SUPPORTING INFORMATION

Novel Germanetellones: XYGe=Te (X, Y=H, F, Cl, Br, I and CN) – Structures and Energetics. Comparison with the First Synthetic Successes

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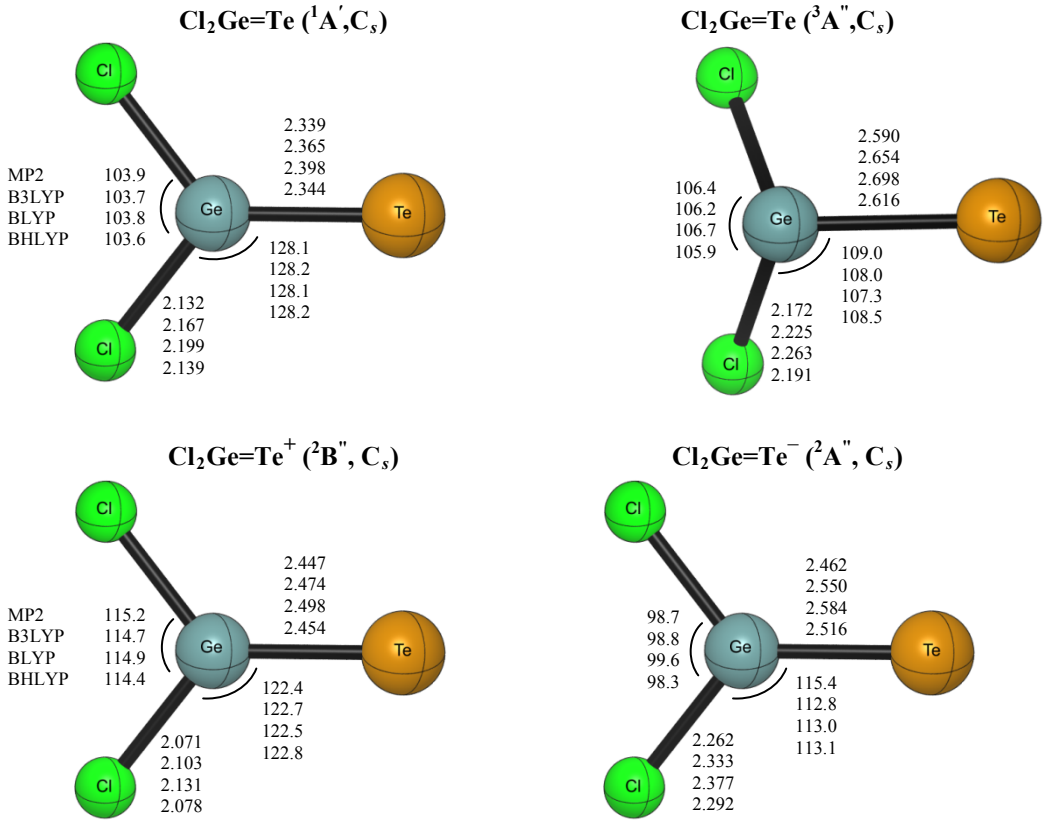

Figure SI 1: Equilibrium geometries (bond lengths in Å, bond angles in °) for the $^{1}A'$ state of $Cl_2Ge=Te$, $^{3}A''$ state of $Cl_2Ge=Te$, $^{2}B''$ state of the $Cl_2Ge=Te^{+}$ cation, and $^{2}B'$ state of the $Cl_2Ge=Te^{-}$ anion.

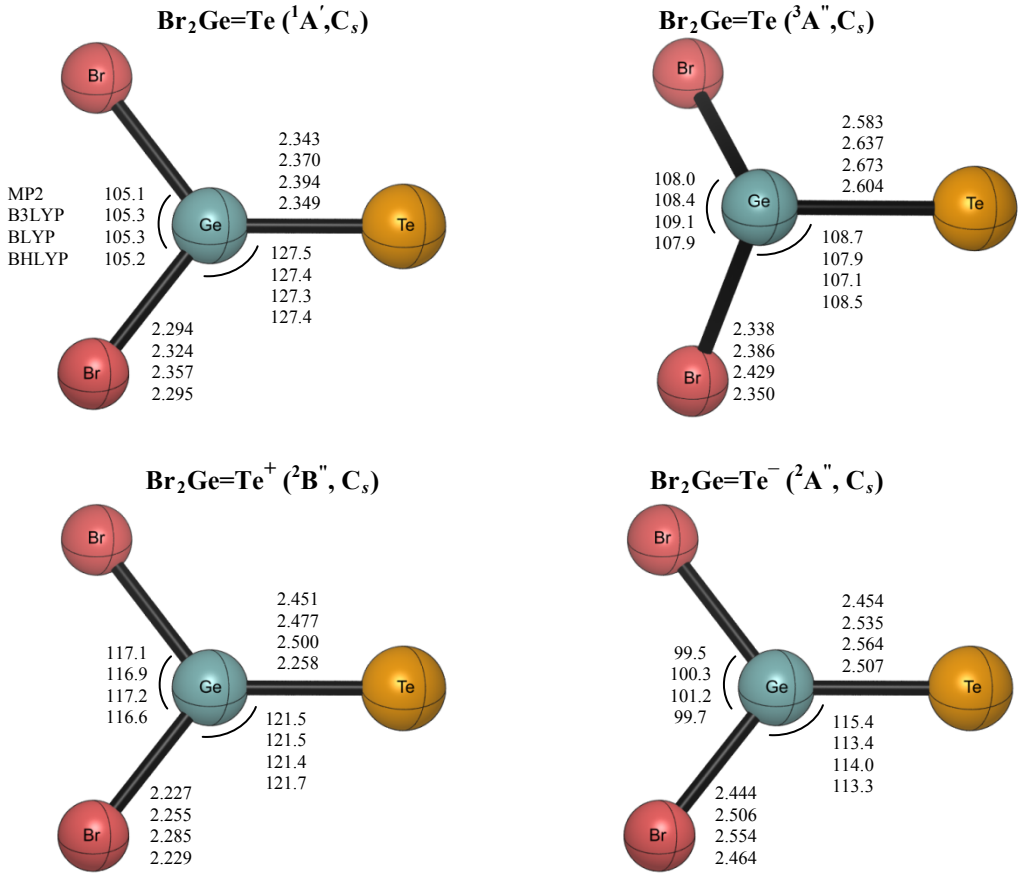

Figure SI 2: Equilibrium geometries (bond lengths in Å, bond angles in °) for the $^1A'$ state of $Br_2Ge=Te$, $^3A''$ state of $Br_2Ge=Te$, $^2B''$ state of the $Br_2Ge=Te^+$ cation, and $^2B'$ state of the $Br_2Ge=Te^-$ anion.

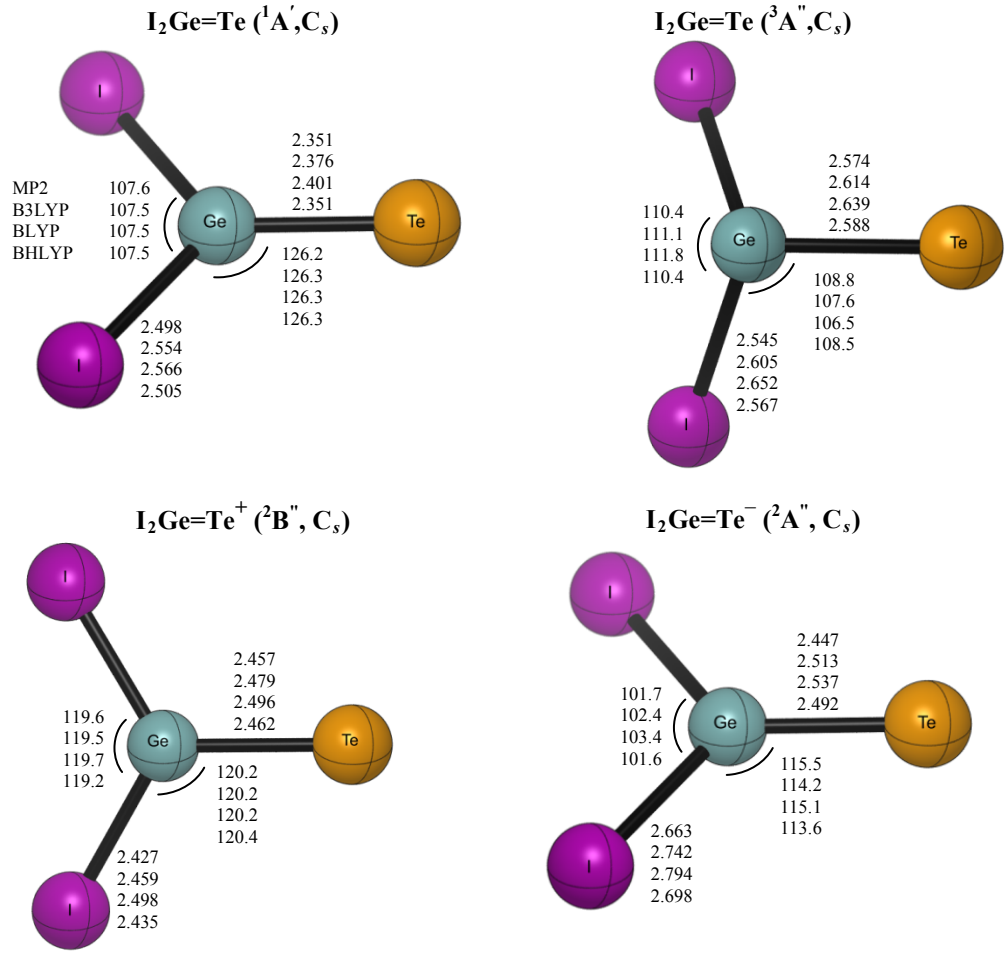

Figure SI 3: Equilibrium geometries (bond lengths in Å, bond angles in °) for the $^{1}A'$ state of $I_2Ge=Te$, $^{3}A''$ state of $I_2Ge=Te$, $^{2}B''$ state of the $I_2Ge=Te^{+}$ cation, and $^{2}B'$ state of the $I_2Ge=Te^{-}$ anion.

