Supporting Information
(Revised Manuscript)

The Interactions Between Carbocations and Anions in Crystals

Thomas Laube

Loker Hydrocarbon Research Institute, University of Southern California, University Park, Los Angeles, CA 90089-1661, USA.

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REFCODE	(Suppl. Mat., page S*x*) *x*	C(*i*)$^{\delta+}$XYZ *i: X, Y [,Z]* (C(*i*)$^{\delta+}$ = [partially charged] cationic C, C2 = Csp^2, C3 = Csp^3)	C(*i*)$^{\delta+}$$_{sp}$···*Nu* *i: Nu [, Nu [...]]*	C(*i*)$^{\delta+}$$_{sp^2}$···*Nu* *i: Nu [, Nu]*	C(*i*)$^{\delta+}$$_{sp^3}$···*Nu* *i: Nu*	*Donor-H···Acc*	*X···Hal* (*X* = N,S,Se)	*Hal*^{1}···*Hal*^{2}	*Z'*
ACCLSB20	11	1: C3,=O	1: 4 × Cl						1
ACETFS	11	1: C3,O,O		1: O,O					1
ACIMDC	12	1: C3,N,N				4 × NH···Cl			1
ACNITR20	12	1: C3,Cl,N		1: Cl,Cl		2 × NH···Cl		Cl···Cl	1
ACTNBR	13	1: C3,Br,N		1: Br,Br		2 × NH···Br		Br···Br	1
ACTRPB	14	1: C2,C2,O 2-7:C2,C2,H		1-7: Br,(O)		6 × NH···Br			1
APCRBP10	14	1: C2,C2,C2		1: C2		3 × NH···O			1
BERTEX	15	7: N,N,S				NH···Cl NH···O			1
CADZUC	16	2: C2,C2,O 3-8: C2,C2,H		2-8: ((F)),O					½
CAFBAM	17	1: N,N,O 6: N,N,O		1: O 6: O					1
CAFBEQ	17	1,2,4,5: C2,C2,N 3,6: C2,C2,O		1-3,5: O 4: O					1
CANWET10	18	3,4: N,N,O		3,4: O					1
CAPRLC	18	1,21: C3,N,O		1,21: Cl		2 × NH···Cl 2 × OH···Cl			2
CBUALC	95	2,2B: C2,C3,C3 3: C2,C2,C3		2,2B: Cl^C,((Cl)) 3: Cl^C,(Cl)					½
CIRLIY	19	1: C3,Se,Se		1: C2			4 × Se···Cl		1
CIRLOE	20	1: C3,S,S		1: C2			4 × S···Cl		1
CLBRPZ	20	1: N,N,N		1: Br				2 × Br···Br	1

REFCODE	(Suppl. Mat., page S*x*) *x*	C(i)$^{\delta+}$*XYZ* ***i: X, Y [,Z]*** (C(i)$^{\delta+}$ = [partially charged] cationic C, C2 = Csp^2, C3 = Csp^3)	C(i)$^{\delta+}_{sp}$···*Nu* ***i: Nu [, Nu [...]]***	C(i)$^{\delta+}_{sp^2}$···*Nu* ***i: Nu [, Nu]***	C(i)$^{\delta+}_{sp^3}$···*Nu* ***i: Nu***	***Donor-H···Acc***	***X···Hal*** (*X* = N,S,Se)	***Hal*** ^{1}***···Hal*** ^{2}	***Z'***
COMBIP	21	2,6: C2,C3,C3 3-5: C2,C2,C3		3-6: Cl					1
COVSUB10	22	10,13: C2,C3,N 11: C2,C2,C3		10: O,((Br)) 13: O 11: O					1
CUGBAH	23	1,2,3,1A,2A, 3A: C2,C2,C2		3,1A,2A: Br					2
DATZIH	24	114: C3,C3,N 214: C3,C3,N		*a*					1
DEGLUW	24	1: Cl,N,N		1: Cl,O		2 × NH···Cl		Cl···Cl	
DEJKEI	25	2,2F: C2,C3,C3 3: C2,C2,C3		*a*					½
DEJKIM	25	2,4: C2,C3,C3 3: C2,C2,C3		*a*		OH···F			1
DIBCAS	26	1: F,S,S		1: F,F	2: F,F		4 × S···F		¼
DIFMEK	26	1: C2,C3,C3		1: (Cl),(Cl)	14,14A: Cl				½
DIJTIZ	27	1,2: C2,C2,C3 3: C2,C2,C2		1-3: C					1
DIJTOF	28	1-3: C2,C2,C3		2: F,F 1,3: F,F					½
DIVXEL	28	1-7: C2,C2,H		1-7: C2 or O					1
DMCPRP10	29	1-3: C2,C2,N 10-12: C2,C2,N		1-3: [Pt]^b 10-12: [Pt]^b					2
DOMFUG	30	2: C2,C3,O		2: Cl,(Cl)		OH···O			1
DONBAJ	30	1: C3,C3,O		1: F,F		OH···F			½

REFCODE	(Suppl. Mat., page S*x*) ***x***	C(i)$^{\delta+}$*XYZ* ***i: X, Y [,Z]*** (C(i)$^{\delta+}$ = [partially charged] cationic C, C2 = Csp^2, C3 = Csp^3)	C(i)$^{\delta+}$$_{sp}$···*Nu* ***i: Nu [, Nu [...]]***	C(i)$^{\delta+}$$_{sp^2}$···*Nu* ***i: Nu [, Nu]***	C(i)$^{\delta+}$$_{sp^3}$···*Nu* ***i: Nu***	***Donor-H···Acc***	***X···Hal*** (*X* = N,S,Se)	***Hal^1···Hal^2***	***Z'***
DONBEN	31	11: C2,C3,O 12: C2,C3,O		11: F 12: F,F		OH···F OH···F			2
DOPRIJ	32	1: C3,C3,C3		1: F					1
DOXYLP	32	1: C3,O,O		1: O,O	2: O 3: O	CH···O			1
DOYBIC	33	7,9: C2,C2,N 8: C2,C2,H				2 × NH···O			1
DOZSOA	34	1: C2,C3,O		1: Cl,C[c]					1
DPMBSB10	34	19: C2,C2,C2 36: C2,C2,C2		19: (Cl) 39: Cl					1
DTHTRO	35	1,4: C2,C2,S 7,9: C2,C2,C2 2,3,8: C2,C2,H		1-4,7-9: ((F))					1
DUVZAV	35	2: H,N,N		2: I		CH···I			1
ENANLC	37	1: C3,N,O		1: Cl		NH···Cl OH···Cl			1
ETOCGA	37	1: C3,=O	1: 5 × Cl, (Cl)			CH···Cl			1
FAFGUO	38	1-3: C2,C2,N		1,2: I					1
FEDZIX	38	21,61,22,62: C2,C3,N 41,42: C2,C2,N (31,51,32,52: C2,C2,H)				2 × CH···Br			2

REFCODE	(Suppl. Mat., page S*x*) ***x***	C(i)$^{\delta+}$*XYZ* ***i: X, Y [,Z]*** (C(i)$^{\delta+}$ = [partially charged] cationic C, C2 = Csp^2, C3 = Csp^3)	C(i)$^{\delta+}$$_{sp}$···*Nu* ***i: Nu [, Nu [...]]***	C(i)$^{\delta+}$$_{sp^2}$···*Nu* ***i: Nu [, Nu]***	C(i)$^{\delta+}$$_{sp^3}$···*Nu* ***i: Nu***	***Donor-H···Acc***	***X···Hal*** (*X* = N,S,Se)	***Hal^1···Hal^2***	***Z'***
FEDZOD	39	2,6: C2,C3,N 4: C2,C2,N (3,5: C2,C2,H)				2 × CH···O			1
FEDZUJ	39	2,6: C2,C3,N 4: C2,C2,N (3,5: C2,C2,H)			7: O	CH···O			1
FIBXAP	40	1: N,N,N 2: N,N,N				5 × NH···F 6 × NH···F			2
FITDIV	41	2: C3,C3,C3		2: F,(F)					1
FIZCAS10	41	11: N,N,N				6 × NH···O			1
FODZAZ	42	2: C3,C3,O		2: F,F		CH···F			1
FOGBIM	43	8: C3,N,O		8: I,I					1
FOSPOS01	44	1: C3,N,N		1: O,O		4 × NH···O			½
FUFRUT	44	1: Cl,N,N		1: Cl,Cl					1
FUFSAA	45	1: N,N,O		1: Cl,O					1
FUXCAC	46	10: N,N,O		10: O		2 × NH···O			1
GADMUT	47	3: C2,N,N				4 × NH···O			1
GEGGAA	47	1-7: C2,C2,H		1-7: O					1
GUHOXM01	48	3: N,N,N				6 × NH···O			1
HEBZCA	48	6,10: C2,C3,C3 7-9: C2,C2,C3		7,8: Cl,Cl					1
IBUSBC20	49	1: C3,=O	1: 2 × Cl 4 × Cl			CH···Cl			½
JAJRIV	50	1: C3,C3,N		1: Cl		2 × NH···Cl 4 × CH···Cl			1

REFCODE	(Suppl. Mat., page S*x*) ***x***	C(i)$^{\delta+}$*XYZ* ***i: X, Y [,Z]*** (C(i)$^{\delta+}$ = [partially charged] cationic C, C2 = Csp^2, C3 = Csp^3)	C(i)$^{\delta+}$$_{sp}$···*Nu* ***i: Nu [, Nu [...]]***	C(i)$^{\delta+}$$_{sp^2}$···*Nu* ***i: Nu [, Nu]***	C(i)$^{\delta+}$$_{sp^3}$···*Nu* ***i: Nu***	***Donor-H···Acc***	***X···Hal*** (*X* = N,S,Se)	***Hal*** ^{1}***···Hal*** ^{2}	***Z'***
JAKBAY	50	8: N,N,N		8: O,O					1
JALSOE	52	11: N,N,S		11: C,O		2 × NH···O 2 × NH···S			1
JECDEA	52	2,3,7: C2,C3,C3		2,7: C2^c, F 3: C2^c					1
JICPOA	53	1: C3,C3,O		1: F,F		OH···F			½
JICPUG	54	1: C3,C3,O		1: F,F		OH···F			1
JICRAO	54	1: C3,C3,O		1: Cl,Cl		OH···Cl			1
JOJXUB	55	6: N,O,O 1,5: C2,H,N		6: F 1,5: O		CH···F			1
JOPSEM	56	5: C3,O,O		5: Cl,Cl					1
JOPSOW	56	5: C3,O,O		5: Cl,Cl					1
JOPSUC	57	5: C3,O,O		5: Cl,(Cl)					1
JUKWAN	58	2: N,N,N				4 × NH···O			1
JUNVAP	58	1: Cl,Cl,N 2: Cl,Cl,N		1: Cl 2: Cl		4 × NH···Cl		2× Cl···Cl, 2× Cl···Cl	2
JUNVET	59	1: C2,N,O 10: C2,C2,N		1: F,F 10: Cl,Cl					1
JUXBEJ	60	1: N,N,S		1: O		4 × NH···O 1 × SH···O			1
JUYYUX	60	1: S,S,S		1: Cl,Cl					1
KAZDEU	61	1: C2,N,N		1: O					1
KECGOO	61	2: C3,N,N				2 × NH···Cl 1 × NH···O			1

REFCODE	(Suppl. Mat., page S*x*) *x*	C(i)$^{\delta+}$*XYZ* ***i: X, Y [,Z]*** (C(i)$^{\delta+}$ = [partially charged] cationic C, C2 = Csp^2, C3 = Csp^3)	C(i)$^{\delta+}$$_{sp}$···*Nu* ***i: Nu [, Nu [...]]***	C(i)$^{\delta+}$$_{sp^2}$···*Nu* ***i: Nu [, Nu]***	C(i)$^{\delta+}$$_{sp^3}$···*Nu* ***i: Nu***	***Donor-H···Acc***	***X···Hal*** (*X* = N,S,Se)	***Hal*** ^{1}***···Hal*** ^{2}	***Z'***
KESDER	62	3: C3,C3,N 17: C3,C3,N 31: C3,C3,N		3: O 17: O 31: F		CH···O,CH···F CH···O,CH···F CH···O			3
KIBPIU	63	9: C3,N,N		9: O		NH···O			1
KIBPOA	64	9: C3,N,N				2 × NH···Cl			1
KIBPUG	65	10: C3,N,N				2 × NH···Cl			1
KOHVOS	65	1: C2,C2,C2		1: Cl					1
KOWGOS	66	1,1C,1D: C2,C2,N		1,1C,1D: Cl,Cl					⅓
KOWGUY	66	1,1C,1D: C2,C2,N		1,1C,1D: Cl,Cl					⅓
KUBLUO	68	1: C2,C2,C2		1: O^c,O^c					1
LAFMEK	68	1: Br,Cl,N 2: Br,Cl,N		1: Cl 2: Cl		2 × NH···Cl 2 × NH···Cl		2× Br···Cl, 2× Cl···Cl	2
LALLOZ	69	1: C3,N,N		1: Cl,Cl		2 × NH···Cl			1
MACPRP10	70	1,2,2B: C2,C2,N		2,2B: O	3,3B: O				½
MAECBA	96	1,3: C2,C3,N 2: C2,C2,C3		3: O					1
MALLPC	70	9,11: C2,N,N 10: C2,C2,H		9,11: ((O))					1
MEGUAN	71	2: N,N,N		2: O,O		5 × NH···O			½
MOCFSB10	71	2: C3,=O	2: 4 × F			CH···F			½
MPOCSB	72	1: C2,=O	1: 2×Cl, 3×Cl,(Cl)						1
MTDXYL	73	1: C3,O,O		1: F,F	2:F, 3:F	CH···F			1
MTDXYP	73	8: C3,O,O		8: O,O	2,3: O,O				1

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MTMCBA	97	1: C2,C3,N 2: C2,C2,C3 3: C2,C3,C3		1: O,O					1
OXLCLI	74	1: C2,O,O		1: Cl,Cl	3,3B: ((I))[a]				½
PCBTEC10	75	1: C2,C2,C2		1: Cl,(Cl)					1
PCCLSB	75	1: N,N,N		1: Cl,Cl					1
PESGID	93	1: C3,C3,C3		1: F,F		9 × CH···F			1
PHPRPC10	76	18-20: C2,C2,C2		18: O,O, 19-20: O,O					1
PMDXLP	77	2: C3,O,O		2: O,O	3,4: ((O))[a]				1
PONHOP	93	2,3: C2,C3,C3 5: C3,C3,C3		2,3:C2[c],Cl 5:C2[c],((Cl))[a]				Cl···Cl	½
PONHUV	94	2,3: C2,C3,C3 5: C3,C3,C3		2,3: C2[c],F 5: C2[c],O[d]					1
SASNOP	77	13-19: C2,C2,H		13-19: C2,C2		CH···F			1
SAXCAV	78	4,6: C2,C3,C3 1-3: C2,C2,C3		2: Cl,Cl 3: Cl					1
SIYDOT	78	11-13: C2,C2,C3		12,13: Cl					1
SODREI	79	9: C2,C2,C3		9: Cl,Cl 4,5,6: Cl,Cl					½
SUNMOD	95	2: C2,C3,C3		2: F					1
TADXOL	80	1: C2,C2,C2 20: C2,C2,C2		1: Cl 20: (Cl)					2
TAFBOR	81	2: C3,N,O		2: O,(O)		NH···O,OH···O			1

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THIURN01	82	1: N,N,S		1: O,O		NH···O,SH···O			½
TIPMEP	83	5: C2,C2,C2		5: O,O (disordered anions with Cl1M, Cl1N)					⅙
TRAZSB	83	1: N,N,N		1: Cl			4 × N···Cl		1
VAPREJ	84	2: H,H,N		2: Cl,Cl	1,1A: Cl	6 × CH···Cl 2 × NH···Cl			¼
VAWXEW10	84	15,15A,15B: C2,C2,C3							⅙
VEKMON	85	6: C3,N,O 1,5: C2,H,N		1,5: O 6: O					1
VIGXUE	85	1: C2,C2,C2		1: (O)					1
VIGYAL	86	1: C2,C2,C2		1: ((O))	21: F				1
VIMPOW	86	1: H,N,N		1: Cl,(Cl)		CH···Cl			1
VIRDAB	87	1: C2,C2,C2		1: Cl,Cl					1
VIRDEF	88	1: C2,C2,C2		1: Br,(Br)					1
VOJGAC	89	2: C3,O,O		2: O,O		2 × OH···O			½
VOJGEG	89	2,4,6,8: C3,O,O		2: O, 6: O 4: O,F 8: F,F		6 × OH···O			2
WABZEE	90	7: N,O,O 1,5: C2,H,N		7: C 1,5: C					1
WABZEE01	91	7: N,O,O 1,5: C2,H,N		7: C 5: C					1

REFCODE	(Suppl. Mat., page S*x*) *x*	C(*i*)$^{\delta+}$*XYZ* ***i: X, Y [,Z]*** (C(*i*)$^{\delta+}$ = [partially charged] cationic C, C2 = Csp^2, C3 = Csp^3)	C(*i*)$^{\delta+}$$_{sp}$···*Nu* ***i: Nu [, Nu [...]]***	C(*i*)$^{\delta+}$$_{sp^2}$···*Nu* ***i: Nu [, Nu]***	C(*i*)$^{\delta+}$$_{sp^3}$···*Nu* ***i: Nu***	***Donor-H···Acc***	***X···Hal*** (*X* = N,S,Se)	***Hal*^{1}···*Hal*^{2}**	***Z'***
WAZYOL	91	17,21: C2,C3,N 19: C2,C2,N 18,20: C2,C2,H				2 × CH···O 3 × NH···O			1
YAMWOY	92	1: C2,C2,Cl		1: F,F 3: F				Cl···Cl[c] Cl···F	1

In C(*i*), *i* is the C atom number from the CSD. The classification of the $atom_1 \cdots atom_2$ interaction, indicated by a marking of the element symbol(s) as given below, is based on the variable *diff*, which is defined as follows:

$$diff = distance(atom_1 \cdots atom_2) - radius_{\text{van der Waals}}(atom_1) - radius_{\text{van der Waals}}(atom_2)$$

The van der Waals radii used here are (in Å): C = 1.70, F = 1.47, Cl = 1.75, Br = 1.85, I = 1.98, O = 1.52, N = 1.55, S = 1.80, Se = 1.90, H = 1.20.

