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Theoretical and experimental study of molecular structure and vibrational spectra of *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide

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Abstract *N*-(2-Pyridylmethyl)-2-pyrazinecarboxamide was prepared and its crystal structure was investigated by X-ray analysis. The compound crystallizes in the triclinic space group $P\bar{1}$ with $a = 4.262(3)$, $b = 12.117(9)$, $c = 20.840(18)$ Å, $\alpha = 91.802(6)$, $\beta = 89.834(7)$, $\gamma = 91.845(6)°$, $V = 1075.2(16)$ Å^3, $Z = 4$, and $D = 1.323\,\mathrm{Mg/m^3}$. The structure was solved by direct method and refined to $R = 0.0699$ and $wR_2 = 0.1268$ by full matrix anisotropic least-squares method. Using the *Hartree-Fock* and density functional method (*B*3*LYP*) with 6-31G(d) basis set, the molecular geometry and vibrational frequencies of the title compound has been investigated and compared with experimental ones from experimental studies. The optimized bond lengths obtained by R*HF* method and bond angles obtained by *B*3*LYP* method show better agreement with the experimental values. The vibrations computed of the title compound by the R*HF* and DFT methods are in good agreement with the observed IR spectra data.

Keywords *Ab initio*; IR spectra; *N*-(2-Pyridylmethyl)-2-pyrazinecarboxamide; Vibrational assignment.

Introduction

The peptide group –C(O)NH– is an important construction unit in chemistry and biology [1, 2]. Consequently, a large variety of pyridine amide ligands have been synthesized for investigating their metal-binding properties [3–6], for providing models from the standpoint of bioinorganic chemistry [7, 8], for use in catalysis [9], and as molecular receptors [10, 11]. In order to understand the structure-activity relationships of proteins, it is desirable to undertake a systematic study of the molecular structure of pyridinecarboxamides, which serve as model systems, and note the effect of varying intra- and intermolecular interactions. In this context, *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide was chosen as an example of a carboxamide for experimental and theoretical investigation.

With the recent development in computer hardware and software it is possible to correctly describe physiochemical properties of relatively small molecules with nearly chemical accuracy using classical ab initio methods based on self-consistent field molecular orbital *Hartree-Fock* theory (SCF-MO *HF*) [12–17]. On the other hand, density functional theory (DFT) calculations are reported to provide excellent vibrational frequencies of organic molecules if the calculated frequencies are scaled to compensate for the approximate treatment of electron correlation, for basic set deficiencies and for the anharmonicity [18–25]. In a systematic study, *Rauhut* and *Pulay* reported the vibrational spectra of 31 molecules by using the *B*3*LYP*/6-31G(d) method [26]. In their work, they have calculated vibrational frequencies of 20 smaller molecules whose experimental

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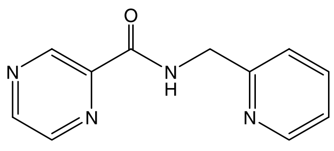

Scheme 1

vibrational frequencies are well assigned, and derived transferable scaling factors by using a least-square method. The scaling factors have been successfully applied to other eleven larger molecules. Thus, vibrational frequencies calculated by using the *B*3*LYP* functional with 6-31G(d) basis could be utilized to eliminate the uncertainties of the fundamental assignments in the infrared and *Raman* spectra [27].

In this work, we synthesized *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide, Scheme 1, and determined its crystal structure, ^{13}C, ^{1}H NMR, and IR spectra. By using the R*HF* and DFT (*B*3*LYP*) methods, we also calculate geometric parameters and vibrational frequencies of *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide in the ground state to distinguish the fundamental from the experimental vibrational frequencies and geometric parameters. These calculations are valuable for providing insight into the molecular parameters, and the vibrational spectra.

