Electronic Structure Predictions of the Energetic Properties of Tellurium Fluorides

Monica Vasiliu,[1] Kirk A. Peterson,[2] Karl O. Christe,[3] and David A. Dixon[1,*]

[1]Department of Chemistry and Biochemistry, Shelby Hall, The University of Alabama, Box 870336, Tuscaloosa, AL 35487-0336

[2]Department of Chemistry, Washington State University, Pullman, Washington 99164-4630

[3]Loker Hydrocarbon Research Institute and Department of Chemistry University of Southern California, Los Angeles, CA 90089-1661

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Table S1. Optimized CCSD(T) Geometry Parameters: Bond Lengths (Å) and Angles (°).[a]

Molecule	**Basis set**	**R_{TeF}**	**∠FTeF**	**∠FTeF**
TeF^+ ($^3\Pi$, $C_{\infty v}$)	aVQZ	1.850		
TeF ($^2\Pi$, $C_{\infty v}$)	aVQZ	1.920		
TeF^- ($^1\Pi$, $C_{\infty v}$)	aVQZ	2.010		
TeF_2^+ ($^2B_1$, C_{2v})	aVQZ	1.837	95.3	
TeF_2 ($^1A_1$, C_{2v})	aVQZ	1.901	93.8	
TeF_2^- ($^2\Sigma_g^+$, $D_{\infty h}$)	aVQZ	2.092	180.0	
TeF_2^- ($^2B_2$, C_{2v})	aVQZ	2.025	76.7	
TeF_3^+ ($^1A_1$, C_{3v})	aVQZ	1.821	95.0	
TeF_3 ($^2B_1$, C_{2v})	aVQZ	1.867eq	83.1	166.2ax
		1.945ax(2)		
TeF_3^- ($^1A_1$, C_{2v})	aVQZ	1.933eq	83.3	166.7ax
		2.044ax(2)		
TeF_4^+ ($^2A_1$, C_{2v})	aVTZ	1.850eq	94.8	99.4eq
		1.879ax		165.2ax
TeF_4 ($^1A_1$, C_{2v})	aVTZ	1.861eq	84.2ax	100.8eq
		1.921ax		161.6ax
TeF_4^- ($^2B_1$, C_{2v})	aVTZ	1.964eq	85.1	78.4eq
		2.000ax		167.3ax
TeF_5^+ ($^1A_1'$, D_{3h})	aVTZ	1.813eq	90.0	120.0eq
		1.820ax		180.0ax
TeF_5 ($^2A_1$, C_{4v})	aVTZ	1.890eq	89.4	90.0eq
		1.840ax		
TeF_5^- ($^1A_1$, C_{4v})	aVTZ	1.974eq	81.9	88.9eq
		1.886ax		
TeF_6 ($^1A_{1g}$, O_h)	aVQZ	1.833	90.0	90.0
TeF_6^- ($^2A_{1g}$, O_h)	aVTZ	1.963	90.0	90.0
TeF_7^- ($^1A_1$, D_{5h})	aVTZ	1.923eq	90.0	72.0eq
		1.862ax		180.0ax
TeF_8^{2-} ($^1A_1$, D_{4d})	aVTZ	1.966	78.3, 114.2	

[a] ax = axial and eq = equatorial. Values in parentheses are from experiment.

Table S2. Total Energies at the CCSD(T) Level of Theory in Atomic Units.

