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Quantum Chemical Calculations on Oxygen Monofluoride (OF) and its Protonated Analogues: Comparison of Methods

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ABSTRACT

Quantum chemical calculations offer the real promise of being able to complement experiment as a means to uncover and explore new areas in chemistry. One of such is its use in the determination of molecular structure, kinetics and reactivity. This work seeks to investigate the molecular properties of Oxygen monofluoride (OF) and its two possible protonated analogues (HOF^+ and HFO^+). Quantum chemical methods; Hartree fock (HF), Becke-3-Lee-Yang-Parr (B3LYP), Moller-Plesset second order (MP2), Coupled Cluster method (CCSD) and Gaussian 04 method (G4) with varying basis sets were employed in the determination of the parameters (Dipole moment, bond distance, IR frequency, zero point vibrational energy, and rotational constants) reported for the three molecular species studied in this work. Bond angle was reported for the two protonated analogues (HOF^+ and HFO^+). From the results as compared to the experimental values, B3LYP/6-311++G** method proves itself as the best method in the optimization and frequencies calculations of the OF, HOF^+ and HFO^+ because it gives better accuracy in most of the calculated parameters and the MP2 method also give relative accuracy in some of the calculated parameters of OF and its protonated analogues, HOF^+ and HFO^+. The optimized geometry shows the OF molecule to be linear while the protonated analogues were non-linear.

Introduction

Quantum chemistry is a branch of chemistry which has as its aim the fundamental characterization of chemical phenomena. Quantum mechanics was developed in 1900 by Max Planck when he unveiled the quantized state of the energy of black body radiation. The reactivity and properties of very small systems like electrons and ions where ordinarily inaccessible with classical mechanics. Quantum mechanics complements the inadequacies of the classical mechanics by providing a reliable route by which the behavior of these systems are being qualified [1]. Amongst the major scientific roles played by quantum mechanics is its use as a bedrock on which most computational chemical calculations are built. Thus, there is a direct relationship between quantum mechanics and computational chemistry. This relationship is an indispensable tool in describing the properties, structure and reactivity of electrons [2].

Computational chemistry is the numerical replication of chemical reactions and structures in a bid to tackle important chemical problems. Computational chemistry is the conglomeration of computing programs, mathematical skills and chemical prowess in investigating chemical phenomena [3]. It involves the use of computer programs to generate data on the properties of molecules which in turn aids the study of the reactivity, structure and kinetics of these molecules.

Oxygen monofluoride (OF) is a diatomic molecule and belongs to the halogen oxides family, it was first discovered in 1937 by Vaidya [4]. The existence of the diatomic OF molecule has been confirmed [5]. Oxygen monofluoride is highly reactive and unstable. Series of reactions have affirmed to the existence of oxygen monofluoride as an unstable intermediate. They include: the thermal decomposition of OF_2 [6]; reaction between OF_2 and SO_3 [7]; and the ionization dissociation of perchloryl fluoride [8]. Unsuccessful efforts in the gas phase detection of OF is a pointer to its short-lived and unstable nature [9]. Consequently, experimental data on the physical properties of the molecule is lacking. Information on the spectroscopic properties of the molecule is available [5]. Streng, 1963 provides detailed information about the bonding system in OF, describing the O-F bond. The knowledge of this bonding scheme is of utmost importance since it facilitates the understanding and estimation of radicals in their intermediary reaction stages [7], and also in polymerization processes [10]. Previously, in the course of examining the thermodynamic properties of the fluorides of group VIA of the periodic table, the dissociation energy for OF was estimated to be 51±3 kcal mol^{-1} (2.2±0.1 eV)[11]. The binding energy for OF, the ionization potential, electron affinity, internuclear distance, and the dipole and quadrupole moments have been determined and available in literature[12].

The equilibrium internuclear separation (r_e) has not been measured experimentally. Series of calculations with *minimal* basis sets for O and F, gave a preliminary value of 2.52 bohr (1.33 A) for $r_e(OF)$.

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Molecular Self consistent field wave functions were also calculated for OF$^+$ ($^3\Sigma$) and OF$^-$($^1\Sigma$) at the OF equilibrium separation.

Though there are a few studies on OF, there is dearth of information on its protonated analogues; HFO$^+$ and HOF$^+$, hence the need for this study. This research work is focused on the computational study of OF, and the protonated analogues. The parameters to be calculated include; optimized geometries, Bond distance, Dipole moment, constant, IR frequency, ZPE, Rotational constants.