Results and discussion

Crystal structure analysis

A single crystal of *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide was obtained from slow diffusion of diethyl ether into a dichloromethane solution at room temperature. The molecular structure with the atomic numbering is shown in Fig. 1. Selected bond lengths, bond angles, and torsion angles are summarized in Table 2. The asymmetric unit of the crystal contains two separate molecules. Since both parts of the asymmetric unit have the same structure, here according to geometric position of two pyridine and pyrazine rings connected to CH_2, we choose one of these two separate moieties in the same geometric position resulted from theoretical calculations. The unit cell-packing diagram of the title compound is presented in Fig. 2. From this packing diagram, the intermolecular bond distances and angle confirms hydrogen bonding formation between two adjacent molecules. As can be seen from the packing diagram in Fig. 2, intermolecular N–H···N (H2b···N1^{i} = 2.26(2), N2···N1^{i} = 3.01(1) Å and N2-H2b···N1^{i} = 142.1(3)°; H6c···N5^{ii} = 2.32(3), N6···N5^{ii} = 3.09(1) Å and N6-H6c···N5^{ii} = 141.0(2)°) hydrogen bonds (symmetry codes: (i) $-x$, $-y$, $1-z$ and (ii) $2-x$, $-y$, $1-z$) link the molecules to form ten-membered rings. These intermolecular hydrogen bonds seem to be an effective factor in the stabilization of the crystal structure. There is also some intramolecular N–H···N (H2b···N4 = 2.38(2), N2···N4 = 2.79(1) Å, and N2–H2b···N4 = 108.2(2)°; H6c···N8 = 2.30(2), N6···N8 = 2.71(1) Å, and N6–H6c···N8 = 107.1(2)°) hydrogen bonds that link two molecules. In the title compound, the pyridine ring (N1/C1–C5) and pyrazine ring (C8–C9/N3/C10–C11/N4) are, of course, planar and the dihedral angles between them are 61.94°. The bond lengths and angles are within normal ranges.

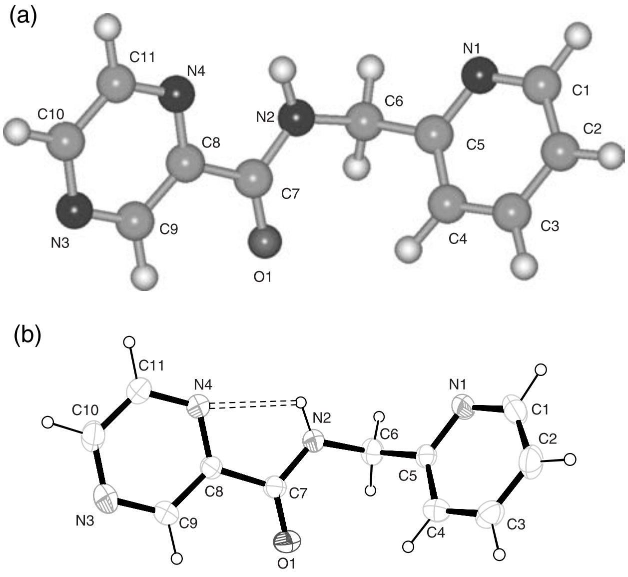

Fig. 1 (a) Optimized geometry of the *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide and (b) thermal ellipsoid plot (30% probability level) showing the numbering scheme. Dashed lines denote the intramolecular hydrogen bond

Computational study

The experimental and optimized geometric parameters (bond lengths, bond angles, and torsion angles) by R*HF* and DFT with 6-31G(d) as the basis set are listed in Table 2. As can be seen from this

