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Molecular Structures and Rotational Potential Energy Surfaces of E and Z Geometrical Isomers of Propionaldehyde Oxime: ab Initio and DFT Studies

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Molecular structure and conformational stability of E and Z geometrical isomers of propionaldehyde oxime ($C(1)H_3C(2)H_2C(3)HNOH$) have been studied by using the ab initio and DFT methods. The molecular geometries were optimized by employing the atomic basis sets 6-31G* at the HF-SCF and MP2 levels of theory in the ab initio method. The basis sets 6-31G and 6-31G* are used in the BLYP method of DFT to optimize the molecule. The optimized structural parameters of the above methods are discussed in the light of the electron diffraction results of the molecule. The variations in C═N bond length, C1C2C3 and C2C3N angles of the sp and ac conformers of E isomer and of the ap conformer of Z isomer have been discussed in terms of nonbonding interactions of CH_3 and NOH groups. The rotational potential energy surfaces of E and Z isomers were obtained for the C2−C3 rotational angle of propionaldehyde oxime at HF/6-31G*, MP2/6-31G*, and BLYP/6-31G* levels of theory. The global minimum occurs at $\phi(\mathrm{CCCN}) = 120°$ and $\phi = 0°$ for the ac and sp conformations of the E isomer and $\phi = 180°$ for the Z isomer. The ac form is found to be more stable than the sp form by 0.16 kcal/mol in HF/6-31G* level of theory; this difference agrees very well with the experimental value of 0.15 kcal/mol. The rotational potential curve of Z form shows that it has large-amplitude motion. The chemical hardness values obtained for the different conformers of the two isomers are in disagreement with the statement that the higher stable conformation has higher chemical hardness, but the trend obeys the general trend of oxime molecules. The Fourier decompositions of the rotational potential of the propionaldehyde oxime are analyzed.

Introduction

The oxime molecules play an important role in the Beckmann rearrangement reaction. Oximes, oxime ethers, and oxazines constitute an important class of substrates in stereoselective carbon−carbon bond-forming reactions. Recently, the pyrolysates of oximes, such as propionaldehyde oxime ($CH_3CH_2CH{=}NOH$) and chloropropanone oxime ($ClCH_2C(CH_3){=}NOH$), have been investigated by mass spectrometry/microwave spectroscopy and it has been found that the pyrolysis mechanisms are different for the different substituent groups.[1,2] NMR study of propionaldehyde oxime reveals that it has two isomers, E and Z, with respect to the C═N bond.[3] Moreover, each form has four possible rotational conformations with respect to the C2−C3 bond (see Figure 1). The rotational constants and structural parameters for the E and Z isomers of the propionaldehyde oxime were studied by microwave spectroscopy.[4,5] By combining the electron diffraction and the microwave spectroscopic data, we have determined the structure and conformation of the molecule.[6,7] These studies have found two rotational conformers, anticlinal (ac) and synperiplanar (sp), for the E isomer and only one conformer, antiperiplanar (ap), for the Z isomer (see Figure 2). The abundance ratios of E-ac, E-sp, and Z-ap forms at 323 K are 0.56, 0.23, and 0.21, respectively.[7] So the ac form is the main conformer of propionaldehyde oxime in the gas phase.

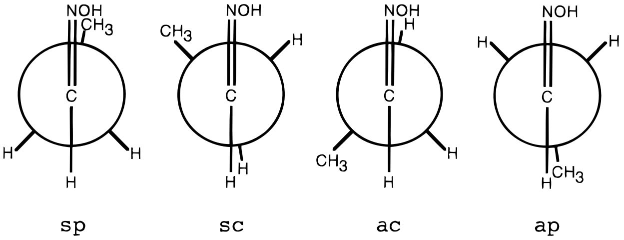

Figure 1. Four possible conformers of propionaldehyde oxime.

