

Theoretical investigations of photolysis for Halon-2402 in stratospheric layer

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Abstract

Photolysis of Halon-2402(1,2-dibromotetrafluoroethane) in stratospheric layer have been investigated theoretically using quantum calculation methods likes DFT, ab-initio and semi-empirical. These methods have been carried out to estimate the depletion of ozone layer. Quantum calculations have been carried out for all suggested chemical moieties that's participated in the photochemical reactions through optimizing geometry by PM3-configuration interaction microstate, HF, MP2 and DFT according to different basis sets.

Calculations shows the photolysis reaction of Halon-2402 occurs through C-Br bond needed energy light equal to 92.3 kcal/mol (309.95 nm) in highly probability than other bonds. The recombination of photolysis radical products ($\dot{\text{C}}_2\text{F}_4\text{Br}$ and $\text{Br}\dot{\text{C}}$) is take out either Cis-addition of the Br radical into radical center to produce the gauche-conformer of TFEDB. The Trans-addition produces the anti-conformer of TFEDB. Clearly $\dot{\text{C}}_2\text{F}_4\text{Br}$ radical has a classical nonbridged structure and the secondary dissociation is more possible than Cis or Trans-addition. The yield of atmospheric fate for TFEDB two radical of bromine and two FCOF fragments by oxidation process with O_2 . Two bromine radicals are responsible for the ozone depletion by direct pathway or indirect pathway through sharing with atmospheric chlorine radicals.

Key Words: Halone-2402 (TFEDB), photolysis, Ozone, tropospheric ozone, potential energy surface, bond dissociation energy, quantum calculation methods.

Introduction

Organic halides act an important role in stratospheric ozone depletion due their providing of anthropogenic halogens atoms into atmospheric layers (Hansen *et al.*1999). The importance of bromine and its chemistry in the atmosphere is receiving renewed interest based on the ability of bromine is almost 100 times more destructive to stratospheric ozone than chlorine atom (McGivern *et al.* 2000, Orkin *et al.*2002). Variety of applicable chemicals being using by industrial developments, the Halons are One of the major sources of anthropogenic bromine in the stratosphere (Hansen *et al.*1999). The measurements of the halogenated species in the tropical tropopause found that 1,2-dibromotetrafluoroethane (CF₂BrCF₂Br(TFEDB)) detected between 30 °S and 30 °N latitudes. Transporting from the troposphere into the stratosphere occurs mainly in this region. Since the concentration of CF₂BrCF₂Br in tropical tropopause provides a good measure of the relative mixing ratio in the stratosphere (Schauffler *et al.*1993). The Halon-2402 has widespread uses as a fire suppressant, flame retardant and fumigating agent although the production of CF₂BrCF₂Br in the development countries has been halted by the Copenhagen Amendment to the Montreal Protocol. The long lifetime of Halone-2402 in the atmosphere reached to 25–40 years, make it a significant

contribution to stratosphere ozone depletion for an extended period of time (Struijs *et al.*2010). The photodissociation of TFEDB in gas phase was studied at wavelengths of 193, 233 and 266 nm by North and Co-workers using photofragment translational energy spectroscopy (Zou *et al.*2000). At 193 and 233 nm, the quantum yield of Br• formation was 1.9 ± 0.1 ; this dropped to 1.4 ± 0.1 at 266 nm. The increasing of quantum yield at shorter wavelengths was attributed to secondary dissociation of the C₂F₄Br radical prior to stabilized collision and the dissociation energy of C-Br bond equal to 16.02 ± 1.92 kcal/mol has been determined for the radical, which is around twice that for bromo-ethyl. There is a little spectroscopic information available for this radical, although it was the focus of a recent theoretical study using gradient-corrected density functional theory (DFT) methods (Ihee *et al.*2001).

In the present work, calculation methods likes Hartree-Fock (HF), DFT and second-order Moller-Plesset perturbation (MP2) methods in combination with 6-31G**, 3-21G+(s,sp,6d) and 3-21++G** basis sets for C, F and Br atoms in addition to PM3-CI(4x4) have been used to estimate the geometry optimization and single point to get on the total energy, dipole moment, HOMO & LUMO, Mullikan charges, bond characters and vibrational analysis .

