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STABILITY OF RJ-5 FUEL

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Abstract. In this work, the stability of a bicyclic high-energy-density fuel, RJ-5 ($C_{14}H_{18}$), has been inspected. The tendency of RJ-5 jet fuel to form hydroperoxide structure under storage conditions has been examined. The negative $\Delta G^{\circ}_{\text{rxn}}$ values showed that oxidation of fuel through hydroperoxidation is a spontaneous process. It was shown that the bridgehead carbon atoms and the carbon atoms that link the norbornane structure with the other ring system are the vulnerable centers to hydroperoxidation because the corresponding hydroperoxides are quite low in total electronic energies. The thermodynamic calculations showed that these hydroperoxide structures may rearrange themselves to minimize their energy forming different molecules. These rearranged molecules have been identified using rearrangement mechanism in the literature. The probable rearrangement products were determined and confirmed by thermodynamic calculations. The heat of combustion values of RJ-5, hydroperoxides and rearrangement products of hydroperoxides have been calculated using T1 heat of formation data. The results showed that the formation of hydroperoxide molecules under storage conditions worsens the performance of RJ-5 jet fuel.

Keywords: jet fuel, RJ-5, oxidation, hydroperoxidation, rearrangement

Introduction

High energy liquid fuel has been employed for rockets along with jet engines such as turbo-jet, ram-jet, pulse jet and etc. In order to improve thrust force of rockets and jet engines, fuel having high combustion energy as much as possible per unit volume, i.e., liquid fuel having ‘high density and high heat of combustion’ is required. Moreover, since liquid fuel is supplied to combustion chambers through pipes, or used in combination with liquid oxygen, or employed for flying objects in ultra-high altitude region at low temperature, suitable viscosity and pour point are required for such liquid fuel. In addition, it is also necessary that liquid fuel should be non-corrosive to engines (Edwards, 2003; Chung et al., 1999; Wucherer & Wilson, 1998; Roy, 2000). RJ-5 is a fuel that satisfies these requirements.

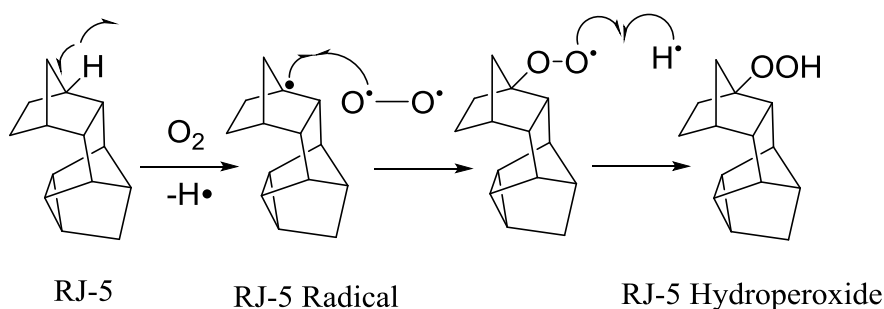


Fig. 1. The formation of hydroperoxide by O_2 molecule

RJ-5 is a bridged polycyclic alkane molecule with the chemical formula $C_{14}H_{18}$ (Fig. 1). It is synthesized by reacting norbornadiene (which can be produced from acetylene and cyclopentadiene) over 15 wt % of a rhodium on carbon catalyst, followed by hydrogenation and isomerization to yield the product endo, endo-dihydronorbornadiene (RJ-5)¹⁾ (Harvey et al., 2010).

Fuel instability is a result of formation of hydroperoxy molecules in the fuel. Hydrocarbon fuels are vulnerable to degradation under long time, low-temperature storage conditions (storage stability) or under short time high-temperature stress (thermal oxidative stability). The major thermal oxidation may arise during flight conditions, where fuel assists as a coolant on its way to the combustion chamber. Minor thermal degradations may happen in nonoxidizing atmospheres, but the presence of oxygen or active species such as hydroperoxides tremendously accelerate the oxidative degradation initiating severe deviations in fuel character. The hydrocarbon structure, heteroatom concentration, oxygen concentration and the temperature are the key parameters in the rate of autooxidation of hydrocarbon fuel. If adequate oxygen is present in the medium, the concentration of hydroperoxides formed reaches to high levels. If the available oxygen is low, but the temperature is high, the hydroperoxide concentration is limited by free-radical decomposition. In this circumstance, fuel degradation can be related to both hydroperoxide formation and rearrangement (Watkins et al., 1999).

