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Bonding analysis of telluroketones H$_2$A=Te (A = C, Si, Ge)

**Naziah B. Jaufeerally · Ponnadurai Ramasami ·
Paul Jerabek · Gernot Frenking**

Abstract Quantum chemical calculations using density functional theory BP86/def2-TZVPP and ab initio methods at CCSD(T)/def2-TZVPP have been carried for the telluroketones H$_2$A=Te (A = C, Si, Ge). DFT calculations have also been carried out for the ketones H$_2$C=E (E = O, S, Se, Te) and for the complexes NHC→[H$_2$A=Te]→B(C$_6$F$_5$)$_3$. The nature of the bonding has been investigated with charge- and energy decomposition analyses. The calculated bond dissociation energies for the double bonds of the H$_2$C=E and H$_2$A=Te molecules show the expected trends O > S > Se > Te for atom E and C > Si > Ge for atom A. Complexation of the telluroketones in NHC→ [H$_2$A=Te]→B(C$_6$F$_5$)$_3$ leads to longer and weaker A-Te bonds which exhibit the surprising trend for the bond dissociation energy Si>Ge>C. The contribution of the π bonding in H$_2$A=Te increases for the heavier atoms with the sequence C < Si < Ge.

Keywords Telluroketones · Molecular orbitals · Natural bond orbital · Energy decomposition analysis

Introduction

Carbonyl (C=O) and thiocarbonyls compounds (C=S) are ubiquitous building blocks in nature and have been explored for their uses from the chemical industry to bioscience [1].

N. B. Jaufeerally · P. Ramasami (✉)
Computational Chemistry Group, Department of Chemistry,
University of Mauritius, Réduit, Mauritius
e-mail: ramchemi@intnet.mu

P. Jerabek · G. Frenking (✉)
Fachbereich Chemie, Philipps-Universität Marburg, 35032 Marburg,
Germany
e-mail: frenking@chemie.uni-marburg.de

P. Jerabek
e-mail: paul.jerabek@chemie.uni-marburg.de

Selenocarbonyls (C=Se) have also been of great interest since selenium-containing fragments can be introduced readily into an organic compound and, after appropriate transformations, the selenium atom can be removed easily by simple processes [2]. Besides, the redox catalytic activity of selenium-containing peptides is found to be switchable, leading to the development of nature-mimicking smart materials with promising properties [3].

The importance of C=O, C=S and C=Se moieties has prompted numerous chemists to synthesize stable heavier-element congeners with double bonds between heavier group 14 and group 16 elements R$_2$A=E (A = Si, Ge, Sn, Pb; E = S, Se,Te), known as "heavy ketones". The considerable progress being made in the chemistry of compounds with multiple bonds with heavier group 14 elements is not merely because of experimental curiosity but also because such compounds are capable of activating small molecules and thus mimic transition elements [4, 5]. However, telluro-ketones have received scant importance compared to oxo-, thio- and seleno-analogues, yet stable and isolable Si=Te [6] and Ge=Te [7] compounds have already been synthesized. Recently, Tiekink reported that compounds with C–Te bonds offer possibilities as therapeutic agents, and their biological functions deserve more attention [8]. Therefore, it is important to gather accurate data for organotellurium compounds.

Attempts to synthesize and isolate heavy ketones have met with great difficulties due to the polarity of both the σ and π bonds of A=E, which contribute to the spontaneous intermolecular oligomerization or polymerization of the heavy ketones [9–14]. Based on the kinetic stabilization concept, some stable heavy ketones with various combinations between heavier group 14/16 elements R$_2$A=E have been synthesized and isolated using bulky substituents R [15–21]. Recently, with the first successful isolation of a germanone (Eind)$_2$Ge=O (Eind = 1,1,3,3,5,5,7,7-octaethyl-s-hydrindacen-4-yl), Li et al. [22] reported that the isomerization process can be inhibited by rigid bulky protecting groups. All these isolatable heavy ketones bear sterically encumbered substituents from group 14 elements while the group 16

elements are left unsupported. Very recently, Ghadwal et al. [23] exploited the stabilization of $R_2A=E$ with N-heterocyclic carbenes (NHCs) and reported the first Lewis donor-acceptor stabilized silacarbonyl halide, $NHC^1\rightarrow[SiH(Cl)=O]\rightarrow B(C_6F_5)_3$ ($NHC^1 = $ 1,3-bis(2,6-diisopropyl-phenyl)imidazol-2-ylidene), in which the oxygen atom is also protected.