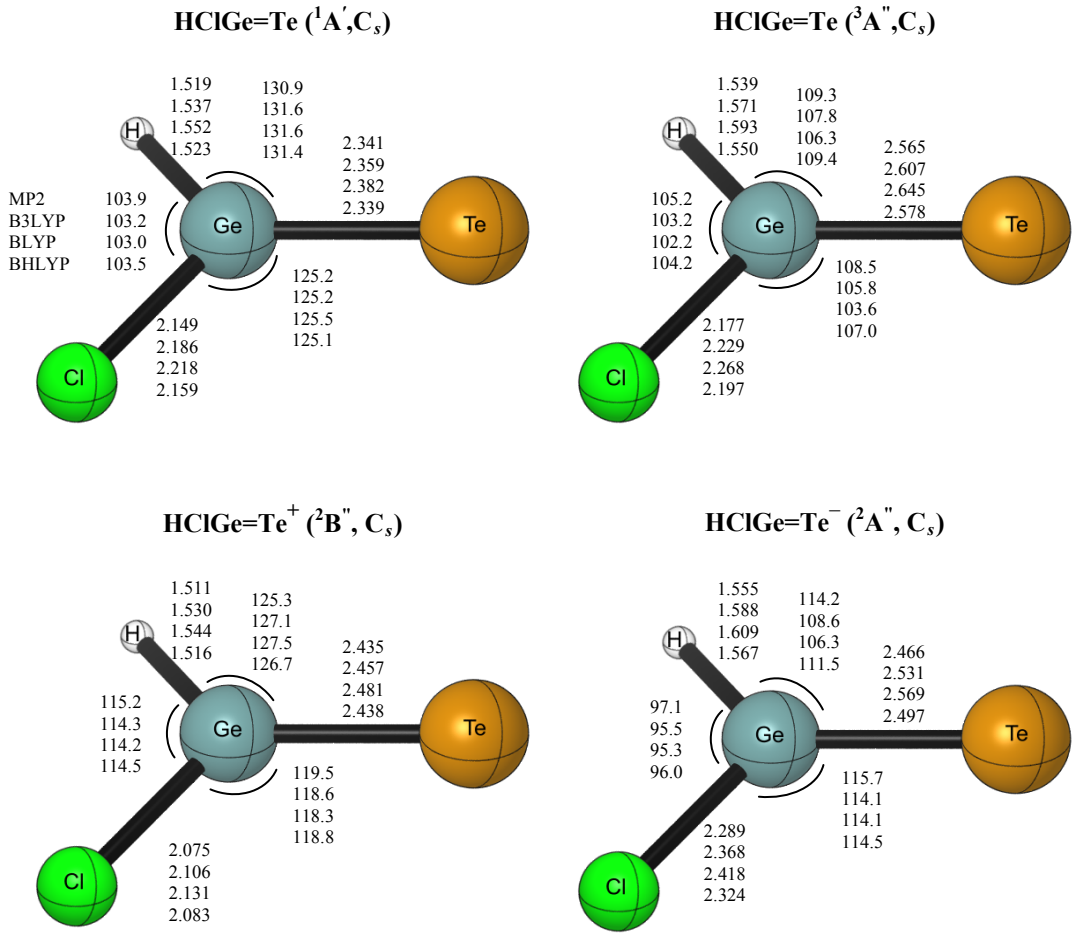

Figure SI 4: Equilibrium geometries (bond lengths in Å, bond angles in °) for the $^{1}A'$ state of HClGe=Te, $^{3}A''$ state of HClGe=Te, $^{2}B''$ state of the HClGe=Te^{+} cation, and $^{2}B'$ state of the HClGe=Te^{-} anion.

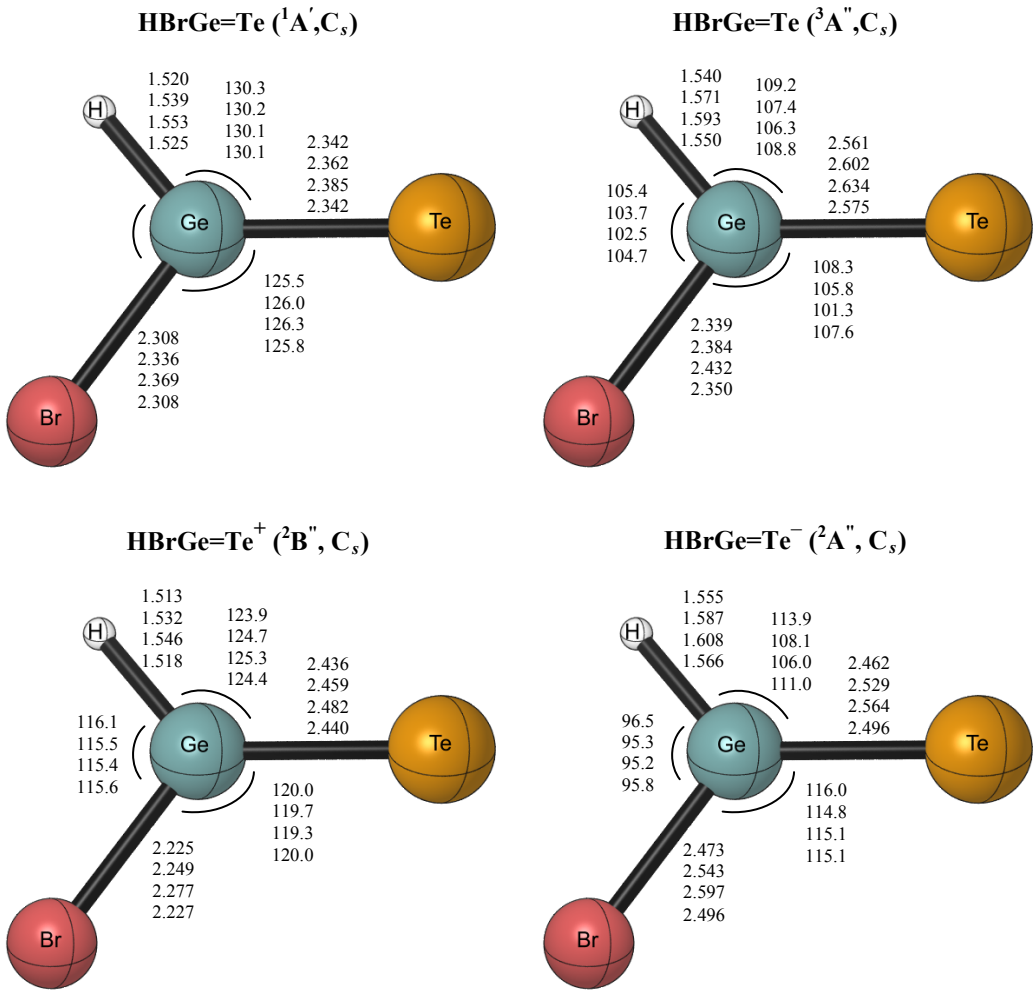

Figure SI 5: Equilibrium geometries (bond lengths in Å, bond angles in °) for the ^{1}A′ state of HBrGe=Te, ^{3}A" state of HBrGe=Te, ^{2}B" state of the HBrGe=Te$^+$ cation, and ^{2}B′ state of the HBrGe=Te$^-$ anion.

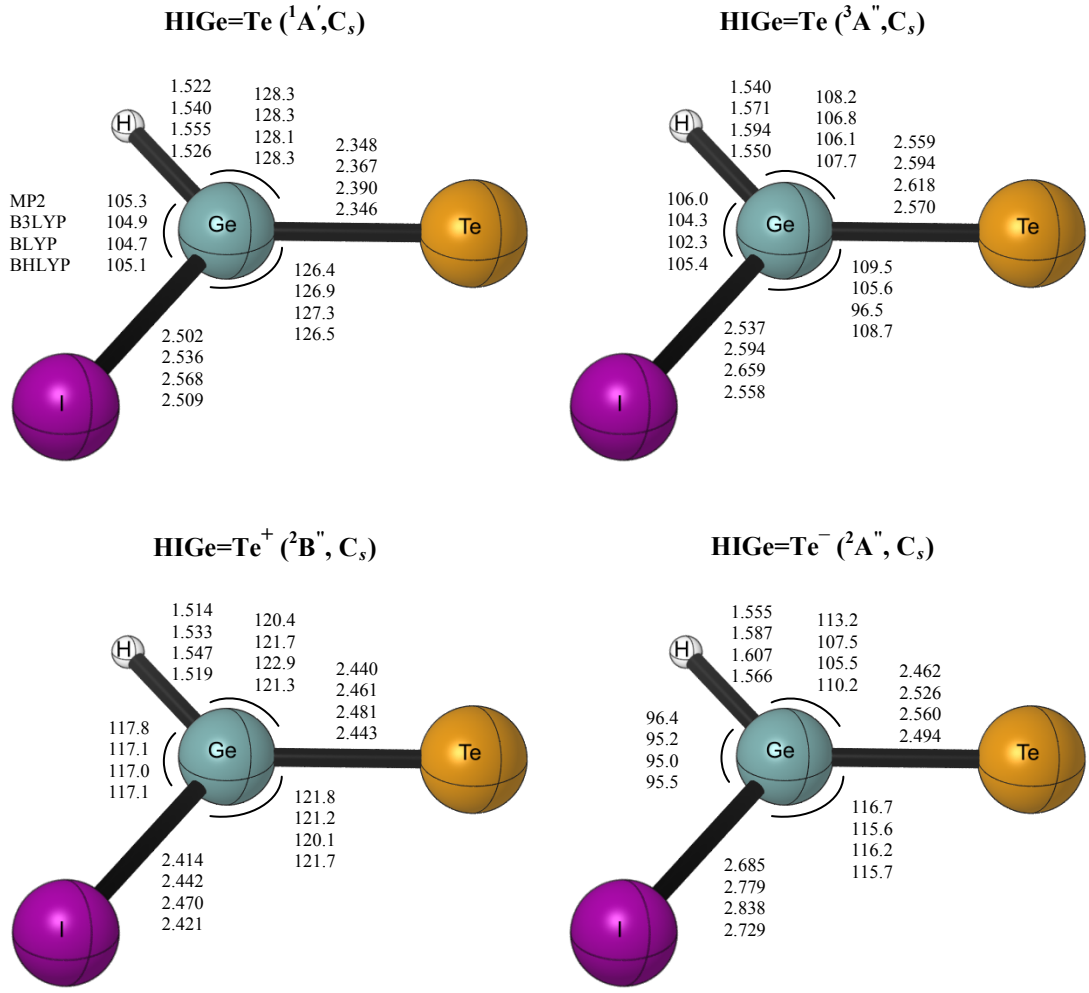

Figure SI 6: Equilibrium geometries (bond lengths in Å, bond angles in °) for the ^{1}A′ state of HIGe=Te, ^{3}A″ state of HIGe=Te, ^{2}B″ state of the HIGe=Te$^+$ cation, and ^{2}B′ state of the HIGe=Te$^-$ anion.

