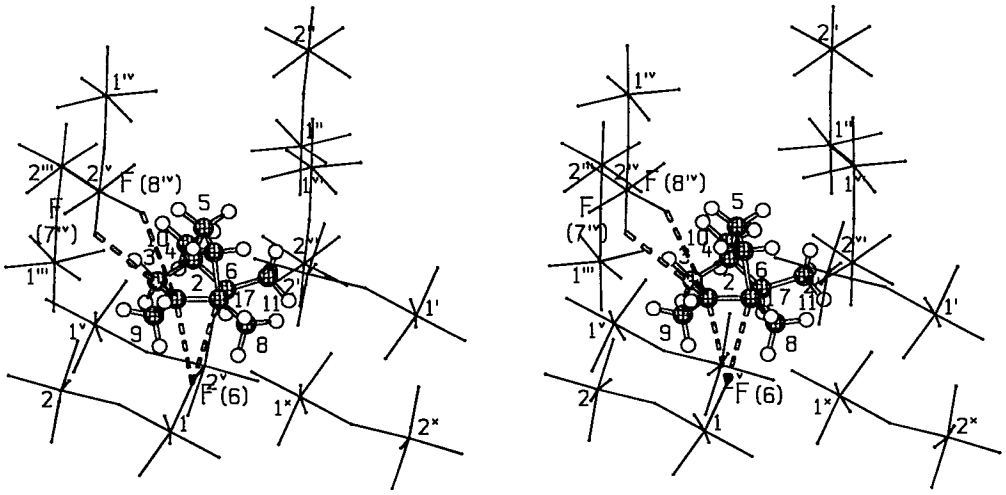
FITDIV

1,2,4,7-anti-Tetramethyl-2-norbornyl (μ_2-fluoro)-bis(pentafluoro-antimony)
at -80 deg.C
C11 H19 1+,F11 Sb2 1-
T.Laube
Angew.Chem.,Int.Ed.Engl., 26, 560,1987
Redetermination at 110 K: see refcode FITDIV01
FITDIV P21/c Z= 4 NATOMS= 43 DIFF AS=3 R-FACTOR= 0.080
19 C-H BONDS: S.D.= 0.026; MEAN = 1.081; RANGE: 1.021 - 1.120

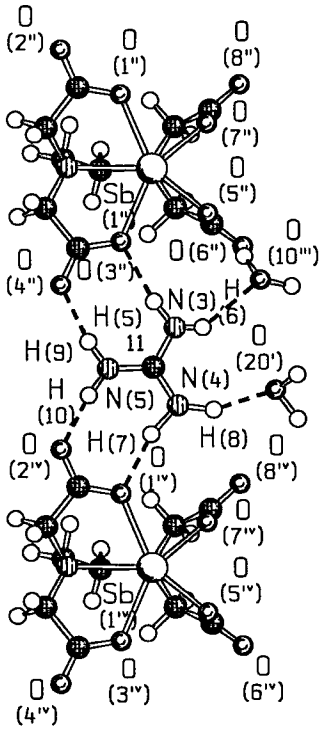


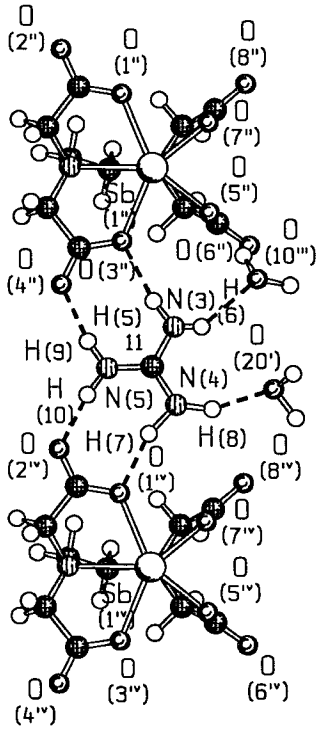
F(6)	- C(1)	3.277	*diff* =	0.107	
F(6)	- C(2)	3.268	*diff* =	0.098	
C(2)	- F(7^{IV})	3.642	*diff* =	0.472	weak
C(2)	- F(8^{IV})	4.332	*diff* =	1.162	very weak

FIZCAS10

Guanidinium (ethylenediaminetetra-acetato)-antimony(iii) dihydrate
C10 H12 N2 O8 Sb1 1-,C1 H6 N3 1+,2(H2 O1)
V.E.Mistryukov,A.V.Sergeev,Yu.N.Mikhailov,R.N.Shchelokov
Koord.Khim., 13, 1129,1987

FIZCAS10 P21/n Z= 4 NATOMS= 49 DIFF AS=0 R-FACTOR= 0.065
ERROR z(H12) should be positive
12 C-H BONDS: S.D.= 0.059; MEAN = 1.070; RANGE: 0.985 - 1.223





H(5)	- $O(3^{II})$	2.066	*diff* = -0.654 (H bond)
H(6)	- $O(10^{III})$	2.263	*diff* = -0.457 (H bond)
H(7)	- $O(1^{IV})$	1.984	*diff* = -0.736 (H bond)
$O(20^{I})$	- H(8)	1.896	*diff* = -0.824 (H bond)
H(9)	- $O(4^{II})$	1.874	*diff* = -0.846 (H bond)
H(10)	- $O(2^{IV})$	1.808	*diff* = -0.912 (H bond)

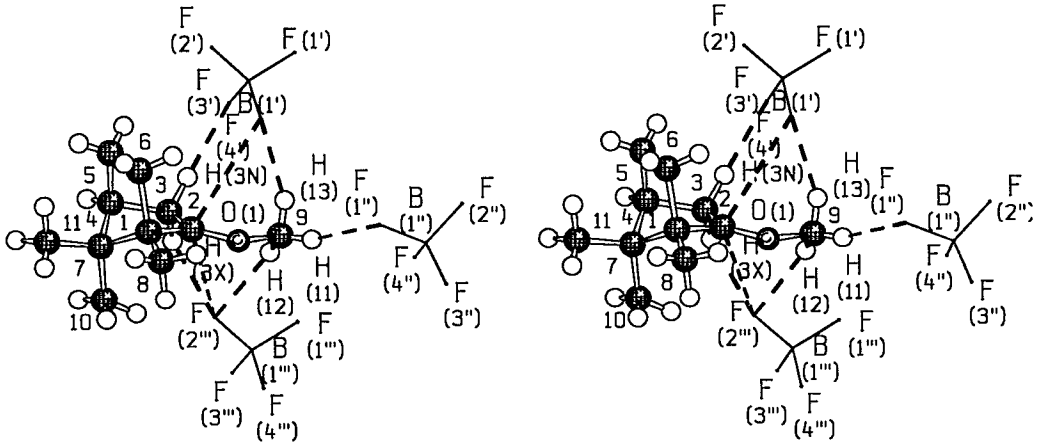
FODZAZ

2-Methoxy-1,7,7-trimethylbicyclo(2.2.1)hept-2-ylium tetrafluoroborate
at -155 deg.C
C11 H19 O1 1+,B1 F4 1-
L.K.Montgomery,M.P.Grendze,J.C.Huffman
J.Am.Chem.Soc., 109, 4749,1987

FODZAZ P21 Z= 0 NATOMS= 36 DIFF AS=2 R-FACTOR= 0.061

REMARK Numbering between paper and supp.data is inconsistent; that in latter was used
19 C-H BONDS: S.D.= 0.088; MEAN = 0.925; RANGE: 0.723 - 1.086

The H atoms H(3X) and H(3N) were newly computed in the present paper.

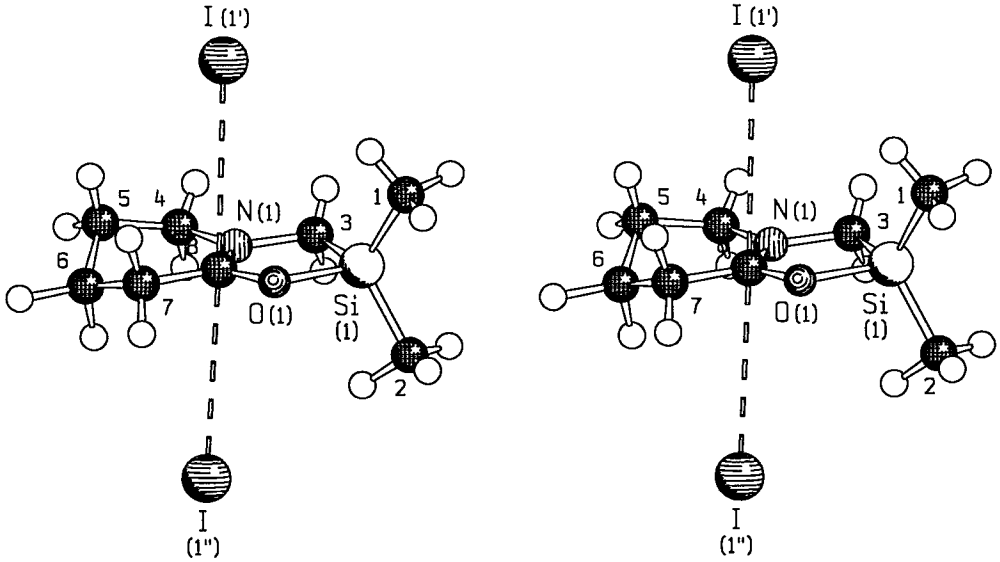


C(2)	- $F(4^{I})$	3.357	*diff* = 0.187	
C(2)	- $F(2^{III})$	3.412	*diff* = 0.242	
H(11)	- $F(1^{II})$	2.309	*diff* = -0.361	(H bond)
H(12)	- $F(2^{III})$	2.378	*diff* = -0.292	(H bond)
H(13)	- $F(4^{I})$	2.261	*diff* = -0.409	(H bond)
$F(2^{III})$	- H(3X)	2.296	*diff* = -0.374	(H bond)
$F(3^{I})$	- H(3N)	2.257	*diff* = -0.413	(H bond)

FOGBIM

(1-(Dimethylsilyl)methyl)-2-piperidone iodide
at -120 deg.C
C8 H16 N1 O1 Si1 1+,I1 1-
A.A.Macharashvili,V.E.Shklover,Yu.T.Struchkov,Yu.I.Baukov,E.P.Kramarova,G.I.Oleneva
J.Organomet.Chem., 327, 167,1987

FOGBIM Pna21 Z= 4 NATOMS= 28 DIFF AS=1 R-FACTOR= 0.018
16 C-H BONDS: S.D.= 0.097; MEAN = 1.052; RANGE: 0.877 - 1.279

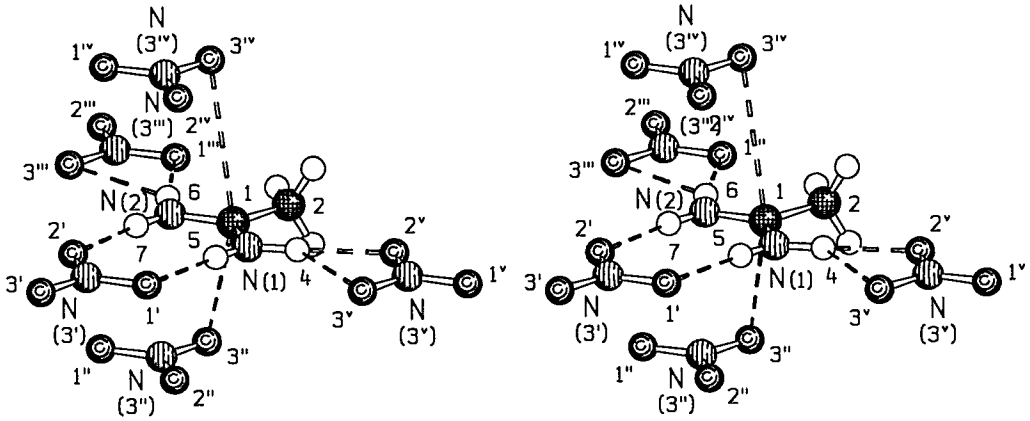


C(8)	- $I(1^{I})$	3.831	*diff* = 0.151	
C(8)	- $I(1^{II})$	3.863	*diff* = 0.183	

FOSPOS01

Acetamidinium nitrate
at 116 deg.K
C2 H7 N2 1+,N1 O3 1-
M.Hjorth,R.Norrestam
Acta Cryst.,C (Cr.Str.Comm.), 43, 1589,1987

FOSPOS P21/m Z= 2 NATOMS= 15 DIFF AS=1 R-FACTOR= 0.035
3 C-H BONDS: S.D.= 0.030; MEAN = 0.849; RANGE: 0.828 - 0.892

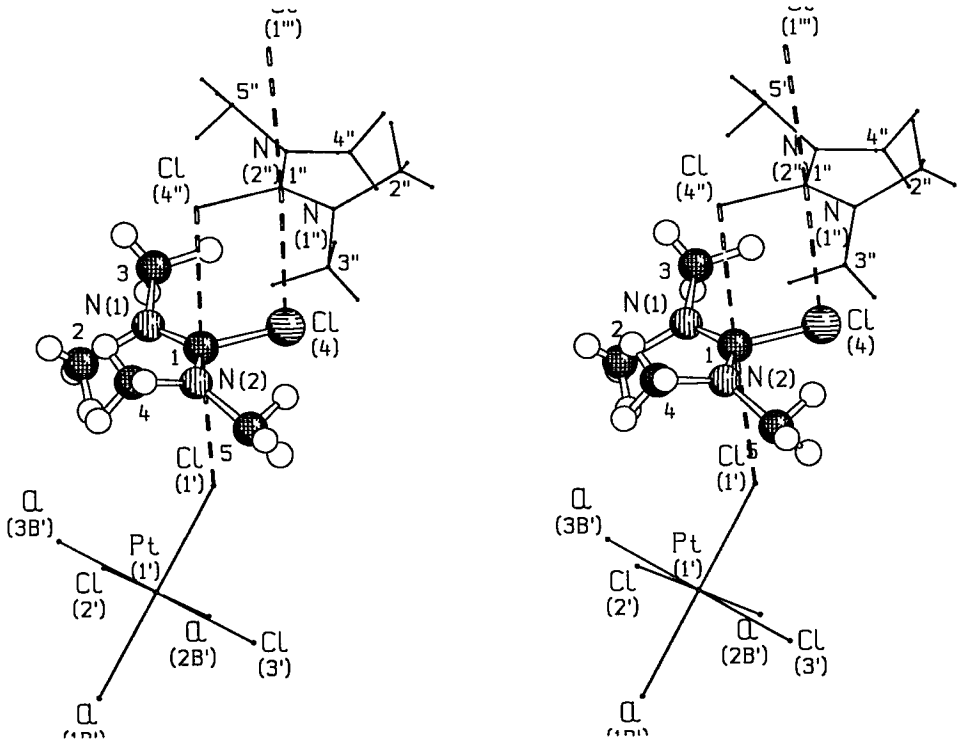


H(4)	- $O(2^{V})$	1.949	*diff* = -0.771	(H bond)
H(4)	- $O(3^{V})$	2.532	*diff* = -0.188	(H bond)
H(5)	- $O(1^{I})$	2.048	*diff* = -0.672	(H bond)
H(6)	- $O(1^{III})$	2.129	*diff* = -0.591	(H bond)
H(6)	- $O(3^{III})$	2.565	*diff* = -0.155	(H bond)
H(7)	- $O(2^{I})$	2.007	*diff* = -0.713	(H bond)
C(1)	- $O(3^{II})$	3.363	*diff* = 0.143	
C(1)	- $O(3^{IV})$	3.362	*diff* = 0.142	

FUFRUT

bis(Chloro-bis(dimethylamino)-carbenium) hexachloro-platinum
2(C5 H12 Cl1 N2 1+),Cl6 Pt1 2-
E.B.Chuklanova,A.I.Gusev,A.S.Zhdanov,Z.V.Belyakova,V.M.Shevchenko,V.D.Sheludyakov
Koord.Khim., 13, 1109,1987

FUFRUT P21/n Z= 2 NATOMS= 27 DIFF AS=2 R-FACTOR= 0.018
12 C-H BONDS: S.D.= 0.087; MEAN = 0.945; RANGE: 0.762 - 1.103



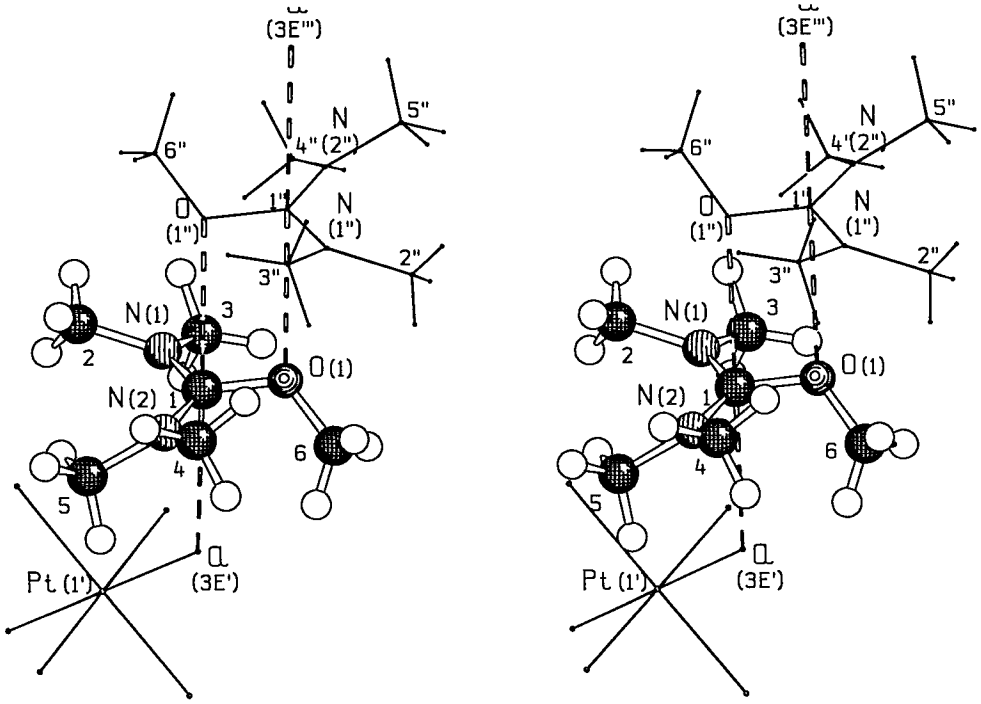
Cl(1^{I})	- C(1)	3.147	*diff* = -0.303	**very strong**
C(1)	- Cl(4^{II})	3.587	*diff* = 0.137	
Cl(4)	- C(1^{II})	3.587	*diff* = 0.137	
Cl(1^{III})	- C(1^{II})	3.147	*diff* = -0.303	**very strong**

FUFSAA

bis(Methoxy-bis(dimethylamino)carbenium) hexachloro-platinum
2(C6 H15 N2 O1 1+),Cl6 Pt1 2-
E.B.Chuklanova,A.I.Gusev,A.S.Zhdanov,Z.V.Belyakova,V.M.Shevchenko,V.D.Sheludyakov
Koord.Khim., 13, 1109,1987

FUFSAA C2/c Z= 4 NATOMS= 31 DIFF AS=2 R-FACTOR= 0.019
ERROR The y coordinate of H9 should be negative
15 C-H BONDS: S.D.= 0.084; MEAN = 1.010; RANGE: 0.750 - 1.123

H atoms at C(5) were newly computed in the present paper.

