SUPPORTING INFORMATION

Synthesis and Structural Characterization of C(OTeF₅)₄, and a Comparative Structural Study of the Isoelectronic B(OTeF₅)₄⁻ Anion

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Figure S1. The two different orientations of the disordered molecules (2) in the unit cell of $\text{C}(\text{OTeF}_5)_4$.

Table S1. Experimental (C_1) and Calculated (C_1 and S_4)^a Te–O–C/B–O Torsion Angles (deg) for C(OTeF₅)₄ and B(OTeF₅)₄[–]

C(OTeF ₅) ₄ ^b					B(OTeF ₅) ₄ [–]			
exptl (C_1)	exptl (C_1)	exptl (C_1)	calcd (C_1)	calcd (S_4)	exptl (C_1)	calcd (C_1)	calcd (S_4) ^c	calcd (S_4)
78.0	77.5	86.6	71.7	71.9	71.3	68.6	89.4	104.8
74.7	76.2	75.0	71.6		70.4	68.6		
72.0	70.7	67.4	71.5		64.1	60.0		
63.5	65.8	66.4	71.4		61.1	60.0		
55.0	51.8	52.3	47.5	47.0	47.3	49.7	29.9	15.2
45.2	45.5	51.0	47.4		48.5	49.8		
43.8	44.8	49.3	47.3		54.0	58.7		
42.2	44.4	28.8	47.2		57.9	58.7		
174.4	171.2	174.0	107.8	169.3	179.7	179.4	151.2	135.3
169.9	168.4	169.4	169.7		176.6	179.3		
169.7	168.3	169.0	169.6		171.2	173.7		
163.5	165.1	155.3	169.5		170.4	173.7		

^a SVWN/(SDB-)cc-pVTZ. ^b The quoted torsion angles are for the non-disordered C(OTeF₅)₄ molecules. ^c Calculated S_4 geometry with one imaginary frequency.

Table S2. Experimental and Calculated Vibrational Frequencies^a for E(OTeF₅)₄⁻⁰ (E = B, C)^c

¹² C(OTeF ₅) ₄		B(OTeF ₅) ₄ ⁻			assgnts (<i>S</i> ₄) ^c
	calcd (<i>S</i> ₄) ^c	exptl ^{b,d}	calcd (<i>S</i> ₄) ^c		
1084(2) 1078 sh } 1070(<1) 1064 sh }	1097(15)	989(7), br	1026(6)	1065[690]	E, v(EO – EO)
	1083(8)	989(7), br	1019(8)	1040[459]	B, v(EO ₂ – EO ₂)
1023(2)	1010(31)	958(4) 951(7) }	981(80)	968[0]	A, v(EO ₄ – 4TeO)
813.5(3)	794(16)	800(7)	787(15)	781[<1]	E, v(2TeO – 2TeO)
756(1)	741(2)	761(4)	774(8)	785[54]	B, v[2(TeO – TeF _a) + 2(TeF _a – TeO) + 4(TeF _{e trans} – TeF _{e trans})] _{small}
747.3(2)	731(1)	754(7)	708(1)	709[225]	E, v[4(TeF _{e trans} – TeF _{e trans})] + δ(EO ₂ – EO ₂) _{small}
	732(1)	746(5)	710(2)	710[322]	B, δ(EO ₂ – EO ₂) + v[(2(TeO – TeF _a) + 2(TeF _a – TeO) + 4(TeF _{e trans} – TeF _{e trans})]
	730(2)	738(4)	704(4)	706[0]	A, v[4(TeF _{e trans} – TeF _{e trans})]
736.8 sh } 734.7(6) }	728(2)	721(7) 718(11) }	707(2)	707[90]	B, δ(EO ₂ – EO ₂) _{small} + v[4(TeF _{e trans} – TeF _{e trans})]
	725(6)		696(9)	700[0]	A, v[4(TeF _{e trans} – TeF _{e trans})]
	720(<1)		698(<1)	699[38]	E, v[2(TeF _{e trans} – TeF _{e trans}) + 2(TeF _{2e cis} – TeF _{2e cis})]
721.0(44)	708(21)	709 sh 702(100) }	675(60)	677[0]	A, v(4TeF _a)
714.5(10) 711(6) }	699(6)	688(8) 682(7) }	660(6)	662[155]	E, v(2TeF _a – 2TeF _a)
705(9)	691(10)	675(7)	659(17)	659[63]	B, δ(EO ₂ – EO ₂) + v(2TeF _a – 2TeF _a)
678(100)	659(91)	649(78) 646 sh }	636(63)	636[0]	A, v(4TeF _{4e})

Table S2. (continued ...)

