 –H10	0.990		
C11 –C12	1.380(7)		
C11 –H11	0.974		
C12 –C13	1.378(7)		
C12 –H12	0.982		
C13 –H13	0.969		
C14 –H14A	0.987		
C14 –H14B	0.946		
C14 –H14C	0.971		
O4 –C15	1.411(5)		
C15 –H15A	0.957		
C15 –H15B	0.974		
C15 –H15C	0.986		
S –O1	1.428(3)		
S –O2	1.430(3)		
S –O3	1.425(4)		
S –C	1.801(5)		
C –F1	1.330(6)		
C –F2	1.328(6)		

Table S IX. (Cont.)

			Angle(°)				Angle(°)
C5	-N1	-C1	120.4(4)	C15	-O4	-C9	119.4(3)
C14	-N1	-C1	118.3(4)	O2	-S	-O1	114.9(2)
C14	-N1	-C5	121.2(4)	O3	-S	-O1	114.7(2)
C2	-C1	-N1	122.2(4)	C	-S	-O1	102.9(2)
H1	-C1	-N1	117.2	O3	-S	-O2	115.9(2)
H1	-C1	-C2	120.7	C	-S	-O2	102.4(2)
C3	-C2	-C1	118.7(4)	C	-S	-O3	103.3(2)
H2	-C2	-C1	118.5	F1	-C	-S	112.1(3)
H2	-C2	-C3	122.8	F2	-C	-S	112.9(4)
C4	-C3	-C2	119.1(4)	F3	-C	-S	112.2(3)
H3	-C3	-C2	119.8	F2	-C	-F1	107.2(4)
H3	-C3	-C4	121.2	F3	-C	-F1	105.7(4)
C5	-C4	-C3	121.9(4)	F3	-C	-F2	106.2(4)
H4	-C4	-C3	118.3				
H4	-C4	-C5	119.8				
C4	-C5	-N1	117.7(4)				
C6	-C5	-N1	119.4(4)				
C6	-C5	-C4	122.9(4)				
C7	-C6	-C5	125.0(4)				
H6	-C6	-C5	118.6				
H6	-C6	-C7	116.3				
C8	-C7	-C6	127.1(4)				
H7	-C7	-C6	115.3				
H7	-C7	-C8	117.6				
C9	-C8	-C7	118.6(4)				
C13	-C8	-C7	123.1(4)				
C13	-C8	-C9	118.3(4)				
C10	-C9	-C8	120.1(4)				
O4	-C9	-C8	115.1(4)				
O4	-C9	-C10	124.7(4)				
C11	-C10	-C9	119.5(5)				
H10	-C10	-C9	119.4				
H10	-C10	-C11	121.2				
C12	-C11	-C10	121.3(5)				
H11	-C11	-C10	115.9				
H11	-C11	-C12	122.8				
C13	-C12	-C11	118.9(5)				
H12	-C12	-C11	117.8				
H12	-C12	-C13	123.3				
C12	-C13	-C8	121.9(5)				

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Table S V. Observed and Calculated Structure Factors for 3′-Methoxy-2-N-Methyl Stilbazolium Triflate.

The columns contain, in order, h, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$.
A minus sign preceeding F_{obs} indicates that F^2_{obs} is negative.

h	0	0	
2	213	222	-54
4	1498	1431	56
6	534	499	79
8	212	219	-40
10	641	631	19
12	456	431	67
14	292	279	54
16	231	228	15
18	156	153	16
20	125	121	24

h	0	2	
-20	115	114	7
-18	52	50	8
-16	308	313	-15
-14	517	504	29
-12	305	311	-20
-10	217	209	37
-8	93	92	8
-6	205	215	-51
-4	1376	1380	-3
-2	1752	1895	-98
0	413	378	93
2	2106	2102	1
4	1143	1124	19
6	346	328	57
8	338	332	19
10	184	181	13
12	547	545	3
14	524	519	11
16	144	138	35
18	254	268	-45
20	34	37	-10

h	0	4	
-20	105	108	-12
-18	101	104	-14
-16	480	475	10
-14	519	519	-1
-12	549	555	-13
-10	119	122	-19
-8	168	169	-1
-6	427	406	55
-4	37	43	-62
-2	1049	1081	-35
0	798	806	-11
2	641	617	43
4	374	362	34
6	694	685	15
8	216	222	-29
10	147	150	-18
12	355	358	-9
14	217	223	-28
16	336	356	-68
18	18	23	-10
20	103	119	-71

h	0	6	
-20	180	183	-12
-18	128	133	-21
-16	155	164	-40
-14	274	273	1
-12	490	477	28
-10	324	317	20
-8	342	325	51
-6	369	359	30
-4	297	313	-63
-2	640	659	-34
0	987	967	22
2	819	741	104
4	757	700	99
6	237	233	19
8	363	367	-14
10	144	141	20
12	409	407	5
14	102	104	-16
16	153	158	-22
18	107	115	-36

h	0	8	
-18	95	103	-33
-16	187	200	-49
-14	306	307	-3
-12	241	214	107
-10	323	300	73
-8	333	318	48
-6	523	527	-8
-4	575	565	18
-2	399	400	-2
0	633	600	43
2	516	508	17
4	177	178	-7
6	127	118	58
8	255	254	4
10	184	166	85
12	315	292	73
14	152	148	18
16	163	159	15