Methodology:

The Gaussian 09 suit of program is applied for all the calculations reported in this work. Different computational methods have been employed in this study; these include the Hartree Fock (HF), B3LYP, the MP2 method, the CCSD and the Gaussian 04 compound method. The choice of these methods is based on experience as some methods perform well for some properties than other methods. Thus there is need for comparison of methods to determine which is better for a particular parameter. The cc-pvdz and the 6-311++G** basis sets are used. The reported results are for stable molecules with no imaginary (negative) frequency [13-18]. This is confirmed with the frequency calculations.

Results and discussion:

In this section, results of quantum chemical calculations carried out on oxygen monofluoride (OF) and the two possible protonated species (HFO$^+$ and HOF$^+$) based on the methods described above are presented and discussed. The results obtained for the different parameters (optimized geometry, dipole moment, bond distance, rotational constants, infrared frequency and zero point vibrational energy) for each of the molecular species are presented and discussed under different subheadings. This makes it easy to compare the computationally calculated data for each parameter with experimental data from literature.

Optimized geometry:

The optimized geometry for the three molecular species (OF, HOF+ and HFO+) considered in this work are as shown in figures 1 to 3 respectively. The OF molecule is linear as seen in fig. 1 while the protonated species (HOF+ and HFO+) were observed to be non-linear (fig. 2 and fig. 3) respectively. This non-linear state of the molecular ions could possibly be attributed to the effect of protonation.

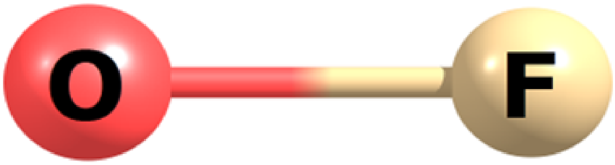

Figure 1. Optimized geometry for OF.

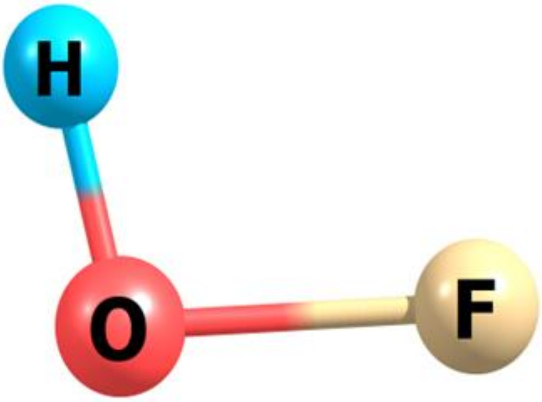

Figure 2. Optimized geometry for HOF^{+}.

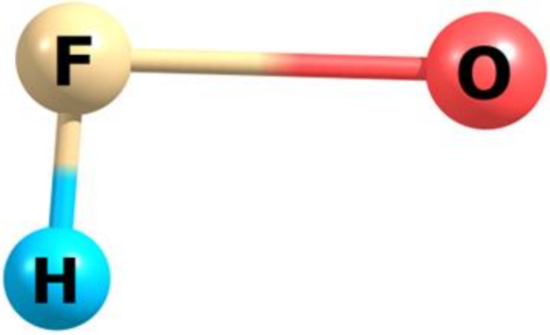

Figure 3. Optimized geometry for HFO$^+$.

Dipole Moment:

Tables 1a to 1c show the value for dipole moment calculated for OF, HOF$^+$ and HFO$^+$ at six different methods which include Hartree Fock (HF), Beckee 3 Lee Yang Parr (B3LYP), Moller Plesset Second Order MP2), Couple Cluster single-double excitation (CCSD) and Gaussian 04 (G4) respectively. The value ranges from 0.0264 to 0.4586 Debye for OF, 2.2169 to 3.9771Debye for HOF$^+$ and 1.9718 to 2.2169Debye for the HFO$^+$. From the result obtained, B3LYP method with the 6-311++G** basis set gives better accuracy for OF with an uncertainty value of 0.0264 as compared to the experimental value of 0.004Debye and HF method gives better accuracy for HOF$^+$ with an uncertainty value of -0.0131 as compared to the experimental value of 2.230Debye and HF method is expected to predict the best value for HFO$^+$ with no experimental value.

Table 1a. Dipole moment for OF molecule.