Telluroformaldehyde ($H_2C=Te$), was first stabilized by coordination to transition-metal centers by Roper et al. in 1983 [24, 25]. The first stable germanetellones, Tbt(Dis)Ge=Te and Tbt(Tip)Ge=Te (Tbt = 2,4,6-tris[bis(trimethylsilyl)methyl]phenyl, Dis = bis(trimethylsilyl)methyl and Tip = 2,4,6-triisopropylphenyl) were reported in 1997 [15–21]. A free telluroketone $R_2C=Te$, where R_2 is cyclic 1,1,3,3-tetramethylindane, has been synthesized in solution but the structure could not be determined by X-ray analysis [26]. The synthesis and isolation of free telluroketones bearing the Si=Te and Ge=Te moieties remains elusive. Recently, we reported the structures and energetics of $R_2A=Te$ and $R^1R^2A=Te$ (A = C and Si and R = H, F, Cl, Br, I and CN) molecules [27, 28]. In this work, we analyze the nature of the bonding in the telluroketones $H_2A=Te$ and $NHC\rightarrow H_2A=Te\rightarrow B(C_6F_5)_3$ (A = C, Si, Ge) complexes with donor-acceptor ligands. The parent ketones $H_2C=E$ (E = O, S and Se) were also investigated for comparison purposes.

Methods

The ketones and complexes were optimized using the BP86 functional [29, 30] using Gaussian 03 [31] in conjunction with the Turbomole 6.3 [32] program package. The RI approximation [33] was applied using auxiliary basis functions [34–36]. The Ahlrichs def2-TVZPP basis sets [37] were used for all the atoms. An effective core potential [38] was used for the tellurium atom. Stationary points were characterized by calculating the Hessian matrix analytically. Frequencies and thermodynamics corrections were calculated with the aoforce [39–41] program of the Turbomole package. The telluroketones were also optimized at the CCSD(T) level [42] with cc-pVTZ basis sets [43–46] using MOLPRO [47]. Atomic partial charges were calculated using the natural bond orbital (NBO) method [48, 49]. The functional BP86 was chosen because numerous studies by our group in the past have shown that it gives quite accurate geometries and energies [50–53].

Energy decomposition analyses (EDA) [54] were carried out using the ADF (2012.02) program package at the BP86/TZ2P+ level of theory [55]. Uncontracted Slater-type orbitals (STOs) were employed as basis functions in self-consistent field (SCF) calculations [56]. Triple-zeta-quality basis sets were used, which were augmented by two sets of polarization functions, i.e., p and d functions for the hydrogen atom and d and f functions for the other atoms. An auxiliary set of s, p, d, f and g STOs was used to fit the molecule densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle [57]. Scalar relativistic effects were considered using the zero-order regular approximation (ZORA) [58–62].