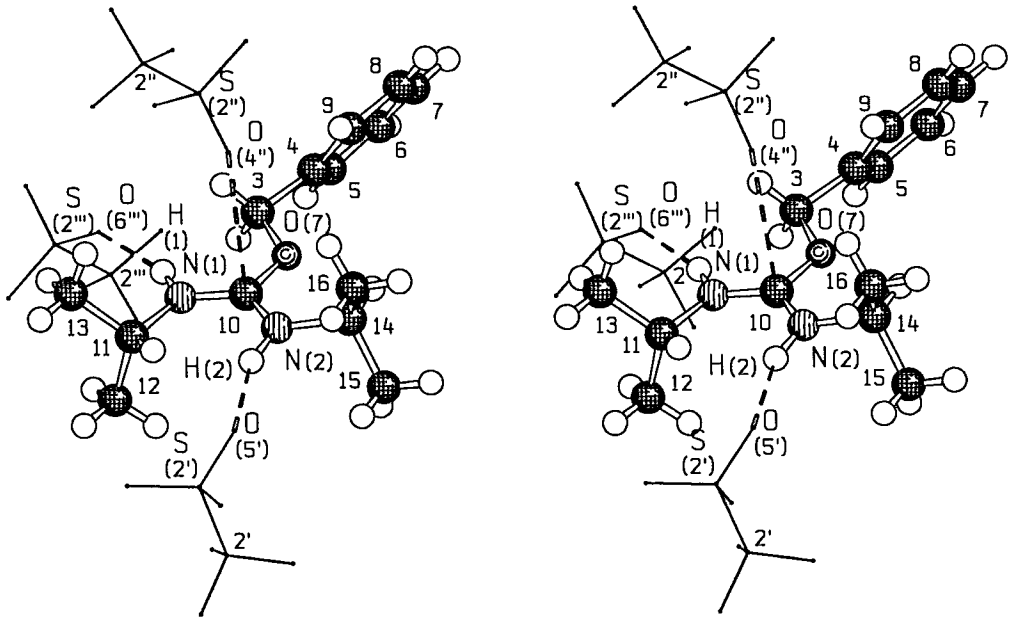


$C(1^{II})$	- $Cl(3E^{III})$	3.431	*diff* =	-0.019
$Cl(3E^{I})$	- C(1)	3.431	*diff* =	-0.019
$C(1^{II})$	- O(1)	3.344	*diff* =	0.124
$O(1^{II})$	- C(1)	3.345	*diff* =	0.125

FUXCAC

Benzyloxy-N,N'-di-isopropyluronium trifluoromethanesulfonate
C14 H23 N2 O1 1+,C1 F3 O3 S1 1-
W.Clegg,S.P.Collingwood,S.M.Hodgson,B.T.Golding
Acta Cryst.,C (Cr.Str.Comm.), 44, 123,1988

FUXCAC P21/c Z= 8 NATOMS= 96 DIFF AS=2 R-FACTOR= 0.061
42 C-H BONDS: S.D.= 0.001; MEAN = 0.960; RANGE: 0.958 - 0.961

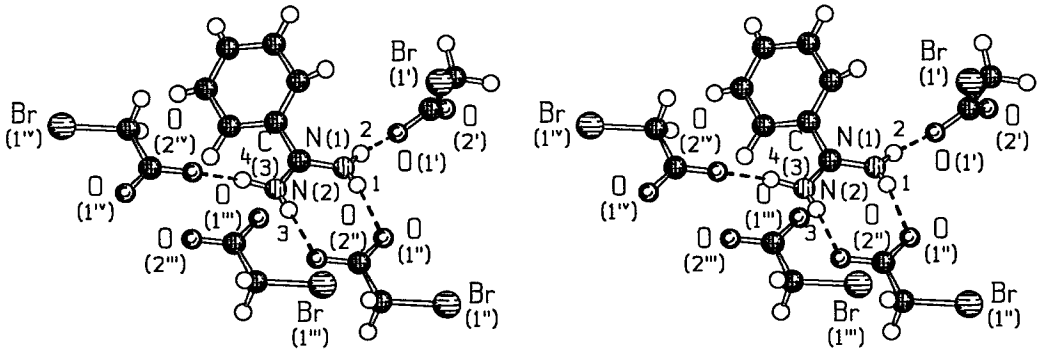


C(10)	- O(4^{II})	3.331	*diff* = 0.111
O(5^{I})	- H(2)	1.963	*diff* = -0.757 (H bond)
H(1)	- O(6^{III})	2.022	*diff* = -0.698 (H bond)

GADMUT

Benzamidinium bromoacetate
C2 H2 Br1 O2 1-,C7 H9 N2 1+
B.Kratochvil,J.Ondracek,K.Maly,L.Csordas
Collect.Czech.Chem.Commun., 53, 294,1988

GADMUT P1121/n Z= 4 NATOMS= 25 DIFF AS=2 R-FACTOR= 0.066
7 C-H BONDS: S.D.= 0.125; MEAN = 0.899; RANGE: 0.733 - 1.058

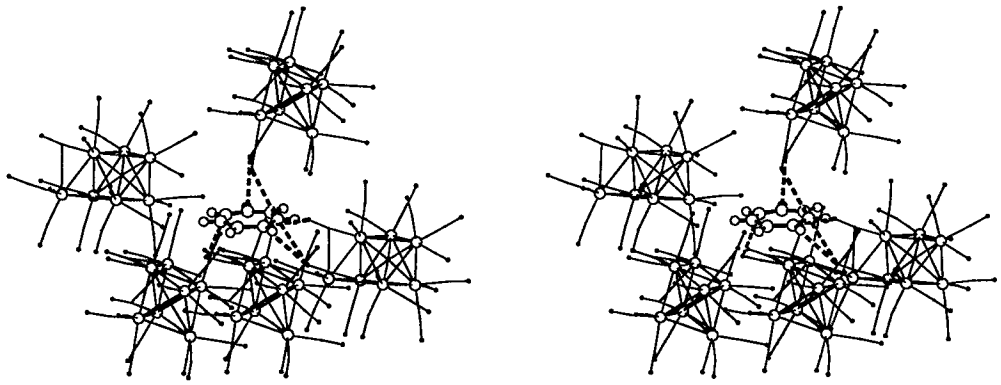


H(1)	- O(1^{II})	2.060	*diff* = -0.660 (H bond)
H(2)	- O(1^{I})	1.949	*diff* = -0.771 (H bond)
H(3)	- O(2^{II})	2.051	*diff* = -0.669 (H bond)
H(4)	- O(2^{IV})	1.920	*diff* = -0.800 (H bond)

GEGGAA

Tropylium tetraethylammonium (μ_6-carbido)-henicosacarbonyl-(μ_2-hydrido)-hepta-rhenium
Cycloheptatrienylium tetraethylammonium (μ_6-carbido)-henicosacarbonyl-(μ_2-hydrido)-hepta-rhenium
isomer b
C7 H7 1+,C8 H20 N1 1+,C22 H1 O21 Re7 2-
T.Beringhelli,G.D'Alfonso,G.Ciani,A.Sironi,H.Molinari
J.Chem.Soc.,Dalton Trans., , 1281,1988

GEGGAA P21 Z= 2 NATOMS= 93 DIFF AS=4 R-FACTOR= 0.025
27 C-H BONDS: S.D.= 0.003; MEAN = 0.951; RANGE: 0.945 - 0.955



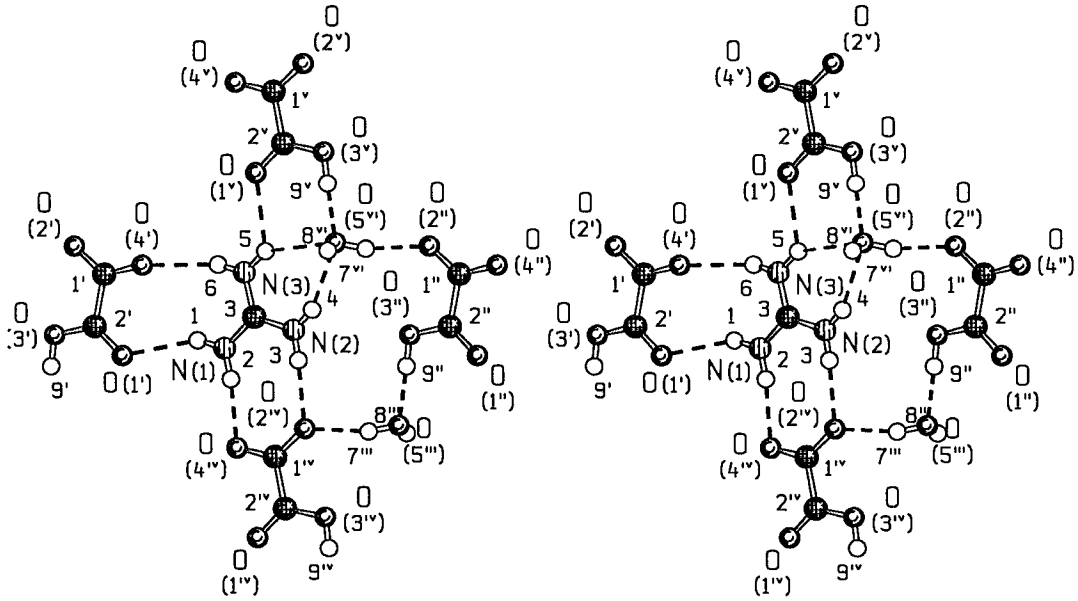
O(53^{II})	- C(1)	3.188	*diff* = -0.032

O(43^{III})	- C(2)	3.142	*diff* = -0.078
O(52^{I})	- C(4)	3.144	*diff* = -0.076
O(23^{III})	- C(4)	3.157	*diff* = -0.063
O(42^{I})	- C(5)	3.165	*diff* = -0.055
O(52^{I})	- C(5)	3.184	*diff* = -0.036

GUHOXM01

Guanidinium hydrogen oxalate monohydrate
C2 H1 O4 1-,C1 H6 N3 1+,H2 O1
L.C.Andrews,B.R.Deroski,J.S.Ricci
J.Cryst.Mol.Struct., 9, 163,1979

GUHOXM P21/c Z= 4 NATOMS= 20 DENS AS=2 R-FACTOR= 0.085

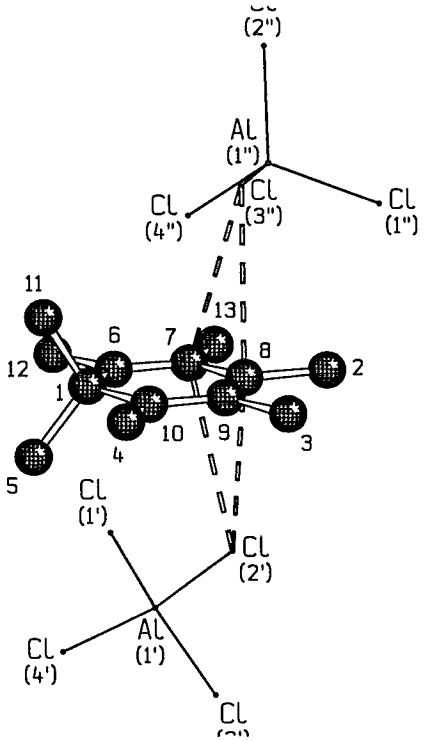


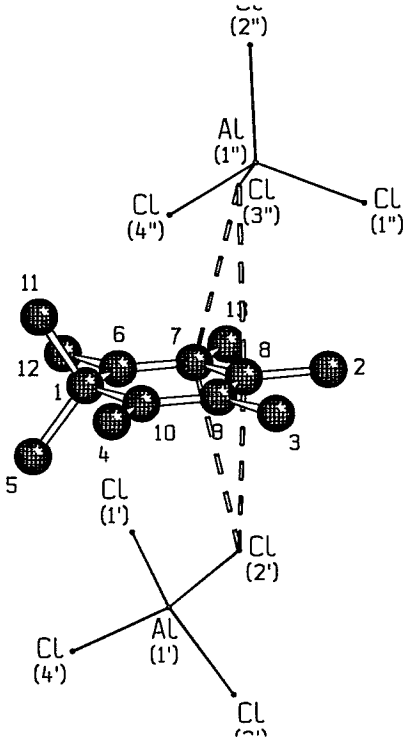
H(2)	- O(4^{IV})	2.020	*diff* = -0.700 (H bond)
H(3)	- O(2^{IV})	2.000	*diff* = -0.720 (H bond)
O(4^{I})	- H(6)	2.166	*diff* = -0.554 (H bond)
O(1^{I})	- H(1)	2.222	*diff* = -0.498 (H bond)
H(5)	- O(1^{V})	2.289	*diff* = -0.431 (H bond)
H(5)	- O(5^{VI})	2.509	*diff* = -0.211 (H bond)
O(2^{II})	- H(7^{VI})	1.861	*diff* = -0.859 (H bond)
H(4)	- O(5^{VI})	2.214	*diff* = -0.506 (H bond)
H(9^{V})	- O(5^{VI})	1.748	*diff* = -0.972 (H bond)
H(9^{II})	- O(5^{III})	1.748	*diff* = -0.972 (H bond)
H(7^{III})	- O(2^{IV})	1.861	*diff* = -0.859 (H bond)

HEBZCA

Heptamethylbenzene tetrachloroaluminate
C13 H21 1+,Al1 Cl4 1-
N.C.Baenziger,A.D.Nelson
J.Am.Chem.Soc., 90, 6602,1968

HEBZCA P21/n Z= 4 NATOMS= 18 PHOT AS=3 R-FACTOR= 0.090





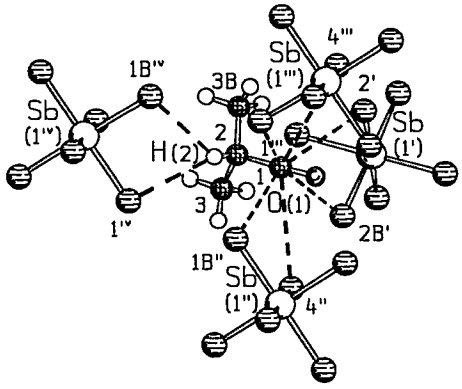
C(7)	- Cl(2^{I})	3.459	*diff* = 0.009
C(7)	- Cl(3^{II})	3.574	*diff* = 0.124
C(8)	- Cl(2^{I})	3.368	*diff* = -0.082
C(8)	- Cl(3^{II})	3.452	*diff* = 0.002

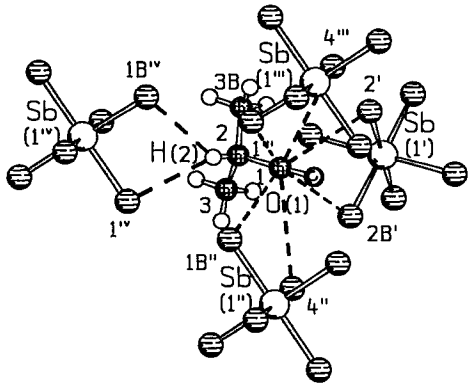
IBUSBC20

Isopropyl-oxocarbonium hexachloroantimonate
C4 H7 O1 1+,Cl6 Sb1 1-
J.-M.Le Carpentier,R.Weiss
Acta Crystallogr.,Sect.B, 28, 1430,1972

IBUSBC20 Pnma Z= 4 NATOMS= 12 DIFF AS=0 R-FACTOR= 0.036

All H atoms were added in the present paper.





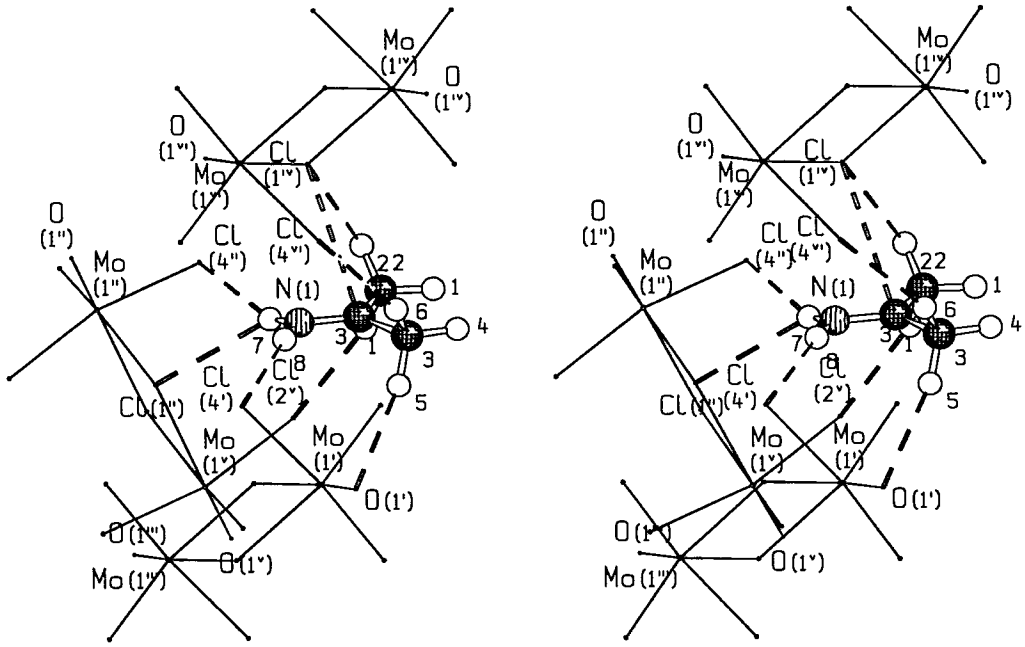
C(1)	- Cl($1B^{II}$)	3.270	*diff* = -0.180	strong
C(1)	- Cl(1^{III})	3.271	*diff* = -0.179	strong
C(1)	- Cl(2^{I})	3.683	*diff* = 0.233	
C(1)	- Cl($2B^{I}$)	3.683	*diff* = 0.233	
C(1)	- Cl(4^{II})	3.722	*diff* = 0.272	
C(1)	- Cl(4^{III})	3.722	*diff* = 0.272	

Cl(1^{IV})	- H(2)	2.918	*diff* = -0.032 (H bond)
Cl($1B^{IV}$)	- H(2)	2.918	*diff* = -0.032 (H bond)

JAJRIV

Isopropylideniminium tetrachloro-oxo-molybdenum(v)
C3 H8 N1 1+,Cl4 Mo1 O1 1-
P.Klinzing,A.El-Kholi,U.Muller,K.Dehnicke,K.Findeisen
Z.Anorg.Allg.Chem., 569, 83,1989

JAJRIV P21/c Z= 4 NATOMS= 18 DIFF AS=2 R-FACTOR= 0.044
6 C-H BONDS: S.D.= 0.000; MEAN = 1.080; RANGE: 1.079 - 1.080

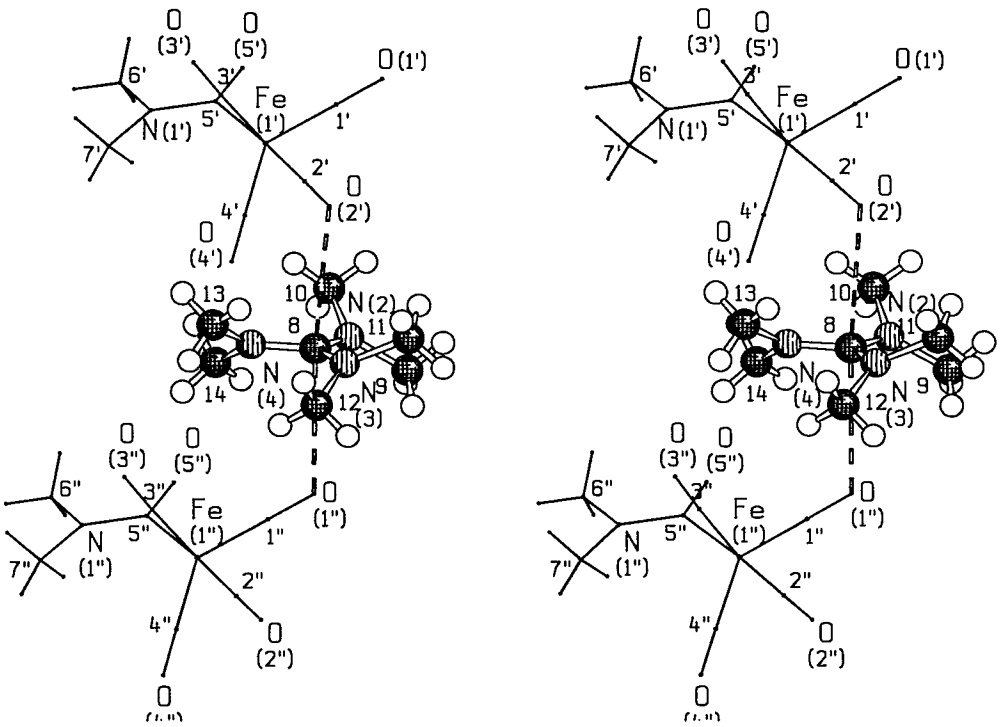


C(1)	- Cl(1^{IV})	3.402	*diff* = -0.048
H(2)	- Cl(1^{IV})	2.824	*diff* = -0.126 (H bond)
H(3)	- Cl(2^{V})	2.476	*diff* = -0.474 (H bond)
H(6)	- Cl(4^{VI})	2.703	*diff* = -0.247 (H bond)
H(7)	- Cl(1^{II})	2.735	*diff* = -0.215 (H bond)
H(7)	- Cl(4^{II})	2.608	*diff* = -0.342 (H bond)
H(8)	- Cl(4^{I})	2.662	*diff* = -0.288 (H bond)
H(5)	- O(1^{I})	2.557	*diff* = -0.163 (H bond)