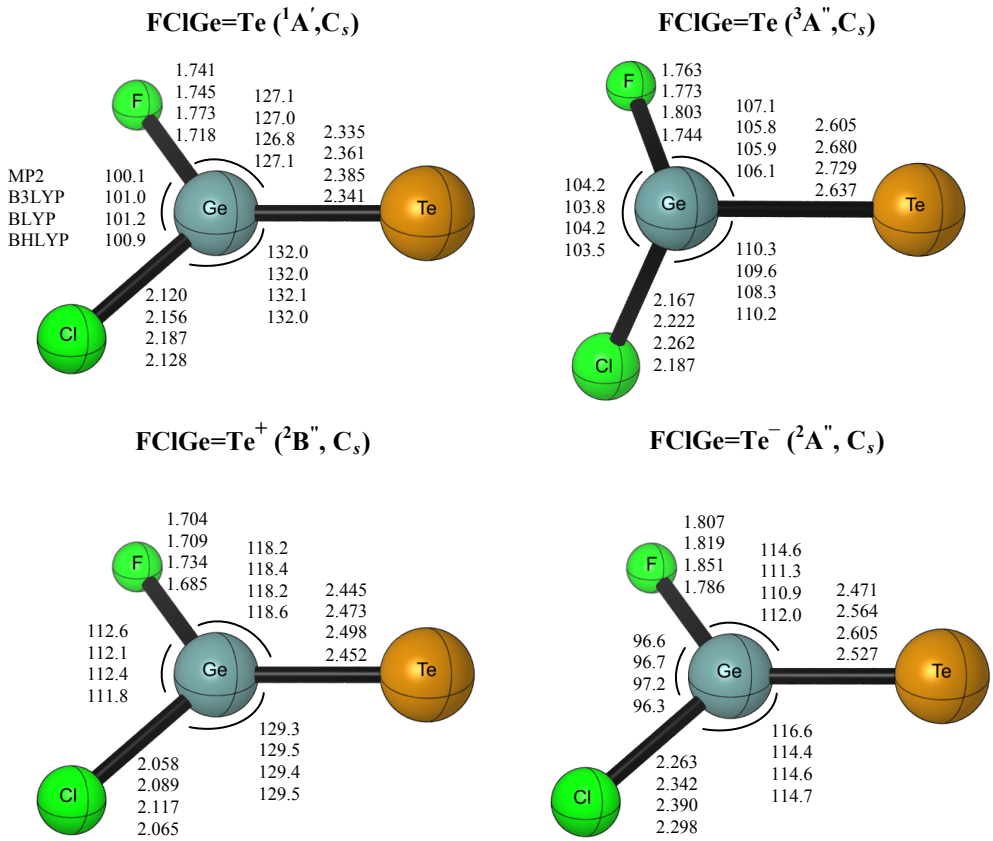

Figure SI 7: Equilibrium geometries (bond lengths in Å, bond angles in °) for the ^{1}A′ state of FClGe=Te, ^{3}A" state of FClGe=Te, ^{2}B" state of the FClGe=Te$^+$ cation, and ^{2}B′ state of the FClGe=Te$^-$ anion.

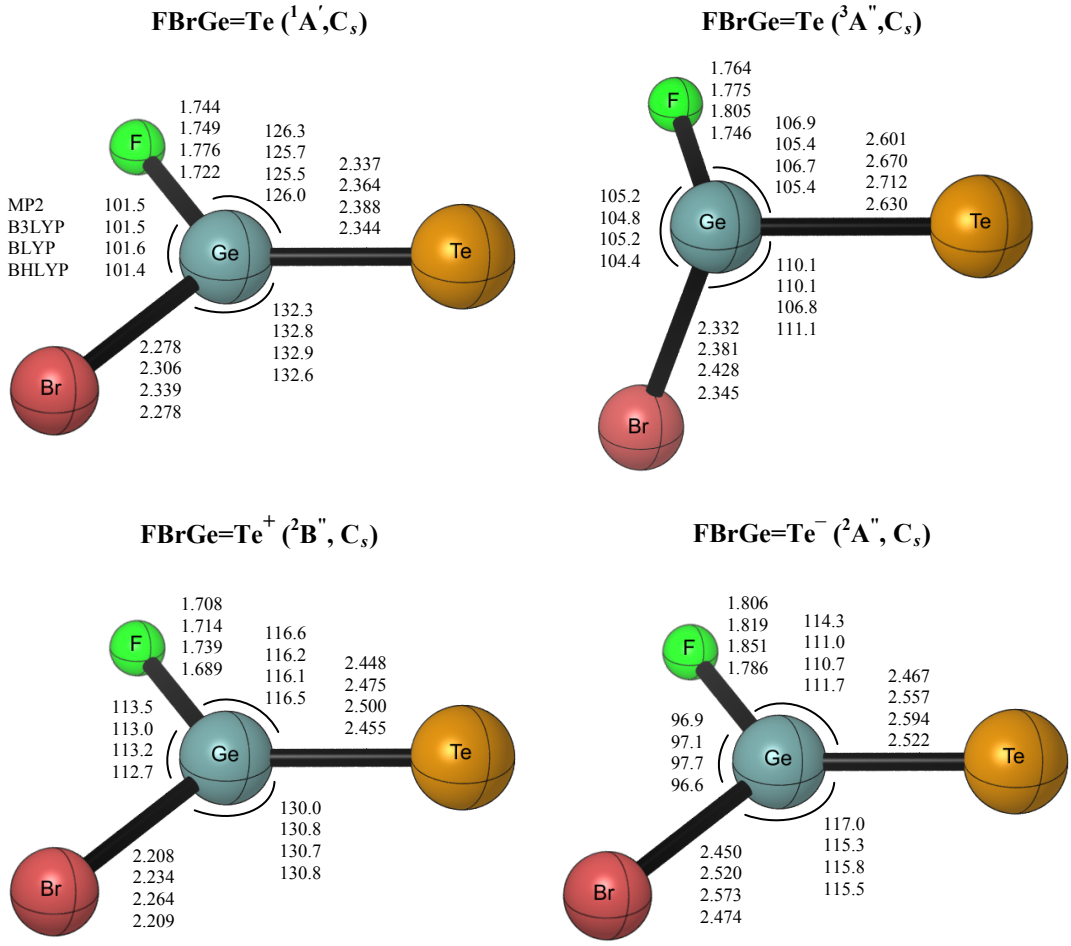

Figure SI 8: Equilibrium geometries (bond lengths in Å, bond angles in °) for the ^{1}A′ state of FBrGe=Te, ^{3}A″ state of FBrGe=Te, ^{2}B″ state of the FBrGe=Te$^+$ cation, and ^{2}B′ state of the FBrGe=Te$^-$ anion.

