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Experimental and theoretical Investigation of the IR spectra and thermochemistry of four isomers of 2-N,N-dimethylaminecyclohexyl 1-N',N'-dimethylcarbamate

A. F. Jalbout[1], Xin-Hua Li[2*], B. Trzaskowski1 and H. Raissi[1]*
[1]*Department of Chemistry, The University of Arizona, Tucson, Arizona, 85721, USA*
[2]*School of Chemistry and Materials Science, Wenzhou University, Zhejiang Wenzhou 325027, P.R.China*
**Corresponding authors. E-mail addresses: ajalbout@u.arizona.edu (A.F. Jalbout);lixinhua01@126.com(Xin-Hua Li)*

Abstract: A combined experimental and Density functional theory (DFT) B3LYP/6-311+G* study on the IR spectra of four stable isomers of 2-N,N-dimethylaminecyclohexyl 1-N',N'-dimethylcarbamate was performed. Our theoretical calculations reveal that two new isomers of this compound exist and may be more stable than the known isomers. In addition the entropy, heat capacity, and the enthalpy content of the stable isomers are computed by fitting the calculated data to a standard Shomate equation and IR spectra for the two new isomers are presented.

Keywords: density functional theory (DFT); B3LYP; C11H22N2O2; IR spectra; thermochemical properties.

Introduction

Carbamates are an important class of biologically active compounds used in the treatment of several diseases, such as myasthenia gravis [1] or Alzheimer [2]. In view of this, many researches have focused on correlating molecular structure of carbamate to their pharmacological activity [3–8]. Earlier investigations on structure–activity relationship by Beers and Reich suggested that the distances between functional groups are the main feature responsible by the pharmacological usefulness [3]. Nevertheless, Furukawa et al. demonstrated that molecular flexibility also plays an important role [5]. They found that (S)-methacholine and (2S,4R,5S)-muscarine change their conformation upon binding to an acetylcholine receptor. Much of this flexibility is dictated by a hindered rotation around chemical bonds, as is the case of conjugated C–N linkages [9–13]. Thus, recently carbamates attracted much attention with respect to their molecular structure [14–19].

Several studies on the C–N rotational barrier in carbamates have also been reported [15-17]. In particular the rotational barrier of the conjugated C-N bond in 2-*N*,*N*-dimethylaminecyclohexyl 1-*N'*,*Ní*-dimethylcarbamate has been studied for two isomers. In isomer 1 the carbamate group lies at the axial position, whereas in isomer 2 it adopts an equatorial arrangement [20]. It is, however, interesting to notice that from the theoretical point of view there may be four different isomers of this compound. Two additional isomers may be created changing the relative position of the N-dimethyl group from equatorial to axial (isomers 3 and 4) [Fig. 1].

In this article, a combined experimental and density functional theory study on the stability and IR spectra of all four isomers of 2-*N*,*N*-

