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### Interaction of difluoromethylene phosphobetaine with heteroatom-centered electrophiles

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**Graphical Abstract** 



Synthesis of difluorinated phosphonium salts by interaction of the phosphobetaine reagent with

halogen and chalcogen electrophiles is described.

### Highlights

- Reactions of difluoromethylene phosphobetaine
- Halogenation of fluorinated ylides
- Synthesis of fluorinated phosphonium salts

Abstract A series of difluorinated phosphonium salts were obtained by reaction of difluoromethylene phosphobetaine with halogenating reagents, as well as arylsulfenyl and arylselenyl chlorides. The reaction proceeds via decarboxylation of the phosphobetaine followed by trapping of the difluorinated phosphorus ylide by heteroatom-centered electrophiles. The crystal structures of the phosphonium salts were studied by X-ray diffraction analysis. For the salt containing the  $CF_2I$  group and iodide counterion, the I...I interaction was identified in the solid state. The nature of this halogen bond was evaluated by quantum chemical calculations.

Keywords: phosphonium salts, phosphobetaine, phosphorus ylide, halogenation, halogen bonding

#### **1. Introduction**

Fluorinated organophosphorus compounds have emerged as valuable targets in medicinal chemistry [1], as well as useful reagents for the synthesis of organofluorine compounds [2]. In 1964, difluorinated phosphorus ylide **1** was proposed as an intermediate generated from the combination of triphenylphosphine and difluorocarbene [3], and since then it has been extensively exploited for olefination of carbonyl compounds [4] (Scheme 1). Despite synthetic applications, ylide **1** has not yet been spectroscopically characterized, presumably, due to its instability associated with facile fragmentation into triphenylphosphine and difluorocarbene [5]. Correspondingly, this ylide must be generated *in situ* in the presence of a suitable electrophile, which can attack at the ylide carbon. We have recently demonstrated that ylide **1** can react with various  $\pi$ -electrophiles such as Michael acceptors [6,7], azomethines [6], and carbonyl compounds [6-8] affording difluorinated phosphonium salts. Salts of this type have numerous applications associated with the cleavage of the carbon-phosphorus bond [9,10]. Herein we report that ylide **1**, generated from an inexpensive precursor, can be trapped by halogenating reagents, as well as sulfur- and selenium-centered electrophiles.



Scheme 1. Chemistry of ylide 1.

#### 2. Results and discussion

#### 2.1. Synthetic studies.

Among various methods for the generation of ylide 1 [3-7,11,12], we were particularly interested in application of difluoromethylene phosphobetaine 2 discovered by Xiao [12]. Reagent 2 can be conveniently prepared on a hundred-gram scale from readily available chemicals - potassium bromodifluoroacetate and triphenylphosphine. This compound is an air stable solid, which can be shelf-stored at room temperature for a long time. However, upon mild heating, reagent 2 undergoes decarboxylation with concomitant generation of ylide 1. Correspondingly, this reagent has found numerous applications [5,6,12,13]. Thus, betaine 2 was combined with halogenating reagents, and the mixture was heated in acetonitrile around 50 °C. The reactions were typically complete within 1.5 hours, as evidenced by cease of gas evolution, as well as dissolution of betaine 2. For chlorination, N-chlorosuccinimide (NCS) was used, and then the mixture was treated with iodomethane to scavenge succinimide counter-ion leading to iodide salt 3a. Bromination and iodination reactions were carried out with elemental halogens affording salts 3b,c in good isolated yields. Interaction of betaine 2 with arylsulfenyl and arylselenyl chlorides also worked well leading to salts 3d,f in reasonable yields. Phenyl disulfide did not react with betaine 2 under standard conditions. However, addition of iodomethane allowed smooth formation of expected salt 3e. The role of iodomethane in this case is believed to methylate the disulfide reagent converting it to a stronger sulfenylating species. Salts 3 are air sensitive solids, which should be stored under inert atmosphere.