Molecule	awCVDZ	awCVTZ	awCVQZ	CBS
Te^+	-267.534177	-267.913262	-268.086156	-268.189946
Te^-	-267.167188	-267.525614	-267.690602	-267.789762
TeF^+	-366.861942	-367.333507	-367.530666	-367.647653
TeF	-367.180745	-367.660807	-367.861296	-367.980240
TeF^-	-367.262297	-367.745763	-367.948975	-368.069643
TeF_2^+	-466.574211	-467.158311	-467.387453	-467.522160
TeF_2	-466.907808	-467.495350	-467.726864	-467.863056
$^2TeF_2^-(D_{\infty h})$	-466.981860	-467.567289	-467.799269	-467.935851
$^2TeF_2^-(C_{2v})$	-466.958624	-467.545509	-467.778031	-467.914928
TeF_3^+	-566.304505	-567.001444	-567.262515	-567.414896
TeF_3	-566.614527	-567.306684	-567.568111	-567.720900
TeF_3^-	-566.722778	-567.414927	-567.677854	-567.831658
TeF_4^+	-665.906698	-666.710988	-667.001882	-667.170703
TeF_4	-666.359760	-667.162806	-667.455726	-667.625962
TeF_4^-	-666.426848	-667.224520	-667.517719	-667.688331
TeF_5^+	-765.604954	-766.526125	-766.848814	-767.035076
TeF_5	-766.000166	-766.913375	-767.236549	-767.423417
TeF_5^-	-766.201722	-767.107408	-767.431520	-767.619286
TeF_6^+	-865.206459	-866.228519	-866.579028	-866.780601
TeF_6	-865.736060	-866.769840	-867.124734	-867.328865
TeF_6^-	-865.858719	-866.869709	-867.223045	-867.426917
TeF_7^+	-964.842105	-965.967228	-966.345972	-966.563059
TeF_7^-	-965.542780	-966.674803	-967.060057	-967.281310
TeF_8^{2-}	-1065.167451	-1066.396796	-1066.812633	-1067.051190

Table S3. Calculated B3LYP Vibrational Frequencies in cm^{-1} for TeF_3 and TeF_7^-.

Molecule	assignment	B3LYP/aVDZ
TeF_3 ($^2B_1$, C_{2v})	ν_1(sym stretch - a_1)	641.5
	ν_2(asym stretch - b_2)	556.9
	ν_3(asym stretch - a_1)	541.8
	ν_4(bending - b_2)	267.7
	ν_5(bending - a_1)	168.0
	ν_6(bending - b_1)	39.4
TeF_7^- ($^1A_1'$, D_{5h})	ν_1(asym stretch - a_2'')	645.2
	ν_2(sym stretch - a_1')	585.2
	ν_3(asym stretch - e_1')	572.8
	ν_4(asym stretch - a_1')	551.1
	ν_5(asym stretch - e_2')	494.6
	ν_6(asym stretch - e_2')	427.3
	ν_7(bending - e_1')	363.2
	ν_8(bending - a_2'')	299.4
	ν_9(bending - e_1'')	260.8
	ν_{10}(bending - e_1')	214.8
	ν_{11}(bending - e_1'')	20.7

Table S4. T1 values from CCSD(T)/awCVQZ(-PP).

Molecule	T1
Te	0.007
Te^+	0.007
Te^-	0.009
Te_2	0.010
TeH_2	0.011
TeO	0.030/0.008(pw91)
TeO^-	/0.014(pw91)
TeO_2	0.025
TeO_2^-	0.024
TeF^+	0.015
TeF	0.013
TeF^-	0.012
TeF_2^+	0.015
TeF_2	0.013
$^2TeF_2^-(D_{\infty h})$	0.014
$^2TeF_2^-(C_{2v})$	0.014
TeF_3^+	0.015
TeF_3	0.015
TeF_3^-	0.013
TeF_4^+	0.017
TeF_4	0.014
TeF_4^-	0.014
TeF_5^+	0.014
TeF_5	0.017
TeF_5^-	0.014
TeF_6^+	0.014
TeF_6	0.012
TeF_6^-	0.014
TeF_7^+	0.014
TeF_7^-	0.013
TeF_8^{2-}	0.014

Table S5. Calculated SO in kcal/mol at BLYP/TZ2P level in ADF.

Molecule	SO correction (SO-Scalar)
Te	-7.77
TeF^+	-1.43
TeF	-6.82
TeF^-	-2.35
TeF_2^+	-1.59
TeF_2	-2.38
$^2TeF_2^-(D_{\infty h})$	-5.90
$^2TeF_2^-(C_{2v})$	-2.23
TeF_3^+	-1.16
TeF_3	-1.42
TeF_3^-	-1.97
TeF_4^+	-1.09
TeF_4	-1.13
TeF_4^-	-1.50
TeF_5^+	-1.03
TeF_5	-1.04
TeF_5^-	-1.07
TeF_6^+	-1.04
TeF_6	-0.98
TeF_6^-	-0.96
TeF_7^+	-1.06
TeF_7^-	-1.00
TeF_8^{2-}	-1.00
FTeTeF	-4.08
F_2TeTe	-3.78
Te_2F_6	-2.74
Te_2F_{10}	-2.16

Table S6. Calculated bond distances at CCSD(T) level with different basis sets for diatomics.