Method	(D)Cal. Value (Debye)	Cal.-Expt. (Debye)
HF/6-311++G**	0.3703	0.3663
B3LYP/6-311++G**	0.0264	0.0224
MP2/6-311++G**	0.4371	0.4331
MP2/cc-pVDZ	0.4586	0.4546
CCSD/cc-pVDZ	0.1237	0.1197
G4	0.3815	0.3775

Experimental determine value; 0.004 (Debye). Ref [19]

Table 1b. Dipole moment for HOF+.

Method	(D) cal. Value	Cal. - Exprt. (Debye)
HF/6-311++G**	2.2169	-0.0131
B3LYP/6-311++G**	3.2480	1.018
MP2/6-311++G**	2.0695	-0.1605
CCSD/cc-pVDZ	3.7716	1.5416
G4	3.9771	1.7471

Dipole moment; 2.230 (Debye) (NIST Triatomic Spectral Database)

Table 1c. Dipole moment for HFO$^+$.

Method	(D) cal. Value (Debye)
B3LYP/6-311++G**	3.2480
MP2/ cc-pVDZ	2.9374
CCSD/cc-pVDZ	2.0533
G4	1.9718

Bond Distance:

Calculated bond distances for OF and its protonated analogue at the six different methods employed in this study are presented in tables 2a to 2c. The value ranges from 1.3106 to 1.3656Å for OF, 0.9469^{R1} to 1.3073^{R1} and 1.0273^{R2} to 1.4359^{R2}Å for HOF$^+$ molecule and 0.9347^{R1} to 1.4933^{R1}Å and 0.9804^{R2} to 1.6945^{R2}Å for HFO$^+$ molecule. From the result obtained, B3LYP method with the 6-311++G** basis set gives the best prediction for OF with an uncertainty value of -0.0011 as compared to the experimental value of 1.354Å. The MP2 method e with the 6-311++G** basis set gives better accuracy for HOF$^+$ with an uncertainty value of 0.0083^{R1} and -0.0108^{R2} as compared to the experimental value of

0.9600^{R1}Å and 1.4420^{R2}Å and MP2 method with the cc-pVDZ basis set is believed to predict the best value for HFO^+ molecule.

Table 2a. Bond distance for OF.

Method	Bond distance cal. Value (Å)	Cal. - Exptl. (Å)
HF/6-311++G**	1.3106	-0.0434
B3LYP/6-311++G**	1.3529	-0.0011
MP2/6-311++G**	1.3317	-0.0223
MP2/cc-pVDZ	1.3374	-0.0166
CCSD/cc-pVDZ	1.3656	0.0116
G4	1.3413	-0.0127

Bond distance Experimental determine value; 1.354 Å. Ref: [20]

Table 2b. Bond distance for HOF^+.

Method	Bond distance Cal. Value (Å)	Cal. - Exprt. (Å)
HF/6-311++G**	0.9469^{R1} 1.3617^{R2}	-0.0131 -0.0810
B3LYP/6-311++G**	0.9722^{R2} 1.4359^{R2}	0.0122 -0.0061
MP2/6-311++G**	0.9683^{R1} 1.4312^{R2}	0.0083 -0.0108
MP2/cc-pVDZ	0.9736^{R1} 1.4375^{R2}	0.0136 -0.0045
CCSD/cc-pVDZ	1.3072^{R1} 1.0293^{R2}	0.3472 -0.4127
G4	1.2834^{R1} 1.0273^{R2}	0.3234 -0.4147

Exptl det. Bond distance in Å OH = 0.9600^{R1} FO = 1.4420^{R2}. Ref: [21]

Table 2c. Bond distance for HFO^+.

Method	**Bond distance Cal. Value (Å)**
B3LYP/6-311++G**	0.9347^{R1} 1.6945^{R2}
MP2/cc-pVDZ	0.933^{R1} 1.6742^{R2}
CCSD/cc-pVDZ	1.4933^{R1} 0.9804^{R2}
G4	1.4497^{R1} 0.9848^{R2}

Bond angle:

Tables 3a and 3b show the bond angle calculated for the protonated analogues of OF (HOF^+ and HFO^+) at six different methods respectively. The value ranges from 100 to 180 degree for HOF^+ and 92.5652 to 180.0 degree for HFO^+ molecule. From the result obtained, MP2/ccpvdz method gives better accuracy with an uncertainty value -0.0126 as compared to the experimental value 97.2 degree. Thus the value of bond angle predicted with the HF/6-311++G** method for HFO^+ with no experimental value is expected to be accurate.

