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Crystal structure and geometry-optimization study of 4-methyl-3′,5′-dinitro-4′-methyl benzylidene aniline

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Abstract

Schiff base 4-methyl-3′,5′-dinitro-4′-methyl benzylidene aniline was synthesized by the condensation of 4-amino-2,6-dinitrotoluene with 4-methylbenzaldehyde. The crystal of the title compound was obtained and it was characterized by X-ray single crystal diffraction analysis, EA, FTIR and ^{1}H NMR. The geometry and normal vibrations have been obtained from the density functional theory (DFT) method with the B3LYP method employing the 6-31G** and 6-311G** basis sets. The calculated results propose that the latter is more accurate to the experimental data. The structural parameters from the theory are close to those of the crystal, and the computational frequencies are in agreement with the experimental data.

Keywords: Crystal structure; Benzylidene aniline; Density functional theory; Geometry-optimization

1. Introduction

Condensation of primary amines with aldehydes or ketones yields Schiff bases containing imine (C=N) function group [1]. Some of these compounds are donor–acceptor benzene derivatives, which can conform conjugated π-electron systems easily, and they are known to exhibit extremely large second-order optical non-linearities, such as 4-nitro-4′-methyl benzylidene aniline (NMBA) [2], 4-nitro-4′-methoxy benzylidene aniline (NMOBA) [3], *N*-2-[3′-(methoxysalicylideneimino) benzyl]-3″-methoxysalicylideneimine [4]. Organic crystals in terms of non-linear optical property possess advantages when compared to their inorganic counterparts, and they have larger structural diversity [5], so the preparation of this kind of materials has gained increasing importance.

With the advance of quantum chemistry method and high performance computers, the structures of some organic compounds can be theoretically predicted in high accuracy. Density functional theory (DFT) method has recently been successfully applied to investigate the structures and predict properties of some compounds [6,7]. Mondal et al. [8] have successfully predicted the properties of the Schiff base of 2-benzyliminiomethylene-4-nitrophenolate, John [9] predicted some structures of benzylidene anilines containing the 4-dimethyl amino group at one end of the molecule and the 4′-nitro group at the other.

In this work, we synthesized 4-methyl-3′,5′-dinitro-4′-methyl benzylidene aniline (MDNMBA) containing the methyl group at one benzene ring of the molecule and two nitro groups at the other, which was alike with NMBA and NMOBA in the molecular structure. We obtained the crystal of MDNMBA, which was also characterized by EA, FTIR, ^{1}H NMR. The geometry and normal vibrations were obtained from the DFT method with the B3LYP method [10,11] employing the 6-31G** and 6-311G** basis sets. All the electronic structure calculations were carried out using GAUSSIAN 98 program [12].

2. Experiment and computational methods

2.1. Synthesis

MDNMBA has been synthesized by the condensation reaction of 4-amino-2,6-dinitrotoluene (ADNT) with 4-methylbenzaldehyde, and the equation of the reaction is shown as follows:

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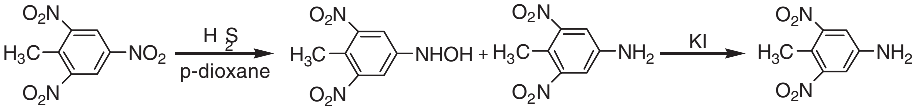
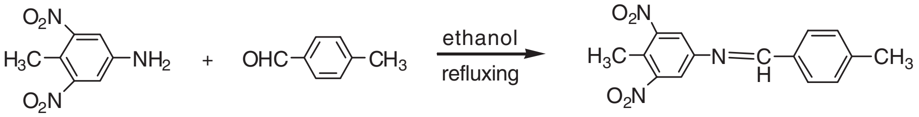
Table 1
Crystallographic and refinement parameters of MDNMBA