Basis set	Te_2 ($^3\Sigma_g$, $D_{\infty h}$) R_{TeTe}	TeO ($^3\Sigma$, $C_{\infty v}$) R_{TeO}	TeO^- ($^2\Sigma$, $C_{\infty v}$) R_{TeO}
aVQZ	2.573	1.836	
aVQZ/PW91		1.835	1.907
awCVQZ	2.540		
awCVQZ/PW91		1.814	1.888
DK-awCVQZ	2.546	1.819	
DK-awCVQZ/PW91		1.819	1.893
Expt.			1.884 ± 0.028

Table S7. NBO6 populations for TeF_x molecules at B3LYP/aug-cc-pVDZ(-PP) level using CCSD(T) optimized geometries.

Molecule	qNBO, Te	qNBO F	5s(α/β)	5p(α/β)	5d
$^3TeF^+$	1.51	-0.51	1.94(0.97/0.97)	2.53(2.20/0.32)	
^2TeF	0.59	-0.59	1.94(0.97/0.97)	3.44(2.19/1.24)	
$^1TeF^-$	-0.33	-0.67	1.95	4.34	
$^2TeF_2^+$	2.07	-0.53	1.86(0.93/0.93)	2.03(1.45/0.57)	
$^1TeF_2$	1.20	-0.60	1.87	2.87	
$^2TeF_2^-(D_{\infty h})$	0.47	-0.74	1.99(1.00/1.00)	3.46(2.18/1.27)	
$^2TeF_2^-(C_{2v})$	0.39	-0.70	1.90(0.95/0.95)	3.61(2.21/1.40)	
$^1TeF_3^+$	2.66	-0.55	1.77	1.51	
$^2TeF_3$	1.93	-0.66(2), -0.60	1.87(0.94/0.93)	2.12(1.48/0.64)	
$^1TeF_3^-$	1.12	-0.73(2), -0.65	1.89	2.90	
$^2TeF_4^+$	2.98	-0.53(2), -0.46(2)	1.52(0.88/0.63)	1.44(0.77/0.67)	
$^1TeF_4$	2.56	-0.67(2), -0.61(2)	1.96	1.61	
$^2TeF_4^-$	1.81	-0.72(2), -0.69(2)	1.81(0.90/0.90)	2.23(1.50/2.73)	0.06
$^1TeF_5^+$	3.52	-0.50(3), -0.51(2)	1.08	1.35	
$^2TeF_5$	2.99	-0.59(4), -0.61	1.44(0.86/0.58)	1.48(0.82/0.67)	
$^1TeF_5^-$	2.52	-0.72(4), -0.66	1.76	1.61	
$^2TeF_6^{+a}$	3.48	-0.51(5), 0.08	1.08(0.54/0.54)	1.37(0.68/0.69)	0.05
$^1TeF_6$	3.57	-0.59	1.01	1.35	0.05
$^2TeF_6^{-b}$	3.02	-0.67	1.58(1.00/0.58)	1.31(0.63/0.68)	0.05
$^1TeF_7^{+c}$	3.42	-0.50(5), -0.02, 0.11	1.13	1.39	0.05
$^1TeF_7^-$	3.49	-0.65(5), -0.63(2)	1.06	1.37	0.05
$^1TeF_8^{2-}$	3.42	-0.68	1.09	1.39	0.05

[a] $^2TeF_6^+$; F: 2s: 1.99(1.00/0.99), 2p: 4.92(2.95/1.97); regular F: 2s 1.95(0.97/0.97), 2p: 5.54(2.77/2.77)

[b] $^2TeF_6^-$; F: 2s: 1.96(0.98/0.98), 2p: 5.70(2.90/2.80);

[c] $^1TeF_7^+$; F: 2s: 1.97, 2p: 4.91; regular F: 2s: 1.95, 2p: 5.53(oneF:5.05);

Table S8. NBO6 populations for SeF_x molecules at B3LYP/aug-cc-pVDZ(-PP) level using CCSD(T) optimized geometries.