JAKBAY

Hexamethyl guanidinium (dimethylaminocarbonyl-C)-tetracarbonyl-iron
C7 H6 Fe1 N1 O5 1-,C7 H18 N3 1+
R.Boese,D.Blaser,W.Petz
Z.Naturforsch.,Teil B, 43, 945,1988

JAKBAY P-1 Z= 2 NATOMS= 48 DIFF AS=2 R-FACTOR= 0.045
24 C-H BONDS: S.D.= 0.000; MEAN = 0.960; RANGE: 0.959 - 0.960

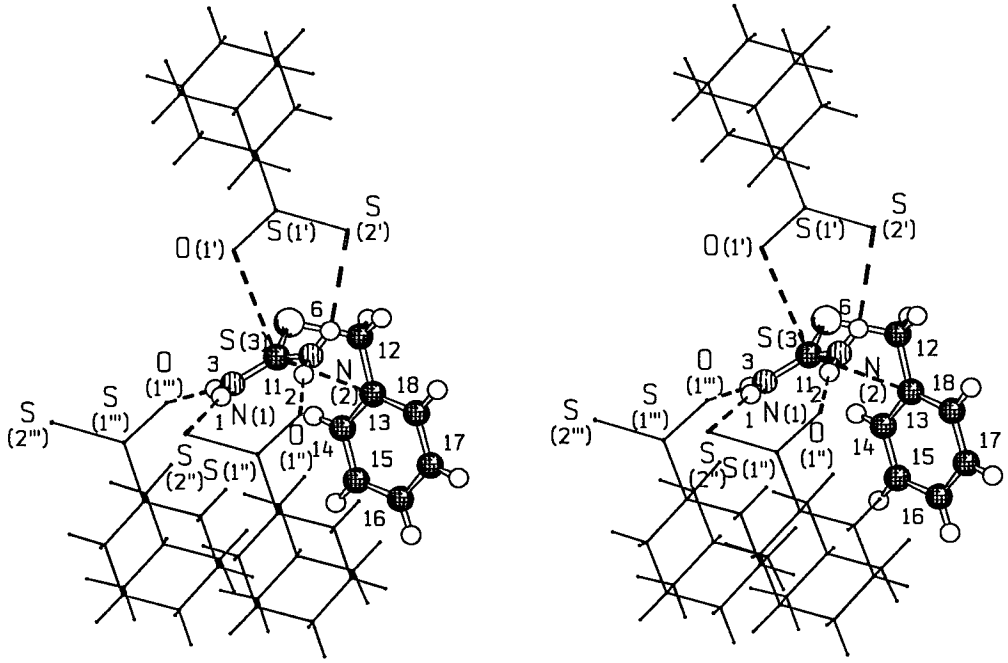


$O(1^{II})$	- C(8)	3.151	*diff* = -0.069
$O(2^{I})$	- C(8)	3.220	*diff* = 0.000

JALSOE

S-Benzylthiuronium adamantanethiosulfinate
C10 H15 O1 S2 1-,C8 H11 N2 S1 1+
M.Mikolajczyk,P.Lyzwa,J.Drabowicz,M.Wieczorek,G.Buyacz
Angew.Chem.,Int.Ed.Engl., 28, 97,1989

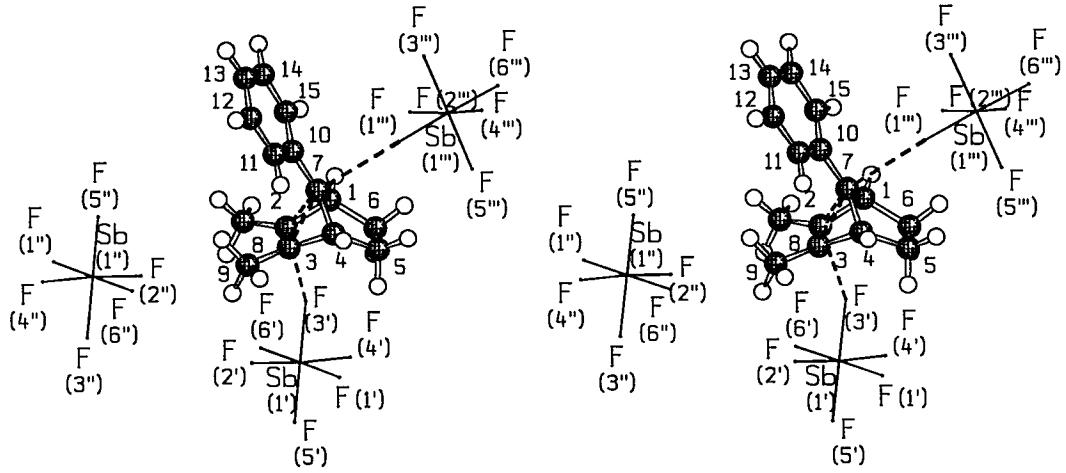
JALSOE P-1 Z= 2 NATOMS= 50 DIFF AS=1 R-FACTOR= 0.033
22 C-H BONDS: S.D.= 0.028; MEAN = 0.984; RANGE: 0.944 - 1.031



$O(1^{I})$	- C(11)	3.191	*diff* = -0.029
H(2)	- $O(1^{II})$	1.805	*diff* = -0.915 (H bond)
H(3)	- $O(1^{III})$	1.992	*diff* = -0.728 (H bond)
$S(2^{I})$	- H(6)	2.667	*diff* = -0.333 (H bond)
H(1)	- $S(2^{II})$	2.494	*diff* = -0.506 (H bond)
C(11)	- C(13)	3.136	*diff* = -0.264 strong

JECDEA

2,3-Dimethyl-7-phenyl-2-norbornen-7-ylium hexafluoroantimonate(v)
at -80 deg.C
C15 H17 1+,F6 Sb1 1-
T.Laube
J.Am.Chem.Soc., 111, 9224,1989
(Improved refinement: T.Laube, C.Lohse, J.Am.Chem.Soc. 116, 9001,1994)
JECDEA P21/n Z= 4 NATOMS= 39 DIFF AS=3 R-FACTOR= 0.084
17 C-H BONDS: S.D.= 0.012; MEAN = 1.080; RANGE: 1.055 - 1.100



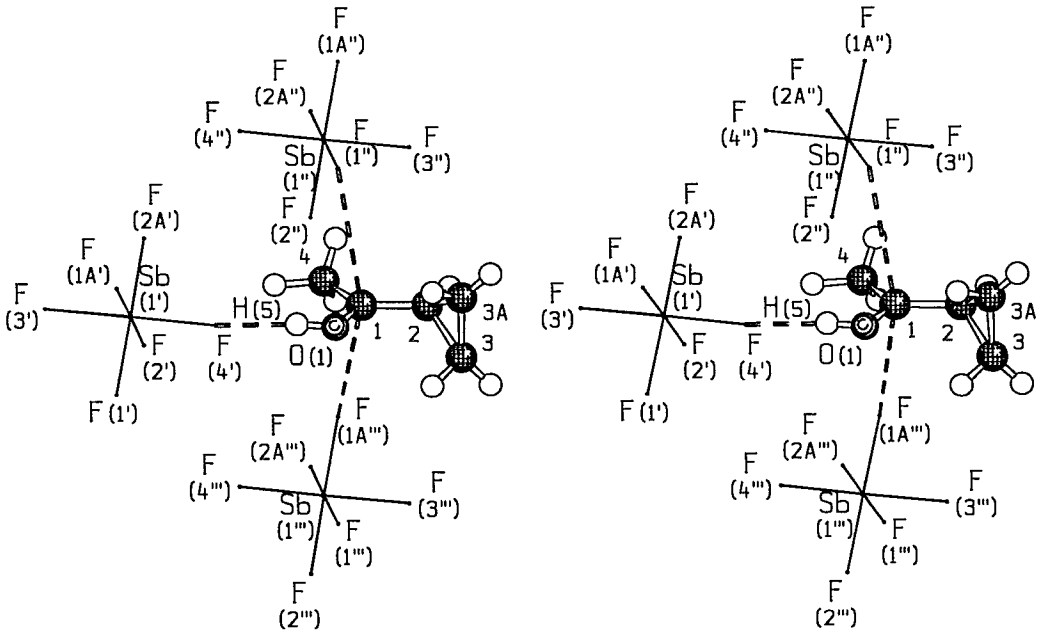
C(2)	- C(7)	1.855	*diff* = -1.545	**extremely strong**
C(3)	- C(7)	1.857	*diff* = -1.543	**extremely strong**
C(2)	- F(3^{I})	3.034	*diff* = -0.136	strong
C(7)	- F(1^{III})	3.013	*diff* = -0.157	strong

JICPOA

1-Cyclopropyl-1-hydroxyethylium hexafluoroantimonate
at -65 deg.C
C5 H9 O1 1+,F6 Sb1 1-
R.F.Childs,M.D.Kostyk,C.J.L.Lock,M.Mahendran
J.Am.Chem.Soc., 112, 8912,1990

JICPOA Pmnb Z= 8 NATOMS= 21 DIFF AS=2 R-FACTOR= 0.037
7 C-H BONDS: S.D.= 0.048; MEAN = 0.952; RANGE: 0.876 - 0.989

H atom at C(2) and H atom in the molecular mirror plane at C(4) were newly computed in the present paper.

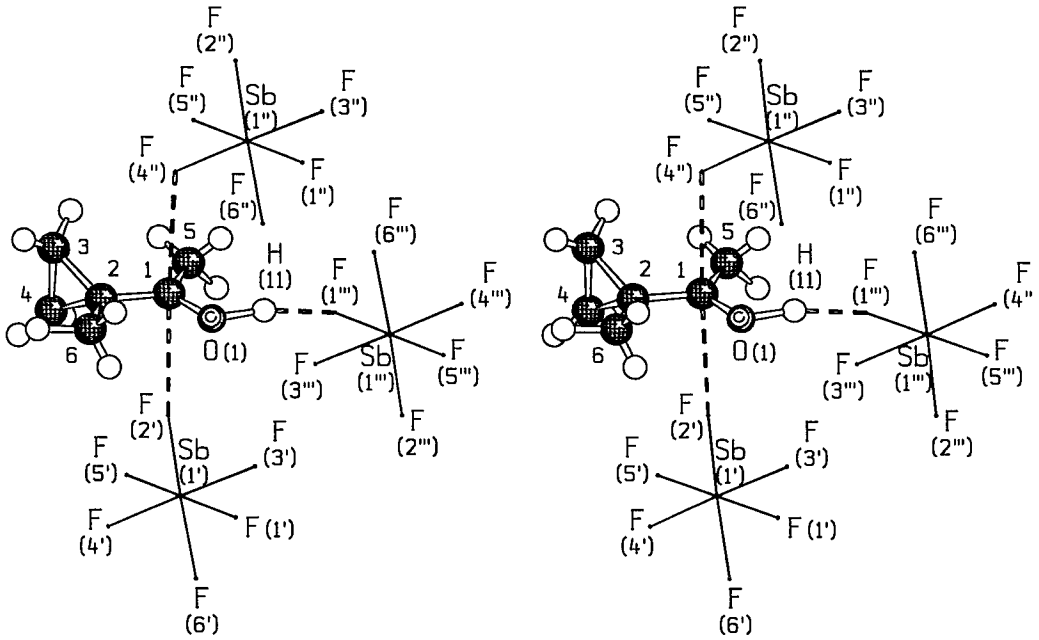


C(1)	- F(1^{II})	3.109	*diff* = -0.061	
C(1)	- F(1A^{III})	3.109	*diff* = -0.061	
F(4^{I})	- H(5)	1.743	*diff* = -0.927	(H bond)

JICPUG

1-(1'-Methylcyclopropyl)-1-hydroxyethylium hexafluoroantimonate
at -65 deg.C
C6 H11 O1 1+,F6 Sb1 1-
R.F.Childs,M.D.Kostyk,C.J.L.Lock,M.Mahendran
J.Am.Chem.Soc., 112, 8912,1990

JICPUG P21/n Z= 4 NATOMS= 25 DIFF AS=2 R-FACTOR= 0.062
10 C-H BONDS: S.D.= 0.088; MEAN = 0.938; RANGE: 0.827 - 1.090

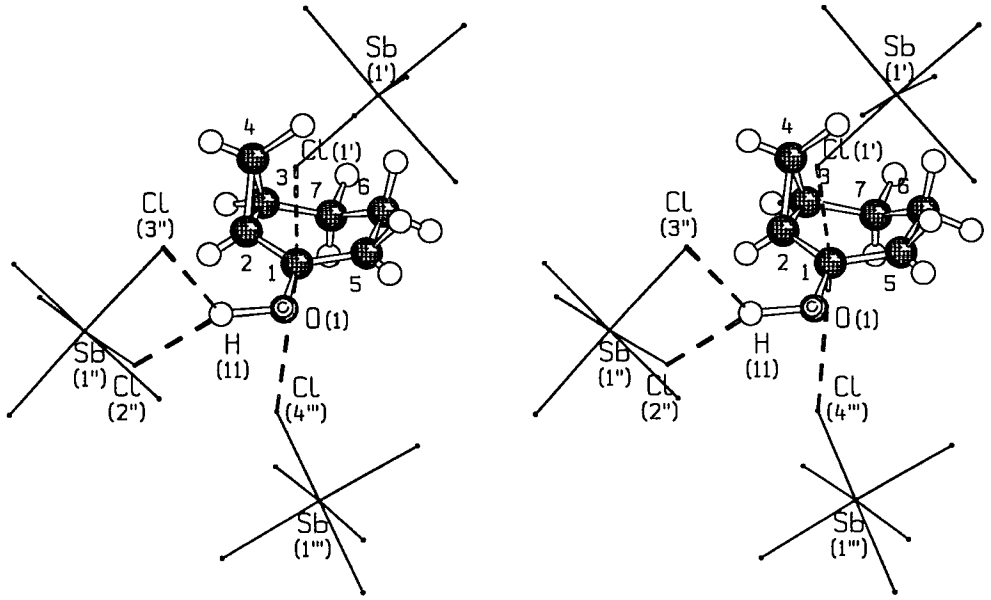


H(11)	- $F(1^{III})$	1.477	*diff* = -1.193	(H bond)
C(1)	- $F(2^{I})$	3.012	*diff* = -0.158	strong
C(1)	- $F(4^{II})$	2.916	*diff* = -0.254	strong

JICRAO

2-Hydroxybicyclo(4.1.0)heptan-2-ylium hexachloroantimonate
at -65 deg.C
C7 H11 O1 1+,Cl6 Sb1 1-
R.F.Childs,M.D.Kostyk,C.J.L.Lock,M.Mahendran
J.Am.Chem.Soc., 112, 8912,1990

JICRAO Pc21b Z= 4 NATOMS= 26 DIFF AS=0 R-FACTOR= 0.030
10 C-H BONDS: S.D.= 0.201; MEAN = 1.052; RANGE: 0.679 - 1.368



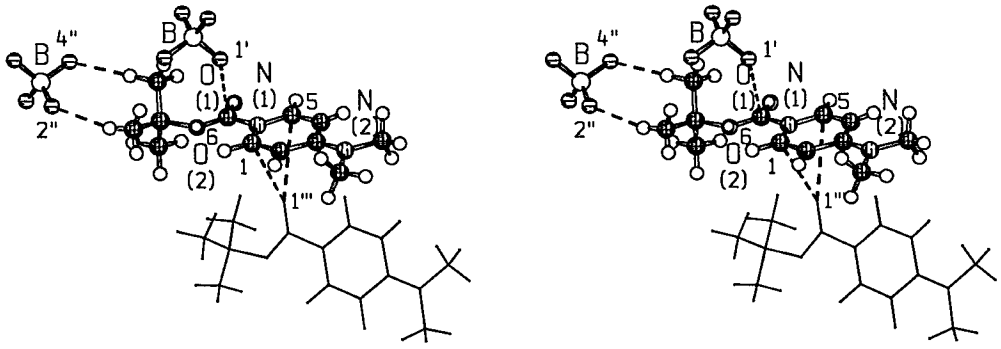
H(11)	- $Cl(2^{II})$	2.142	*diff* = -0.808 (H bond)
H(11)	- $Cl(3^{II})$	2.401	*diff* = -0.549 (H bond)
C(1)	- $Cl(1^{I})$	3.465	*diff* = 0.015
C(1)	- $Cl(4^{III})$	3.586	*diff* = 0.136

JOJXUB

N-(t-Butyloxycarbonyl)-4-(dimethylamino)-pyridinium tetrafluoroborate at -30 deg.C
C12 H19 N2 O2 1+,B1 F4 1-
C.Lohse,S.Hollenstein,T.Laube
Angew.Chem.,Int.Ed.Engl., 30, 1656,1991

JOJXUB P21/c Z= 4 NATOMS= 40 DIFF AS=2 R-FACTOR= 0.043
19 C-H BONDS: S.D.= 0.093; MEAN = 1.031; RANGE: 0.812 - 1.141

Several N hydrogens were newly computed.