Computational Details:

Theoretical calculations in this work were performed using computational implemented in the Hyperchem package 8.02 (HyperChem 8.02, 2007). Optimized geometries of TFEDB have been done using 3-21G+(s,sp,6d), 3-21++G**(p,d) (Christopher 2002, Jensen 2007, Obies *et al.*2012) with B3LYP (Cerkovnik *et al.*2009) and 6-31G**(p,d) (Wu and Carr 2003, Rassolov *et al.*1998, Castillo and Boyd 2006, Ciancetta *et al.*2011, Brudnik *et al.*2011) with ROHF, also PM3-CI(4x4). Vibrational frequencies carried out through same methods to characterization the nature of stationary points with zero point energy. Potential energy stability had been performed at B3LYP/3-21G+(s,sp,6d)/MP2/3-21G(s,sp,6d) level of theory for length, angle and torsion of bond angle in C₂F₄Br₂. Potential energy surface performed by mapping reactants into products in order to calculate the energy barrier at PM3. First and second dissociation reaction for C-Br bonds in C₂F₄Br₂ had been studied by HF, MP2 and DFT(B3LYP,B3PW91) combining with 6-31G(LAV3P), 6-31G* (LAV3P (p)), 6-31G**(LAV3P(p,d)), 4-31G(MSV), 4-31G*(MSV(d)) (Gordon 1980), 3-21G(s,sp,6d) and 3-21++G** basis sets in addition to PM3-CI(4x4) microstate.

Results and discussion:

1,2-dibromotetrafluoroethane is a weak polar molecule shown in table 1. Both of PM3 and ROHF//6-31G**(p,d) given approach in the zero point energy (17.03 and 17.01 kcal/mol respectively) and dipole moment (0.0002 and 0.0001 D respectively) with positive imaginary frequency sign. B3LYP,MP2//3-21G+(s,sp,6d) and B3LYP//3-21++G**(p,d) are given lowest zero point energy and more stable with negative imaginary frequency sign. HOMO has high energy value to occupy the electrons. The ability of electrons losses is larger than LUMO, that's considerably larger ability to accept the electrons (Hypercup 2002). In addition, the energy band gap according to B3LYP//3-21++G**(p,d) given lowest energy band gap equal to 163.7 kcal/mol therefore any excitation process occurrence will be needed this value of energy (Hameed 2005). The calculated atomic charge for Bromine atom by all methods have positive excess charge except B3LYP, MP2//3-21+G(s,sp,6d) level gave negative excess charge, while the fluorine atom have negative excess charge with all methods and also the carbon atom C₁ and C₂ have positive excess charge by all methods that's means the C-F bond are more stronger than C-Br bond (Hameed 2006).

Table (1) Energetic properties of C₂F₄Br₂ calculated at units of kcal/mol, Debye for dipole moment and coulomb for charges.

Method		PM3- CI(4x4)	ROHF//6-31G** (p,d)	B3LYP, MP2// 3-21G+(s,sp,6d)	B3LYP// 3-21++G** (p,d)
Energy calculation					
Total energy		-62408.829	-3522413.3	-3490277.7	-3512026.4
Zero point energy		17.03	17.001	15.212	14.95
Dipole moment		0.0002	0.0001	0.0056	0.000102
Imaginary frequency		+	+	-	-
Molecular Orbital Energy	HOMO	-277.411	-260.33	-115.531	-183.4
	LUMO	-53.176	-60.4	70.794	-19.7
	ΔE	224.235	199.93	186.325	163.7
Mullikan Charges	C1	0.163070	0.267547	0.180457	0.305404
	C2	0.163070	0.267547	0.180553	0.305350
	Br3	0.009109	0.030108	-0.020653	0.205613
	Br4	0.009109	0.030108	-0.020678	0.205641
	F5	-0.086080	-0.148787	-0.079961	-0.255517
	F6	-0.086100	-0.148867	-0.079889	-0.255481
	F7	-0.086080	-0.148787	-0.079905	-0.255514
	F8	-0.086100	-0.148867	-0.079922	-0.255495

Vibrational analysis has been calculated at different levels of basis set as shown in table 2. They found that's only several frequencies

have intensities larger than 15 km/mol units, with highly accuracy value that's estimate the real significant values.