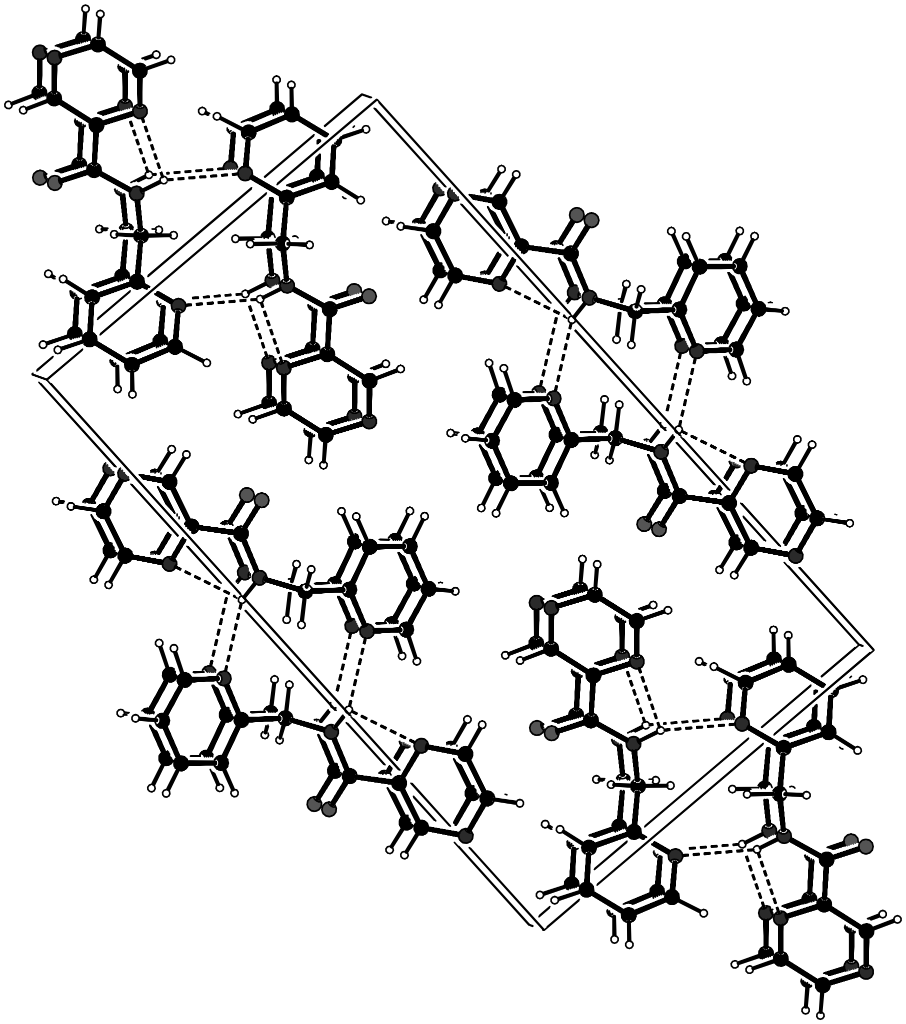

Fig. 2 A view of *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide along the *a* direction, showing two adjacent molecules linked by intermolecular hydrogen bonds (dashed lines)

table the calculated values are in good agreement with the experimental values. It is to be noted that calculated data were for the gaseous phase and experimental results were obtained for the solid phase. The title molecule contains two planar rings; a pyridine ring (atoms; N1, C1, C2, C3, C4, and C5) and a pyrazine ring (atoms; N3, N4, C8, C9, C10, and C11). The bond angles of C1–N1–C5, C8–N4–C11, and C9–N3–C10 were determined at 117.8(2), 114.9(2), and 114.8(2)° angles were calculated at 118.4, 117.3, and 117.0 for R*HF*, and at 117.8, 116.5, and 116.2° for *B*3*LYP*. The C–N bonds were observed/calculated at: 1.332(3)/1.320 (for R*HF*), 1.341 Å (for *B*3*LYP*) and 1.324(4)/1.317 (for R*HF*), 1.338 Å (for *B*3*LYP*) for C8–N4 and C10–N3 in pyrazine ring and 1.340(3)/1.324 (for R*HF*), 1.341 Å (for *B*3*LYP*) C5–N1 in the pyridine ring in two different methods. The observed C=O bond length (1.224(3) Å) is also in agreement with the calculated one (1.205 Å for R*HF* and 1.231 Å for *B*3*LYP*). It is well known that R*HF* methods underestimate some bond lengths [28–31]. The correlation between the experimental and calculated geometric parameters from different methods is shown in Fig. 3. The optimized geometric parameters obtained by the two methods are similar. Owing to our calculations, between methods considered (R*HF* and *B*3*LYP*) a reasonable accuracy have been achieved with R*HF*/6-31G(d) method/basis set for the bond lengths (Table 2 and Fig. 3a). For the bond angles, the DFT method correlates slightly better than the R*HF* method. The vibrational bands as-

