

Table S1. Experimental and Calculated Frequencies (cm^{-1}), Raman Intensities^a and Assignments^b for CX_3^+ and BX_3 (X = F, Cl, Br, I)

CF_3^+

assgnts	expt ^c	6-31G(2d)		cc-pVTZ	
		HF	MP2	HF	MP2
$\nu_1(\text{A}_1')$, $\nu_s(\text{C}-\text{F})$		1145(4)	1048(7)	1161(4)	1072(7)
$\nu_2(\text{A}_2'')$, $\pi(\text{C}-\text{F}_3)$	798.1	912(0)	843(0)	895(0)	825(0)
$\nu_3(\text{E}')$, $\nu_{as}(\text{C}-\text{F})$	1662.4	1835(<1)	1692(<1)	1847(<1)	1717(<0)
$\nu_4(\text{E}')$, $\delta_d(\text{F}-\text{C}-\text{F})$		642(<1)	595(1)	648(<1)	601(1)

CCl_3^+

assgnts	expt	6-31G(2d)		cc-pVTZ	
		HF	MP2	HF	MP2
$\nu_1(\text{A}_1')$, $\nu_s(\text{C}-\text{Cl})$	554(28) ^d	574(8)	559(18)	579(8)	568(17)
$\nu_2(\text{A}_2'')$, $\pi(\text{C}-\text{Cl}_3)$	-	566(0)	538(0)	571(0)	541(0)
$\nu_3(\text{E}')$, $\nu_{as}(\text{C}-\text{Cl})$	1035, ^e 1037 ^f	1112(1)	1072(<1)	1114(1)	1086(<1)
$\nu_4(\text{E}')$, $\delta_d(\text{Cl}-\text{C}-\text{Cl})$	326.9(9)	329(2)	318(4)	329(3)	317(4)

CBr_3^+

assgnts	Expt	6-31G(2d)		cc-pVTZ	
		HF	MP2	HF	MP2
$\nu_1(\text{A}_1')$, $\nu_s(\text{C}-\text{Br})$	321.4(27)	346(6)	341(13)	336(5)	340(13)
$\nu_2(\text{A}_2'')$, $\pi(\text{C}-\text{Br}_3)$		479(0)	461(0)	470(0)	454(0)
$\nu_3(\text{E}')$, $\nu_{as}(\text{C}-\text{Br})$		963(3)	932(3)	936(4)	931(2)
$\nu_4(\text{E}')$, $\delta_d(\text{Br}-\text{C}-\text{Br})$	183.5(15) 187.0(12)	198(1)	193(3)	190(2)	186(3)

CI_3^+

assgnts	Expt ^g	(SDB-)cc-pVTZ	
		HF	MP2
$\nu_1(\text{A}_1')$, $\nu_s(\text{C}-\text{I})$		231(3)	240(14)
$\nu_2(\text{A}_2'')$, $\pi(\text{C}-\text{I}_3)$	339, w	395(0)	384(0)
$\nu_3(\text{E}')$, $\nu_{as}(\text{C}-\text{I})$	739, vs	800(24)	807(10)
$\nu_4(\text{E}')$, $\delta_d(\text{I}-\text{C}-\text{I})$		128(2)	127(3)

BF_3

assgnts	expt ^h	6-31G(2d)		cc-pVTZ	
		HF	MP2	HF	MP2
$\nu_1(\text{A}_1')$, $\nu_s(\text{B}-\text{F})$	888.0	938(2)	883(4)	952(2)	895(4)
$\nu_2(\text{A}_2'')$, $\pi(\text{B}-\text{F}_3)$	691.5	760(0)	723(0)	741(0)	698(0)
$\nu_3(\text{E}')$, $\nu_{as}(\text{B}-\text{F})$	1453.5	1554(<1)	1475(<1)	1566(<1)	1484(<1)
$\nu_4(\text{E}')$, $\delta_d(\text{F}-\text{B}-\text{F})$	480.4	515(<1)	491(<1)	513(<1)	481(<1)

Table S1. (continued ...)