Molecular formula	$C_{15}H_{13}N_3O_4$
Formula weight	299.28
Crystal color	Yellow
Size	0.54×0.34×0.24 mm
Crystal system	Monoclinic
Space group	$P2(1)/n$
Unit cell parameters	$a=19.441(4)$ Å
	$b=7.544(1)$ Å
	$c=19.997(3)$ Å
	$\beta=99.68(1)°$
Volume	2891.16(94) $Å^3$
Z	8
$F(000)$	1248
Density (calculated)	1.375 g cm^{-3}
Theta range for data collection	1.35–25.50°
Limiting indices	$0\leq h\leq 23$, $0\leq k\leq 9$, $-24\leq l\leq 23$
Reflections collected	6212
Absorption coefficient	0.102 mm^{-1}
Reflections collected	6212
Data/restraints/parameters	5386/0/400
Independent reflections	5386 [R(int)=0.0162]
Extinction coefficient	0.0068(5)
Final R indices [$I>2\sigma(I)$]	$R1=0.0520$, $wR2=0.1127$
R indices (all data)	$R1=0.1396$, $wR2=0.1340$
Largest diff. peak and hole	0.266 and −0.210 e $Å^{-3}$


Equation 1


Equation 2

The ADNT was prepared by adopting the method of Mehilal et al. [13]. Fifty grams of 2,4,6-trinitrotoluene was dissolved in 100 ml of *p*-dioxane. One millilitre concentrated ammonium hydroxide solution (0.25 ml, four times) was added giving a deep red solution. Hydrogen sulfide gas was bubbled into the stirred solution at a rate sufficient to maintain the temperature below 35 °C, after 1 h H_2S addition was stopped. The precipitated sulfur was filtered and dried giving a mixture of 4-amino-2,6-dinitrotoluene and the partial reduction product 4-hydroxylamino-2,6-dinitrotoluene.

Ten grams of this mixture was suspended in 500 ml of 3 mol L^{-1} hydrochloric acid, 3.12 g of potassium iodide was added, and the stirred solution was heated to reflux. After 1 h an additional 1.56 g KI was added. Following additional half an hour at reflux, the hot solution was filtered to give a clear red solution. The cooled solution was neutralized to pH 8 by addition of concentrated ammonium hydroxide solution. The precipitated yellow solid was filtered and dried.

Recrystallization from methanol gave the pure 4-amino-2,6-dinitrotoluene with the yield ∼58%, m.p. 169–171 °C. IR (KBr): νNH_2: 3478, 3380 cm^{-1}, νNH: 1658 cm^{-1}, νNO_2: 1536, 1352 cm^{-1}.

To a solution of 0.04 mol aldehyde in 100 ml ethanol was added a solution of 0.04 mol amine in 75 ml ethanol. The resulting solution was boiled under reflux for 3 h, then concentrated and cooled in an ice bath until crystallization was observed, which was the title compound. The yellow solid was suction filtered, dried and recrystallized from dichloromethane–methanol with the yield 86%, m.p. 147–149 °C. IR (KBr): νC=N: 1632 cm^{-1}, νNO_2: 1602, 1533, 1362 cm^{-1}. ^1H NMR (acetone): 8.77 ppm (s, 1H, HC=N), 8.05 ppm (s, 2H, Ar-H), 7.90 ppm (d, 2H, Ar-H), 7.39 ppm (d, 2H, Ar-H), 2.52 ppm (s, 3H, CH_3), 2.43 ppm (s, 3H, CH_3). Elemental analysis for MDNMBA: calcd: C 60.20, H 4.35, N 14.05; found: C 59.91, H 4.49, N 14.06.

2.2. Physical measurements

FTIR spectra for MDNMBA were recorded by KBr pellet technique between the range of 400 and 4000 cm^{-1} using Bruker Equinox 55 FTIR spectrometer. ^1H NMR spectra were obtained with acetone as solvent and internal TMS as standard using an AV400 spectrometer. Elemental analysis of C, H and N were carried out on a Perkin–Elmer 2400 (USA)