Table 1 Crystallographic and structure refinement data

Formula	$C_{11}H_{10}N_4O_1$
Formula weight	214.23
Temperature/K	293(2)
Wavelength λ/Å	0.71073
Crystal system	Triclinic
Space group	$P\bar{1}$
Crystal size/mm^3	$0.40 \times 0.06 \times 0.03$
a/Å	4.262(3)
B/Å	12.117(9)
c/Å	20.840(18)
α/°	91.802(6)
β/°	89.834(7)
γ/°	91.845(6)
V/$Å^3$	1075.2(16)
Z	4
$D_{calc}/g \cdot cm^{-3}$	1.323
θ ranges for data collection/°	1.68–29.41
$F(000)$	448
Absorption coefficient μ/mm^{-1}	0.091
Index ranges	$-4 \leq h \leq 5$ $-16 \leq k \leq 16$ $-28 \leq l \leq 28$
Data collected	12957
Unique data (R_{int})	5641, (0.0713)
Observed data ($I > 2\sigma(I)$)	5641
Parameters, restrains	369, 0
Final R_1, wR_2[a] (obs. data)	0.0699, 0.1268
Final R_1, wR_2[a] (all data)	0.1163, 0.1436
Goodness of fit on F^2 (S)	1.166
Largest diff peak and hole/e.$Å^3$	0.192, −0.152

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma(w(F_o{}^2 - F_c{}^2)^2)/\Sigma w(F_o{}^2)^2]^{1/2}$

Table 2 Optimized and experimental geometries of the title compound

Parameters	X-Ray analysis	Calculated	
		R*HF*/ 6-31G(d)	*B*3*LYP*/ 6-31G(d)
Bond lengths/Å			
C(5)–N(1)	1.340(3)	1.324	1.341
C(7)–N(2)	1.345(3)	1.339	1.354
C(8)–N(4)	1.332(3)	1.320	1.341
C(10)–N(3)	1.324(4)	1.317	1.338
C(7)–O(1)	1.224(3)	1.205	1.231
Bond angles/°			
C(1)–N(1)–C(5)	117.8(2)	118.4	117.8
C(2)–C(1)–N(1)	124.4(3)	123.6	123.7
C(5)–C(6)–N(2)	114.7(2)	112.6	113.3
C(6)–C(5)–N(1)	116.5(2)	116.1	116.4
C(7)–C(8)–C(9)	119.4(2)	119.6	119.7
C(8)–C(7)–O(1)	119.6(2)	120.3	121.0
C(8)–N(4)–C(11)	114.9(2)	117.3	116.5
C(9)–N(3)–C(10)	114.8(2)	117.0	116.2
N(2)–C(7)–O(1)	125.3(2)	124.5	124.6
Dihedral angles/°			
C(1)–N(1)–C(5)–C(6)	179.9(2)	178.8	179.6
C(7)–C(8)–N(4)–C(11)	−178.8(2)	−179.8	−179.7
C(5)–C(6)–N(2)–C(7)	96.6(3)	90.7	93.6
C(6)–N(2)–C(7)–C(8)	175.2(2)	176.7	179.0
C(7)–C(8)–C(9)–N(3)	178.8(2)	179.9	179.8
C(9)–C(8)–C(7)–O(1)	−0.9(3)	−1.6	−1.8
N(2)–C(7)–C(8)–N(4)	−2.0(3)	−2.5	−2.5
N(4)–C(8)–C(7)–O(1)	177.8(2)	178.2	177.9

signments were made by using the *Gauss*-View molecular visualization program [16]. We calculated the theoretical vibrational spectra of *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide. We compared these calculations with their experimental results and these frequencies are listed in Table 3. To make comparison with experiment, a correlation graph is presented in Fig. 4. The correlation coefficients between the calculated and experimental vibration frequencies are both higher than 0.999 for R*HF* and DFT methods. As can be seen from Table 3, the C=O vibration was calculated by using the R*HF* and *B*3*LYP* method with 6-31G(d) basis set at 1936 and 1762 cm^{-1}. The experimental C=O stretching was observed in 1669 cm^{-1}. The C–H vibrations of the title compound are between 2980 and 3240 cm^{-1}, Table 3. The calculated C–H vibrations are in the same range – especially in the *B*3*LYP* theoretical level – and there is a good agreement between theoretical and experimental values. The NH_2 stretching has been calculated at 3880 and 3594 cm^{-1} with R*HF* and *B*3*LYP* methods Table 3. According to experimental vibration of NH_2 at 3465 cm^{-1}, it is clear that there is better agreement with the DFT method in this frequency range.

In conclusion, the molecular structure of *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide was determined by X-ray structure analysis and computation by using R*HF* and *B*3*LYP* with 6-31G(d) basis set. The optimized bond lengths obtained by R*HF* and bond angles obtained by DFT show better agreement with the experimental values. The vibrations of the *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide computed by the R*HF* and DFT methods are in good agreement with the experimental IR spectra values, but the *B*3*LYP* method gave a better fit to experimental frequencies.