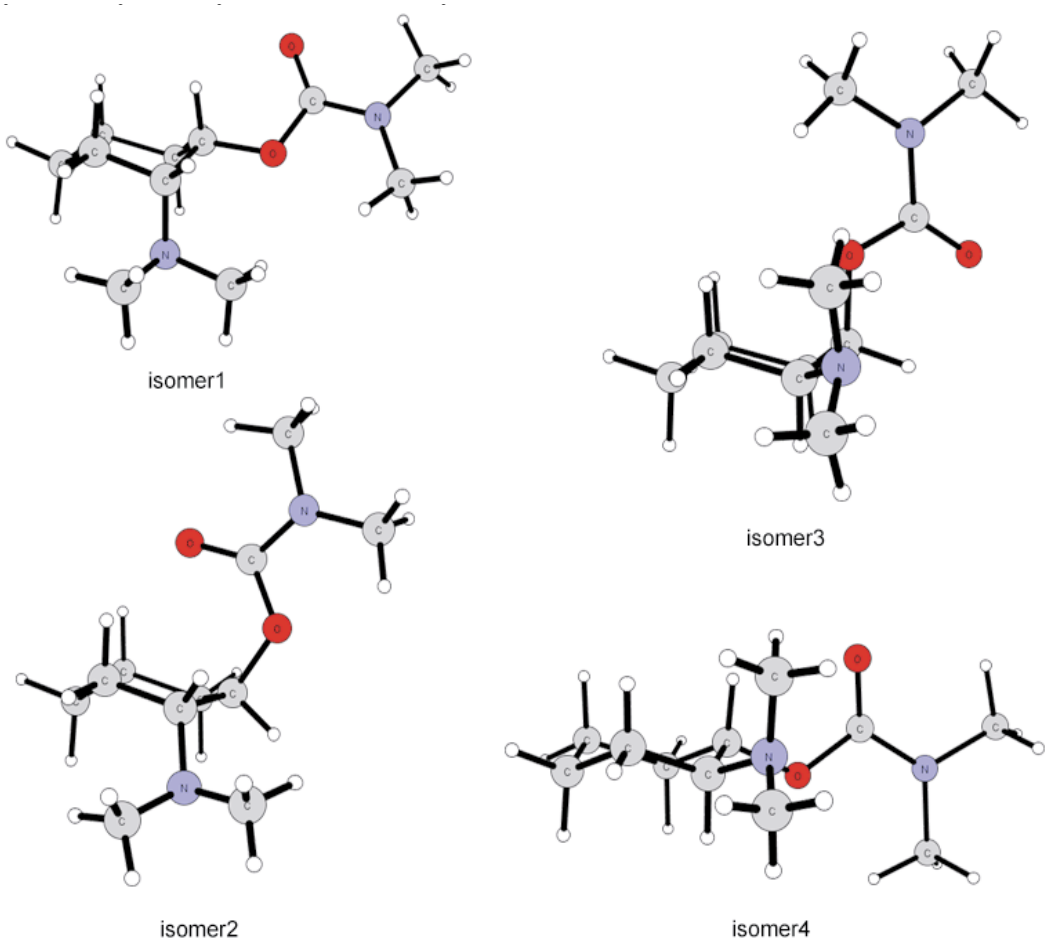

Figure 1. Optimized geometries od molecular models of four different isomers of 2-*N*,*N*-dimethylaminecyclohexyl 1-*N*',*Ní*-dimethylcarbamate.

dimethylaminecyclohexyl 1-*N*',*Ní*-dimethylcarbamate was performed. In addition the entropy, heat capacity, and the enthalpy of the four stable isomers are estimated by fitting to a standard Shomate equation.

Experimental methods

IR measurements

Isomers 3 and 4 were obtained according the procedure described elsewhere [6]. IR spectra for those isomers (900-4000cm^{-1}) were recorded in CCl_4 solution on a FTIR spectrophotometer.

Computational methods

Quantum chemical calculations were performed by using the Gaussian 98 [21] software package. Full geometry optimizations and frequency calculations of these species were carried out at the B3LYP level of theory [22,23] with the standard 6-311+G* and 6-311++G** basis sets. The DFT approach was chosen due to the large size of the molecule and the good experimental correlations with the IR frequencies. Zero-point energy corrections scaled by 0.96 were added to the final DFT energies. Additionally the final molecular energy of the isomers was calculated at MP2 level of theory [24]. The thermodynamical properties were computed using the simple but

reasonably accurate rigid rotor harmonic oscillator (RRHO) approximation.

Results and summary

The theoretical molecular energies of the four isomers (Table 1) reveal interesting information. The computational approach predicts that the new isomers should be more stable than the other two isomers. The results suggest, that isomer 4 is the most stable of all the isomers of 2-*N*,*N*-dimethylaminecyclohexyl 1-*N'*,*Ní*-dimethylcarbamate. The energy of isomer 3 is ~2 kcal/mol higher than the energy of isomer 4, what is well within the standard error of the B3LYP method (estimated to be ~2.2 kcal/mol). Isomer 1 is also quite close on the energy scale with only 4.6 kcal/mol (2.7 kcal/mol on the MP2 level of theory) more than isomer 4. The least stable of the isomers is compound 2, with ~10.5 kcal/mol more than isomer 4. The high stability of isomers 1, 3 and 4 may be caused by favorable interactions between the N-dimethyl group and carbamate moiety, which in those three isomers are relatively close to each other, allowing overlap of

Table 1. Theoretical relative energies and HOMO/LUMO energies of four 2-*N*,*N*-dimethylaminecyclohexyl 1-*N'*,*N'*-dimethylcarbamate isomers calculated at different levels of theory.

	isomer 1	**isomer 2**	**isomer 3**	**isomer 4**
$HOMO^{DFT}$(Hartree)	-0.21928	-0.21808	-0.21129	-0.20853
$LUMO^{DFT}$(Hartree)	-0.00211	-0.00260	-0.00481	-0.00172
ΔE^{DFT} (kcal/mol)	4.15	10.24	2.42	0.0
$HOMO^{MP2}$(Hartree)	-0.35227	-0.35081	-0.34	-0.34
$LUMO^{MP2}$(Hartree)	0.06420	0.06472	0.06	0.06
ΔE^{MP2} (kcal/mol)	2.67	10.47	1.76	0.0