BCl₃

assgnts	Expt ⁱ	6-31G(2d)		cc-pVTZ	
		HF	MP2	HF	MP2
v ₁ (A ₁ ')	467.3	487(7)	477(9)	489(6)	483(8)
v ₂ (A ₂ ''), π(B-Cl ₃)	447.3 ^j	481(0)	465(0)	482(0)	465(0)
v ₃ (E'), v _{as} (B-Cl)	931	989(<1)	970(<1)	989(<1)	984(<1)
v ₄ (E'), δ _d (Cl-B-Cl)	254.5	267(2)	257(3)	268(2)	259(2)

BBr₃

assgnts	Expt ^k	6-31G(2d)		cc-pVTZ	
		HF	MP2	HF	MP2
v ₁ (A ₁ ')	279.6	297(6)	292(7)	290(5)	292(6)
v ₂ (A ₂ ''), π(B-Br ₃)	377.3 ^j	425(0)	414(0)	409(0)	401(0)
v ₃ (E'), v _{as} (B-Br)	794.4	867(<1)	849(<1)	848(<1)	853(<1)
v ₄ (E'), δ _d (Br-B-Br)	153.4	161(1)	155(1)	160(1)	157(2)

BI₃

assgnt.	expt. ^k	(SDB-)cc-pVTZ	
		HF	MP2
v ₁ (A ₁ ')	194.5	200(5)	203(6)
v ₂ (A ₂ ''), π(B-I ₃)	307.9 ^j	346(0)	336(0)
v ₃ (E'), v _{as} (B-I)	681.0	738(1)	741(<1)
v ₄ (E'), δ _d (I-B-I)	105.3	108(1)	106(2)

^a Values in parentheses represent experimental uncorrected relative Raman intensities (see Table S3) or calculated Raman intensities (in Å⁴ amu⁻¹). ^b Frequencies have been calculated for D_{3h} symmetry and have been assigned under this symmetry. ^c From ref. 10. ^d The v₁ band is split as a result of the mass effect of the ³⁵Cl and ³⁷Cl isotopes: 554.1(100) (C³⁵Cl₃), 549.1(96) (C³⁵Cl₂³⁷Cl), 544.1(32) (C³⁵Cl³⁷Cl₂) and 538.8(3) (C³⁷Cl₃) cm⁻¹; the most intense band has been scaled to 100 (see Figure 4). ^e From ref. 6. ^f From ref. 4 and ref. 5. ^g From ref. 14. ^h From ref. 64. ⁱ From ref. 65. ^j Observed as 2v₂(A₂''). ^k From ref. 66.

Table S2. Experimental and Calculated Frequencies (cm^{-1}) and Intensities for CX_4 (T_d)^a
 CF_4

assignt.	expt. ^b	6-31G(2d)		cc-pVTZ	
		HF	MP2	HF	MP2
$\nu_1(\text{A}_1), \nu_s$	908.4	995(5)	904(6)	1012(4)	925(5)
$\nu_2(\text{E}), \delta_s$	434.5	476(<1)	435(<1)	480(<1)	440(<1)
$\nu_3(\text{T}_2), \nu_{\text{as}}$	1283.0	1435(1)	1295(<1)	1448(1)	1312(<1)
$\nu_4(\text{T}_2), \delta_{\text{as}}$	631.2	684(1)	626(1)	694(1)	640(1)

 CCl_4

assignt.	expt. ^c	6-31G(2d)		cc-pVTZ	
		HF	MP2	HF	MP2
$\nu_1(\text{A}_1), \nu_s$	459(100) ^d		494(18)	463(15)	496(17) 471
$\nu_2(\text{E}), \delta_s$	220(58)		238(2)	222(3)	237(3) 221
$\nu_3(\text{T}_2), \nu_{\text{as}}$	794(20), 761(16)		891(9)	796(3)	889(8) 810
$\nu_4(\text{T}_2), \delta_{\text{as}}$	317(68)		340(3)	321(3)	340(4) 321

 CBr_4

assignt.	expt. ^c	6-31G(2d)		cc-pVTZ	
		HF	MP2	HF	MP2
$\nu_1(\text{A}_1), \nu_s$	269(100)		302(16)	285	292(16) 282
$\nu_2(\text{E}), \delta_s$	128(33)		145(2)	135	138(2) 129
$\nu_3(\text{T}_2), \nu_{\text{as}}$	673(15), 664(15), 658(10)		789(13)	713	770(17) 708
$\nu_4(\text{T}_2), \delta_{\text{as}}$	182(41), 184(47)		208(2)	196	201(3) 190