Within the EDA, bond formation between the interacting fragments is divided into three steps: in the first step, fragments calculated with the frozen geometry of the entire molecule were superimposed without electronic relaxation to yield the quasiclassical electrostatic attraction ΔE_{elstat}. In the second step, the product wave function becomes antisymmetrized and renormalized, which gave the repulsive term ΔE_{Pauli}, named Pauli repulsion. The third step consists of relaxation of the molecular orbitals to their final form to yield the stabilizing orbital interaction ΔE_{orb}. The sum of the three terms $\Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb}$ gives the total interaction energy ΔE_{int}. The orbital interactions ΔE_{orb} can be divided into pairwise contributions of the interacting fragments with the extended EDA-natural orbitals for chemical valence (NOCV) method [63]. Further details and examples of EDA and EDA-NOCV calculations are available from the literature [64–68].
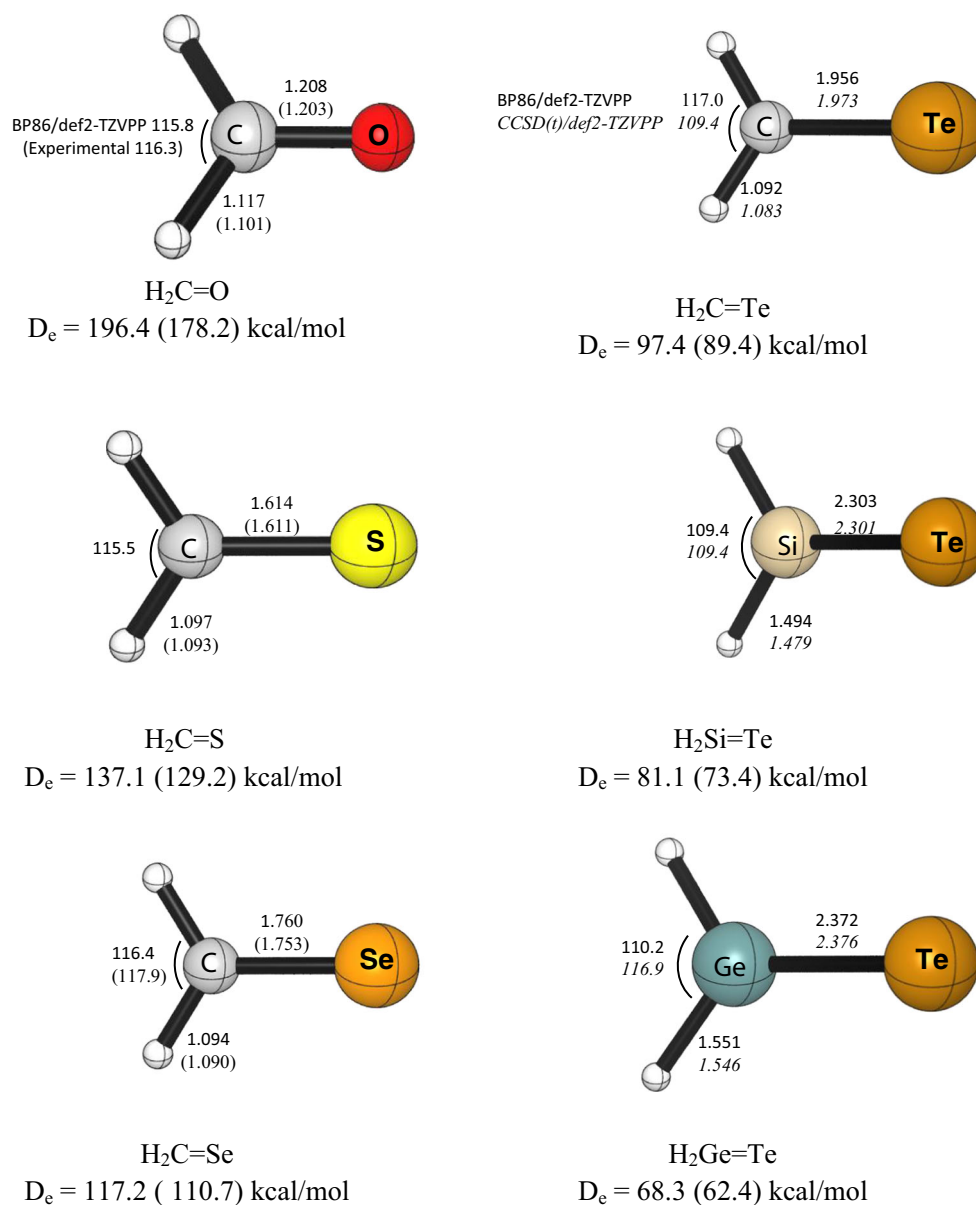
Results and discussion

Geometries and energies

Figure 1 shows the calculated BP86/def2-TZVPP geometries for $H_2C=E$ (E = O, S, Se) alongside the experimentally known bond lengths and bond angles. The agreement of the experimental values with the calculated data was very good. No experimental data are available for $H_2C=Te$. We calculated the geometry of the telluroketones $H_2A=Te$ at the BP86/def2-TZVPP and CCSD(T)/def2-TZVPP levels of theory. The agreement between the two levels of theory was reasonable. The H–E–H angle at CCSD(T)/def2-TZVPP is more acute for E = C but it is wider for E = Ge compared with the BP86/def2-TZVPP values, while the A–Te distances agree quite well. The calculated bond dissociation energies (BDEs) for the $H_2C=E$ and $H_2A=Te$ bonds at CCSD(T)/def2-TZVPP and BP86/def2-TZVPP show the expected trends for $D_e = O > S > Se > Te$ for atom E and C > Si > Ge for atom A. The latter values are a bit higher than the former but the differences are not relevant for this work. The calculated D_e values are in good agreement with previous high-level calculations [69].