h	0	10	
-16	73	95	-105
-14	8	24	-25
-12	340	338	5
-10	107	103	23
-8	290	280	37
-6	268	279	-43
-4	599	590	16
-2	183	193	-57
0	281	284	-11
2	276	283	-28
4	107	110	-18
6	186	192	-27
8	229	219	41
10	172	162	52
12	145	134	43
14	126	128	-5

h	0	12	
-14	73	75	-6
-12	10	15	-5
-10	7	10	-3
-8	127	125	9
-6	109	105	22
-4	204	198	24
-2	123	132	-60
0	153	162	-55
2	213	215	-6
4	264	296	-134
6	167	163	19
8	76	87	-52
10	111	118	-30
12	51	46	18

h	0	14	
-10	59	62	-10
-8	95	81	56
-6	79	73	25
-4	109	113	-15
-2	29	34	-14
0	74	70	17
2	72	78	-27
4	96	93	13
6	67	76	-38
8	29	26	6

h	1	0	
1	87	76	126
3	195	207	-81
5	191	198	-40
7	463	470	-18
9	477	494	-46
11	179	185	-37
13	70	67	28
15	132	135	-16
17	133	130	18
19	86	79	40
21	38	39	-3

h	1	1	
-21	75	76	-4
-19	44	43	1
-17	105	106	-11
-15	320	305	48
-13	286	285	1
-11	258	259	-2
-9	268	259	38
-7	508	485	52
-5	528	502	54
-3	1371	1337	28
-1	871	846	32
1	888	886	2
3	1105	1084	21
5	619	616	5
7	883	829	68
9	951	878	84
11	506	473	71
13	308	304	12
15	243	227	64
17	148	146	10
19	91	83	33
21	126	128	-7

h	1	2	
-21	64	51	43
-19	72	67	18
-17	69	64	29
-15	146	142	25
-13	149	151	-12
-11	326	341	-52
-9	522	546	-54
-7	493	520	-66
-5	311	340	-110
-3	106	109	-28
-1	214	232	-97
1	334	372	-134
3	307	338	-120
5	189	214	-149
7	237	245	-36
9	54	55	-7
11	163	165	-13
13	215	222	-35
15	223	223	0
17	164	164	-1
19	74	75	-5

h	1	3	
-21	164	155	31
-19	47	48	-3
-17	269	260	27
-15	238	245	-28
-13	488	481	16
-11	157	144	73
-9	158	156	9
-7	410	389	59
-5	460	422	91
-3	251	261	-42
-1	1005	1016	-12
1	913	875	47
3	279	269	41
5	108	104	26
7	280	273	30
9	582	545	71
11	361	349	37
13	211	200	49
15	218	203	65
17	200	194	21
19	83	81	9

h	1	4	
-19	68	54	49
-17	129	118	48
-15	83	72	72
-13	94	90	21
-11	194	199	-26
-9	346	353	-21
-7	185	190	-24
-5	136	125	70
-3	379	405	-79
-1	269	290	-90
1	111	113	-17
3	329	345	-54
5	310	324	-50
7	195	206	-57
9	262	259	11
11	231	239	-38
13	257	264	-29
15	195	196	-5
17	147	147	2
19	75	79	-16

h	1	5	
-19	62	61	4
-17	146	135	45
-15	323	331	-27
-13	181	168	67
-11	82	81	8
-9	583	540	81
-7	621	548	127
-5	945	908	44
-3	261	252	37
-1	139	128	78
1	582	553	56
3	298	270	98
5	297	290	28
7	146	142	26
9	107	101	44
11	335	334	4
13	248	247	3
15	192	186	30
17	73	81	-37
19	57	65	-34

h	1	6	
-19	42	39	6
-17	54	48	21
-15	69	73	-27
-13	93	102	-64
-11	164	166	-10
-9	145	145	2
-7	80	76	32
-5	389	400	-32
-3	470	500	-74
-1	282	316	-142
1	215	242	-147
3	161	163	-7
5	221	219	9
7	196	198	-11
9	217	220	-9
11	114	123	-57
13	188	195	-34
15	142	145	-14
17	88	99	-50
19	31	42	-30

h	1	7	

-19	107	117	-45
-17	103	105	-7
-15	134	135	-5
-13	255	250	18
-11	298	300	-7
-9	248	248	0
-7	305	282	80
-5	144	148	-26
-3	414	411	9
-1	471	485	-35
1	275	265	40
3	324	314	34
5	75	73	19
7	218	226	-37
9	799	790	12
11	456	464	-19
13	374	368	16
15	85	91	-25
17	85	83	6

h 1 8

-17	30	32	-3
-15	64	70	-25
-13	94	90	23
-11	153	149	26
-9	139	136	14
-7	38	37	3
-5	89	91	-16
-3	189	191	-9
-1	119	120	-12
1	81	87	-48
3	169	173	-23
5	192	195	-15
7	154	156	-10
9	121	132	-73
11	169	177	-40
13	50	57	-30
15	76	79	-15
17	49	55	-23

h 1 9

-17	70	75	-21
-15	142	148	-23
-13	275	289	-46
-11	141	149	-48
-9	211	215	-19
-7	331	327	15
-5	304	290	49
-3	356	363	-22
-1	345	341	12
1	239	229	41
3	190	193	-18
5	285	275	35
7	220	215	24
9	124	132	-55
11	459	444	35
13	35	35	0
15	93	85	35