Hydroperoxide formation in fuel deteriorates elastomeric structure in aircraft fuel tank systems, which resulted in the loss of an airplane during the 1970s. After that accident, a project was proposed to shed some light on the hydroperoxide forming tendency of a hydrocarbon jet fuel under storage conditions (Nadler, 1980).

The partial oxidation of hydrocarbons through hydroperoxide formation is an initial point for the understanding of the cracking mechanisms in alkane compounds (Jensen et al., 1979; Blaine & Savage, 1991). We supposed that RJ-5 is a potential substance susceptible to oxidation through hydroperoxide formation. This has inspired us to investigate hydroperoxide formation of RJ-5, computationally.

The biradical O_2 molecule may easily cause any of C-H group to lose hydrogen radical and adds itself to the carbon radical of the molecule. The formed peroxy radical abstracts the hydrogen radical to form a hydroperoxide molecule as indicated in Fig. 1.

Method

The initial structure optimizations of RJ-5, hydroperoxide derivatives and rearrangement products were achieved by following the order: MM2 method, PM3 method, STO and HF 6-31G(d,p) and finally DFT-B3LYP at the level of 6-31G(d,p) were applied (Leach, 1997; Stewart, 1989a; 1989b; Kohl & Sham, 1965; Parr & Weetao, 1989). No imaginary frequencies have been observed in single point calculations. The total electronic energies were corrected for zero point vibrational energies (ZPE). The heat of formation of all the molecules were calculated by a T1 Thermochemical Recipe implemented in Spartan'08 (Ohlinget et al., 2009). All these computations were performed by using Spartan'08 package program at standard conditions of 298.15 K and 1.00 atm.²⁾

Results and discussion

The hydrogen and carbon atoms of RJ-5 are numbered as shown in Fig. 2. Numberings of the hydroperoxides have been done in the same manner. Table 1 indicates the labeling of the hydroperoxide molecules derived from the corresponding atoms.

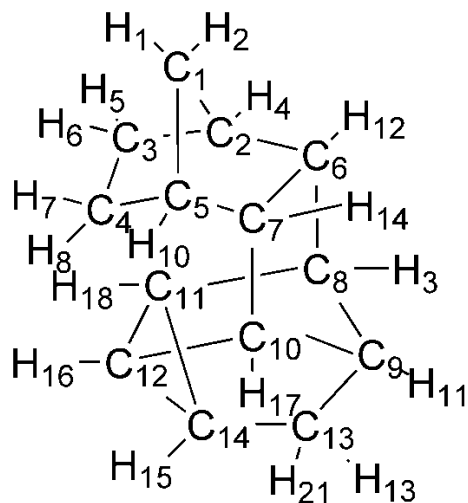


Fig. 2. Labeling of hydrogen and carbon atoms of RJ-5

The point group of RJ-5 molecule is C_1 . The molecule lacks symmetry and all the hydrogen atoms of the molecule are different (18 different hydrogen atoms). For that reason, in the present study, RJ-5 itself, 18 different hydroperoxides originated from RJ-5 and 12 rearrangement products have been considered theoretically. T_1 thermochemical recipe has been utilized to calculate the heat of formation of RJ-5 (Ohlinget et al., 2009). The T_1 heat of formation value of RJ-5 has been calculated as $130.81 \text{ kJ.mol}^{-1}$, which indicates that the formation of the compound from its elements is an endothermic process. We have calculated the dipole moment of RJ-5 as 0.12 Debye. The fuel has been thought to be an almost nonpolar molecule.

Table 1. Labeling of the hydroperoxides derived from RJ-5, ZPE corrected total electronic energy and G° values of the molecules calculated at B3LYP 6-31G(d,p) level

The Atoms	Hydroperoxide Label	E_{total} (kJ/mol)	G° (kJ/mol)
C ₁ -OOH ₁	A	-1823001.13	-1823094.38
C ₁ -OOH ₂	B	-1823002.78	-1823095.96
C ₂ -OOH ₄	C	-1823010.94	-1823103.54
C ₃ -OOH ₅	D	-1822989.80	-1822958.26
C ₃ -OOH ₆	E	-1823005.88	-1823099.14
C ₄ -OOH ₇	F	-1822989.77	-1823082.42
C ₄ -OOH ₈	G	-1823005.97	-1823099.25
C ₅ -OOH ₁₀	H	-1823010.87	-1823103.43
C ₆ -OOH ₁₂	I	-1823000.90	-1823092.93
C ₇ -OOH ₁₄	J	-1823001.08	-1823093.12
C ₈ -OOH ₃	K	-1823011.33	-1823104.08
C ₉ -OOH ₁₁	L	-1823005.16	-1823097.98
C ₁₀ -OOH ₁₇	M	-1823011.54	-1823104.36
C ₁₁ -OOH ₁₈	N	-1822987.30	-1823080.12
C ₁₂ -OOH ₁₆	O	-1823017.14	-1823079.99
C ₁₃ -OOH ₁₃	P	-1823000.97	-1823094.14
C ₁₃ -OOH ₂₁	R	-1823000.95	-1823093.98
C ₁₄ -OOH ₁₅	S	-1823003.30	-1823096.35