Table (2) The calculated vibrational frequencies of the C₂F₄Br₂ in cm⁻¹ (intensities in km/mol).

Method		PM3- CI(4x4)	ROHF// 6-31G** (p,d)	B3LYP,MP2// 3-21G+ (s,sp,6d)	B3LYP// 3-21++G** (p,d)
normal mode	v ₁₁	578.86 (13.328)	637.30 (16.28797)	557.48 (23.19464)	534.61 (25.42543)
	v ₁₃	774.09 (97.4347)	855.13 (144.1580)	849.70 (224.33689)	706.93 (222.79838)
	v ₁₅	1476.13 (121.38)	1283.22 (211.821)	1231.75 (203.2332)	1194.78 (208.6001)
	v ₁₇	1593.15 (95.657)	1381.26 (84.0125)	1329.82 (8.02341)	1280.42 (10.00267)
	v ₁₈	---	---	1330.99 (169.0578)	1318.07 (150.6503)

Table 3 shows the bonds parameters of $C_2F_4Br_2$ by using different calculation methods. The C-Br bond in $C_2F_4Br_2$ has length equal to 1.9211 Å according to ROHF//6-31G**(p,d) level whereas 1.9390, 1.9393 and 1.8893 Å by PM3, B3LYP,MP2//3-21G+(s,sp,6d) and B3LYP//3-21++G**(p,d) levels respectively. These results are closer to experimental value (1.922 Å) (Thomassen *et al.*1993). The same thing for C-C bond, was 1.5441 Å of the length by B3LYP//3-21++G**(p,d) method than experimental value (1.548 Å). The C-F bond have 1.3363 Å according to B3LYP,MP2//3-21G(s,sp,6d) method more little than experimental (1.332 Å) (Ihee *et al.*1997). Previous investigation (Ihee *et al.*2001) refers that C-Br bond is more favorable toward the photolysis reaction than other bonds due to the C-Br bond is the of the electrostatic potential displayed negative electrostatic potential regions are diffuse on some atoms therefore there are incomplete distribution of electrostatic potential on the atoms and also in total charge. Also geometry optimization shapes at the two and three dimension for Halon-2402 described the frontal orbital's (HOMO and LUOM) calculated at B3LYP/3-21G+//MP2/3-21G+(s,sp,6d) level of theory (Jalbout *et al.*2006). Estimation the bond

longer subsequently required less energy in order to scission into two free radical Br^{\bullet} and $\bullet C_2F_4Br$ than C-C and C-F bond. There are three types of bond angles is F-C-C, Br-C-C, F-C-F and Br-C-F angles. The calculated F-C-C angle found 109.2° by ROHF//6-31G**(p,d) whereas the experimental value is 109.9° (Fossey *et al.*1995). The Br- C-C angle equal to 110.6259° calculated by ROHF//6-31G**(p,d) while the experimental value equal to 110.5° (Ihee *et al.*1997). The F-C-F angle is 108.8178° by ROHF//6-31G**(p,d) which is closer to the experimental value 108.4° (Ihee *et al.*2001). The calculated Br-C-F angle is equal to 109.48° according to ROHF//6-31G**(p,d). The torsion angle of Br- C₁-C₂-Br is 180.00° calculated by B3LYP,MP2//3-21G+(s,sp,6d) .

Figure 1 represented the structural and electronic properties Halon-2402. Isosurface reactivity of Halon-2402 has been done through calculations of potential energy stability (Drea 2010). Figure 2 illustrates the stability compares of C-Br, C- F and C- C bond, was found C-Br bond is more reactive toward the reactions than C-F and C-C bond. The length of C-Br bond equal to 1.93 Å (-3500260.5 kcal/mol) is equilibrium but at 3.4 Å (-3500204.06 kcal/mol) is broken down. The bond dissociation energy equal to 56.44 kcal/mol

Table (3) Bonds parameters of C₂F₄Br₂ calculated at different quantum methods.