h 1 10

-17	27	29	-5
-15	33	38	-15
-13	98	96	7
-11	140	136	22
-9	155	151	22
-7	121	128	-41
-5	101	113	-81
-3	99	102	-21
-1	126	138	-81
1	204	209	-21
3	246	248	-5
5	194	199	-21
7	172	172	-1
9	99	99	0
11	54	53	3
13	73	70	9
15	58	58	-2

h 1 11

-15	92	94	-5
-13	49	50	-1
-11	90	92	-7
-9	133	134	-5
-7	217	213	18
-5	609	610	-2
-3	499	468	67
-1	288	281	25
1	140	140	0
3	183	186	-15
5	64	54	61
7	127	131	-22
9	110	112	-8
11	81	66	59
13	54	57	-9

h 1 12

-13	47	51	-14
-11	59	60	-7
-9	88	91	-13
-7	30	40	-34
-5	95	99	-30
-3	60	74	-96
-1	116	128	-75
1	150	153	-18
3	192	193	-2
5	154	151	16
7	91	94	-16
9	73	75	-5
11	52	52	1

h 1 13

-13	68	62	23
-11	82	82	2
-9	62	64	-7
-7	48	41	22
-5	53	58	-19
-3	139	137	6
-1	61	50	40
1	22	20	5
3	63	64	-3
5	100	94	24
7	50	54	-15
9	83	79	13

h 1 14

-9	47	47	0
-7	-17	20	-39
-5	23	28	-12
-3	29	37	-23
-1	52	60	-34
1	77	77	0
3	63	68	-18
5	73	74	-3
7	29	41	-35

h 1 15

-7	81	73	30
-5	28	31	-9
-3	47	50	-9
-1	69	62	26
1	43	36	20
3	114	105	36
5	35	45	-27

h 2 0

0	2210	2224	-7
2	2282	2231	27
4	136	140	-38
6	292	293	-4
8	328	314	49
10	283	273	38
12	207	192	84
14	57	58	-5
16	88	85	23
18	60	60	-1
20	61	63	-7

h 2 1

-20	65	63	8
-18	88	84	17
-16	112	118	-34
-14	185	185	0
-12	165	177	-69
-10	189	208	-102
-8	352	375	-78
-6	335	343	-28
-4	472	456	39
-2	515	522	-16
0	827	808	25
2	990	1024	-39
4	388	424	-110
6	100	106	-50
8	125	125	1
10	219	221	-10
12	226	233	-31
14	212	218	-25
16	148	145	12
18	110	112	-8
20	73	75	-7

h 2 2

-20	94	92	10
-18	44	49	-18
-16	232	228	15
-14	273	281	-28
-12	201	183	88
-10	366	355	35
-8	266	253	55
-6	-12	20	-81
-4	155	158	-25
-2	427	422	14
0	1570	1529	29
2	539	533	11
4	510	517	-16
6	98	96	18
8	596	551	83
10	-21	1	-33
12	146	126	112
14	122	115	39
16	161	177	-94
18	132	136	-18
20	49	64	-59

h 2 3

-20	68	59	33
-18	74	72	10
-16	201	190	48
-14	85	82	23
-12	263	273	-40
-10	230	248	-88
-8	322	345	-81
-6	203	209	-34
-4	296	298	-7
-2	497	500	-8
0	612	614	-4
2	456	497	-107
4	492	532	-97
6	327	336	-32
8	245	253	-35
10	273	271	6
12	220	233	-62
14	221	225	-14
16	255	264	-30
18	95	84	46
20	100	103	-13

h 2 4

-20	76	70	22
-18	91	91	-1
-16	359	339	48
-14	459	465	-13
-12	286	282	14
-10	128	117	72
-8	243	222	86
-6	254	239	61
-4	265	265	0
-2	118	117	11
0	333	308	80
2	544	524	40
4	327	333	-20
6	337	321	50
8	505	494	24
10	193	187	30
12	156	149	40
14	114	107	42
16	165	157	29
18	72	88	-71

h 2 5

-20	63	58	16
-18	61	52	30
-16	129	128	6
-14	245	244	3
-12	99	102	-21
-10	199	201	-10
-8	161	163	-12
-6	205	207	-10
-4	350	350	0
-2	281	299	-74
0	149	150	-6
2	393	394	-4
4	369	352	48
6	253	246	29
8	117	123	-41
10	181	178	18
12	249	256	-29
14	193	199	-29
16	158	157	7
18	96	104	-33

h 2 6

-18	48	51	-8
-16	19	13	9
-14	72	66	34
-12	134	137	-21
-10	113	113	-1
-8	116	120	-27
-6	264	268	-15
-4	232	232	0
-2	88	90	-15
0	415	384	83
2	779	735	62
4	549	516	66
6	386	398	-37
8	142	140	11
10	83	83	3
12	152	143	48
14	129	131	-7
16	79	73	23
18	88	93	-19

h 2 7

-18	95	89	24
-16	62	64	-9
-14	108	108	0

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-12	160	168	-44
-10	208	205	15
-8	219	207	53
-6	85	84	7
-4	169	167	9
-2	269	279	-41
0	286	284	6
2	156	149	44
4	223	219	17
6	139	133	38
8	166	160	33
10	106	103	16
12	147	144	17
14	142	151	-39
16	86	87	-4

h 2 8

-18	39	30	22
-16	69	74	-22
-14	47	46	5
-12	100	107	-48
-10	60	52	49
-8	26	35	-43
-6	150	149	5
-4	20	20	0
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9	429	407	56
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9	261	248	50
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13	201	206	-23
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-9	158	163	-26
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6	170	174	-27
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16	187	189	-7
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6	135	142	-44
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12	82	82	-2
14	121	125	-18
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0	204	204	-3
2	153	151	10
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11	165	166	-7
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h 6 7