The tendency of formation of RJ-5 hydroperoxides

RJ-5 is vulnerable to oxidation through hydroperoxide formation like all hydrocarbons (Hayashi et al., 1998) under storage conditions. This has directed us to study hydroperoxide formation of RJ-5, computationally. The route adopted in the current study is as follows: the biradical O₂ molecule simply causes any C-H group of RJ-5 to lose a hydrogen radical forming RJ-5 radical and then bonds itself to that radical. The formed peroxy radical combines with the eliminated hydrogen radical to yield the hydroperoxide molecule as shown in Fig. 1.

Table 1 shows the labeling of the hydroperoxides originated from the corresponding atoms, their zero point energy (ZPE) corrected total electronic energies calculated at (B3LYP/6-31G(d,p)) level of theory. A molecule is supposed

to be stable when total electronic energy value is low. When total electronic energy values of hydroperoxides are considered, the stability order is as follows: O>M>K>C>H>G>E>L>S>B>A>J>P>R>I>D>F>N. The molecules having hydroperoxy groups at tertiary carbon centers are lower in energy when compared to ones holding hydroperoxy groups at secondary carbon centers. The comparison of the total electronic energies of the hydroperoxide molecules enables to assign the “the most feasible carbon centers”. These are the potent carbons to be oxidized through hydroperoxidation. The bridgehead carbon atoms C₂ and C₅, the carbon centers that link the norbornane structure with the other ring system C₈, C₁₀ and C₁₂ are very prone to oxidation through hydroperoxidation because the corresponding hydroperoxides C, H, K, M and O are quite low in total electronic energies (Table 1). The carbon center C₁₁ seems to be the least reasonable position for oxidation as a result of the highest total electronic energy of all.

Table 2 displays the $\Delta G^{\circ}_{\text{rxn}}$ values for the transformation of RJ-5 to hydroperoxide molecules. $\Delta G^{\circ}_{\text{rxn}}$ has been calculated as the difference between the G° values of the products (hydroperoxide molecule) and the reactants (RJ-5 ($G^{\circ} = -1428379.67$ kJ/mol) and O₂ ($G^{\circ} = -392584.96$ kJ/mol) molecule) at B3LYP/6-31G(d,p) level. According to the negative $\Delta G^{\circ}_{\text{rxn}}$ values shown in Table 2, hydroperoxidation of any site of RJ-5 is a spontaneous process. The probability of formation of hydroperoxides C, H, K and M is high due to larger negative $\Delta G^{\circ}_{\text{rxn}}$ values than those of other structures. Although “hydroperoxide O” seems to be thermodynamically the most stable of all, $\Delta G^{\circ}_{\text{rxn}}$ value is not as low as those of C, H, K and M molecules. These hydroperoxides have one mutual point. They all have the hydroperoxy groups on tertiary position.

Table 2. The $\Delta G^{\circ}_{\text{rxn}}$ values for the hydroperoxidation of RJ-5 and relative $\Delta G^{\circ}_{\text{rxn}}$ values

Hydroperoxide Label	$\Delta G^{\circ}_{\text{rxn}}$ (kJ/mol)	Relative $\Delta G^{\circ}_{\text{rxn}}$ (kJ/mol)
M	-2139.72	0.00
K	-2139.45	0.28
C	-2138.91	0.81
H	-2138.79	0.93
G	-2134.62	5.11
E	-2134.51	5.22
L	-2133.35	6.37
S	-2131.72	8.01
B	-2131.33	8.39

A	-2129.75	9.98
P	-2129.50	10.22
R	-2129.35	10.38
J	-2128.48	11.24
I	-2128.29	11.43
F	-2117.78	21.94
N	-2115.48	24.24
O	-2115.36	24.36
D	-1993.63	146.09

Rearrangement of RJ-5 hydroperoxides

In this part of the study, the rearrangement of the most feasible hydroperoxides has been inspected. The hydroperoxides whose relative $\Delta G^{\circ}_{\text{rxn}}$ values with respect to $\Delta G^{\circ}_{\text{rxn}}$ of hydroperoxide M (from RJ-5 to the corresponding hydroperoxide molecule) are within the limit of 1 kJ/mol have been selected. The probabilities of formation of these hydroperoxide molecules are close to each other.