Method		PM3- microstate	ROHF// 6-31G**	B3LYP,MP2// 3-21G+	B3LYP// 3-21++G**
Bond length A° units	C1-Br3	1.9390	1.9211	1.9393	1.8893
	C2-Br4	1.9392	1.9211	1.9393	1.8893
	C1-C2	1.55373	1.535	1.5536	1.5441
	C1-F5	1.3366	1.3166	1.3363	1.4134
	C1-F6	1.3368	1.3166	1.3363	1.4134
	C2-F7	1.3361	1.3166	1.3363	1.4134
	C2-F8	1.3366	1.3166	1.3363	1.4134
Bond angle Degree units	F8-C2-F7	106.3305	108.8178	106.302	106.8401
	F8-C2-Br4	112.4243	109.4825	112.484	110.4296
	F8-C2-C1	112.2887	109.2	112.26	107.4420
	F7-C2-Br4	112.4369	109.4836	112.483	110.4307
	F7-C2-C1	112.2997	109.2	112.26	107.4424
	Br4-C2-C1	101.2127	110.6259	101.209	113.9482
	F5-C1-Br3	112.4349	109.4830	112.483	110.4303
	F5-C1-F6	106.3187	108.8182	106.302	106.8394
	F5-C1-C2	112.2931	109.2	112.26	107.4430
	Br3-C1-F6	112.4305	109.4839	112.484	110.4314
	Br3-C1-C2	101.2107	110.6249	101.209	113.9474
	F6-C1-C2	112.3016	109.1999	112.26	107.4415
Torsion angle Degree units	F6-C1-C2-Br4	-59.8738	-59.4399	-59.8432	-57.3226
	F6-C1-C2-F7	-179.999	179.9993	180.000	179.9997
	F6-C1-C2-F8	60.2284	61.1194	60.3136	60.3535
	Br3-C1-C2-	-179.9924	-179.999	180.0000	-180.0000
	Br3-C1-C2-F7	59.8823	59.4393	59.8447	57.3223
	Br3-C1-C2-F8	-59.8902	-59.4408	-59.8432	-57.3239
	F5-C1-C2-Br6	59.8878	59.4398	59.8447	57.3229
	F5-C1-C2-F7	-60.2376	-61.1211	-60.3106	-65.3548
F5-C1-C2-F8	179.9900	179.9991	180.000	179.9990	
Bond order	C1-Br3	0.91569	1.052	1.00	1.001
	C2-Br4	0.9157	1.052	1.00	1.001
	C1-C2	0.89102	0.907	0.901	0.835
	C1-F5	1.0013	0.9	0.922	0.977
	C1-F6	1.0012	0.9	0.922	0.977
	C2-F7	1.0012	0.9	0.922	0.977
	C2-F8	1.0012	0.9	0.922	0.977

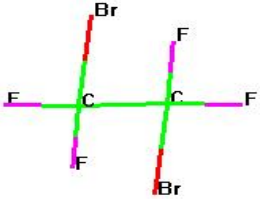
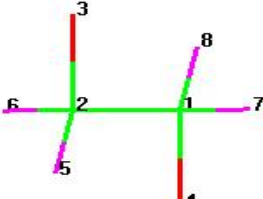
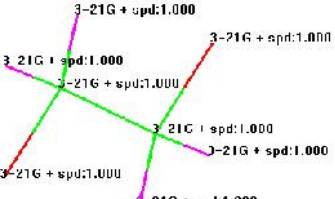
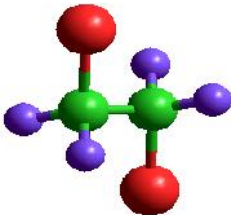
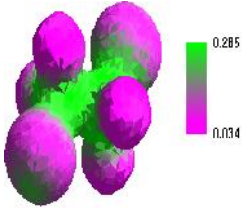
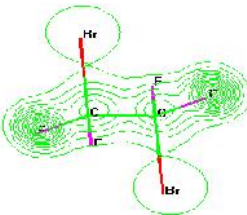


		
a-Atomic symbol	b-Atomic serial number	c-Basis set of calculation
		
d-Ball and stick view	e-Electrostatic Potential at three dimensions	f-Total charge density at 2D contours
		
g- HOMO at 3D contours		h-LUMO at 3D contours

Figure (1) Structural and electronic properties of optimized Halon-2402 calculated at B3LYP/3-21G+//MP2/3-21G+(s,sp,6d) level of theory.