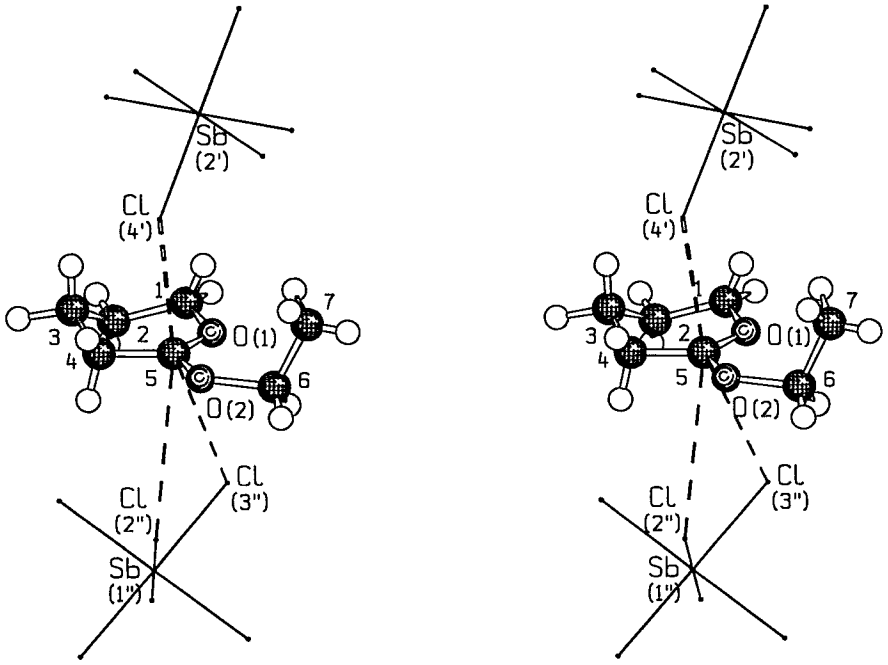


C(6)	- $F(1^{I})$	3.063	*diff* = -0.107 strong
C(1)	- $O(1^{III})$	3.204	*diff* = -0.016
C(5)	- $O(1^{III})$	3.269	*diff* = 0.049
$F(4^{II})$	- H(7)	2.588	*diff* = -0.082 (H bond)
$F(2^{II})$	- H(10)	2.673	*diff* = 0.003 (H bond)

JOPSEM

6-Ethoxy-2,3,4,5-tetrahydropyrylium hexachloroantimonate
at -65 deg.C
C7 H13 O2 1+,Cl6 Sb1 1-
R.F.Childs,M.D.Kostyk,C.J.L.Lock,M.Mahendran
Can.J.Chem., 69, 2024,1991

JOPSEM P1 Z= 2 NATOMS= 30 DIFF AS=2 R-FACTOR= 0.037
13 C-H BONDS: S.D.= 0.160; MEAN = 0.939; RANGE: 0.679 - 1.265

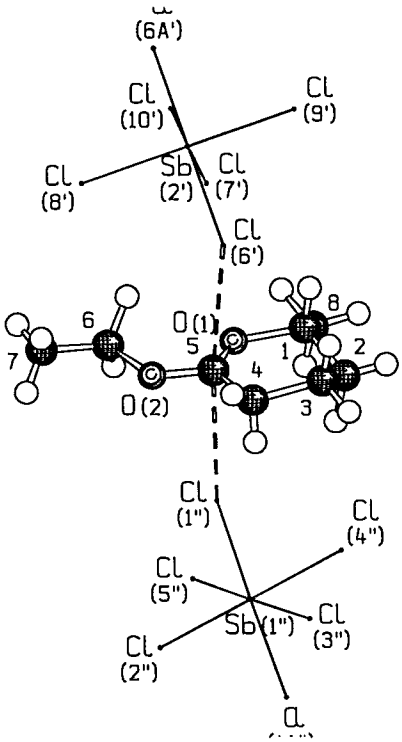


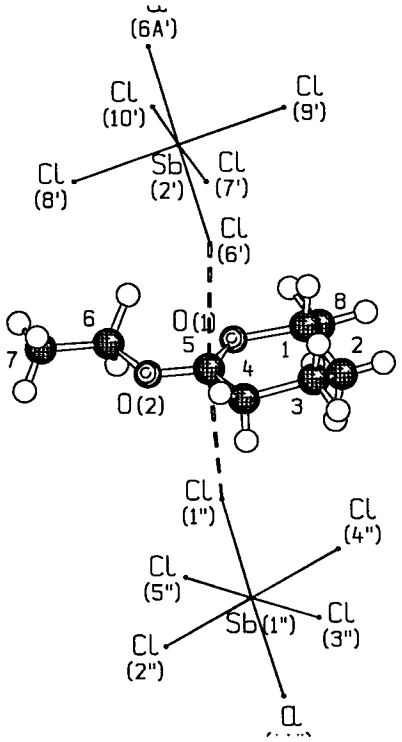
C(5)	- $Cl(4^{I})$	3.200	*diff* = -0.250	strong
C(5)	- $Cl(2^{II})$	3.865	*diff* = 0.415	weak
C(5)	- $Cl(3^{II})$	3.710	*diff* = 0.260	

JOPSOW

6-Ethoxy-2-methyl-2,3,4,5-tetrahydropyrylium hexachloroantimonate
at -65 deg.C
C8 H15 O2 1+,Cl6 Sb1 1-
R.F.Childs,M.D.Kostyk,C.J.L.Lock,M.Mahendran
Can.J.Chem., 69, 2024,1991

JOPSOW Pmnb Z= 8 NATOMS= 39 DIFF AS=2 R-FACTOR= 0.031
15 C-H BONDS: S.D.= 0.090; MEAN = 0.956; RANGE: 0.818 - 1.114



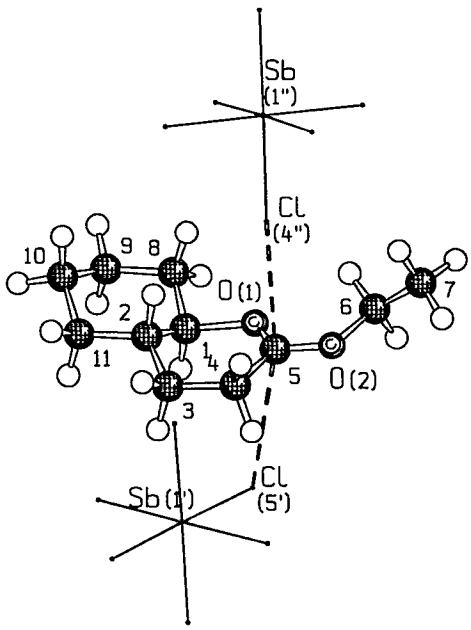


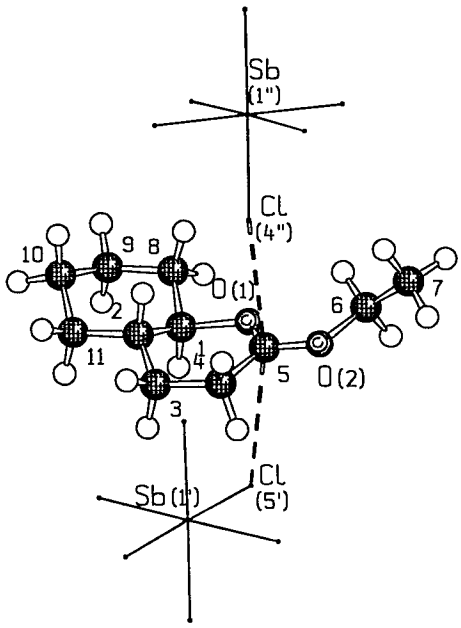
C(5) - Cl(6^{I}) 3.336 | *diff* = -0.114 strong
C(5) - Cl(1^{II}) 3.533 | *diff* = 0.083

JOPSUC

2-Ethoxy-3,4,4a,5,6,7,8,8a-octahydro-1-benzopyrylium hexachloroantimonate
C11 H19 O2 1+,Cl6 Sb1 1-
R.F.Childs,M.D.Kostyk,C.J.L.Lock,M.Mahendran
Can.J.Chem., 69, 2024,1991

JOPSUC Pca21 Z= 4 NATOMS= 39 DIFF AS=0 R-FACTOR= 0.035
19 C-H BONDS: S.D.= 0.123; MEAN = 1.047; RANGE: 0.794 - 1.300



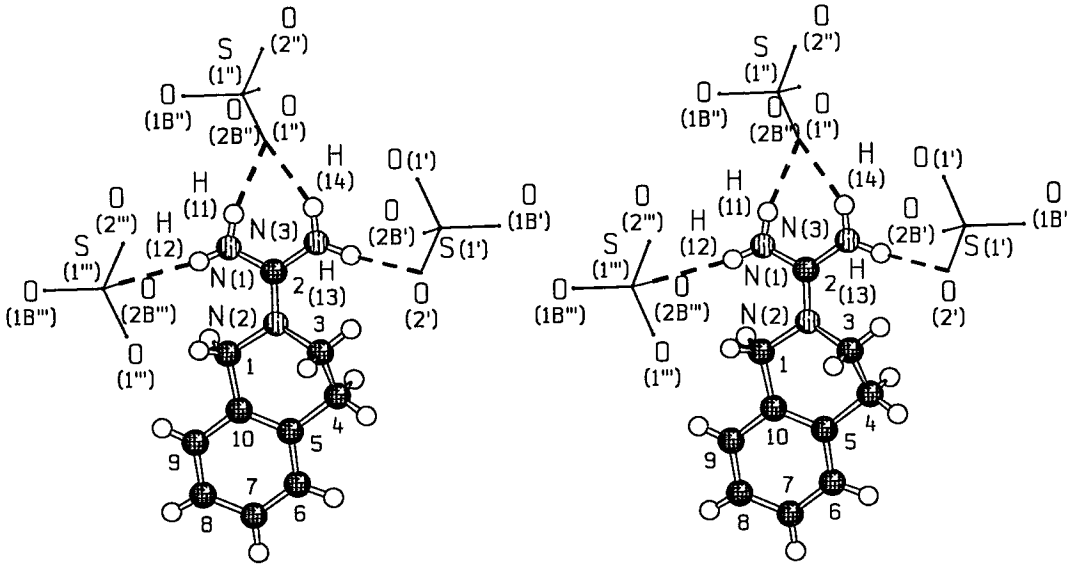


C(5)	- Cl(4^{II})	3.287	*diff* = -0.163	strong
C(5)	- Cl(5^{I})	3.766	*diff* = 0.316	weak

JUKWAN

bis(3,4-Dihydro-2(1H)-isoquinolinecarboxamidinium) sulfate
antihypertensive drug activity
2(C10 H14 N3 1+),O4 S1 2-
P.A.Bates,S.A.Islam,M.J.E.Sternberg
Acta Cryst.,C (Cr.Str.Comm.), 49, 300,1993

JUKWAN C2/c Z= 4 NATOMS= 32 DIFF AS=1 R-FACTOR= 0.042
REMARK CIF entry LI1020
10 C-H BONDS: S.D.= 0.054; MEAN = 0.988; RANGE: 0.901 - 1.073



H(11)	- O(1^{II})	2.002	*diff* = -0.718	(H bond)
H(12)	- O($2B^{III}$)	2.091	*diff* = -0.629	(H bond)
O(2^{I})	- H(13)	1.994	*diff* = -0.726	(H bond)
H(14)	- O(1^{II})	2.110	*diff* = -0.610	(H bond)

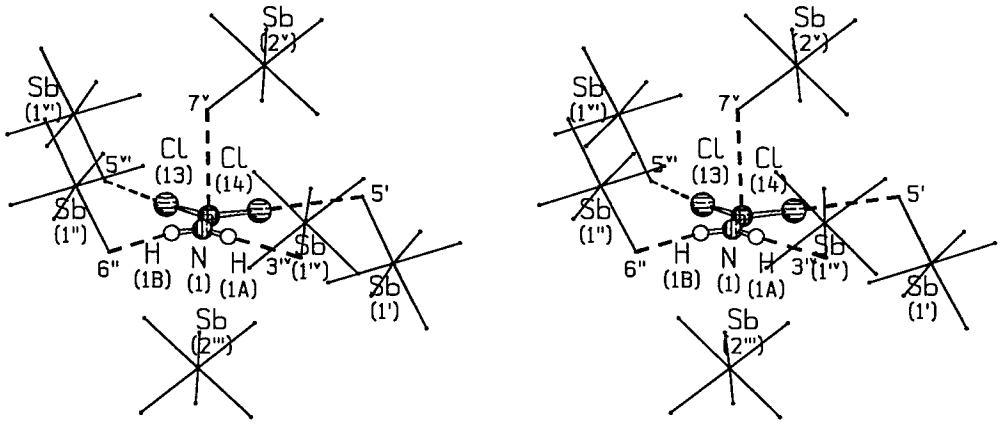
JUNVAP

Dichloromethyleneiminium hexachloroantimonate
C1 H2 Cl2 N1 1+,Cl6 Sb1 1-
R.Minkwitz,W.Meckstroth,H.Preut
Z.Anorg.Allg.Chem., 617, 136,1992

JUNVAP P21/c Z= 8 NATOMS= 22 DIFF AS=2 R-FACTOR= 0.042
REMARK CSD 56548 contains no further data for this compound

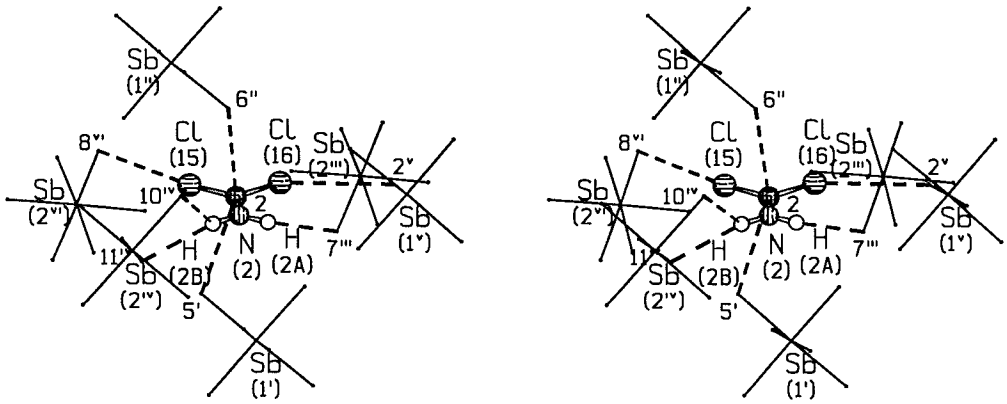
H atoms were added in the present paper.

cation #1:



H(1B)	- Cl(6^{II})	2.315	*diff* = -0.635	(H bond)
H(1A)	- Cl(3^{IV})	2.414	*diff* = -0.536	(H bond)
C(1)	- Cl(7^{V})	3.436	*diff* = -0.014	
Cl(14)	- Cl(5^{I})	3.264	*diff* = -0.236	strong
Cl(13)	- Cl(5^{VI})	3.648	*diff* = 0.148	

cation #2:

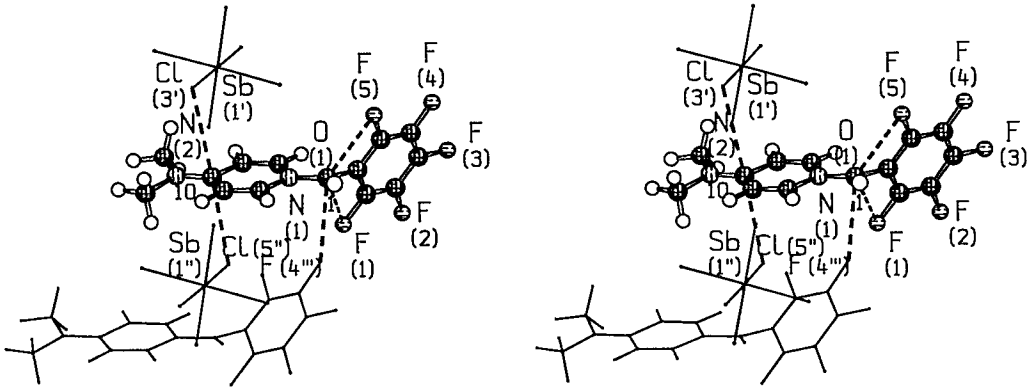


H(2A)	- Cl(7^{III})	2.287	*diff* = -0.663	(H bond)
H(2B)	- Cl(10^{IV})	2.639	*diff* = -0.311	(H bond)
H(2B)	- Cl(11^{IV})	2.579	*diff* = -0.371	(H bond)
C(2)	- Cl(6^{II})	3.511	*diff* = 0.061	
Cl(16)	- Cl(2^{V})	3.631	*diff* = 0.131	
Cl(15)	- Cl(8^{VI})	3.325	*diff* = -0.175	strong
C(2)	- Cl(5^{I})	3.597	*diff* = 0.147	

JUNVET

N-Pentafluorobenzoyl-4-dimethylaminopyridinium hexachloroantimonate
at -80 deg.C
C14 H10 F5 N2 O1 1+,Cl6 Sb1 1-
S.Hollenstein,C.Lohse,T.Laube
Croat.Chem.Acta, 65, 727,1992

JUNVET P1 Z= 1 NATOMS= 39 DIFF AS=2 R-FACTOR= 0.029
10 C-H BONDS: S.D.= 0.002; MEAN = 1.080; RANGE: 1.076 - 1.084

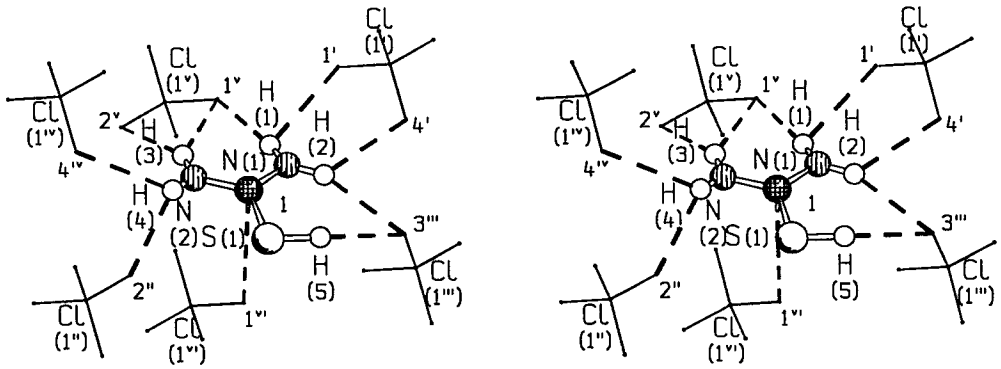


Cl(5^{II})	- C(10)	3.290	*diff* = -0.160	strong
Cl(3^{I})	- C(10)	3.383	*diff* = -0.067	
F(4^{III})	- C(1)	3.037	*diff* = -0.133	strong
C(1)	- F(1)	2.844	*diff* = -0.326	**very strong**
C(1)	- F(5)	2.800	*diff* = -0.370	**very strong**

JUXBEJ

Thiourea hydrogen perchlorate
at -70 deg.C
C1 H5 N2 S1 1+,Cl1 O4 1-
Kh.M.Eskudero,V.M.Akimov,M.Yu.Antipin,S.V.Lindeman,Yu.T.Struchkov
Zh.Neorg.Khim., 37, 767,1992

JUXBEJ P-1 Z= 2 NATOMS= 14 DIFF AS=1 R-FACTOR= 0.044

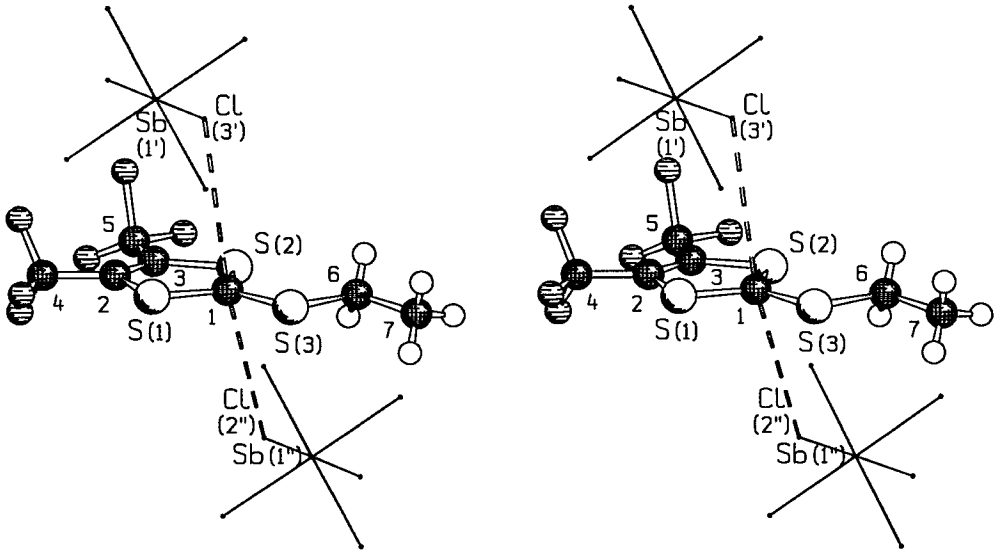


H(1)	- O(1^{V})	2.142	*diff* = -0.578	(H bond)
O(2^{II})	- H(4)	2.354	*diff* = -0.366	(H bond)
O(3^{III})	- H(5)	2.249	*diff* = -0.471	(H bond)
O(4^{I})	- H(2)	2.513	*diff* = -0.207	(H bond)
O(3^{III})	- H(2)	2.446	*diff* = -0.274	(H bond)
H(3)	- O(1^{V})	2.482	*diff* = -0.238	(H bond)
H(3)	- O(2^{V})	2.463	*diff* = -0.257	(H bond)
O(1^{I})	- H(1)	2.774	*diff* = 0.054	(H bond)
O(4^{IV})	- H(4)	2.624	*diff* = -0.096	(H bond)
C(1)	- O(1^{VI})	3.384	*diff* = 0.164	

JUYYUX

2-Ethylthio-4,5-bis(trifluoromethyl)-1,3-dithiolium hexachloroantimonate
C7 H5 F6 S3 1+,Cl6 Sb1 1-
M.Frasch,S.Mono,H.Pritzkow,W.Sundermeyer
Chem.Ber., 126, 273,1993

JUYYUX P21/c Z= 4 NATOMS= 28 DIFF AS=2 R-FACTOR= 0.037
REMARK CSD 56695 used
DISORD One trifluoromethyl group is disordered
5 C-H BONDS: S.D.= 0.051; MEAN = 0.913; RANGE: 0.818 - 0.950