The quantum-chemical calculations for the oximes have been reported.[8−15] Nguyen and Ha[12] have studied the aldoximes (RCH═NOH, R = H, CH_3, NH_2, OH, and F) by ab initio SCF techniques, employing the double-zeta (DZ) basis sets. Glaser and Streitwieser[14] performed ab initio studies for several conformers of acetaldoxime and carbanions of acetaldoxime. It has been observed that the addition of polarization function of the HF-SCF level of theory significantly shortens the N−O bond length in the formaldoxime. The geometrical isomers of acetaldoxime differ to a significant extent only in their tilt angles. We have found no theoretical reports published on propionaldehyde oxime. The experimental results have shown that three conformers were identified; the C═N bond length and C1C2C3 and C2C3N bond angles of E-ac and E-sp forms differ appreciably for the two conformers. These points prompt us to probe further the rotational conformer of the geometrical isomer of the propionaldehyde oxime molecule by using the ab initio and DFT (density functional theory) methods.

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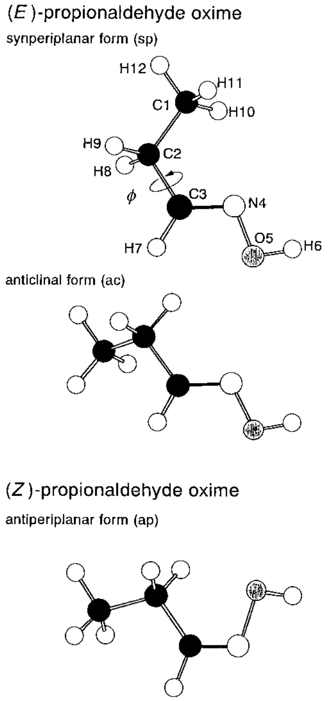

Figure 2. Rotational isomerism structure and conformational definitions of E and Z isomers of propionaldehyde oxime. ϕ denotes C1C2C3N4 dihedral angle. ϕ is defined to be zero when the C1−C2 bond eclipses the C3−N4 bond and takes a positive value when C1 rotates clockwise from the eclipsed position.

Computational Procedure

The calculations were performed with Gaussian 94 program.[16] The geometries were optimized by using the restricted Hartree−Fock (HF-SCF) theory, second-order Møller−Plesset perturbation theory[17] (MP2) and DFT method for the ac and sp forms of the E and ap form of the Z geometrical isomer. In HF-SCF method, the 6-31G* basis set was used. To study the electron correlation effects, the MP2 method was used, implementing the 6-31G* basis set. In DFT method, Becke−Lee−Yang−Parr (BLYP) gradient-corrected density functional[18] was used. In order to see the polarization function effect on the DFT method, we have used 6-31G and 6-31G* basis sets. The nonlocal BLYP results are better than those from HF and are comparable in quality with the results of MPn ab initio calculations.[19] Since this method is less sensitive to the basis set, the 6-31G* basis set is competitive to produce results which are comparable in quality with the higher level of ab initio theory. The fine grid procedure as implemented in the Gaussian 94 program was applied to integrate the function numerically. To study the different conformations of the molecule, the potential energy scans (PES) were performed for the E isomer in HF/6-31G*, MP2/6-31G*, and BLYP/6-31G* levels of theory. For the Z isomer, the PES was performed in the HF/6-31G* level. The torsional angle ϕ(CCCN) is varied in steps of 30° between $\phi = 0°$ and $\phi = 180°$; at each step of angle, the geometry was optimized.

To derive the potential function for the internal rotation, the six-term truncated Fourier expansion[20,21] was considered for the potential function, $V(\phi)$, as

$$V(\phi) = \sum_{i=1}^{6} 1/2V_i(1 - \cos(i\phi))$$

$V(\phi)$ is the relative energy at the rotational angle ϕ with the sp form defined as an origin ($\phi = 0°$). The conformational stability of the E and Z isomers are discussed using the ab initio and DFT methods.

Results and Discussion

In this section, we present the structural parameters of the sp and ac conformations of the E isomer and of the ap conformation of the Z isomer obtained at different levels of theory. The results of the joint analysis of gas-phase electron diffraction data and rotational constants[6,7] are compared with the present theoretical values and are discussed in the light of correlation effects and the inclusion of polarization function in the DFT method. The conformational stability of the E and Z isomers were studied by using the relative energies computed for different conformers. The barrier heights and the relative stability obtained by the present investigation were discussed with the experimental joint analysis work.