The meta stable hydroperoxide molecules tend to transform themselves to molecules having less total electronic energies. The carboxylic acid (ester) – alkane, alcohol - aldehyde and alcohol - ketone mechanisms have been suggested for hydroperoxide rearrangement in the literature (Türker & Varış, 2014; 2015; Türker et al., 2013) and have been taken into account in this work. Due to structural limitation of hydroperoxide molecules in the current study, only alcohol-ketone rearrangement mechanism has been applied to the RJ-5 Hydroperoxide molecules. In this mechanism, as the name designates, rearrangement of the hydroperoxide group yields an alcohol and an aldehyde group. This mechanism arises for the rearrangement of tertiary peroxides just as the ones in the present study. The choice of this mechanism is based on analytic information along with the distribution of products formed from the oxidative cracking of hydroperoxides (Câmara et al., 2006).

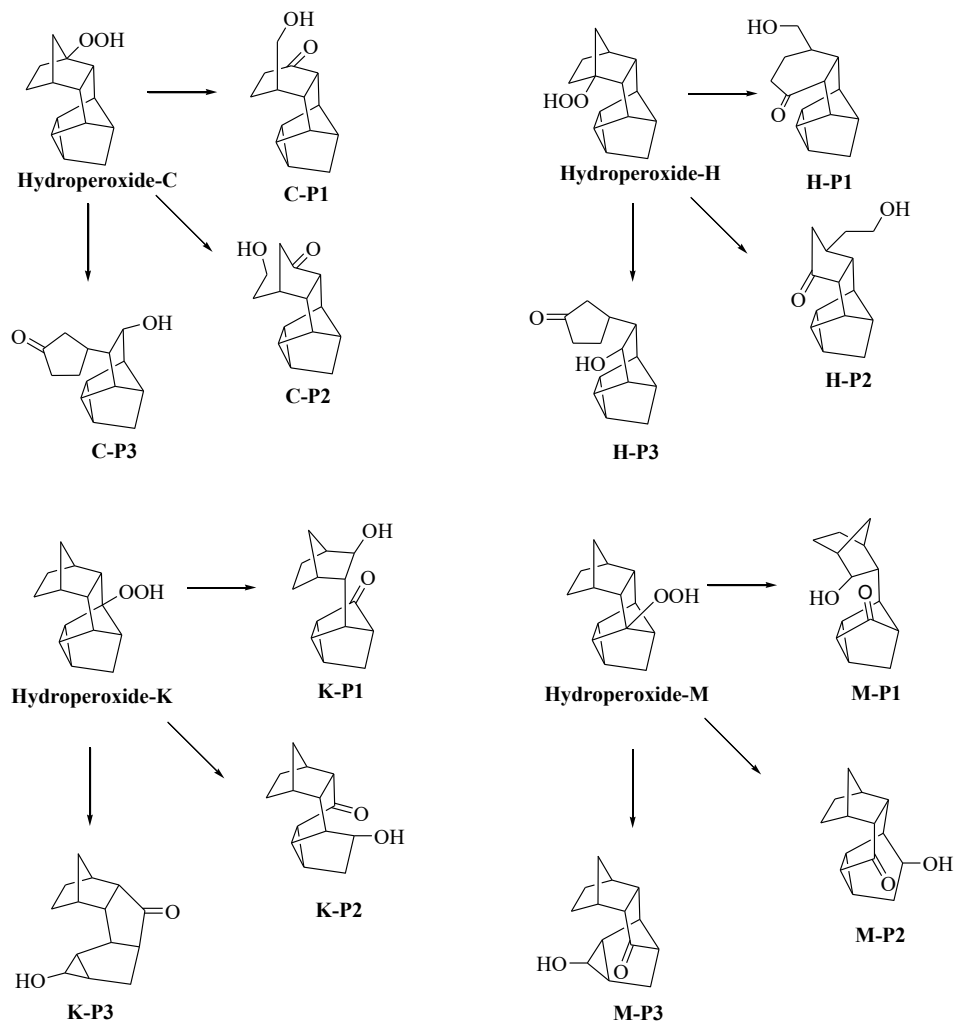


Fig. 3. The rearrangement products of hydroperoxide molecules C, H, K and M

Presently, the rearrangements of the hydroperoxides C, H, K and M have been considered in view of the proposed mechanisms as previously stated. As seen from Fig. 3, we have made thermodynamic energy calculations on these twelve products over DFT optimized structures using B3LYP method and 6-31G(d,p) basis set. The $\Delta G^{\circ}_{\text{rxn}}$ values for the conversion of hydroperoxide molecules to the products are shown in Table 3. $\Delta G^{\circ}_{\text{rxn}}$ values have been calculated as the difference between