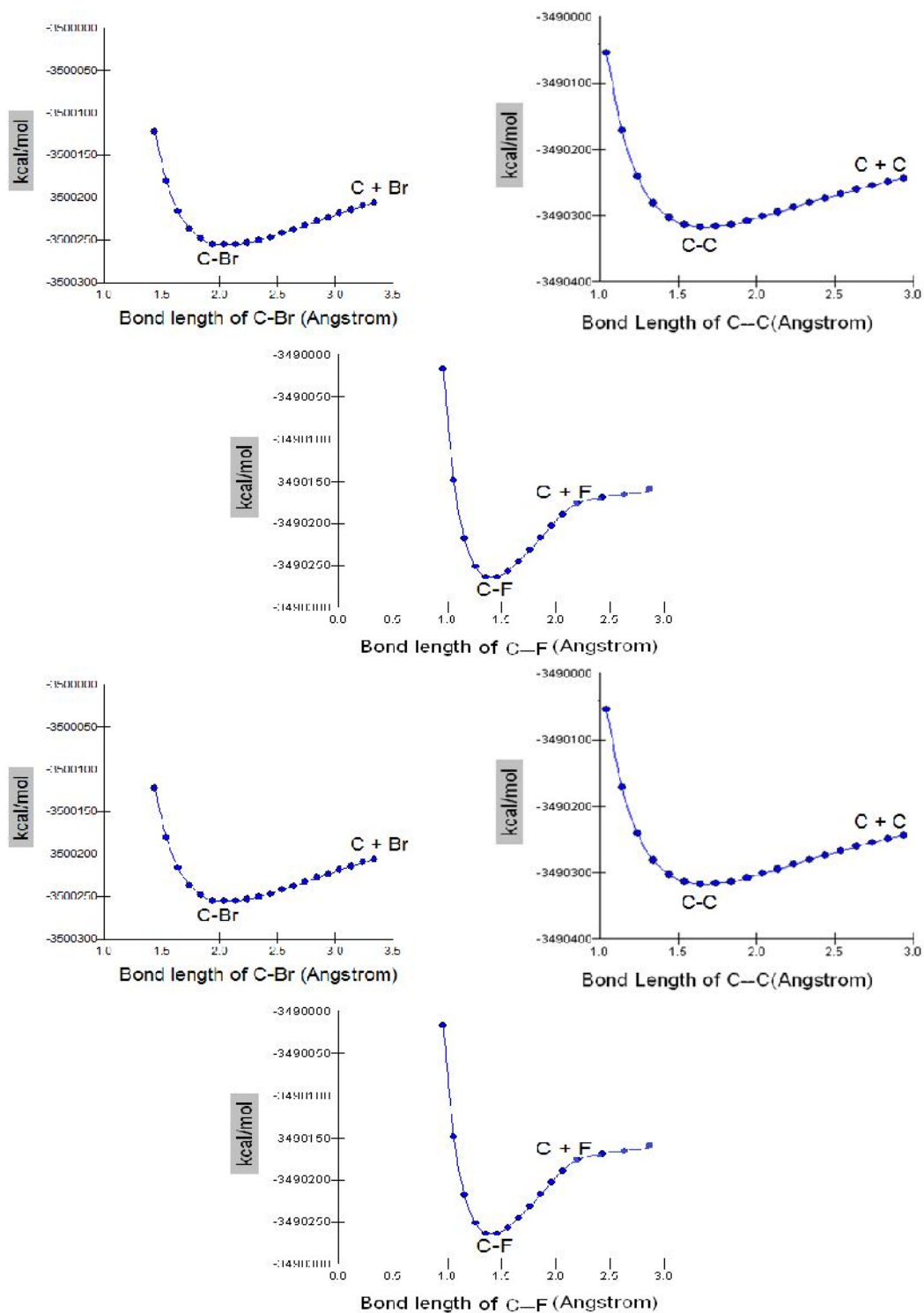


Figure (2) Potential energy stability calculations of Halon-2402 at B3LYP/3-21G+//MP2/3-21G+(s,sp,6d) level of theory.

calculated by B3LYP//3-21G+(s,sp,6d) level of theory. The F-C bond is stable at 1.338 Å (-3490270.44 kcal/mol) and broken down at 2.93 Å (-3490130.55 kcal/mol) that's refer to the bond dissociation energy equal to 139.89 kcal/mol according to B3LYP/3-21G+//MP2/3-21G+(s,sp,6d) level of theory.