1. Geometries. The optimized geometrical parameters and energies of propionaldehyde oxime at different levels of theory are given in Table 1 along with the experimental values. The microwave−electron diffraction joint analysis[7] showed that the distances of C1−C2, C2−C3, and N−O bonds are the same in both ac and sp forms of the E isomer. But the C═N bond distances, r_g(C═N), of ac and sp forms were found to be 1.284(2) and 1.291(3) Å, respectively. In this study, we have not observed such large differences of r_e(C═N) in these two forms in all levels of theory. The HF-SCF level of theory underestimated and BLYP/6-31G level of theory overestimated the C═N bond length, compared with the experimental values. The difference of r_g(C═N) between E and Z isomers may be due to the nonbonding interactions of CH_3CH_2 and NOH groups. Due to the lone pair electrons of the N atom, the ab initio and DFT methods could not clearly distinguish the r(C═N) differences in the conformations.

The differences of N−O bond length between the theory and the experiment are 0.077 and 0.010 Å in BLYP/6-31G and BLYP/6-31G* levels of theory, respectively. This implies that the addition of polarization functions to the basis set in the DFT method improves the accuracy of the N−O bond length. Similar trends have been found for the related compounds, formaldoxime[14] and acetamidoxime,[22] in the HF-SCF level. The addition of polarization functions to the atomic basis sets shortens the N−O bond and at the same time the unpolarized basis sets lengthen the same bond.[14] In general, the computation of a bond length adjacent to the atom with lone pair electrons is a difficult problem in the ab initio theory.[23] As suggested by Glaser and Streitwieser,[14] there was no intercorrelation between the C═N and N−O bonds. The close inspection of atomic charges of the N and O atoms reveal that net charge transfer between the atoms is the same for the two isomers. Since the Mulliken population analysis is sensitive to the basis set, the net charge transfer between the two atoms is found to be quite different in different basis sets. So this may be the reason for the difference of r(N−O) from ab initio and DFT methods.

The C2−C3 bond lengths of sp and ac forms of E isomer are shorter than that of C1−C2 bond length by 0.029 and 0.04 Å, respectively, in BLYP/6-31G* level of theory. In the Z isomer, the r(C2−C3) was found to be shorter than the r(C1−C2) by 0.027 Å in the same level of theory. We have obtained the similar value and trends for these bonds in MP2/6-31G* level. In chloroacetaldehyde oxime also, the r(C2−C3) is shorter than the r(C1−C2) by 0.05 Å.[24] These predictions are consistent with the general trend that the C−C bond next to a double bond is shortened.[25] In all the conformations, the DFT methods predicts the O−H and C−H bond lengths more accurately than the ab initio method.

TABLE 1: Principal Geometric Parameters and Total Energies for E and Z Isomers of Propionaldehyde Oxime[a]

E-ac form parameters	ab initio MO[b]		DFT		
	HF/6-31G*	MP2/6-31G*	BLYP/6-31G	BLYP/6-31G*	GED + MW[c]
C1−C2	1.532	1.531	1.557	1.551	1.552(3)
C2−C3	1.500	1.494	1.513	1.510	1.493(2)
C3−N4	1.251	1.286	1.300	1.290	1.284(2)
N4−O5	1.375	1.417	1.506	1.439	1.429(2)
C1−C2−C3	112.11	111.73	112.52	112.66	111.5(3)
C2−C3−N4	120.79	119.36	119.63	119.86	119.0(11)
C3−N4−O5	111.87	110.05	109.32	110.50	109.4(2)
N4−O5−H6	104.26	101.66	101.22	101.04	95.7(20)
C1−C2−C3−N4	119.77	117.09	119.20	118.25	
C2−C3−N4−O5	−180.00	−179.11	−179.68	−179.68	
E	−246.91906	−247.64974	−248.28118	−248.34803	

E-sp form parameters	ab initio MO[b]		DFT		
	HF/6-31G*	MP2/6-31G*	BLYP/6-31G	BLYP/6-31G*	GED + MW[c]
C1−C2	1.526	1.525	1.547	1.541	1.550(3)
C2−C3	1.502	1.497	1.515	1.512	1.490(2)
C3−N4	1.251	1.285	1.300	1.289	1.290(3)
N4−O5	1.376	1.419	1.505	1.439	1.428(2)
C1−C2−C3	114.98	114.37	115.35	115.42	112.6(9)
C2−C3−N4	121.82	120.22	120.59	120.84	122.6(11)
C3−N4−O5	111.79	109.93	109.24	110.50	109.4(2)
N4−O5−H6	104.26	101.60	101.18	101.07	95.7(20)
C1−C2−C3−N4	0.00	0.00	0.00	0.00	
C2−C3−N4−O5	180.00	180.00	180.00	180.00	
E	−246.91880	−247.64962	−248.28067	−248.34750	

