ORIGINAL PAPER

Synthesis, Molecular Structure and DFT Study of 2-(*N*-Benzoylbenzamido)pyridine-3-yl benzoate

Çiğdem Yüksektepe · Canan Kazak · Cem Özdoğan · Ziya B. Güvenç · Orhan Büyükgüngör · Figen Arslan · Mustafa Odabaşoğlu

Received: 12 June 2010/Accepted: 28 May 2011/Published online: 11 June 2011 © Springer Science+Business Media, LLC 2011

Abstract The biologically important 2-amino-3-hydroxypyridine reacts with benzoyl chloride to give 2-(N-benzoylbenzamido)pyridine-3-yl benzoate. This synthesized compound has been studied by elemental analysis, X-ray crystallography and also theoretically by density functional theory (DFT) framework with B3LYP/6-311++G(d, p)level of theory. The molecules of this compound crystallize in the orthorhombic space group of $P2_12_12_1$ and the crystal packing involves both hydrogen-bonding and C-H $\cdots\pi$ interaction. The vibrational normal modes of the molecular structure are investigated by ab initio method for both infrared intensities (IR) and for Raman activities. Furthermore, the corresponding assignments are discussed. Hydrogen and carbon atoms of the benzene rings are found to be highly active. Also, experimentally obtained IR spectrum is presented and compared with the available

Ç. Yüksektepe (⊠)

Department of Physics, Faculty of Science, Cankiri Karatekin University, 18100 Ballica, Cankiri, Turkey e-mail: yuksekc@yahoo.com; yuksektepe.c@karatekin.edu.tr

C. Kazak · O. Büyükgüngör Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayis University, 55139 Kurupelit, Samsun, Turkey

C. Özdoğan · Z. B. Güvenç

Department of Materials Science and Engineering, Faculty of Engineering and Architecture, Cankaya University, 06530 Balgat, Ankara, Turkey

F. Arslan Department of Chemistry, Faculty of Arts and Sciences, Karabuk University, Karabuk, Turkey

M. Odabaşoğlu

Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayis University, 55139 Kurupelit, Samsun, Turkey theoretical data. Experimentally and theoretically obtained IR spectrum are in good agreement.

Keywords Crystal structure · DFT calculation · Pyridylbenzoate · Benzoylaminopyridyne

Introduction

2-Amino-3-hydroxypyridines have been the focus of a great deal of attention [1-10]. 3,4-Dihydro-2H-1,4-benzoxazine-2-carboxylatederivatives are often found embedded in compounds exhibiting a wide range of biological activities [11-15]. Ethyl 3,4-dihydro-2H-1,4-benzoxazine-2-carboxylate derivatives andethyl 3,4-dihydro-2H-pyrido [3,2-b][1,4] oxazine-2-carboxylate derivatives synthesized from 2-amino-3-hydroxypyridine are potential templates for bioactive compounds [1]. In addition, 2-amino-3hydroxypyridine is biologically important in preparation of clinical anti inflammatory analgesics [16]. 2-Amino-3-hydroxypyridineis of interest since its anion chelates metal ions as a bidentate N, O donor form five-member rings. This compound and its derivatives have been also reported as an effective corrosion inhibitors for aluminum and copper [2]. Because of the importance of 2-amino-3-hydroxypyridines in industry as raw materials, intermediate and finished products, their biological properties and use in variety of chemical researches, 2-amino-3-hydroxypyridine derivatives are synthesized and their spectroscopic properties reinvestigated.

In this work, we investigated the crystallographic and molecular structure of 2-(N,N-dibenzoylamino)-3-pyr-idylbenzoate synthesized on the expectation that the N,N,O-threebenzoyl derivatives of 2-amino-3-hydroxypyr-idine should have similar properties with those mentioned

above. The experimental infrared spectrum for this sample is also obtained and compared with the theoretical findings. We are not aware of any other experimental data to compare for the reported vibrational modes. We believe that our detailed quantum chemical study will aid in clarifying the experimentally obtained data.