#### 3. Structural studies

The structures of compounds **3a,c,f** were studied by single crystal X-ray diffraction analysis (Figure 1). For compound **3d**, we have not been able to obtain crystals of satisfactory quality. However, in attempt to perform counter ion exchange from chloride to iodide, we were fortunate to identify a crystal containing the cationic fragment of salt **3d** [14]. For salt **3b**, the crystal structure was reported in the literature [15]. Therefore, it is possible to compare structural parameters of all types of phosphonium cations of salts **3**. (Table 1).



**Figure 1.** General views of cation of **3a**, salt **3c**, cations of **3d** and **3f** (from left to right). Atoms are presented as ellipsoids of anisotropic displacement (50% probability). Hydrogen atoms are omitted for clarity.

The phosphonium cations have similar structural parameters. In particular, C-P bond distances are close for the whole series irrespective of the nature of heteroatom group E. One of the most noticeable features in salt **3c** is a cation-anion interaction via I...I contact. The corresponding I...I distance is 3.2674(9) Å that is 0.55 Å larger than I-I bond in solid iodine (2.7179(2) Å [16]). The angle C-I...I of 172.06(18)° is close to linear and the angle P-C-I is 115(1)°, which is indicative of halogen-halogen contact of type II [17]. The latter contacts are classified as true halogen bonds [18].

The characteristics of halogen bond in 3c were studied using quantum chemical calculations. Starting coordinates of cation and anion were taken from its X-ray structure. All calculations were

carried out with all-electron TZVPP basis set and PBE0 functional implemented into ORCA 3.0.3 program [19]. Relativistic effects were accounted using ZORA approximation. To save computation time, RI (resolution of identity) approximation was utilized. Two models were calculated to find structure that is most similar to that obtained from X-ray analysis. The first model is a simple calculation of isolated cation-anion pair. In the second one, cation-anion pair was placed into solvation continuum (COSMO model, dielectric constant 79). After optimization of atomic coordinates, the resulted geometries were checked for the presence of negative eigenvalues of hessian matrix. As a result, in the first model I...I distance was found to be 3.030 Å, while in the second one this distance is 3.385 Å, with the latter being closer to the experimental value of 3.2674(9) Å. Correspondingly, the second model was used for further discussion.

Bond length and angles in optimized structure of the cation are in good agreement with experimental values. For instance, C-I and F<sub>2</sub>C-P bonds are equal to 2.173 and 1.890 Å, respectively, that reproduced experimental values within 0.02 Å.

According to analysis in terms of quantum theory of atoms in molecules (QTAIM) [20], bond critical point (*bcp*) was found between the iodine atoms (Figure 2, (a)). In addition, the presence of several C-H...F and C-H...I interactions was revealed. The value of electron density  $\rho(\mathbf{r})$  in *bcp* of I...I bond is rather small (0.02 a.u.), while its Laplacian is positive (0.042 a.u). This is indicative of a closed-shell interaction. The energy of I...I bond was estimated by correlation formula proposed by Espinosa [21] affording the value of 3.3 kcal/mol, which is on the same scale as weak hydrogen bonds.



**Figure 2.** (a) Molecular graph of cation-anion pair **3c**. Green points correspond to bond critical points. (b) Isosurfaces of RDG function colorized according to the sign of  $\lambda_2$ .

Finally, the presence of halogen bond was illustrated by non-covalent interaction (NCI) analysis [22]. This method utilizes dimensionless reduced density gradient (RDG). The sign of eigenvector  $\lambda_2$  serves as a descriptor of the nature of non-covalent interactions (attractive or repulsive). Isovalues of RDG colorized according to its value and sign of  $\lambda_2$  were used in our study to reveal the character of weak intermolecular bonds. The presence of separate isosurfaces in regions of small values of electron density and its gradient is indicative for weak interatomic bonds and can be described as an analog of *bcp*. Areas of negative values is indicative of attractive interactions responsible for stabilization of particular atomic configuration in the crystal structure, and such an area is clearly identified in the case of I...I bond in cation **3c**. Indeed, small oblate disk-shaped region is located between the iodine atoms (Figure 2, (b)). The similar attractive character of intermolecular interactions is also demonstrated in the case of C-H...F and C-H...I interactions.