Z-ap form parameters	ab initio MO[b]		DFT		
	HF/6-31G*	MP2/6-31G*	BLYP/6-31G	BLYP/6-31G*	GED + MW[c]
C1−C2	1.528	1.526	1.547	1.542	1.549(3)
C2−C3	1.506	1.500	1.514	1.515	1.497(2)
C3−N4	1.253	1.289	1.303	1.292	1.295(1)
N4−O5	1.375	1.418	1.510	1.443	1.430(2)
C1−C2−C3	112.45	112.52	113.11	113.22	109.4(4)
C2−C3−N4	126.71	126.21	127.70	127.46	127.5(3)
C3−N4−O5	112.14	109.73	109.34	110.41	109.3(3)
N4−O5−H6	104.10	101.42	100.86	100.76	94.0(14)
C1−C2−C3−N4	180.00	180.00	180.00	180.00	
C2−C3−N4−O5	0.00	0.00	0.00	0.00	
E	−246.91781	−247.64931	−248.28101	−248.34722	

[a] The numbering of the atoms is given in Figure 2. Bond lengths are in angstroms and bond angles are in degrees. Total energies, E, are in hartrees. [b] r_e structure. [c] Results from the joint analysis of electron diffraction data and rotational constants from refs 7 and 6 for E and Z isomers, respectively (r_g and $\angle_\alpha$).

The experimental bond angles, C1C2C3 and C2C3N, were found to be different in the ac and sp forms of the E isomer. The C1C2C3 angle is the largest in the E-sp form and the smallest in the Z-ap form. This is due to the fact that the repulsion between the NOH and CH_3 groups is maximum in the E-sp form, owing to the short distance between two groups. The ab initio and DFT methods reproduced the difference in the above bond angle between the two conformers of the E isomer. The bond angles obtained by the MP2/6-31G* level agree well with the experimental values of the ac form. The C2C3N angle obtained by the DFT method is in close agreement with the experimental value.

The values of CNO angle determined by electron diffraction were not different among the three stable conformers. Generally, the values of CNO angle of oximes are confined to a narrow interval (111°−114°).[25] In the present investigation, BLYP/6-31G* level of theory reproduced the CNO angle very accurately for the E and Z isomers.

It is important that the NOH bond angle obtained by the theories and from experiment are very different. There may be two reasons for such a large deviation. The electron diffraction experiment could not correctly locate the hydrogen atom. Moreover, two lone pair electrons and one lone pair electron are found in the oxygen and nitrogen atoms, respectively. So, the fact that the theories were inadequate to treat the lone pair electrons produced the large deviation between the theory and the experiment.

The computed rotational constants for both the isomers fairly agree with the experimental values in MP2/6-31G* level of theory. All levels of calculation predict that the E-ac form is the most stable conformer, in which the value of dihedral angle, ϕ, is around 120°. The next stable conformer is the E-sp form where $\phi = 0°$. These angles agree well with the gas-phase electron diffraction values. The minimum energy structure of the Z form is obtained at the dihedral angle of 180°.

2. Torsional Potential. The relative energies obtained at different dihedral angles, ϕ, of the E and Z isomers of propionaldehyde oxime are presented in Table 2. They are calculated for each 30° rotation around C2−C3 bond. The results for the E isomer show that the most stable conformation is the ac form at $\phi = 120°$ and the next stable conformation is the sp form at $\phi = 0°$. The energy differences between the ac and sp conformers are 0.16, 0.06, and 0.33 kcal/mol in HF/6-31G*, MP2/6-31G*, and BLYP/6-31G* levels of theory, respectively. These results are in agreement with the electron diffraction experiment[7] where the ac form is more stable than the sp form by 0.15 kcal/mol.