the G° values of the products and the reactants. The first rearrangement product of hydroperoxide C is labeled as C-P1, second product is C-P2 and third one is C-P3. Other ones are labeled in the same way.

Hydroperoxide C holds the peroxy group at bridgehead carbon numbered as 2 (Fig. 2). It may transform itself to three different products (C-P1, C-P2 and C-P3). Since Gibbs free energy change ($\Delta G^\circ_{\text{rxn}}$) for the formation of C-P1 (Fig. 3) is more negative than those of other reactions, Hydroperoxide-C molecule thermodynamically prefers to convert itself to that molecule. Also, the total electronic energy of C-P1 is lower than those of the C-P2 and C-P3. Therefore, C-P1 has been found to be the most feasible rearrangement product of Hydroperoxide C in terms of the thermodynamic considerations.

Table 3. The ZPE corrected total energy values and $\Delta G^\circ_{\text{rxn}}$ values of the reactions in Fig. 3

Rearrangement Products	E_{total} (kJ/mol)	$\Delta G^\circ_{\text{rxn}}$ (kJ/mol)
C-P1	-1823294.44	-285.62
C-P2	-1823293.51	-285.16
C-P3	-1823292.23	-282.97
H-P1	-1823293.39	-284.91
H-P2	-1823275.58	-267.16
H-P3	-1823293.80	-285.38
K-P1	-1823264.48	-254.86
K-P2	-1823282.38	-271.93
K-P3	-1823228.61	-219.07
M-P1	-1823263.00	-252.54
M-P2	-1823284.42	-273.81
M-P3	-1823261.87	-251.45

Another bridgehead hydroperoxide is “H”. There are also three rearrangement products for hydroperoxide-H. Since $\Delta G^\circ_{\text{rxn}}$ for the formation of C-P3 is more negative than those of other products, this hydroperoxide molecule prefers to change itself to C-P3. Furthermore, the total electronic energy of C-P3 is lower than other molecules, which shows the stability of C-P3 molecule.

The hydroperoxide K holds the hydroperoxy group on the tertiary carbon that connects the norbornane structure with the other ring system. This hydroperoxide tends to transform itself to K-P2 molecule due to more negative $\Delta G^\circ_{\text{rxn}}$. Also, this product seems more stable than other ones considering the total electronic energy.

Likewise, hydroperoxide M also has the peroxy group on the other tertiary carbon that connects the norbornane structure with the other ring system. It is likely to rearrange itself to M-P2 molecule considering $\Delta G_{\text{rxn}}^{\circ}$ values.

The effect of hydroperoxidation on the heat of combustion of RJ-5

The heat of combustion (ΔH_c°) is the energy released as heat when a compound undergoes complete combustion with O_2 under standard conditions. The chemical reaction is typically a hydrocarbon reacting with oxygen to produce carbon dioxide, water and heat. The heat released is expressed in kJ/mol. ΔH_c° can be calculated taking the difference between the heat of formation (ΔH_f°) of the products and the reactants considering stoichiometry of the combustion reaction.

The complete combustion of RJ-5 ($C_{14}H_{18}$) and RJ-5 hydroperoxide ($C_{14}H_{18}O_2$) is as follows:



The heat of formation (ΔH_f°) values of each species in above reactions should be known for the determination of the ΔH_c° . ΔH_f° has been calculated by T₁ Thermochemical Recipe implemented in Spartan'08 (Ohlimg et al, 2009). It follows the G3(MP2) recipe, by substituting an HF/6-31G(d) for the MP2/6-31G* geometry, eliminating both the HF/6-31G(d) frequency and QCISD(T)/6-31G(d) energy and approximating the MP2/G3MP2 large energy using dual basis set RI-MP2 techniques (Ohlimg et al, 2009). It produces reasonable results which are comparable to experimental values. Table 4 shows the T₁ heat of formation values of the molecules. The data in the parenthesis are the literature values. The calculated values for CO_2 , H_2O and RJ-5 are quite close to the actual values. This consistency increases the reliability of the T₁ method employed in the present work.