### 4. Conclusions

Difluorinated phosphonium salts bearing an additional halogen atom or a halcogen fragment can be obtained from the readily accessible phosphobetaine reagent. The process involves the interaction of transient difluorinated ylide with a source of electrophilic halogen, as well as sulfenyl and selenyl based regents. Analysis of crystals of obtained salts suggested similar structural parameters of cationic fluorinated phosphonium fragments. However, for the salt containing the CF<sub>2</sub>I group and iodide counterion, the I...I interaction was observed, which was assigned to a typical halogen bond with the estimated energy of 3.3 kcal/mol.

#### 5. Experimental

#### 5.1 General Experimental Procedures

All reactions were performed under an argon atmosphere. Dichloromethane was distilled from CaH<sub>2</sub> prior to use. Acetonitrile was distilled twice: from P<sub>2</sub>O<sub>5</sub> and CaH<sub>2</sub> successively and stored over MS 3Å. High resolution mass spectra (HRMS) were measured using electrospray ionization (ESI) and time-of-flight (TOF) mass analyzer. The measurements were done in a positive ion mode (interface capillary voltage – 4500 V) or in a negative ion mode (3200 V); mass range from m/z 50 to m/z 3000. Phosphobetaine **2** was obtained according to a literature procedure [12]. NMR spectra were recorded on a Bruker AM300 instrument in dry CDCl<sub>3</sub> at 27 °C.

### 5.2. 4-Chlorophenylsulfenyl chloride [23].

A solution of 4-chlorobenzenethiol (30 mmol, 4.32 g) in thionyl chloride (75 mmol, 6.06 ml) was heated with stirring in water bath at 70 °C until the formation of gas has stopped (about 1.5 h). The resulting mixture was distilled under reduced pressure affording wine-red liquid. Bp 96-97 °C (8 mbar). Yield 4.75 g (89%).

### 5.3. Phenylselenyl chloride [24].

A mixture of diphenyl diselenide (3000 mg, 9.62 mmol) and thionyl chloride (780  $\mu$ L, 9.62 mmol) in carbon tetrachloride (5 mL) was stirred at room temperature for 30 min. The resulting

suspension was dissolved upon heating with a heat gun. Then, the mixture was cooled to -20 °C, and kept for 2 h at this temperature without stirring. The solvent was decanted affording orange crystals. Yield 2042 mg (94%). Mp 63-64 °C.

#### 5.4. (Chlorodifluoromethyl)triphenylphosphonium iodide (3a).

A suspension of reagent **2** (1068 mg, 3.0 mmol), *N*-chlorosuccinimide (400 mg, 3.0 mmol) in acetonitrile (2.0 mL) was heated with stirring in water bath at 50 °C for 1.25 h (until bubbling stopped). The mixture was cooled to room temperature, methyl iodide (375 µL, 6.0 mmol) was added, and the reaction mixture was stirred for 10 min at 40 °C. The solvent was evaporated under vacuum to a half of its volume, and methyl *tert*-butyl ether (1.5 mL) was added. The mixture was cooled to -20 °C, and kept for 16 h at this temperature without stirring. The solvent was decanted, the residue was washed with methyl *tert*-butyl ether (3×1.5 mL), and the solid was recrystallized from acetonitrile affording 1011 mg (yield 71%) of salt **3a** as colorless crystals. Mp 156-157 °C (dec.) <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>),  $\delta$ : 7.58-7.69 (m, 6H), 7.69-7.78 (m, 6H), 7.82-7.90 (m, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>),  $\delta$ : 109.7 (d, *J* = 86.2 Hz), 124.2 (td, *J* = 324.0, 110.6 Hz), 131.0 (d, *J* = 13.3 Hz), 134.1 (d, *J* = 9.9 Hz), 137.2 (d, *J* = 2.2 Hz). <sup>19</sup>F NMR (282 MHz, CDCl<sub>3</sub>),  $\delta$ : -52.5 (d, *J* = 87.2 Hz). <sup>31</sup>P{<sup>1</sup>H} NMR (121 MHz, CDCl<sub>3</sub>),  $\delta$ : 33.9 (t, *J* = 87.2 Hz). HRMS (ESI): calcd for C<sub>19</sub>H<sub>15</sub>ClF<sub>2</sub>P (M<sup>+</sup>) 347.0562, found 347.0564.