Results and Discussion

X-Ray Crystallography

A suitable single crystal was mounted on a glass fiber and data collection was performed on a STOE IPDSII image plate detector using Mo K α radiation ($\lambda = 0.71073$ Å). Details of the crystal structure are given in Table 1. Data collection and cell refinement: Stoe X-AREA [17]. Data reduction: Stoe X-RED [17]. Molecular drawings: ORTEP-III and PLATON [18, 19]. Software used to prepare this material for the publication: WinGX [20].

The structure was solved by direct-methods using SHELXS-97 [21] and anisotropic displacement parameters were applied to non-hydrogen atoms in a full-matrix least-squares refinement based on F^2 using SHELXL-97 [21]. All carbon hydrogens were positioned geometrically and refined by a riding model with U_{iso} 1.2 times that of attached atoms. 1800 Friedel pairs were averaged before the final refinement.

Computational Procedure

All calculations were carried out by solving the Kohn– Sham equations in the DFT framework. We have employed the generalized gradient approximations (GGA) using the functionals of Becke's three-parameter hybrid exchange functional [22] and the Lee–Yang–Parr (LYP) non-local correlation functional [23].

The appropriateness of the DFT based quantum chemical studies for calculation of geometries, total energies, fundamental normal modes (in terms of infrared-absorption intensities and Raman-scattering activities) to serve as an indirect probe for the experimental studies is discussed in the literature [24, 25]. The suitability of the GGA and LDA (Local Density Approximations) methods for the aimed physical and chemical properties and importance of the polarization basis functions and well converged wave functions are outlined in these studies. In the present study, 6-311++G(d, p) basis set is employed in order to optimize the geometry. This size of basis set (diffuse functions together with polarization functions) fulfills the necessary requirements. Since the used basis set is large and results as $O(N^4)$ computation expense (with N is the system size), the starting geometry for a long lasting optimization procedure should represent a better point on the potential energy surface. In order to fulfill this requirement, we applied three-stage procedure for all of our calculations. First, relatively small 6-31G basis set was employed for a linear (tight self consistent field (SCF) convergence criteria) search for local minima on the potential energy surface of the system to obtain reliable initial guesses and reasonable geometries. Second, starting from these equilibrium structures, the stable method [26, 27] was used to establish a stable wave function but using the larger 6-311++G(d, p)basis set. Finally, geometry optimization, natural bond orbital (NBO) analysis (NBO 3.1 version included into Gaussian package [28]) and frequency calculations (a procedure to evaluate the vibrational normal modes) were performed. Both of the infrared intensities and Raman activities are reported since some of the infrared inactive vibrations (because of the lack of change in dipole moment) are active in Raman spectroscopy because Raman activity is associated with the polarizability of the molecule, and infrared is associated with the change of a dipole moment. The experimental infrared spectrum for this sample is also obtained and reported. We are not aware of any other experimental data to compare for the reported vibrational modes, we believe that the presented detailed quantum chemical study will aid in clarifying the experimental data available. Quadratically convergent SCF procedure was used for the optimization at the B3LYP/6-311++G(d, p) level of theory. The vibrational frequencies, calculated at the same level, were used for the characterization of stationary points and for zero-point energy (ZPE) corrections. The zero-point vibrational energy ZPVE (or ZPE) results from the vibrational motion of the molecular systems even at 0 K and is calculated from a harmonic oscillator model as a sum of contributions from all the vibrational modes of the system. Most partition function formulae assume that the zero of energy is the energy of the ground state of the studied system $(E_{TOTAL} = E_{ELEC})$ $_{\text{TRONIC}}$ + E_{ZPE}). All the stationary points were positively identified for the minima (no imaginary frequency) or transition states (only one imaginary frequency) or higherorder saddle points (more than one imaginary frequency). All of the obtained molecular orbitals (Highest Occupied Molecular Orbital; HOMO and Lowest Unoccupied Molecular Orbital; LUMO) are depicted at the same level of theory (see Fig. 3). Chemcraft [29] program is made use of for analyzing the outputs of the Gaussian package and also for drawing MO energy levels, HOMO-LUMO pictures and NBO analysis with dipole moment figures; namely 3 and 4. Computations were carried out using the program package Gaussian-03 [28] installed on our parallel computing laboratory (linux cluster with ×86 CPUs at Cankaya university) and because of the time complexity, Linda package was utilized for parallel computations.