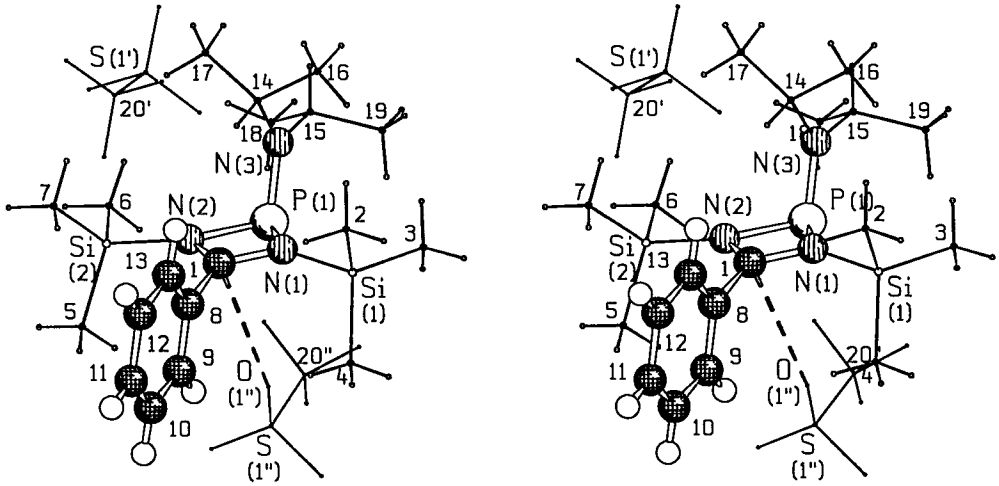


C(1) - Cl(2^{II}) 3.629 | *diff* = 0.179
C(1) - Cl(3^{I}) 3.722 | *diff* = 0.272

KAZDEU

2-Di-isopropylamino-1,3-bis(trimethylsilyl)-4-phenyl-1,3-diaza-2-phosphetine trifluoromethanesulfonate
C19 H37 N3 P1 Si2 1+,C1 F3 O3 S1 1-
C.Roques,M.-R.Mazieres,J.-P.Majoral,M.Sanchez,J.Jaud
Inorg.Chem., 28, 3931,1989

KAZDEU P21/n Z= 4 NATOMS= 70 DIFF AS=3 R-FACTOR= 0.073
37 C-H BONDS: S.D.= 0.003; MEAN = 0.970; RANGE: 0.955 - 0.978

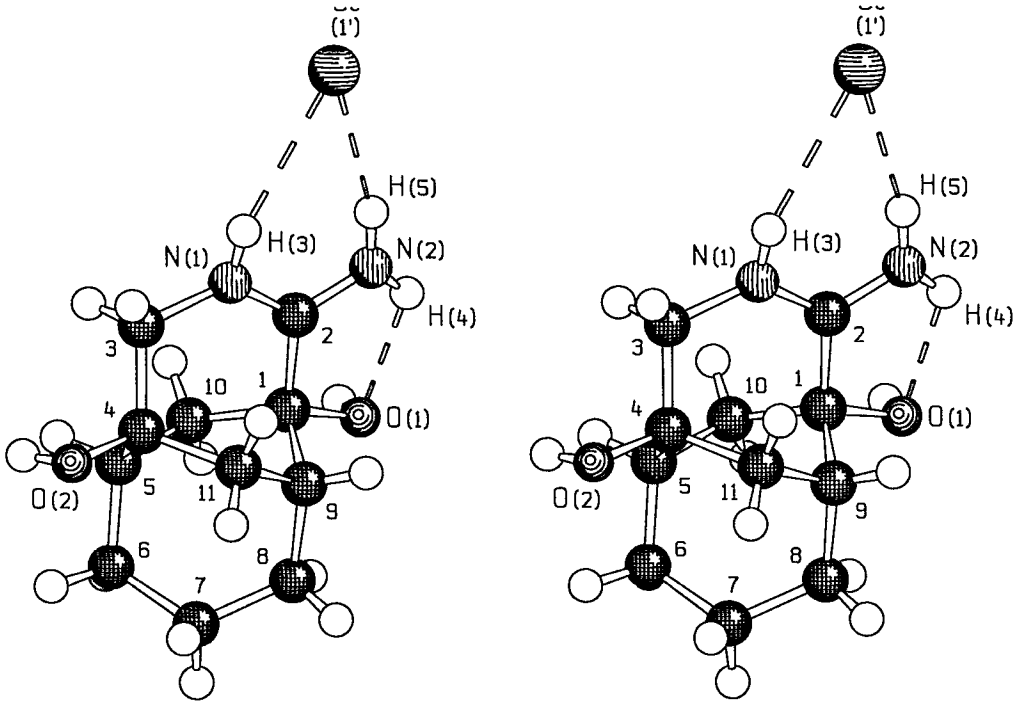


C(1) - O(1^{II}) 3.375 | *diff* = 0.155

KECGOO

4-Amino-5-azatricyclo[5.5.0.$0^{3,9}$]dodec-4-ene-3,7-diol hydrochloride
C11 H19 N2 O2 1+,Cl1 1-
Sungho Kim,R.Bishop,D.C.Craig,I.G.Dance,M.L.Scudder
J.Org.Chem., 55, 355,1990

KECGOO P21 Z= 2 NATOMS= 35 DIFF AS=1 R-FACTOR= 0.024
14 C-H BONDS: S.D.= 0.029; MEAN = 0.979; RANGE: 0.928 - 1.024



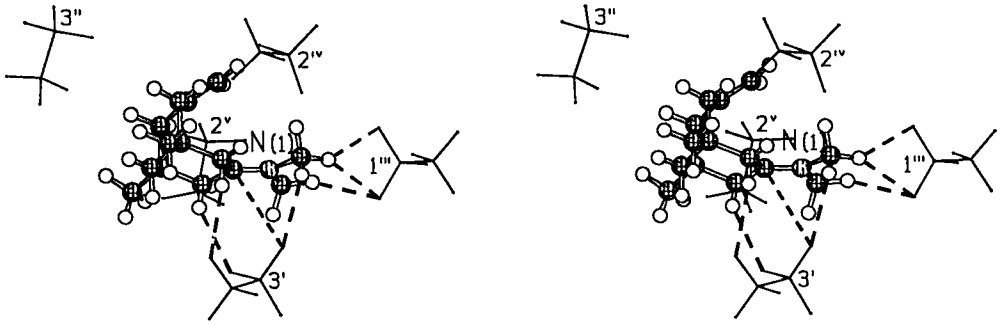
H(3) - Cl(1^{I}) 2.675 | *diff* = -0.275 (H bond)
H(5) - Cl(1^{I}) 2.336 | *diff* = -0.614 (H bond)
O(1) - H(4) 2.086 | *diff* = -0.634 (H bond)

KESDER

3-Dimethyliminium-7-methylene-1,5-dimethyl-bicyclo(3.3.1)-nonane trifluoromethanesulfonate
at -80 deg.C
C14 H24 N1 1+,C1 F3 O3 S1 1-
S.Hollenstein,T.Laube
Angew.Chem.,Int.Ed.Engl., 29, 188,1990

KESDER Pna21 Z= 12 NATOMS=141 DIFF AS=2 R-FACTOR= 0.047
72 C-H BONDS: S.D.= 0.047; MEAN = 1.066; RANGE: 0.842 - 1.161

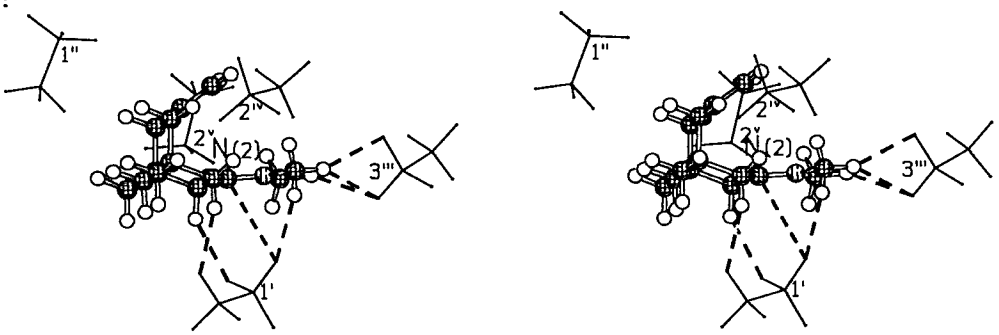
cation #1:



C(3) - O(7^{I}) 3.345 | *diff* = 0.125

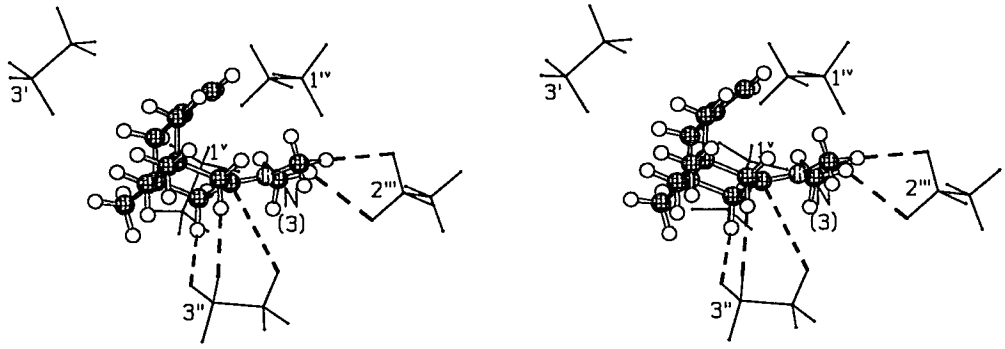
H(1)	- $F(8^{I})$	2.662	*diff* = -0.008 (H bond)
H(3)	- $O(9^{I})$	2.541	*diff* = -0.179 (H bond)
H(19)	- $O(1^{III})$	2.700	*diff* = -0.020 (H bond)
H(19)	- $O(3^{III})$	2.531	*diff* = -0.189 (H bond)
H(20)	- $O(7^{I})$	2.659	*diff* = -0.061 (H bond)
H(22)	- $O(1^{III})$	2.405	*diff* = -0.315 (H bond)

cation #2:



H(25)	- $F(2^{I})$	2.360	*diff* = -0.310 (H bond)
H(28)	- $O(2^{I})$	2.424	*diff* = -0.296 (H bond)
H(43)	- $O(7^{III})$	2.618	*diff* = -0.102 (H bond)
H(43)	- $O(8^{III})$	2.365	*diff* = -0.355 (H bond)
H(44)	- $O(1^{I})$	2.498	*diff* = -0.222 (H bond)
H(46)	- $O(7^{III})$	2.449	*diff* = -0.271 (H bond)
C(17)	- $O(1^{I})$	3.381	*diff* = 0.161

cation #3:



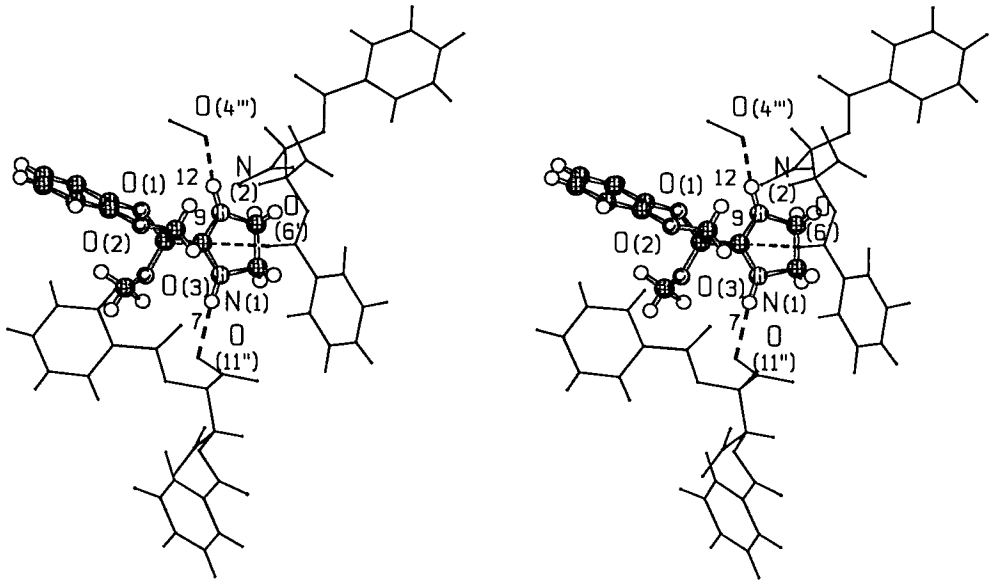
H(67)	- $O(6^{III})$	2.538	*diff* = -0.182 (H bond)
H(70)	- $O(5^{III})$	2.681	*diff* = -0.039 (H bond)
H(49)	- $O(8^{II})$	2.518	*diff* = -0.202 (H bond)
H(52)	- $O(9^{II})$	2.328	*diff* = -0.392 (H bond)
C(31)	- $F(7^{II})$	3.470	*diff* = 0.300

The names of the anions I and II in the environment of cation #3 are interchanged in Fig. 31c *of the manuscript.*

KIBPIU

(+)-2-(2-Methoxy-2,3-dihydro-1,4-benzodioxin-2-yl)-4,5-dihydroimidazolium hydrogen dibenzoyltartrate methanol solvate
C12 H15 N2 O3 1+,C18 H13 O8 1-,C1 H4 O1
A.A.Freer,G.A.Sim
J.Chem.Soc.,Perkin Trans.2, , 1717,1990

KIBPIU P21 Z= 2 NATOMS= 72 DIFF AS=2 R-FACTOR= 0.043
25 C-H BONDS: S.D.= 0.081; MEAN = 0.957; RANGE: 0.764 - 1.159

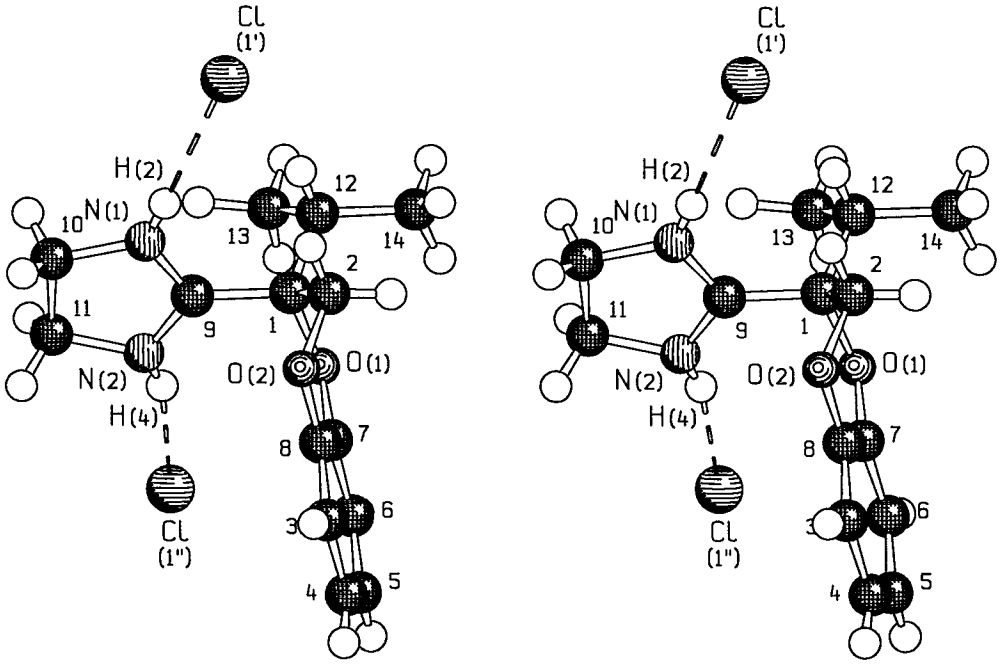


O(6^{I})	- C(9)	3.082	*diff* = -0.138	strong
H(7)	- O(11^{II})	1.998	*diff* = -0.722	(H bond)
O(4^{III})	- H(12)	1.765	*diff* = -0.955	(H bond)

KIBPOA

2-(2-Isopropyl-2,3-dihydro-1,4-benzodioxin-2-yl)-4,5-dihydroimidazolium chloride
C14 H19 N2 O2 1+,Cl1 1-
A.A.Freer,G.A.Sim
J.Chem.Soc.,Perkin Trans.2, , 1717,1990

KIBPOA P21/n Z= 4 NATOMS= 38 DIFF AS=2 R-FACTOR= 0.063
17 C-H BONDS: S.D.= 0.068; MEAN = 0.949; RANGE: 0.853 - 1.092

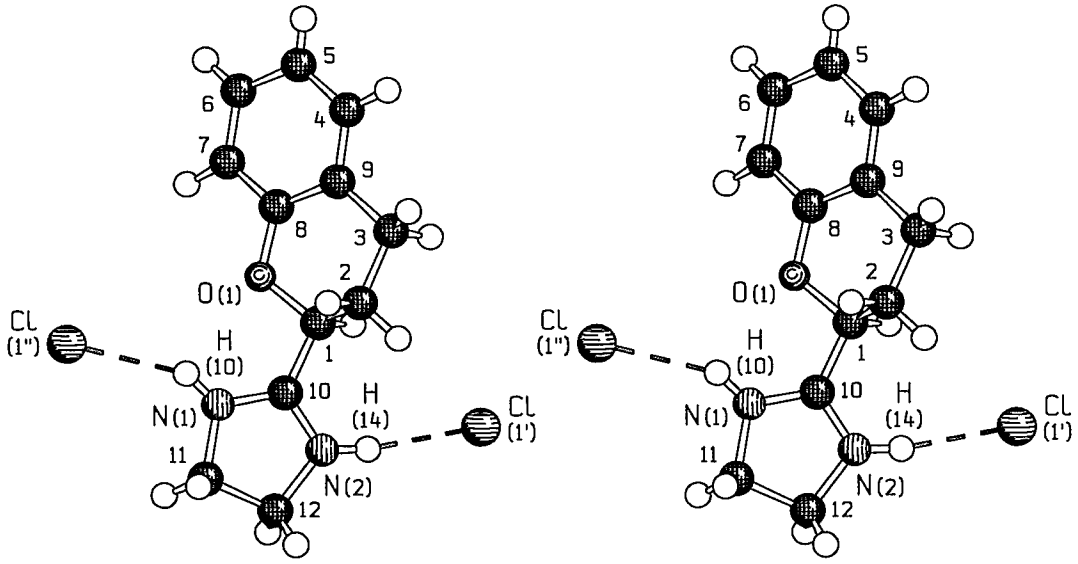


Cl(1^{I})	- H(2)	2.369	*diff* = -0.581	(H bond)
H(4)	- Cl(1^{II})	2.359	*diff* = -0.591	(H bond)

KIBPUG

2-(2,3-Dihydro-1-benzopyran-2-yl)-4,5-dihydroimidazolium chloride
C12 H15 N2 O1 1+,Cl1 1-
A.A.Freer,G.A.Sim
J.Chem.Soc.,Perkin Trans.2, , 1717,1990

KIBPUG P-1 Z= 2 NATOMS= 31 DIFF AS=1 R-FACTOR= 0.051
13 C-H BONDS: S.D.= 0.037; MEAN = 0.975; RANGE: 0.891 - 1.036

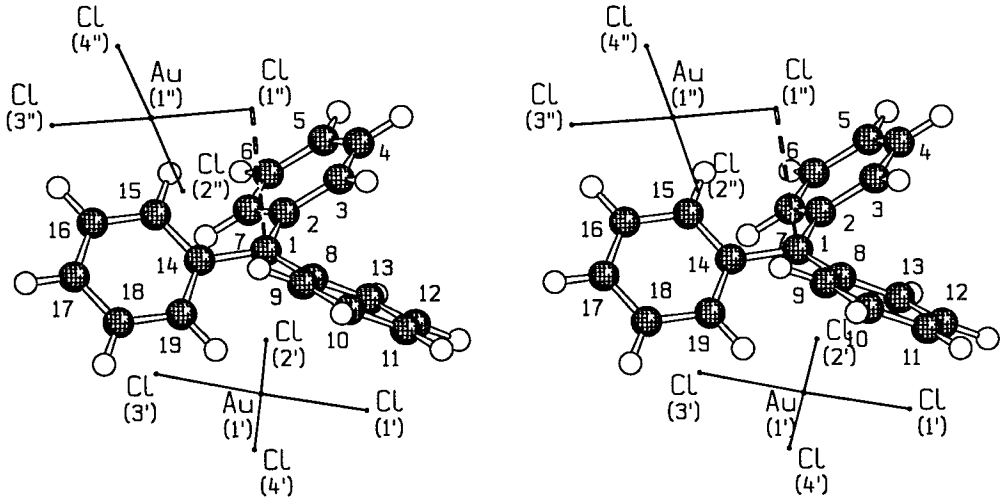


H(10) - Cl(1^{II}) 2.348 | *diff* = -0.602 (H bond)
H(14) - Cl(1^{I}) 2.239 | *diff* = -0.711 (H bond)