### 5.5. Synthesis of compounds **3b**, *c*.

A mixture of reagent **2** (3.6 mmol, 1282 mg) and bromine (for **3b**, 155  $\mu$ L, 3.0 mmol) or iodine (for **3c**, 762 mg, 3.0 mmol) in acetonitrile (2.0 mL) was heated with stirring in water bath at 53 °C for 1 h (until bubbling stopped). The mixture was cooled to room temperature, the solvent was decanted, the residue was washed with acetonitrile (3×1.5 mL), and the resulting solid was dried under vacuum with heating at 50 °C.

### 5.5.1. (Bromodifluoromethyl)triphenylphosphonium bromide (3b) [15].

Yield 1019 mg (72%). Pale-yellow crystals. Mp 169-170 °C (dec.). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>),  $\delta$ : 7.57-7.81 (m, 12H), 7.81-7.95 (m, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>),  $\delta$ : 111.2 (d, J = 85.1

Hz), 116.3 (td, J = 333.9, 95.1 Hz), 131.2 (d, J = 14.4 Hz), 134.5 (d, J = 9.9 Hz), 137.4 (d, J = 3.3 Hz). <sup>19</sup>F NMR (282 MHz, CDCl<sub>3</sub>),  $\delta$ : -52.0, (d, J = 83.4 Hz). <sup>31</sup>P{<sup>1</sup>H} NMR (121 MHz, CDCl<sub>3</sub>),  $\delta$ : 32.4, (t, J = 83.4 Hz).

#### 5.5.2. (Difluoroiodomethyl)triphenylphosphonium iodide (3c)

Yield 81% (1375 mg). Pale-brown crystals. Mp 172-173 °C (dec.). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>),  $\delta$ : 7.68-7.82 (m, 12H), 7.88-7.98 (m, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>),  $\delta$ : 99.4 (td, J = 339.5, 50.9 Hz), 112.9 (d, J = 84.0 Hz), 130.8 (d, J = 12.1 Hz), 134.5 (d, J = 10.0 Hz), 136.6 (d, J = 3.3Hz). <sup>19</sup>F NMR (282 MHz, CDCl<sub>3</sub>),  $\delta$ : -62.3 (d, J = 82.8 Hz). <sup>31</sup>P{<sup>1</sup>H} NMR (121 MHz, CDCl<sub>3</sub>),  $\delta$ : 25.2 (t, J = 82.8 Hz). HRMS (ESI): calcd for C<sub>19</sub>H<sub>15</sub>F<sub>2</sub>IP (M<sup>+</sup>) 438.9919, found 438.9921.

### 4.6. [Difluoro(4-chlorophenylthio)methyl]triphenylphosphonium chloride (3d).

A suspension of reagent 1 (5909 mg, 16.6 mmol) and 4-chlorophenylsulfenyl chloride (2980 mg, 16.6 mmol) in acetonitrile (10.0 mL) was heated with stirring in water bath at 50 °C for 1 h (until bubbling stopped). The mixture was cooled to room temperature, the solvent was evaporated under vacuum to a half of its volume, methyl tert-butyl ether (7 ml) was added. The mixture was cooled to -20 °C, and kept for 16 h at this temperature without stirring. The solvent was decanted, the residue was washed with methyl *tert*-butyl ether (3×5 mL), and the resulting solid was dried under vacuum with heating at 50 °C. Yield 5542 mg (68%). Colorless crystals. Mp 74-75 °C. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>),  $\delta$ : 6.95 (d, 2H, J = 8.1 Hz), 7.15 (d, 2H, J = 8.1 Hz), 7.31-7.84 (m, 15H). <sup>13</sup>C{<sup>1</sup>H} NMR  $(75 \text{ MHz}, \text{CDCl}_3), \delta: 110.6 \text{ (d}, J = 84.0 \text{ Hz}), 118.5, 125.5 \text{ (td}, J = 309.6, 87.7 \text{ Hz}), 129.3, 130.5 \text{ (d}, J = 309.6, 87.7 \text{ Hz})$ = 13.3 Hz), 133.9 (d, J = 11.1 Hz), 136.7 (d, J = 3.3 Hz), 137.4, 137.5. <sup>19</sup>F NMR (282 MHz, CDCl<sub>3</sub>),  $\delta$ : -70.3 (d, J = 91.1 Hz). <sup>31</sup>P{<sup>1</sup>H} NMR (121 MHz, CDCl<sub>3</sub>),  $\delta$ : 30.5, (t, J = 91.1 Hz). HRMS (ESI): calcd for C<sub>25</sub>H<sub>19</sub>ClF<sub>2</sub>PS (M<sup>+</sup>) 455.0596, found 455.0609. In an attempt to effect counter ion exchange, the reaction mixture obtained after heating of reagent 1 with 4chlorophenylsulfenyl chloride was cooled to room temperature. Then, methyl iodide (1.5 equiv) was added and the mixture was stirred at 40 °C 10 min. The mixture was analyzed by <sup>19</sup>F NMR with 4-fluorotoluene as internal standard, which suggested the yield of 19% of cation of 3d. The