The C-C bond have length stability equal to 1.546 Å (-3490320.33 kcal/mol) whereas 3.00 Å (-3490237.6 kcal/mol) therefore the bond dissociation energy is 82.73 kcal/mol. There for, indication proof that the reaction of C₂F₄Br₂ molecule occurs through C-Br bond scission with high probability than C-C, C-F bonds scission.

The photolysis of C-Br bonds has been used to calculated the first dissociation energy (D₁) for the reaction of CF₂BrCF₂Br into CF₂BrC•F₂ and Br• according to different calculation methods. The same thing are doing for second dissociation to give up the final products CF₂=CF₂ and Br• (second dissociation energy (D₂)). Table 5 show lists the calculated dissociation energy for each

reaction. There are no direct measurements of these dissociation energies. Nathanson *et al.*1989, they achieved the measurements using the photofragment translational spectroscopy that's estimate the upper limits of dissociation energies 22.3 ±2.5 kcal/mol for D₀ (CF₂CF₂-Br). These values were obtained by assuming that the C-I bond energies in the CF₂BrCF₂I and CF₂ICF₂I molecules are the same. The dissociation energies for CF₂CF₂Br were also estimated by Krajnovich *et al.*1984 using the available thermodynamic data for the related molecules and halogen atoms. They are obtained D₀ (CF₂CF₂-Br) of 16 kcal/mol by assuming that the C-F bond dissociation energies in CF₂ICF₂ and CF₂BrCF₂ radical are the same as in C₂F₆. Also, they are obtained upper limit of D₀ (CF₂CF₂-Br) to 19.3 kcal/mol based on their experimental results. Photolysis energy value of the B3PW91(MSV(d)) method equal to 92.3 kcal/mol (309.95 nm) gave the best value compared with experimental value (Ihee *et al.*2001).

Table (5) Dissociation energies calculations of C₂F₄Br₂ and CF₂BrC[•]F₂ Radicals in

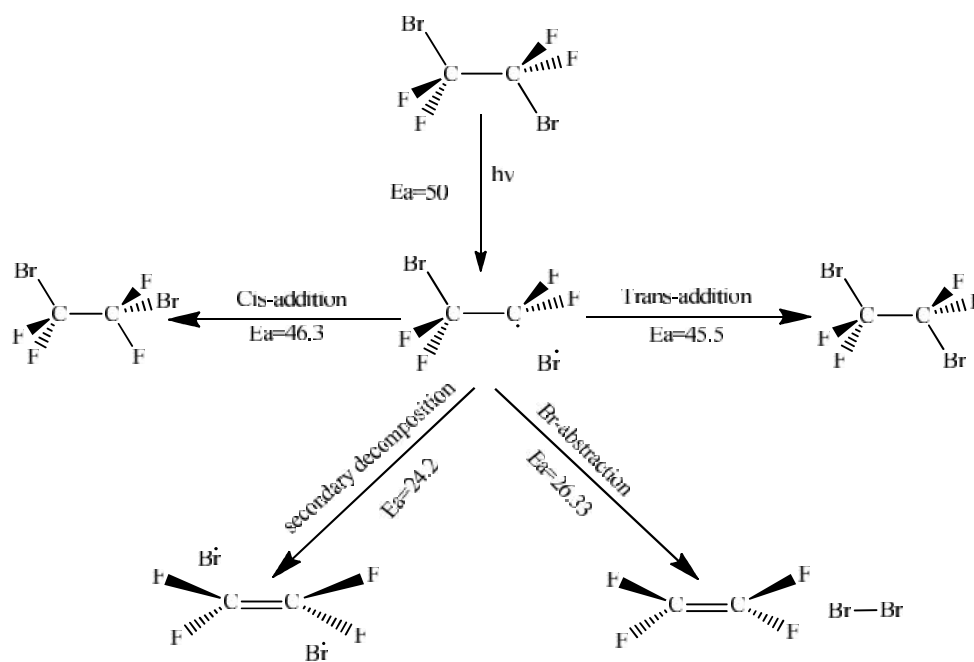
Energy Method	total dissociation energy(TD) C ₂ F ₄ Br ₂ →	first dissociation energy (D1) C ₂ F ₄ Br ₂ →	second dissociation energy (D2) CF ₂ BrC [•] F ₂ →	D ₁ - D ₂
PM3-CI(4x4)	75.4	51	24.4	26.6
HF//LAV3P	30	28.4	1.6	26.8
HF (LAV3P(d))	44.2	35.33	8.7	26.63
HF// LAV3P(p,d)	50.44	38.22	12.22	26
MP2//HF(LAV3P)	63.2	56.33	6.8	49.53
MP2//HF(LAV3P(d))	78.33	60.2	18.13	42.07
B3PW91//LAV3P	65.6	54.11	11.49	42.62
B3PW91//LAV3P(d)	80.4	62.9	17.5	45.4
B3PW91//MSV	77.1	58.26	8.8	49.46
B3PW91//MSV(d)	92.3	68.3	24	44.3
B3LYP//3-21G+(s,sp,6d)	79.3	56.44	22.86	33.58
B3LYP//3-21++G**(p,d)	78.53	55.33	23.2	32.13
Experiment	—	67.6 ± 1.6	22.3 ± 2.5	45