Description of the Crystal Structure

The compound (1) crystallizes in the orthorhombic, space group of $P2_12_12_1$ with unit cell parameters a = 8.9054(3) Å, b = 11.8974(5) Å, c = 20.2347(8) Å, $\alpha = \beta = \gamma = 90^{\circ}$. The title compound contains pyridine, phenyl, ester (O–C=O) and amide (N–C=O) moieties. Details of crystal parameters, data collection, structure solution and refinement are given in Table 1 and the crystal structure with the formula, $C_{26}H_{18}N_2O_4$ (1) shown in Fig. 1. The central sixmember pyridine ring is essentially planar, to within 0.0008 Å. The dihedral angles between the pyridine ring

 Table 1 Crystallographic data of the title compound (1)

Chemical formula	$C_{26}H_{18}N_2O_4$
Formula weight	422.42
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a (Å)	8.9054(3)
b (Å)	11.8974(5)
c (Å)	20.2347(8)
α (°), β (°), γ (°)	90.00
Unit cell volume V $(\text{\AA})^3$	2143.89(15)
Z	4
Calculated density D _x (Mg/m ³)	1.309
Electron number (F ₀₀₀)	880
Linear absorption coefficient μ (mm ⁻¹)	0.089
Crystal colour, shape	Colourless, prism
Crystal dimensions (mm)	$0.58 \times 0.51 \times 0.46$
X-ray and wavelength	Μο Κα, 0.71073
Data collection temperature, T (K)	296
R _{int}	0.1536
h, k, l intervals (°)	$-10 \rightarrow 10, -14 \rightarrow 14,$ $-24 \rightarrow 24$
θ_{\max} (°)	25.99
Data collection device	STOE IPDS II
Data collection method	ω scan
Reflections with $(I > 2\sigma(I))$	2093
Measured reflections	30114
Independent reflections	2402
Used programs	Wingx, SHELXS–97, SHELXL–97, ORTEP III
Structure refinement	Full matrix (F ²)
Weight function	$1/[\sigma^{2}(F_{o}^{2}) + (0.0599P)^{2} + 0.0106P],$ P = (F_{o}^{2} + 2F_{c}^{2})/3
Parameter number refined	289
R, R _W (I > σ (I))	0.033, 0.089
S	1.130
$\Delta \rho_{\min}, \Delta \rho_{\max} \ (e/Å^3)$	-0.150, 0.091



Fig. 1 An ORTEPIII [8] view of the title compound, showing the atom numbering scheme, 20% probability displacement ellipsoids

A(N1 through C5), phenyl rings B(C7 through C12), C(C14 through C19) and D(C21 through C26) are equal to 79.27(11)° (A/B), 69.52(07)° (A/C), 72.87(08)° (A/D), 77.68(09)° (B/C), 36.70(12)° (B/D) and 89.93(07)° (C/D). Selected bond lengths and angles are listed in Table 2. The C=O bond distances of ester and amide groups are almost the same, with C6-O2 being 1.198(3) Å, C13-O3 being 1.213(2) Å and C20–O4 being 1.207(2) Å, all of which are lower than those reported earlier, such as 1.244(10) Å [30], 1.235(2) Å [31], 1.218(2) Å [32] and 1.238(6) Å [33]. As can seen in Table 2, due to substituent groups, the bond lengths of N2-C13 and N2-C20 of amide group are slightly differ from those found in related amide groups (1.356(6) and 1.369(3) Å) [33, 34]. On the other hand, the C–O bond distance of ester group is 1.368(3) Å and this bond distance is in good agreement with those found in related structures including ester group, such as 1.353(3) Å [35] and 1.360(2) Å [32]. The bond angles of O3–C13–N2, O4–C20– N2 and O1–C6–O2 are 119.3(2)°, 119.4(2)° and 121.5(2)°, respectively. Other bond lengths and bond angles in the phenyl rings and pyridine ring conform with literature values [36, 37].