TABLE 2: Relative Energies of E and Z Isomers Calculated at Different Torsional Angles (ϕ)[a]

	E isomer			Z isomer
ϕ (deg)	HF/6-31G*	MP2/6-31G*	BLYP/6-31G*	HF/6-31G*
0[b]	0.000	0.000	0.000	0.000
30	0.929	0.816	0.872	−0.402
60	1.826	1.644	1.613	−2.422
90	0.715	0.621	0.452	−3.571
120	−0.163	−0.063	−0.333	−3.558
150	0.778	1.010	0.646	−3.633
180	1.889	2.190	1.788	−3.803

[a] Relative energies are in kcal/mol. ϕ denotes the dihedral angle of C1C2C3N4 (see Figure 2). The total energies for the E isomer at the HF/6-31G*, MP2/6-31G*, and BLYP/6-31G* levels are −246.918 80, −247.649 62, and −248.347 50 hartrees, respectively. The total energy for the Z isomer at the HF/6-31G* level is −246.911 75 hartrees.

TABLE 3: Fourier-Fitted Torsional Potentials of Propionaldehyde Oxime[a]

	E isomer			Z isomer
parameter	HF/6-31G*	MP2/6-31G*	BLYP/6-31G*	HF/6-31G*
V_1	−0.120	0.273	−0.183	−3.512
V_2	−0.167	−0.397	−0.374	−1.761
V_3	1.956	1.868	1.893	−0.510
V_4	0.017	−0.008	0.036	0.310
V_5	0.054	0.049	0.078	0.220
V_6	−0.062	−0.076	−0.068	0.092

[a] V_i are the potential coefficients of the Fourier expansion in kcal/mol (see text).

The experimental observation shows that the (*Z*)-propionaldehyde oxime exists in one rotational conformer, the ap form. The experimental barrier height obtained by the electron diffraction data was found to be 1.5 kcal/mol for the Z isomer.[6] The present study predicted the barrier height as 3.803 kcal/mol in the HF/6-31G* level of theory. We have performed the calculations in MP2/6-31G* level at $\phi = 0°$ and $180°$ to determine the barrier height, 3.916 kcal/mol, which is very high compared with the experimental one.

Wiberg and Martin[26] reported that conformational equilibria may involve a contribution from the attractive portion of the interaction between nonbonded atoms. The simplest view is that the oxygen has little net effect on the rotational barrier; this is supported by other calculations on acetaldoxime.[14] So the potential barrier height in this compound does not necessarily depend on the repulsive force between atoms. Figure 3 shows the potential energy curves of E and Z isomers of propionaldehyde oxime as a function of ϕ. The greater stability of the E-ac conformer compared with the E-sp conformer should be attributed to the interactions between NOH and CH_3 groups. The energy difference between the two conformers is small enough to justify the presence of the planar structure in the solid state due to the packing forces. The small energy difference further suggests the coexistence of the ac and sp conformers in the gas and liquid phases. The intramolecular interaction between CH_3 group and the H7 atom also induces a comparatively moderate increase in the energy of the sp form relative to the ac form. The similar trends exhibited when interacting groups approach each other reveal the importance of steric repulsions in determining the basic shape of the torsional potential in this molecule.

The potential energy function for the internal rotation can be obtained by fitting the energies calculated for different conformers to a truncated Fourier expansion. The six-term potential coefficients, V_1-V_6, for the E and Z isomers of propionaldehyde oxime have been calculated in HF, MP2 and BLYP levels of