KOHVOS

Triphenylmethylium tetrachloro-gold(iii)
C19 H15 1+,Au1 Cl4 1-
D.B.Dell'Amico,F.Calderazzo,A.Morvillo,G.Pelizzi,P.Robino
J.Chem.Soc.,Dalton Trans., , 3009,1991

KOHVOS P21/c Z= 4 NATOMS= 39 DIFF AS=3 R-FACTOR= 0.060
15 C-H BONDS: S.D.= 0.000; MEAN = 1.080; RANGE: 1.079 - 1.080

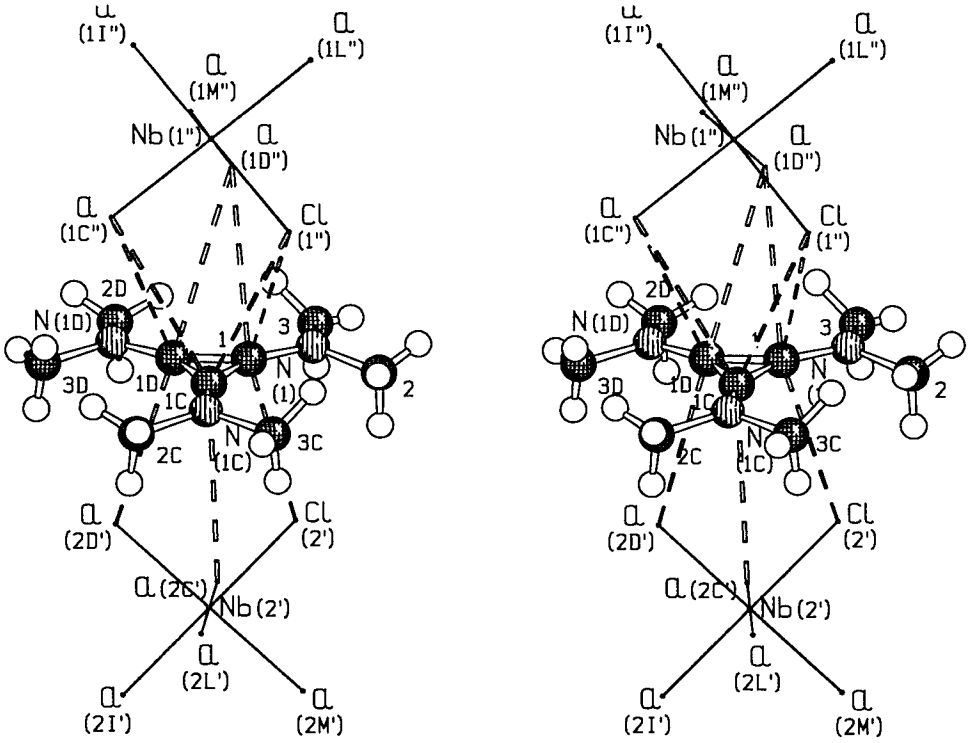


C(1) - Cl(1^{II}) 3.650 | *diff* = 0.200

KOWGOS

1,2,3-tris(Dimethylamino)cyclopropenylium hexachloro-niobium(v)
C9 H18 N3 1+,Cl6 Nb1 1-
H.N.Schafer,H.Burzlaff,A.M.H.Grimmeiss,R.Weiss
Acta Cryst.,C (Cr.Str.Comm.), 48, 795,1992

KOWGOS R-3 Z= 6 NATOMS= 44 DIFF AS=1 R-FACTOR= 0.025
18 C-H BONDS: S.D.= 0.134; MEAN = 0.937; RANGE: 0.666 - 1.090

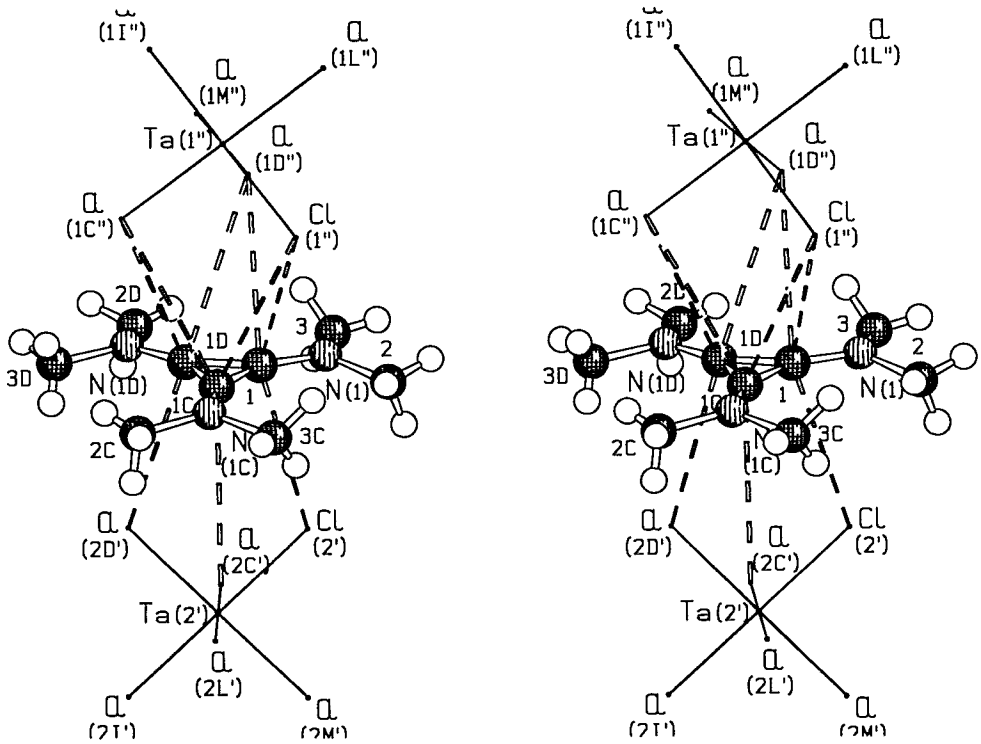


$Cl(1D^{II})$	- C(1)	3.619	*diff* =	0.169
$Cl(1^{II})$	- C(1C)	3.619	*diff* =	0.169
$Cl(1C^{II})$	- C(1D)	3.619	*diff* =	0.169
$Cl(1^{II})$	- C(1)	3.739	*diff* =	0.289
$Cl(2^{I})$	- C(1)	3.736	*diff* =	0.286
$Cl(1C^{II})$	- C(1C)	3.739	*diff* =	0.289
$Cl(2C^{I})$	- C(1C)	3.736	*diff* =	0.286
$Cl(1D^{II})$	- C(1D)	3.739	*diff* =	0.289
$Cl(2D^{I})$	- C(1D)	3.736	*diff* =	0.286

KOWGUY

1,2,3-tris(Dimethylamino)cyclopropenylium hexachloro-tantalum(v)
C9 H18 N3 1+,Cl6 Ta1 1-
H.N.Schafer,H.Burzlaff,A.M.H.Grimmeiss,R.Weiss
Acta Cryst.,C (Cr.Str.Comm.), 48, 795,1992

KOWGUY R-3 Z= 6 NATOMS= 44 DIFF AS=1 R-FACTOR= 0.023
18 C-H BONDS: S.D.= 0.089; MEAN = 0.883; RANGE: 0.769 - 0.995

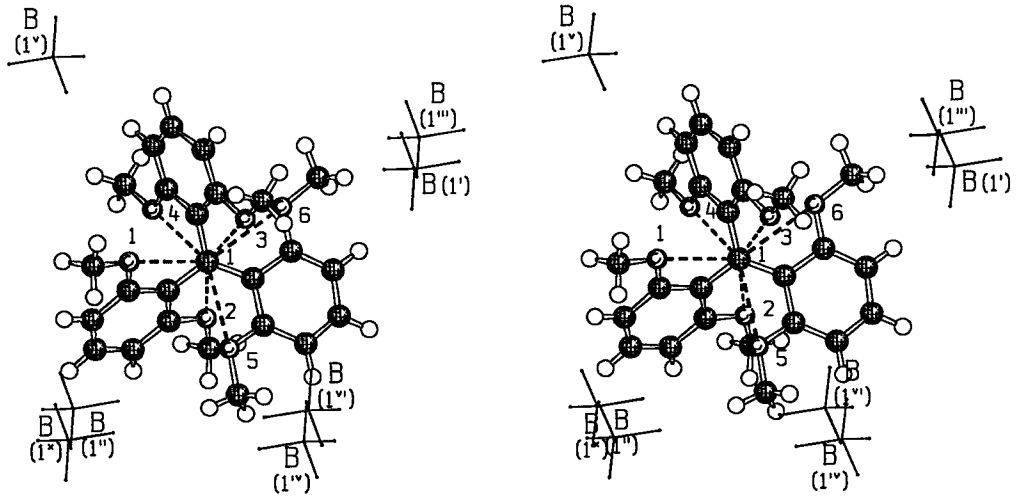


Cl(1D^{II})	- C(1)	3.626	*diff* =	0.176
Cl(1^{II})	- C(1C)	3.626	*diff* =	0.176
Cl(1C^{II})	- C(1D)	3.627	*diff* =	0.177
Cl(1^{II})	- C(1)	3.745	*diff* =	0.295
Cl(2^{I})	- C(1)	3.744	*diff* =	0.294
Cl(1C^{II})	- C(1C)	3.745	*diff* =	0.295
Cl(2C^{I})	- C(1C)	3.744	*diff* =	0.294
Cl(1D^{II})	- C(1D)	3.745	*diff* =	0.295
Cl(2D^{I})	- C(1D)	3.744	*diff* =	0.294

KUBLUO

tris(2,6-Dimethoxyphenyl)methyl tetrafluoroborate
at 110 deg.K
C25 H27 O6 1+,B1 F4 1-
B.Kahr,J.E.Jackson,D.L.Ward,Sei-Hum Jang,J.F.Blount
Acta Cryst.,B (Str.Sci.), 48, 324,1992

KUBLUO P-1 Z= 2 NATOMS= 63 DIFF AS=1 R-FACTOR= 0.056
27 C-H BONDS: S.D.= 0.012; MEAN = 1.005; RANGE: 0.985 - 1.029



C(1)	- O(1)	2.771	*diff* = -0.449	**very strong**
C(1)	- O(2)	2.769	*diff* = -0.451	**very strong**
C(1)	- O(3)	2.758	*diff* = -0.462	**very strong**
C(1)	- O(4)	2.757	*diff* = -0.463	**very strong**
C(1)	- O(5)	2.776	*diff* = -0.444	**very strong**
C(1)	- O(6)	2.779	*diff* = -0.441	**very strong**

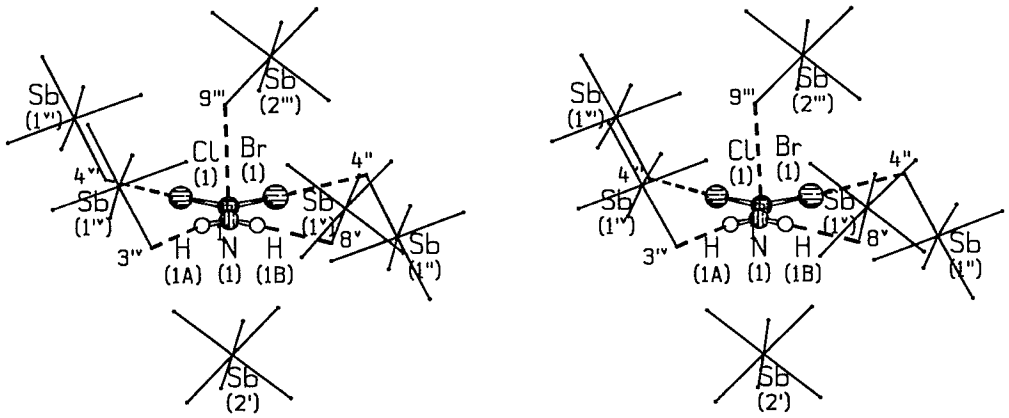
LAFMEK

Bromochloromethyleneiminium hexachloro-antimony
C1 H2 Br1 Cl1 N1 1+,Cl6 Sb1 1-
R.Minkwitz,W.Meckstroth,H.Preut
Z.Naturforsch.,Teil B, 48, 19,1993

LAFMEK P21/c Z= 8 NATOMS= 22 DIFF AS=2 R-FACTOR= 0.038
REMARK CSD 56551 duplicates publication
DISORD One of the cations is disordered

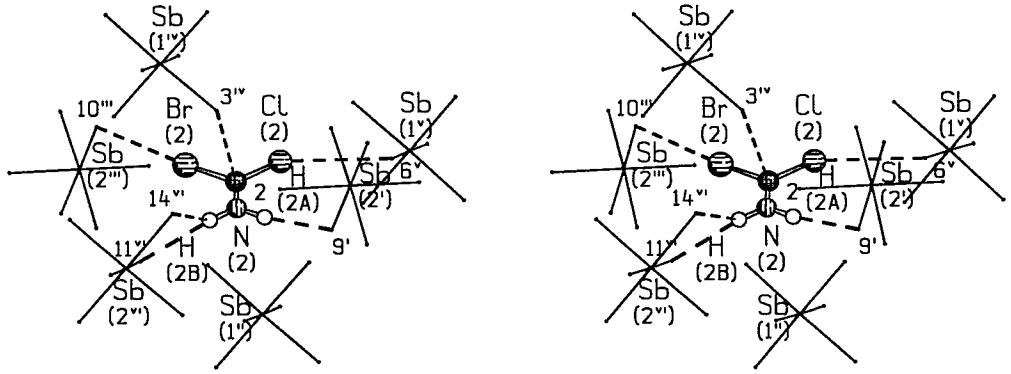
H atoms were added in the present paper.

cation #1:



H(1A)	- Cl(3^{IV})	2.314	*diff* = -0.636	(H bond)
H(1B)	- Cl(8^{V})	2.437	*diff* = -0.513	(H bond)
C(1)	- Cl(9^{III})	3.487	*diff* = 0.037	
Cl(1)	- Cl(4^{VI})	3.532	*diff* = 0.032	
Br(1)	- Cl(4^{II})	3.219	*diff* = -0.381	**very strong**

cation #2:



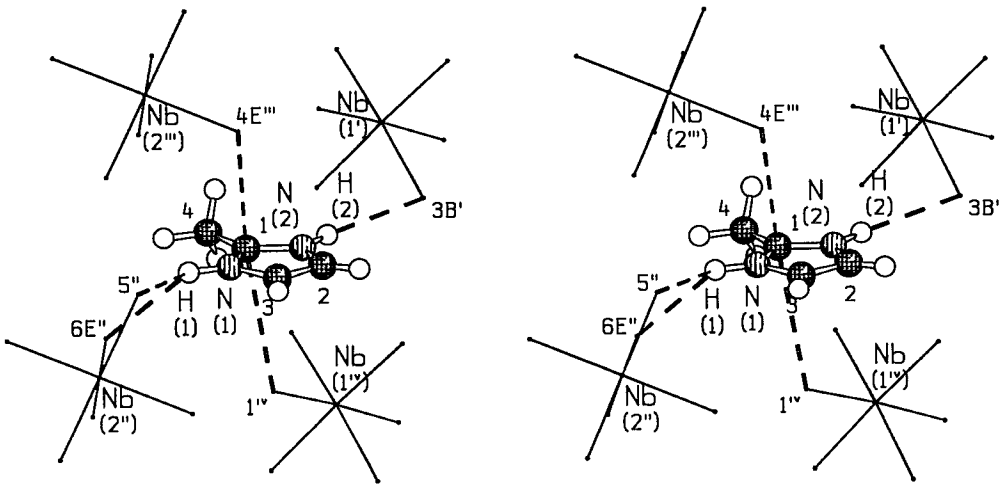
H(2A)	- Cl(9^{I})	2.282	*diff* = -0.668	(H bond)
H(2B)	- Cl(11^{VI})	2.630	*diff* = -0.320	(H bond)
H(2B)	- Cl(14^{VI})	2.583	*diff* = -0.367	(H bond)
C(2)	- Cl(3^{IV})	3.553	*diff* = 0.103	
Br(2)	- Cl(10^{III})	3.268	*diff* = -0.332	**very strong**
Cl(2)	- Cl(6^{V})	3.568	*diff* = 0.068	

LALLOZ

2-Methylimidazolium hexachloro-niobium(v)
at 200 deg.K
C4 H7 N2 1+,Cl6 Nb1 1-
B.Therrien,A.L.Beauchamp
Acta Cryst.,C (Cr.Str.Comm.), 49, 1303,1993

LALLOZ C2/c Z= 8 NATOMS= 27 DIFF AS=2 R-FACTOR= 0.030
REMARK CIF entry CD1013
5 C-H BONDS: S.D.= 0.089; MEAN = 1.006; RANGE: 0.892 - 1.082

H(1) and H(2) were newly computed in the present paper.

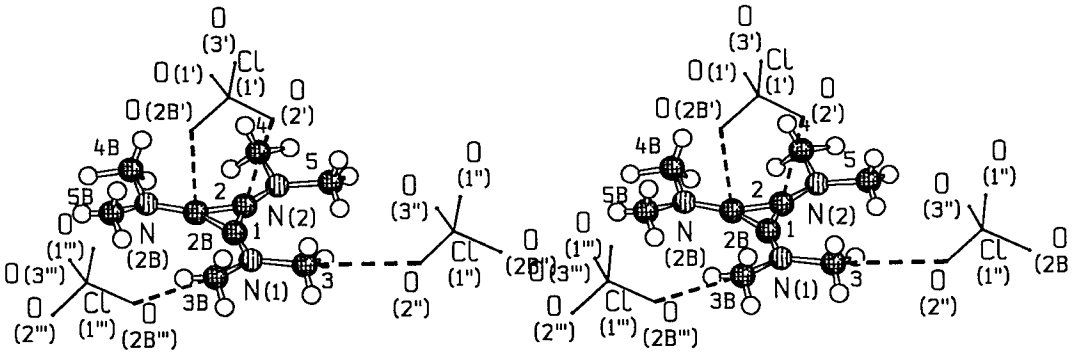


Cl(5^{II})	- H(1)	2.587	*diff* = -0.363	(H bond)
Cl($6E^{II}$)	- H(1)	2.619	*diff* = -0.331	(H bond)
Cl($3B^{I}$)	- H(2)	2.548	*diff* = -0.402	(H bond)
C(1)	- Cl($4E^{III}$)	3.517	*diff* = 0.067	
C(1)	- Cl(1^{IV})	3.478	*diff* = 0.028	

MACPRP10

1,2,3-tris(Dimethylamino)cyclopropenium perchlorate
C9 H18 N3 1+,Cl1 O4 1-
A.T.Ku,M.Sundaralingam
J.Am.Chem.Soc., 94, 1688,1972

MACPRP10 Pnma Z= 4 NATOMS= 35 DIFF AS=0 R-FACTOR= 0.076
18 C-H BONDS: S.D.= 0.104; MEAN = 0.941; RANGE: 0.821 - 1.156



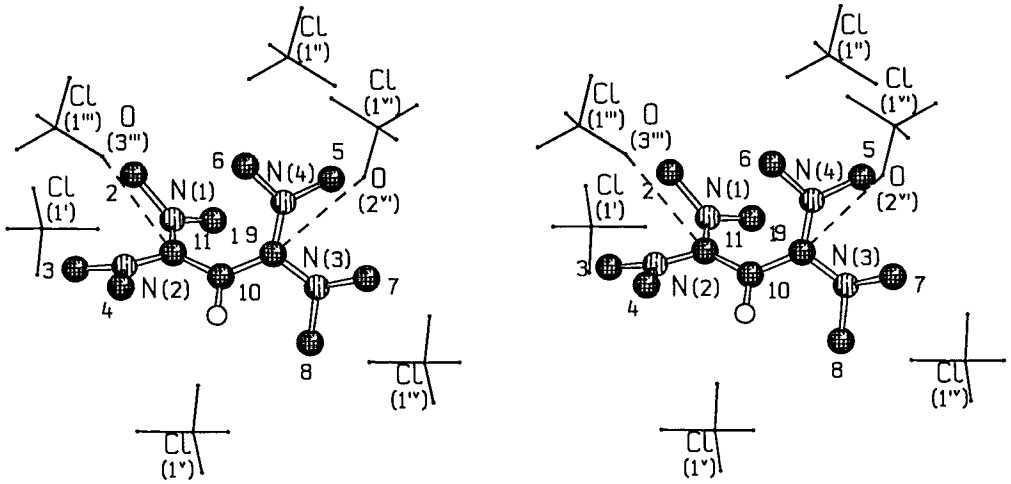
O(2^{I})	- C(2)	3.160	*diff* = -0.060	
C(3)	- O(2^{II})	3.100	*diff* = -0.120	strong
O($2B^{I}$)	- C(2B)	3.160	*diff* = -0.060	
C(3B)	- O($2B^{III}$)	3.100	*diff* = -0.120	strong

MALLPC

1,1,3,3-Tetra(dimethylamino)allyl perchlorate
C11 H25 N4 1+,Cl1 O4 1-
E.Oeser
Chem.Ber., 107, 627,1974

MALLPC P21/c Z= 4 NATOMS= 20 DIFF AS=2 R-FACTOR= 0.104

H atom at C(10) was added in the present paper.