Figure 2 shows the theoretically predicted equilibrium geometries of the complexes $NHC\rightarrow[H_2A=Te]\rightarrow B(C_6F_5)_3$ (A = C, Si, Ge), which possess an antiperiplanar arrangement

Fig. 1 Calculated geometries of $H_2A=E$. Bond dissociation energies (D_e) at BP86/def2-TZVPP and at CCSD(T)/cc-pVTZ (*in parentheses*). Bond lengths are in Ångstroms and angles are in degrees. References for experimental data: $H_2C=O$ [75]; $H_2C=S$ [76]; $H_2C=Se$ [77]

BP86/def2-TZVPP 115.8
(Experimental 116.3)

1.208
(1.203)

1.117
(1.101)

$H_2C=O$
D_e = 196.4 (178.2) kcal/mol

BP86/def2-TZVPP 117.0
CCSD(t)/def2-TZVPP 109.4

1.956
1.973

1.092
1.083

$H_2C=Te$
D_e = 97.4 (89.4) kcal/mol

115.5

1.614
(1.611)

1.097
(1.093)

$H_2C=S$
D_e = 137.1 (129.2) kcal/mol

109.4
109.4

2.303
2.301

1.494
1.479

$H_2Si=Te$
D_e = 81.1 (73.4) kcal/mol

116.4
(117.9)

1.760
(1.753)

1.094
(1.090)

$H_2C=Se$
D_e = 117.2 (110.7) kcal/mol

110.2
116.9

2.372
2.376
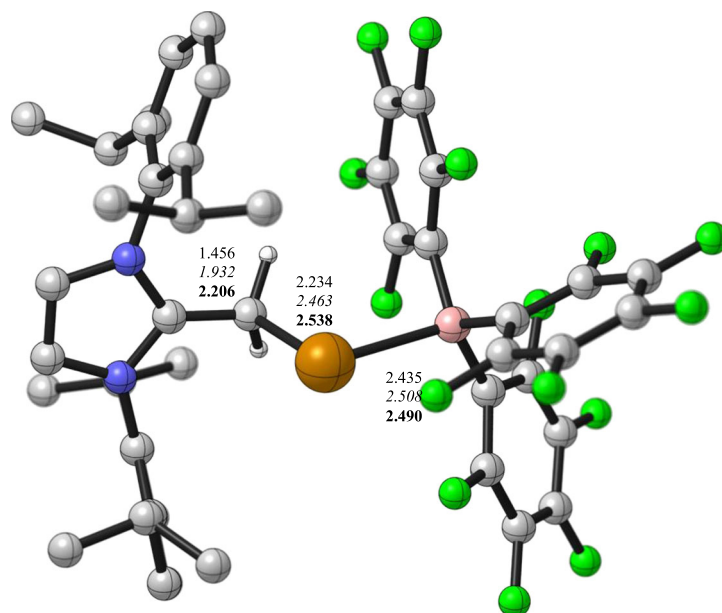
1.551
1.546

$H_2Ge=Te$
D_e = 68.3 (62.4) kcal/mol

of the donor and acceptor moieties. The torsion angle C–A–Te–B for all complexes is 180°. The comparison with the free telluroketones makes it obvious that the A–Te bonds become significantly longer between 0.27 Å (A = C) and 0.16 Å (A = Si, Ge) [70, 71][1]. The same trend is also calculated for the BDEs of the A–Te bonds in the complexes, which are clearly weaker than in the free compounds. Note that the theoretically predicted A–Te bond strength in the complexes NHC→