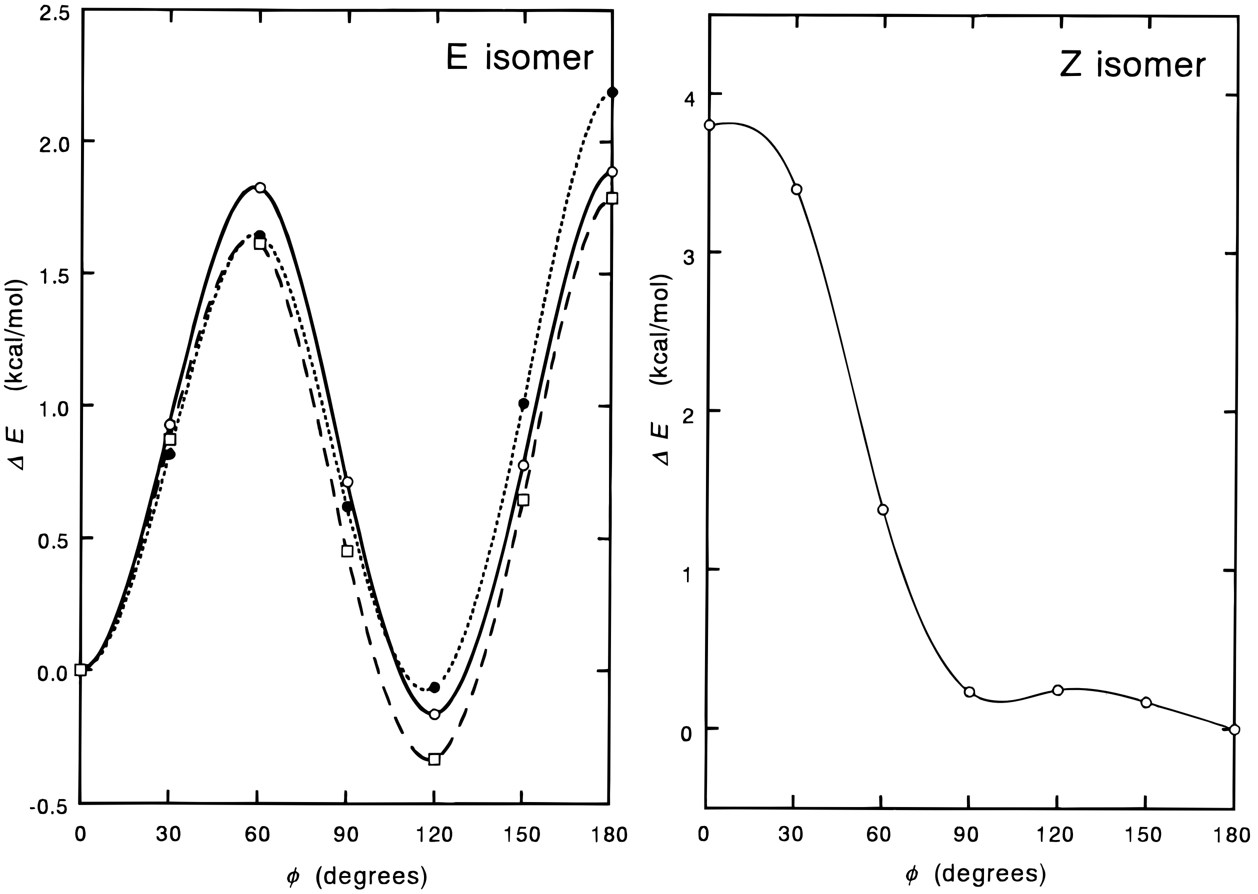

Figure 3. Torsional potential curves of propionaldehyde oxime as a function of the dihedral angle ϕ: plots of the E isomer calculated at HF/6-31G* (—), MP2/6-31G* (···) and BLYP/6-31G* (- - -) levels (left); plot of the Z isomer calculated at HF/6-31G* level (right).

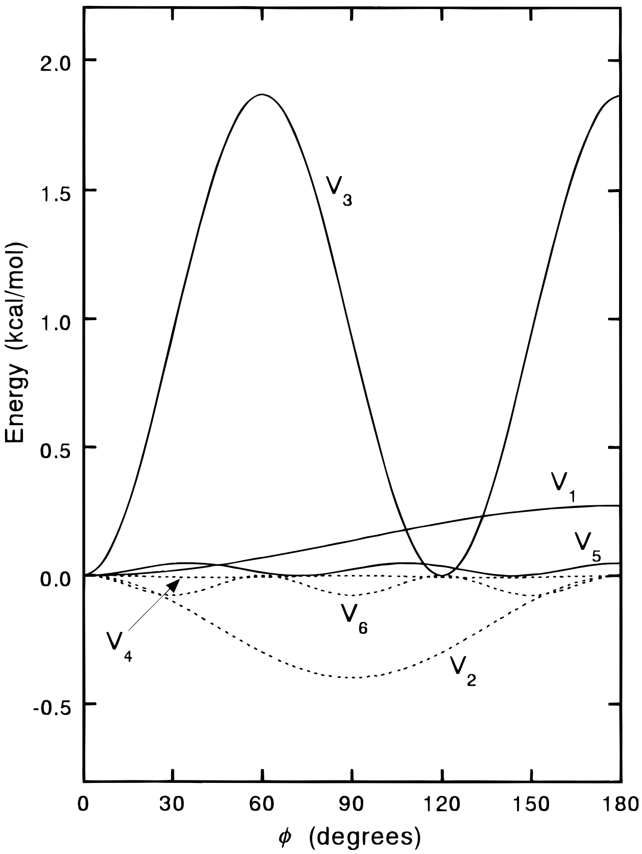

Figure 4. Fourier decomposition of the torsional potential, $V(\phi)$, of propionaldehyde oxime calculated at the MP2/6-31G* level of theory.