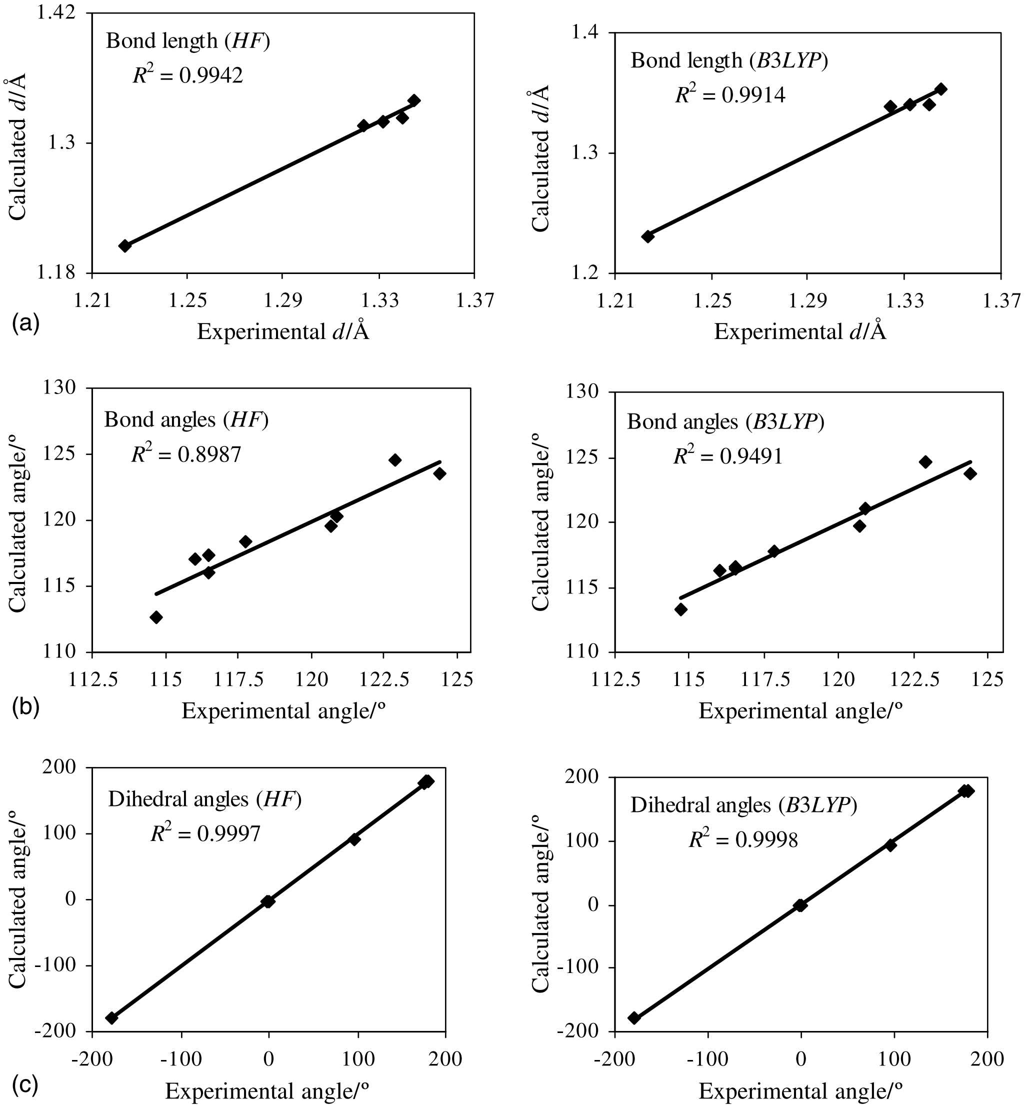

Fig. 3 Correlation graphs of experimental (from X-ray diffraction analysis) and calculated (from R*HF*/6-31G(d) and *B3LYP*/6-31G(d) levels) molecular bond lengths (a), molecular bond angles (b), and molecular dihedral angles (c) of *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide