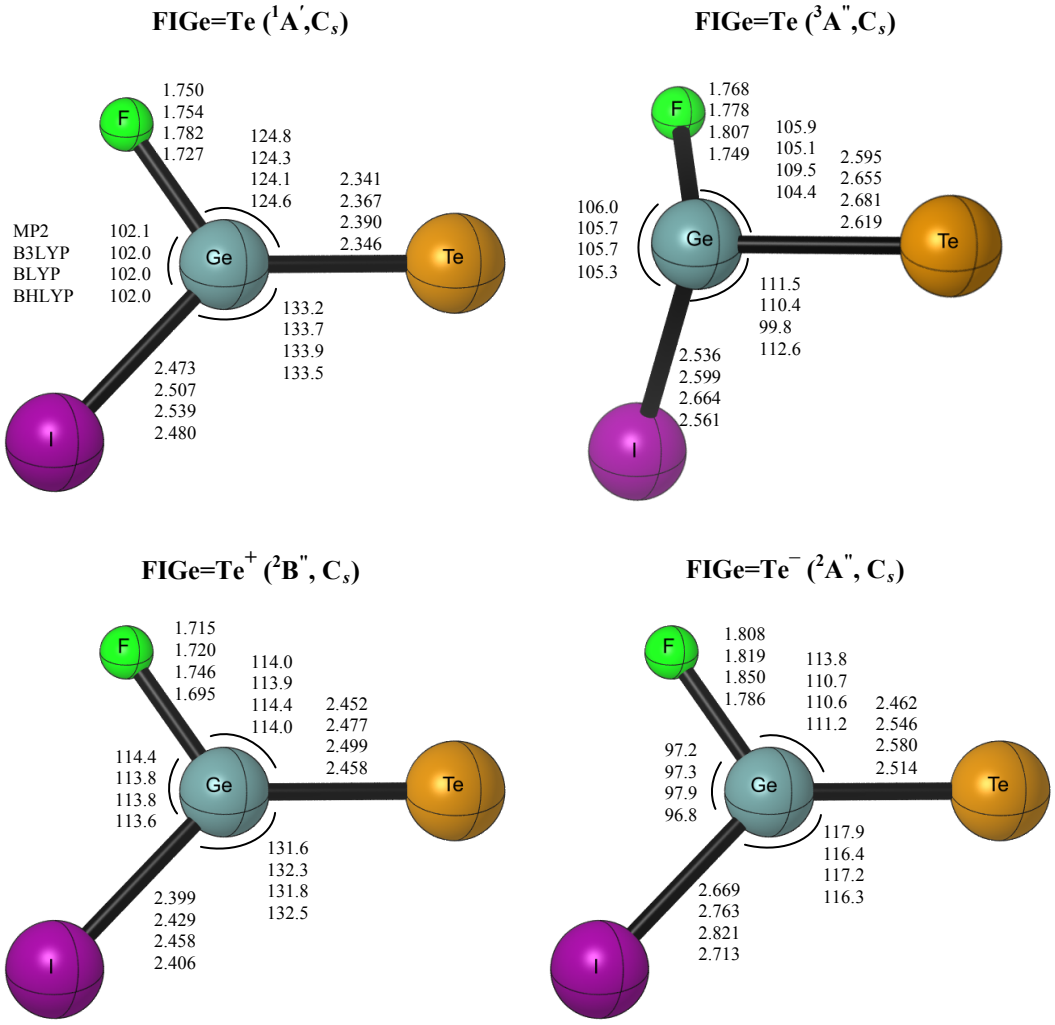

Figure SI 9: Equilibrium geometries (bond lengths in Å, bond angles in °) for the $^{1}A'$ state of FIGe=Te, $^{3}A''$ state of FIGe=Te, $^{2}B''$ state of the FIGe=Te^{+} cation, and $^{2}B'$ state of the FIGe=Te^{-} anion.

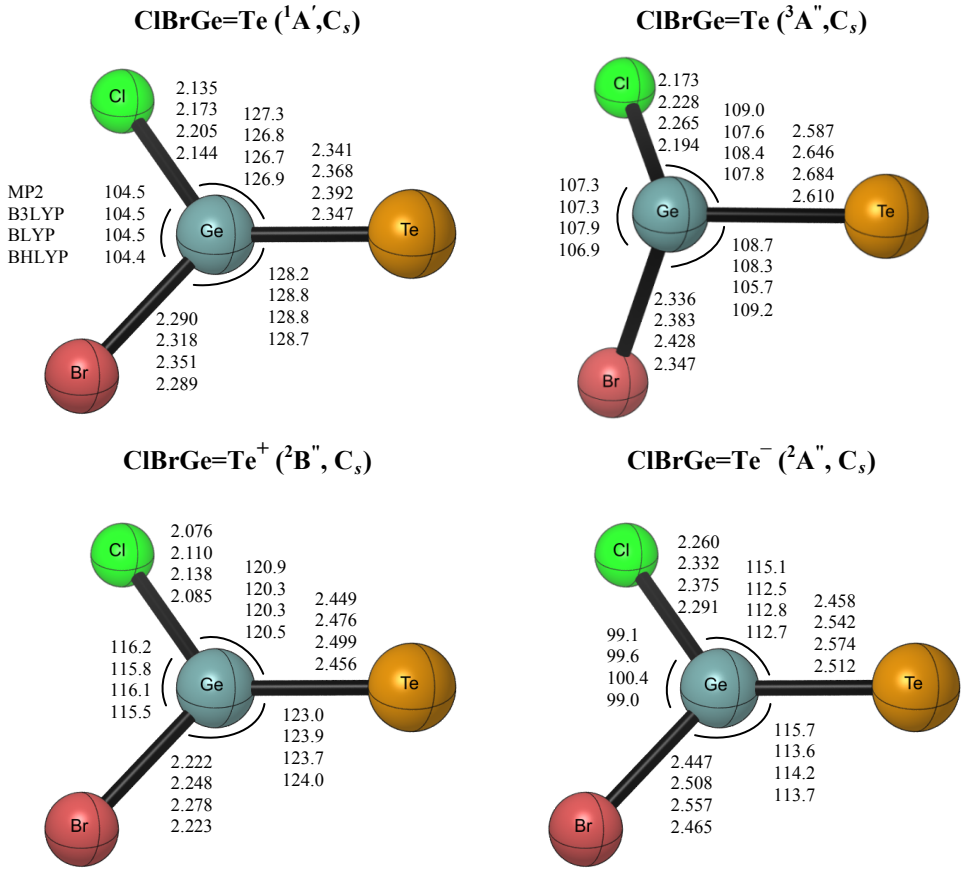

Figure SI 10: Equilibrium geometries (bond lengths in Å, bond angles in °) for the ^{1}A′ state of ClBrGe=Te, ^{3}A″ state of ClBrGe=Te, ^{2}B″ state of the ClBrGe=Te$^+$ cation, and ^{2}B′ state of the ClBrGe=Te$^-$ anion.

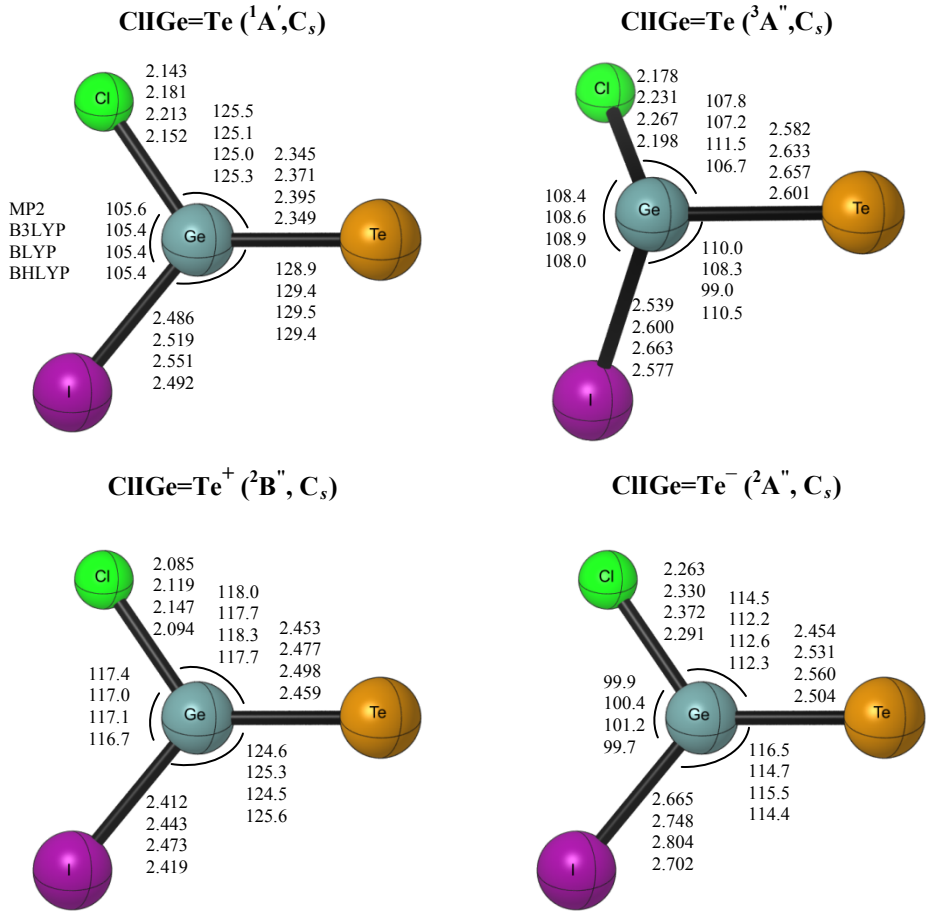

Figure SI 11: Equilibrium geometries (bond lengths in Å, bond angles in °) for the $^1A'$ state of ClIGe=Te, $^3A''$ state of ClIGe=Te, $^2B''$ state of the ClIGe=Te$^+$ cation, and $^2B'$ state of the ClIGe=Te$^-$ anion.