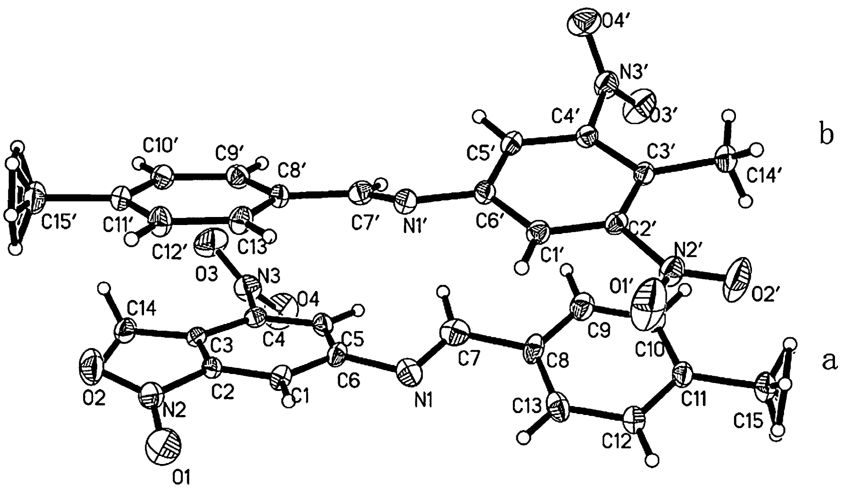


Fig. 1. The ORTEP view of the molecular structure of MDNMBA.

microanalyzer. Single crystal X-ray diffraction analysis was performed for MDNMBA crystal using a Siemens P4 four-circle diffractometer with graphite monochromatized Mo K_α radiation ($\lambda = 0.71073$ Å) at 296(2) K using ω scan mode. The crystals suitable for X-ray diffraction analysis were obtained from a saturated solution of dry acetone. Crystallographic and refinement parameters are given in Table 1. The structure was solved by direct methods. Anisotropic displacement parameters were applied to all non-hydrogen atoms in full-matrix least-squares refinements based on F^2. All hydrogen atoms were calculated using a riding model. ORTEP view of the molecular structure of the title compound is given in Fig. 1, which shows the experimental geometry of MDNMBA. The crystallographic-information-file (CIF) has been deposited with the Cambridge Crystallographic Database Center as a supplementary publication No. CCDC 282113.

2.3. Computational methods

Geometry optimization and frequency analysis of 4-methyl-2′,6′-dinitro-4′-methyl benzylidene aniline were performed using the B3LYP hybrid density functional method of theory with the 6-31G** and 6-311G** basis sets. Here, B3LYP denotes the combination of the Becke's three parameter exchange with the Lee–Yang–Parr (LYP) correlation functional. All the electronic structure calculations were carried out using the GAUSSIAN 98 program packages.

3. Results and discussion

3.1. Molecular and crystal structure

From the molecular structure, it is found that there are two crystallographically independent but structurally very similar molecules in the unit cell of the title compound, and the selected bond distances, bond angles of the two molecules are given in Tables 2 and 3, respectively. The hydrogen of CH_3 are different for C14 and C15. The sites of H atoms of C14 methyl are ascertained, while those of C15 methyl are unascertained, and the occupancy of every site is 0.5.

From the data of the crystal, the N–O bond lengths in all the nitro groups are around the normal N–O double bond in nitro group (about 1.20 Å) [14]. The lengths of C–C bond in benzene ring are as normal length, and all of the C–N bond lengths except for N1–C7 are in the range of 1.46–1.48 Å and are around the normal C–N single bond which is referred to 1.47 Å, while the bond length of N1–C7 is 1.189 or 1.244 Å, which is smaller than those of N3–C4 and N2–C2, showing that the bond between N1 and C7 is double bond.

The endocyclic angles have a rule that if the C of the benzene ring has methyl substitute it has smaller angles (less than 120°) than that has nitro group substitute (more than 120°) [15]. For the title compound, the endocyclic angles of C1–C2–C3 (about 124°) and C3–C4–C5 (about 125°) are larger than those of C2–C3–C4 (about 112°) and C10–C11–C12 (about 118°), which is expected due to the nitro groups attraction affect and the methyl repulsion affect.

From the crystal data, it is found that the two N atoms of the two nitro groups are almost co-planar to the benzene ring, and the largest torsion angle is only 2.6°. The two C atoms of the two methyl groups at the two ends of the molecule are also co-planar to the benzene ring, and the largest torsion angle is 4.0°.