-12	51	43	22
-10	14	25	-20
-8	-7	9	-7
-6	65	62	11
-4	8	19	-15
-2	121	119	11
0	26	47	-73
2	197	199	-7
4	74	81	-33
6	58	58	0
8	-2	17	-14
10	84	69	54

h 6 8

-10	30	41	-32
-8	62	62	0
-6	69	62	28
-4	86	77	37
-2	102	94	31
0	83	80	11
2	44	49	-19
4	18	23	-10
6	95	92	9
8	53	54	-1

h 6 9

-8	29	37	-21
-6	121	114	27
-4	53	53	0
-2	142	127	59
0	56	46	35
2	58	53	16
4	28	30	-5
6	58	54	14

h 6 10

-6	101	103	-7
-4	113	102	41
-2	139	134	16
0	83	72	41
2	73	74	-2
4	43	46	-10

h 6 11

-2	35	24	24
0	61	56	14

h 7 0

1	66	67	-6
3	108	91	97
5	40	32	31
7	195	180	66
9	48	40	36
11	126	122	21

h 7 1

-11	54	48	20
-9	11	4	4
-7	21	13	13
-5	12	26	-27
-3	145	154	-39
-1	56	61	-19
1	45	60	-63
3	-13	9	-13
5	28	29	-3
7	69	70	-2
9	82	80	8
11	26	33	-17

h 7 2

-11	125	115	38
-9	65	60	18
-7	37	44	-22
-5	54	52	10
-3	59	52	25
-1	40	32	23
1	92	87	20
3	39	35	13
5	149	138	44
7	42	33	25
9	198	188	35
11	56	37	54

h 7 3

-11	53	59	-22
-9	53	44	29
-7	62	64	-9
-5	29	40	-32
-3	38	48	-33
-1	26	21	11
1	7	11	-4
3	27	33	-15
5	44	43	4
7	35	25	25
9	21	16	9

h 7 4

-9	81	81	-1
-7	127	125	5
-5	101	105	-19
-3	90	91	-4
-1	-15	17	-29
1	64	57	25
3	70	67	12
5	61	54	25
7	116	109	29
9	36	27	22

h 7 5

-9	42	51	-29
-7	46	56	-37
-5	53	56	7
-3	65	69	-15
-1	-13	8	-13
1	22	29	-17
3	43	50	-26
5	64	65	-4
7	27	29	-3
9	16	11	5

h 7 6

-9	56	52	11
-7	68	65	9
-5	89	88	0
-3	48	38	31
-1	52	49	10
1	88	90	-9
3	81	76	20
5	74	68	21
7	75	68	27

h 7 7

-7	14	22	-12
-5	33	36	-9
-3	31	31	0
-1	50	54	-16
1	26	25	1
3	24	24	0
5	-4	20	-20

h 7 8

-5	40	25	34
-3	73	64	33
-1	91	75	60
1	73	59	48
3	67	57	35

h 8 0

0	93	100	-33
2	49	55	-31
4	68	72	-20
6	40	30	34

h 8 1

-6	94	83	41
-4	53	49	14
-2	162	173	-43
0	172	189	-64
2	124	137	-54
4	96	92	17
6	89	78	43

h 8 2

-4	35	33	5
-2	46	45	1
0	24	8	22
2	97	92	17
4	63	55	26

h 8 3

-4	57	44	42
-2	31	33	-6
0	21	25	-8
2	76	76	2
4	56	46	31

h 8 4

-2	58	57	4
0	22	12	14
2	46	46	0

Table S X. Observed and Calculated Structure Factors for 2′-Methoxy-2-N-Methyl Stilbazolium Triflate.

The columns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceding F_{obs} indicates that F^2_{obs} is negative.

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-10 0 1

4	111	113	-10

-10 1 1

3	126	120	24
4	185	189	-7

-9 0 1

3	45	44	1
5	243	240	6

-9 1 1

3	32	28	4
4	175	180	-12
5	253	249	8
6	85	85	0

-9 2 1

3	74	74	0
4	54	61	-26
5	106	106	-1
6	46	54	-25

-9 3 1

3	48	43	15
4	231	237	-13
5	22	34	-26

-9 4 1

3	6	0	1
4	105	106	-5
5	35	22	12

-9 5 1

3	-21	4	-8

-8 0 1

4	33	20	32
6	77	80	-13

-8 1 1

3	89	90	-4
4	181	172	20
5	86	91	-23
6	91	88	15
7	-29	14	-22

-8 2 1

3	207	215	-19
4	-27	8	-20
5	140	139	2
6	55	62	-24
7	180	181	-1

-8 3 1

3	60	55	21
4	3	5	0
5	310	309	2
6	82	84	-5
7	188	172	37

-8 4 1

3	26	13	9
4	-15	31	-26
5	95	95	1
6	-26	11	-17

-8 5 1

3	180	179	2
4	261	266	-9
5	311	305	11
6	252	250	4

-8 6 1

3	-3	26	-13
4	36	54	-59
5	23	13	6

-7 0 1

3	159	145	37
5	227	217	22

-7 1 1

5	249	251	-4
8	168	167	2

-7 2 1

6	173	175	-3
8	320	311	17

-7 3 1

4	162	165	-10

-7 4 1

3	116	110	26
4	195	197	-3

-7 5 1

3	270	272	-3
4	305	285	41
5	360	350	18
6	207	186	42
7	89	85	18

-7 6 1

3	87	76	47

-7 7 1

5	247	245	4

-6 0 1

2	192	198	-16
4	228	221	17
6	171	163	18
8	243	241	3

-6 1 1

2	169	178	-25
3	251	248	8
4	157	167	-29
5	297	282	32
6	418	418	0
7	80	83	-13
8	119	129	-42