theory, using the 6-31G* basis set tabulated in Table 3. Figure 4 shows the Fourier decomposition of the potential energy curve for the E isomer. The obtained potential curve of the E isomer shows the fact that the V_1 to V_3 coefficients significantly contribute to the torsional potential. The first V_1 potential coefficient corresponds to the interaction of the CH_3 and NOH groups and accounts for the main part in the ac and sp forms. The V_2 term may be the interaction between the lone pairs of oxygen and the CH_3 group of the molecule. The V_3 term reflects the CH and CH_3 repulsion which makes the main contribution to the total potential curve. This tendency is almost the same in all the levels of theory.

Recently we have made an attempt to study the chemical hardness and chemical potential of isomers of XC(O)OX (X = F, Cl), C_2H_3NO, C_2H_2, and HCNC molecules and the hardness profiles of hydrogen bond systems, HF···HCN, HF···HCl, and $CH_3OH\cdots H_2O$.[27] In most of the cases, the chemical hardness is found to be a good indicator for predicting the most stable isomer. The same conclusion, that the minimum energy conformer has the maximum hardness value, was obtained for the SiC_2 molecule.[28] So it is interesting to study the stability of isomer through the chemical hardness and chemical potential of the E and Z isomers of the propionaldehyde oxime.

The chemical hardness (η) and chemical potential (μ) are defined as

$$\eta = 1/2(\mathrm{d}^2E/\mathrm{d}N^2)_{V(r)};\quad \mu = (\mathrm{d}E/\mathrm{d}N)$$

where E is the total energy; $V(r)$ is the external potential, and N is the number of electrons, in a finite difference approximation, with the assumption that the energy varies quadratically with the number of electrons. These two quantities can be expressed with an orbital basis as

$$\eta = (I - A)/2;\quad \mu = -(I + A)/2$$

where I is the ionization potential and A is the electron affinity of a system. From Koopmans' theorem, these two quantities are obtained on an orbital basis:

$$I = -E_{\mathrm{HOMO}}$$

$$A = -E_{\mathrm{LUMO}}$$

where E_{HOMO} and E_{LUMO} are the energies of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). By applying the above equations, the chemical hardness and chemical potential have been computed for the different conformations of the E and Z isomers. The calculated values are given in Table 4. Further, we have examined the hardness profiles for the different dihedral angles of the two conformers of the E isomer, given in Figure 5.

From Table 4 and Figure 5, it is clear that the chemical hardness value could not predict the most stable conformation of this molecule. In the earlier study of C_2H_3NO molecule,[27] the higher chemical hardness value could not predict the more stable isomer. In all the cases except for $NH_2CH{=}NOH$ molecule, the same trends of results have been obtained. Now it is very interesting to probe further on this subject. Nguyen and Ha[12] obtained the HOMO and LUMO energies for a few aldoximes. Further, the ionization potential (HOMO) of the aldoximes obtained by the photoelectron spectrum including propionaldehyde oxime and nitrosoethylene are of π type except for $NH_2CH{=}NOH$, where the LUMO is of σ type. The two lowest ionization potentials (HOMO) which represent the "n ionization (lone pair)" and "π ionization (C=N)" in these molecules are in the reverse order to those found for nonconjugated imines. The HOMO values are also strongly affected by the substituent groups. Due to the substituents, the C=N double bond was found to be affected and the C=N overlap population to be high, except for the $NH_2CH{=}NOH$ molecule. The net π charges of the nitrogen atom in the E and Z isomers may be more abundant and quite different compared with the charge of the $NH_2CH{=}NOH$ molecule. So, the chemical hardness values of (*E*)-propionaldehyde oxime were unable to indicate the most stable conformer of the molecule. Thus, we could not generalize this concept that the most stable isomer has the maximum hardness values. A more detailed study is needed to get more information on this subject.