Table 2
Selected bond distances (Å) of crystal data and theoretical calculations of MDNMBA

Distance	MDNMBA-a	MDNMBA-b	B3LYP/ 6-31G**	B3LYP/ 6-311G**
O(1)–N(2)	1.180(3)	1.165(3)	1.229	1.222
O(2)–N(2)	1.202(3)	1.169(3)	1.229	1.222
O(3)–N(3)	1.204(4)	1.203(3)	1.220	1.222
O(4)–N(3)	1.218(4)	1.230(3)	1.230	1.222
N(1)–C(7)	1.189(4)	1.244(3)	1.280	1.270
N(1)–C(6)	1.462(4)	1.428(3)	1.390	1.390
N(2)–C(2)	1.483(4)	1.473(4)	1.470	1.480
N(3)–C(4)	1.468(4)	1.476(4)	1.470	1.480
C(3)–C(14)	1.500(4)	1.504(4)	1.510	1.500
C(7)–C(8)	1.529(4)	1.469(4)	1.460	1.460
C(11)–C(15)	1.512(4)	1.503(4)	1.500	1.500

Table 3
Selected bond angles (°) of crystal data and theoretical calculations of MDNMBA

Angles	MDNMBA-a	MDNMBA-b	B3LYP/6-31G**	B3LYP/6-311G**
C(7)–N(1)–C(6)	116.2(4)	118.0(3)	120.04	120.38
C(2)–C(1)–C(6)	120.1(3)	120.7(3)	120.34	120.28
C(1)–C(2)–C(3)	124.8(3)	124.3(3)	124.23	124.28
C(1)–C(2)–N(2)	114.8(3)	115.4(3)	114.97	115.04
C(3)–C(2)–N(2)	120.4(3)	120.4(3)	120.79	120.66
C(4)–C(3)–C(2)	112.4(3)	112.4(3)	113.22	113.22
C(4)–C(3)–C(14)	122.7(3)	121.7(3)	123.43	123.48
C(2)–C(3)–C(14)	124.8(3)	125.8(3)	123.18	123.16
C(5)–C(4)–C(3)	125.0(3)	125.3(3)	124.24	124.25
C(5)–C(4)–N(3)	115.5(3)	115.2(3)	114.83	114.87
C(3)–C(4)–N(3)	119.5(3)	119.4(3)	120.92	120.86
C(6)–C(5)–C(4)	118.9(3)	119.7(3)	124.24	120.23
C(1)–C(6)–C(5)	118.8(3)	117.6(3)	117.64	117.64
C(1)–C(6)–N(1)	116.0(3)	118.0(3)	118.22	118.28
C(5)–C(6)–N(1)	124.9(3)	124.2(3)	124.06	123.98
N(1)–C(7)–C(8)	120.0(4)	122.4(3)	122.89	122.98
C(9)–C(8)–C(13)	119.4(3)	118.2(3)	118.81	118.76
C(9)–C(8)–C(7)	117.7(4)	119.4(3)	119.48	119.54
C(13)–C(8)–C(7)	122.9(4)	122.4(3)	121.70	121.68
C(10)–C(11)–C(12)	118.5(3)	118.2(3)	118.27	118.24

For most of the benzylidene anilines, the central four atoms of C–C=N–C is almost co-planar [16–18], which is the same with the title compound, and the torsion of C6–N1–C7–C8 for molecular a and b are both 176.2°.

As a rule, the aromatic ring containing the donor group is essentially co-planar with the central –C=N-double bond with typical torsion angles of 5–10°, however, the ring containing the acceptor group is twisted by around 30–50° from the C–C=N–C plane, such as the four polymorphs of 4-(*N*, *N*-dimethyl-amino) benzylidene-4′-nitroaniline [16,17], which is in agreement with the crystal data of the title compound. For molecular a and b the angles between the C–C=N–C plane and the C1–C6 benzene ring are 33.6 or 31.1°, the torsion angles of C7–N1–C6–C1 are 151.0 or 152.4°, C7–N1–C6–C5 are 35.4 or 33.3°, while the angles between the C–C=N–C plane and the C8–C13 benzene ring for molecular a and b are 7.2 or 8.6°, the torsion angles of N1–C7–C8–C9 are 172.4 or 170.9°, N1–C7–C8–C13 are 8.4 or 9.6°.

The plane of C1–C6 benzene ring for molecular a is almost in parallel with that of C8–C13 benzene ring for molecular b, and the angle is 2.9°, and the distance of the two planes is 3.444 Å, which is in the range of π–π stacking interaction (3.3–3.7 Å) [19], may be the existence of π–π stacking interaction benefits for the formation of the crystals.