668(11)	}	658(2)	640(18)	627(1)	628[1]	B, $\delta(4\text{EOTe}) + \nu(2\text{TeF}_{4\text{e}} - 2\text{TeF}_{4\text{e}})$
664(11)		654(4)		632(4)	633[3]	B, $\nu[4(\text{TeF}_{2\text{e trans}} - \text{TeF}_{2\text{e trans}})]$
		651(5)		630(<1)	631[1]	E, $\nu[(2\text{TeF}_{2\text{e trans}} - 2\text{TeF}_{2\text{e trans}})]$
		651(7)		629(7)	629[0]	A, $\nu[4(\text{TeF}_{2\text{e trans}} - \text{TeF}_{2\text{e trans}})]$
		650(2)		628(2)	628[<1]	E, $\nu[(\text{TeF}_{4\text{e}} - \text{TeF}_{4\text{e}}) + 2(\text{TeF}_{2\text{e trans}} - \text{TeF}_{2\text{e trans}})]$
633(<1)		640(3)	461(3)	479(12)	516[<<1]	B, $\delta(2\text{EOTe} - 2\text{EOTe}) + \nu(4\text{TeF}_{4\text{e}})$
533(11)	}	540(56)	521(13)	524(39)	522[0]	A, $\delta(4\text{EOTe})$
512 sh			514 sh			
			506(8)			
			500 sh			
442(2)		444(5)	333(10)	353(3)	383[0]	A, $\rho_t(4\text{EOTe})$
428(3)		430(2)	396(3)	457(<1)	446[71]	E, $\rho_w(\text{EO}_2)$
			375(3)			
			370 sh			
			348(3)			
339(<1)		361(<1)	311 sh	317(6)	331[157]	B, $\rho_w(\text{EO}_4)$
324(9)		326(<1)	318(6)	323(<1)	329[0]	A, $\rho_r(\text{EO}_2 - \text{EO}_2) + \delta(2\text{TeF}_{4\text{e umbrella}} - 2\text{TeF}_{4\text{e umbrella}})$
320(14)	}	307(1)	304(14)	315(1)	315[23]	strongly coupled deformations and torsion modes involving both OTeF_5 and EOTe moieties
313(16)		306(1)		313(3)	314[21]	
302(1)		303(2)		312(<1)	313[0]	
		302(<1)		310(18)	311[7]	
		300(1)		310(<1)	309[18]	
		299(1)		306(<1)	306[0]	
		298(<1)		307(<1)	308[56]	
		296(<1)		307(<1)	306[137]	

Table S2. (continued ...)

269(<1)	$\left\{ \begin{array}{l} 292(1) \\ 286(2) \\ 284(<1) \\ 282(1) \end{array} \right.$	284 (1)	$\left\{ \begin{array}{l} 291(4) \\ 279(<1) \\ 276(<1) \\ 276(<1) \end{array} \right.$	$\left. \begin{array}{l} 295[26] \\ 278[<1] \\ 277[0] \\ 277[<1] \end{array} \right\}$	strongly coupled deformations and torsion modes involving both OTeF ₅ and EOTe moieties
252(11)	$\left. \begin{array}{l} \left\{ \begin{array}{l} 236(<1) \\ 234(<1) \\ 234(2) \\ 233(2) \\ 230(<1) \end{array} \right\} \\ \left\{ \begin{array}{l} 248 \text{ sh} \\ 246(5) \\ 236(3) \\ 233(3) \end{array} \right\} \end{array} \right\}$		$\left\{ \begin{array}{l} 234(<1) \\ 231(<1) \\ 228(1) \\ 220(<1) \\ 211(<1) \end{array} \right.$	$\left. \begin{array}{l} 234[0] \\ 230[8] \\ 228[2] \\ 222[0] \\ 217[4] \end{array} \right\}$	
249(11)					
244 sh					
184(<1)	$\left\{ \begin{array}{l} 200(<1) \\ 194(<1) \\ 193(<1) \\ 190(<1) \end{array} \right.$		$\left\{ \begin{array}{l} 204(<1) \\ 200(<1) \\ 200(<1) \\ 189(<1) \end{array} \right.$	$\left. \begin{array}{l} 202[<1] \\ 199[0] \\ 199[<<1] \\ 189[<1] \end{array} \right\}$	
145(4)	$\left. \begin{array}{l} \left\{ \begin{array}{l} 134(1) \\ 130(<1) \\ 128(1) \\ 123(<1) \\ 120(<1) \end{array} \right\} \\ \left\{ \begin{array}{l} 145(4) \\ 138(4) \\ 136 \text{ sh} \\ 127(4) \\ 126 \text{ sh} \end{array} \right\} \end{array} \right\}$		$\left\{ \begin{array}{l} 135(1) \\ 131(<1) \\ 126(<1) \\ 124(<1) \\ 105(<1) \end{array} \right.$	$\left. \begin{array}{l} 133[0] \\ 130[<<1] \\ 124[0] \\ 121[<1] \\ 108[<1] \end{array} \right\}$	
142(4)					
135(4)					
108(1)	$\left\{ \begin{array}{l} 98(1) \\ 93(<1) \end{array} \right.$		$\left\{ \begin{array}{l} 93(<1) \\ 96(<1) \end{array} \right.$	$\left. \begin{array}{l} 87[0] \\ 92[<1] \end{array} \right\}$	
	47(<1)		47(<1)	37[<1]	
	39(<1)		36(<1)	35[0]	
	33(<1)		42(<1)	35[<1]	
	32(<1)		41(<1)	33[<1]	
	27(<1)		28(<1)	10[<1]	
	22(<1)		28(<1)	9[<1]	
	17(<1)		8(<1)	-9[0]	

Table S2. (continued ...)

^a Frequencies are given in cm^{-1} . ^b Values in parentheses denote experimental uncorrected relative Raman intensities. The abbreviation denotes a shoulder (sh). ^c SVWN/(SDB-)cc-pVTZ. Raman intensities (in $\text{\AA}^4 \text{amu}^{-1}$) are given in parentheses. ^d The abbreviations denote stretch (ν), bend (δ), twist (ρ_t), wag (ρ_w), and rock (ρ_r). Bond elongations and angle openings are denoted by plus (+) signs and bond contractions and angle closings are denoted by minus (−) signs. The notations, F_a and F_e , refer to the axial fluorine atom and the four equatorial fluorine atoms of the OTeF_5 group; the notations TeF_{2e} and TeF_{4e} indicate that 2 or 4, respectively, $\text{Te}-F_e$ bond stretching motions are in phase. The notations, $F_{e \text{ trans}}$ and $F_{e \text{ cis}}$, indicate that the fluorine atoms are trans or cis to each other.