 Cl_4

assgnt.	expt. ^e	(SDB-)cc-pVTZ	
		HF	MP2
$\nu_1(\text{A}_1), \nu_s$	178(10)	201(16)	195
$\nu_2(\text{E}), \delta_s$	90(4)	94(2)	87
$\nu_3(\text{T}_2), \nu_{\text{as}}$	555, vs ^f	672(27)	618
$\nu_4(\text{T}_2), \delta_{\text{as}}$	123(5)	137(3)	129

^a Values in parentheses represent observed or calculated Raman intensities. ^b From R.J.H. Clark, D.M. Rippon *Chem. Commun.*, **1971**, 1295. ^c This work, pure solid compound (-120 °C). ^d The ν_1 band is split as a result of the mass effect of the ^{35}Cl and ^{37}Cl isotopes: 462(95) (C^{35}Cl_3), 459(100) ($\text{C}^{35}\text{Cl}_2^{37}\text{Cl}$), 456(51) ($\text{C}^{35}\text{Cl}^{37}\text{Cl}_2$) and 453(19) (C^{37}Cl_3) cm^{-1} . ^e From H. Stammreich, Y. Tavares, D. Bassi *Spectrochim. Acta* **1961**, 17, 661. ^f This band was only observed in the infrared spectrum; vs denotes very strong.

Table S3. Raman Frequencies and Assignments for $[CCl_3][Sb(OTeF_5)_6]$ and $[CBr_3][Sb(OTeF_5)_6] \cdot nSO_2ClF$ and Related Species

frequencies (cm^{-1})			assgnts				
CCl_3^+ ^{a,b}	CBr_3^+ ^{c,d,e}	CBr_3^+ ^{d,e,f}	CX_3^+	CBr_4	$OTeF_5^g$	non-coordinated SO_2ClF	coordinated SO_2ClF^h
554(19)							
549(19)							
544(6)	321(33)	321(33)			$v_1(A_1')$		
539(<1)							
327(9)	188(48)	187(15)					
	184(54)	184(18)			$v_4(E')$		
673(24)							
668, sh							
653, sh	654(28)				$v_3(F_2)$		
188(48)	187(15)				$v_4(F_2)$		
184(54)	184(18)						
269(93)					$v_1(A_1)$		
128(36)					$v_2(E)$		
1454(2)							
1449(3)							
1095(2), br					$v(CO)^i$		
1444(4)							
1433(14)	1433(18)						
1427, sh						$v_{\text{asym}}(SO_2)$	
1224(32)	1224(42)					$v_{\text{sym}}(SO_2)$	
1219(26)	1218(39)						
847(5)						$v(SF)$	
839(6)							

Table S3. (continued...)

$\text{CCl}_3^{+ \text{a},\text{b}}$	$\text{CBr}_3^{+ \text{c},\text{d},\text{e}}$	$\text{CBr}_3^{+ \text{d},\text{e},\text{f}}$	CX_3^{+}	CBr_4	OTeF_5^{g}	non-coordinated SO_2ClF	coordinated $\text{SO}_2\text{ClF}^{\text{h}}$
	1415(4)	1415(11)					$\nu_{\text{asym}}(\text{SO}_2)$
	1407(4)						
	1166(8)	1168(14)					$\nu_{\text{sym}}(\text{SO}_2)$
	819, sh						$\nu(\text{SF})$
822(5)	827(7), br	830(10),br			j		
751(3)	749(11)						
	745(11)	745(21)			$\nu_8(\text{E}), \nu_{\text{as}}(\text{TeF}_4)$		
724(17)	721(21)						
	717(21)	716(32)					
712(7)	714(22)				$\nu_1(\text{A}_1), \nu(\text{TeF})$		
702(100)	703(67)	703(60)			+ $\nu_s(\text{TeO} + \text{XeO})^k$		
690(8)	693(24)	693(25)					
	690, sh						
686(2)	682(9)	685(18)					
	677(9)	679(19)					
665(8)	668, sh	669(55)			$\nu_2(\text{A}_1), \nu_s(\text{TeF}_4)$		
659(40)	663(100)	663(100)					
653(19)	653, sh	654(28)					
641(10)	648(24)	648(26),br			$\nu_5(\text{B}_1), \nu_{\text{as}}(\text{TeF}_4)$		
	633(14)	635(18),br					
519(<1)		515(6)			j		
505(<1)	503(13)	503(21)			j		
	494(7)	495(10)					
	485, sh						
	480(16)	480(21)			$\nu_s(\text{TeO} + \text{XeO})^k$		
	476, sh						
464(2)	460(5), br						

Table S3. (continued...)