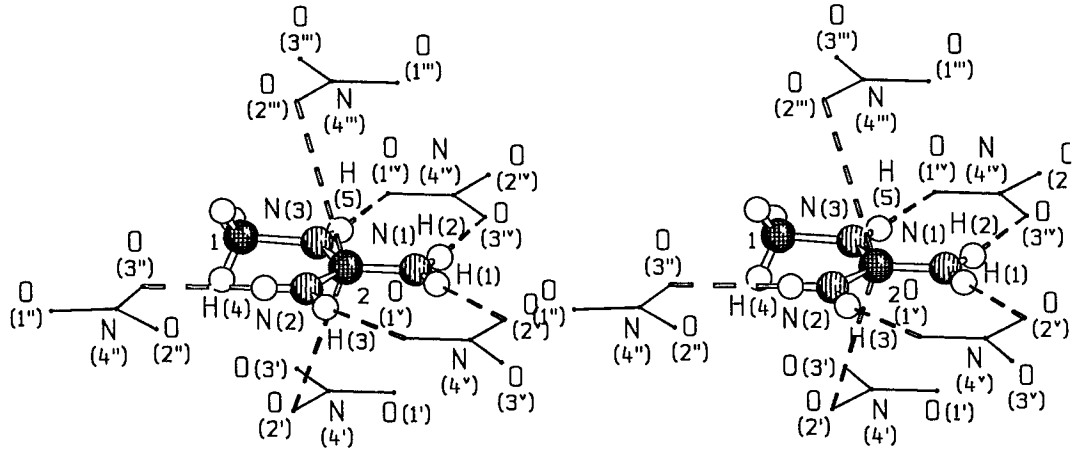


C(11)	- O(3^{III})	3.972	*diff* =	0.752	very weak
C(9)	- O(2^{VI})	4.136	*diff* =	0.916	very weak

MEGUAN

Methylguanidinium nitrate
C2 H8 N3 1+,N1 O3 1-
R.M.Curtis,R.A.Pasternak
Acta Crystallogr., 8, 675,1955

MEGUAN Pnma Z= 4 NATOMS= 17 PHOT AS=2 R-FACTOR= 0.000
3 C-H BONDS: S.D.= 0.001; MEAN = 0.897; RANGE: 0.896 - 0.898



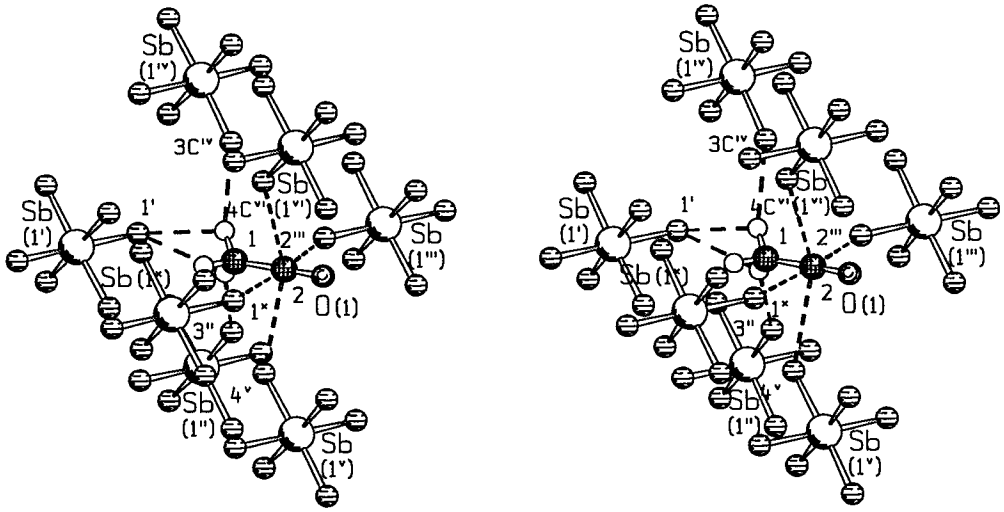
H(1)	- O(2^{V})	2.179	*diff* = -0.541	(H bond)
H(2)	- O(3^{IV})	2.213	*diff* = -0.507	(H bond)
H(3)	- O(1^{V})	2.127	*diff* = -0.593	(H bond)
H(4)	- O(3^{II})	2.295	*diff* = -0.425	(H bond)
H(5)	- O(1^{IV})	2.094	*diff* = -0.626	(H bond)
C(2)	- O(2^{I})	3.418	*diff* = 0.198	
C(2)	- O(2^{III})	3.418	*diff* = 0.198	

MOCFSB10

Methyloxocarbonium hexafluoroantimonate
C2 H3 O1 1+,F6 Sb1 1-
F.P.Boer

J.Am.Chem.Soc., 90, 6706,1968

MOCFSB10 P21/m Z= 2 NATOMS= 13 PHOT AS=3 R-FACTOR= 0.056
3 C-H BONDS: S.D.= 0.057; MEAN = 0.926; RANGE: 0.846 - 0.966

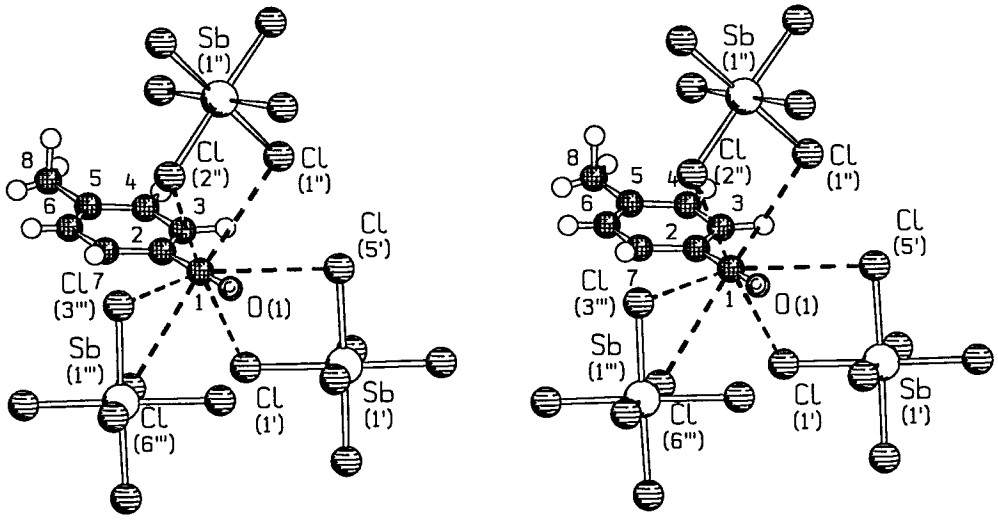


C(2)	- F(2^{III})	2.638	*diff* = -0.532	**extremely strong**
C(2)	- F(4^{V})	2.724	*diff* = -0.446	**very strong**
C(2)	- F($4C^{VI}$)	2.724	*diff* = -0.446	**very strong**
C(2)	- F(1^{X})	2.773	*diff* = -0.397	**very strong**
H(2)	- F(1^{I})	2.647	*diff* = -0.023	(H bond)
H(2)	- F(3^{II})	2.335	*diff* = -0.335	(H bond)
H(2C)	- F(1^{I})	2.647	*diff* = -0.023	(H bond)
H(2C)	- F($3C^{IV}$)	2.335	*diff* = -0.335	(H bond)

MPOCSB

4-Methylphenyl-oxocarbonium hexachloroantimonate
C8 H7 O1 1+,Cl6 Sb1 1-
B.Chevrier,J.-M.Le Carpentier,R.Weiss
J.Am.Chem.Soc., 94, 5718,1972

MPOCSB P21/c Z= 4 NATOMS= 23 DIFF AS=0 R-FACTOR= 0.042
7 C-H BONDS: S.D.= 0.091; MEAN = 0.989; RANGE: 0.812 - 1.135



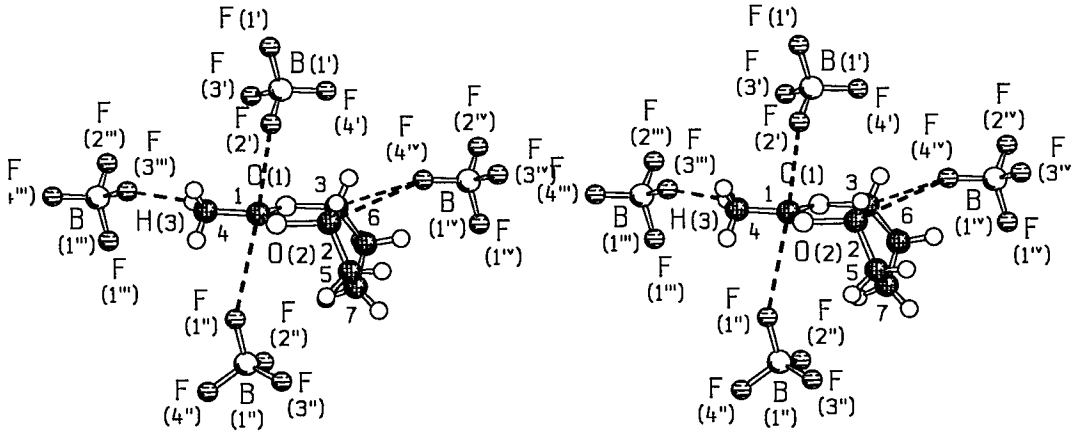
C(1)	- Cl(1^{I})	3.375	*diff* = -0.075	

C(1)	- Cl(5^{I})	3.718	*diff* = 0.268	
C(1)	- Cl(1^{II})	3.410	*diff* = -0.040	
C(1)	- Cl(2^{II})	3.298	*diff* = -0.152	strong
C(1)	- Cl(3^{III})	3.814	*diff* = 0.364	weak
C(1)	- Cl(6^{III})	3.321	*diff* = -0.129	strong

MTDXYL

Endo-2-Methyl-cis-4,5-trimethylene-1,3-dioxolan-2-ylium tetrafluoroborate
C7 H11 O2 1+,B1 F4 1-
H.Paulsen,E.Schuttpelz
Chem.Ber., 112, 3214,1979

MTDXYL P21/c Z= 4 NATOMS= 25 DIFF AS=1 R-FACTOR= 0.082
11 C-H BONDS: S.D.= 0.079; MEAN = 0.948; RANGE: 0.814 - 1.106

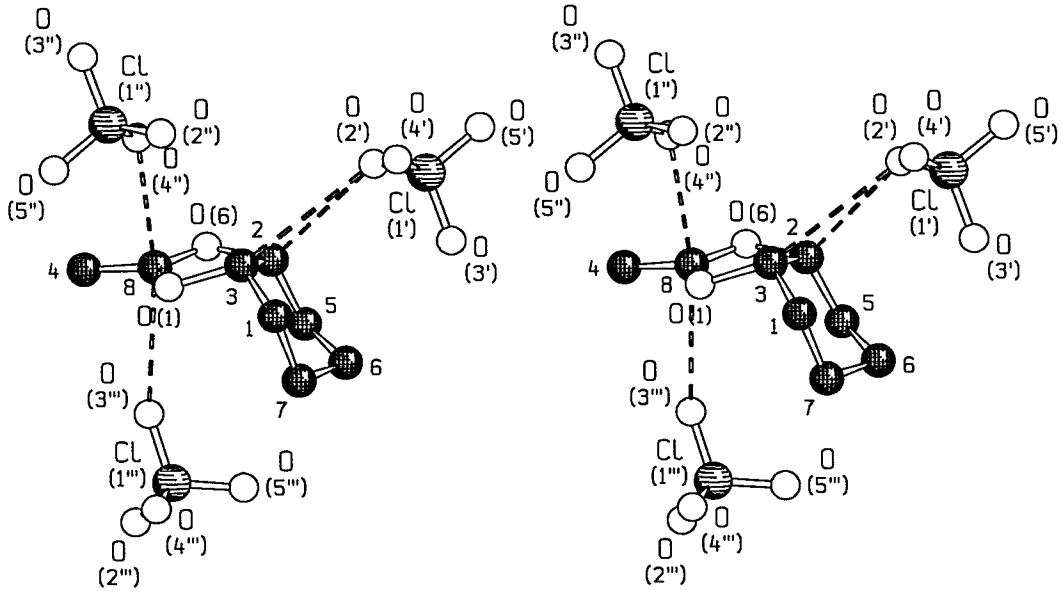


C(1)	- F(2^{I})	2.696	*diff* = -0.474	**very strong**
C(1)	- F(1^{II})	3.113	*diff* = -0.057	
C(2)	- F(4^{IV})	2.962	*diff* = -0.208	strong
C(3)	- F(4^{IV})	3.209	*diff* = 0.039	
H(3)	- F(3^{III})	2.655	*diff* = -0.015	(H bond)

MTDXYP

2-Methyl-4,5-tetramethylene-1,3-dioxolan-2-ylium perchlorate
C8 H13 O2 1+,Cl1 O4 1-
H.Paulsen,R.Dammeyer
Chem.Ber., 109, 605,1976

MTDXYP P21/c Z= 4 NATOMS= 15 DIFF AS=1 R-FACTOR= 0.067
REMARK ALL HYDROGENS REMOVED, THEY GIVE STRANGE GEOMETRY

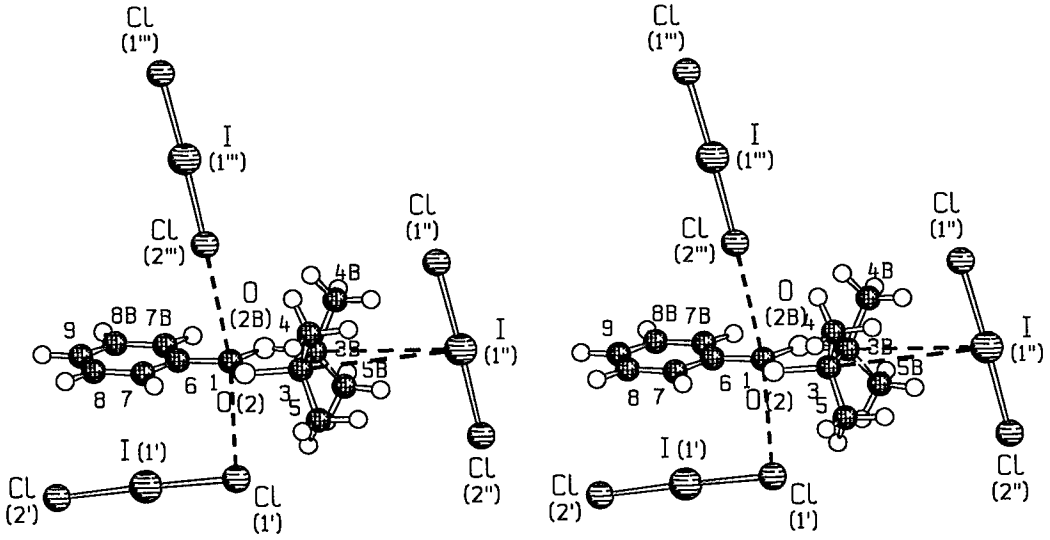


C(8)	- O(4^{II})	2.768	*diff* = -0.452	**very strong**
C(8)	- O(3^{III})	3.086	*diff* = -0.134	strong
C(2)	- O(2^{I})	3.186	*diff* = -0.034	
C(3)	- O(2^{I})	3.252	*diff* = 0.032	

OXLCLI

4,4,5,5-Tetramethyl-2-phenyl-1,3-dioxolan-2-ylium dichloro-iodate(i)
C13 H17 O2 1+,Cl2 I1 1-
M.R.Caira,J.F.de Wet
Acta Crystallogr.,Sect.B, 37, 709,1981

OXLCLI Pnma Z= 4 NATOMS= 35 DIFF AS=3 R-FACTOR= 0.039
17 C-H BONDS: S.D.= 0.003; MEAN = 1.078; RANGE: 1.073 - 1.082

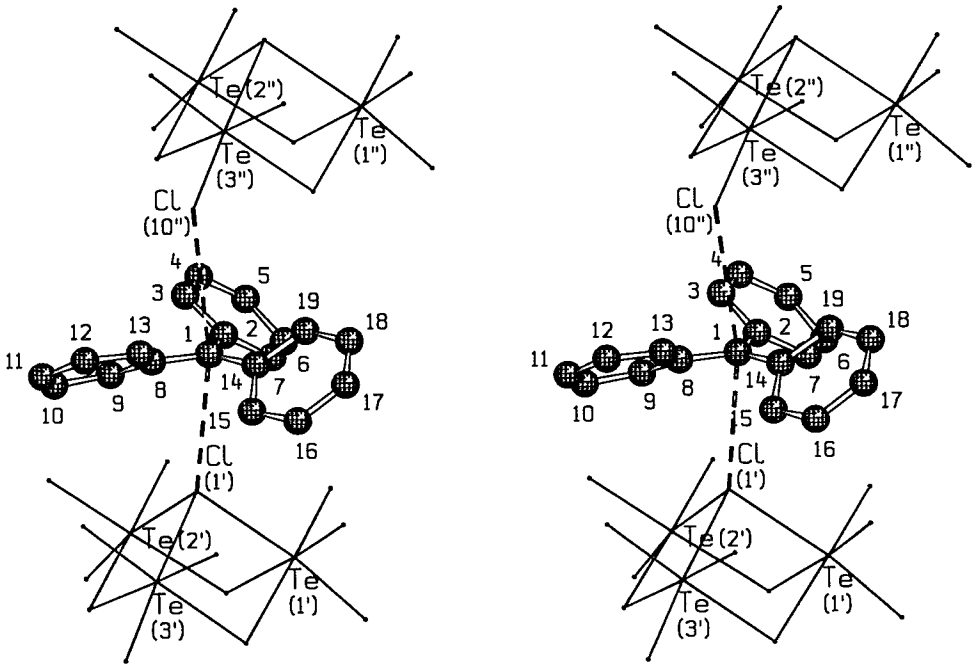


C(1)	- Cl(1^{I})	3.420	*diff* = -0.030	
C(1)	- Cl(2^{III})	3.407	*diff* = -0.043	
C(3)	- I(1^{II})	4.407	*diff* = 0.727	very weak
C(3B)	- I(1^{II})	4.407	*diff* = 0.727	very weak