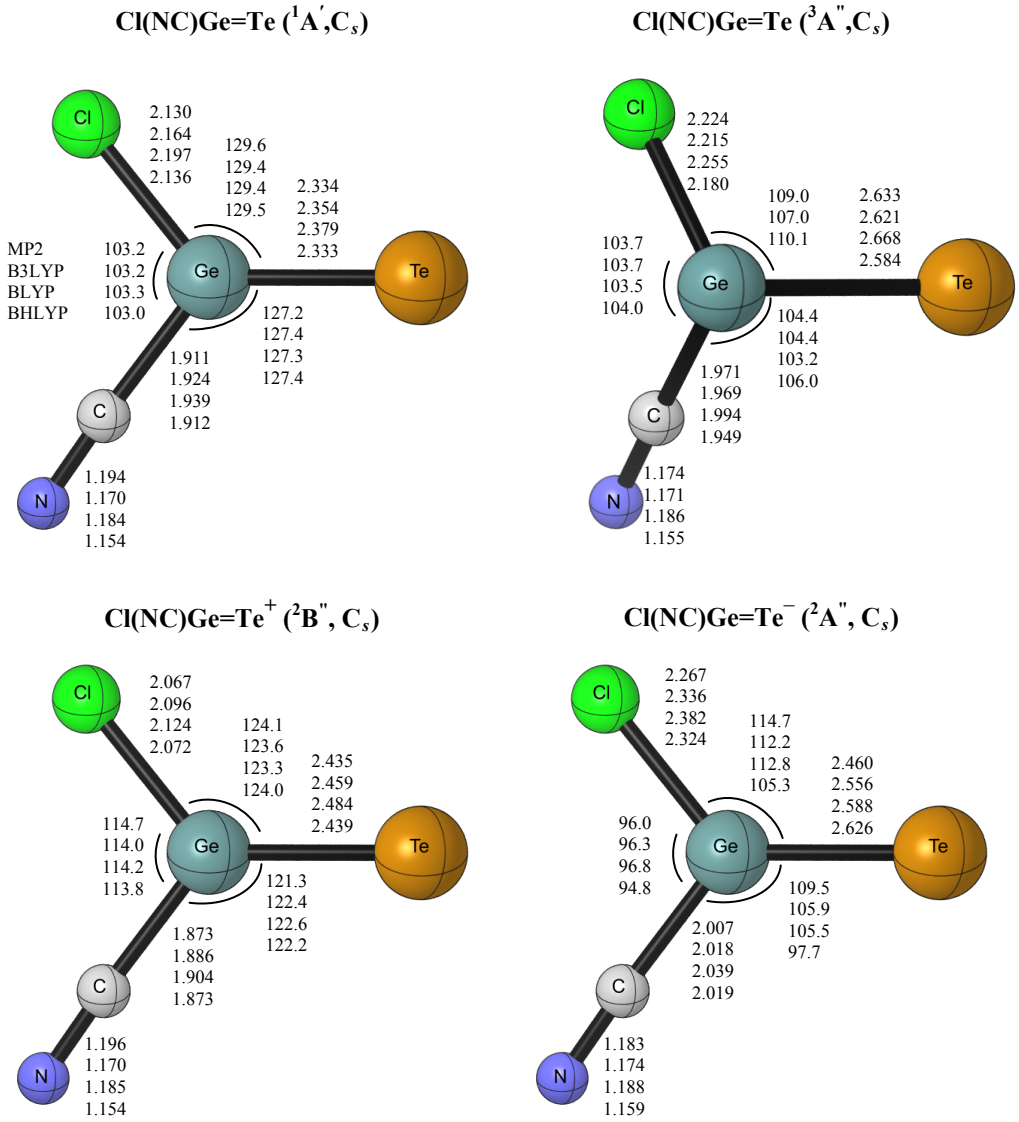

Figure SI 12: Equilibrium geometries (bond lengths in Å, bond angles in °) for the ^{1}A′ state of Cl(NC)Ge=Te, ^{3}A″ state of Cl(NC)Ge=Te, ^{2}B″ state of the Cl(NC)Ge=Te$^+$ cation, and ^{2}B′ state of the Cl(NC)Ge=Te$^-$ anion.

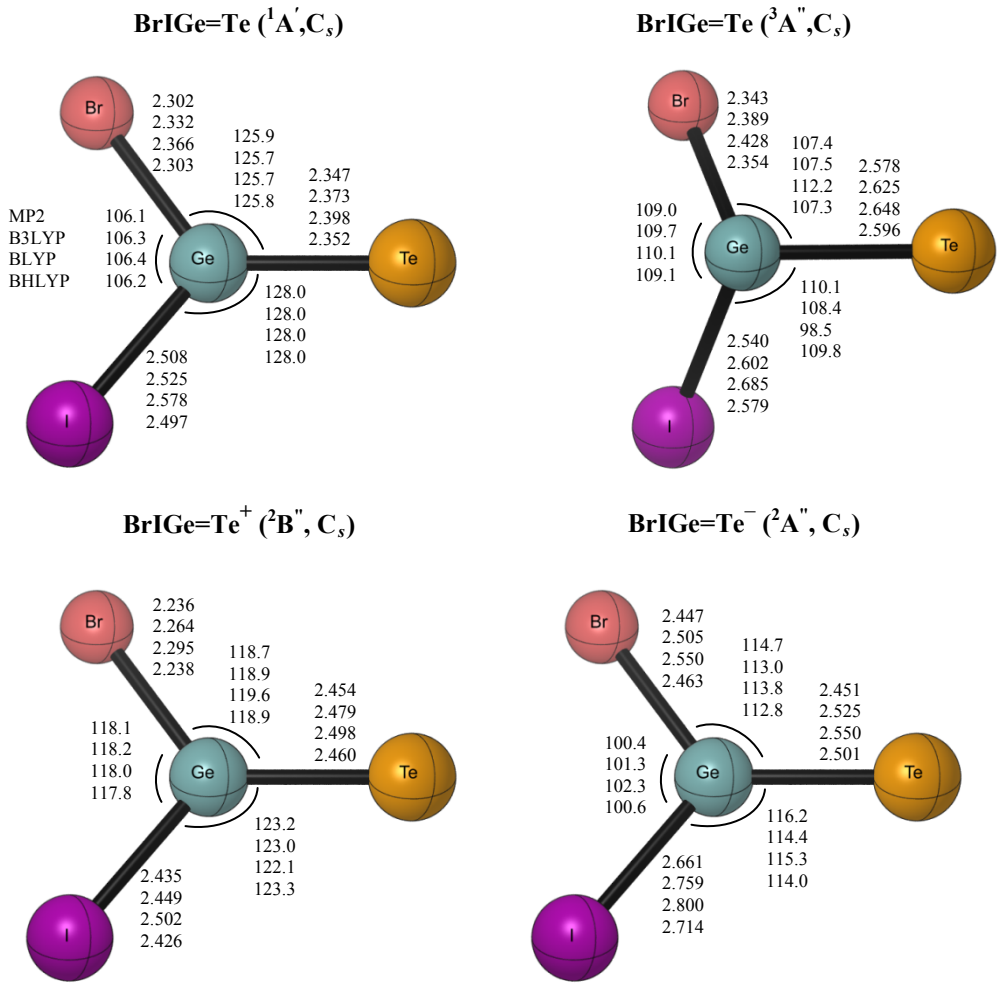

Figure SI 13: Equilibrium geometries (bond lengths in Å, bond angles in °) for the $^{1}A'$ state of BrIGe=Te, $^{3}A''$ state of BrIGe=Te, $^{2}B''$ state of the BrIGe=Te^{+} cation, and $^{2}B'$ state of the BrIGe=Te^{-} anion.

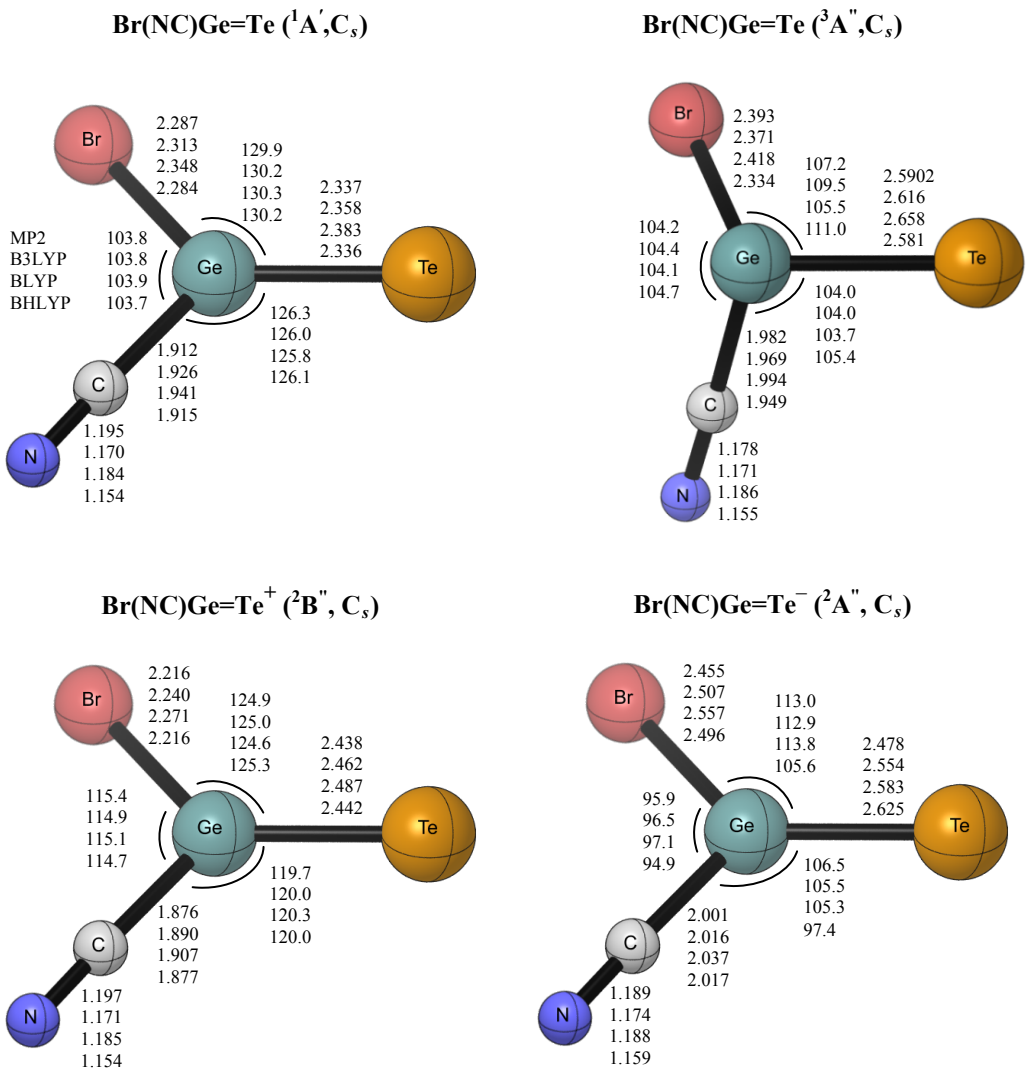

Figure SI 14: Equilibrium geometries (bond lengths in Å, bond angles in °) for the ^{1}A′ state of Br(NC)Ge=Te, ^{3}A″ state of Br(NC)Ge=Te, ^{2}B″ state of the Br(NC)Ge=Te$^+$ cation, and ^{2}B′ state of the Br(NC)Ge=Te$^-$ anion.