-6 2 1

2	236	244	-21
3	265	263	4
4	122	126	-18
5	365	353	23
6	13	9	2
7	22	11	7
8	152	147	13

-6 3 1

2	120	121	-6
3	302	293	19
4	63	65	-10
5	378	381	-6
6	105	106	-3
7	22	23	-2
8	205	201	6

-6 4 1

2	117	114	9
3	39	38	4
4	245	245	1
5	223	216	14
6	193	192	1
7	171	171	0
8	199	201	-3

-6 5 1

2	19	23	-5
3	112	108	17
4	-24	0	-15
5	38	35	8
6	98	96	6
7	84	71	48

-6 6 1

2	78	82	-18
3	16	17	0
4	23	8	9
5	66	65	5
6	178	172	13
7	211	196	29

-6 7 1

2	-14	9	-6
3	35	41	-18
4	130	132	-6
5	133	136	-10
6	73	71	10

-6 8 1

2	119	112	26
3	-22	6	-25
4	-12	20	-25
5	33	40	-8

-6 9 1

2	43	46	-8
3	159	158	2

-5 0 1

3	99	106	-28
5	404	411	-12
7	298	302	-9
9	304	290	27

-5 1 1

2	229	230	-1
3	488	485	5
5	705	690	19
7	327	311	32

-5 2 1

3	342	350	-18
4	689	674	20
5	299	297	3
8	321	345	-47

-5 3 1

3	107	107	0
8	336	356	-37

-5 4 1

2	247	258	-28

-5 5 1

3	471	480	-15

-5 6 1

3	527	525	2
4	364	356	15
5	441	423	30

-5 7 1

5	216	207	18

-5 9 1

4	104	109	-22

-4 0 1

2	151	145	20
4	332	337	-10
6	558	564	-10
8	162	148	38

-4 1 1

2	137	125	37
3	112	113	-5
4	623	623	0
5	120	122	-8
6	299	298	2
7	174	176	-5
8	307	319	-24
9	115	120	-18

-4 2 1

2	133	135	-6
3	632	634	-2
4	103	115	-48
5	94	94	-2
6	336	339	-5
7	60	61	-6
8	135	123	36
9	136	138	-8

-4 3 1

2	184	189	-12
3	165	152	35
4	45	42	12
5	133	135	-5
6	207	211	-8
7	122	117	16
8	125	125	0

-4 4 1

2	207	213	-14
3	244	251	-17
4	-15	24	-24
5	31	30	1

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6	50	54	-17
7	75	76	-6
8	31	27	8

-4 5 l

2	47	54	-37
3	99	102	-11
4	184	170	33
5	79	79	-3
6	50	55	-21
7	106	109	-13
8	250	249	3

-4 6 l

2	340	341	-2
3	52	50	8
4	38	33	16
5	110	109	2
6	164	162	3
7	15	19	-5

-4 7 l

2	72	75	-12
3	-23	12	-18
4	12	17	-3
5	100	98	7
6	77	77	0
7	59	61	-7

-4 8 l

2	77	75	7
3	70	67	12
4	133	130	7
5	177	169	19
6	24	40	-17

-4 9 l

2	-27	16	-23
3	115	119	-15
4	21	12	5
5	40	52	-37

-4 10 l

2	41	39	5
3	66	61	17

-3 0 l

1	457	457	0
3	512	532	-35
5	555	558	-4
7	278	287	-19
9	184	173	25

-3 1 l

1	735	747	-15
2	16	17	-3
3	398	401	-6
4	393	382	22
5	95	91	23
6	68	70	-13
7	265	276	-26
8	15	0	4
9	245	252	-13

-3 2 l

1	232	231	1
2	463	476	-25
3	278	273	13
4	119	108	39
5	192	198	-17
6	167	163	9
7	135	134	4
8	63	61	6
9	134	127	23

-3 3 l

1	700	692	11
2	224	226	-6
3	50	48	14
4	357	361	-7
5	116	117	-3
6	247	245	4
7	7	4	0
8	106	108	-9
9	51	55	-10

-3 4 l

1	562	569	-11
2	482	495	-23
3	274	276	-3
4	14	3	11
5	163	168	-14
6	69	67	6
7	150	160	-27
8	101	102	-7

-3 5 l

1	279	288	-22
2	188	182	16
3	-12	8	-7
4	65	69	-18
5	-13	4	-5
6	166	171	-15
7	64	64	0
8	202	188	28

-3 6 l

1	303	303	0
2	432	438	-10
3	353	343	20
4	39	43	-17
5	128	127	2
6	-29	11	-26
7	140	135	13

-3 7 l

1	154	150	12
2	84	90	-28
3	-16	4	-17
4	70	63	29
5	-23	12	-18
6	-5	19	-18
7	82	80	9