Conclusions

Ab initio and DFT studies of propionaldehyde oxime were performed to obtain the molecular structures and conformational properties of E and Z geometrical isomers. The molecular geometries were optimized at the HF/6-31G*, MP2/6-31G*, BLYP/6-31G, and BLYP/6-31G* levels of theory. The potential energy curves were obtained for the C2−C3 rotational angle at HF/6-31G*, MP2/6-31G*, and BLYP/6-31G* levels of theory. The energy minima were found at $\phi = 120°$, 0°, and 180° for the E-ac, E-sp, and Z-ap conformers, respectively. In the E isomer, the ac form was found to be more stable than the sp form at all levels of theory. These results are consistent with the experimental data in the gas phase. The theoretical results predict that the C=N bond lengths of the three conformers are almost the same in contrast with the experimental results. The accuracy of the N−O bond length was improved by the addition of the polarization function in the DFT method. Other differences of the structural parameters among the E-ac, E-sp, and Z-ap conformers agreed with the experimental data qualitatively at the MP2/6-31G* and BLYP/6-31G* levels of theory. In the

TABLE 4: Chemical Hardness and Chemical Potential for the E and Z Isomers of Propionaldehyde Oxime[a]

	HF/6-31G*	MP2/6-31G*
E-sp form		
η	7.75226	7.52613
μ	−2.64985	−2.82400
E-ac form		
η	7.64722	7.43320
μ	−2.74264	−2.89815
Z-ap form		
η	7.66436	7.43987
μ	−2.76876	−2.92686

[a] η and μ (eV) denote the chemical hardness and chemical potential, respectively (see text).

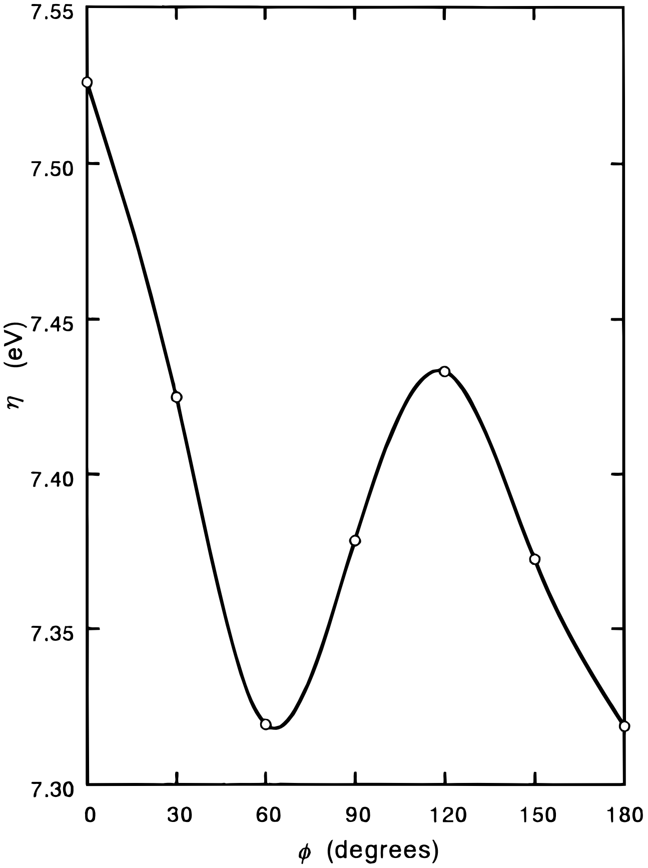

Figure 5. Plot of the chemical hardness of E isomer of propionaldehyde oxime calculated at the MP2/6-31G* level as a function of the dihedral angle ϕ.

Z isomer, the values of barrier height obtained by the ab initio calculations are very high compared with the experimental one. An analysis of the potential curve of the E isomer by using truncated Fourier expansion showed that the V_1 to V_3 terms were the main contributions. In propionaldehyde oxime, the analysis of chemical hardness could not predict the conformational stability because of the nature of the net charge on nitrogen atom.

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Supporting Information Available: Listing of optimized geometric parameters, total energies (Table S1) and Cartesian coordinates (Table S2) for the E and Z isomers of propionaldehyde oxime (6 pages). See any current masthead page for ordering information.

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