$\text{CCl}_3^{+ \text{a},\text{b}}$	$\text{CBr}_3^{+ \text{c},\text{d},\text{e}}$	$\text{CBr}_3^{+ \text{d},\text{e},\text{f}}$	CX_3^+	CBr_4	OTeF_5^{g}	non-coordinated SO_2ClF	coordinated $\text{SO}_2\text{ClF}^{\text{h}}$
451(1)	438(25) ^m 435(27) ^m 432(26) ^m 428(29) ^m 420(13)	440(14) ^m 430(54),br ^m				$\nu_3(\text{A}_1)$, $\nu(\text{TeO})$ also coupled with $\nu_s(\text{Sb-O})^l$	
414(23)	413, sh						
395(5)	408(29)	409(31),br					
369(7)	367(11)	367(15)					
342(5)	341, sh	340(19)			$\nu_9(\text{E})$, $\delta(\text{FTeF}_4)$		
339(14)	333(20)	332(23)					
320(7)					$\nu_{10}(\text{E})$, $\nu(\text{OTeF}_5)$		
310(19)	309(26)	309(44)			$\nu_4(\text{A}_1)$, $\delta_s(\text{FTeF}_4)$		
306(16)	305, sh ⁿ	298(50) ⁿ			$\nu_7(\text{B}_2)$, $\delta_{\text{sciss}}(\text{TeF}_4)$		
	257(7)	258(13)					
	253(9)	254(13)					
246(9)	249(9)				$\nu_{11}(\text{E})$, $\delta_{\text{as}}(\text{TeF}_4)$		
243(6)	240(16)	240(18)					
231(4)	231, sh						
	228(6)	230(10)			$\delta(\text{TeOSb})^l$		
	215(4)	215(8)					
	173(9)	173(14)			$\delta(\text{FTeO})^k$		
	167, sh						
148(14)	145, sh	146(16)			$\tau(\text{TeOSb})^l$		
	141(19)	141(19)					
137(10)	134(12)	136(14)					
123(7)	128(36)				$\delta(\text{XeOTe})^k$		
118(3)	120(12)	121(15)					
100(1)	111(13)	110(14)			lattice modes		

Table S3. (continued...)

^a The Raman spectrum of the solid obtained from the reaction of excess CCl₄ with [XeOTeF₅][Sb(OTeF₅)₆] in SO₂ClF at -78 °C (eq 1). ^b Experimental Raman intensities are given in parentheses. ^c The Raman spectrum of the solid obtained from the reaction of excess CBr₄ with [XeOTeF₅][Sb(OTeF₅)₆] in SO₂ClF at -78 °C (eq 2-7). ^d Infrared intensities, in km mol⁻¹, are given in square brackets. ^e The symbol, sh, denotes a shoulder and br denotes a broad line. ^f The Raman spectrum of the solid obtained from the reaction of excess [XeOTeF₅][Sb(OTeF₅)₆] with CBr₄ in SO₂ClF at -78°C (eq 2-7). ^g The OTeF₅ group assignments for OTeF₅ derivatives resulting from the reactions of CBr₄ with [XeOTeF₅][Sb(OTeF₅)₆] are tentative due to overlap of their Raman bands. The vibrational modes of the OTeF₅ groups are assigned under C_{4v} symmetry (ref. 54). ^h Free SO₂ClF was observed, along with coordinated SO₂ClF, in sample mixtures that were incompletely pumped at -78 °C. ⁱ These modes are most likely assigned to the CBr_{3-n}(OTeF₅)_n⁺ cations (n = 1-3). ^j Unassigned modes. ^k These modes are most likely assigned to the XeOTeF₅⁺ cation (ref. 69). ^l These modes are most likely assigned to the Sb(OTeF₅)₆⁻ anion. ^m These bands may overlap with v₅(S-Cl) of SO₂ClF. ⁿ These bands may overlap with Br₂ which occurs at 296.5 and 302.5 cm⁻¹.