Classification:

extremely strong:	*diff* < -0.5 Å	(double underline)
very strong:	-0.5 Å < *diff* < -0.3 Å	(double underline)
strong:	-0.3 Å < *diff* < -0.1 Å	(single underline)
normal:	-0.1 Å < *diff* < 0.3 Å	(no marking)
weak:	0.3 Å < *diff* < 0.5 Å	(single parentheses)
very weak:	0.5 Å < *diff*	(double parentheses).

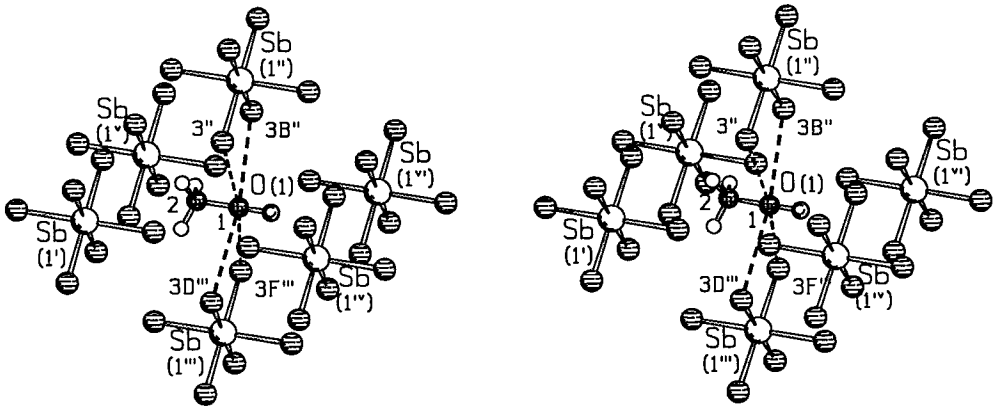
[a] Sterically hindered. [b] Type of the interaction not known; the C_3 ring could also act as e-donor. [c] Intramolecular. [d] Nearly weak (*diff* = 0.28 Å).

ACCLSB20

Methyl-oxocarbonium hexachloroantimonate
C2 H3 O1 1+,Cl6 Sb1 1-
J.-M.Le Carpentier,R.Weiss
Acta Crystallogr.,Sect.B, 28, 1421,1972

ACCLSB20 Imm2 Z= 2 NATOMS= 10 DIFF AS=0 R-FACTOR= 0.029

H atoms were added in the present work

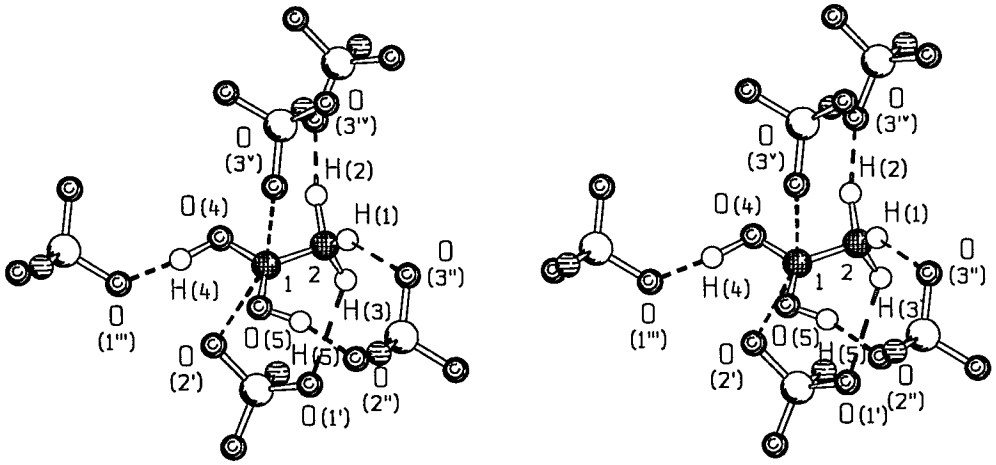


C(1)	- Cl(3^{II})	3.350	*diff* = -0.100	strong
C(1)	- Cl($3B^{II}$)	3.350	*diff* = -0.100	strong
C(1)	- Cl($3D^{III}$)	3.350	*diff* = -0.100	strong
C(1)	- Cl($3F^{III}$)	3.350	*diff* = -0.100	strong

ACETFS

Acetate acidium fluorosulfate
at -57deg.C
C2 H5 O2 1+,F1 O3 S1 1-
A.Kvick,P.-G.Jonsson,I.Olovsson
Inorg.Chem., 8, 2775,1969

ACETFS P21/c Z= 4 NATOMS= 14 PHOT AS=2 R-FACTOR= 0.090
3 C-H BONDS: S.D.= 0.100; MEAN = 1.093; RANGE: 0.981 - 1.224



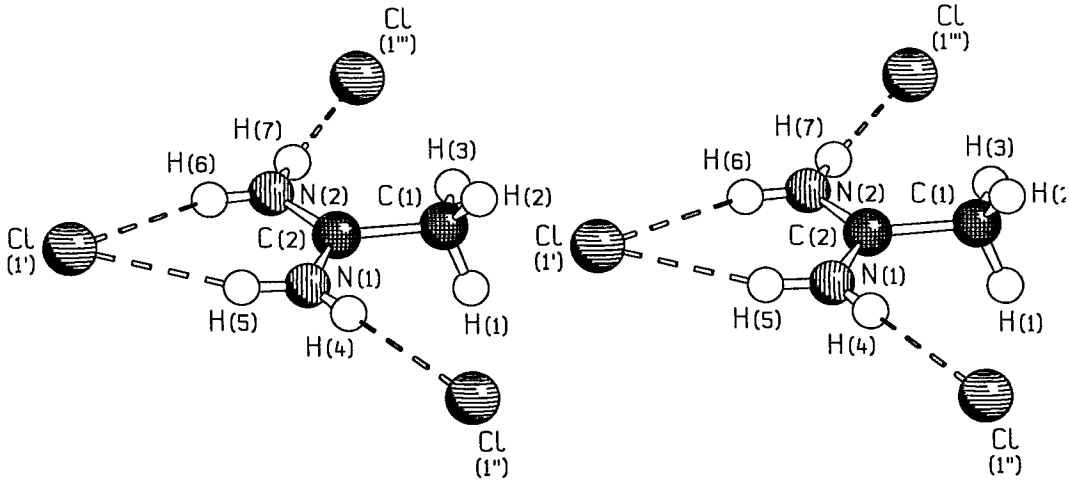
H(4)	- O(1^{III})	1.507	*diff* = -1.213	(H bond)
C(1)	- O(2^{I})	3.149	*diff* = -0.071	
C(1)	- O(3^{V})	2.911	*diff* = -0.309	**very strong**
H(1)	- O(3^{II})	2.591	*diff* = -0.129	(H bond)

H(2)	- $O(3^{IV})$	2.346	*diff* = -0.374 (H bond)
H(5)	- $O(2^{II})$	1.582	*diff* = -1.138 (H bond)
H(3)	- $O(1^{I})$	2.649	*diff* = -0.071 (H bond)

ACIMDC

Acetamidinium chloride
C2 H7 N2 1+,Cl1 1-
J.R.Cannon,A.H.White,A.C.Willis
J.Chem.Soc.,Perkin Trans.2, , 271,1976

ACIMDC C2/c Z= 8 NATOMS= 12 DIFF AS=1 R-FACTOR= 0.037
3 C-H BONDS: S.D.= 0.037; MEAN = 0.949; RANGE: 0.904 - 0.994

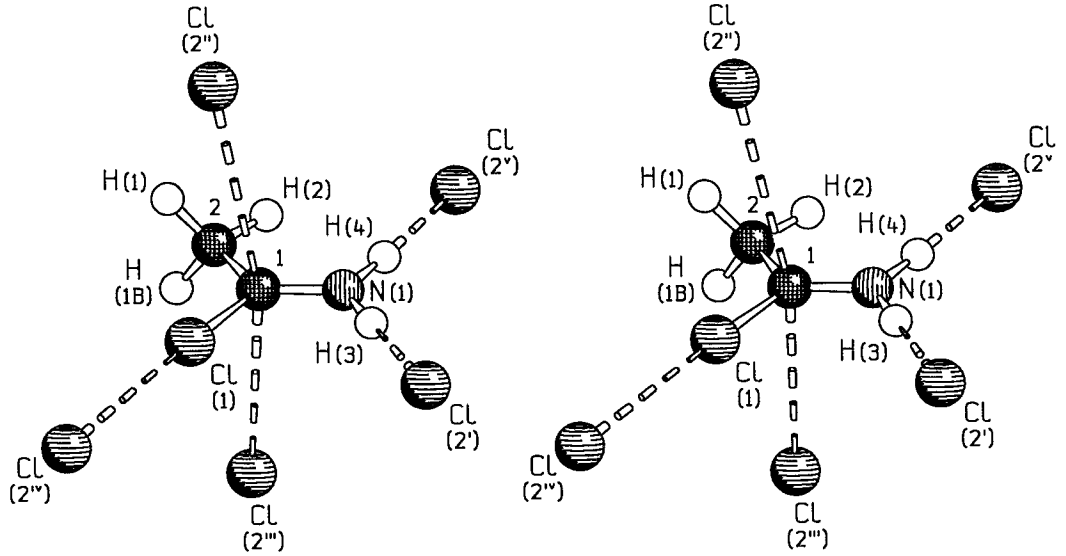


H(4)	- $Cl(1^{II})$	2.434	*diff* = -0.516 (H bond)
H(5)	- $Cl(1^{I})$	2.376	*diff* = -0.574 (H bond)
H(6)	- $Cl(1^{I})$	2.461	*diff* = -0.489 (H bond)
H(7)	- $Cl(1^{III})$	2.329	*diff* = -0.621 (H bond)

ACNITR20

Chloroacetiminium chloride
Acetonitrile dihydrochloride
at -5 deg.C, neutron study
C2 H5 Cl1 N1 1+,Cl1 1-
J.M.Williams,S.W.Peterson,G.M.Brown
Inorg.Chem., 7, 2577,1968

ACNITR20 Pnma Z= 4 NATOMS= 10 DIFF AS=2 R-FACTOR= 0.085
3 C-H BONDS: S.D.= 0.021; MEAN = 1.034; RANGE: 1.019 - 1.063



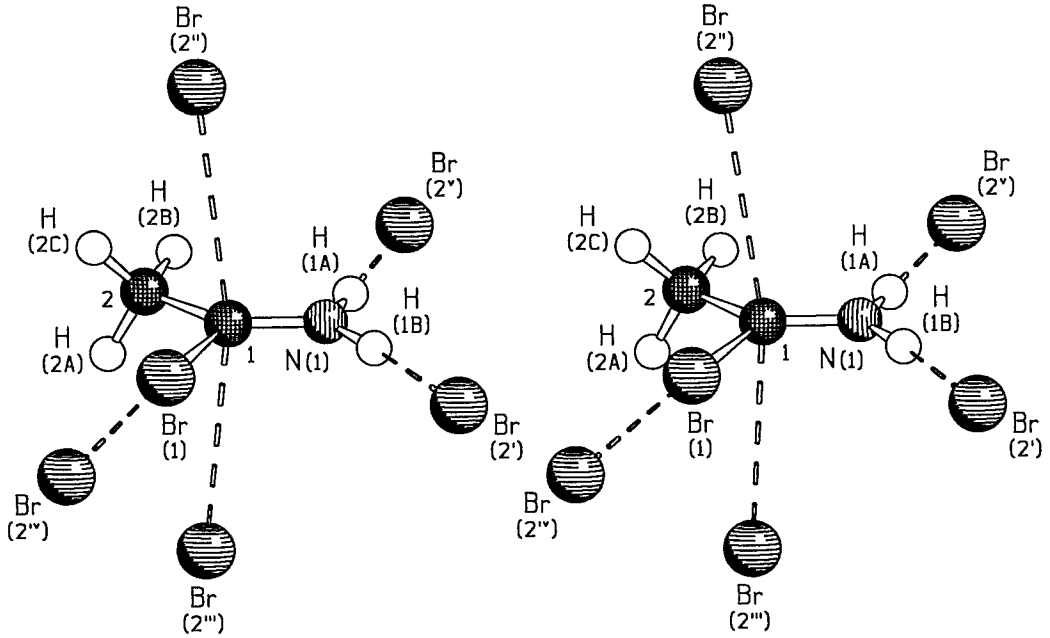
Cl(2^{I})	- H(3)	2.011	*diff* = -0.939	(H bond)
H(4)	- Cl(2^{V})	2.035	*diff* = -0.915	(H bond)
C(1)	- Cl(2^{II})	3.498	*diff* = 0.048	
C(1)	- Cl(2^{III})	3.498	*diff* = 0.048	
Cl(1)	- Cl(2^{IV})	3.329	*diff* = -0.171	strong

ACTNBR

Acetonitrile dihydrobromide
C2 H5 Br1 N1 1+,Br1 1-
B.Matkovic,S.W.Peterson,J.M.Williams
Croat.Chem.Acta, 39, 139,1967

ACTNBR Pnma Z= 4 NATOMS= 5 DIFF AS=0 R-FACTOR= 0.147

H atoms were added in the present work



Br(2^{I})	- H(1B)	2.178	*diff* = -0.872	(H bond)
Br(2^{V})	- H(1A)	2.312	*diff* = -0.738	(H bond)

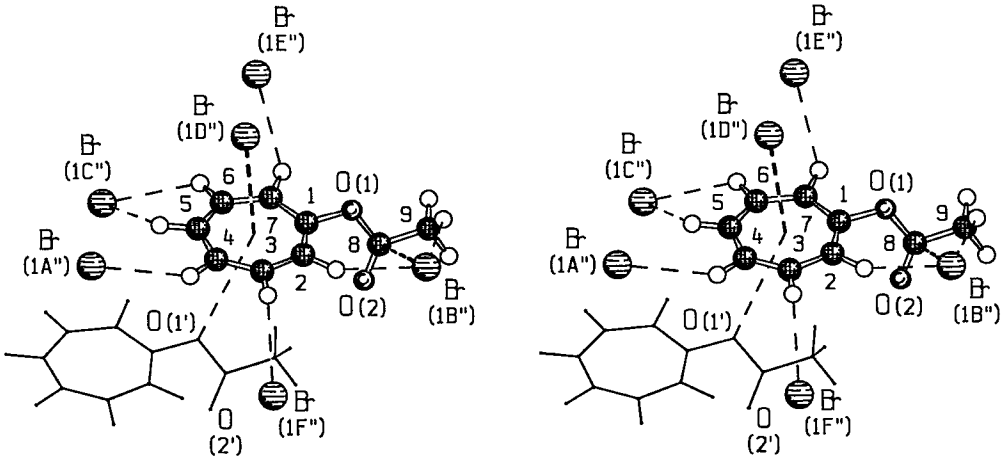
C(1)	- Br(2^{II})	3.643	*diff* = 0.093	
C(1)	- Br(2^{III})	3.643	*diff* = 0.093	
Br(1)	- Br(2^{IV})	3.404	*diff* = -0.296	strong

ACTRPB

Acetoxytropylium bromide
C9 H9 O2 1+,Br1 1-
P.Engel,U.M.Keller,P.Bigler,M.Neuenschwander
Helv.Chim.Acta, 59, 2344,1976

ACTRPB P21/c Z= 4 NATOMS= 12 DIFF AS=4 R-FACTOR= 0.150

Z(1) is the center of the seven-membered ring.
H atoms were added in the present work.



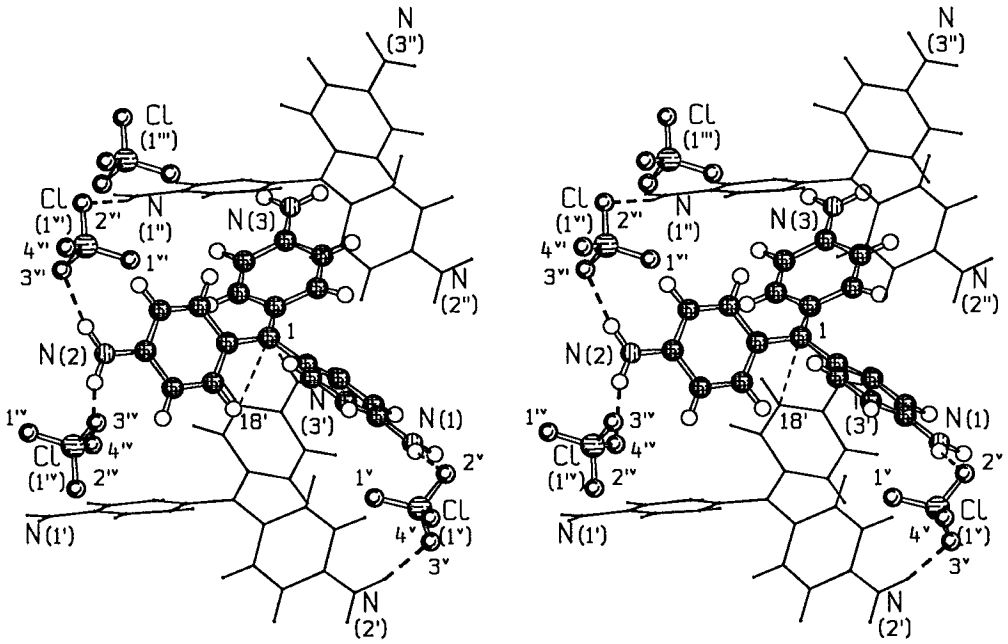
C(8)	- Br(1B^{II})	3.743	*diff* = 0.193
Br(1D^{II})	- Z(1)	3.779	(Z is a center of several atoms)
O(1^{I})	- Z(1)	3.648	(Z is a center of several atoms)
H(2)	- Br(1B^{II})	2.773	*diff* = -0.277 (H bond)
H(3)	- Br(1F^{II})	2.921	*diff* = -0.129 (H bond)
H(4)	- Br(1A^{II})	2.859	*diff* = -0.191 (H bond)
H(5)	- Br(1C^{II})	3.015	*diff* = -0.035 (H bond)
H(6)	- Br(1C^{II})	2.938	*diff* = -0.112 (H bond)
H(7)	- Br(1E^{II})	2.923	*diff* = -0.127 (H bond)
H(9B)	- Br(1B^{II})	3.047	*diff* = -0.003 (H bond)

APCRBP10

Tri-(p-aminophenyl)carbonium perchlorate
Pararosaniline perchlorate
C19 H18 N3 1+,Cl1 O4 1-
L.L.Koh,K.Eriks
Acta Crystallogr.,Sect.B, 27, 1405,1971

APCRBP10 P21/c Z= 4 NATOMS= 45 PHOT AS=0 R-FACTOR= 0.097
12 C-H BONDS: S.D.= 0.032; MEAN = 1.021; RANGE: 0.964 - 1.076

H atoms at C(6) and at all N atoms were newly computed in the present paper.