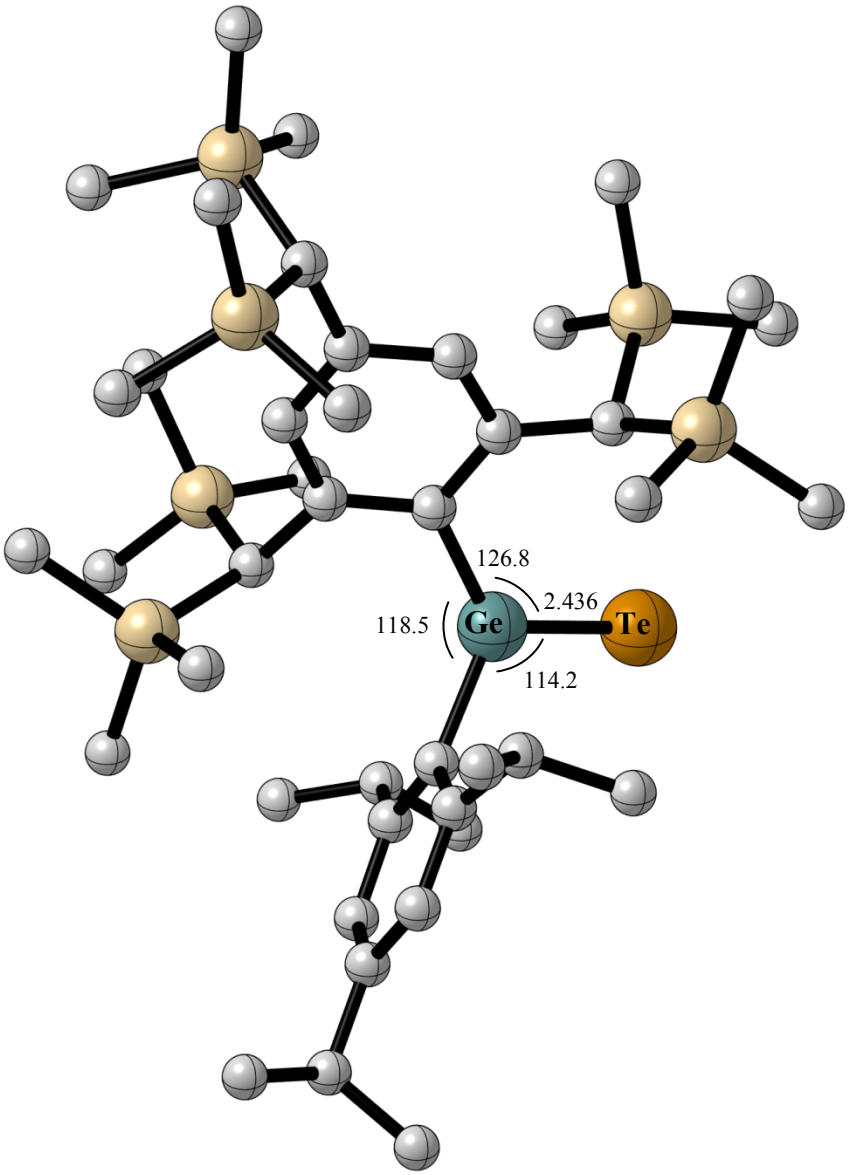

Figure SI 15: Equilibrium geometry (bond lengths in Å, bond angles in °) for the $^{1}A'$ state of Tbt(Tip)Ge=Te (all the H atoms are omitted for clarity) optimized using the BP86/TZVP method.

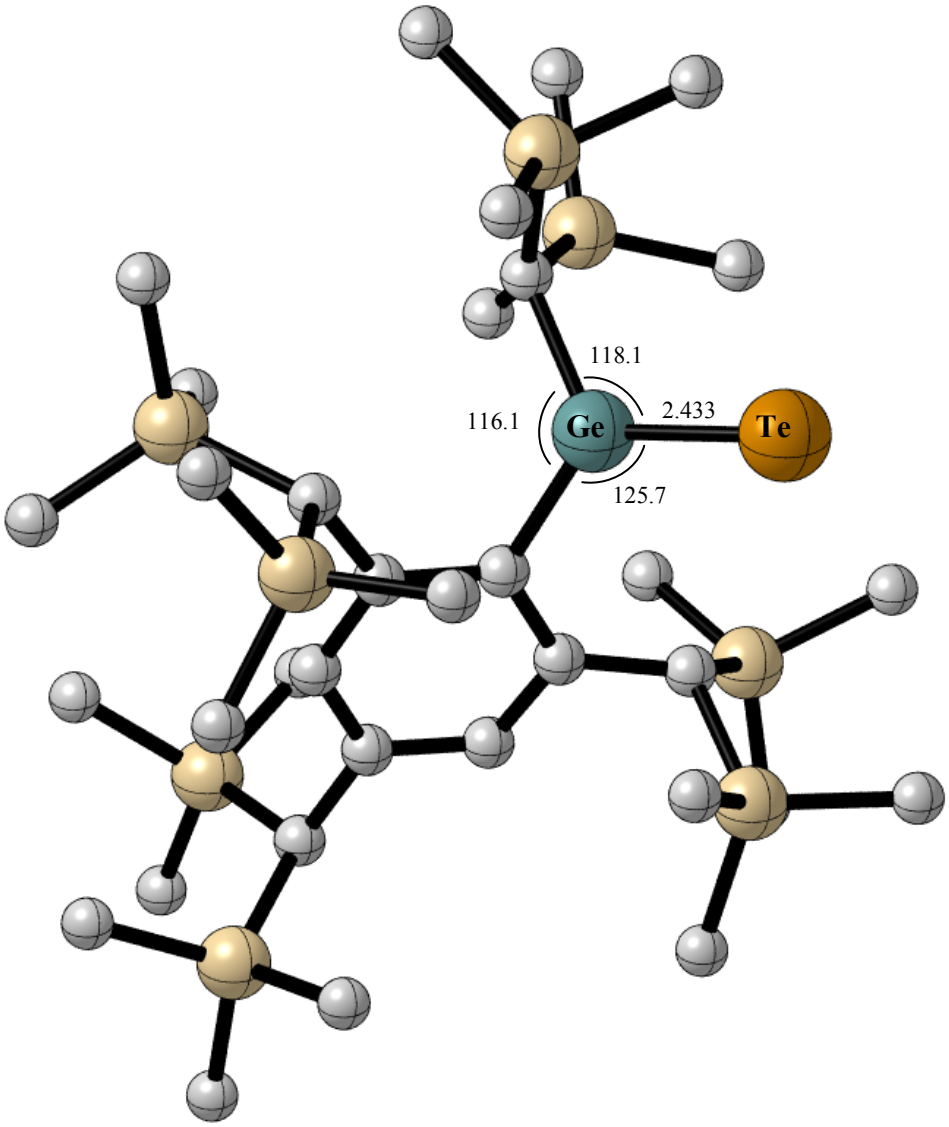

Figure SI 16: Equilibrium geometry (bond lengths in Å, bond angles in °) for the $^{1}A'$ state of Tbt(Dis)Ge=Te (all the H atoms are omitted for clarity) optimized using the BP86/TZVP method.

Table SI 1: Structural parameters for germanium containing heavy ketones.

	r(Ge=E)	r(Ge–X)
$H_2Ge=O$	1.644[a]	1.546[a]
$F_2Ge=O$	1.630[a]	1.726[a]
$Cl_2Ge=O$	1.634[a]	2.142[a]
$Br_2Ge=O$	1.638[a]	2.300[a]
$(Eind)_2Ge=O$	1.676[b]	
$H_2Ge=S$	2.051[c] 2.041[d] 2.051[e]	1.518[c] 1.544[d] 1.518[e]
$F_2Ge=S$	2.021[d]	1.730[d]
$Cl_2Ge=S$	2.029[d]	2.150[d]
$Br_2Ge=S$	2.034[d]	2.308[d]
Tbt(Tip)Ge=S	2.049[f]	
$H_2Ge=Se$	2.171[g] 2.160[h]	1.533[g] 1.527[h]
$F_2Ge=Se$	2.143[g]	1.753[g]
$Cl_2Ge=Se$	2.153[g]	2.129[g]
$Br_2Ge=Se$	2.158[g]	2.289[g]
Tbt(Tip)Ge=Se	2.180[i]	
Tbt(Dis)Ge=Se	2.173[i]	
Tbt(Tip)Ge=Te	2.398[j]	
Tbt(Dis)Ge=Te	2.384[j]	

a=ref 36, b=ref 30 c=ref 34, d=ref 12, e=ref 38, f=ref 18, g=ref 11, h=ref 13, i=ref 37, j=ref 41

Table SI 2: Vertical Electron Affinities (VEA) in eV (kcal mol^{-1} in parentheses) for the XYGe=Te (X, Y=H, F, Cl,Br , I and CN) molecules.