Molecule	qNBO, Se	qNBO F	4s(α/β)	4p(α/β)	4d
$^3SeF^+$	1.40	-0.40	1.93(0.97/0.96)	2.65(2.24/0.41)	
^2SeF	0.51	-0.51	1.94(0.97/0.97)	3.53(2.23/1.30)	
$^1SeF^-$	-0.39	-0.61	1.95	4.40	
$^2SeF_2^+$	1.85	-0.43	1.85(0.93/.0.92)	2.25(1.54/0.71)	
$^1SeF_2$	1.04	-0.52	1.86	3.03	
$^2SeF_2^-$	0.36	-0.68	2.00(1.00/1.00)	3.57(2.23/1.34)	
$^1SeF_3^+$	2.36	-0.45	1.75	1.82	
$^2SeF_3$	1.69	-0.59(2), -0.51	1.88(0.94/0.93)	2.35(1.56/0.78)	
$^1SeF_3^-$	0.95	-0.69(2), -0.58	1.90	3.06	
$^2SeF_4^+$	2.60	-0.43(2), -0.37(2)	1.54(0.88/0.66)	1.77(0.94/0.83)	0.06
$^1SeF_4$	2.25	-0.52(2), -0.60(2)	1.76	1.90	0.05
$^2SeF_4^-$	1.56	-0.62(2), -0.66(2)	1.83(0.92/0.92)	2.48(1.61/0.87)	0.06
$^1SeF_5^+$	3.06	-0.43(2), -0.40(3)	1.15	1.70	0.08
$^2SeF_5$	2.58	-0.52	1.50(0.87/0.63)	1.81(0.98/0.84)	0.07
$^1SeF_5^-$	2.19	-0.65(4), -0.57	1.80	1.90	0.06
$^2SeF_6^{+a}$	2.93	-0.40(5),0.07	1.23(0.61/0.61)	1.75(0.87/0.88)	0.07
$^1SeF_6$	3.04	-0.51	1.14	1.71	0.08
$^2SeF_6^{-b}$	2.57	0.59	1.64(1.00/0.64)	1.69(0.82/0.87)	0.06
$^1SeF_7^{+c}$	3.01	-0.39(3), -0.42(2), 0.01, -0.01	1.18	1.71	0.08
$^1SeF_7^-$	2.88	-0.57(5), -0.52(2)	1.23	1.77	0.08

[a] $^2SeF_6^+$; F: 2s: 2.00(1.00/1.00), 2p: 4.93(2.97/1.96); regular F: 2s 1.94(0.97/0.97), 2p: 5.44(2.72/2.72)

[b] $^2SeF_6^-$; F: 2s: 1.95(0.97/0.97), 2p: 5.64 (2.88/2.76);

[c] $^1SeF_7^+$; F: 2s: 1.95, 2p: 5.02; regular F: 2s: 1.95, 2p: 5.45(oneF:5.05);

Table S9. Optimized x,y,z coordinates in angstroms at CCSD(T)/aVQZ level for all the Te compounds up to tetratomics and TeF_6, and at CCSD(T)/aVTZ level for the rest.

TeO_2

Te	0.0000000000	0.0000000000	0.2430726553
O	0.0000000000	1.4982611629	-0.7818873276
O	0.0000000000	-1.4982611629	-0.7818873276

TeO_2^-

Te	0.0000000000	0.0000000000	0.2509739012
O	0.0000000000	1.5301077578	-0.8184004506
O	0.0000000000	-1.5301077578	-0.8184004506

TeH_2

Te	0.0000000000	0.0000000000	0.0395027018
H	0.0000000000	1.1793405830	-1.1317348508
H	0.0000000000	-1.1793405830	-1.1317348508

TeF^+

Te	0.0000000000	0.0000000000	-0.2397583034
F	0.0000000000	0.0000000000	1.6103016404