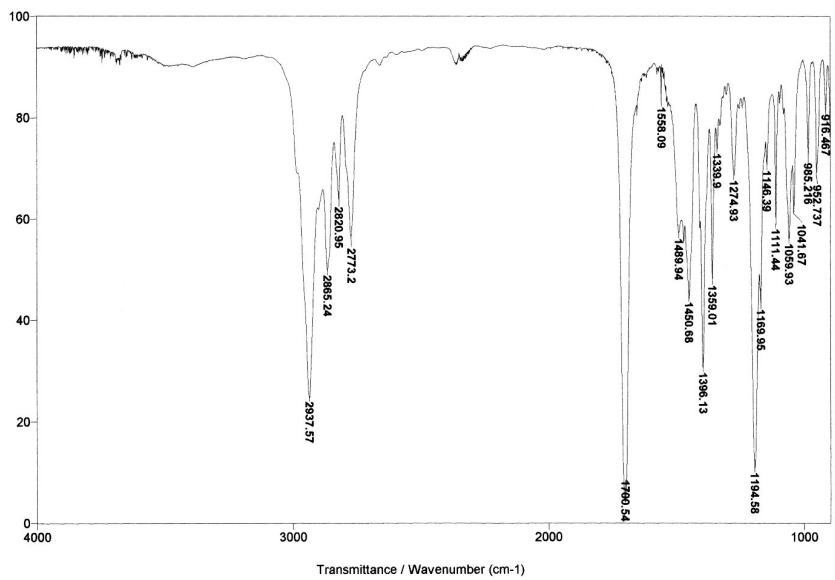

Figure 2. Experimental IR spectrum of isomer 3 in 3.00 X 10^{-2} M CCl_4 solution.

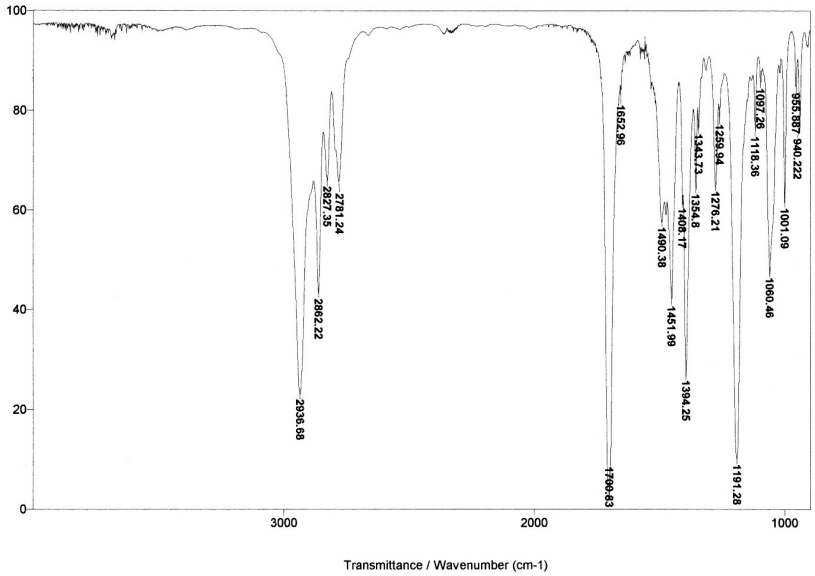

Figure 3. Experimental IR spectrum of isomer 4 in 3.00 X 10^{-2} M CCl_4 solution.

Table 2. Theoretical and experimental frequencies (n, in cm^{-1}) for isomer 3 and the relative theoretical-experimental absolute errors (in cm^{-1}) at different levels of theory.

ν	Assignment	experimental	B3LYP/ 6-311+G*	B3LYP/ 6-311++G**
ν_1	Ring vibration	916.5	886.7	883.0
ν_2	Ring vibration	952.7	907.5	904.2
ν_3	Ring vibration	985.2	949.2	945.7
ν_4	Amine C-N stretching	1059.9	1010.9	984.5
ν_5	Amine CH_3 deformation	1111.4	1070.5	1061.7
ν_6	CH_2 twist	1146.3	1109.0	1067.0
ν_7	Amide CH_3 wag	1169.9	1122.1	1102.7
ν_8	C-O stretching	1194.5	1137.0	1132.5
ν_9	CH_2 twist	1274.9	1217.3	1209.4
ν_{10}	CH_2 twist	1339.9	1272.8	1265.1
ν_{11}	CH_2 wag	1359.0	1288.8	1296.3
ν_{12}	Amide CH_3 deformation	1396.1	1322.8	1325.6
ν_{13}	Amine CH_3 deformation	1450.6	1380.1	1371.6
ν_{14}	Amine C-H stretching	1489.9	1415.1	1414.8
ν_{15}	Amine C-H stretching	1558.0	1475.2	1463.0
ν_{16}	C=O stretching	1700.5	1666.8	1664.2
ν_{17}	Ring C-H stretching	2773.2	2771.9	2766.1
ν_{18}	Ring C-H stretching	2820.9	2784.6	2778.5
ν_{19}	Ring vibration	2865.2	2853.6	2854.8
ν_{20}	Ring vibration	2937.5	2920.8	2917.5
average error			3.56	4.20

Table 3. Theoretical and experimental frequencies (n, in cm^{-1}) for isomer 4 and the relative theoretical-experimental absolute errors (in cm^{-1}) at different levels of theory.