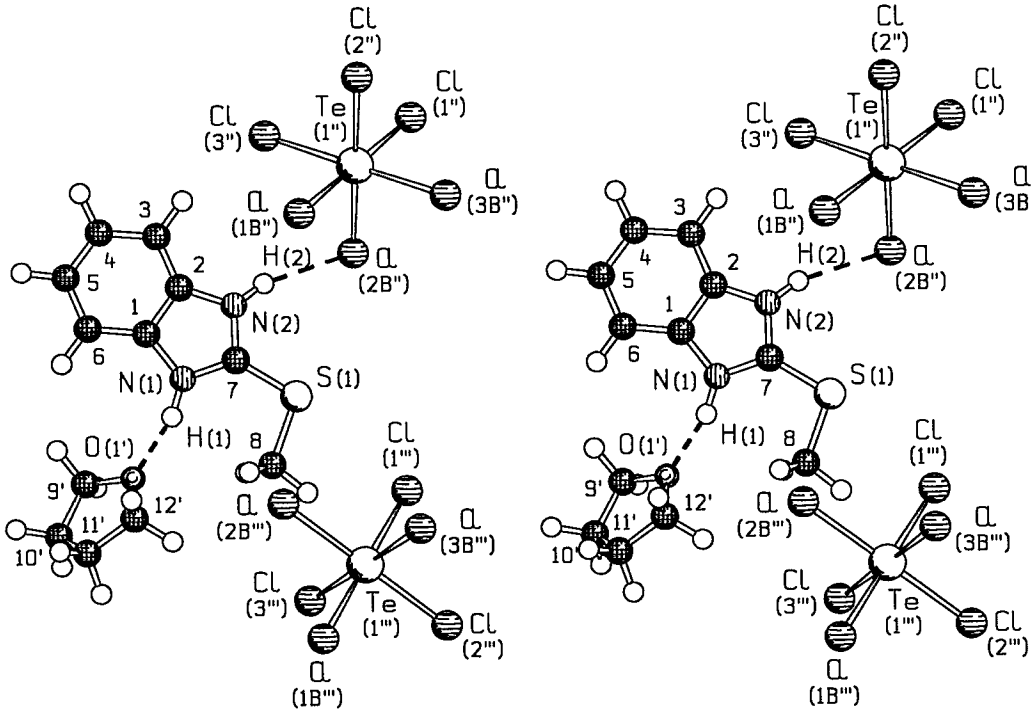
H(1A)	- O(2^{V})	2.038	*diff* = -0.682 (H bond)
H(2A)	- O(3^{VI})	2.083	*diff* = -0.637 (H bond)
H(2B)	- O(4^{IV})	2.079	*diff* = -0.641 (H bond)
H($2A^{I}$)	- O(3^{V})	2.082	*diff* = -0.638 (H bond)
H($1A^{II}$)	- O(2^{VI})	2.038	*diff* = -0.682 (H bond)
C(1)	- C(18^{I})	3.682	*diff* = 0.282

BERTEX

bis(2-Methylmercapto-benzimidazolium) hexachloro-tellurium(iv) tetrahydrofuran solvate
2(C8 H9 N2 S1 1+),Cl6 Te1 2-,2(C4 H8 O1)
W.Hinrichs,D.Mandak,G.Klar
Cryst.Struct.Commun., 11, 309,1982

BERTEX P21/n Z= 2 NATOMS= 25 DIFF AS=3 R-FACTOR= 0.049

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

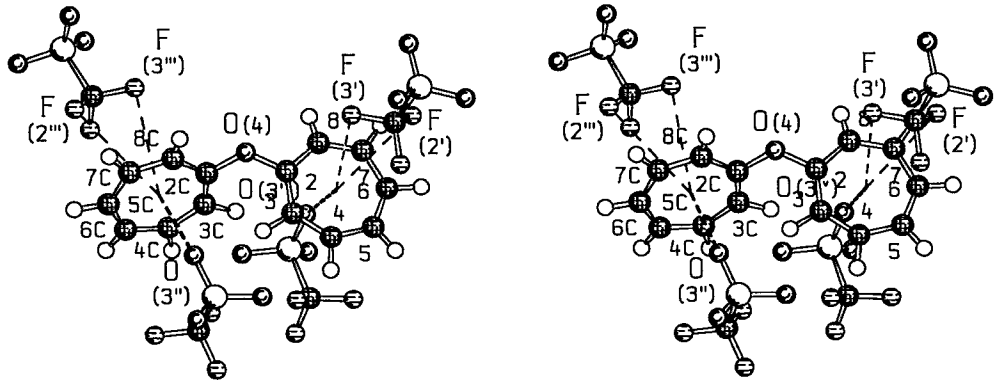


H(1)	- O(1^{I})	1.792	*diff* = -0.928 (H bond)
H(2)	- Cl($2B^{II}$)	2.387	*diff* = -0.563 (H bond)

CADZUC

Ditropenyliumyl-ether bis(trifluoromethanesulfonate)
at -55 dec.C
C14 H12 O1 2+,2(C1 F3 O3 S1 1-)
R.F.Childs,R.Faggiani,C.J.L.Lock,C.V.Rogerson
J.Org.Chem., 48, 3043,1983

CADZUC Pcnb Z= 4 NATOMS= 35 DIFF AS=2 R-FACTOR= 0.042
ERROR Position labelled L1 in atom table should be labelled O1
12 C-H BONDS: S.D.= 0.075; MEAN = 1.039; RANGE: 0.908 - 1.125

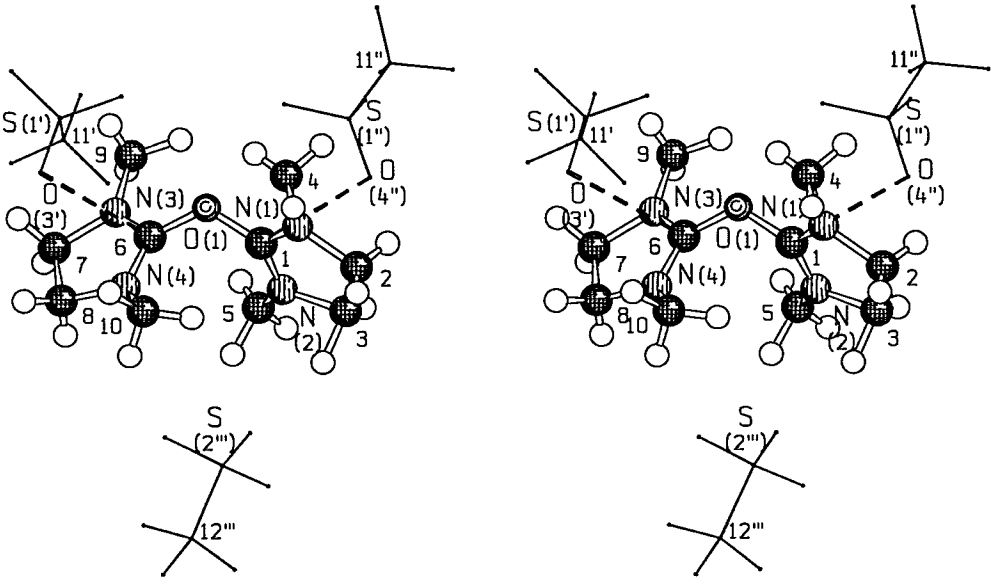


O(3^{II})	- Z(2)	3.052	(Z is a center of several atoms)
O(3^{IV})	- Z(1)	3.052	(Z is a center of several atoms)
F(2^{I})	- Z(1)	3.730	(Z is a center of several atoms)
F(3^{I})	- Z(1)	3.740	(Z is a center of several atoms)
F(2^{III})	- Z(2)	3.730	(Z is a center of several atoms)
F(3^{III})	- Z(2)	3.740	(Z is a center of several atoms)

CAFBAM

bis(1,3-Dimethyl-2-imidazoliniumyl)-ether bis(trifluoromethanesulfonate)
C10 H20 N4 O1 2+,2(C1 F3 O3 S1 1-)
G.Maas,P.J.Stang
J.Org.Chem., 48, 3038,1983

CAFBAM P21/c Z= 4 NATOMS= 51 DIFF AS=3 R-FACTOR= 0.069
20 C-H BONDS: S.D.= 0.123; MEAN = 0.967; RANGE: 0.737 - 1.189



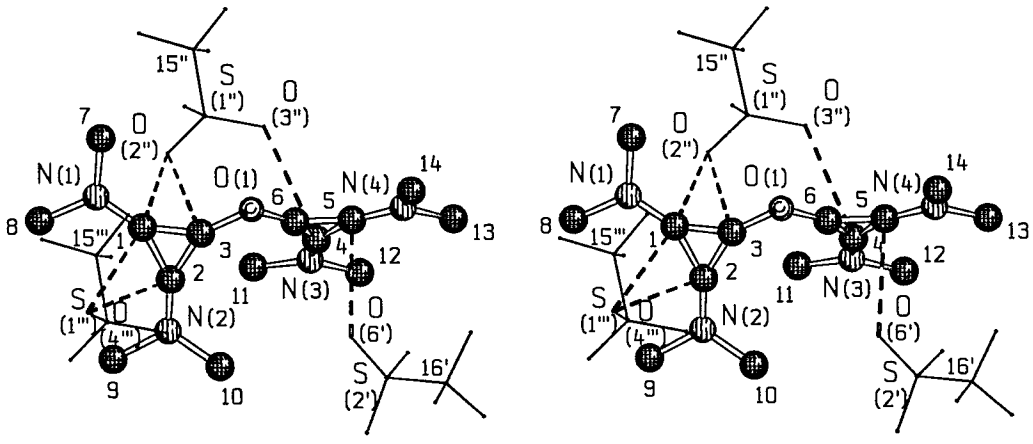
C(1) - O(4^{II}) 3.182 | *diff* = -0.038
C(6) - O(3^{I}) 3.116 | *diff* = -0.104 strong

CAFBEQ

bis(1,2-bis(Dimethylamino)-3-cyclopropenyliumyl)-ether
bis(trifluoromethanesulfonate)
C14 H24 N4 O1 2+,2(C1 F3 O3 S1 1-)
G.Maas,P.J.Stang
J.Org.Chem., 48, 3038,1983

CAFBEQ P-1 Z= 2 NATOMS= 35 DIFF AS=3 R-FACTOR= 0.087

DISORD Fluorines and oxygens in one anion are disordered; positions of 0.88 occupancy are retained

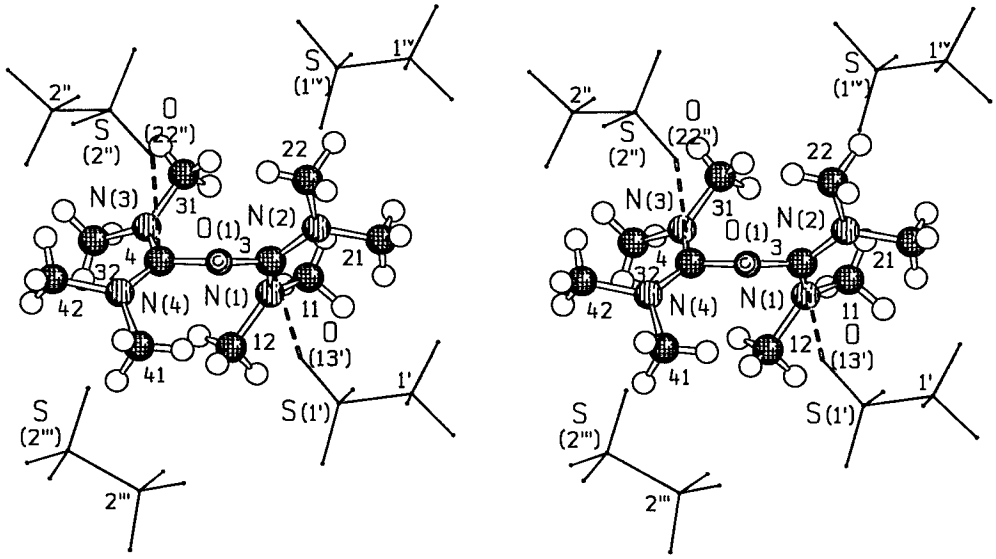


C(1)	- O(2^{II})	2.934	*diff* = -0.286	strong
C(1)	- O(4^{III})	3.059	*diff* = -0.161	strong
C(2)	- O(4^{III})	3.074	*diff* = -0.146	strong
C(3)	- O(2^{II})	3.093	*diff* = -0.127	strong
C(4)	- O(3^{II})	3.122	*diff* = -0.098	
C(5)	- O(6^{I})	3.111	*diff* = -0.109	strong

CANWET10

bis(bis(Dimethylamino)methyl)-ether bis(trifluoromethanesulfonate) at -135 deg.C
C10 H24 N4 O1 2+,2(C1 F3 O3 S1 1-)
T.Gramstad,S.Husebye,K.Maartmann-Moe,J.Saebo
Acta Chem.Scand.Ser.B, 39, 35,1985

CANWET10 P21/n Z= 4 NATOMS= 55 DIFF AS=2 R-FACTOR= 0.052
REMARK dx reported as 1.53, we calculate 1.56
24 C-H BONDS: S.D.= 0.059; MEAN = 0.947; RANGE: 0.818 - 1.050

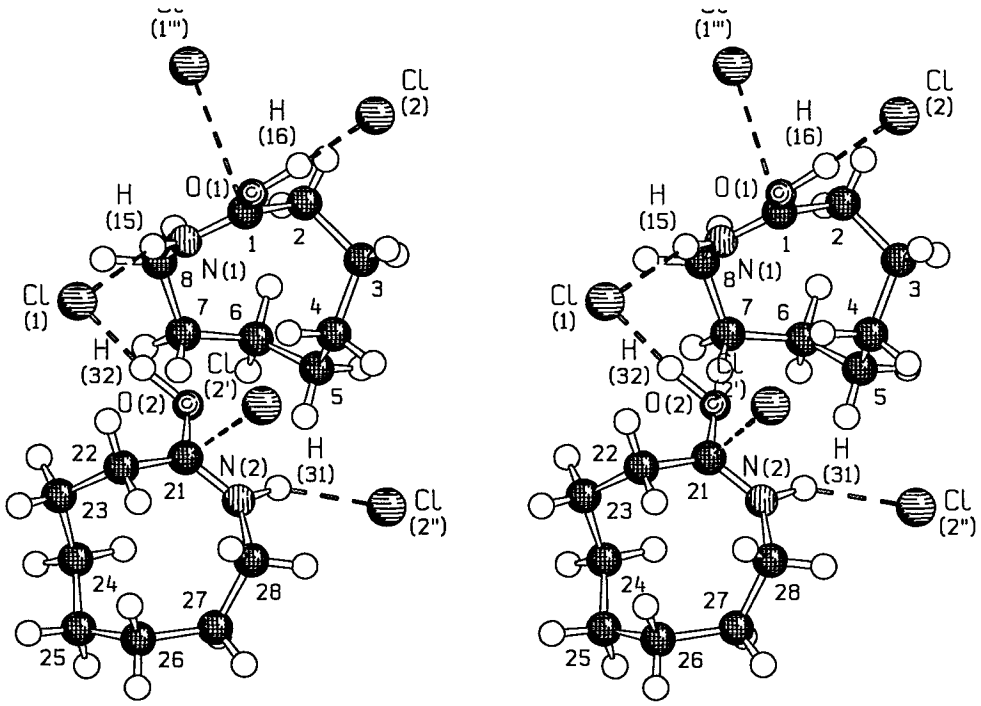


C(3)	- O(13^{I})	3.078	*diff* = -0.142	strong
C(4)	- O(22^{II})	2.967	*diff* = -0.253	strong

CAPRLC

Caprylolactam hydrochloride
C8 H16 N1 O1 1+,Cl1 1-
F.K.Winkler,J.D.Dunitz
Acta Crystallogr.,Sect.B, 31, 278,1975