Table S4. Experimental and Calculated Geometrical Parameters and NBO Study (MP2) for CX₄ (*T*_d)

CF ₄		CCl ₄														
	expt.	6-31G(2d)				cc-pVTZ			C-Cl	6-31G(2d)				cc-pVTZ		
		HF	MP2	HF	MP2	CCSD(T)	HF	MP2		HF	MP2	HF	MP2	CCSD(T)		
C-F	1.315(3) ^d	1.296	1.323	1.296	1.319	1.319			1.77(6) ^a	1.768	1.781	1.764	1.768	1.777		
F-C-F	109.6(3) ^d								1.751(13) ^c							
F ... F	2.148(4) ^d	2.117	2.161	2.116	2.154	2.154	Cl-C-Cl		2.89(12) ^a	2.888	2.908	2.881	2.887	2.902		
							Cl ... Cl		2.859(6) ^c							
CBr ₄		CI ₄														
	expt.	6-31G(2d)				cc-pVTZ			C-I	(SDB-)cc-pVTZ						
		HF	MP2	HF	MP2	CCSD(T)	HF	MP2		HF	MP2	CCSD(T)				
C-Br	1.91(4) ^b	1.923	1.931	1.934	1.928	1.940	2.155(1)	2.131	2.127	2.137						
Br-C-Br							109.5(1)									
Br ... Br	3.12(7) ^b	3.140	3.154	3.158	3.148	3.168	I-C-I									
							I ... I	3.518(1)	3.480	3.473	3.489					
CF ₄		6-31G(2d)				CCl ₄		6-31G(2d)								
charge	C	1.37	1.25	valency	C	charge	C	-0.29	-0.19							
	F	-0.34	-0.31				Cl	0.07	0.05							
valency	C	3.30	2.82	F	C	valency	C	3.36	3.56							
	F	0.75	0.61				Cl	0.71	0.76							
bond order	C-F	0.82	0.70	C-Br	C	bond order	C-Cl	0.84	0.89							
	F---F	-0.02	-0.03				Cl---Cl	-0.04	-0.04							
CBr ₄		6-31G(2d)				CI ₄		(SDB-)cc-pVTZ								
charge	C	-0.63	-0.55	valency	C	charge	C	-1.19								
	Br	0.16	0.14				I	0.30								
valency	C	3.13	3.34	Br	C	valency	C	3.16								
	Br	0.68	0.71				I	0.69								
bond order	C-Br	0.78	0.83	C-Br	C	bond order	C-I	0.79								
	Br---Br	-0.03	-0.04				I---I	-0.03								

^a Neutron diffraction from P. Jóvári, G. Mészáros, L. Pusztai, E. Sváb, *J. Chem. Phys.* **2001**, *114*, 8082. ^b X-ray diffraction M. More, F. Baert, J. Lefebvre *Acta Cryst.* **1977**, *B33*, 3681. (Phase I). ^c X-ray diffraction S. Cohen, R. Powers, R. Rudman, *Acta Cryst.* **1979**, *B35*, 1670.
^d A.N. Fitch, J.K. Cockcroft *Z. Kristallogr.* **1993**, *203*, 29. ^e S. Pohl *Z. Kristallogr.* **1982**, *159*, 211

Table S5. Calculated^a Natural Atomic Charges, Mayer Bond Orders and Mayer Natural Atomic Orbital Valencies, for CX_3^+ , CX_4 , and BX_3 ($\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$)

$\text{CX}_3^+ (D_{3h})$		F	Cl	Br	I
natural Charge q	C (X)	1.37 (-0.12)	-0.09 (0.36)	-0.45 (0.48)	-1.10 (0.70)
bond order	C-X (X…X)	0.88 (-0.04)	1.09 (-0.05)	1.04 (-0.05)	0.99 (-0.06)
valency	C (X)	2.64 (0.81)	3.28 (0.99)	3.12 (0.93)	2.97 (0.88)
p_π populations	C (X)	0.59 (1.77)	0.91 (1.65)	1.00 (1.62)	1.13 (1.57)
σ donation (π donation) ^b	C→X (X→C)	0.32 (0.19)	-0.06 (0.31)	-0.15 (0.33)	-0.32 (0.38)