PCBTEC10

Triphenylmethyl tridecachloro-tri-tellurium
C19 H15 1+,Cl13 Te3 1-
B.Krebs,V.Paulat
Z.Naturforsch.,Teil B, 34, 900,1979

PCBTEC10 P21/c Z= 4 NATOMS= 35 DIFF AS=0 R-FACTOR= 0.065

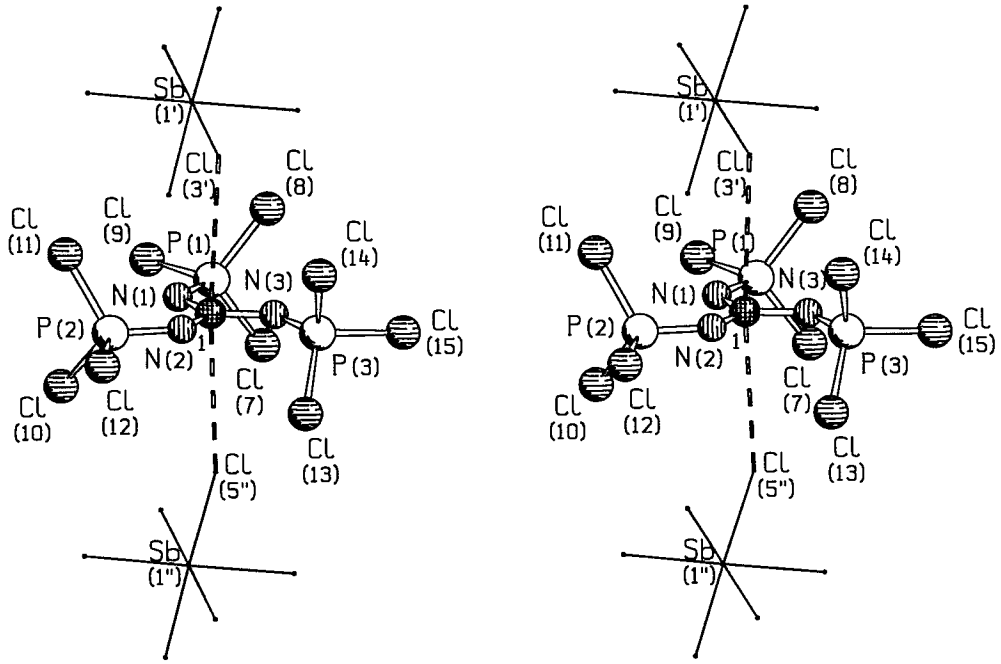


$Cl(1^{I})$	- C(1)	3.480	*diff* =	0.030	
$Cl(10^{II})$	- C(1)	3.918	*diff* =	0.468	weak

PCCLSB

tris(Trichlorophosphazeno)-carbenium hexachloro-antimony
C1 Cl9 N3 P3 1+,Cl6 Sb1 1-
U.Muller
Z.Anorg.Allg.Chem., 463, 117,1980

PCCLSB P-1 Z= 0 NATOMS= 23 DIFF AS=0 R-FACTOR= 0.027
ERROR Cl(11) y 0.3470, not 0.0347

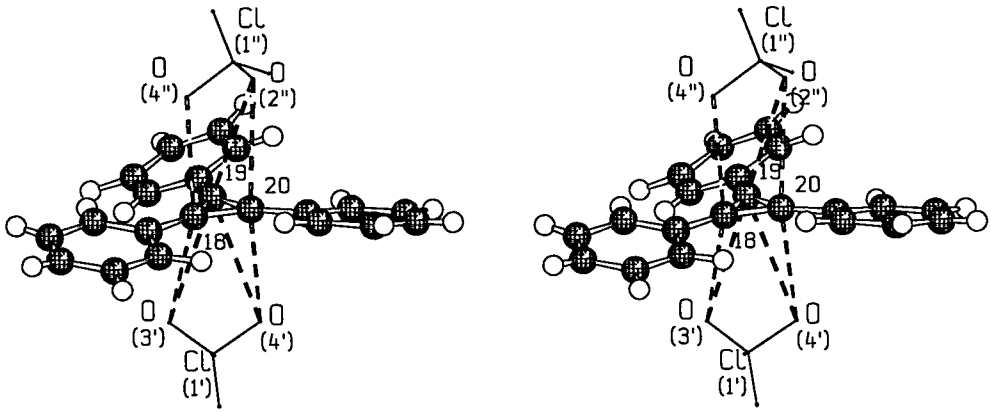


Cl(3^{I})	- C(1)	3.522	*diff* =	0.072
Cl(5^{II})	- C(1)	3.614	*diff* =	0.164

PHPRPC10

sym-Triphenylcyclopropenium perchlorate
C21 H15 1+,Cl1 O4 1-
M.Sundaralingam,L.H.Jensen
J.Am.Chem.Soc., 88, 198,1966

PHPRPC10 P21/c Z= 4 NATOMS= 41 DENS AS=0 R-FACTOR= 0.075
15 C-H BONDS: S.D.= 0.085; MEAN = 0.981; RANGE: 0.845 - 1.155



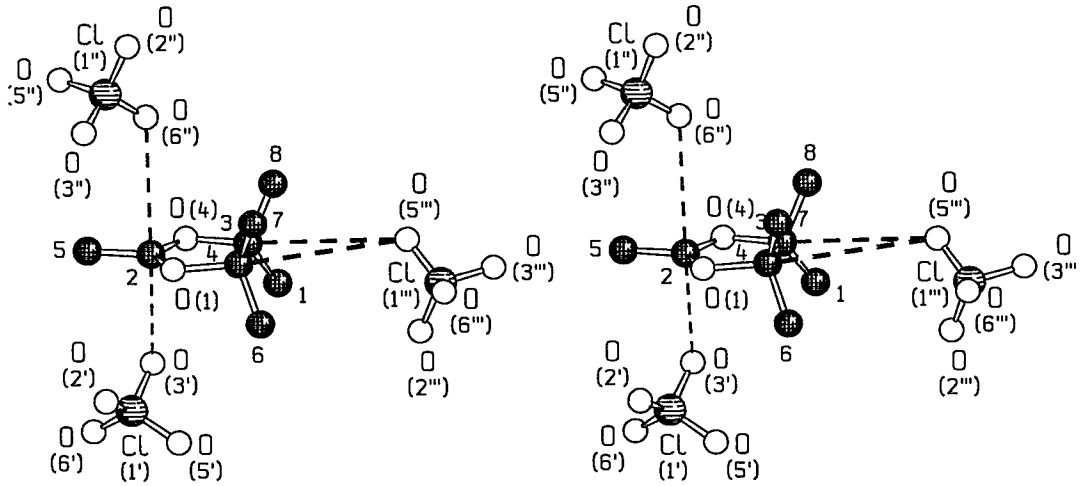
C(18)	- O(4^{II})	3.093	*diff* =	-0.127	strong
C(19)	- O(2^{II})	3.131	*diff* =	-0.089	
C(20)	- O(4^{I})	3.155	*diff* =	-0.065	
C(20)	- O(2^{II})	3.191	*diff* =	-0.029	
C(18)	- O(3^{I})	3.275	*diff* =	0.055	
C(19)	- O(3^{I})	3.287	*diff* =	0.067	
C(19)	- O(4^{I})	3.269	*diff* =	0.049	

PMDXLP

2,4,4,5,5-Pentamethyl-1,3-dioxolan-2-ylium perchlorate
C8 H15 O2 1+,Cl1 O4 1-
H.Paulsen,R.Dammeyer
Chem.Ber., 106, 2324,1973

PMDXLP Pbca Z= 8 NATOMS= 15 DIFF AS=3 R-FACTOR= 0.099

ERROR In Table 1, z(C6) should read 0.5385 rather than 0.3585; y(C6) should read 0.2178 rather than 0.2878



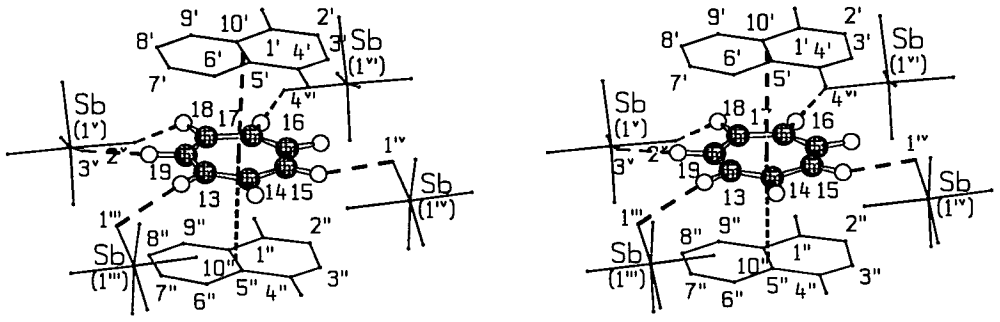
C(2)	- $O(6^{II})$	3.279	*diff* = 0.059	
C(2)	- $O(3^{I})$	3.022	*diff* = -0.198	strong
C(3)	- $O(5^{III})$	3.829	*diff* = 0.609	very weak
C(4)	- $O(5^{III})$	3.997	*diff* = 0.777	very weak

SASNOP

1,4-Dimethylnaphthlene tropylium hexafluoroantimonate
C12 H12,C7 H7 1+,F6 Sb1 1-
Y.Takahashi,S.Sankararaman,J.K.Kochi
J.Am.Chem.Soc., 111, 2954,1989

SASNOP P21 Z= 2 NATOMS= 26 DIFF AS=3 R-FACTOR= 0.027

H atoms and centers of the tropylium ring [Z(1)] and of the naphthalene ring systems [Z(2), top; Z(3), bottom] were added in the present paper.



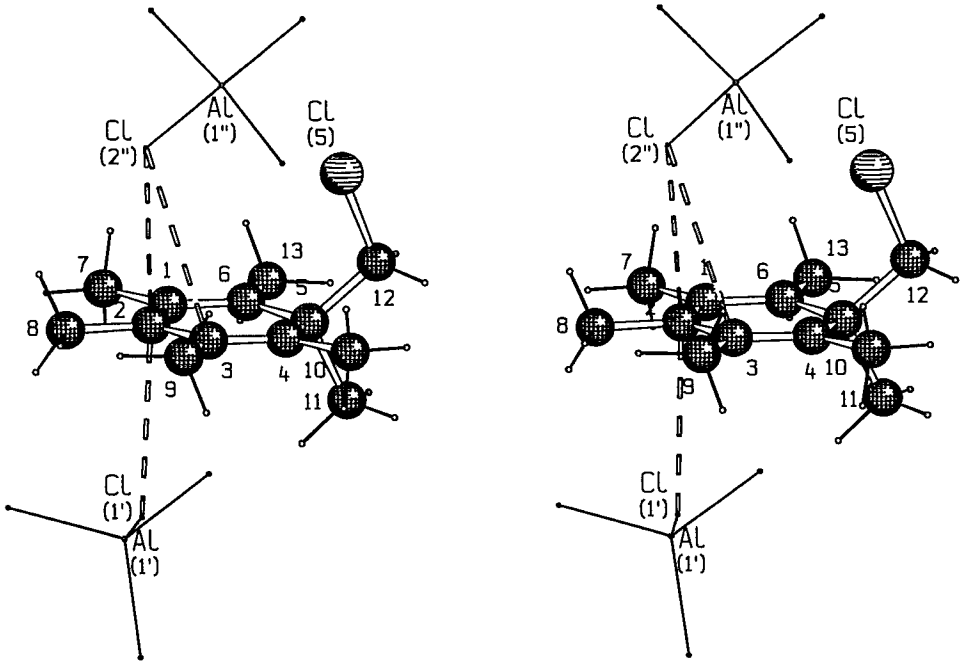
$F(1^{III})$	- H(13)	2.428	*diff* = -0.242	(H bond)
$F(1^{IV})$	- H(15)	2.288	*diff* = -0.382	(H bond)
$F(4^{VI})$	- H(17)	2.341	*diff* = -0.329	(H bond)
$F(2^{V})$	- H(18)	2.517	*diff* = -0.153	(H bond)

F(3^{V})	- H(19)	2.661	*diff* = -0.009 (H bond)
Z(1)	- Z(2)	3.390	
Z(1)	- Z(3)	3.384	

SAXCAV

1-Chloromethyl-1,2,3,4,5,6-hexamethylbenzenium tetrachloro-aluminium
C13 H20 Cl1 1+,Al1 Cl4 1-
M.J.Zaworotko,T.S.Cameron,A.Linden,K.C.Sturge
Acta Cryst.,C (Cr.Str.Comm.), 45, 996,1989

SAXCAV P21/n Z= 4 NATOMS= 39 DIFF AS=2 R-FACTOR= 0.056
20 C-H BONDS: S.D.= 0.001; MEAN = 1.080; RANGE: 1.079 - 1.081

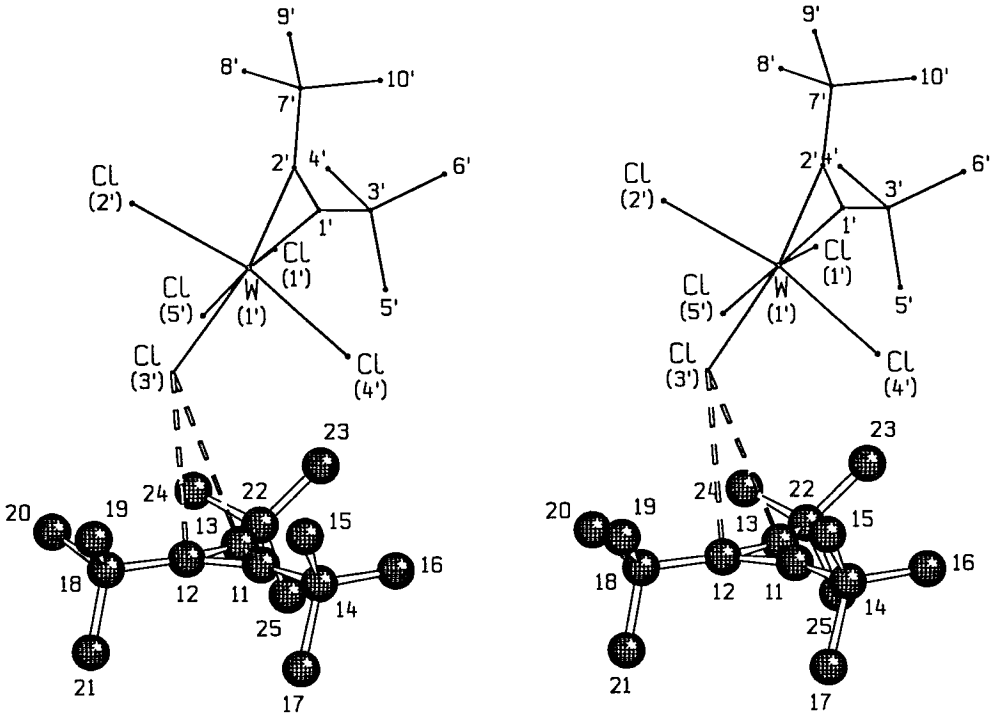


C(2)	- Cl(1^{I})	3.479	*diff* = 0.029
C(2)	- Cl(2^{II})	3.541	*diff* = 0.091
C(3)	- Cl(2^{II})	3.592	*diff* = 0.142

SIYDOT

Tri-t-butylcyclopropenium (η^2-di-t-butylethyne)-pentachloro-tungsten
C10 H18 Cl5 W1 1-,C15 H27 1+
F.Weller,I.Pauls,K.Dehnicke,G.Becker
Z.Naturforsch.,Teil B, 46, 519,1991

SIYDOT P21/c Z= 4 NATOMS= 31 DIFF AS=3 R-FACTOR= 0.052
REMARK CSD 54959 contains no further data



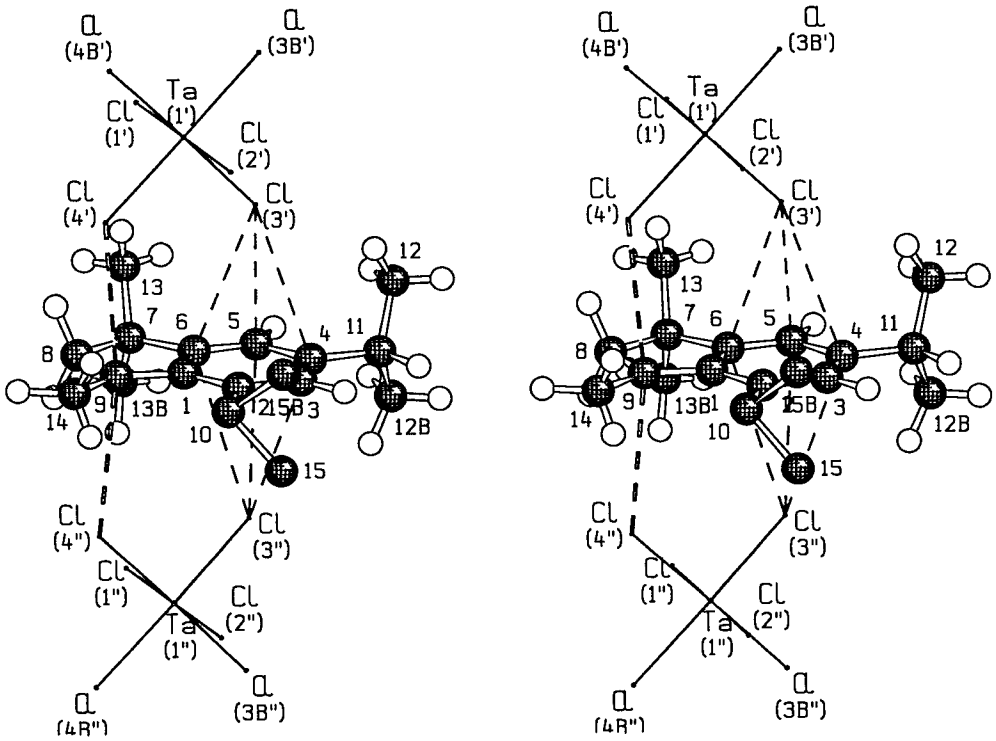
Cl(3^{I})	- C(12)	3.359	*diff* = -0.091
Cl(3^{I})	- C(13)	3.478	*diff* = 0.028

SODREI

5,7-Di-isopropyl-1,3,3-trimethylindan-1-yl hexachloro-tantalum
C18 H27 1+,Cl6 Ta1 1-
E.Solari,C.Floriani,A.Chiesi-Villa,C.Rizzoli
J.Chem.Soc.,Chem.Comm., , 841,1991

SODREI Cmca Z= 8 NATOMS= 45 DIFF AS=3 R-FACTOR= 0.040

DISORD Methyl carbon C11 of an isopropyl group is disordered over two positions with occupancies of 0.52 and 0.48 for A and B
20 C-H BONDS: S.D.= 0.095; MEAN = 1.033; RANGE: 0.863 - 1.182



Cl(4^{I})	- C(9)	3.461	*diff* =	0.011
C(9)	- Cl(4^{II})	3.461	*diff* =	0.011
Cl(3^{I})	- C(4)	3.635	*diff* =	0.185
C(4)	- Cl(3^{II})	3.634	*diff* =	0.184
Cl(3^{I})	- C(5)	3.602	*diff* =	0.152
C(5)	- Cl(3^{II})	3.602	*diff* =	0.152
Cl(3^{I})	- C(6)	3.672	*diff* =	0.222
C(6)	- Cl(3^{II})	3.672	*diff* =	0.222

TADXOL

bis(Triphenylmethylium) bis((μ$_2$-chloro)-tetrachloro-hafnium(iv))
2(C19 H15 1+),Cl10 Hf2 2-
F.Calderazzo,P.Pallavicini,G.Pampaloni,P.F.Zanazzi
J.Chem.Soc.,Dalton Trans., , 2743,1990

TADXOL P-1 Z= 2 NATOMS= 92 DIFF AS=2 R-FACTOR= 0.031
30 C-H BONDS: S.D.= 0.004; MEAN = 1.080; RANGE: 1.071 - 1.087