TeF

Te	0.0000000000	0.0000000000	-0.2488487474
F	0.0000000000	0.0000000000	1.6713562802

TeF^-

Te	0.0000000000	0.0000000000	-0.2604439176
F	0.0000000000	0.0000000000	1.7492335483

TeF_2^+

Te	0.0000000000	0.0000000000	-0.2840145594
F	0.0000000000	1.3570551147	0.9537711613
F	0.0000000000	-1.3570551147	0.9537711613

TeF_2

Te	0.0000000000	0.0000000000	-0.2980359188
F	0.0000000000	1.3879648813	1.0008573678
F	0.0000000000	-1.3879648813	1.0008573678

TeF_2^-(D_{2d})

Te	0.0000000000	0.0000000000	0.0000000000
F	0.0000000000	0.0000000000	2.0915453534
F	0.0000000000	0.0000000000	-2.0915453534

TeF_2^-(C_{2v})

Te	0.0000000000	0.0000000000	-0.3645189824
F	0.0000000000	-1.2558287218	1.2241192629
F	0.0000000000	1.2558287218	1.2241192629

TeF_3^+

F	0.6605724071	0.0000000000	-1.5506176473
Te	-0.2950231840	0.0000000000	-0.0000286427
F	0.6604538677	1.3428534722	0.7754050108
F	0.6604538677	-1.3428534722	0.7754050108

TeF_3

Te	0.0000000000	0.0000000000	-0.2403140046
F	0.0000000000	1.9309886889	-0.0064859033
F	0.0000000000	0.0000000000	1.6270057329
F	0.0000000000	-1.9309886889	-0.0064859033

TeF_3^-

Te	0.0000000000	0.0000000000	-0.2478137180
F	0.0000000000	2.0302712787	-0.0102132973
F	0.0000000000	0.0000000000	1.6848312511
F	0.0000000000	-2.0302712787	-0.0102132973

TeF_4^+

F	0.0000000000	1.3882540178	-0.9711287895
F	0.0000000000	-1.3882540178	-0.9711287895
F	-1.8629721743	0.0000000000	0.4473269046
F	1.8629721743	0.0000000000	0.4473269046
Te	0.0000000000	0.0000000000	0.2055577701

TeF_4

F	0.0283613132	-0.0000683822	-1.8960657961
Te	-0.2785581960	-0.0000254030	-0.0000283428
F	0.9071485581	1.4344406150	-0.0001181396
F	0.0282261231	0.0002807469	1.8960309650
F	0.9071594600	-1.4344823643	0.0003433312

TeF_4^-

F	0.0000000000	1.9872721893	0.1456854011
F	0.0000000000	-1.9872721893	0.1456854011
F	1.2416172214	0.0000000000	-1.1548194121
F	-1.2416172214	0.0000000000	-1.1548194121
Te	0.0000000000	0.0000000000	0.3673510220

TeF_5^+

Te	0.0000000000	0.0000000000	0.0000000000

F	1.8129362304	0.0000000000	0.0000000000
F	-0.9064681152	-1.5700488309	0.0000000000
F	-0.9064681152	1.5700488309	0.0000000000
F	0.0000000000	0.0000000000	1.8202040945
F	0.0000000000	0.0000000000	-1.8202040945

TeF_5

Te	0.0000000000	0.0000000000	-0.1631947446
F	0.0000000000	0.0000000000	1.6763442161
F	1.8897790862	0.0000000000	-0.1450676350
F	0.0000000000	1.8897790862	-0.1450676350
F	0.0000000000	-1.8897790862	-0.1450676350
F	-1.8897790862	0.0000000000	-0.1450676350

TeF_5^-

Te	0.0000000000	0.0000000000	-0.2558116359
F	0.0000000000	0.0000000000	1.6306563164
F	1.9546950614	0.0000000000	0.0218662970
F	0.0000000000	1.9546950614	0.0218662970
F	0.0000000000	-1.9546950614	0.0218662970
F	-1.9546950614	0.0000000000	0.0218662970