	MP2	**B3LYP**	**BLYP**	**BHLYP**
H_2Ge=Te	0.80 (18.47)	1.22 (28.11)	1.03 (23.87)	1.14 (26.28)
F_2Ge=Te	0.29 (6.68)	2.71 (62.59)	1.44 (33.17)	0.97 (22.33)
Cl_2Ge=Te	0.33 (7.72)	1.62 (37.37)	1.70 (39.22)	1.20 (27.67)
Br_2Ge=Te	0.64 (14.78)	1.82 (41.96)	1.87 (43.16)	1.44 (33.11)
I_2Ge=Te	0.95 (21.89)	2.04 (47.66)	2.05 (47.33)	1.71 (39.47)
$(NC)_2$Ge=Te	1.52 (35.23)	2.65 (61.18)	2.45 (56.43)	2.59 (59.68)
HFGe=Te	0.82 (18.87)	1.10 (25.36)	0.92 (21.29)	1.98 (45.57)
HClGe=Te	0.52 (12.05)	0.58 (13.46)	1.11 (25.65)	0.17 (3.92)
HBrGe=Te	0.42 (9.77)	0.75 (17.20)	1.15 (26.56)	0.35 (8.18)
HIGe=Te	1.04 (24.06)	1.43 (32.87)	1.22 (28.18)	1.37 (31.59)
H(NC)Ge=Te	1.63 (37.66)	1.96 (45.24)	1.77 (40.72)	1.89 (43.59)
FClGe=Te	0.26 (6.08)	1.46 (33.75)	1.54 (35.61)	1.05 (24.18)
FBrGe=Te	0.41 (9.50)	1.56 (36.00)	1.63 (37.54)	1.16 (26.78)
FIGe=Te	0.56 (12.91)	1.67 (38.52)	1.72 (39.56)	1.30 (29.97)
F(NC)Ge=Te	1.59 (36.69)	1.91 (43.98)	1.73 (39.79)	1.81 (41.81)
ClBrGe=Te	0.49 (11.38)	1.72 (39.77)	1.79 (41.30)	1.32 (30.52)
ClIGe=Te	0.67 (15.38)	1.85 (42.57)	1.89 (43.56)	1.48 (34.04)
Cl(NC)Ge=Te	1.70 (39.22)	2.04 (47.06)	1.85 (42.63)	1.96 (45.27)
BrIGe=Te	0.80 (18.47)	1.93 (44.60)	1.96 (45.31)	1.58 (36.42)
Br(NC)Ge=Te	1.75 (40.27)	2.06 (47.46)	1.86 (42.89)	1.99 (45.88)

Table SI 3: Vertical Detachment Energies (VDE) in eV (kcal mol^{-1} in parentheses) for the XYGe=Te (X, Y=H, F, Cl, Br , I and CN) molecules.

	MP2	**B3LYP**	**BLYP**	**BHLYP**
H_2Ge=Te	2.06 (47.49)	2.46 (56.65)	2.29 (52.80)	2.38 (54.79)
F_2Ge=Te	3.33 (76.86)	3.67 (84.71)	3.51 (81.07)	3.61 (83.36)
Cl_2Ge=Te	3.37 (77.70)	3.86 (89.06)	3.09 (71.35)	3.82 (88.02)
Br_2Ge=Te	3.40 (78.39)	3.81 (87.82)	3.59 (82.85)	3.79 (87.48)
I_2Ge=Te	3.31 (76.25)	3.73 (85.99)	3.50 (80.63)	4.01 (92.39)
$(NC)_2$Ge=Te	4.16 (95.84)	4.25 (98.07)	4.84 (111.76)	4.53 (104.57)
HFGe=Te	2.63 (60.63)	2.73 (62.99)	2.78 (64.08)	2.34 (54.02)
HClGe=Te	2.76 (63.67)	3.20 (73.83)	3.02 (69.54)	3.13 (72.15)
HBrGe=Te	2.83 (65.20)	3.23 (74.53)	3.03 (69.95)	3.17 (73.09)
HIGe=Te	2.85 (65.63)	3.27 (75.32)	3.06 (70.49)	3.22 (74.14)
H(NC)Ge=Te	3.12 (71.88)	3.34 (77.13)	3.13 (72.23)	3.29 (75.90)
FClGe=Te	3.36 (77.40)	3.78 (87.21)	3.58 (82.56)	3.73 (85.96)
FBrGe=Te	3.38 (77.91)	3.76 (86.71)	3.62 (83.89)	3.72 (85.81)
FIGe=Te	3.33 (76.72)	3.72 (85.85)	3.51 (80.87)	3.69 (85.16)
F(NC)Ge=Te	3.63 (83.72)	3.94 (90.83)	3.71 (85.46)	3.90 (89.94)
ClBrGe=Te	3.39 (78.07)	3.83 (88.39)	3.61 (83.20)	3.80 (87.74)
ClIGe=Te	3.34 (77.02)	3.79 (87.45)	3.57 (82.23)	3.77 (87.03)
Cl(NC)Ge=Te	3.71 (85.58)	4.08 (94.15)	3.82 (88.01)	4.54 (104.77)
BrIGe=Te	3.35 (77.35)	3.77 (86.83)	3.53 (81.45)	3.58 (86.72)
Br(NC)Ge=Te	3.84 (88.56)	4.07 (93.76)	3.79 (87.29)	4.55 (104.83)

Table SI 4: HOMO-LUMO gap for the Singlet Ground States of all the Scrutinized Germanetellones.

	HOMO (a.u.)	LUMO (a.u.)	ΔE_{H-L} (eV)
$H_2Ge=Te$	-0.22	-0.12	2.88
$F_2Ge=Te$	-0.26	-0.12	3.73
$Cl_2Ge=Te$	-0.25	-0.13	3.36
$Br_2Ge=Te$	-0.24	-0.13	3.10
$I_2Ge=Te$	-0.24	-0.14	2.79
$(NC)_2Ge=Te$	-0.27	-0.16	2.79
HFGe=Te	-0.24	-0.11	3.55
HClGe=Te	-0.24	-0.12	3.33
HBrGe=Te	-0.24	-0.12	3.26
HIGe=Te	-0.24	-0.12	3.15
H(NC)Ge=Te	-0.25	-0.14	2.85
FClGe=Te	-0.25	-0.12	3.57
FBrGe=Te	-0.25	-0.13	3.43
FIGe=Te	-0.25	-0.13	3.27
F(NC)Ge=Te	-0.27	-0.14	3.39
ClBrGe=Te	-0.25	-0.13	3.22
ClIGe=Te	-0.24	-0.13	3.05
Cl(NC)Ge=Te	-0.26	-0.14	3.18
BrIGe=Te	-0.24	-0.13	2.94
Br(NC)Ge=Te	-0.26	-0.14	3.12

Tbt(Tip)Ge=Te

E(RBP86) =-5733.3018363 au

C	-1.98785000	-1.39080700	-0.23338700
C	-2.97033100	-0.55287600	0.34239300
C	-2.62087600	0.80056400	0.52568500
C	-1.35188000	1.33535500	0.20700800
C	-0.33461700	0.42970900	-0.27067000
C	-0.68176600	-0.93993300	-0.55146400
H	-2.24376700	-2.43877700	-0.45179600
H	-3.38262400	1.48902000	0.92752300
C	-1.18156500	2.83377600	0.35547000
H	-0.12239100	3.10803800	0.14548000
C	0.26342000	-1.91846300	-1.23713100
C	-4.35529500	-1.03317300	0.73790100
H	-4.88872200	-0.14572100	1.15830600
H	1.29400100	-1.48986800	-1.24056300
Ge	1.55795600	1.03164900	-0.43482500
Te	2.33689300	3.20978400	-1.19794500
C	2.22763800	-4.31668700	-0.72578500
H	2.38361200	-5.25128800	-0.14469200
H	2.35459100	-4.56690700	-1.79805600
H	3.02844500	-3.60431100	-0.43598700
C	0.46331800	-3.32919500	1.55389000
H	1.34218900	-2.72303400	1.85725600
H	-0.45022600	-2.79249000	1.88040500
H	0.51187200	-4.29645400	2.09790600
C	-0.77500300	-4.93600400	-0.79403400
H	-1.81929200	-4.63663900	-0.57060500
H	-0.72121500	-5.20280300	-1.86996100
H	-0.56937900	-5.86190000	-0.21465900
C	-1.95281300	-2.52115700	-3.45858500
H	-2.12243900	-2.57346700	-4.55561100
H	-2.21756600	-3.51049400	-3.03257700
H	-2.65395300	-1.76936900	-3.04558400
C	0.92071200	-3.39197100	-3.99254200
H	0.70761800	-4.41692300	-3.62549400
H	0.68883700	-3.37607300	-5.07949200
H	2.00797200	-3.20559600	-3.88457900
C	0.22272600	-0.40271000	-3.97451100
H	-0.35614700	0.42808300	-3.52233000
H	1.29819700	-0.13339400	-3.91144600
H	-0.04379400	-0.45235900	-5.05220600
C	-7.32155600	-1.23174400	-0.24600600
H	-7.97430000	-1.35948600	-1.13638300
H	-7.66303600	-1.95203300	0.52410800
H	-7.49468700	-0.20699400	0.14632700
C	-5.29699000	-3.26967900	-1.36636200
H	-4.24695500	-3.50328800	-1.63666500
H	-5.62925000	-4.00688500	-0.60596200