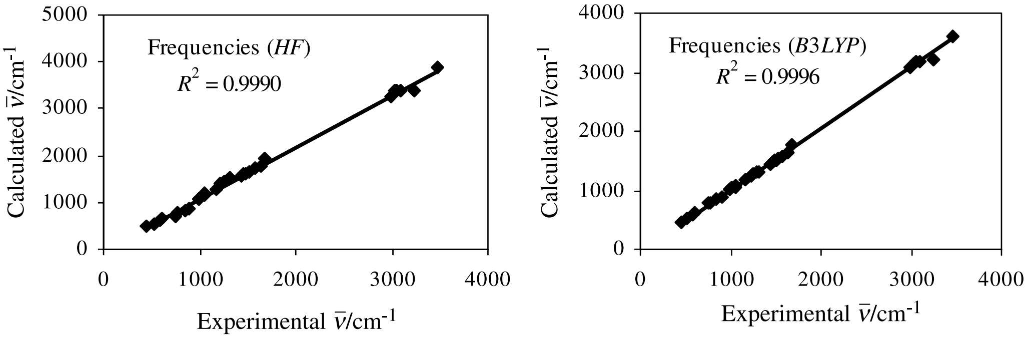

Fig. 4 Correlation graphs of experimental and calculated frequencies (from R*HF*/6-31G(d) and *B3LYP*/6-31G(d) levels) of the *N*-(2-pyridylmethyl)-2-pyrazinecarboxamide

Table 3 Comparison of the experimental and calculated vibrational frequencies ($\bar{\nu}/\text{cm}^{-1}$) of the title compound

Assignment	Experimental IR (KBr)	Calculated	
		HF(6-31G(d))	*B3LYP*(6-31G(d))
N–H str.	3465	3880	3594
Ring $_{\text{pyrz}}$ C–H sym. str.	3240	3402	3200
Ring $_{\text{py}}$ C–H asym. str.	3096	3395	3193
Ring $_{\text{pyrz}}$ C–H asmy. str.	3064	–	3182
Ring $_{\text{py}}$ C–H asmy. str.	3056	3372	3172
CH_2 asym. str.	3023	3369	3146
CH_2 sym. str.	2987	3274	3092
C=O str.	1669	1936	1762
Ring $_{\text{py}}$ C–C,C–N str.	1639	1784	1648
C–N $_{\text{py}}$ str. + N–H rock.	–	1771	1592
N–H rock.	1573	1730	1574
Ring $_{\text{py}}$ C–H rock.	1518	1662	1525
Ring $_{\text{pyrz}}$ C–H rock.	1515	1657	1513
CH_2 sei.	1482	1628	1493
Ring $_{\text{py}}$ C–C str. + C–H rock.	1461	1607	1481
Ring $_{\text{pyrz}}$ C–C str. + C–H rock.	1438	1567	1442
CH_2 twist	1384	–	1398
Ring $_{\text{py}}$ C–H rock. + CH_2 rock.	1349	–	1361
Ring $_{\text{Pyrz}}$ C–H rock. + CH_2 rock.	1319	1533	1326
Ring$_{\text{py}}$ C–N str. + Ring$_{\text{py}}$ N–H rock. + CH_2 rock.	1286	1468	1310
N–H rock. + CH_2 rock.	1249	1432	1272
Ring$_{\text{pyrz}}$ C–N str. + Ring$_{\text{py}}$ N–H rock. + CH_2 rock.	1220	1391	1251
Ring$_{\text{pyrz}}$ C–H rock. + N–H rock.	1166	1295	1194
Ring$_{\text{pyrz}}$ C–H rock.	1054	1192	1085
CH_2 rock. + C–N (NH_2) rock.	1048	1139	1048
Ring$_{\text{pyrz}}$ bend.	1020	1127	1040
Ring$_{\text{py}}$ C–C str. + C–N rock. + CH_2 rock.	999	1095	1014
Ring$_{\text{py}}$ C–H twist	993	1075	1001
Ring$_{\text{pyrz}}$ C–H bend.	897	868	880
Ring$_{\text{py}}$ C–H bend. + C–C str.	839	844	851
Ring$_{\text{py}}$ C–H bend. + C–C str.	774	796	794
Ring$_{\text{py}}$ C–H bend. + C–N str.	752	692	771
Ring$_{\text{py}}$ bend. + N–H wag.	610	671	620
N–H bend.	590	623	604
CH_2 wag. + Ring$_{\text{py}}$ wag.	526	520	534
Ring$_{\text{pyrz}}$ bend.	443	514	461

Experimental

Materials and instruments

All chemicals were purchased from Merck and Aldrich. Infrared spectra (4000–250 cm^{-1}) of solid sample were taken as 1% dispersion in KBr pellets using a Shimadzu-470 spectrometer. ^{1}H NMR spectra were recorded on a Bruker AC-300 MHz spectrometer operating in the quarter mode. Melting point was obtained by a *Kofler* Heizbank *Reichart* type 7841 melting point apparatus and corrected. The elemental analyses were performed using a Heracus CHN–O-Rapid analyzer.