ν	Assignment	experimental	B3LYP/ 6-311+G*	B3LYP/ 6-311++G**
ν_1	Ring Vibration	940.2	910.7	906.8
ν_2	Ring Vibration	955.9	918.6	915.8
ν_3	Ring Vibration	1001.0	965.7	962.4
ν_4	Ring Vibration	1060.4	998.3	1010.2
ν_5	Ring Vibration	1097.2	1042.6	1039
ν_6	Amine CH_3 deformation	1118.3	1070.4	1061.1
ν_7	Amine C-N stretching	1191.2	1127.5	1119.1
ν_8	Amine C-N stretching	1259.9	1182.6	1176.2
ν_9	Amine C-N stretching	1276.2	1224.1	1215.9
ν_{10}	CH_2 wag	1343.7	1266.6	1280
ν_{11}	CH_3 amide deformation	1354.8	1289.3	1298.4
ν_{12}	CH_3 amide deformation	1394.2	1321.4	1316.8
ν_{13}	Amine C-H stretching	1408.1	1325.6	1351.4
ν_{14}	Amine C-H stretching	1451.9	1381.2	1377.6
ν_{15}	Amine C-H stretching	1490.3	1416.8	1418.2
ν_{16}	C=O stretching	1652.9	1476.4	1464.3
ν_{17}	Ring C-H stretching	1700.8	1662.7	1660.1
ν_{18}	Ring Vibration	2781.2	2771.7	2765.6
ν_{19}	Ring Vibration	2827.3	2790.0	2784.6
ν_{20}	Ring Vibration	2862.2	2857.0	2854.9
ν_{21}	Ring Vibration	2936.7	2864.4	2869.1
average error			4.28	4.34

the molecular orbitals. On the other hand in isomer 2 those two groups are on the opposite sides of the cyclohexyl ring, preventing any interactions between them.

The IR spectra [Fig. 2 and 3] of the two new isomers are very similar but show small differences. A thorough analysis of the most important vibrations [Table 2 and 3] allowed us to assign specific modes to particular vibrations. It is clear that, while the IR spectra are similar, the small differences existing may be useful in analyzing the occurrence of the isomers in the sample. It is also interesting to notice a good agreement between the experimental and the theoretical spectra, which allow us to validate the computational approach presented in this study.

Table 4 presents the estimation of the thermodynamic properties (entropy, heat capacity at constant pressure, enthalpy) of all 4 isomers at different temperatures. The calculated data was fit to the Shomate equations, as implemented by the National Institute of Standards and Technology (NIST) [25] to yield the best values. It is interesting to notice that, while isomers 1 and 4 are close on the energetical scale, the predicted thermochemical properties of these compounds are substantially different. On the other hand the thermochemical properties of isomer 2 and 4 are quite similar in spite of the large differences in their molecular energy. The data obtained using Shomate equations allow to predict different values of some of the thermochemical properties of all four isomers at different temperatures, thus

Table 4. Thermodynamic properties of isomers 1-4 at different temperatures.