Scheme 1 summarized the suggested mechanism of the Halon-2402 photolysis which that investigated through mapping the reactants into products then measured the activation energy. The energy barrier required for transformation of Halon-2402 into [•]C₂F₄Br and Br[•] radical is 50 kcal/mol (51 and 68.3 kcal/mol by PM3 and B3PW91//MSV(d) respectively from geometry optimized as show in table 5.). The [•]C₂F₄Br radical would be obey to different reactions. The first is obeying to Cis-addtion or Trans-addition by

equal ratio approximately with 46.3 and 45.5 kcal/mol of activation energy. The second is undergoes to either secondary dissociation to form C₂F₄ and 2Br radicals by 24.2 kcal/mol of activation energy or Br-abstraction to form C₂F₄ and Br₂ molecule with 26.33 kcal/mol of activation energy. Scheme 1 shows the stability of [•]C₂F₄Br radical with low possibility to recombination for Br[•] with [•]C₂F₄Br by Cis,Trans-addition reaction or second dissociation because of high energy barrier value. Kalume *et al.*2010, studied

significantly different behavior in the 1,2-dibromoethanes (EDB) and TFEDB in Argon matrixes at 5 K. They found recombination reaction of radical are observed in annealing experiments that's occurs via either Cis-addition of the Br^\bullet to

photolysis of two atmospherically important radical center producing the gauche-conformer of Halon-2402, or Trans-addition producing the anti-conformer of Halon-2402. The $\text{C}_2\text{F}_4\text{Br}$ radical clearly has a classical no bridged structure (Ihee *et al.*1999).



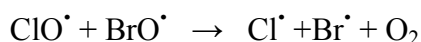
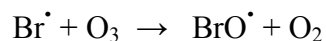
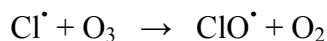
Scheme (1) Suggested mechanism of Halon-2402 photolysis calculated by PM3-microstate.

Photolysis of Halon-2402 under atmospheric conditions will form the $\text{C}_2\text{F}_4\text{Br}$ radical and Br^\bullet . The $\text{C}_2\text{F}_4\text{Br}$ radical undergoes secondary decomposition depends upon the energy light of photolysis. The solar flux in the upper troposphere is largely concentrated at wavelengths longer than 290 nm and photolysis at this wavelength (in this work at 309.95 nm) resulting stable radical respected to secondary decomposition. The suggested