-3 8 l

1	97	100	-13
2	26	17	18
3	20	20	0
4	48	48	-2
5	-28	0	-18
6	6	26	-28

-3 9 l

1	24	21	2
2	8	20	-8
3	57	64	-31
4	5	36	-59
5	75	76	-6

-3 10 l

1	79	85	-24
2	205	197	18
3	138	142	-16
4	108	104	15

-2 0 l

2	1135	1147	-11
4	179	178	3
6	28	13	35
8	460	445	25

-2 1 l

1	242	239	7
2	738	752	-18
3	364	343	48
4	125	152	-27
6	42	53	-47
7	88	69	82
8	340	340	0
9	104	111	-30

-2 2 l

1	672	656	23
2	512	523	-20
3	37	45	-38
4	-15	7	-10
5	17	12	9
6	19	2	21
7	78	78	0
8	49	51	-7
9	44	35	24

-2 3 l

1	646	639	11
2	179	175	11
3	163	161	4
4	47	47	2
5	130	128	4
6	22	7	11
7	196	202	-15
8	71	70	3

-2 4 l

1	513	526	-22
2	512	515	-5
3	139	139	0
4	109	110	-5
5	256	245	25
6	121	125	-17
7	49	46	10
8	205	206	-2

-2 5 l

1	373	373	1
2	-1	23	-17
3	150	155	-14
4	96	100	-22
5	196	202	-16
6	30	39	-13
7	78	68	37
8	153	156	-7

-2 6 l

1	241	240	3
2	412	429	-33
3	141	140	1
4	115	112	10
5	148	147	2
6	204	195	19
7	59	62	-13

-2 7 l

1	76	75	3
2	182	179	8
3	-35	11	-47
4	76	78	-13
5	80	82	-7
6	-8	34	-26
7	88	93	-17

-2 8 l

1	145	136	29
2	4	2	0
3	92	90	8
4	45	46	-4
5	101	101	-2
6	-12	29	-19

-2 9 l

1	115	113	6
2	26	31	-14
3	70	69	6
4	-5	15	-5
5	66	73	-25

-2 10 l

1	104	100	14
2	61	61	0
3	186	174	27
4	56	60	-12

-2 11 l

1	196	198	-3
2	60	56	14

-1 0 l

1	103	114	-59
3	1227	1224	2
5	506	510	-5
7	94	86	37
9	142	148	-21

-1 1 l

1	112	104	35
2	323	331	-21
3	232	236	-10
4	437	428	16
5	69	71	-12
6	202	188	33
7	319	320	0
8	193	195	-6
9	331	333	-3

-1 2 l

1	1066	1052	12
2	565	560	8
3	44	55	-65
4	144	154	-31
5	321	318	7
6	510	480	48
7	22	15	12
8	59	54	17

-1 3 l

1	494	494	0
2	353	351	4
3	73	72	4
4	324	325	-2
5	76	78	-13

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6	109	109	0
7	67	68	-5
8	228	227	2

-1 4 l

1	944	937	7
2	321	330	-21
3	644	654	-14
4	125	133	-29
5	514	518	-7
6	39	46	-25
7	20	6	7
8	109	110	-4

-1 5 l

1	354	365	-25
2	45	43	10
3	147	143	11
4	136	141	-15
5	444	437	11
6	240	244	-10
7	161	160	3
8	25	29	-3

-1 6 l

1	433	432	3
2	80	81	-4
3	17	6	7
4	125	120	15
5	167	159	17
6	87	89	-9
7	58	60	-8

-1 7 l

1	50	55	-23
2	67	66	4
3	-27	15	-30
4	93	91	8
5	115	114	3
6	144	150	-19
7	127	119	24

-1 8 l

1	393	392	1
2	362	359	5
3	99	103	-15
4	211	204	16
5	86	92	-27
6	23	38	-36

-1 9 l

1	103	100	10
2	106	102	17
3	48	50	-8
4	-22	8	-28
5	245	247	-4

-1 10 l

1	28	11	12
2	205	203	4
3	-10	4	-2
4	141	144	-6

-1 11 l

1	15	8	6
2	24	21	1

0 0 l

2	1773	1827	-31
4	58	53	28
6	23	24	-1
8	91	90	1

0 1 l

1	138	135	15
2	850	841	10
3	325	314	27
4	281	272	22
5	505	482	40
6	146	145	0
7	-20	21	-22
8	237	242	-12

0 2 l

0	1001	982	18
1	510	485	45
2	560	560	0
3	225	221	13
4	99	99	0
5	615	613	2
6	249	249	-1
7	102	98	21
8	57	44	46

0 3 l

1	536	540	-6
2	254	245	27
3	276	276	0
4	304	303	3
5	414	415	-2
6	170	167	8
7	196	189	16
8	149	149	1

0 4 l

0	2540	2524	6
1	1178	1164	11
2	604	601	5
3	71	75	-25
4	-14	3	-13
5	18	26	-11
6	-15	33	-34
7	83	87	-15
8	13	29	-14

0 5 l

1	15	4	16
2	168	169	-3
3	47	49	-10
4	97	91	26
5	27	32	-8
6	84	84	0
7	200	192	17

0 6 l

0	67	63	25
1	76	73	15
2	260	263	-9
3	55	54	4
4	251	245	13
5	108	105	11
6	239	238	1
7	-28	3	-17

0 7 l

1	286	292	-14
2	8	2	5
3	13	14	-2
4	77	80	-16
5	-22	6	-28
6	7	32	-49

0 8 l

0	109	105	22
1	562	573	-17
2	120	125	-19
3	96	101	-21
4	-28	8	-22
5	112	109	13
6	54	63	-38