Table 4. The T1 heat of formation (ΔH_f°), heat of combustion (ΔH_c°) and Relative (ΔH_c°) values for the molecules in (kJ/mol)

Molecule	Formula	T1 ΔH_f° (kJ/mol)	ΔH_c° (kJ/mol)	Relative ΔH_c° (kJ/mol)
Carbon Dioxide	CO ₂	-406.42 (-393.52)*	-	-
Water	H ₂ O	-237.61 (-241.83)*	-	-
RJ-5	C ₁₄ H ₁₈	130.81 (134.7)**	-7959.18 (7.8x103kJ/mol)**	0.00
C	C ₁₄ H ₁₈ O ₂	33.62	-7861.99	97.19

H	C ₁₄ H ₁₈ O ₂	33.63	-7862.00	97.18
K	C ₁₄ H ₁₈ O ₂	32.22	-7860.59	98.59
M	C ₁₄ H ₁₈ O ₂	32.06	-7860.43	98.75
C-P1	C ₁₄ H ₁₈ O ₂	-239.98	-7588.39	370.79
C-P2	C ₁₄ H ₁₈ O ₂	-236.53	-7591.84	367.34
C-P3	C ₁₄ H ₁₈ O ₂	-233.68	-7594.69	364.49
H-P1	C ₁₄ H ₁₈ O ₂	-239.84	-7588.53	370.65
H-P2	C ₁₄ H ₁₈ O ₂	-217.75	-7610.62	348.56
H-P3	C ₁₄ H ₁₈ O ₂	-228.30	-7600.07	359.11
K-P1	C ₁₄ H ₁₈ O ₂	-231.11	-7597.26	361.92
K-P2	C ₁₄ H ₁₈ O ₂	-228.09	-7600.28	358.90
K-P3	C ₁₄ H ₁₈ O ₂	-169.07	-7659.30	299.88
M-P1	C ₁₄ H ₁₈ O ₂	-208.8	-7619.57	339.61
M-P2	C ₁₄ H ₁₈ O ₂	-226.99	-7601.38	357.80
M-P3	C ₁₄ H ₁₈ O ₂	-201.59	-7626.78	332.40

*Experimental values (Atkins & De Paola, 2006)

** Experimental values (Osmont et al., 2006)

The heat of combustion (ΔH_c°) value for RJ-5 is calculated as -7959.18 kJ/mol. The literature value has been reported as -7.8×10^3 kJ/mol (Osmont et al., 2006). As seen from the table, formation of hydroperoxide molecules decreases the heat of combustion by 97 kJ/mol. The formation of rearrangement products (containing ketone and alcohol groups) from corresponding hydroperoxides causes a decrease of about 330 – 370 kJ/mol in the heat of combustion. The results in Table 4 numerically indicate the deterioration of performance of RJ-5 jet fuel due to hydroperoxidation.

Conclusion

In this work, the stability of RJ-5 (C₁₄H₁₈), which is a bicyclic high-energy-density fuel, has been inspected. Since hydroperoxide concentration has been found to be a factor in fuel instability, oxidation of RJ-5 through hydroperoxidation mechanism has been discussed based on Density Functional Theory (DFT) calculations. The results showed that the bridgehead carbon atoms (C₂ and C₅) and the carbons that link the norbornane structure with the other ring system (C₈ and C₁₀) are found susceptible to oxidation through hydroperoxidation because the corresponding hydroperoxides C, H, K and M are quite low in total electronic energies. The hydroperoxide whose relative ΔG_{rxn}° values (from RJ-5 to the hydroperoxide C, H, K and M) are within the limit of 1 kJ/mol have been considered. The rearrangement of these molecules has been questioned. The meta stable hydroperoxide molecules tend to convert themselves to molecules having both ketone and alcohol group of lower energy. The most feasible rearrangement products have been determined considering

$\Delta G^{\circ}_{\text{rxn}}$ values. The heat of combustion of RJ-5, hydroperoxides and rearrangement products of hydroperoxides have been calculated using T_1 heat of formation data. The calculations showed that the formation of hydroperoxide molecules during storage conditions deteriorates the heat of combustion of RJ-5 jet fuel.

NOTES

1. U.S. Patent 3,377,398; Apr. 9, 1968.
2. http://downloads.wavefun.com/Spartan08Manual_New.pdf

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