In the crystal packing, there exist inter and intra molecular C-H···O hydrogen bonding and C-H··· π interaction. In the intermolecular hydrogen bonding, the atom C4 of pyridine ring in the molecule at (x, y, z) acts as hydrogen-bond donor, via atom H4, to atom O3 of the amide group at (x - 1, y, z) (see Fig. 2), resulting in the formation of a nearly linear C4-H4···O3ⁱ hydrogen bond (see Table 3). This intermolecular hydrogen bond forms a C(8) graph-set chain [38], viz. C4-H4···O3-C13-N2-C1-N1-C5, running along the [100] and [-100] directions. Eventually, as shown in Fig. 2, adjacent molecules are linked by intermolecular C-H···O hydrogen bonding and C-H··· π interaction to one another.

Table 2 Selected bond lengths (Å) and angles (°) of compound (1)

	Experimental	Calculated
Bond lenghts (Å)		
C1-N1	1.323(3)	1.328
C5-N1	1.345(3)	1.335
C1-N2	1.429(2)	1.427
C13-N2	1.416(2)	1.437
C20-N2	1.424(3)	1.434
C201	1.393(2)	1.390
C601	1.368(3)	1.374
C6–O2	1.198(3)	1.206
C13-O3	1.213(2)	1.210
C20-O4	1.207(2)	1.211
Bond angles (°)		
C2C1N1	123.1(2)	122.0
C5-N1-C1	116.9(2)	118.9
C2C1N2	119.9(2)	120.9
C1-N2-C13	119.3(2)	118.3
C1-N2-C20	115.5(2)	116.7
C13-N2-C20	119.1(2)	118.5
C21-C20-N2	117.3(2)	117.5
N1C1N2	116.9(2)	117.2
O3-C13-N2	119.3(2)	120.0
O4-C20-N2	119.4(2)	120.3
O1-C6-O2	121.5(2)	22.7
Torsion angles (°)		
O3-C13-N2-C1	142.8(2)	133.5
O3-C13-N2-C20	-8.5(3)	-17.6
O4-C20-N2-C13	135.3(2)	135.9
O4-C20-N2-C1	-17.1(3)	-15.7
C14-C13-N2-C20	169.9(2)	159.7
C1-N2-C20-C21	158.6(2)	160.3
C201C6C7	169.9(2)	178.0
C1C2O1C6	-94.2(2)	-99.1
C2-O1-C6-O2	-8.5(3)	2.2
N1-C1-N2-C20	112.1(2)	120.1
C2-C1-N2-C13	140.4(2)	148.1

Density Functional Study

As mentioned in computational procedure, in addition to the crystal structure from X-ray experiment, the molecular geometry, spectroscopic properties, and frontier molecular orbital analysis of the title compound have been calculated by using the B3LYP/6-311++G(d, p) quantum chemical method. Some selected geometric parameters experimentally obtained and theoretically calculated by B3LYP/6-311++G(d, p) method are listed in Table 2. We noted that the experimental results belong to solid phase and theoretical calculations belong to gaseous phase. In the solid state, the existence of the crystal field along with the intermolecular interactions have connected the molecules together, which result in the differences of bond parameters between the calculated and experimental values. As a result, as can be seen in Table 2, the optimized bond lengths, bond angles and torsion angles obtained by B3LYP method are in good agreement with the experimental values. In addition to Table 2, the C–C distance in phenyl groups and the pyridine C–C distance are calculated as of 1.389–1.401 and 1.384–1.401 Å ranges, respectively.

The calculated zero-point vibration energy (ZPE) correction is found to be 10.3712 eV. The ground state of the system used in the total energy calculation is singlet and the electronic state of the system is ¹A. The highest occupied molecular orbital (HOMO) energies, the lowest unoccupied molecular orbital (LUMO) energies, the energy gap for mentioned molecule in above have calculated. The calculated HOMO-LUMO gap of molecule is 0.18295 eV. This small gap value shows that this system is chemically reactive since the larger HOMO-LUMO gap generally refers to a higher value of the chemical hardness. The molecular orbital pictures for the HOMO-LUMO are depicted in Fig. 3. The obtained values for the orbital energies from HOMO-1 to HOMO-5 are very close to each other and could be interpreted as nearly degenerate. This degeneracy in HOMO levels could also explain the small HOMO-LUMO gap. The calculated dipole moments (with field-independent basis, Debye) are -2.4447, -2.5657, 2.5307 and 4.3548 for x, y, z directions and in total magnitudes, respectively (see Fig. 4).