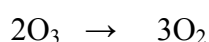
troposphere's reaction including $\text{C}_2\text{F}_4\text{Br}$ radical formation, that's rapidly react with O_2 to form a peroxy radical ($\text{C}_2\text{F}_4\text{BrO}_2$). The radical $\text{C}_2\text{F}_4\text{BrO}_2$ will react primarily with NO to produce $\text{C}_2\text{F}_4\text{BrO}$ and NO_2 . The alkoxy radical $\text{C}_2\text{F}_4\text{BrO}$ undergo C-C bond scission give up CF_2Br and CF_2O (Kalume *et al.*2010). However, since the C-F bond is significantly stronger than the C-Cl bond. Little C-F bond cleavage channel would be

expected for C_2F_4BrO radical dissociation (Mogelberg *et al.*1995). The C-C bond breakage has been previously reported for C_2F_5O radicals (Sehested *et al.*1993). The $\cdot CF_2Br$ undergo subsequent oxidation to yield CF_2O and $\cdot Br$ (Brasseur *et al.*1999). As a result, may be expected that both $\cdot Br$ in the CF_2BrCF_2Br will be released as active bromine upon absorption of UV energy, that's

leads to the ozone depletion process by conversion of O_3 into O_2 . It's been shared with active ion ClO in order to ozone depletion as show in the following equation. Irrespective of the photolysis energy, therefore bromine radical has be very important in ozone layer destroy Kawa *et al.*2009, Harris *et al.*2010).



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Conclusions

- Photolysis reaction of Halon-2402(1,2-dibromotetrafluoroethane) occurs through C-Br bond ,which needed 92.3 kcal/mol (309.95 nm) with highly probability than other bonds.
- Radical recombination of photolysis reaction products ($\cdot C_2F_4Br$ and $\cdot Br$) is take out either in Cis-addition of the Br radical into radical center to producing the gauche-conformer of TFEDB, or in Trans-addition to producing the anti-conformer of TFEDB.

- The secondary dissociation of $\cdot C_2F_4Br$ radical occurs with high probability than Cis or Trans-addition because it has classical nonbridged structure.
- Investigated results refers the atmospheric fate of Halon-2402 to yielding two $\cdot Br$ radicals that's responsible for ozone depletion process in direct or share with $Cl\cdot$ radicals and two CF_2O fragments through oxidation process of $\cdot C_2F_4Br$ radical with O_2 .

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تحقيقات نظرية عن التحلل الضوئي للهالون-2042 في طبقة الستراتوسفير

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الخلاصة

أجريت التحقيقات النظرية عن التحلل الضوئي لجزيئة 2،1- ثنائي برومورباعي فلوروايثان في طبقة الستراتوسفير باستخدام طرائق الكم الحسابية مثل الحسابات الشبه التجريبية والحسابات الأساسية الأولية وحسابات نظرية الكثافة الوظيفية وذلك لتخمين التحطم الحاصل لطبقة الأوزون. تم اجراء الحسابات الكمية لجميع الأصناف الكيميائية المقترحة التي تشارك في التفاعلات الكيميائية الضوئية من خلال الوضعية الهندسية المثلى وبواسطة PM3 و HF و MP2 و DFT باستخدام مجاميع قاعدة مختلفة. الحسابات توضح إن التحلل الضوئي لجزيئة الهالون يحدث من خلال الأصرة C-Br وبطاقة 92.3 كيلو سرعة لكل مول (309.95 نانوميتر) ذات الاحتمالية الكبرى مقارنة ببقية الاواصر. يحدث إعادة الاتحاد لنواتج التحلل الضوئي (C₂F₄Br, Br^{*}) إما من خلال الإضافة ترانس معطيا الشكل المضاد أو الإضافة سس معطيا الشكل الغير مضاد. وجد ان الجذر الحر C₂F₄Br^{*} لا يمتلك تركيب جسري ويكون التفكك الثانوي هو أكثر احتمالية من الإضافة سس أو ترانس. يكون المصير الاموسفيري لجزيئة الهالون هو اثنين من جذور البروبين الحرة وجزيئين من FCOF من خلال الاكسدة بواسطة O₂، حيث ان جذور البروبين هي المسؤولة عن تحطيم الأوزون مباشرة أو من خلال الاشتراك مع جذور الكلورين.

الكلمات المفتاحية: للهالون-2042، التحلل الضوئي، الأوزون، التروبوسفير، الأوزون، سطح طاقة الجهد، طاقة تكسر الاصرة، طرق حسابات الكم.