TeF_6^+

F	0.0000000000	0.0000000000	1.9698127440
F	0.0000000000	1.7695744438	-0.2657047196
F	0.0000000000	-1.7695744438	-0.2657047196
F	-1.8053063139	0.0000000000	-0.0661713494
F	1.8053063139	0.0000000000	-0.0661713494
F	0.0000000000	0.0000000000	-2.2495424241
Te	0.0000000000	0.0000000000	0.1645018180

TeF_6

Te	0.0000000000	0.0000000000	0.0000000000
F	0.0000000000	0.0000000000	1.8333949110
F	1.8333949110	0.0000000000	0.0000000000
F	0.0000000000	-1.8333949110	0.0000000000
F	0.0000000000	0.0000000000	-1.8333949110
F	-1.8333949110	0.0000000000	0.0000000000
F	0.0000000000	1.8333949110	0.0000000000

TeF_6^-

Te	0.0000000000	0.0000000000	0.0000000000
F	0.0000000000	0.0000000000	1.9633267911
F	1.9633267911	0.0000000000	0.0000000000
F	0.0000000000	-1.9633267911	0.0000000000
F	0.0000000000	0.0000000000	-1.9633267911

F	-1.9633267911	0.0000000000	0.0000000000
F	0.0000000000	1.9633267911	0.0000000000

TeF_7^+

F	2.1341918561	0.5583253308	0.0216549369
F	-0.2829047891	0.9858182456	1.4235900971
F	0.4694446028	-1.4561626252	1.1015330327
F	-1.9089177523	-0.7794894291	-0.0589989280
F	-2.7777631406	0.3801872598	0.0965250179
F	-0.3359701196	1.3039370434	-1.1302288616
F	0.4146316628	-1.1394867324	-1.4471866932
Te	0.3816606799	0.0214949070	-0.0076056017

TeF_7^-

F	-0.0000000000	0.0000000000	-1.8623887890
Te	-0.0000000000	0.0000000000	0.0000000000
F	1.9232022842	0.0000000000	0.0000000000
F	-0.0000000000	0.0000000000	1.8623887890
F	0.5943021895	1.8290740646	0.0000000000
F	-1.5559033316	1.1304299399	0.0000000000
F	-1.5559033316	-1.1304299399	0.0000000000
F	0.5943021895	-1.8290740646	0.0000000000

TeF_8^{2-}

F	0.0000000000	1.6509353692	1.0683351021
F	1.1673895249	-1.1673895249	-1.0683348926
F	1.1673895249	1.1673895249	-1.0683348926
F	-1.1673895249	-1.1673895249	-1.0683348926
F	0.0000000000	-1.6509353692	1.0683351021
F	1.6509353692	0.0000000000	1.0683351021
F	-1.6509353692	0.0000000000	1.0683351021
F	-1.1673895249	1.1673895249	-1.0683348926
Te	0.0000000000	0.0000000000	-0.0000008375

FTeTeF

Te	1.236267	-0.424530	-0.197877
Te	-1.236267	0.424530	-0.197877
F	1.236267	-1.877768	1.143288
F	-1.236267	1.877768	1.143288

F_2TeTe

Te	0.419967	-1.498727	0.000000
Te	-0.565340	0.856904	0.000000
F	0.419967	1.854155	1.377602
F	0.419967	1.854155	-1.377602

Te_2F_6

F	1.140082	1.465487	1.446573
F	-1.436719	0.811770	-1.449988
F	-1.436719	1.953719	0.957498
Te	0.008209	1.417242	-0.165130
Te	-0.008209	-1.417242	-0.165130
F	1.436719	-0.811770	-1.449988
F	1.436719	-1.953719	0.957498
F	-1.140082	-1.465487	1.446573

Te_2F_{10}

F	0.000000	1.907204	1.509995
F	0.000000	-1.907204	1.509995
F	-1.907204	0.000000	1.509995
Te	0.000000	0.000000	1.491499
Te	0.000000	0.000000	-1.491499
F	0.000000	1.907204	-1.509995
F	-1.907204	0.000000	-1.509995
F	0.000000	-1.907204	-1.509995
F	0.000000	0.000000	-3.364660
F	0.000000	0.000000	3.364660
F	1.907204	0.000000	1.509995
F	1.907204	0.000000	-1.509995