$\text{CX}_4 (T_d)$		F	Cl	Br	I
natural Charge q	C (X)	1.25 (-0.31)	-0.11 (0.03)	-0.56 (0.14)	-1.19 (0.30)
bond order	C-X (X…X)	0.70 (-0.03)	0.90 (-0.04)	0.83 (-0.04)	0.79 (-0.03)
valency	C (X)	2.82 (0.61)	3.61 (0.79)	3.34 (0.71)	3.16 (0.69)

$\text{BX}_3 (D_{3h})$		F	Cl	Br	I
natural Charge q	B (X)	1.39 (-0.46)	0.34 (-0.11)	0.06 (-0.02)	-0.49 (0.16)
bond order	B-X (X…X)	0.86 (-0.02)	1.08 (-0.04)	1.09 (-0.04)	1.16 (-0.04)
valency	B (X)	2.58 (0.81)	3.24 (1.00)	3.27 (1.00)	3.47 (1.07)
p_π populations at	B (X)	0.32 (1.86)	0.48 (1.79)	0.53 (1.78)	0.63 (1.74)
σ donation (π donation) ^b	B→X (X→B)	0.57 (0.11)	0.27 (0.16)	0.20 (0.18)	0.04 (0.21)

^a MP2/(SDB-)cc-pVTZ. ^b The value given is per bond; a negative sign indicates donation in reversed order.

Table S6. Valence Natural Atomic Orbital (NAO) Populations in the Calculated Species

CX₃⁺		MP2/cc-pVTZ				BX₃				MP2/cc-pVTZ				
		F	Cl	Br	I	B	s	0.40	0.75	0.85	I	F	Cl	Br
C	s	0.67	1.11	1.23	1.37	B	s	0.40	0.75	0.85	1.01			
	p _y	0.64	0.97	1.04	1.22		p _y	0.40	0.67	0.72	0.85			
	p _x	0.64	0.97	1.04	1.22		p _x	0.40	0.67	0.72	0.85			
	p _z	0.59	0.91	1.00	1.13		p _z	0.32	0.48	0.53	0.63			
X(1)	s	1.83	1.80	1.81	1.81	X(1)	s	1.84	1.81	1.81	1.78			
	p _y	1.54	1.19	1.08	0.90		p _y	1.76	1.49	1.42	1.30			
	p _x	1.90	1.88	1.89	1.89		p _x	1.92	1.89	1.89	1.88			
	p _z	1.77	1.65	1.62	1.57		p _z	1.86	1.79	1.78	1.74			
X(2)	s	1.83	1.80	1.81	1.81	X(2)	s	1.84	1.81	1.81	1.78			
	p _y	1.81	1.71	1.69	1.64		p _y	1.88	1.79	1.78	1.74			
	p _x	1.63	1.36	1.28	1.14		p _x	1.80	1.59	1.54	1.42			
	p _z	1.77	1.65	1.62	1.57		p _z	1.86	1.79	1.78	1.74			
X(3)	s	1.83	1.80	1.81	1.81	X(3)	s	1.84	1.81	1.81	1.78			
	p _y	1.81	1.71	1.69	1.64		p _y	1.88	1.79	1.78	1.74			
	p _x	1.63	1.36	1.28	1.14		p _x	1.80	1.59	1.54	1.42			
	p _z	1.77	1.65	1.62	1.57		p _z	1.86	1.79	1.78	1.74			
CF₃⁺		HF/cc-pVTZ				BF₃				HF/cc-pVTZ				
C	s	0.65				B	s	0.37						
	p _y	0.63					p _y	0.38						
	p _x	0.63					p _x	0.38						
	p _z	0.46					p _z	0.26						
F(1)	s	1.83				F(1)	s	1.85						
	p _y	1.57					p _y	1.79						
	p _x	1.94					p _x	1.95						
	p _z	1.83					p _z	1.91						
F(2)	s	1.83				F(2)	s	1.85						
	p _y	1.85					p _y	1.91						
	p _x	1.66					p _x	1.83						
	p _z	1.83					p _z	1.91						
F(3)	s	1.83				F(3)	s	1.85						
	p _y	1.85					p _y	1.91						
	p _x	1.66					p _x	1.83						
	p _z	1.83					p _z	1.91						

Table S6. (continued ...)