N-(2-Pyridylmethyl)-2-pyrazinecarboxamide ($C_{11}H_{10}N_4O_1$)

A solution of 1.02 cm^3 2-(aminomethyl)pyridine in 10 cm^3 pyridine was added to a solution of 1.24 g pyrazine-2-carboxylic acid in 10 cm^3 pyridine. The resulting solution was stirred at 40°C for 20 min, then 2.6 cm^3 triphenyl phosphite was added dropwise, and the reaction mixture was stirred at 100°C for 5 h and at ambient temperature for 24 h. A brown solution resulted, which after volume reduction yielded a brown oil. This was taken up in chloroform, washed 3 × with H_2O, 5 × with saturated Na_2CO_3, and 4 × with H_2O. The resulting solution was dried ($MgSO_4$), filtered, and the solvent removed. The resultant light brown oil was taken up in a small amount of $CHCl_3$ and added dropwise to ice-cold diethyl ether with vigorous stirring. The mixture was stirred in an ice bath for 2 h. A white solid resulted with a yield of 80%, mp 145°C. X-ray quality crystals were obtained by slow diffusion of diethyl ether into a CH_2Cl_2 solution at room temperature. ^{1}H NMR (300 MHz, $CDCl_3$): $\delta = 4.81$ (d, $J = 5.3$ Hz, CH_2), 7.24 (m, 1H), 7.35 (m, 1H), 7.70 (m, 1H), 8.61 (m, 2H), 8.76 (m, 1H), 8.86 (s, NH), 9.44 (m, 1H) ppm; ^{13}C NMR (300 MHz, $CDCl_3$): $\delta = 163.2$, 156.1, 149.3, 147.3, 144.5, 144.4, 142.8, 137.0, 122.6, 122.1, 44.5 ppm.

Crystal structure determination and refinement of N-(2-pyridylmethyl)-2-pyrazinecarboxamide

The X-ray diffraction measurements were made on a STOE IPDS-II diffractometer with graphite monochromated Mo–K_α radiation. A colorless needle crystal with a dimension of $0.40 \times 0.06 \times 0.03$ mm was mounted on a glass fiber and used for data collection. Cell constants and an orientation matrix for data collection were obtained by least-squares refinement of diffraction data from 5641 unique reflections. Data were collected at a temperature of 293(2) K to a maximum 2θ value of 58.82° and in a series of ω scans in 1° oscillations and integrated using the Stoe X-AREA [32] software package. The numerical absorption coefficient, μ, for Mo–K_α radiation is 0.091 mm^{-1}. A numerical absorption correction was applied using X-RED [33] and X-SHAPE [34] software's. The data were corrected for *Lorentz* and polarizing effects. The structures were solved by direct methods [35] and subsequent difference *Fourier* map and then refined on F^2 by a full-matrix least-squares procedure using anisotropic displacement parameters [35]. All of the hydrogen atoms were located in a difference *Fourier* map and then after refined isotropically. Subsequent refinement then converged with *R* factors and parameters errors significantly better than for all attempts to model the solvent disorder. Atomic factors are from International Tables for X-ray Crystallography [36]. All refinements were performed using the X-STEP32 crystallographic software package [37]. A summary of the crystal data, experimental details and refinement results is given in Table 1. Full crystallographic details are deposited with Cambridge Structural Database (CCDC No. 664358). Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK.

Computational procedure

All calculations were carried out by using Gaussian-98 (R-A.9) software [16]. In order to obtain local minima geometries of the title molecule in the ground state (*in vacuo*), two different *ab initio* methods, *HF* [38, 39] and *B3LYP* [40] were employed with 6-31G(d) basis set [41]. All initial geometries were assumed as *C1* point group with no special symmetry constraints imposed. Two sets of vibrational frequencies for these species were calculated with these methods for 298.15 K and 101.3 kPa with global minimum conformation. Gaussian program defaults were used as appropriate optimization criteria.

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