

Inorganic Chemistry

including bioinorganic chemistry

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Bond lengths (Angstr.)

Cs1	-	F1	2.924(2)	Cs1	-	F1a	2.924(2)
Cs1	-	F1b	2.924(2)	Ga1	-	F1	1.970(4)
Ga1	-	C1	1.998(5)	C1	-	C11	1.514(7)
C1	-	C12	1.518(8)	C1	-	H1	0.99(1)
C11	-	H111	0.97(1)	C11	-	H112	0.97(1)
C11	-	H113	0.97(1)	C12	-	H121	0.97(1)
C12	-	H122	0.97(1)	C12	-	H123	0.97(1)

Bond angles (deg.)

F1	-	Cs1	-	F1a	79.70(6)	F1	-	Ga1	-	C1	101.3(2)
C1	-	Ga1	-	C1a	116.2(2)	Cs1	-	F1	-	Ga1	118.25(9)
Cs1	-	F1	-	Cs1a	99.43(7)	Ga1	-	C1	-	C11	113.3(4)
Ga1	-	C1	-	C12	111.9(4)	C11	-	C1	-	C12	109.9(4)
Ga1	-	C1	-	H1	107.3(4)	C11	-	C1	-	H1	106.6(5)
C12	-	C1	-	H1	107.4(5)	C1	-	C11	-	H111	109.7(6)
C1	-	C11	-	H112	109.9(7)	C1	-	C11	-	H113	108.8(6)
H111	-	C11	-	H112	109.5(8)	H111	-	C11	-	H113	109.5(8)
H112	-	C11	-	H113	109.5(7)	C1	-	C12	-	H121	109.2(7)
C1	-	C12	-	H122	109.6(7)	C1	-	C12	-	H123	109.6(8)
H121	-	C12	-	H122	109.5(9)	H121	-	C12	-	H123	109.5(9)
H122	-	C12	-	H123	109.5(8)						

Atom	x	y	z	Ueq/Uiso
Cs1	-0.11295(2)	0.11295(2)	0.11295(2)	0.0410(1)
Ga1	0.17634(3)	0.17634(3)	0.17634(3)	0.0387(1)
F1	0.0949(2)	0.0949(2)	0.0949(2)	0.0413(6)
C1	0.2030(3)	0.0886(3)	0.2862(3)	0.052(2)
C11	0.2856(4)	0.1213(5)	0.3483(4)	0.079(2)
C12	0.1147(5)	0.0723(5)	0.3474(5)	0.093(3)
H1	0.2218(3)	0.0258(3)	0.2589(3)	0.099(8) *
H111	0.3420(4)	0.1313(5)	0.3090(4)	0.099(8) *
H112	0.2994(4)	0.0733(5)	0.3966(4)	0.099(8) *
H113	0.2681(4)	0.1810(5)	0.3792(4)	0.099(8) *
H121	0.0625(5)	0.0507(5)	0.3070(5)	0.099(8) *
H122	0.0968(5)	0.1317(5)	0.3787(5)	0.099(8) *
H123	0.1283(5)	0.0240(5)	0.3956(5)	0.099(8) *

* refined isotropically

Atom	U11	U22	U33	U23	U13	U12
Cs1	0.0410(2)	0.0410(2)	0.0410(2)	-0.0041(1)	0.0041(1)	0.0041(1)
Ga1	0.0387(2)	0.0387(2)	0.0387(2)	-0.0043(2)	-0.0043(2)	-0.0043(2)
F1	0.041(1)	0.041(1)	0.041(1)	-0.005(1)	-0.005(1)	-0.005(1)
C1	0.064(3)	0.045(3)	0.047(3)	-0.005(2)	-0.009(2)	-0.006(2)
C11	0.093(4)	0.083(4)	0.061(3)	0.000(4)	-0.031(3)	-0.004(4)
C12	0.109(5)	0.092(4)	0.077(4)	0.032(4)	0.012(5)	-0.019(5)

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Bond lengths (Angstr.)