In terms of NBO analysis, the effective valance electron configuration (natural electron configuration) promoted configuration of sp³ hybridization for the carbon atoms, configuration of sp⁴ hybridization for the nitrogen atoms, and configuration of s²p⁵ hybridization for the oxygen atoms. The second order perturbation theory analysis of Fock matrix in NBO basis of the alpha spin orbitals reports donor-acceptor (bond-antibond) interactions and that suggests the existence of multi-centered bonds. This can be concluded as the delocalization of the electrons. This delocalized and multi-centered π bonding nature of the chemical bonding can be also seen from the molecular orbital pictures in Fig. 3. Accepted Lewis structure by the NBO analysis demonstrates the number of occupied BD bonds (2-center bonds) as 68 and occupied LP bonds (lone pair) as 10. The charges found from an electrostatic fit are reported as; all the hydrogen atoms have positive values while the oxygen and nitrogen atoms have negative charges, and both positive and negative charge values are for the carbon atoms. There are three double BD bonds in the hexagons as in the order of single BD and double BD bonds (see benzene rings in Fig. 4). Three oxygen atoms have made bonding only with a carbon atom and these are also double BD bonds.

Fig. 2 The packing of crystal, viewed along the b axis. Dashed lines indicate hydrogen bonds. Symmetry code (i): -1 + x, *y*, *z*, Cg(4) ring: C21 through C26



Table 3 Hydrogen bond interactions of compound (1) (Å, °)

D–H···A	D–H	H···A	D····A	D−H…A
C4–H4····O3 ⁱ	0.930	2.450	3.107(2)	128.0
C15–H15…O2	0.930	2.420	3.333(3)	167.0

Symmetry code: (i) -1 + x, y, z

All the calculated frequencies identify the stationary points since there is no imaginary frequency found. The obtained spectrums for infrared intensities and Raman activities are given in Fig. 5. The bands are broadened with Lorentzian broadening (band width of half-height is 48.43). The experimental infrared spectrum is given as inset of the figure and the first twelve frequencies having the highest

MO energy levels (Alpha MOs)

Fig. 3 Obtained molecular orbitals (the energy values in vertical axes are in Hartree and numbers in the squares show the number of the occupied states at the molecular energy levels) and HOMO–LUMO pictures



Fig. 4 The dipole moment and chemical bonding structure obtained by the NBO analysis



Fig. 5 Plots for the calculated infrared intensities and Raman activities with Lorentzian broadening (band width of half-height is 48.43). Experimentally obtained infrared spectrum is given at *inset* of upper panel

transmittance percentages are also given in Table 4. It should be noted that the experimental and calculated data show close resemblance. This could be interpreted as the convenience and suitability of the utilized computational approach. The major peaks for the calculated infrared intensities and Raman activities and corresponding assignments are also given in Table 4. All the presented normal modes are assigned to one of the following motion; C-H stretch, C-O stretch, C-N stretch, H-C-C bend, and H-C-N bend. The most intense peak for the infrared intensities is found at 1255 cm^{-1} (see Fig. 5, upper without Lorentzian broadening and Table 4), this frequency and the other peaks at nearby frequencies correspond to in-plane scissoring and in-plane rocking bending vibrations for H–C–C at benzene rings. The following two peaks (at 1782 and 1753 cm^{-1}) are assigned as C6-O2 and C13-O3/C20-O4 (see Fig. 1 for numbering notation of the atoms) stretching, respectively. The next peak is at the frequency value of 1313 cm⁻¹ and two active modes are observed as in-plane scissoring bending vibration for the H-C-C at benzene rings and C1-N2 stretch. The asymmetric stretching mode is observed at 1324 cm^{-1} in the nitrogen containing benzene rings.