CAPRLC P21/c Z= 8 NATOMS= 54 DIFF AS=1 R-FACTOR= 0.056
28 C-H BONDS: S.D.= 0.046; MEAN = 1.016; RANGE: 0.942 - 1.135

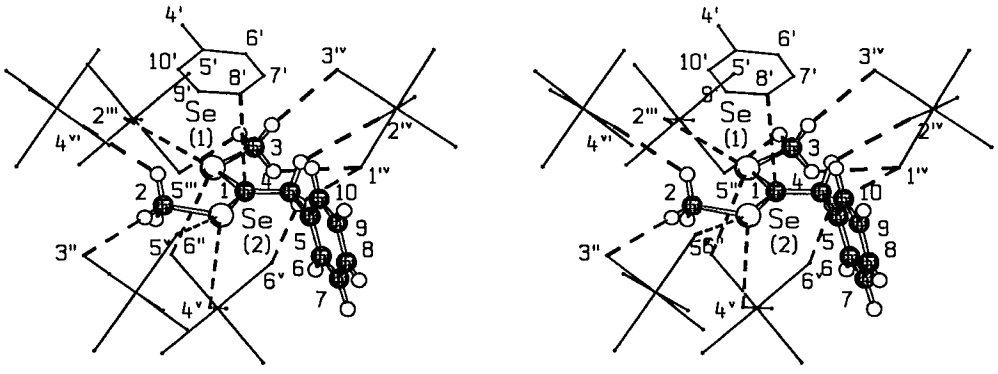


Cl(1)	- H(15)	2.233	*diff* = -0.717	(H bond)
H(16)	- Cl(2)	1.804	*diff* = -1.146	(H bond)
Cl(1)	- H(32)	1.771	*diff* = -1.179	(H bond)
C(1)	- Cl(1^{III})	3.562	*diff* = 0.112	
Cl(2^{I})	- C(21)	3.445	*diff* = -0.005	
H(31)	- Cl(2^{II})	2.218	*diff* = -0.732	(H bond)

CIRLIY

bis(Methylseleno)benzylcarbenium hexachloro-antimonate
at 173 deg.K
C10 H13 Se2 1+,C16 Sb1 1-
L.Hevesi,S.Desauvage,B.Georges,G.Evrard,P.Blanpain,A.Michel,S.Harkema,G.J.van Hummel
J.Am.Chem.Soc., 106, 3784,1984

CIRLIY Pbca Z= 8 NATOMS= 19 DIFF AS=3 R-FACTOR= 0.060



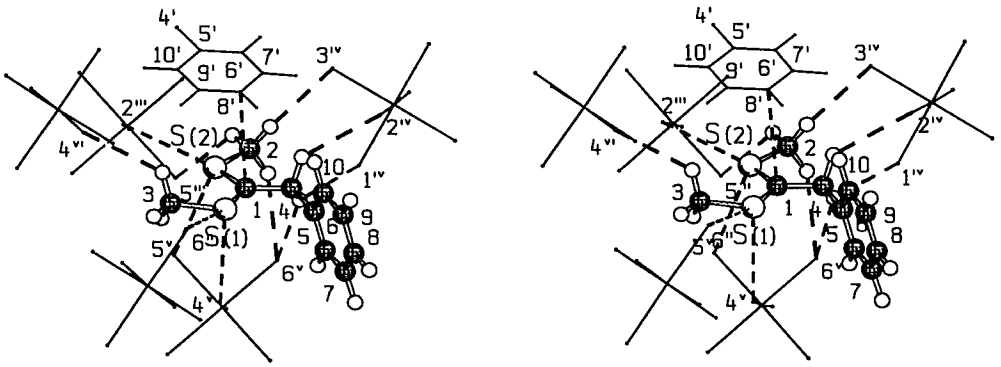
Cl(3^{II})	- H(2A)	2.985	*diff* = 0.035	(H bond)
H(2C)	- Cl(4^{VI})	2.923	*diff* = -0.027	(H bond)
H(3A)	- Cl(5^{III})	2.836	*diff* = -0.114	(H bond)
H(3B)	- Cl(1^{IV})	2.881	*diff* = -0.069	(H bond)
H(3C)	- Cl(3^{IV})	2.884	*diff* = -0.066	(H bond)
H(4A)	- Cl(2^{IV})	2.964	*diff* = 0.014	(H bond)

H(4B)	- $Cl(6^{V})$	2.740	*diff* = -0.210	(H bond)
H(4B)	- $Cl(1^{IV})$	2.970	*diff* = 0.020	(H bond)
Se(1)	- $Cl(5^{V})$	3.757	*diff* = 0.107	
Se(1)	- $Cl(2^{III})$	3.606	*diff* = -0.044	
$Cl(6^{II})$	- Se(2)	3.724	*diff* = 0.074	
Se(2)	- $Cl(4^{V})$	3.782	*diff* = 0.132	
C(1)	- $C(8^{I})$	3.578	*diff* = 0.178	

CIRLOE

bis(Methylthio)benzylcarbenium hexachloro-antimonate
at 163 deg.K
C10 H13 S2 1+,Cl6 Sb1 1-
L.Hevesi,S.Desauvage,B.Georges,G.Evrard,P.Blanpain,A.Michel,S.Harkema,G.J.van Hummel
J.Am.Chem.Soc., 106, 3784,1984

CIRLOE Pbca Z= 8 NATOMS= 32 DIFF AS=3 R-FACTOR= 0.050
13 C-H BONDS: S.D.= 0.005; MEAN = 1.088; RANGE: 1.077 - 1.096



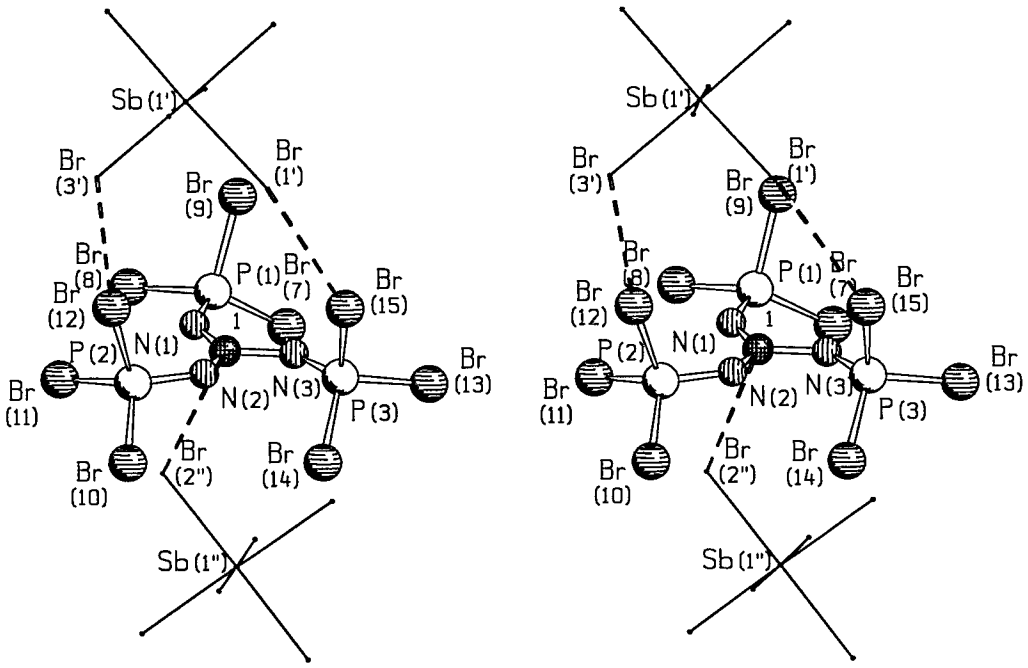
C(1)	- $C(8^{I})$	3.520	*diff* = 0.120	
H(3)	- $Cl(4^{VI})$	2.896	*diff* = -0.054	(H bond)
H(4)	- $Cl(1^{IV})$	2.901	*diff* = -0.049	(H bond)
H(4)	- $Cl(6^{V})$	2.781	*diff* = -0.169	(H bond)
H(5)	- $Cl(2^{IV})$	2.930	*diff* = -0.020	(H bond)
H(11)	- $Cl(5^{III})$	2.854	*diff* = -0.096	(H bond)
H(12)	- $Cl(6^{V})$	2.932	*diff* = -0.018	(H bond)
H(13)	- $Cl(3^{IV})$	2.890	*diff* = -0.060	(H bond)
S(1)	- $Cl(6^{II})$	3.619	*diff* = 0.069	
S(1)	- $Cl(4^{V})$	3.678	*diff* = 0.128	
S(2)	- $Cl(2^{III})$	3.593	*diff* = 0.043	
S(2)	- $Cl(5^{V})$	3.695	*diff* = 0.145	

CLBRPZ

tris(Chlorobromophosphazeno)-carbenium hexabromo-antimony
C1 Br9 N3 P3 1+,Br6 Sb1 1-
U.Muller,F.Schmock
Z.Anorg.Allg.Chem., 468, 165,1980

CLBRPZ Pbca Z= 8 NATOMS= 23 DIFF AS=0 R-FACTOR= 0.052

DISORD The halogen atoms are statistically disordered such that each site contains 0.78 Br and 0.22 Cl

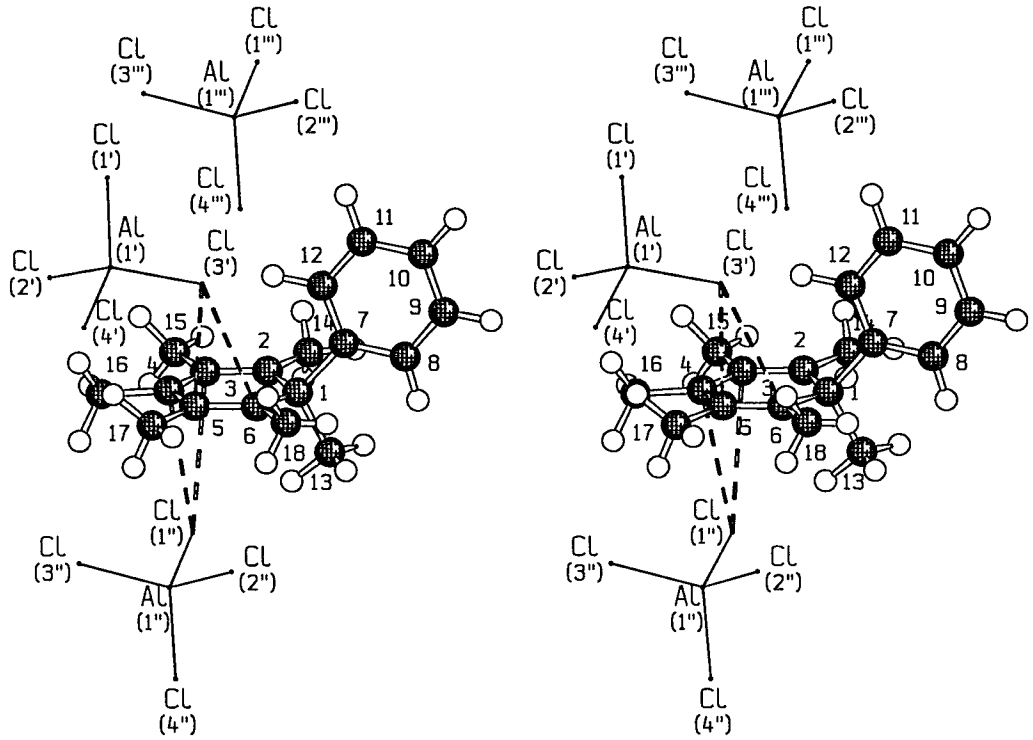


C(1)	- Br(2^{II})	3.805	*diff* = 0.255	
Br(12)	- Br(3^{I})	3.550	*diff* = -0.150	strong
Br(15)	- Br(1^{I})	3.570	*diff* = -0.130	strong

COMBIP

1-Phenyl-1,2,3,4,5,6-hexamethyl-benzenium tetrachloro-aluminium
at -110 deg.C
C18 H23 1+,Al1 Cl4 1-
G.I.Borodkin,Sh.M.Nagi,I.Yu.Bagryanskaya,Yu.V.Gatilov
Zh.Strukt.Khim., 25, 114-3,1984

COMBIP Pbca Z= 8 NATOMS= 46 DIFF AS=3 R-FACTOR= 0.088
23 C-H BONDS: S.D.= 0.097; MEAN = 1.027; RANGE: 0.811 - 1.212



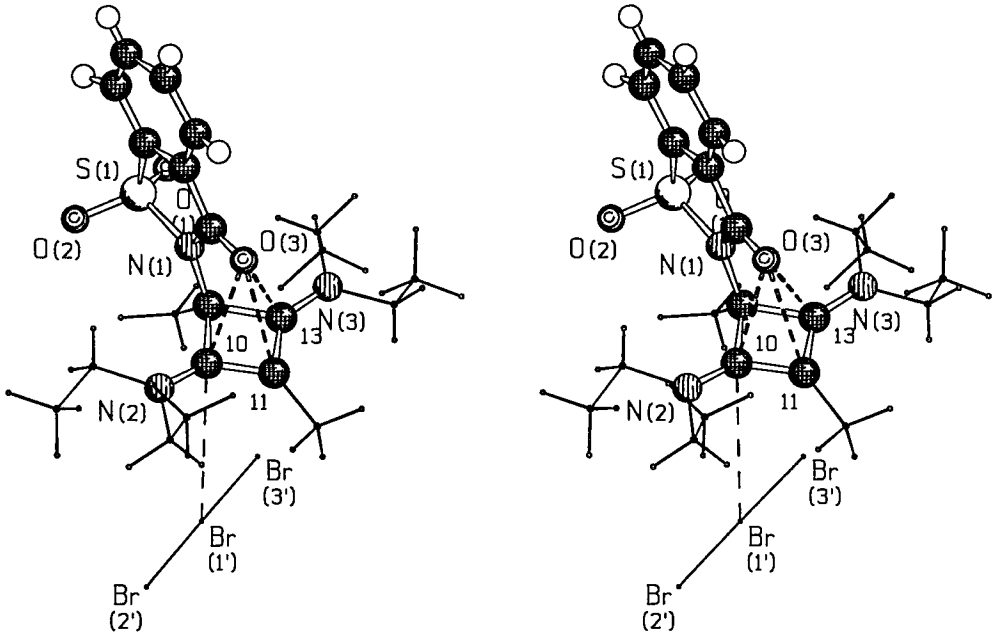
C(3)	- Cl(1^{II})	3.682	*diff* =	0.232
C(4)	- Cl(1^{II})	3.635	*diff* =	0.185
C(5)	- Cl(3^{I})	3.571	*diff* =	0.121
C(6)	- Cl(3^{I})	3.650	*diff* =	0.200

COVSUB10

1,3-bis(Diethylamino)-2,4-dimethyl-2-(1,1,3-trioxo-2H-1λ^6,3-benzothiazol-2-yl)-cyclobutenium tribromide
C21 H30 N3 O3 S1 1+,Br3 1-
J.Estienne
Acta Cryst.,C (Cr.Str.Comm.), 42, 1614,1986

COVSUB10 P21/c Z= 4 NATOMS= 59 DIFF AS=3 R-FACTOR= 0.035
REMARK H"(C15) and H'(C17) are deleted for suspected coordinate errors
28 C-H BONDS: S.D.= 0.129; MEAN = 0.949; RANGE: 0.597 - 1.232

H atoms at three methyl groups were newly computed in the present paper.

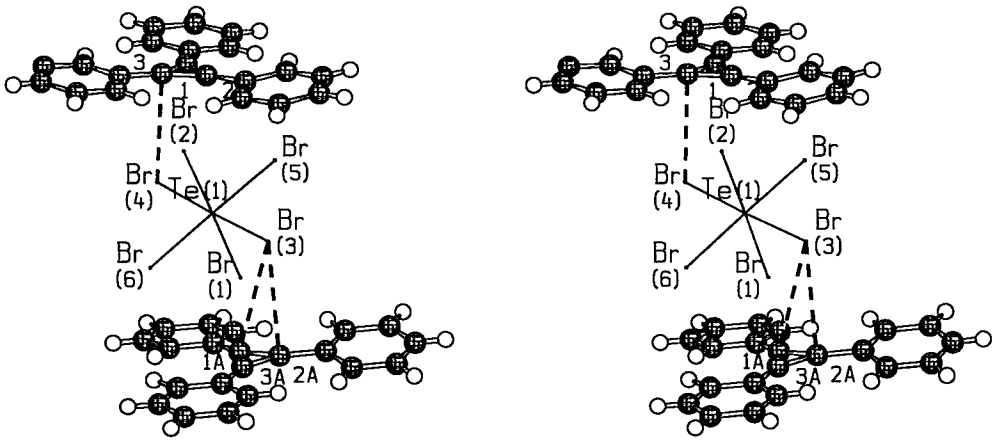


O(3)	- C(10)	2.898	*diff* = -0.322	**very strong**
O(3)	- C(13)	2.985	*diff* = -0.235	strong
O(3)	- C(11)	3.129	*diff* = -0.091	
Br(1^{I})	- C(10)	3.995	*diff* = 0.445	weak

CUGBAH

bis(sym-Triphenylcyclopropenylium) hexabromo-tellurium(iv)
2(C21 H15 1+),Br6 Te1 2-
B.A.Borgias,R.C.Scarrow,M.D.Seidler,W.P.Weiner
Acta Cryst.,C (Cr.Str.Comm.), 41, 476,1985

CUGBAH P21/c Z= 4 NATOMS= 78 DIFF AS=2 R-FACTOR= 0.026
REMARK Coordinates for H20 have not been retained due to illegibility
29 C-H BONDS: S.D.= 0.013; MEAN = 0.951; RANGE: 0.939 - 1.021