3.2. Computational results and discussion

The calculated data of selected bond distances, bond angles of MDNMBA are given in Tables 2 and 3, respectively. It is found that the computation results obtained at B3LYP/6-31G** and B3LYP/6-311G** level of theories are similar, but on the whole the latter is closer to the data of the crystal structure from the experiment.

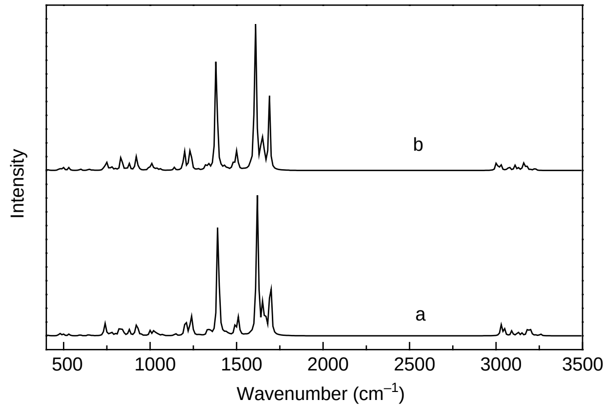


Fig. 2. The calculated FTIR spectra of MDNMBA, a and b are the calculated results by using B3LYP/6-31G** and B3LYP/6-311G** level of theory, respectively.

It is found that the bond lengths and bond angles have subtle differences between the data obtained at B3LYP/6-311G** level and the average values of crystal, in which all bond distances deviate by less than 0.055 Å, and the largest bond-angle error is 3.280°.

The calculated results obtained at B3LYP/6-311G** level predict that the angles of C11–C2–C2, C2–C3–C4, C3–C4–C5, C4–C5–C6 and C5–C6–C1 are 120.38, 124.28, 113.22, 124.25, 120.23 and 117.64°, which is in agreement with the rule of endocyclic angles mentioned above.

The computational results show that C3, N2 and N3 are co-planar to the aniline ring, and C15 is co-planar to the aldehyde ring. The four atoms of C6, N1, C7 and C8 are almost co-planar (176.81°), and the aldehyde ring is almost co-planar to the C6–N1–C7–C8 axis (N1–C7–C8–C9 179.10°, and N1–C7–C8–C13 0.97°), and the aniline ring is twisted from the C6–N1–C7–C8 plane (C7–N1–C6–C1 143.74°, and C7–N1–C6–C5 39.65°), which is in line with the data of the crystal, therefore, the DFT calculations can give a remarkably good description of the molecular geometry.

Vibrational frequencies were calculated using two levels of theories for MDNMBA. The predicted IR spectra using B3LYP/6-31G** and B3LYP/6-311G** level of theory

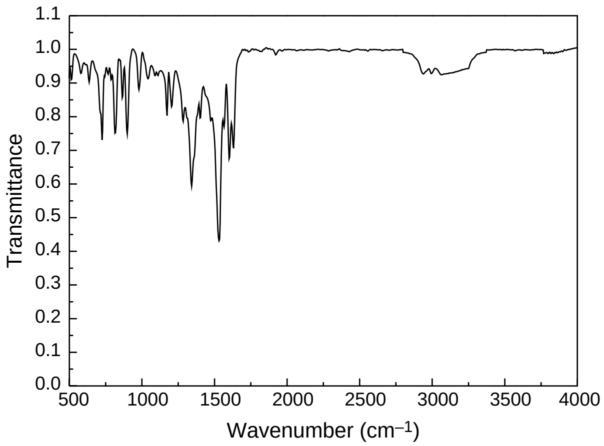


Fig. 3. FTIR spectra of MDNMBA.

for MDNMBA are shown in Fig. 2 a and b, respectively. Comparing the two methods, we can find that B3LYP/6-311G** method is more accurate to predict the experimental IR spectra, which is shown in Fig. 3 so the predicted frequencies and intensities for MDNMBA are listed in Table 4 at the B3LYP/6-311G** level of theory. All theoretical frequencies reported here are listed as calculated, as no scale factor is available for the B3LYP method with the 6-311G** basis set. We assigned the main vibrational frequencies of some main function groups.