$[H_2A=Te]→B(C_6F_5)_3$ has the trend Si > Ge > C, which is clearly different than for free $H_2A=Te$. The calculations predict that the carbon complex NHC→$[H_2C=Te]→B(C_6F_5)_3$ has the weakest bond to Te and that the silicon species NHC→$[H_2Si=Te]→B(C_6F_5)_3$ has the strongest bond. The peculiar bond weakening of the A–E bonds may be related to the strength of the donor-acceptor interactions in the complexes. Figure 2 shows that the complexation energies for the reaction NHC→$[H_2A=Te]→B(C_6F_5)_3→H_2A=Te$ + NHC + $B(C_6F_5)_3$, which exhibit the trend C > Si > Ge, are rather high. The very large strong donor-acceptor interactions of the carbon complex apparently weakens the C–Te bond to such an extent that it becomes weaker than the other two A–Te bonds.
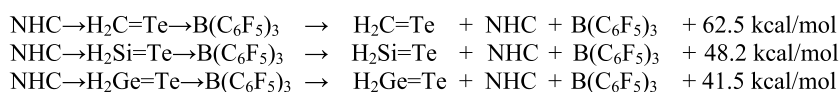
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[1] The calculated bond length and the bonding analysis indicates that the A–Te bonds in the complexes are single bonds. We keep the formal notation with double bonds NHC→$[H_2A=Te]→B(C_6F_5)_3$, which sketches the bonding situation between the isolated fragments. For a discussion of using arrows for chemical bonds.

Fig. 2 Calculated geometries (BP86/def2-TZVPP) of the complexes NHC→[H$_2$E=Te] →B(C$_6$F$_6$)$_3$ (E = C, Si, Ge) and bond dissociation energies D_e. Bond lengths are in Ångstroms and angles are in degrees

1.456
1.932
2.206

2.234
2.463
2.538

2.435
2.508
2.490

D_e (C-Te) = 41.0 kcal/mol
D_e (Si-Te) = 63.3 kcal/mol
D_e (Ge-Te) = 53.9 kcal/mol

NHC→H$_2$C=Te→B(C$_6$F$_5$)$_3$ → H$_2$C=Te + NHC + B(C$_6$F$_5$)$_3$ + 62.5 kcal/mol
NHC→H$_2$Si=Te→B(C$_6$F$_5$)$_3$ → H$_2$Si=Te + NHC + B(C$_6$F$_5$)$_3$ + 48.2 kcal/mol
NHC→H$_2$Ge=Te→B(C$_6$F$_5$)$_3$ → H$_2$Ge=Te + NHC + B(C$_6$F$_5$)$_3$ + 41.5 kcal/mol

Bonding analysis

Inspection of the molecular orbitals of the telluroketones H$_2$A=Te shows that the highest occupied molecular orbital (HOMO) is the A=Te π orbital while the lowest unoccupied molecular orbital (LUMO) is the A=Te π^* orbital (Fig. 3). The NBO analysis is in agreement with the expected Lewis picture of the A–Te bonds, i.e., there is a σ and a π bond (Table 1). According to the NBO results, the C–Te σ bond is clearly polarized toward the carbon end, while the π bond is nearly unpolar. The Si–Te and Ge–Te σ bonds are nearly unpolar but the π bonds are polarized towards Te. This leads to a positive partial charge at Te in H$_2$C=Te while the tellurium atoms in H$_2$A=Te (A = Si, Ge) carry a negative charge (Table 1).

The antiperiplanar arrangement of the donor and acceptor fragments in NHC→[H$_2$A=Te]→B(C$_6$F$_5$)$_3$ indicate that the donation NHC→H$_2$A=Te takes place into the vacant A=Te π^* orbital while the Te→B(C$_6$F$_5$)$_3$ donation occurs through the occupied A=Te π MO. This is in agreement with the NBO analysis of the complexes NHC→[H$_2$A=Te]→B(C$_6$F$_5$)$_3$, which show that there is no occupied A=Te π orbital (Table 2). Thus, the bonding situation in the complexes should be described either in terms of donor-acceptor bonds NHC→ H$_2$A=Te→B(C$_6$F$_5$)$_3$ or, alternatively, as zwitterion NHC(+)-H$_2$A-Te-(−)B(C$_6$F$_5$)$_3$. This is in agreement with the calculated

partial charges, which indicate that the fragments TeB(C$_6$F$_5$)$_3$ and B(C$_6$F$_5$)$_3$ are acceptor moieties (Table 2). The NBO results