Cs1	-	F1	2.889(2)	Cs1	-	F1a	2.889(2)
Cs1	-	F1b	2.889(2)	In1	-	F1	2.168(3)
In1	-	C1	2.199(4)	C1	-	C11	1.505(7)
C1	-	C12	1.501(8)	C1	-	H1	0.99(1)
C11	-	H111	0.97(1)	C11	-	H112	0.97(1)
C11	-	H113	0.97(1)	C12	-	H121	0.97(1)
C12	-	H122	0.97(1)	C12	-	H123	0.97(1)

Bond angles (deg.)

F1	-	Cs1	-	F1a	77.77(5)	F1	-	In1	-	C1	100.0(1)
C1	-	In1	-	C1a	117.1(2)	Cs1	-	F1	-	In1	116.99(7)
Cs1	-	F1	-	Cs1a	101.02(6)	In1	-	C1	-	C11	111.9(3)
In1	-	C1	-	C12	111.3(4)	C11	-	C1	-	C12	111.4(4)
In1	-	C1	-	H1	107.2(4)	C11	-	C1	-	H1	107.4(5)
C12	-	C1	-	H1	107.4(5)	C1	-	C11	-	H111	109.0(5)
C1	-	C11	-	H112	109.9(7)	C1	-	C11	-	H113	109.5(6)
H111	-	C11	-	H112	109.5(8)	H111	-	C11	-	H113	109.5(9)
H112	-	C11	-	H113	109.5(7)	C1	-	C12	-	H121	109.6(7)
C1	-	C12	-	H122	109.4(7)	C1	-	C12	-	H123	109.3(8)
H121	-	C12	-	H122	109.5(9)	H121	-	C12	-	H123	109.5(9)
H122	-	C12	-	H123	109.5(8)						

Atom	x	y	z	Ueq/Uiso
Cs1	-0.11126(1)	0.11126(1)	0.11126(1)	0.0495(1)
In1	0.17884(2)	0.17884(2)	0.17884(2)	0.0434(1)
F1	0.0905(1)	0.0905(1)	0.0905(1)	0.0485(5)
C1	0.2025(3)	0.0825(3)	0.2982(3)	0.061(2)
C11	0.2846(4)	0.1132(5)	0.3581(3)	0.098(2)
C12	0.1146(6)	0.0707(5)	0.3561(5)	0.117(3)
H1	0.2184(3)	0.0200(3)	0.2714(3)	0.135(9) *
H111	0.3399(4)	0.1201(5)	0.3184(3)	0.135(9) *
H112	0.2970(4)	0.0664(5)	0.4065(3)	0.135(9) *
H113	0.2701(4)	0.1732(5)	0.3877(3)	0.135(9) *
H121	0.0630(6)	0.0509(5)	0.3158(5)	0.135(9) *
H122	0.0988(6)	0.1303(5)	0.3858(5)	0.135(9) *
H123	0.1255(6)	0.0234(5)	0.4043(5)	0.135(9) *

* refined isotropically

Atom	U11	U22	U33	U23	U13	U12
Cs1	0.0495(1)	0.0495(1)	0.0495(1)	-0.0063(1)	0.0063(1)	0.0063(1)
In1	0.0434(1)	0.0434(1)	0.0434(1)	-0.0040(1)	-0.0040(1)	-0.0040(1)
F1	0.049(1)	0.049(1)	0.049(1)	-0.007(1)	-0.007(1)	-0.007(1)
C1	0.081(3)	0.051(2)	0.052(2)	0.001(2)	-0.010(2)	0.005(2)
C11	0.115(4)	0.115(5)	0.063(3)	-0.007(3)	-0.034(3)	0.014(4)
C12	0.124(5)	0.115(5)	0.112(5)	0.053(4)	0.018(4)	-0.018(4)