The most intense peak for the Raman activities is observed at 3220 cm⁻¹ and corresponds to C-H stretchings at the benzene rings. This peak and the other peaks nearby to this frequency value (see Table 4) show that hydrogen and carbon atoms in the benzene rings are highly active. The next most intense peak is observed at 1758 cm^{-1} (see Fig. 5, lower without Lorentzian broadening) and is assigned for the C-O stretching (for both C13-O3 and C20-O4, see Fig. 1). This mode is also observed for the infrared intensities. The next peak is at the frequency value of 1295 cm^{-1} and two active modes are observed as in-plane scissoring bending vibration for the H-C-C at benzene rings and C1-N2 stretch. This mode is also observed for the infrared intensities. Another calculated in-plane scissoring bending vibration for the H-C-C at benzene rings is at the frequency value of 1649 cm^{-1} .

Experimental Section

Synthesis of Compound of 2-(*N*-Benzoylbenzamido)pyridine-3-yl benzoate

The compound was synthesized as in Scheme 1 by the following procedure. 2-(*N*-Benzoylbenzamido)pyridine-3-yl benzoate was synthesized using 2-amino-3-hydroxypyridine obtained commercially (Aldrich). A solution of sodium hydroxide(1.8 mmol) in water was added drop wise with stirring to a solution of 2-amino-3-hydroxypyridine (1.8 mmol) in hot water. The mixture was stirred for 1 h and the solvent was removed. The resulting precipitation was dissolved in THF and benzoyl chloride (5.4 mmol) was added drop wise with stirring. The mixture was heated to 60 °C in a temperature controlled bath and

Exp. Freq. (cm ⁻¹)	Trans. (%)	Calculated frequency (cm ⁻¹)	IR intensity (km/mol)	Assignment	Calculated frequency (cm ⁻¹)	Raman activity (Å ⁴ /amu)	Assignment
1232.43	54.35	1255.11	502.44	H-C-C bend	3220.25	306.69	C-H stretch
1020.27	61.07	1782.14	330.61	C-O stretch	3221.01	260.98	C-H stretch
1687.12	62.20	1753.07	310.32	C-O stretch	1758.39	227.11	C-O stretch
1172.64	62.92	1294.55	276.75	H–C–C bend/ C–N stretch	3207.10	163.20	C-H stretch
1044.38	64.29	1199.54	195.14	H–C–C bend	1294.55	159.99	H–C–C bend/ C–N stretch
1054.51	65.02	1267.66	193.06	H-C-C bend	3204.42	158.97	C-H stretch
1287.40	65.37	1312.87	189.89	C-N stretch	3210.87	150.79	C-H stretch
1181.80	66.67	1758.39	162.17	C-O stretch	3195.07	148.11	C-H stretch
1739.19	67.37	1477.51	161.59	H-C-N bend	1649.53	146.99	H-C-C bend
1101.28	69.51	1145.17	152.47	H-C-C bend	3207.72	131.55	C-H stretch
1436.39	70.15	1210.24	135.44	H-C-C bend	3193.51	129.54	C-H stretch
1122.01	70.23	1323.65	101.27	C-N stretch	1647.75	119.26	H-C-C bend

Table 4 Experimentally obtained and calculated infrared intensities and Raman activities and corresponding assignments



Scheme 1 The chemical diagram of 2-(N-benzoylbenzamido)pyridine-3-yl benzoate

stirred for 2 h. The reaction mixture was then cooled to room temperature and the solvent was removed. The resulting white powder was recrystallized in acetonitrile. Yield for the investigated structure is 30%; mp 150 °C. Elemental analysis found as (calculated for $C_{26}H_{18}N_2O_4$): C, 74.05(73.92); H, 4.56(4.29); N, 6.75(6.63).

Conclusions

In conclusion, the *N*,*N*,*O*-threebenzoyl derivative of biologically and industrially important 2-amino-3-hydroxypyridine is synthesized and crystallographic, molecular structure and spectroscopic properties of the compound are investigated in both experimentally and with detailed quantum chemical study. The similarities of the experimental and calculated results for the infrared intensities gives us confidence of the suitability of the applied density function level of theory and the basis set used. The bonding nature of the molecule is mostly due to the delocalized multi-centered π electrons with the exception of one benzene ring. This could also leads to a non-homogeneous charge distribution and resulting dipole moment towards to this benzene ring. The calculated HOMO–LUMO gap is 0.18295 eV with nearly degenerate orbital energies from HOMO-1 to HOMO-5. This small gap value shows that this system is chemically reactive.