Molecule	HOMO	LUMO
H$_2$C=Te		
H$_2$Si=Te		
H$_2$Ge=Te		

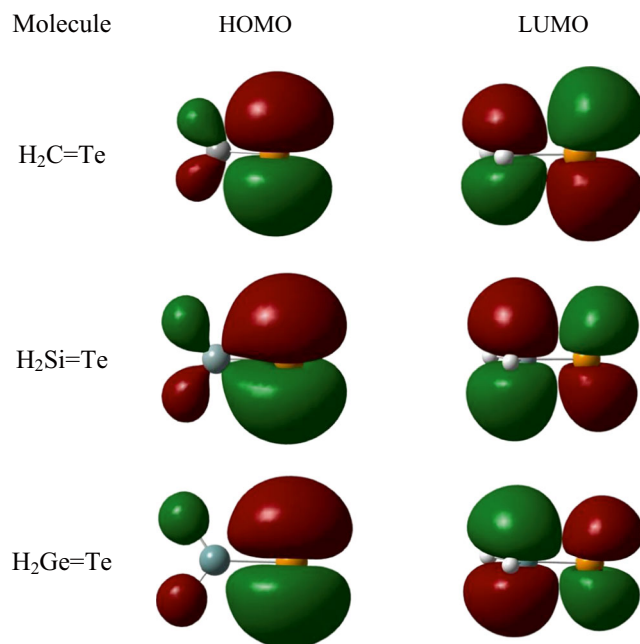**Fig. 3** Shape of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of H$_2$A=Te

Table 1 Natural bond orbital (NBO) partial charges (q) and results of the relevant occupied orbitals of $H_2A=Te$ (A = C, Si, Ge) at BP86/def2-TZVPP

Orbital	Occupation	Contributions of atom to the orbital (%)	Composition %		q(Te)
			s	p	
$H_2C=Te$					+0.26
BD(1) C–Te (σ)	1.998	C: 61.8	34.2	65.8	
		Te: 38.2	13.4	86.4	
BD(1) C–Te (π)	1.999	C: 48.8	0.0	99.8	
		Te: 51.2	0.0	99.7	
LP(1) Te (σ)	1.995		87.8	12.2	
LP(2) Te (π)	1.952		0.0	100.0	
$H_2Si=Te$					-0.24
BD(2) Si–Te (σ)	1.976	Si: 47.5	37.0	62.6	
		Te: 52.5	12.6	87.2	
BD(1) Si–Te (π)	1.999	Si: 32.4	0.0	98.9	
		Te: 67.6	0.0	99.7	
LP(1) Te (σ)	1.988		87.6	12.4	
LP(2) Te (π)	1.859		0.0	99.9	
$H_2Ge=Te$					−0.23
BD(2) Ge–Te (σ)	1.898	Ge: 49.9	37.0	62.8	
		Te: 50.2	10.4	89.1	
BD(1) Ge–Te (π)	1.999	Ge: 32.2	0.0	99.3	
		Te: 67.8	0.0	99.7	
LP(1) Te (σ)	1.984		89.7	10.4	
LP(2) Te (π)	1.891		0.0	99.9	

Table 2 NBO partial charges (q) and results of the relevant occupied orbitals of NHC→$[H_2A=Te]$→$B(C_6F_5)_3$ (A = C, Si, Ge) at BP86/def2-TZVPP

Orbital	Occupation	Contributions of atom to the orbital (%)	Composition %		q	q
			s	p	Te	TeB($C_6F_5)_3$
NHC→$[H_2C=Te]$→$B(C_6F_5)_3$					+0.21	−1.06
BD(1) C–Te (σ)	1.889	C: 65.3	18.6	81.3		
		Te: 34.8	6.6	93.2		
LP(1) Te (σ)	1.980		81.1	18.9		
LP(2) Te (π)	1.914		0.1	99.9		
NHC→$[H_2Si=Te]$→$B(C_6F_5)_3$					−0.10	−1.30
BD(2) Si–Te (σ)	1.946	Si: 48.3	22.6	71.7		
		Te: 51.7	10.0	89.9		
LP(1) Te (σ)	1.967		78.1	21.9		
LP(2) Te (π)	1.844		0.1	99.9		
NHC→$[H_2Ge=Te]$→$B(C_6F_5)_3$					−0.07	−0.26
BD(2) Ge–Te (σ)	1.934	Ge: 50.8	28.3	71.6		
		Te: 49.2	8.0	81.7		
LP(1) Te (σ)	1.967		79.8	20.2		
LP(2) Te (π)	1.870		0.1	99.9		

suggest that Te has two electron lone pairs and that the polarity of the A–Te σ bond changes only slightly in the complexes.