C(OTeF₅)₃⁺ HF/SDB-cc-pVTZ**B(OTeF₅)₃** HF/SDB-cc-pVTZ

C	<i>s</i>	0.65			B	<i>s</i>	0.37		
	<i>p_y</i>	0.72				<i>p_y</i>	0.43		
	<i>p_x</i>	0.72				<i>p_x</i>	0.43		
	<i>p_z</i>	0.56				<i>p_z</i>	0.27		
		(1)	(2)	(3)			(1)	(2)	(3)
O	<i>s</i>	1.67	1.67	1.67	O	<i>s</i>	1.70	1.70	1.70
	<i>p_y</i>	1.52	1.72	1.82		<i>p_y</i>	1.70	1.74	1.88
	<i>p_x</i>	1.85	1.65	1.55		<i>p_x</i>	1.85	1.81	1.67
	<i>p_z</i>	1.80	1.80	1.80		<i>p_z</i>	1.88	1.88	1.88
		(1)	(2)	(3)			(1)	(2)	(3)
Te	<i>s</i>	0.72	0.72	0.72	Te	<i>s</i>	0.71	0.71	0.71
	<i>p_y</i>	0.38	0.37	0.37		<i>p_y</i>	0.38	0.37	0.37
	<i>p_x</i>	0.37	0.37	0.38		<i>p_x</i>	0.37	0.37	0.38
	<i>p_z</i>	0.37	0.37	0.37		<i>p_z</i>	0.37	0.37	0.37
		(1)	(2)	(3)			(1)	(2)	(3)
F	<i>s</i>	1.92	1.92	1.92	F	<i>s</i>	1.92	1.92	1.92
	<i>p_y</i>	1.87	1.79	1.96		<i>p_y</i>	1.87	1.81	1.97
	<i>p_x</i>	1.88	1.95	1.79		<i>p_x</i>	1.90	1.96	1.80
	<i>p_z</i>	1.97	1.97	1.97		<i>p_z</i>	1.97	1.97	1.97
		(5)	(6)	(7)			(5)	(6)	(8)
F	<i>s</i>	1.92	1.92	1.92	F	<i>s</i>	1.92	1.92	1.92
	<i>p_y</i>	1.96	1.88	1.92		<i>p_y</i>	1.97	1.89	1.94
	<i>p_x</i>	1.89	1.97	1.93		<i>p_x</i>	1.89	1.97	1.92
	<i>p_z</i>	1.87	1.87	1.88		<i>p_z</i>	1.88	1.88	1.88
		(9)	(10)	(11)			(9)	(10)	(11)
F	<i>s</i>	1.92	1.92	1.92	F	<i>s</i>	1.92	1.92	1.92
	<i>p_y</i>	1.89	1.93	1.96		<i>p_y</i>	1.89	1.93	1.97
	<i>p_x</i>	1.96	1.91	1.89		<i>p_x</i>	1.97	1.92	1.89
	<i>p_z</i>	1.88	1.87	1.87		<i>p_z</i>	1.88	1.88	1.88
		(13)	(14)	(15)			(13)	(14)	(15)
F	<i>s</i>	1.92	1.92	1.92	F	<i>s</i>	1.92	1.92	1.92
	<i>p_y</i>	1.92	1.97	1.89		<i>p_y</i>	1.94	1.97	1.89
	<i>p_x</i>	1.92	1.88	1.97		<i>p_x</i>	1.92	1.90	1.97
	<i>p_z</i>	1.88	1.88	1.88		<i>p_z</i>	1.88	1.88	1.88

CX₄ MP2/cc-pVTZ**F Cl Br I**

C	<i>s</i>	0.71	1.15	1.27	1.41
	<i>p_y</i>	0.64	0.96	1.04	1.20
	<i>p_x</i>	0.64	0.96	1.04	1.20
	<i>p_z</i>	0.64	0.96	1.04	1.20
X(all)	<i>s</i>	1.85	1.83	1.84	1.84
	<i>p_y</i>	1.80	1.71	1.63	1.57
	<i>p_x</i>	1.80	1.71	1.63	1.57
	<i>p_z</i>	1.80	1.71	1.63	1.57