	Property	*Fitted Thermodynamic Equation (T/1000=t)*	*100*K	*298.15K*	*1000K*
1[a]	S (J/mol*K)[c]	-19.27684*ln(t) + 1046.38976*t -308.15331*t²/2 -72.17832*t³/3+0.60117/(2*t²) + 233.31191			
	C_p (kJ/mol*K)[d]	279.67304+942.65658*t -63.49214*t^2-57.42896*t^3 -0.22514*t^{-2}			
	H° - H°$_{298.15}$ (kJ/mol)[e]	1.67269*t + 959.98678*t²/2 -181.65772*t³/3 -131.70779*t⁴/4+0.40953/t			
2[a]	S (J/mol*K)	-18.01857*ln(t) + 1043.7303*t -308.09809*t²/2 - 70.85667*t³/3+0.58322/(2*t²) + 238.11687	353.26	553.67	1103.98
	C_p (kJ/mol*K)	281.45185+ 946.76815*t -69.3773*t^2-54.81026*t^3 -0.22109*t^{-2}	124.06	268.66	653.64
	H° - H°$_{298.15}$ (kJ/mol)	1.66451*t + 963.73597*t²/2 -192.11685*t³/3 -124.90469*t⁴/4+0.40169/t	7.8	46.65	393.38
3[a]	S (J/mol*K)	4.12198*ln(t) -42.55898*t +1132.49684*t²/2 -444.20905*t³/3+ 0.0491/(2*t²) + 18.60524	354.61	557.18	1108.23
	C_p (kJ/mol*K)	8.6918 -20.37762*t+546.87866*t^2-140.93425*t^3 -0.04068*t^{-2}	126.47	269.62	654.04
	H° - H°$_{298.15}$ (kJ/mol)	2.02177*t +965.52164*t²/2 -194.1014*t³/3 -124.42143*t⁴/4+0.44725/t	7.92	47.13	394.25
3[b]	S (J/mol*K)	-18.75968 *ln(t) 1055.99732 *t -322.42927 *t²/2 -66.43605 *t³/3+0.6207 /(2*t²) + 237.73775			
	C_p (kJ/mol*K)	282.85511 -955.04707 *t-73.0603 *t^2-54.61964 *t^3			
	H° - H°$_{298.15}$ (kJ/mol)	1.75634 *t +972.25178 *t²/2 -200.43501 *t³/3 -123.49363 *t⁴/4+0.43362 /t	7.91	47.24	395.58
4[a]	S (J/mol*K)	4.87376*ln(t) -45.73716*t +1135.1577*t²/2 - 444.56315*t³/3+0.04159/(2*t²) + 20.16502	353.17	555.38	1105.97
	C_p (kJ/mol*K)	8.44355-19.51033*t+544.67639*t^2-139.75091*t^3 -0.03987*t^{-2}	125.38	269.47	653.85
	H° - H°$_{298.15}$ (kJ/mol)	1.98603*t + 965.55544*t²/2 -197.60318*t³/3 -120.88774*t⁴/4+0.44389/t	7.82	46.99	393.85
4[b]	S (J/mol*K)	-15.1279649*ln(t) + 1038.10267*t - 297.015371*t²/2 - 77.7776121*t³/3+0.578806606/(2*t²) + 243.541614			
	C_p (kJ/mol*K)	279.92463+ 956.69556*t -77.4193*t^2-52.11341*t^3 -0.2302*t^{-2}			
H°	H° - $_{298.15}$ (kJ/mol)	1.92868*t + 971.55095*t²/2 -201.71088*t³/3 -121.53117*t⁴/4+0.42767/t	7.79	47.05	395.12

[a]at B3LYP/6-311+G* level of theory
[b]at B3LYP/6-311++G** level of theory
[c] Entropy
[d] Heat capacity at constant pressure
[e] Enthalpy content

providing additional means of detecting different isomers. These methods allow for distinction of isomers to be performed under various thermodynamical conditions. They are very useful for indexing purposes by government agencies.

Conclusions

Experimental IR spectra and theoretical calculations were used to inspect the stability of two new isomers of 2-*N*,*N*-dimethylaminecy-

clohexyl 1-*N',Ní*-dimethylcarbamate. The results of this study reveals that both new isomers are stable and can be detected using standard spectroscopic approaches. The results aloww us to predict that the termodynamic properties of all four isomers should be similar as well as the new isomers may be more stable than the known ones.

Aknowledgements

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A. F. Jalbout, Xin-Hua Li, B. Trzaskowski and H. Raissi. Estudo teórico e experimental dos espectros no IR e da termoquímica de quatro isômeros do 2-*N,N*-dimetilaminacicloexil 1-*N',Ní*-dimetilcarbamato.

Resumo: Foi realizado um estudo combinado, experimental e teórico utilizando a teoria da função de densidade (DFT) B3LYP/6-311+G* para os espectros de IR de quatro isômeros estáveis do 2-*N,N*-dimetilaminaciclohexil 1-*N',Ní*-dimetilcarbamato. Os cálculos teóricos mostraram a existência de dois novos isômeros deste composto, que parecem ser mais estáveis que os isômeros conhecidos. Além disso, os valores da entropia, capacidade calorífica e entalpia dos isômeros estáveis foram calculados a partir do ajuste dos dados à equação padrão de Shomate, e foram obtidos os espectros de IR para os dois novos isômeros.

Palavras-chave: teoria da função de densidade (DFT); B3LYP; $C_{11}H_{22}N_2O_2$; espectros no IR; propriedades termoquímicas.