Table 3a. Bond angle for HOF^+.

Method	Bond angle Cal. Value (degree)	Cal. - Expt. (degree)
HF/6-311++G**	100.9218	3.7218
B3LYP/6-311++G**	98.6828	1.4828
MP2/6-311++G**	98.2348	1.0348
MP2/cc-pVDZ	97.1874	-0.0126
CCSD/cc-Pvdz	180.0	82.8
G4	180.0	82.8

Experimental value; 97.2 degree. Ref: [21]

Table 3b. Bond angle for HFO^+.

Method	Bond angle (degree) cal. Values
B3LYP/6-311++G**	92.5652
MP2/cc-pvdz	93.1764
CCSD/cc-pVDZ	180.0
G4	180.0

Rotational constants:

Tables 4a to 4b show the data calculated for rotational constant for OF, and its protonated analogues (HOF^+ and HFO^+) at the six different methods respectively. The values ranges from 31.2073 to 33.8815GHz for OF, 584.6683^a to 629.0677^aGHz, 26.7230^b to 29.7783^bGHz and 25.55502^c to 28.4324^cGHz for HOF^+ and 584.6683^a to 629.0677^aGHz, 19.7340^b to 29.7783^bGHz and 19.1330^c to 28.4324^cGHz for HFO^+.

Table 4a. Rotational constant for OF.

Method	Rotational constant cal. Value (GHz)	Cal. - Expt. (GHz)
HF/6-311++G**	33.881469	2.142239
B3LYP/6-311++G**	31.794701	0.055431
MP2/6-311++G**	32.818234	1.078964
MP2/cc-pVDZ	32.536112	0.796842
CCSD/cc-pVDZ	31.207323	-0.531947
G4	32.3467726	0.6075026

Rotational Constants Experimental determine value; 31.73927 GHz. Ref: [22]

Table 4b. Rotational constant for HOF^+

Method	Rotational constant Cal. Value (GHz)	Cal. - Expt. (GHz)
HF/6-311++G**	629.06771^a 29.77834^b 28.43243^c	40.05947 2.78613 2.6227
B3LYP/6-311++G**	586.08910^a 26.89778^b 25.71751^c	-2.91914 -0.09443 -0.09222
MP2/6-311++G**	589.00169^a 27.09751^b 25.90570^c	-0.00655 0.1053 0.09597
MP2/cc-pVDZ	578.72992^a 26.90773^b 25.71225^c	-10.27832 -0.08448 -0.09748
CCSD/cc-pVDZ	584.66825^a 26.72305^b 25.55502^c	-4.340 -0.26916 -0.25471
G4	587.87512^a 27.45841^b 26.23311^c	-1.13312 0.4662 0.42338

Rotational constant in GHz; 589.00824^a 26.99221^b 25.80973^c. ref: [23]

Table 4c. Rotational constant for HFO^+

Method	Rotational constant Cal. Value (GHz)
B3LYP/6-311++G**	607.66224^a 19.73401^b 19.11330^c
MP2/ cc-pVDZ	611.02218^a 20.20172^b 19.55518^c
CCSD/cc-pVDZ	0.0000000^a 22.5013689^b 22.5013689^c
G4	0.0000000^a 24.1690087^b 24.1690087^c

From the result obtained, the B3LYP/6-311++G** method gives better accuracy for OF with an uncertainty value of 0.0554 as compared to the experimental value of 31.7393GHz and MP2/6-311++G** method give better accuracy for HOF$^+$ with an uncertainty value of -0.0066^a, 0.1053^b and 0.0959^c as compared to the experimental value 589.0082^a, 26.9922^b and 25.8097^{c}GHz. Thus the values of 611.022^a, 20.201^b, 19.555^{c}GHz predicted with the MP2/cc-pVDZ method for the HFO$^+$ with no experimental value are believed to be accurate.

Vibrational frequencies

Zero point vibrational energy

Tables 5a to 5c show the values calculated for the vibrational zero point energy for OF and its protonated analogues (HOF$^+$ and HFO$^+$) at six different methods respectively. The values range from 1.43092 to 2.08034Kcal/mol for OF, 5.98050 to 9.83124Kcal/mol for HOF$^+$ and 5.72269 to 7.24409 Kcal/mol for HFO$^+$. From the result obtained, the B3LYP/6-311++G** method gives better accuracy for both OF and HOF$^+$ with an uncertainty value of 0.37449 and 0.05611 respectively as compared to the experimental value 8.30857Kcal/mol and the value of HFO$^+$ predicted with the B3LYP/6-311++G** method are expected to be accurate for the HFO$^+$ with no experimental value.