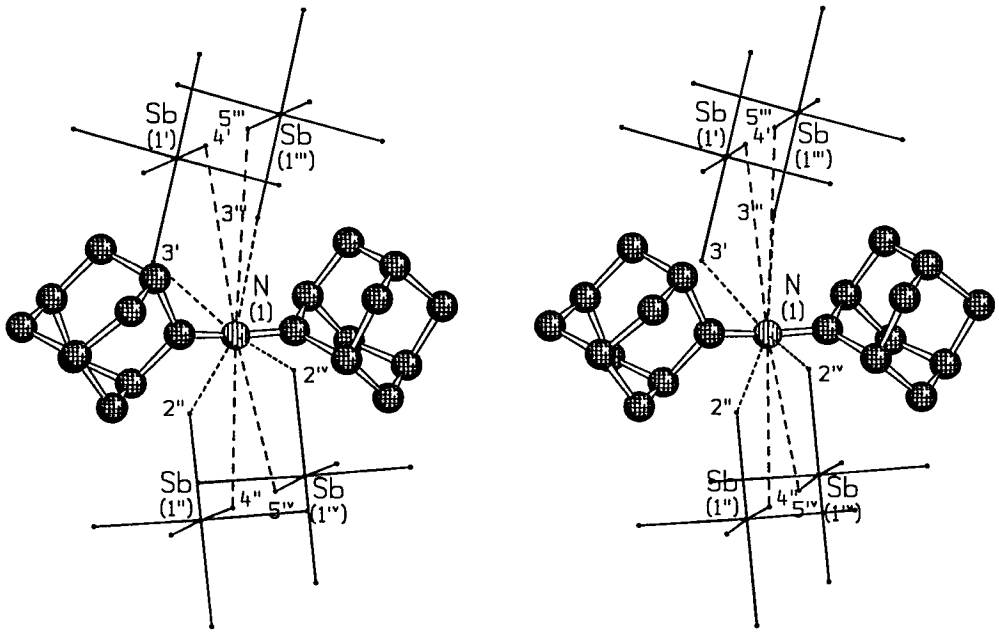
C(3)	- Br(4)	3.531	*diff* = -0.019	
C(1A)	- Br(3)	3.588	*diff* = 0.038	
C(2A)	- Br(3)	3.562	*diff* = 0.012	

DATZIH

bis(2-Adamantylidene)-ammonium hexachloro-antimony
C20 H28 N1 1+,Cl6 Sb1 1-
E.-U.Wurthwein,R.Kupfer,P.H.M.Budzelaar,C.Strobel,H.P.Beck
Angew.Chem.,Int.Ed.Engl., 24, 340,1985

DATZIH Pna21 Z= 4 NATOMS= 28 DIFF AS=0 R-FACTOR= 0.092

DISORD The crystals are disordered, mainly with respect to rotations around the C=N=C axis of the cation

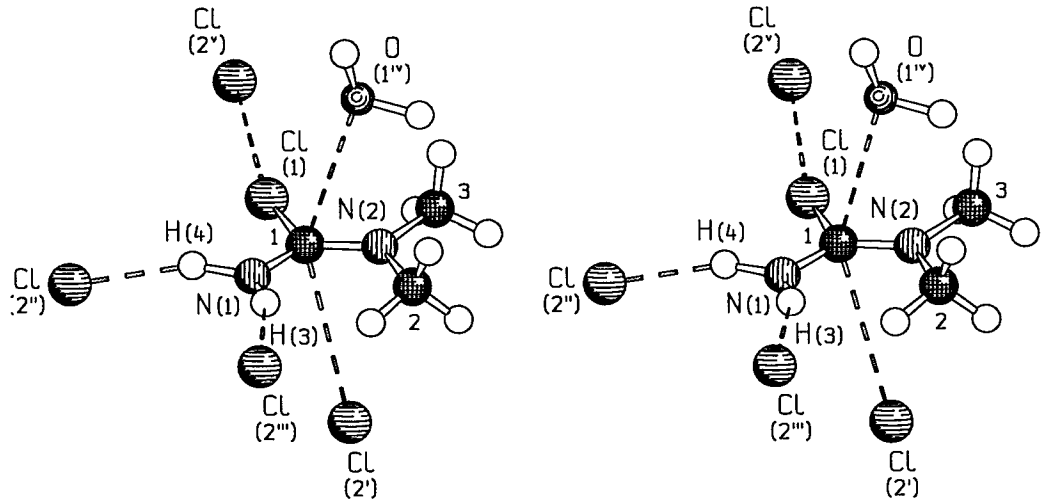


N(1)	- Cl(4^{II})	3.953	*diff* =	0.653	very weak
N(1)	- Cl(3^{I})	4.438	*diff* =	1.138	very weak
N(1)	- Cl(2^{II})	4.096	*diff* =	0.796	very weak
N(1)	- Cl(2^{IV})	4.231	*diff* =	0.931	very weak
N(1)	- Cl(5^{IV})	4.023	*diff* =	0.723	very weak
N(1)	- Cl(4^{I})	4.614	*diff* =	1.314	very weak
N(1)	- Cl(3^{III})	4.596	*diff* =	1.296	very weak
N(1)	- Cl(5^{III})	4.631	*diff* =	1.331	very weak

DEGLUW

N,N-Dimethyl-chloroformamidinium chloride monohydrate
C3 H8 Cl1 N2 1+,Cl1 1-,H2 O1
T.Chivers,J.F.Richardson,N.R.M.Smith
Inorg.Chem., 24, 2353,1985

DEGLUW P21/c Z= 4 NATOMS= 18 DIFF AS=2 R-FACTOR= 0.038
6 C-H BONDS: S.D.= 0.013; MEAN = 1.002; RANGE: 0.984 - 1.024

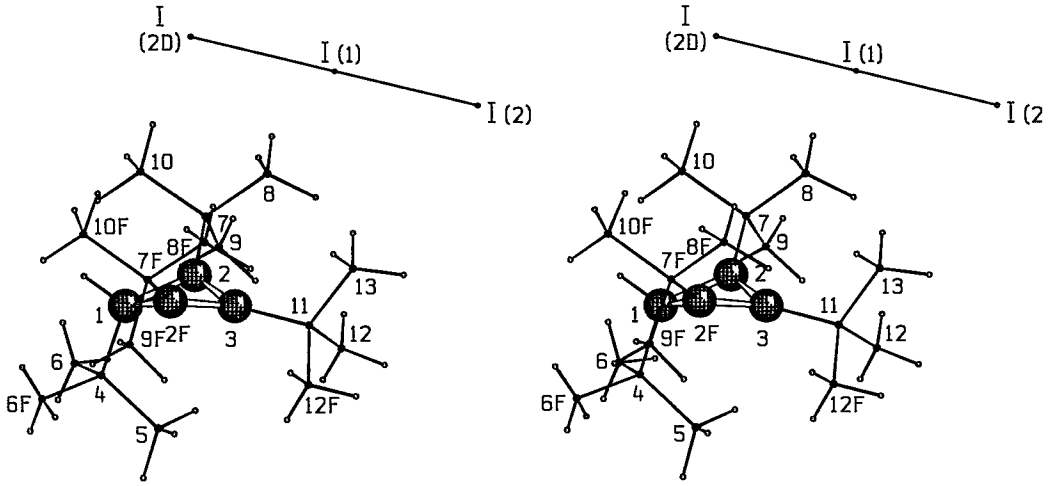


H(3)	- $Cl(2^{III})$	2.299	*diff* = -0.651	(H bond)
H(4)	- $Cl(2^{II})$	2.127	*diff* = -0.823	(H bond)
C(1)	- $Cl(2^{I})$	3.550	*diff* = 0.100	
C(1)	- $O(1^{IV})$	3.319	*diff* = 0.099	
Cl(1)	- $Cl(2^{V})$	3.465	*diff* = -0.035	

DEJKEI

1,2,3,4-Tetra-t-butyl-cyclobut-2-en-1-ylium tri-iodide
C20 H37 1+,I3 1-
G.Maier,R.Emrich,K.-D.Malsch,K.-A.Schneider,M.Nixdorf,H.Irngartinger
Chem.Ber., 118, 2798,1985

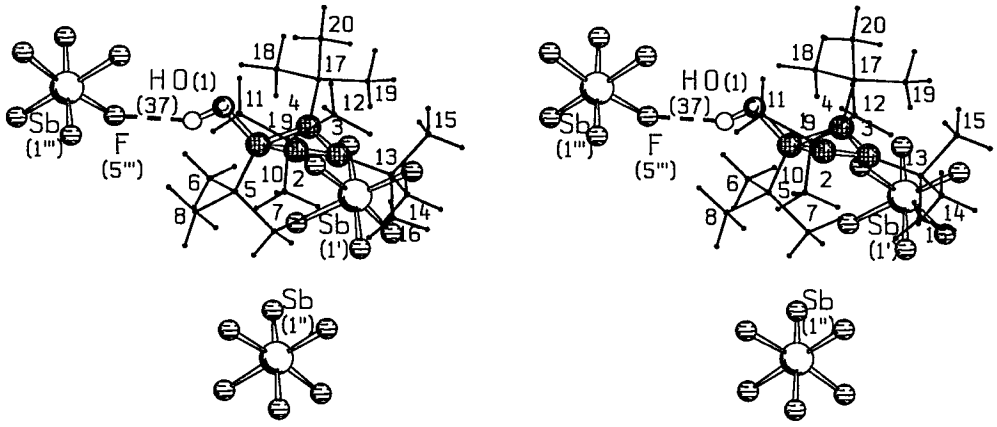
DEJKEI C2/m Z= 4 NATOMS= 63 DIFF AS=2 R-FACTOR= 0.048
37 C-H BONDS: S.D.= 0.084; MEAN = 0.941; RANGE: 0.800 - 1.088



DEJKIM

1,2,3,4-Tetra-t-butyl-4-hydroxy-cyclobut-2-en-1-ylium hexafluoro-antimony
C20 H37 O1 1+,F6 Sb1 1-
G.Maier,R.Emrich,K.-D.Malsch,K.-A.Schneider,M.Nixdorf,H.Irngartinger
Chem.Ber., 118, 2798,1985

DEJKIM P21/c Z= 4 NATOMS= 65 DIFF AS=2 R-FACTOR= 0.041
ERROR beta=113.33 not 133.33
36 C-H BONDS: S.D.= 0.063; MEAN = 0.974; RANGE: 0.837 - 1.092

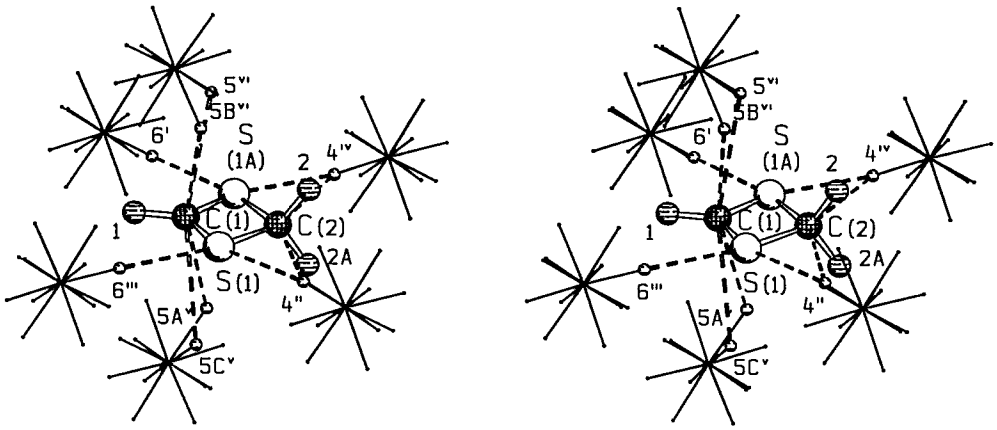


H(37) - F(5^{III}) 2.069 | *diff* = -0.601 (H bond)

DIBCAS

2,4,4-Trifluoro-1,3-dithietan-2-ylium hexafluoroarsenate
C2 F3 S2 1+,As1 F6 1-
J.Antel,K.Harms,P.G.Jones,R.Mews,G.M.Sheldrick,A.Waterfeld
Chem.Ber., 118, 5006,1985

DIBCAS Pmmn Z= 2 NATOMS= 5 DIFF AS=0 R-FACTOR= 0.045
DISORD The anion is two-fold disordered



C(2)	- F(4^{IV})	2.910	*diff* = -0.260	strong
C(1)	- F($5A^{V}$)	3.224	*diff* = 0.054	
C(1)	- F($5C^{V}$)	3.224	*diff* = 0.054	
C(1)	- F(5^{VI})	3.224	*diff* = 0.054	
C(1)	- F($5B^{VI}$)	3.224	*diff* = 0.054	
C(2)	- F(4^{II})	2.910	*diff* = -0.260	strong
S(1)	- F(4^{II})	2.633	*diff* = -0.637	**extremely strong**
S(1)	- F(6^{III})	2.653	*diff* = -0.617	**extremely strong**
S(1A)	- F(6^{I})	2.653	*diff* = -0.617	**extremely strong**
S(1A)	- F(4^{IV})	2.633	*diff* = -0.637	**extremely strong**

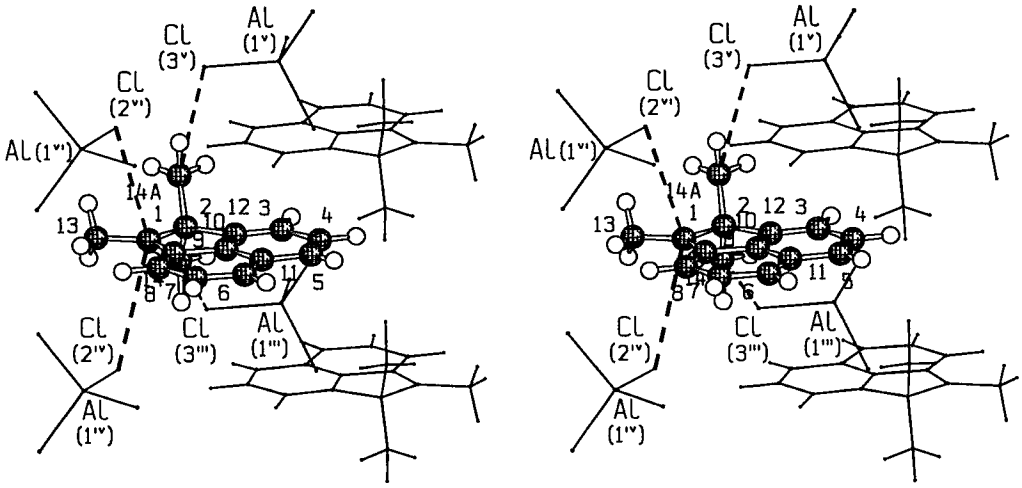
DIFMEK

1,1,2-Trimethyl-2-acenaphthenium tetrachloro-aluminium
at -20 deg.C
C15 H15 1+,Al1 Cl4 1-
G.I.Borodkin,Sh.M.Nagi,Yu.V.Gatilov,V.G.Shubin

Dokl.Akad.Nauk SSSR, 280, 881,1985

DIFMEK Pmcn Z= 4 NATOMS= 35 DIFF AS=3 R-FACTOR= 0.073
15 C-H BONDS: S.D.= 0.150; MEAN = 0.974; RANGE: 0.656 - 1.196

H atom at C(4) newly computed in the present paper.

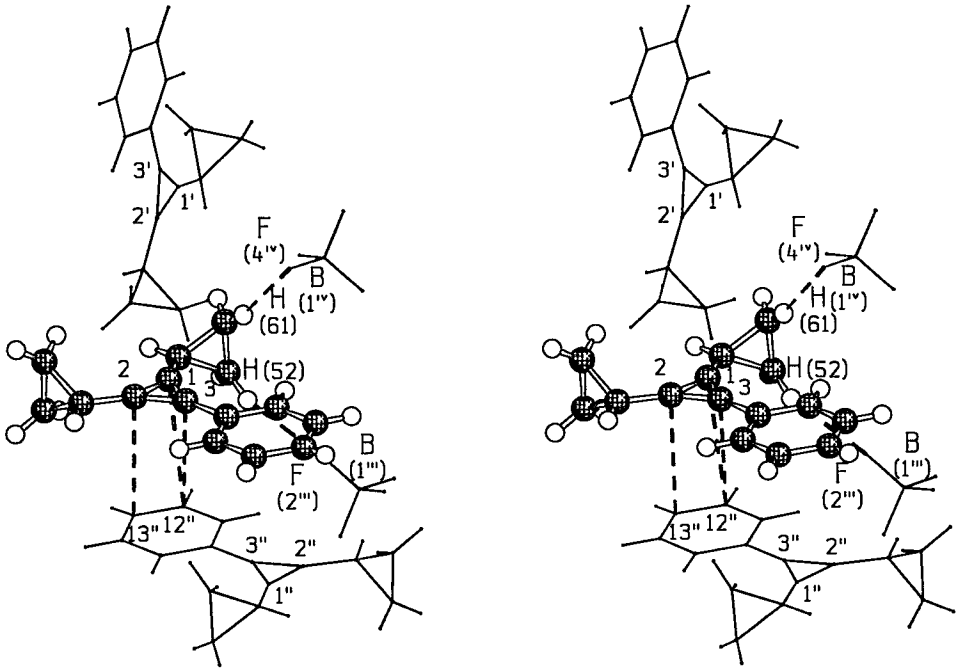


C(1)	- Cl(2^{IV})	3.775	*diff* =	0.325	weak
C(1)	- Cl(2^{VI})	3.775	*diff* =	0.325	weak
C(14)	- Cl(3^{III})	3.590	*diff* =	0.140	
C(14A)	- Cl(3^{V})	3.590	*diff* =	0.140	

DIJTIZ

1,2-Dicyclopropyl-3-phenylcyclopropenium tetrafluoroborate
C15 H15 1+,B1 F4 1-
R.A.Moss,S.Shen,K.Krogh-Jespersen,J.A.Potenza,H.J.Schugar,R.C.Munjal
J.Am.Chem.Soc., 108, 134,1986