Supplementary Data

Crystallographic data (excluding structure factors) for the structure reported in this article have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 777466. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

References

- 1. Aral A, Trousseau F, Guillemot G et al (2002) Tetrahedron 53:8145
- 2. Mostafa SI, Maksoud SAA (1998) Monatshefte für Chemie 129:455
- 3. Zatar NA, Abu-Zuhri AZ, Abu-Shaweesh AA (1998) Talanta 47:883–890

- 4. Kaya I, Koc S (2004) Polymer 45:1743-1753
- 5. Gerber TIA, Luzipo D, Mayer P (2004) J Coord Chem 57:1419–1423
- 6. Woydowski K, Liebscher J (1999) Tetrahedron 55:9205-9220
- 7. Yang QZ, Siri O, Brisset H et al (2006) Tetrahedron Lett 47:5727–5731
- 8. Gillard M, Chatelain P (2006) Eur J Pharmacol 530:205-214
- 9. Boyland E, Sims P (1958) J Chem Soc 4198-4199
- 10. Moore JA, Marascia FJ (1959) J Am Chem Soc 81:6049-6056
- 11. Bourlot AS, Sanchez I, Dureng G et al (1998) J Med Chem 41:3142–3158
- Baurin N, Vangrevelinghe E, Morin Allory L et al (2000) J Med Chem 43:1109–1122
- 13. Baxter EW, Reitz AB (1997) Bioorg Med Chem Lett 7:763-768
- 14. Matsuoka H, Ohi N, Mihara M et al (1997) J Med Chem 40:105-111
- 15. Largeron M, Lockart B, Pfeiffer B et al (1999) J Med Chem 42:5043–5052
- Flouzat C, Bresson Y, Mattio A et al (1993) J Med Chem Bioorg 36:497–503
- 17. Stoe & Cie (2002) X-AREA and X-RED32. Stoe & Cie, Darmstadt
- Burnett MN, Johnson CK (1996) ORTEPIII report ORNL-6895. Oak Ridge National Laboratory, Oak Ridge
- 19. Spek AL (1997) PLATON. University of Utrecht, Utrecht
- 20. Farrugia LJ (1999) J Appl Cryst 32:837-838

- Sheldrick GM (1997) SHELXS97 and SHELXL97. University of Göttingen, Göttingen
- 22. Becke AD (1993) J Chem Phys 98:5648-5652
- 23. Lee C, Yang W, Parr RG (1988) Phys Rev B 37:785-789
- 24. Porezag D, Pederson MR (1996) Phys Rev B 54:7830-7836
- 25. Jackson K (2000) Phys Stat Sol 217:293
- 26. Seeger R, Pople JA (1977) J Chem Phys 66:3045-3050
- 27. Bauernschmitt R, Ahlrichs R (1996) J Chem Phys 104: 9047–9052
- 28. Frisch MJ, Trucks GW, Schlegel HB et al (2004) Gaussian 03, revision C.02. Gaussian, Inc., Wallingford
- 29. http://www.chemcraftprog.com
- 30. Dasari BK, Srikrishnan T (2002) J Chem Cryst 12:499-504
- 31. Bathori NB, Bourne SA (2009) J Chem Cryst 39:539-543
- 32. Mahendra M, Doreswamy BH, Sridhar MA et al (2005) J Chem Cryst 6:463–467
- 33. Shan DH, Dong WD, Qiong JC (2005) J Chem Cryst 11:897-901
- Caleta I, Cincic D, Zamola GK et al (2008) J Chem Cryst 38:775–780
- 35. Jian FF, Wang KF, Zhao PS et al (2006) J Struct Chem 17:539–545
- 36. Ancın N, Öztaş SG, İde S (2007) J Struct Chem 18:667-675
- 37. Tamilvendan D, Prabhu GV, Fronczek FR et al (2010) J Chem Cryst 40(11):981–984
- Bernstein J, Davis RE, Shimoni L et al (1995) Angew Chem Int Ed Engl 34:1555–1573