Table 3 shows the results of the EDA calculations of the systems $H_2A=E$. The intrinsic C=E bond strength of the carbon systems $H_2C=E$, which is given by the interaction energy ΔE_{int} between the frozen fragments H_2C and E in the triplet state, decreases in the expected order O > S > Se > Te. The C=E bonds are more covalent than electrostatic in character but the degree of covalence, which is given by the percentage contribution of ΔE_{orb} to the total attraction, decreases also with the same trend O > S > Se > Te. Note that the π contribution of $\Delta E(b_1)\pi_\perp$ to the orbital term remains nearly the same for the chalcogen atoms. It has been shown before that the alleged weakening of π bonds of heavier main group atoms, which is sometimes stated to be the reason for the lower stability of molecules that have multiple bonds between main group elements is a myth [72–74]. The calculated trend of the bond dissociation energies, D_e, is very similar to the ΔE_{int} values, which agrees quite well with previous results

[69]. This is because the rather small preparation energies ΔE_{prep} do not change very much along the series.

The strength of the interaction energies ΔE_{int} for the telluroketones $H_2A=Te$ decreases in the order C > Si > Te but the differences are not very large. In contrast, the D_e values have a much larger slope with decreasing values for D_e (Table 3). This is because the preparation energies of the heavier systems become significantly larger. The ΔE_{prep} values of H_2Si and H_2Ge include the electronic excitation energy from the singlet ground state to the triplet excited state, which is the reference state for $H_2Si=Te$ and $H_2Ge=Te$. We want to draw attention to the increase in π bonding in the series $H_2A=Te$ when A becomes bigger. Table 3 shows that the percentage contribution of $\Delta E(b_1)\pi_\perp$ to ΔE_{orb} in $H_2A=Te$ becomes larger with the trend C < Si < Te. This is in agreement with analysis of the bonding in E_2 (E = N – Bi) which shows that the relative contribution of π bonding in the heavier species P_2 and As_2 is bigger than in N_2 [73].

We also analyzed the A–Te bonds in the complexes NH→$[H_2A=Te]$→$B(C_6F_5)_3$ with the EDA method in order to investigate the change in bonds between the free molecules $H_2A=Te$ and the complexes. Table 4 shows the results of the EDA-NOCV calculations. The EDA-NOCV makes it possible to separate the specific contributions of the σ- and

Table 3 Energy decomposition analyses (EDA) calculations of the compounds $H_2A=E$ (A = C, Si, Ge; E = O, Si, Se, Te) at BP86/def2-TVZPP. The interacting fragments are AH_2 and E in the electronic triplet states. Energy values are in kcal mol^{-1}

	$H_2C=O$	$H_2C=S$	$H_2C=Se$	$H_2C=Te$	$H_2Si=Te$	$H_2Ge=Te$
ΔE_{int}	−196.6	−141.3	−122.2	−103.1	−100.7	−94.5
ΔE_{Pauli}	488.3	290.8	247.2	205.2	168.2	153.9
ΔE_{elstat}	−199.5 (29.1 %)	−166.1 (38.4 %)	−155.8 (42.2 %)	−139.0 (45.1 %)	−119.8 (44.6 %)	−110.2 (44.4 %)
ΔE_{orb}	−485.4 (70.9 %)	−266.0 (61.6 %)	−213.6 (57.8 %)	−169.3 (54.9 %)	−149.1 (55.4 %)	−138.2 (55.6 %)
$\Delta E(a_1)\sigma^b$	−348.4 (71.8 %)	−190.9 (71.8 %)	−156.6 (73.3 %)	−127.6 (75.4 %)	−94.6 (63.4 %)	−90.2 (65.3 %)
$\Delta E(a_2)\delta^b$	0	0	0	0	0	0
$\Delta E(b_1)\pi_\perp{}^b$	−109.5 (22.6 %)	−61.0 (22.9 %)	−47.4 (22.2 %)	−34.9 (20.6 %)	−41.4 (27.7 %)	−38.9 (28.1 %)
$\Delta E(b_2)\pi_\parallel{}^b$	−27.5 (5.7 %)	−14.1 (5.3 %)	−9.7 (4.5 %)	−6.7 (4.0 %)	−13.1 (8.8 %)	−9.1 (6.6 %)
ΔE_{prep}	0.2	4.2	5.0	5.7	19.6	26.2
D_e	196.4 (181.4)^c	137.1 (133.8)^c	117.2 (114.0)^c	97.4	81.1	68.3