Table 5a. Zero point vibrational energy for OF.

Method	ZPE cal. Value (Kcal/Mol)	Cal.- Exprt. (Kcal/Mol)
HF/6-311++G**	1.72220	0.21791
B3LYP/6-311++G**	1.56040	0.05611
MP2/6-311++G**	2.01990	0.51561
MP2/cc-pVDZ	2.08034	0.57605
CCSD/cc-pVDZ	1.43092	-0.07337
G4	1.64557	014128

ZPE Experimental determine value; 526.5 cm^{-1} = 1.50429 Kcal/mol. Ref: [22]

Table 5b. Zero point vibrational energy for HOF$^+$

Method	ZPE Cal. Value (Kcal/mol)	Cal. – Exptl (Kcal/Mol)
HF/6-311++G**	9.83124	1.52267
B3LYP/6-311++G**	8.68306	0.37449
MP2/6-311++G**	8.7S7623	0.46766
MP2/cc-pVDZ	8.75341	0.44484
CCSD/cc-pVDZ	5.98050	-2.32807
G4	6.17565	-2.13292

Experimental value: 2908.0 cm^{-1} = 8.30857 Kcal/mol. Ref: [24]

Table 5c. Zero point vibrational energy for HFO+ Molecule.

Method	ZPE Cal. Value (Kcal/mol)
B3LYP/6-311++G**	7.12926
MP2/cc-pVDZ	7.24409
CCSD/cc-pVDZ	5.72269
G4	5.83788

IR frequency

Tables 6a to 6c show the values calculated for IR frequency for OF and its protonated analogues (HOF$^+$ and HFO$^+$) at the six different methods respectively. The values range from 1000.9441 to1455.2213cm^{-1} for OF molecule, 931.0134 to 1168.2862, 1389.3654 to 1599.9554 and 3737.3537 to 4108.8095 for HOF$^+$ and 488.3605 to 51.1015^{n1}, 557.0922 to 591.3539^{n2} and 3924.7975 to 3987.5974^{n3}. From the result obtained, B3LYP/6-311++G** method gives better accuracy for OF with an uncertainty value of 38.5141 as compared to the experimental value 1053cm^{-1} and B3LYP6-311++G** method gives better accuracy for HOF$^+$ with an uncertainty value 0f -2591.654, 3.4019 and 2845.7437cm^{-1} as compared to the experimental value 3537, 1393 and 886cm^{-1}. Thus the B3LYP/6-311++G** method is expected to predict the best value for HFO$^+$ with no experimental value.

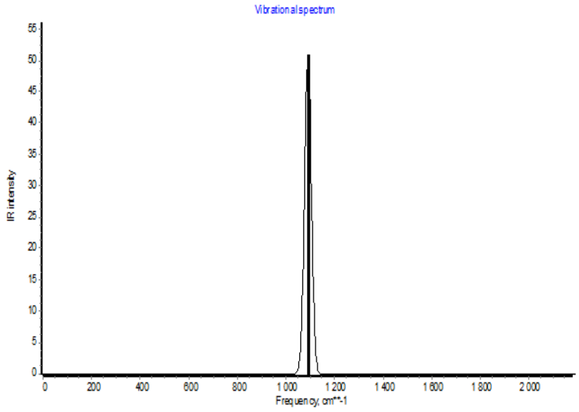

Figure 4. IR Spectrum for OF Molecule.

IR frequency

Table 6a. IR frequency for OF molecule.