0 9 l

1	144	150	-18
2	30	39	-14
3	87	87	0
4	108	106	8
5	43	42	0

0 10 l

0	78	70	34
1	424	411	23
2	38	30	21
3	60	56	15
4	162	158	10

0 11 l

1	187	174	34
2	104	99	22

1 0 l

1	63	63	-4
3	171	176	-15
5	84	83	7
7	67	58	35

1 1 l

0	420	420	-1
1	289	266	64
2	37	37	1
3	504	500	7
4	-18	3	-10
5	284	298	-33
6	27	9	15
7	372	382	-19
8	182	182	0

1 2 l

0	120	106	57
1	622	624	-2
2	406	421	-33
3	94	92	7
4	136	133	10
5	39	32	25
6	163	162	0
7	119	118	4
8	136	145	-30

1 3 l

0	354	363	-21
1	828	842	-16
2	160	167	-23
3	229	223	14
4	52	49	16
5	64	61	14
6	40	36	16
7	45	42	10
8	228	236	-17

1 4 l

0	1565	1552	8
1	197	202	-17
2	357	358	-1
3	26	31	-20
4	246	236	23
5	211	210	1
6	96	94	11
7	-18	16	-12

1 5 l

0	524	530	-18
1	177	177	0
2	49	52	-14
3	325	325	0
4	65	64	5
5	175	172	7
6	68	64	18
7	171	178	-18

1 6 l

0	126	134	-26
1	546	545	1
2	114	117	-12
3	140	144	-12
4	326	323	6
5	157	154	6
6	129	131	-7
7	92	93	-7

1 7 l

0	633	629	6
1	60	64	-22
2	229	225	7
3	58	55	15
4	107	112	-20
5	126	128	-5
6	24	38	-35

1 8 l

0	856	867	-12
1	103	95	31
2	178	181	-6
3	34	34	-1
4	102	103	-1
5	35	44	-26

1 9 l

0	125	111	51
1	118	124	-27
2	133	133	0
3	63	66	-11
4	77	81	-13
5	-10	26	-32

1 10 l

0	197	191	15
1	73	71	11
2	159	155	11
3	42	50	-25

1 11 l

0	96	97	-2
1	118	116	7

2 0 l

0	1071	1038	30
2	58	55	19
4	200	196	9
6	346	341	10
8	183	178	11

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2 1 1

0	1198	1183	12
1	188	185	9
2	837	853	-26
3	10	2	3
4	604	613	-12
5	57	62	-25
6	395	394	1
7	175	163	28
8	120	114	20

2 2 1

0	118	111	26
1	777	779	-3
2	48	52	-22
3	232	227	13
4	83	85	-12
5	32	38	-21
6	133	135	-4
7	78	66	48

2 3 1

0	130	117	42
1	205	199	17
2	396	409	-27
3	7	10	-1
4	11	30	-22
5	14	17	-2
6	127	112	45
7	214	217	-6

2 4 1

0	708	700	11
1	440	447	-13
2	116	119	-12
3	84	84	-1
4	71	70	1
5	156	149	19
6	51	55	-19
7	100	102	-7

2 5 1

0	282	286	-11
1	150	141	23
2	347	343	8
3	48	49	-2
4	196	185	28
5	39	44	-17
6	102	94	28
7	98	94	15

2 6 1

0	503	512	-15
1	224	231	-18
2	218	218	0
3	84	82	7
4	16	36	-24
5	66	63	4
6	-26	11	-17

2 7 1

0	-5	2	0
1	169	174	-12
2	-16	21	-19
3	-24	12	-20
4	42	46	-14
5	23	32	-21
6	13	21	-12

2 8 1

0	201	200	3
1	112	109	10
2	82	79	13
3	66	61	20
4	-14	32	-25
5	-25	23	-24

2 9 1

0	57	55	8
1	107	107	3
2	-20	9	-11
3	155	153	5
4	41	35	6

2 10 1

0	12	44	-36
1	28	41	-17
2	52	55	-12
3	35	41	-16

2 11 1

0	72	71	6

3 0 1

1	285	279	15
3	756	737	23
5	545	545	0
7	197	198	-3

3 1 1

0	378	379	-1
1	546	553	-12
2	33	36	-12
3	767	767	0
4	38	18	26
5	208	206	4
6	182	184	-3
7	67	60	23

3 2 1

0	800	794	10
1	90	88	5
2	275	275	0
3	172	178	-15
4	273	275	-4
5	248	247	3
6	84	85	-6
7	58	44	43

3 3 1

0	44	46	-8
1	596	595	1
2	-2	1	0
3	105	98	24
4	34	25	27
5	144	152	-25
6	69	72	-10
7	171	181	-23

3 4 1

0	876	867	9
1	70	68	12
2	362	355	15
3	176	159	42
4	49	46	13
5	48	50	-7
6	67	62	16
7	146	152	-16

3 5 1

0	84	79	23
1	374	370	7
2	115	117	-8
3	302	303	-1
4	-5	13	-5
5	228	226	4
6	280	278	4

3 6 1

0	420	414	10
1	341	356	-31
2	170	175	-13
3	53	54	-4
4	40	41	-5
5	24	21	6
6	24	36	-11