solvent was evaporated under vacuum to a half of its volume, the mixture was cooled to -20 °C, and kept for 16 h at this temperature without stirring, and the resulting crystals were withdrawn and studied by X-ray diffraction.

### 5.7. [Difluoro(phenylthio)methyl]triphenylphosphonium iodide (3e).

A suspension of reagent **2** (7.2 mmol, 2.563 g), phenyl disulfide (8.0 mmol, 1.744 g) and methyl iodide (12 mmol, 744 µL) in acetonitrile (4.0 mL) was heated with stirring in water bath at 55 °C for 2 h (until bubbling stopped). The mixture was cooled to room temperature, the solvent was evaporated under vacuum to a half of its volume, and the mixture was cooled to -20 °C, and kept for 16 h at this temperature without stirring. The solvent was decanted, the residue was washed with methyl *tert*-butyl ether (3×2 mL), and the resulting solid was dried under vacuum at 50 °C affording 3.153 g (yield 72%) of salt **3e** as pale-yellow crystals. Mp 194-195 °C (dec.). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>),  $\delta$ : 7.24-7.33 (m, 2H), 7.35-7.46 (m, 3H), 7.63-7.85 (m, 12H), 7.89-7.98 (m, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>),  $\delta$ : 111.4 (d, *J* = 84.3 Hz), 120.7 (m), 126.3 (td, *J* = 310.3, 90.2 Hz), 129.7, 131.1 (d, *J* = 13.2 Hz), 131.6, 134.6 (d, *J* = 10.5 Hz), 136.6, 137.2 (d, *J* = 3.0 Hz). <sup>19</sup>F NMR (282 MHz, CDCl<sub>3</sub>),  $\delta$ : -69.1 (d, *J* = 92.8 Hz). <sup>31</sup>P{<sup>1</sup>H} NMR (121 MHz, CDCl<sub>3</sub>),  $\delta$ : 29.8 (t, *J* = 92.8 Hz). HRMS (ESI): calcd for C<sub>25</sub>H<sub>20</sub>F<sub>2</sub>PS (M<sup>+</sup>) 421.0986, found 455.0979.

### 5.8. [Difluoro(phenylselenyl)methyl]triphenylphosphonium iodide (3f).

A suspension of reagent **2** (3.240 g, 9.1 mmol), phenylselenyl chloride (1.744 g, 9.1 mmol) in acetonitrile (4.0 mL) was heated with stirring in water bath at 50 °C for 1.5 h (until bubbling stopped). The mixture was cooled to room temperature, and methyl iodide (850  $\mu$ L, 13.65 mmol) was added. The reaction mixture was stirred at 40 °C 10 min, then the solvent was evaporated under vacuum to a half of its volume, methyl *tert*-butyl ether (3.0 ml) was added. The mixture was cooled to -20 °C, and kept for 16 h at this temperature without stirring. The solvent was decanted, the residue was washed with methyl *tert*-butyl ether (3×2 mL), and the resulting solid was dried under vacuum with heating at 50 °C. Yield 3302 mg (61%). Pale-yellow crystals. Mp 153-154 °C (dec.). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>),  $\delta$ : 6.96-7.04 (m, 2H), 7.09-7.17 (m, 1H), 7.18-7.23 (m, 2H), 7.44-7.63