H	-5.91619700	-3.42795500	-2.27530200
C	-5.15733800	-0.27361900	-2.17369800
H	-5.43374300	0.76215100	-1.88407900
H	-4.08760300	-0.26223200	-2.46628300
H	-5.75552800	-0.54201000	-3.07040600
C	-6.11125200	-2.47324100	2.91202900
H	-6.65270300	-1.51378300	3.04950700
H	-6.71736400	-3.11420900	2.23876000
H	-6.07183200	-2.97893000	3.90087400
C	-3.33349900	-1.37251300	3.64147300
H	-2.29139800	-1.17231600	3.31672900
H	-3.78671800	-0.40306200	3.93847600
H	-3.29037100	-2.01471600	4.54702200
C	-3.58492400	-3.92264400	1.92902200
H	-2.51304700	-3.85670200	1.65486000
H	-3.65264000	-4.54114100	2.84999700
H	-4.11424400	-4.46694700	1.12065900
C	-1.55078900	5.59985300	-1.05471600
H	-1.96626200	6.12654900	-1.94048500
H	-1.90856900	6.13608100	-0.15124800
H	-0.44477200	5.68866100	-1.09716200
C	-3.98008100	3.68080900	-1.01131400
H	-4.33354200	2.63129000	-1.07810800
H	-4.41315500	4.13556500	-0.09877900
H	-4.39500200	4.22433900	-1.88791100
C	-1.57106000	3.01424800	-2.74640100
H	-0.46793700	3.02015000	-2.86868900
H	-1.92821400	1.96637200	-2.82611800
H	-2.01846500	3.58865200	-3.58589700
Si	-4.33983100	-2.21466900	2.26867700
Si	-5.50532300	-1.48376500	-0.75259500
Si	0.51086800	-3.61201000	-0.32076500
Si	-0.14049100	-2.06461700	-3.13586100
Si	-2.08069500	3.77534800	-1.08698300
Si	-1.47063400	3.57967000	2.12004400
C	-3.19364200	4.34017900	2.40843100
H	-3.24412800	4.72067900	3.45168400
H	-3.40324400	5.19613800	1.73434200
H	-4.01294500	3.60095100	2.28712500
C	-0.17524600	4.94370200	2.38981600
H	-0.27271600	5.76311900	1.64854300
H	-0.28351100	5.38824600	3.40238100
H	0.85464400	4.53805300	2.30284100
C	-1.23241000	2.25510000	3.45838300
H	-1.96325400	1.42680600	3.36171300
H	-0.21761500	1.81246900	3.40955400
H	-1.35690700	2.70701300	4.46571900
C	3.00246500	-0.14788700	0.29849100
C	4.00662200	-0.70145600	-0.54610700
C	3.09480000	-0.31579400	1.71158600
C	5.03179700	-1.47613500	0.03918500
C	4.13691200	-1.10194400	2.24289000

C	5.11156900	-1.70466000	1.42422700
H	5.80727400	-1.91530600	-0.61043000
H	4.19889700	-1.23079800	3.33543900
C	2.17827900	0.44831900	2.66975400
H	1.25990200	0.72547200	2.09472300
C	6.23609300	-2.55344800	2.01415000
H	6.85172200	-2.90659400	1.15645300
C	4.06710600	-0.43470100	-2.05240600
H	3.07563200	-0.01657900	-2.35152700
C	2.86444200	1.76257900	3.10870800
H	3.79039000	1.54396600	3.68169600
H	3.14606500	2.38591100	2.23508300
H	2.19421800	2.36154800	3.76095900
C	1.71542400	-0.36422700	3.89297600
H	1.24196100	-1.32184400	3.59828500
H	2.56092500	-0.59444300	4.57515100
H	0.97609000	0.21453100	4.48400800
C	7.15864600	-1.72482500	2.93323700
H	6.61242900	-1.35135500	3.82556000
H	8.00856900	-2.34032800	3.29695200
H	7.57472700	-0.84431200	2.40199900
C	5.69528800	-3.80296100	2.74020600
H	5.07934900	-3.52479700	3.62188600
H	5.06190700	-4.41877900	2.06919100
H	6.52945500	-4.43925900	3.10459900
C	5.12745100	0.64098800	-2.37221800
H	5.14484300	0.86102500	-3.46087000
H	4.91506900	1.58685800	-1.83399100
H	6.14007900	0.29065000	-2.07855900
C	4.31406300	-1.69996800	-2.89603100
H	4.20623500	-1.47110700	-3.97678300
H	5.34229900	-2.09356800	-2.75122900
H	3.60791300	-2.51428800	-2.64056300

Tbt(Dis)Ge=Te

E(RBP86) =-6005.080845au

C	-2.12594600	-0.99879100	-0.09620900
C	-2.82214100	0.18333200	0.24531000
C	-2.07173300	1.37702800	0.28016300
C	-0.68126200	1.43655600	0.02975100
C	0.01805000	0.19650600	-0.18838500
C	-0.72580500	-1.02740400	-0.31416300
H	-2.69097000	-1.93767000	-0.19996500
H	-2.59865600	2.32113200	0.49449200
C	-0.04375300	2.81251400	-0.04878200
H	1.05547600	2.69848300	-0.19650800
C	-0.08830300	-2.34454400	-0.74145400
C	-4.31037200	0.21685500	0.54361300
H	-4.56870600	1.28447300	0.75022200
C	2.88276300	-1.12725200	1.04381800
H	2.12374400	-1.92317300	1.22939100
H	1.02246700	-2.25541200	-0.66301900
Ge	2.01068100	0.14371400	-0.22861800
Te	3.44177200	1.58367100	-1.56902900
Si	3.11293200	-0.30167500	2.78363800
Si	4.44642000	-2.01528400	0.31892400
C	4.35091800	-1.23114300	3.89111600
H	5.38501500	-1.23714300	3.49135600
H	4.37830900	-0.71746600	4.87679200
H	4.04181800	-2.28102100	4.07331400
C	3.71732600	1.48887500	2.63366000
H	3.90719200	1.90966500	3.64439700
H	4.65928100	1.55057800	2.05002200
H	2.98099700	2.14499700	2.12571800
C	1.44924300	-0.37924600	3.69618300
H	0.60315100	-0.01953000	3.07653700
H	1.22267000	-1.42336900	3.99958800
H	1.48095900	0.23399400	4.62175200
C	5.99646400	-0.92976000	0.40904300
H	6.28111600	-0.68253500	1.45263300
H	6.85319600	-1.46493700	-0.05396600
H	5.84050600	0.01918400	-0.14530200
C	4.74787200	-3.61768900	1.30423900
H	5.58526000	-4.17840800	0.83530400
H	5.01929100	-3.43358200	2.36198600
H	3.85925700	-4.28333600	1.29045200
C	4.16829400	-2.55640500	-1.48222000
H	4.05012000	-1.69084000	-2.16541100
H	5.04502600	-3.14454400	-1.82967100
H	3.27393900	-3.20751800	-1.58234500
C	0.93885300	-5.12389900	0.28668100
H	0.75045900	-5.95751300	0.99700500
H	1.06553200	-5.56515300	-0.72154500

H	1.90314500	-4.65592000	0.57511600
C	-0.63719500	-3.33530600	2.19349300
H	0.33978500	-2.97755200	2.57834700
H	-1.36791200	-2.51372300	2.33389500
H	-0.95342700	-4.19152500	2.82666400
C	-2.08503600	-4.79872300	-0.11199400
H	-2.98920700	-4.15625400	-0.09059800
H	-2.01403400	-5.24995400	-1.12354900
H	-2.25609900	-5.62881500	0.60689600
C	-2.12463600	-2.60966100	-3.18312700
H	-2.19165800	-2.78144200	-4.27885500
H	-2.73154100	-3.39167500	-2.68367400
H	-2.58839500	-1.62591300	-2.96869300
C	0.41393500	-4.34280700	-3.16136800
H	-0.13598700	-5.20109500	-2.72405300
H	0.34522100	-4.43482900	-4.26679600
H	1.48562500	-4.44485500	-2.89105700
C	0.64413600	-1.32658000	-3.61263800
H	0.27420100	-0.30414700	-3.39698000
H	1.72877000	-1.34444500	-3.37681400
H	0.53555300	-1.50119600	-4.70494300
C	-7.14719900	0.63110700	-0.71644000
H	-7.74089900	0.55871200	-1.65305100
H	-7.72838300	0.13448000	0.08637400
H	-7.06506700	1.70846000	-0.45882300
C	-5.67022600	-2.00466000	-1.33941200
H	-4.70438600	-2.53475800	-1.46924700
H	-6.23513300	-2.51234000	-0.53048500
H	-6.24723000	-2.13436800	-2.28013000
C	-4.66658000	0.68414900	-2.50805200
H	-4.66145200	1.78840300	-2.39124000
H	-3.61835500	0.36215700	-2.67600900
H	-5.24969800	0.44597900	-3.42299700
C	-6.51703700	-0.11467200	2.75550700
H	-6.68546000	0.98024500	2.67879700
H	-7.29546400	-0.62167200	2.14881700
H	-6.68478200	-0.40414300	3.81531000
C	-3.55403400	0.08259700	3.54405300
H	-2.49800300	-0.14500100	3.29033200
H	-3.64771200	1.18548400	3.63597700
H	-3.76743500	-0.35740000	4.54163300
C	-4.63603000	-2.49693100	2.23549700
H	-3.61937800	-2.85198600	1.97271500
H	-4.87021800	-2.88368400	3.25064600
H	-5.35317100	-2.95867300	1.52664800
C	0.51206200	5.24812500	-1.95025000
H	0.32195200	5.67021200	-2.96043800
H	0.29178100	6.04700000	-1.21167000
H	1.59299200	5.00314800	-1.88716800
C	-2.39065600	4.20008900	-1.78060200
H	-3.05414200	3.31264000	-1.72999700
H	-2.69469300	4.90723000	-0.98465800

H	-2.57618900	4.69381400	-2.75932400
C	-0.27763100	2.52127100	-3.16738200
H	0.77290900	2.16513500	-3.20612200
H	-0.94642100	1.63851300	-3.09448900
H	-0.50803600	3.04182000	-4.12182200
Si	-4.75222500	-0.60198500	2.23885500
Si	-5.43508100	-0.15239900	-0.98653300
Si	-0.49265900	-3.87678300	0.37952300
Si	-0.30481900	-2.65481200	-2.65351700
Si	-0.55700500	3.69502000	-1.70682200
Si	-0.16027500	3.93575100	1.52639100
C	-1.62911800	5.14967500	1.55199000
H	-1.61812300	5.69417100	2.52106600
H	-1.57414800	5.91075100	0.74639800
H	-2.61106600	4.63836300	1.47257300
C	1.43391400	4.96522000	1.64243700
H	1.56667400	5.63494400	0.76899000
H	1.41241300	5.59924000	2.55473800
H	2.33345400	4.31762100	1.70467400
C	-0.29976100	2.88228800	3.09737300
H	-1.18158100	2.20967300	3.07191100
H	0.60029800	2.25373000	3.24634800
H	-0.39858200	3.54240800	3.98571100

Complete citation for reference 44.

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, R. A. Gaussian 09, I. Gaussian, Wallingford CT, 2009.