DIJTIZ P21/n Z= 4 NATOMS= 35 DIFF AS=2 R-FACTOR= 0.062
15 C-H BONDS: S.D.= 0.065; MEAN = 0.952; RANGE: 0.809 - 1.015

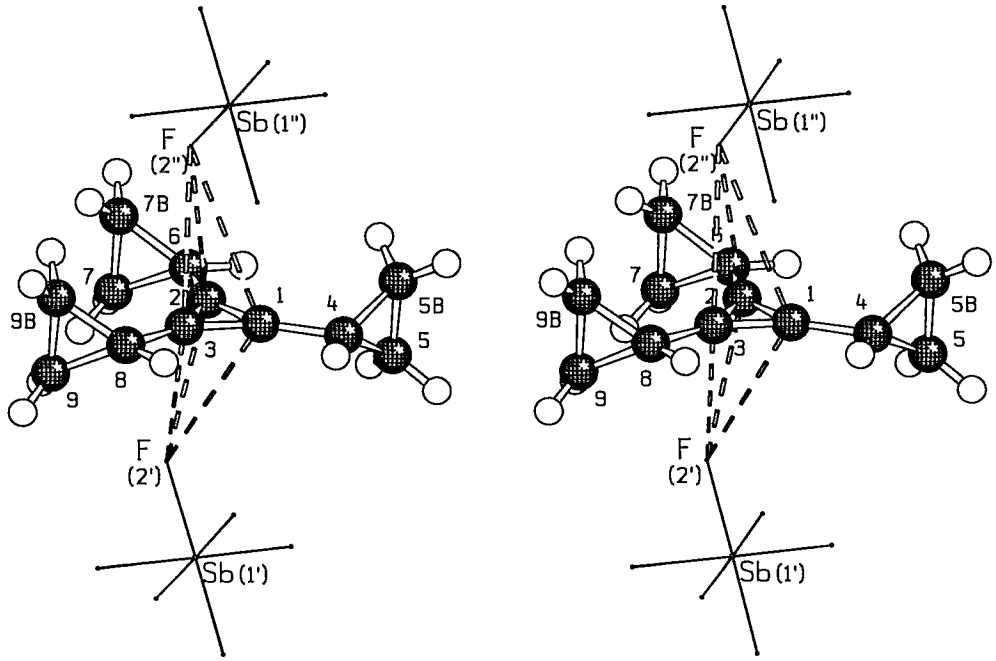


C(1)	- C(12^{II})	3.540	*diff* = 0.140	
C(2)	- C(13^{II})	3.537	*diff* = 0.137	
C(3)	- C(12^{II})	3.580	*diff* = 0.180	
H(52)	- F(2^{III})	2.461	*diff* = -0.209	(H bond)
H(61)	- F(4^{IV})	2.383	*diff* = -0.287	(H bond)

DIJTOF

Tricyclopropyl-cyclopropenium hexafluoroantimonate
C12 H15 1+,F6 Sb1 1-
R.A.Moss,S.Shen,K.Krogh-Jespersen,J.A.Potenza,H.J.Schugar,R.C.Munjal
J.Am.Chem.Soc., 108, 134,1986

DIJTOF Pnma Z= 4 NATOMS= 34 DIFF AS=3 R-FACTOR= 0.041
REMARK fw reported as 349.99, we calculate 394.99
15 C-H BONDS: S.D.= 0.016; MEAN = 0.979; RANGE: 0.947 - 1.005



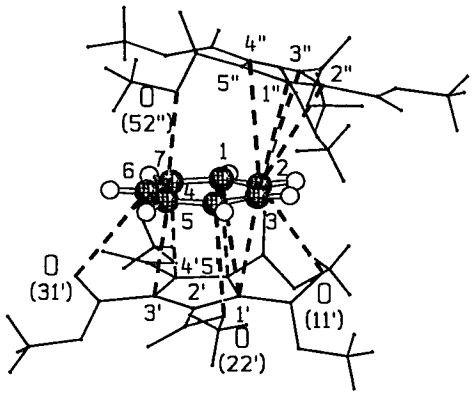
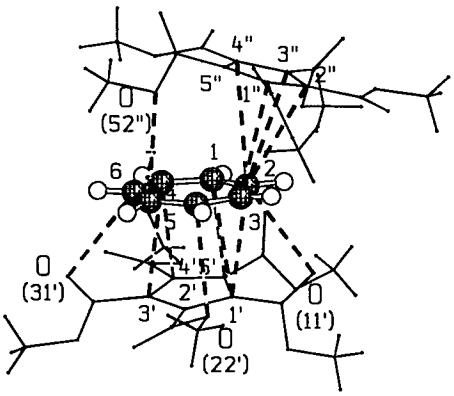
F(2^{I})	- C(2)	3.047	*diff* = -0.123	strong
C(2)	- F(2^{II})	3.047	*diff* = -0.123	strong
F(2^{I})	- C(3)	3.174	*diff* = 0.004	
C(3)	- F(2^{II})	3.174	*diff* = 0.004	
F(2^{I})	- C(1)	3.376	*diff* = 0.206	
C(1)	- F(2^{II})	3.376	*diff* = 0.206	

DIVXEL

Tropylium pentakis(methoxycarbonyl)-cyclopentadienide
C7 H7 1+,C15 H15 O10 1-
M.I.Bruce,P.A.Humphrey,B.W.Skelton,A.H.White
Aust.J.Chem., 39, 165,1986

DIVXEL Pbcn Z= 8 NATOMS= 54 DIFF AS=3 R-FACTOR= 0.047
22 C-H BONDS: S.D.= 0.032; MEAN = 0.985; RANGE: 0.888 - 1.035

The dashs from the tropylium C atom numbers were removed.

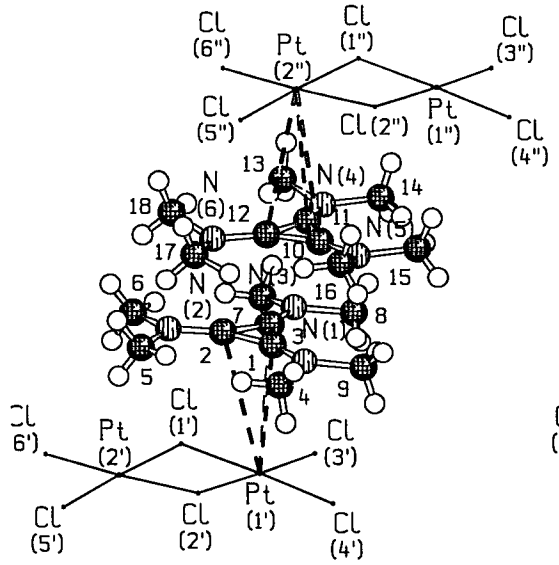
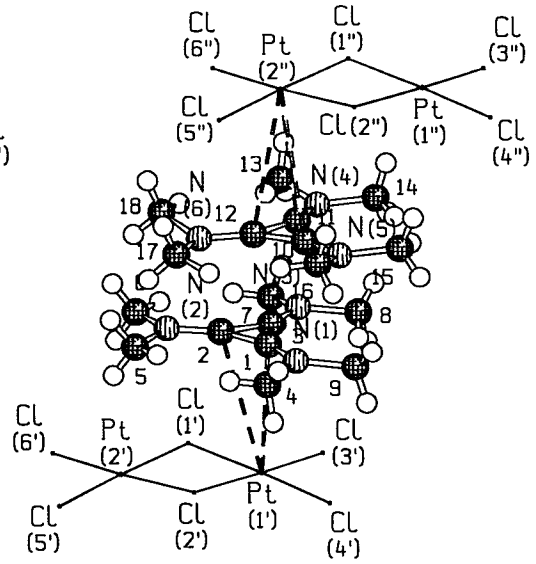



C(1)	- C(1^{I})	3.296	*diff* = -0.104	strong
C(2)	- C(1^{I})	3.407	*diff* = 0.007	
C(7)	- C(3^{I})	3.306	*diff* = -0.094	
C(7)	- C(4^{I})	3.406	*diff* = 0.006	
C(1)	- C(5^{I})	3.266	*diff* = -0.134	strong
C(3)	- C(1^{II})	3.357	*diff* = -0.043	
C(2)	- C(2^{II})	3.401	*diff* = 0.001	
C(2)	- C(3^{II})	3.299	*diff* = -0.101	strong
C(2)	- C(4^{II})	3.416	*diff* = 0.016	
C(2)	- O(11^{I})	3.112	*diff* = -0.108	strong
C(4)	- O(22^{I})	3.161	*diff* = -0.059	
C(5)	- O(52^{II})	3.251	*diff* = 0.031	
C(6)	- O(31^{I})	3.216	*diff* = -0.004	

DMCPRP10

1,2,3-tris(Dimethylamino)cyclopropenium hexachlorodiplatinum
2(C9 H18 N3 1+),Cl6 Pt2 2-
C.D.Cowman,J.C.Thibeault,R.F.Ziolo,H.B.Gray
J.Am.Chem.Soc., 98, 3209,1976

DMCPRP10 P21/c Z= 4 NATOMS= 67 DIFF AS=0 R-FACTOR= 0.058
REMARK H31 REMOVED FOR SUSPECTED COORD. ERROR
ERROR Z/C OF H21 GIVEN AS .523 SHOULD BE .0523
35 C-H BONDS: S.D.= 0.069; MEAN = 0.902; RANGE: 0.513 - 0.945

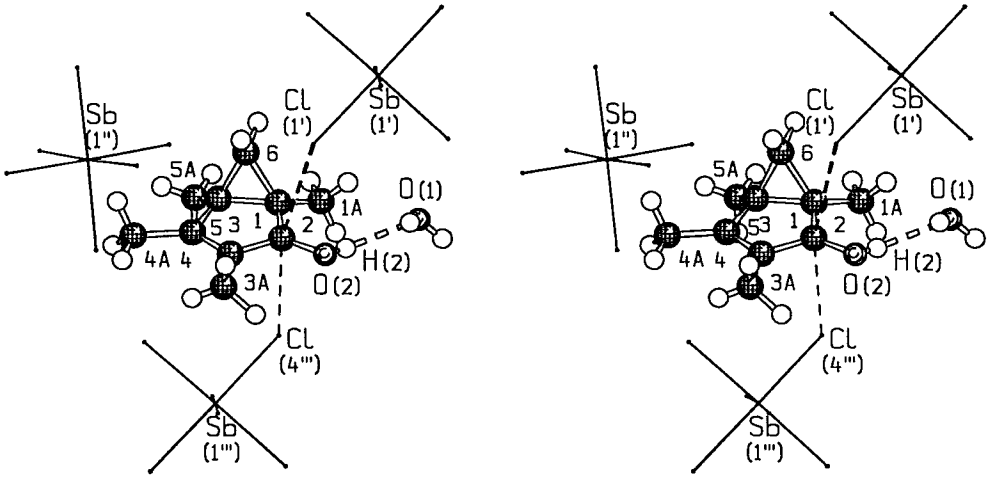
Pt(1^{I})	- C(1)	3.589	*diff* = 0.509	(metal radius of Pt: 1.38)
Pt(1^{I})	- C(2)	3.752	*diff* = 0.672	(metal radius of Pt: 1.38)

Pt(1^{I})	- C(3)	3.672	*diff* =	0.592 (metal radius of Pt: 1.38)
C(10)	- Pt(2^{II})	3.576	*diff* =	0.496 (metal radius of Pt: 1.38)
C(11)	- Pt(2^{II})	3.794	*diff* =	0.714 (metal radius of Pt: 1.38)
C(12)	- Pt(2^{II})	3.699	*diff* =	0.619 (metal radius of Pt: 1.38)

DOMFUG

2-Hydroxy-1,3,4,5-tetramethylbicyclo(3.1.0)hex-3-enium hexachloro-antimony monohydrate
C10 H15 O1 1+,Cl6 Sb1 1-,H2 O1
S.K.Chadda,R.F.Childs,R.Faggiani,C.J.L.Lock
J.Am.Chem.Soc., 108, 1694,1986

DOMFUG P21/c Z= 4 NATOMS= 36 DIFF AS=2 R-FACTOR= 0.041
ERROR X and z coordinates for H11 should be positive
14 C-H BONDS: S.D.= 0.070; MEAN = 0.941; RANGE: 0.837 - 1.064

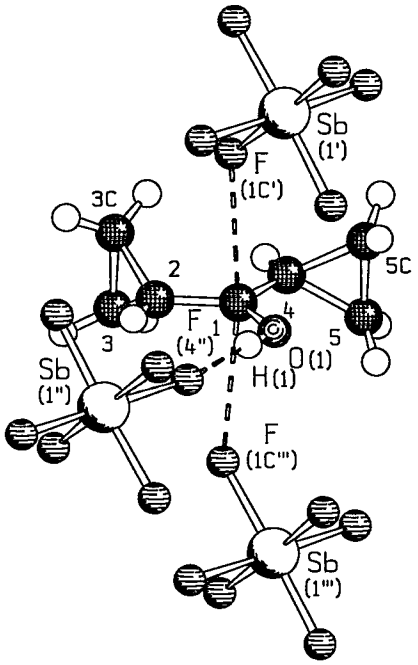


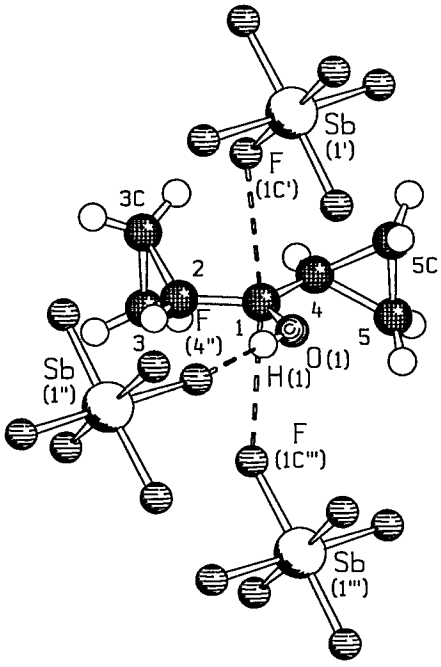
C(2)	- Cl(1^{I})	3.604	*diff* =	0.154
C(2)	- Cl(4^{III})	3.910	*diff* =	0.460 weak
H(2)	- O(1)	1.968	*diff* =	-0.752 (H bond)

DONBAJ

Hydroxy-dicyclopropylmethylium hexafluoro-antimony
C7 H11 O1 1+,F6 Sb1 1-
R.F.Childs,R.Faggiani,C.J.L.Lock,M.Mahendran,S.D.Zweep
J.Am.Chem.Soc., 108, 1692,1986

DONBAJ P21/m Z= 2 NATOMS= 26 DIFF AS=2 R-FACTOR= 0.025
10 C-H BONDS: S.D.= 0.060; MEAN = 0.947; RANGE: 0.794 - 1.002





H(1)	- $F(4^{II})$	1.826	*diff* = -0.844 (H bond)
C(1)	- $F(1C^{I})$	3.007	*diff* = -0.163 strong
C(1)	- $F(1C^{III})$	3.007	*diff* = -0.163 strong

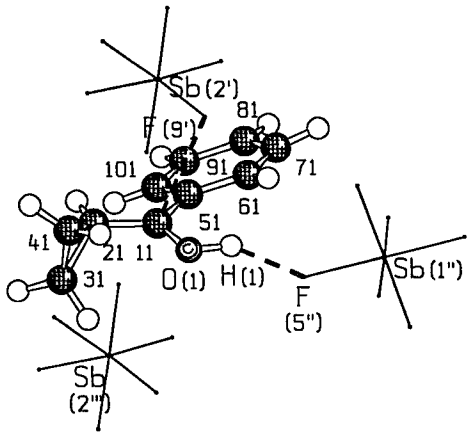
DONBEN

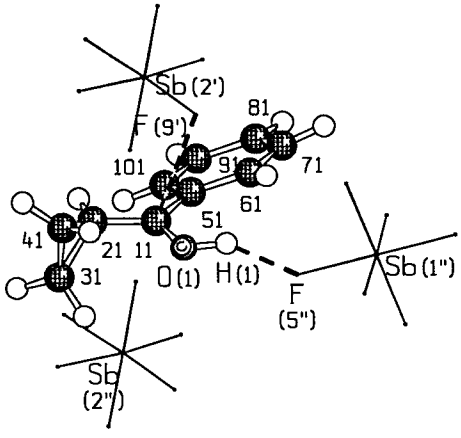
Hydroxy-cyclopropyl-phenylmethylium hexafluoro-antimony
C10 H11 O1 1+,F6 Sb1 1-
R.F.Childs,R.Faggiani,C.J.L.Lock,M.Mahendran,S.D.Zweep
J.Am.Chem.Soc., 108, 1692,1986

DONBEN P21/c Z= 8 NATOMS= 55 DIFF AS=2 R-FACTOR= 0.036
18 C-H BONDS: S.D.= 0.072; MEAN = 0.994; RANGE: 0.878 - 1.160

H atoms at C(31) and C(41) were newly computed in the present paper. H(2) was computed in the present paper with a conformation similar to that of H(1).