^{a} Values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb}$

^{b} Values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}

^{c} Ref. [69]

π bonding, which come from the pairwise interactions between the fragments NHC(H_2A) and TeB(C_6F_5)$_3$. The calculated data show that the much lower BDE of the carbon species NHC→[$H_2C=Te$]→B(C_6F_5)$_3$ comes from weakening of the C–Te interaction energy. The ΔE_{int} value in the complex is much smaller (−79.3 kcal mol^{-1}) than in free $H_2C=Te$ (−103.1 kcal mol^{-1}, Table 3). Inspection of the energy terms of the EDA-NOCV calculations suggests that the weakening is mainly due to the loss of π bonding in NHC→[$H_2C=Te$]→B(C_6F_5)$_3$, which contributes only −9.6 kcal mol^{-1} to ΔE_{orb} (Table 4) while it is −34.9 kcal mol^{-1} in free $H_2C=Te$. A surprising result comes from the EDA-NOCV data for the

silicon system NHC→[$H_2Si=Te$]→B(C_6F_5)$_3$. The data in Table 4 show that the intrinsic interaction ΔE_{int} in the complex is not much weaker (−99.4 kcal mol^{-1}) than in free $H_2Si=Te$ (−100.7 kcal mol^{-1}, Table 3). Inspection of the energy terms in NHC→[$H_2Si=Te$]→B(C_6F_5)$_3$ revels that the Si–Te σ orbital interactions in the complex (−159.0 kcal mol^{-1}) are stronger than the total orbital interactions in the Si=Te double bond of free $H_2Si=Te$ (−149.1 kcal mol^{-1}, Table 3). A similar situation is found for the Ge-Te bonds in NHC→[$H_2Ge=Te$]→B(C_6F_5)$_3$ and $H_2Ge=Te$. The Ge-Te σ orbital interactions in the complex (−142.3 kcal mol^{-1}) are stronger than the total orbital interactions in the Ge=Te double bond of free $H_2Ge=Te$ (−138.2 kcal mol^{-1}, Table 3). The smaller BDEs for the A–Te bonds in the latter two complexes compared with the free species $H_2A=Te$ (A = Si, Ge) comes from the bigger preparation energies ΔE_{prep} in the adducts.

Summary and conclusions

The results of this work can be summarized as follows. The calculated bond dissociation energies for the $H_2C=E$ and $H_2A=Te$ show the expected trends O > S > Se > Te for atom E and C > Si > Ge for atom A. Complexation of the telluroketones in NHC→[$H_2A→Te$]→B(C_6F_5)$_3$ leads to longer and weaker A–Te bonds, which exhibit a surprising trend for the bond dissociation energy of Si > Ge > C. The contribution of the π bonding in $H_2A=Te$ increases for the heavier atoms with the sequence C < Si < Ge.

Table 4 EDA-natural orbitals for chemical valence (NOCV) calculations (BP86/TZ2P+) of the A–Te bonds in the complexes NHC→[$H_2A=Te$]→B(C_6F_5)$_3$ using the fragments: NHC(H_2A) and TeB(C_6F_5)$_3$ in the singlet state. The energy values are in kcal mol^{-1}

NHC→[$H_2A=Te$]→B(C_6F_5)$_3$

	A = C	A = Si	A = Ge
ΔE_{int}	−79.3	−99.4	−90.4
ΔE_{Pauli}	195.0	256.4	219.5
$\Delta E_{elstat}{}^a$	−130.9 (47.6 %)	−170.1 (47.8 %)	−147.6 (47.6 %)
$\Delta E_{orb}{}^a$	−144.0 (52.4 %)	−185.7 (52.2 %)	−162.3 (52.4 %)
$\Delta E_{orb, (\sigma)}{}^b$	−122.0 (84.7 %)	−159.0 (85.6 %)	−142.3 (87.6 %)
$\Delta E_{orb, (\pi)}{}^b$	−9.6 (6.7 %)	−11.6 (6.2 %)	−8.8 (5.4 %)
$\Delta E_{orb, rest}{}^b$	−12.4 (8.6 %)	−15.1 (8.1 %)	−11.2 (6.9 %)
ΔE_{prep}	38.3	36.1	36.5
D_e	41.0	63.3	53.9

^{a} Values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb}$

^{b} Values in parentheses gives the percentage contribution to the total orbital interactions ΔE_{orb}

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