3 7 1

0	267	262	12
1	44	39	19
2	167	167	0
3	116	114	8
4	30	37	-9
5	225	227	-4

3 8 1

0	45	50	-21
1	-23	14	-19
2	196	191	13
3	39	38	2
4	-35	1	-29

3 9 1

0	-31	28	-47
1	-16	0	-5
2	117	112	23
3	-24	7	-13

3 10 1

0	114	123	-37
1	116	124	-27
2	-37	20	-41

4 0 1

0	379	370	20
2	377	366	22
4	547	545	1
6	415	402	22

4 1 1

-1	129	128	0
0	362	351	25
1	-14	3	-7
2	8	9	0
3	54	53	4
4	38	28	33
5	239	242	-6
6	87	87	0

4 2 1

-1	137	136	5
0	410	404	13
1	237	236	1
2	173	176	-10
3	69	68	6
4	384	384	0
5	20	22	-2
6	35	18	35

4 3 1

-1	174	181	-28
0	82	80	10
1	495	485	16
2	310	296	30
3	216	219	-5
4	-13	3	-4
5	336	351	-31
6	169	164	15

4 4 1

-1	678	683	-8
0	-12	2	-5
1	77	77	-3
2	364	370	-11
3	217	223	-15
4	-13	6	-5
5	37	42	-14
6	312	301	20

4 5 1

-1	430	427	6
0	339	340	-2
1	421	425	-7
2	152	153	-3
3	308	310	-4
4	156	156	1
5	151	158	-20

4 6 1

-1	325	329	-10
0	379	388	-17
1	63	60	13
2	78	80	-8
3	-11	14	-8
4	168	158	23
5	92	92	0

4 7 1

-1	98	104	-39
0	131	131	0
1	211	217	-12
2	278	282	-9
3	74	74	0
4	177	175	3

4 8 1

-1	162	162	2
0	123	120	12
1	94	91	12
2	78	78	0
3	222	222	0
4	73	75	-6

4 9 1

-1	99	105	-33
0	140	137	11
1	112	121	-29
2	-14	16	-21
3	164	167	-6

4 10 1

-1	77	79	-7
0	77	77	0
1	10	0	2

5 0 1

-1	760	752	10

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1	774	753	25
3	775	777	-3
5	46	41	14

5 1 l

1	388	376	24

5 2 l

-1	432	428	8
3	216	206	24
6	132	137	-18

5 3 l

-1	49	55	-28
3	89	89	0
4	289	291	-5

5 4 l

0	186	179	17
3	301	308	-14
4	206	203	6

5 5 l

3	188	182	12
4	191	182	22

5 6 l

-1	162	161	3

5 7 l

-1	157	161	-14

5 8 l

0	269	253	32
2	279	273	11

5 9 l

-1	148	154	-15

6 0 l

0	230	220	25
2	-8	10	-4
4	132	130	4

6 1 l

-1	158	158	0
0	241	249	-18
1	72	69	13
2	171	171	0
3	33	36	-8
4	-39	0	-41
5	67	72	-20

6 2 l

-1	8	13	-7
0	150	149	1
1	-23	6	-17
2	103	112	-34
3	136	142	-18
4	-22	18	-38
5	298	300	-3

6 3 l

-1	111	118	-26
0	101	103	-8
1	70	72	-9
2	46	48	-8
3	188	178	23
4	77	81	-18
5	151	159	-22

6 4 l

-1	93	95	-8
0	71	60	46
1	222	209	28
2	29	25	10
3	372	353	34
4	202	199	7

6 5 l

-1	120	117	9
0	128	130	-8
1	205	204	2
2	295	287	17
3	218	219	-1
4	36	28	8

6 6 l

-1	121	117	12
0	103	100	12
1	84	86	-12
2	204	206	-4
3	217	206	22

6 7 l

-1	133	133	-1
0	94	95	-2
1	33	34	-3
2	161	158	8

6 8 l

-1	120	108	44
0	-31	15	-25
1	137	148	-33

6 9 l

-1	103	101	7

7 0 l

3	96	92	14

7 2 l

-1	93	95	-8
0	225	226	-4
1	143	144	-2
3	65	68	-10

7 3 l

-1	202	206	-8

7 6 l

0	30	40	-29

7 7 l

0	133	127	18

8 0 l

-2	66	62	21
0	209	206	5
2	199	207	-16

8 1 l

-2	152	154	-9
-1	30	38	-26
0	41	50	-32
1	82	86	-13
2	255	258	-6
3	54	57	-9

8 2 l

-2	235	232	8
-1	354	364	-18
0	113	119	-22
1	188	184	9
2	66	71	-18

8 3 l

-2	59	60	-1
-1	53	50	10
0	-32	23	-38
1	124	122	6
2	20	19	0

8 4 l

-2	76	77	-11
-1	-27	2	-17
0	75	76	-5
1	144	140	11
2	99	96	15

8 5 l

-2	257	256	4
-1	103	99	13
0	60	61	-3
1	-27	21	-25

8 6 l

-2	242	241	3
-1	129	123	17
0	150	153	-6

8 7 l

-2	54	50	11

9 0 l

-1	145	133	32
1	134	139	-15

9 1 l

-2	171	160	27
-1	101	101	0
0	74	77	-12
1	57	58	-4

9 2 l

-2	526	537	-15
-1	65	68	-11
0	127	129	-4
1	98	106	-30

9 3 l

-2	122	117	21
-1	219	214	10
0	73	77	-16

9 4 l

-2	32	4	17
-1	78	73	19
0	126	120	19

9 5 l

-2	66	68	-7

10 0 l

-2	59	58	5

10 1 l

-2	197	206	-22