(m, 12H), 7.68-7.89 (m, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>),  $\delta$ : 110.7 (d, J = 84.0 Hz), 120.3 (m), 120.3 (td, J = 326.2, 78.5 Hz), 129.0, 130.1, 130.3 (d, J = 13.3 Hz), 133.7 (d, J = 9.9 Hz), 136.3, 136.4 (d, J = 2.2 Hz). <sup>19</sup>F NMR (282 MHz, CDCl<sub>3</sub>),  $\delta$ : -71.5 (d, J = 89.3 Hz). <sup>31</sup>P{<sup>1</sup>H} NMR (121 MHz, CDCl<sub>3</sub>),  $\delta$ : 28.4 (t, J = 89.3 Hz). HRMS (ESI): calcd for C<sub>25</sub>H<sub>20</sub>F<sub>2</sub>PSe (M<sup>+</sup>) 469.0432, found 469.0424.

#### 6. X-ray analysis.

The structures were solved by direct method and refined in anisotropic approximation for nonhydrogen atoms. Hydrogens atoms of methyl, methylene and aromatic fragments were calculated according to those idealized geometry and refined with constraints applied to C-H and N-H bond lengths and equivalent displacement parameters ( $U_{eq}(H) = 1.2U_{eq}(X)$ , X - central atom of XH<sub>2</sub> group;  $U_{eq}(H) = 1.5U_{eq}(Y)$ , Y - central atom of YH<sub>3</sub> group. All structures were solved with the ShelXT<sup>1</sup> program and refined with the ShelXL<sup>2</sup> program. Molecular graphics was drawn using OLEX2<sup>3</sup> program.

Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication [for **3a**, CCDC 1887171; for **3c**, CCDC 1887168; for **3d**, CCDC 1887169; for **3f**, CCDC 1887170]. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44 1223 336033 or e-mail: deposit@ccdc.cam.ac.uk).

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O Ph₃P, ↓ e	lectrophile (0.8-1 equiv)	Ph <sub>3</sub> P <sup>+</sup> E	
2 F F M	leCN, 50-53 °C, 1-1.5 h	3 F F X	
Electrophile	Product		Yield of <b>3</b> , % <sup>a</sup>
NCS; MeI	Ph <sub>3</sub> P <sup>+</sup> Cl F F I <sup>-</sup>	<b>3</b> a	71
Br <sub>2</sub>	Ph <sub>3</sub> P <sup>+</sup> Br F F Br	3b	72
I <sub>2</sub>	Ph <sub>3</sub> P <sup>+</sup> F F I <sup>-</sup>	3c	81
4-ClC <sub>6</sub> H <sub>4</sub> SCl	Ph <sub>3</sub> P <sup>+</sup> S F F CI	3d	68
Ph <sub>2</sub> S <sub>2</sub> ; MeI	Ph <sub>3</sub> P <sup>+</sup> S F F I	3e	72
PhSeCl; MeI	Ph <sub>3</sub> P <sup>+</sup> Se F F I	3f	61
<sup>a</sup> Isolated yield.			

**Table 1.** Synthesis of phosphonium salts 3.

	E	F <sub>2</sub> C-P	C <sub>Ph</sub> -P	C-F	F <sub>2</sub> C-E
<b>3</b> a	Cl	1.901(3)	1.785(3)	1.382(4)	1.695(4)
<b>3b</b> <sup><i>a</i></sup>	Br	1.883	1.783	1.347	1.923
3c	Ι	1.870(7)	1.787(6)	1.362(7)	2.195(7)
3d	SAr	1.884(6)	1.783(6)	1.368(6)	1.786(6)
3f	SePh	1.878(2)	1.785(2)	1.360(2)	1.968(2)

Table 2. Selected structural parameters of cations Ph<sub>3</sub>P<sup>+</sup>CF<sub>2</sub>E, Å.

<sup>*a*</sup> Data from ref. [15].