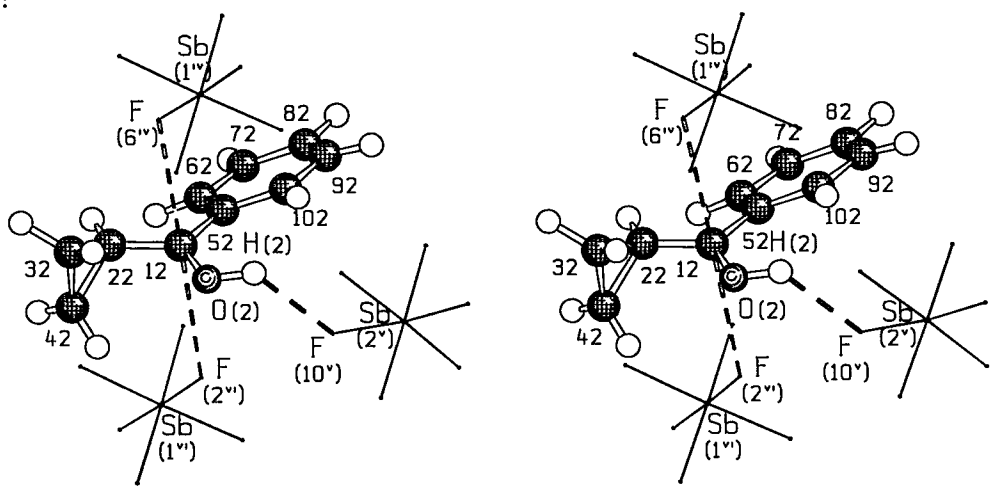
cation #1:





C(11)	- $F(9^{I})$	3.200	*diff* = 0.030
H(1)	- $F(5^{II})$	1.788	*diff* = -0.882 (H bond)

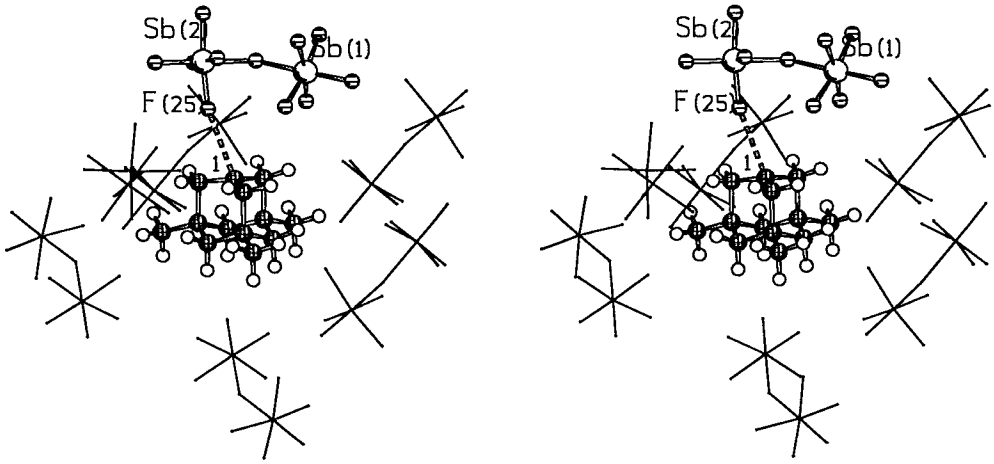
cation #2:



C(12)	- $F(2^{VI})$	3.245	*diff* = 0.075
C(12)	- $F(6^{IV})$	3.097	*diff* = -0.073
$F(10^{V})$	- H(2)	2.050	*diff* = -0.620 (H bond)

DOPRIJ

3,5,7-Trimethyl-adamantyl (μ_2-fluoro)-bis(pentafluoro-antimony)
at -160deg.C
C13 H21 1+,F11 Sb2 1-
T.Laube
Angew.Chem.,Int.Ed.Engl., 25, 349,1986
(Redetermination: T.Laube, E.Schaller, Acta Crystallogr. B51, 177, 1995)
DOPRIJ Pbca Z= 8 NATOMS= 47 DIFF AS=3 R-FACTOR= 0.070
21 C-H BONDS: S.D.= 0.080; MEAN = 1.069; RANGE: 0.813 - 1.254



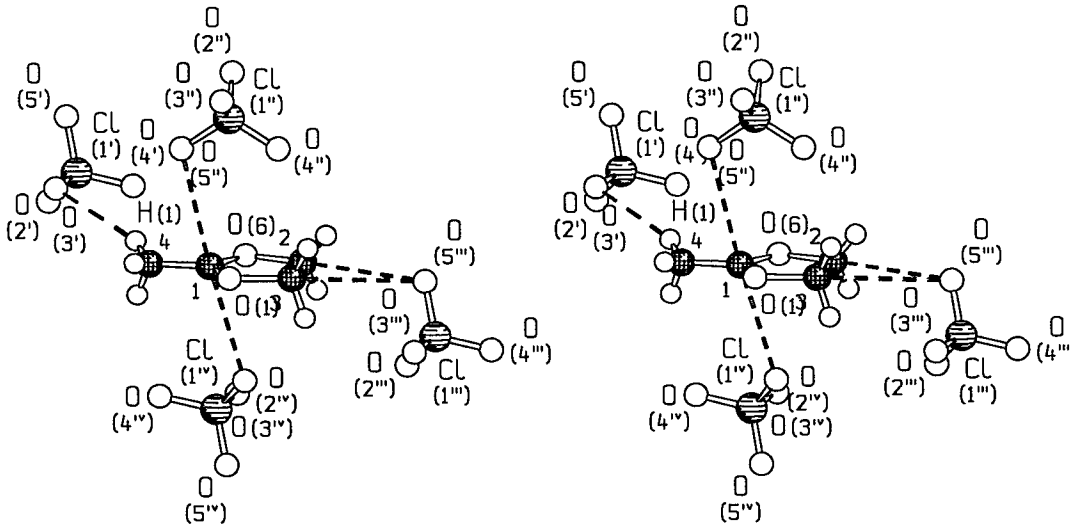
F(25)	- C(1)	2.879	*diff* = -0.291 strong

DOXYLP

2-Methyl-1,3-dioxolan-2-ylium perchlorate
C4 H7 O2 1+,Cl1 O4 1-
H.Paulsen,R.Dammeyer
Chem.Ber., 109, 1837,1976

DOXYLP P21/c Z= 4 NATOMS= 18 DIFF AS=2 R-FACTOR= 0.077

REMARK dm 1.460; dc 1.61
7 C-H BONDS: S.D.= 0.111; MEAN = 0.884; RANGE: 0.683 - 1.035

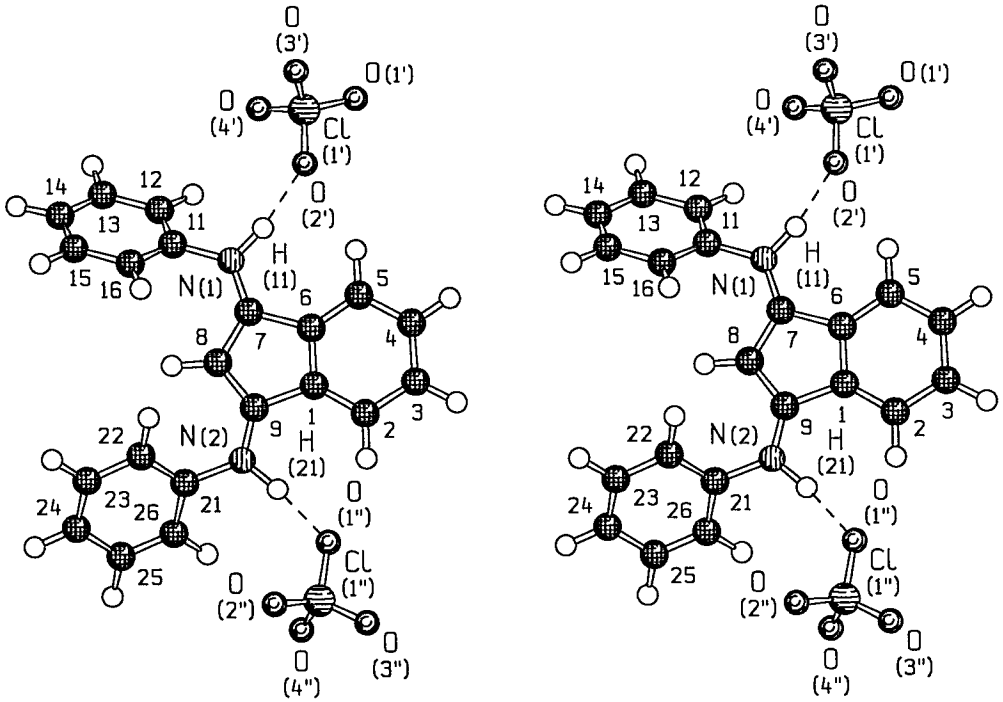


C(1)	- $O(5^{II})$	3.014	*diff* = -0.206	strong
C(1)	- $O(2^{IV})$	2.954	*diff* = -0.266	strong
C(2)	- $O(5^{III})$	3.097	*diff* = -0.123	strong
C(3)	- $O(5^{III})$	3.185	*diff* = -0.035	
H(1)	- $O(3^{I})$	2.615	*diff* = -0.105	(H bond)

DOYBIC

1,3-bis(Phenylamino)-indenium perchlorate
C21 H17 N2 1+,Cl1 O4 1-
G.Ferguson,M.Parvez,D.Lloyd,D.Marshall,D.Potter
Acta Cryst.,C (Cr.Str.Comm.), 42, 912,1986

DOYBIC Pc21b Z= 4 NATOMS= 45 DIFF AS=3 R-FACTOR= 0.033
15 C-H BONDS: S.D.= 0.002; MEAN = 1.079; RANGE: 1.075 - 1.083

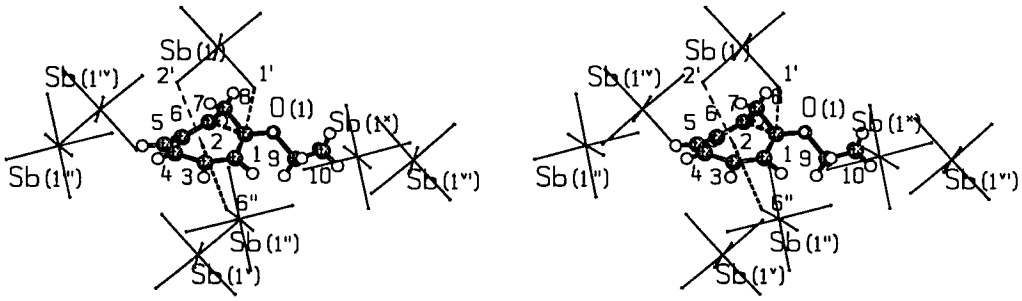


O(2^{I})	- H(11)	1.870	*diff* = -0.850 (H bond)
H(21)	- O(1^{II})	1.856	*diff* = -0.864 (H bond)

DOZSOA

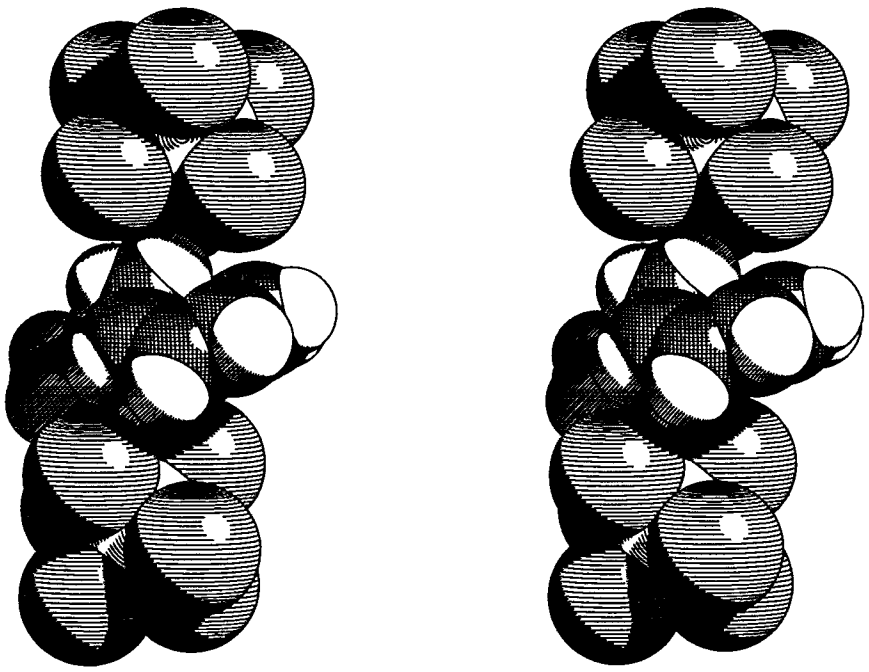
1-Ethoxy-homotropylium hexachloro-antimony
at -67 deg.C
C10 H13 O1 1+,Cl6 Sb1 1-
R.F.Childs,R.Faggiani,C.J.L.Lock,M.Mahendran
J.Am.Chem.Soc., 108, 3613,1986

DOZSOA P21/c Z= 4 NATOMS= 31 DIFF AS=2 R-FACTOR= 0.043
13 C-H BONDS: S.D.= 0.063; MEAN = 0.954; RANGE: 0.829 - 1.082



Cl(6^{II})	- Z(1)	3.527	(Z is a center of several atoms)
Cl(2^{I})	- Z(1)	4.162	(Z is a center of several atoms)
C(1)	- Cl(1^{I})	3.685	*diff* = 0.235
C(1)	- C(7)	2.284	*diff* = -1.116 **extremely strong**

space-filling model:

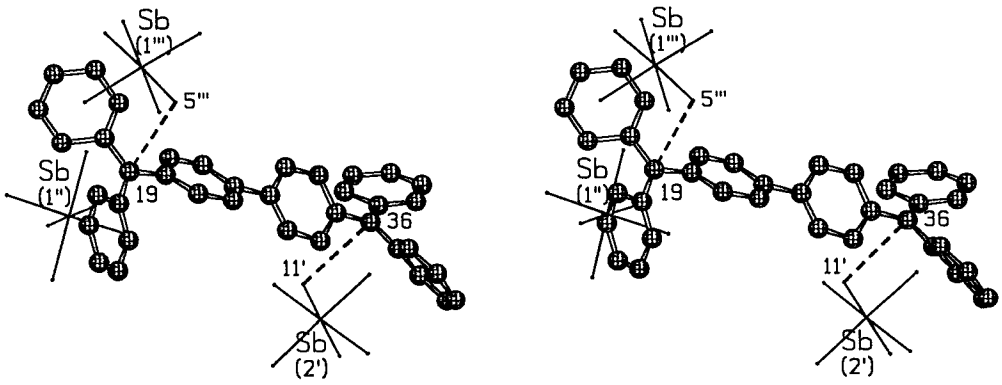


DPMBSB10

Biphenyl-4,4'-bis(diphenylmethylium) hexachloroantimonate

C38 H28 2+,2(Cl6 Sb1 1-)
J.S.McKechnie,I.C.Paul
J.Chem.Soc.B, , 918,1971

DPMBSB10 P21/c Z= 4 NATOMS= 52 PHOT AS=4 R-FACTOR= 0.100



C(19) - Cl(5^{III}) 3.870 | *diff* = 0.420 weak
Cl(11^{I}) - C(36) 3.469 | *diff* = 0.019

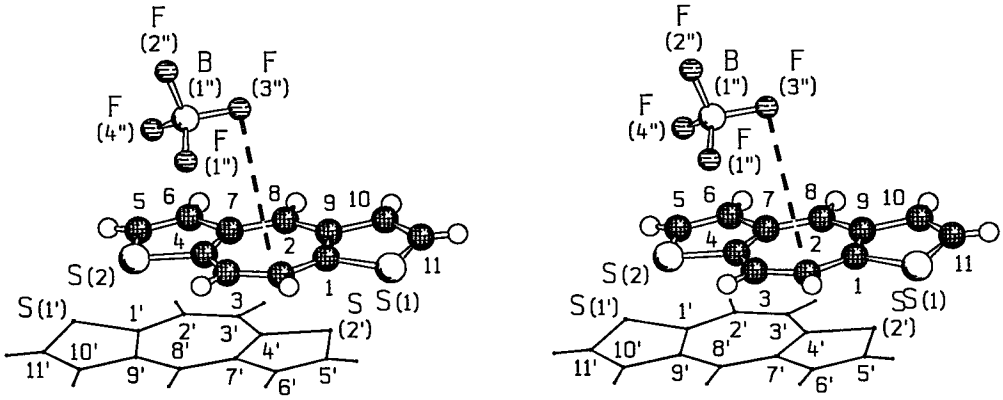
DTHTRO

Dithieno(1,2-b:5,4-b')tropylium tetrafluoroborate
at 143 deg.K
C11 H7 S2 1+,B1 F4 1-
J.-E.Andersson
Acta Crystallogr.,Sect.B, 35, 1349,1979

DTHTRO P-1 Z= 2 NATOMS= 25 DIFF AS=1 R-FACTOR= 0.043

DISORD The fluorines of the tetrafluoroborate anions are disordered over 2 orientations with occupancies 0.64,0.36. Positions for the former have been retained
7 C-H BONDS: S.D.= 0.061; MEAN = 0.911; RANGE: 0.791 - 1.018

Z(1) is the center of the tropylium ring.