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Supplementary Information

Cartesian Coordinates of Optimized Structures

Isomer **1**
B3LYP/6-311+G*:

C,0,-2.6251681585,-0.6671181404,-1.4070723528
C,0,-2.9539716409,-1.6680290962,-0.2888166607
C,0,-2.3804367785,-1.2144495823,1.0619442764
C,0,-0.8492500005,-0.9892618994,0.9932246548
C,0,-0.6761778315,0.1298748633,-0.0544676202
C,0,-1.1294042073,-0.3077603782,-1.4453706374
N,0,-0.1402048385,-2.2456158372,0.6805271884
C,0,-0.4607176415,-3.3186476742,1.6177542495
C,0,1.3106345806,-2.1060418878,0.5830751541
O,0,0.6859880044,0.6359010052,-0.0661816394
C,0,0.8335085302,1.9662379453,-0.3215731198
O,0,-0.0955857737,2.7157911377,-0.5598617564
N,0,2.1447539747,2.3480266243,-0.2606423163
C,0,2.4988833451,3.6978649232,-0.6714536415
C,0,3.2448900402,1.4158178767,-0.0638364503
H,0,-3.2041556752,0.2523086284,-1.2522553294
H,0,-2.9375229754,-1.066204305,-2.3775255468
H,0,-2.5441915998,-2.6498425615,-0.5460673616
H,0,-4.0394414493,-1.7911923471,-0.2061719389
H,0,-2.6357624447,-1.9222312067,1.8525707419
H,0,-2.8435459163,-0.2668081489,1.3596721685
H,0,-0.5041919618,-0.5940534798,1.9685540033
H,0,-1.3013986916,0.9630902379,0.269692033
H,0,-0.9564435746,0.5073696024,-2.1528558846
H,0,-0.5384900364,-1.1686664259,-1.771012316
H,0,0.1446802578,-4.194497967,1.3769142111
H,0,-1.5051642251,-3.6200292242,1.5416312582
H,0,-0.2562165252,-3.0484210575,2.6709558448
H,0,1.7460667383,-3.0856147726,0.3730940889
H,0,1.7679464976,-1.7245343691,1.5151016226
H,0,1.5858880121,-1.4353561695,-0.2257018517
H,0,3.1606102406,4.1543499891,0.0707044156
H,0,1.5951296679,4.2942846829,-0.7594010858
H,0,3.0167957358,3.6925148072,-1.638581186
H,0,4.0422267739,1.9202416758,0.4880162318
H,0,3.6585060306,1.0670851262,-1.0189435897
H,0,2.9168718971,0.5548729323,0.5103154193

Isomer **2**
B3LYP/6-311+G*:

C,0,0.0159667198,-0.8676607866,-2.5051918022
C,0,-1.3882228775,-1.3455210069,-2.1228346927
C,0,1.0114560759,-1.1582631636,-1.3762461762
C,0,-1.8366473703,-0.6859485455,-0.8129178769
C,0,0.5921909773,-0.7604096593,0.0504369611
C,0,-0.9157366593,-0.9733369507,0.3868974422
O,0,1.1071698939,0.5361240318,0.5010292891
N,0,-1.0367388105,-2.3511966578,0.9351338186
C,0,0.7426887288,1.71752803,-0.0467958787
C,0,-2.3417639559,-2.9877243102,0.8039423768
C,0,-0.6171145056,-2.3999964557,2.3326266286
O,0,-0.0147648911,1.8421178593,-0.992544314
N,0,1.3276083812,2.7686065234,0.6086872072
C,0,1.1533117667,4.1099016236,0.0746294826
C,0,2.3226458469,2.6174207595,1.6600098724
H,0,-0.0108798239,0.2015895128,-2.7190151589
H,0,0.3565028854,-1.3746635293,-3.4153450663
H,0,-1.3951362633,-2.4391106069,-2.0320505306
H,0,-2.1001362651,-1.0960331221,-2.9170793755
H,0,1.9904903269,-0.7147141152,-1.5843920203
H,0,1.1736266941,-2.242125201,-1.336647692
H,0,-2.865779686,-0.9568652717,-0.5651382301
H,0,-1.8335843725,0.3947524994,-0.9586825605
H,0,1.1576320967,-1.4053379163,0.7181278582
H,0,-1.1790053351,-0.2499338152,1.1783861957
H,0,-2.2847745647,-3.9863491539,1.2439182102
H,0,-2.6226246255,-3.1100002497,-0.2409616364
H,0,-3.1528573827,-2.4436408767,1.3215491961
H,0,-0.5607389245,-3.4382535736,2.6685807109
H,0,-1.3156303888,-1.8608729699,2.9993796717
H,0,0.3704328497,-1.9566772526,2.4673106272
H,0,0.8863475925,4.8008058676,0.8801145146
H,0,0.360331636,4.1016604177,-0.6677203852
H,0,2.0762502553,4.47117902,-0.3962013129
H,0,2.1618780051,3.3860600109,2.4214928427
H,0,3.3412778788,2.7343805648,1.2678344354
H,0,2.2384019139,1.6404083653,2.1245747024

Isomer **3** (CIS)
B3LYP/6-311+G*:

C,-2.1841955694,0.9096746105,-0.5174513443
C,-3.4407436892,0.0644378367,-0.2783679648
C,-3.2622784966,-1.3557780984,-0.825513096
C,-2.0110407342,-2.017222274,-0.2349840173
C,-0.7351567804,-1.1799738181,-0.4877356836
C,-0.9320937762,0.2464193794,0.0584264492
H,-2.0372405548,1.0589704936,-1.5943825336
H,-4.3071581651,0.5498560094,-0.7393983471
H,-3.6523894084,0.0158379156,0.7976419095
H,-3.1775630877,-1.3175054836,-1.9196139859
H,-4.1471545867,-1.963529095,-0.6073437349
H,-1.8775920439,-3.0198901203,-0.6539207296
H,-2.154942253,-2.150769334,0.8437371494
H,-0.6157080955,-1.0728900684,-1.5734170139
N,0.5195373016,-1.7774745489,-0.0106680869
O,0.1952264094,1.0635513397,-0.3253860315
C,1.0442891757,-2.8073135028,-0.8925277165
C,0.5362094676,-2.2025544766,1.3837333295
H,1.1063999919,-2.4304279001,-1.9165882825
H,0.4472600963,-3.7377977957,-0.9060957006
H,2.0558029092,-3.0758963597,-0.5753743271
H,-0.0803627265,-3.096424967,1.582465825
H,1.5644053058,-2.4424229767,1.667264968
H,-2.2934386869,1.9048670371,-0.0758348407
H,-0.9823991843,0.2366708966,1.1480852383
H,0.2074163821,-1.3946334209,2.0370793673
C,1.0994871366,1.3905561497,0.6352839382
O,0.937854295,1.1735570043,1.8231931381
N,2.1923584688,2.0155783242,0.105530494
C,3.2098802301,2.5393231059,1.0006030194
C,2.3733263356,2.2895899886,-1.3107470407
H,2.952887691,2.2838492076,2.0246616068
H,1.6522514531,1.7321511394,-1.8989503195
H,4.1884387264,2.110532508,0.758572573
H,3.281580618,3.6298641288,0.9107811032
H,2.2530752579,3.3591291885,-1.5242143723
H,3.3824145365,1.9939124127,-1.6159684937

Isomer **3** (CIS)
B3LYP/6-311++G**:

C,0,-0.5253678022,1.9826653807,-0.9853488117
C,0,-0.9042284356,2.6358355042,0.3520825366
C,0,-2.202111208,2.0453644592,0.9190534655
C,0,-2.1235160362,0.5144070568,1.0338541551
C,0,-1.7652279908,-0.1225841067,-0.3260123027
C,0,-0.4550358011,0.4535498859,-0.8877823194
H,0,0.4322781604,2.3584163518,-1.3540896041
H,0,-1.2729951544,2.2356771735,-1.7472339638
H,0,-1.1041762573,3.7179117314,0.2203425701
H,0,-0.092001713,2.4825106084,1.0712881145
H,0,-3.0400054967,2.314802653,0.2622801857
H,0,-2.4224746465,2.4847091034,1.8974812356
H,0,-3.0794381162,0.1161513463,1.3887284144
H,0,-1.3697952277,0.2435431398,1.7799412893
H,0,-2.5171374574,0.225098989,-1.0450413993
N,0,-1.8282258195,-1.5929951321,-0.3992104126
O,0,0.6445913439,0.0809731673,-0.0051853913
H,0,-0.2563126762,0.0123156928,-1.8633720221
C,0,-3.176908152,-2.0895477874,-0.6431777365
C,0,-1.1969733325,-2.3259567424,0.6947013367
H,0,-3.5983214668,-1.6155674668,-1.5330575652
H,0,-3.8727016976,-1.9231594896,0.2002091218
H,0,-3.1370582646,-3.1666260746,-0.8268825025
H,0,-1.7498413797,-2.2542830521,1.6484041215
H,0,-0.1826460756,-1.9677451702,0.854266511
H,0,-1.1441534712,-3.3842896031,0.424334574
C,0,1.8725459838,-0.0358434474,-0.5800568462
O,0,2.0806677132,0.1282199247,-1.7676882677
N,0,2.8319633416,-0.3749360762,0.3349161718
C,0,2.6087207312,-0.426322347,1.7725057041
H,0,1.5463248348,-0.4705300352,1.989356601
C,0,4.2163276285,-0.4623094052,-0.1057167527
H,0,4.2459194485,-0.4548436024,-1.1920343864
H,0,4.6664519848,-1.3887899834,0.2642015627
H,0,4.8036694841,0.383396668,0.2734098074
H,0,3.0345848318,0.4546952964,2.2701980526
H,0,3.092241734,-1.3169712576,2.1857036655

Isomer **4** (TRANS)
B3LYP/6-311+G*:

C,-1.0276540783,1.339936444,-1.5250340691
C,-2.3700934956,0.6081790801,-1.3855620228
C,-2.3066038562,-0.8048756232,-1.9788307155
C,-1.1467511009,-1.617861733,-1.3831215879
C,0.1945929593,-0.8751347304,-1.5588598787
C,0.1409050797,0.5336621582,-0.9450982367
H,-1.057508474,2.3206291244,-1.0429523535
H,-0.8142486575,1.5263623849,-2.5852936261
H,-3.1613388439,1.1895619703,-1.8707670278
H,-2.6406391165,0.5454652256,-0.3252965894
H,-2.178072955,-0.7365482083,-3.0677547866
H,-3.2553423574,-1.3277729976,-1.8156933488
H,-1.0930664693,-2.6006569246,-1.8633399808
H,-1.3362837572,-1.7987351662,-0.3200407455
H,0.3050545409,-0.673858358,-2.6318179647
N,1.4109611376,-1.6200030772,-1.1894841801
O,-0.0264255531,0.4180518949,0.4980440081
H,1.0877198351,1.040650712,-1.1252701681
C,1.8855163974,-2.4932770509,-2.2542694748
C,1.373626092,-2.3309598961,0.083891572
H,2.0196407732,-1.9263068473,-3.1786728557
H,1.2132434683,-3.345130868,-2.4667566805
H,2.8584365475,-2.9075873087,-1.9767756073
H,0.719213247,-3.2207223566,0.0724922721
H,1.0411280629,-1.6681833853,0.8792213765
H,2.3835852217,-2.6710018687,0.3292272903
C,0.4817390006,1.4299164305,1.2528846056
O,1.0759202245,2.3852703016,0.790037892
N,0.2591112231,1.2284366295,2.5885048203
C,-0.5803580785,0.1688545615,3.1256869362
H,-0.733776865,-0.6085996473,2.3846280564
C,0.669208709,2.2605568401,3.5273229325
H,1.3170411414,2.9704659527,3.020980822
H,1.2114780032,1.8100604668,4.3643544178
H,-0.1999075672,2.7966488045,3.9286580746
H,-1.5593287325,0.5573171903,3.4352432753
H,-0.098256712,-0.2716492175,4.0037661037

Isomer **4** (TRANS)
B3LYP/6-311++G**:

C,0,-1.2454614128,-2.0706843416,0.1151371455
C,0,-2.7171330989,-2.1024260068,-0.3149350297
C,0,-3.4931091754,-0.931559867,0.2988036836
C,0,-2.8307027665,0.4065475725,-0.0538938827
C,0,-1.3479925589,0.4572512231,0.3865317014
C,0,-0.5824211907,-0.733277799,-0.2202793258
H,0,-1.1728564697,-2.2328949041,1.1974713165
H,0,-3.1669256569,-3.0574969704,-0.0264074958
H,0,-2.7808987193,-2.0456062762,-1.4089260482
H,0,-3.5258362984,-1.0490209008,1.3896721759
H,0,-4.5321492348,-0.9390712742,-0.0463940943
H,0,-3.3752486724,1.2341789868,0.4110591806
H,0,-2.8948390921,0.5597059937,-1.1373971628
H,0,-1.3168443621,0.3140675523,1.4739902421
N,0,-0.6580819431,1.7304388606,0.1371868859
O,0,0.7522312259,-0.772208517,0.3325529153
C,0,-0.9697754265,2.7601743753,1.1167312104
C,0,-0.7303426523,2.2418727078,-1.2273883158
H,0,-0.8169698598,2.3734826019,2.1276631937
H,0,-2.0032074846,3.1480348775,1.0498589689
H,0,-0.2938002675,3.6084374272,0.9767216231
H,0,-1.7326026179,2.6076327256,-1.5114333917
H,0,-0.0332390658,3.0784269435,-1.3254491383
H,0,-0.6810770617,-2.8753090595,-0.3649291441
H,0,-0.4930935603,-0.6194376216,-1.3017370463
H,0,-0.4150910831,1.4787539689,-1.9393062821
C,0,1.7814307626,-0.3902781316,-0.4690284686
O,0,1.6666628101,-0.1647074933,-1.6610994374
N,0,2.957903652,-0.3201505941,0.2206107805
C,0,4.1854772872,-0.0343423481,-0.5045050405
C,0,3.0947202591,-0.6098417049,1.639938115
H,0,3.9468427281,0.1517654603,-1.5482937453
H,0,2.1177324604,-0.6561314722,2.1097818141
H,0,4.6783996212,0.8487476993,-0.0833791246
H,0,4.8794672313,-0.8809768808,-0.4389665451
H,0,3.6115981708,-1.5647531649,1.7986558311
H,0,3.6825948824,0.180160427,2.1188626272