Method	IR frequency Cal. Value (cm $^{-1}$)	Cal. – Exptl (cm $^{-1}$)
HF/6-311++G**	1204.6962	151.6962
B3LYP/6-311++G**	**1091.5141**	**38.5141**
MP2/6-311++G**	1412.9394	359.9394
MP2/cc-pVDZ	1455.2213	402.2213
CCSD/cc-pVDZ	1000.9441	-52.0559
G4	1151.0951	98.0951

Experimental value: 1053.0 cm^{-1}. Ref: [22]

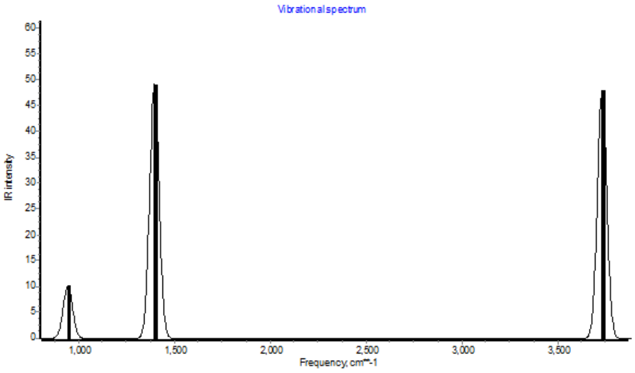

Figure 5. IR spectrums for HOF$^+$.

Table 6b IR frequency for HOF$^+$.

Method	IR frequency Cal. Value (cm $^{-1}$)	Cal. – Exptl (cm $^{-1}$)
HF/6-311++G**	1168.2862 ^{n1} 1599.9554 ^{n2} 4108.8095 ^{n3}	-2368.7138 206.9554 3222.8095
B3LYP/6-311++G**	945.3446 ^{n1} 1396.8 ^{n2} 3731.7437 ^{n3}	-2591.654 3.4019 2845.7437
MP2/6-311++G**	931.0134^{n1} 1395.4019^{n2} 3812.6486^{n3}	-2605.9866 2.4019 2926.6486
MP2/cc-pVDZ	947.5116 ^{n1} 1389.3654 ^{n2} 3786.2192 ^{n3}	-2589.4884 -3.6346 2900.2192
CCSD/cc-pVDZ	914.2857 ^{n1} 1390.3232 ^{n2} 3746.1486 ^{n3}	-2622.7143 -2.678 2860.1486
G4	1006.0931 1417.7473 ^{n2} 3737.3537 ^{n3}	-2530.9069 24.7473 2851.3537

Experimental value: 3537^{n1} 1393^{n2} and 886^{n3} Ref: [22]

Keys; n1 = node 1, n2 = node 2 and n3 = node 3

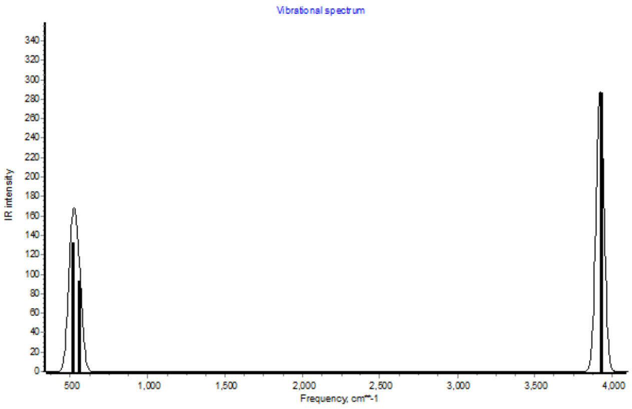

Figure 6. IR spectrum of HFO+.

Table 6c. IR frequency for HFO$^+$.

Method	IR frequency Cal. Value
B3LYP/6-311++G**	511.1015^{n1} 551.0922^{n2} 3924.7975^{n3}
MP2/cc-pVDZ	488.3605^{n1} 591.3539^{n2} 3987.5974^{n3}

Keys; n1 = node 1, n2 = node 2 and n3 = node 3

Conclusion

From the results obtain in the geometry optimization and frequency calculations of OF molecule and its protonated analogue (HOF$^+$ and HFO$^+$ molecule) using different methods of computational chemical calculation [Hartree-Fock (HF), Becke-3-Lee-Yang-Parr (B3LYP), Moller-Plesset second order (MP2), Coupled Cluster method (CCSD), and Gaussian 04 method (G4)]. These Levels of theories or methods are used to compare the following parameters of OF molecule, HOF$^+$ and HFO$^+$ molecules; Dipole moment, Bond distance and Bond angle, Rotational constant, and vibrational frequencies. From the results as compared to the experimental values, it shows that the B3LYP/6-311++G** method is the best method in the optimization and frequencies calculations of the OF, HOF$^+$ and HFO$^+$ because it gives better accuracy in most of the calculated parameters and the MP2 method also give relative accuracy in some of the calculated parameters of OF and its protonated analogues HOF$^+$ and HFO$^+$.

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