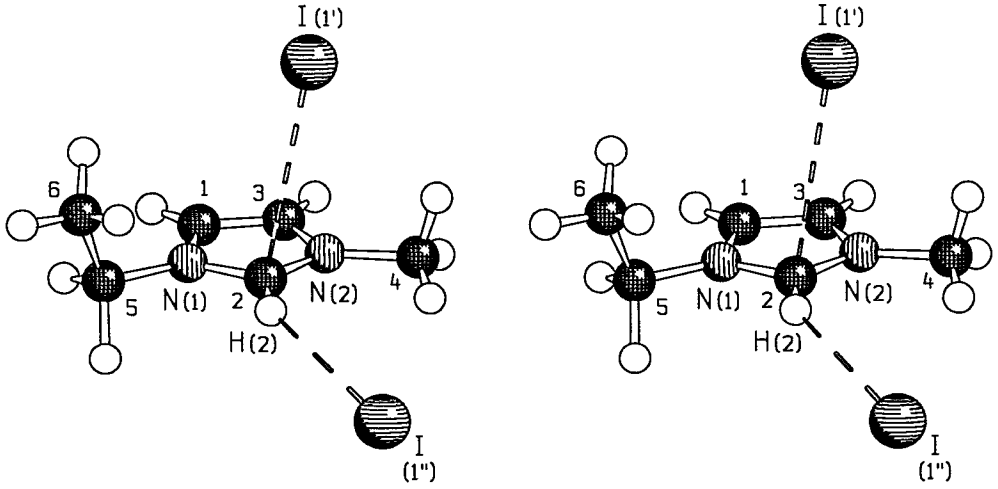
F(3^{II}) - Z(1) 3.768 | (Z is a center of several atoms)

DUVZAV

1-Methyl-3-ethyl-imidazolium iodide
C6 H11 N2 1+,I1 1-
A.K.Abdul-Sada,A.M.Greenway,P.B.Hitchcock,T.J.Mohammed,K.R.Seddon,J.A.Zora

J.Chem.Soc.,Chem.Comm., , 1753,1986

DUVZAV P21/c Z= 4 NATOMS= 19 DIFF AS=2 R-FACTOR= 0.023
REMARK H(6c) has been deleted due to a suspected coordinate error
10 C-H BONDS: S.D.= 0.127; MEAN = 1.019; RANGE: 0.739 - 1.240

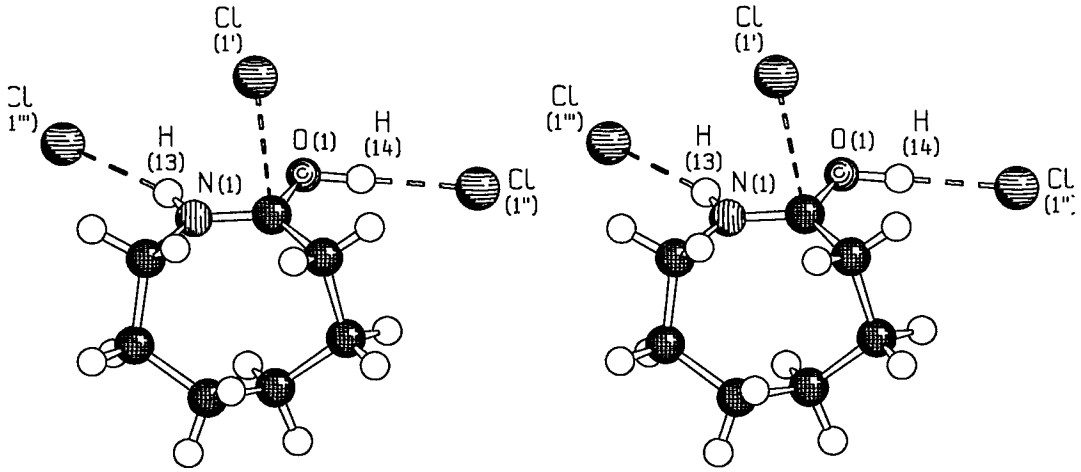


H(2)	- $I(1^{II})$	2.928	*diff* = -0.252 (H bond)
C(2)	- $I(1^{I})$	3.766	*diff* = 0.086

ENANLC

Enantholactam hydrochloride
C7 H14 N1 O1 1+,Cl1 1-
F.K.Winkler,J.D.Dunitz
Acta Crystallogr.,Sect.B, 31, 273,1975

ENANLC P21/c Z= 4 NATOMS= 24 DIFF AS=1 R-FACTOR= 0.044
12 C-H BONDS: S.D.= 0.030; MEAN = 1.005; RANGE: 0.945 - 1.049



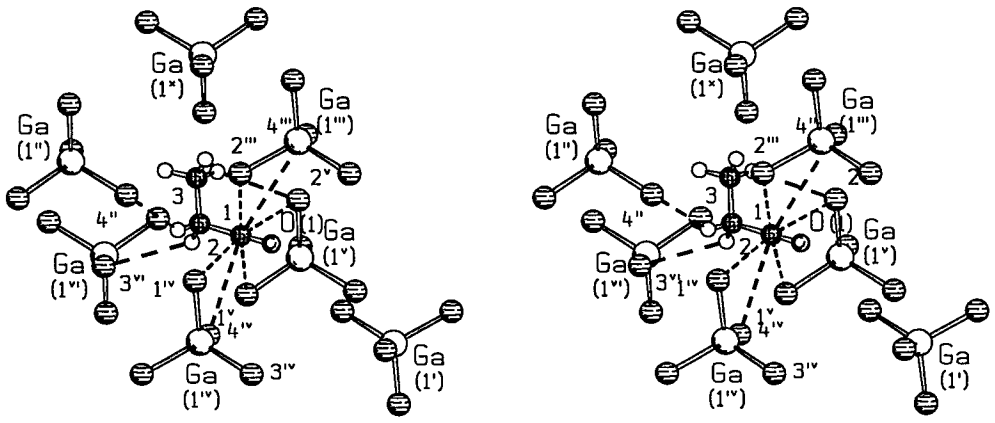
H(13)	- $Cl(1^{III})$	2.350	*diff* = -0.600 (H bond)
H(14)	- $Cl(1^{II})$	1.964	*diff* = -0.986 (H bond)
C(1)	- $Cl(1^{I})$	3.338	*diff* = -0.112 strong

ETOCGA

Ethyl-oxocarbonium tetrachlorogallate
C3 H5 O1 1+,Cl4 Ga1 1-
J.-M.Le Carpentier,R.Weiss
Acta Crystallogr.,Sect.B, 28, 1430,1972

ETOCGA P21/c Z= 4 NATOMS= 9 DIFF AS=0 R-FACTOR= 0.051

H atoms were added in the present paper.



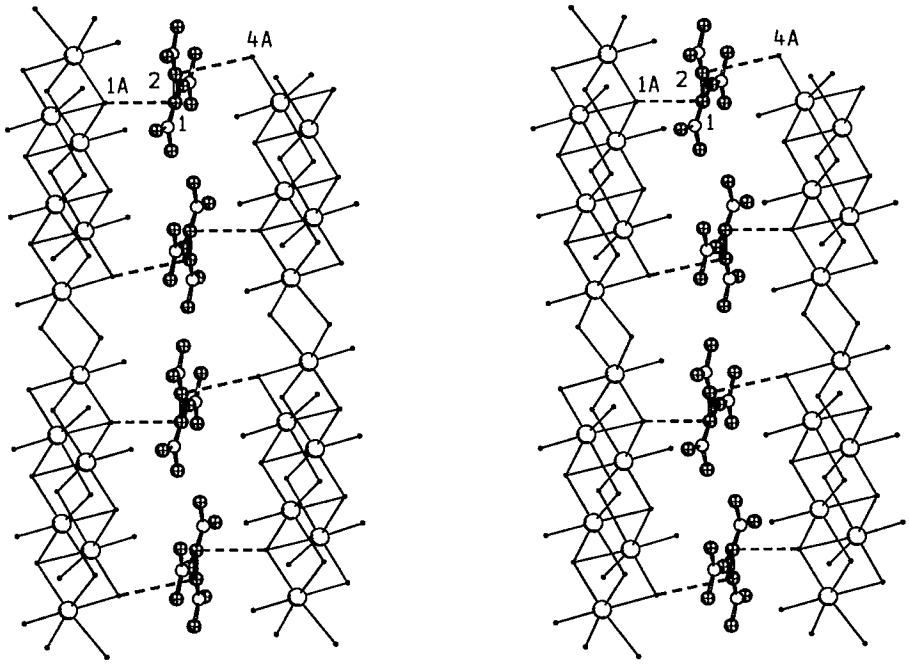
C(1)	- $Cl(4^{IV})$	3.424	*diff* = -0.026
C(1)	- $Cl(2^{V})$	3.428	*diff* = -0.022
C(1)	- $Cl(2^{III})$	3.506	*diff* = 0.056
C(1)	- $Cl(1^{IV})$	3.548	*diff* = 0.098
C(1)	- $Cl(1^{V})$	3.708	*diff* = 0.258
C(1)	- $Cl(4^{III})$	3.923	*diff* = 0.473 weak

H(2A)	- Cl(4^{II})	2.805	*diff* = -0.145 (H bond)
H(2B)	- Cl(3^{VI})	2.925	*diff* = -0.025 (H bond)
H(3A)	- Cl(2^{V})	2.917	*diff* = -0.033 (H bond)

FAFGUO

1,2,3-tris(Dimethylamino)-cyclopropenylium catena-(decaiodo-tri-antimony(iii))
(C9 H18 N3 1+)n,n(I10 Sb3 1-)
S.Pohl,W.Saak,P.Mayer,A.Schmidpeter
Angew.Chem.,Int.Ed.Engl., 25, 825,1986

FAFGUO P-1 Z= 0 NATOMS= 61 DIFF AS=3 R-FACTOR= 0.060
18 C-H BONDS: S.D.= 0.004; MEAN = 0.960; RANGE: 0.952 - 0.973

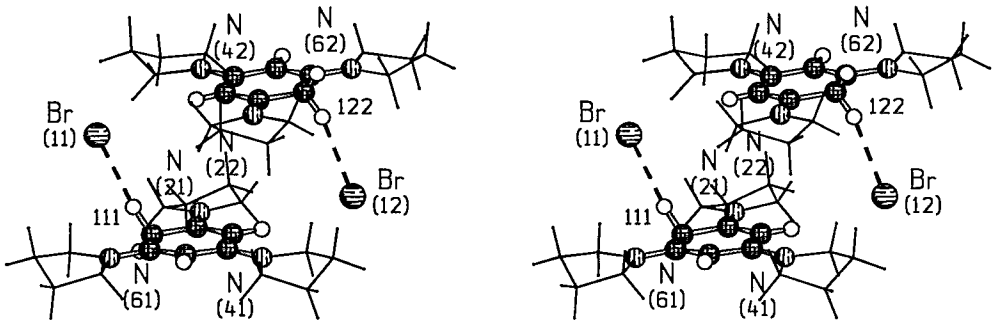


C(1)	- I(1A)	3.710	*diff* = 0.030
C(2)	- I(4A)	3.799	*diff* = 0.119

FEDZIX

2,4,6-Tripyrrolidino-cyclohexadienylium bromide
at 120 deg.K
C18 H28 N3 1+,Br1 1-
F.Effenberger,F.Reisinger,K.H.Schonwalder,P.Bauerle,J.J.Stezowski,K.H.Jogun,K.Sc
hollkopf,W.-D.Stohrer
J.Am.Chem.Soc., 109, 882,1987

FEDZIX P21/c Z= 8 NATOMS=100 DIFF AS=3 R-FACTOR= 0.082
ERROR In bond table N6-C62 should be N6-C64
56 C-H BONDS: S.D.= 0.046; MEAN = 1.018; RANGE: 0.920 - 1.122

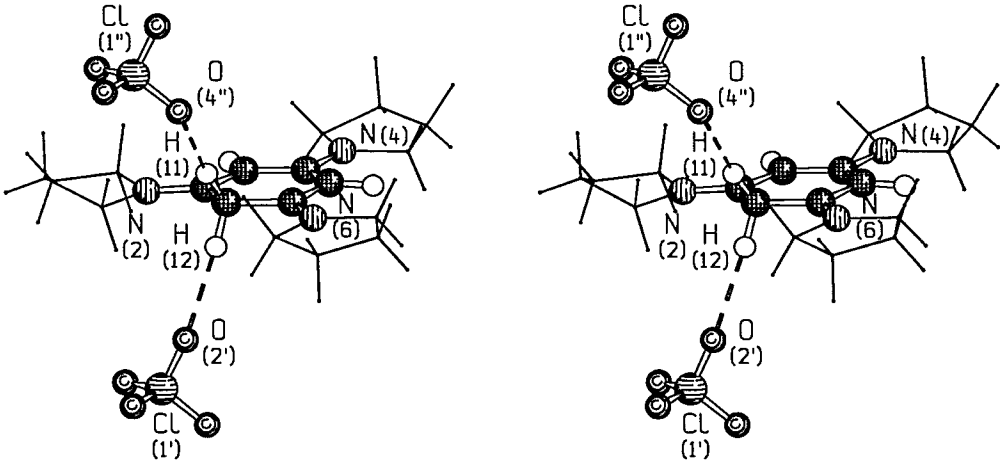


Br(11) - H(111) 2.587 | *diff* = -0.463 (H bond)
Br(12) - H(122) 2.717 | *diff* = -0.333 (H bond)

FEDZOD

2,4,6-Tripyrrolidino-cyclohexadienylium perchlorate
C18 H28 N3 1+,Cl1 O4 1-
F.Effenberger,F.Reisinger,K.H.Schonwalder,P.Bauerle,J.J.Stezowski,K.H.Jogun,K.Sc
hollkopf,W.-D.Stohrer
J.Am.Chem.Soc., 109, 882,1987

FEDZOD Pn21a Z= 4 NATOMS= 54 DIFF AS=3 R-FACTOR= 0.094
ERROR In bond table N2-C62 should be N2-C64
28 C-H BONDS: S.D.= 0.069; MEAN = 1.043; RANGE: 0.922 - 1.210

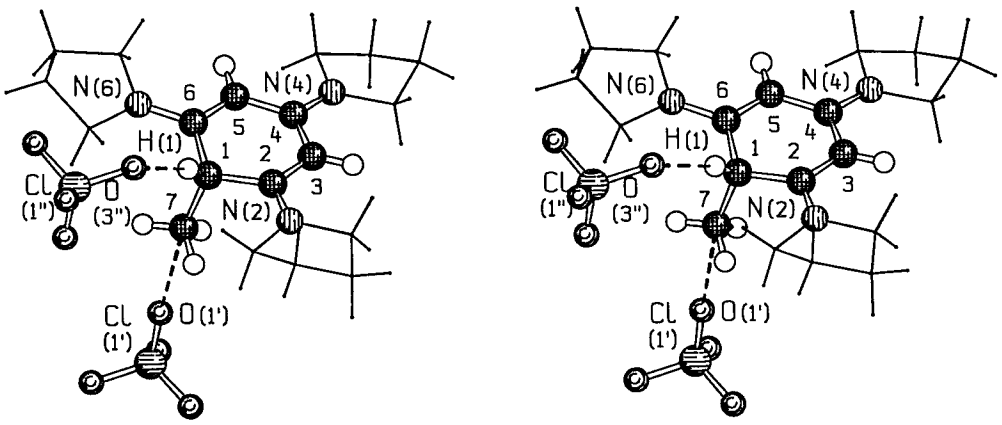


H(11) - O(4^{II}) 2.236 | *diff* = -0.484 (H bond)
O(2^{I}) - H(12) 2.306 | *diff* = -0.414 (H bond)

FEDZUJ

1-Methyl-2,4,6-tripyrrolidino-cyclohexadienylium perchlorate
at 120 deg.K
C19 H30 N3 1+,Cl1 O4 1-
F.Effenberger,F.Reisinger,K.H.Schonwalder,P.Bauerle,J.J.Stezowski,K.H.Jogun,K.Sc
hollkopf,W.-D.Stohrer
J.Am.Chem.Soc., 109, 882,1987

FEDZUJ P21/c Z= 4 NATOMS= 57 DIFF AS=1 R-FACTOR= 0.049
ERROR In bond table N2-C62 should be N2-C64
30 C-H BONDS: S.D.= 0.036; MEAN = 0.989; RANGE: 0.909 - 1.073



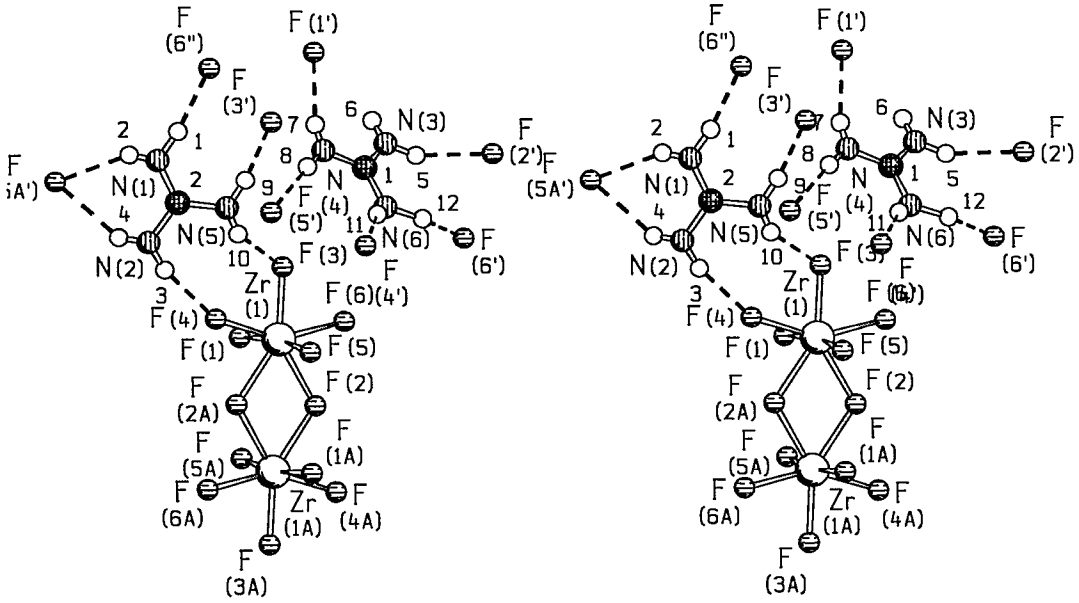
C(7)	- $O(1^{I})$	3.096	*diff* = -0.124 strong
H(1)	- $O(3^{II})$	2.703	*diff* = -0.017

FIBXAP

tetrakis(Triaminocarbonium) bis(μ_2-fluoro)-decafluoro-di-zirconium
4(C1 H6 N3 1+),F12 Zr2 4-
B.V.Bukvetskii,A.V.Gerasimenko,I.P.Kondratyuk,R.L.Davidovich,M.A.Medkov
Koord.Khim., 13, 661,1987

FIBXAP P-1 Z= 1 NATOMS= 34 DIFF AS=2 R-FACTOR= 0.034

All isolated F atoms in the drawing belong to $Zr_2F_{12}^{4-}$ *ions.*



H(1)	- $F(6^{II})$	1.944	*diff* = -0.726 (H bond)
H(2)	- $F(5A^{I})$	2.186	*diff* = -0.484 (H bond)
H(3)	- F(4)	1.988	*diff* = -0.682 (H bond)
H(4)	- $F(5A^{I})$	2.296	*diff* = -0.374 (H bond)
H(9)	- $F(3^{I})$	1.876	*diff* = -0.794 (H bond)
H(10)	- F(3)	2.248	*diff* = -0.422 (H bond)
H(5)	- $F(2^{I})$	2.085	*diff* = -0.585 (H bond)
H(7)	- $F(1^{I})$	2.242	*diff* = -0.428 (H bond)
H(8)	- $F(5^{I})$	1.925	*diff* = -0.745 (H bond)
H(11)	- $F(4^{I})$	2.080	*diff* = -0.590 (H bond)
H(12)	- $F(6^{I})$	1.740	*diff* = -0.930 (H bond)