Aromatic nitro compounds have strong absorptions due to the asymmetric and symmetric vibrations of the NO_2 group. From Table 4, it is found that the absorption bands at 1608 and 1379 cm^{-1} can be designated to asymmetric stretching and

Table 4
Selected vibrational assignment of MDNMBA based on the B3LYP/6-311G** frequencies and assignment

ν	Energy (cm^{-1})	Intensity	Assignment
1	27.8	0.16	τC15H$_3$
2	52.3	0.23	τN2O$_2$ (twist.), τN3O$_2$ (twist.)
3	128.8	2.96	δC7–N1
4	178.4	0.98	γring1
5	202.1	3.98	γring2
6	214.7	7.53	γC7–N1, γring1
7	350.4	1.67	δC3–C14, δC11–C15
8	471.7	1.50	γN2O$_2$ (wag.), γN3O$_2$ (wag.), γring1
9	484.3	8.66	δring1, δring2
10	500.5	9.72	γring1, γring2, γC7–N1
11	531.0	10.60	γring2
12	645.9	5.29	τring1, γC6–N1, δring2
13	732.9	6.99	τring2
14	746.5	40.76	δring1, δN2O$_2$ (sciss.), δN3O$_2$ (sciss.)
15	777.6	9.43	γN3O$_2$ (wag.), δring2, γC1–H, γC5–H
16	784.0	4.12	γring1, γN2O$_2$ (wag.)
17	832.8	31.45	γC9–H, γC10–H, γC12–H, γC13–H
18	834.5	38.56	δN2O$_2$ (sciss.), δN3O$_2$ (sciss.), δring1, δring2
19	878.5	25.34	δC7–N1, δring2, γC1–H, γC5–H
20	918.3	40.93	γC1–H, γC5–H, δring1, νC2–N2, νC4–N3
21	924.8	24.93	γC1–H, γC5–H
22	966.0	1.07	γC9–H, γC10–H, γC7–H
23	994.8	14.85	δring1, δring2, δC6–N1
24	1009.4	21.78	δC15H$_3$ (rock.)
25	1017.7	6.38	γC7–H
26	1035.2	9.02	δring2, δC9–H, δC10–H, δC12–H, δC13–H
27	1043.9	3.60	δC14H$_3$ (rock.)
28	1139.4	10.77	δC9–H, δC10–H, δC12–H, δC13–H
29	1197.3	85.17	δC9–H, δC10–H, δC12–H, δC13–H
30	1227.6	59.78	δring1, δring2, δC7– C8, δC6–N1, δC7–N1
31	1237.4	44.16	δring2, δC1–H, δC5–H
32	1319.2	14.64	δring1, δring2, δC7– C8, δC6–N1
33	1335.9	21.56	δring2, δC7–C8
34	1379.5	351.94	ν_sN2O$_2$, ν_sN3O$_2$, νC2–N2, νC4–N3
35	1387.5	146.77	ν_sN2O$_2$, ν_sN3O$_2$, νC2–N2, νC4–N3
36	1404.7	12.25	δC7–H
37	1430.1	8.64	δring1, δC1–H, δC5–H, δC7–H, δC14–H$_3$ (sciss.)
38	1477.9	16.79	δC14–H$_3$ (sciss.)
39	1495.8	13.24	δC15–H$_3$ (sciss.)
40	1502.6	74.16	δring1, νC6–N1, δC14–H$_3$ (sciss.)
41	1578.8	10.58	δring1, δC6–N1
42	1604.9	136.69	νC7–N1, δring2
43	1608.5	471.52	ν_aN2O$_2$, ν_aN3O$_2$, δring1, δring2
44	1616.9	78.30	ν_aN2O$_2$, ν_aN3O$_2$, δring1
45	1645.9	166.18	νC7–N1, δring1, δring2
46	1661.0	44.81	νC7–N1, δring1, δring2
47	1689.2	272.27	νC7–N1, δring1, δring2
48	3003.6	38.02	νC7–H
49	3026.8	26.30	νC15–H$_3$
50	3109.3	18.01	ν_aC15–H$_3$
51	3128.2	9.26	ν_aC14–H$_3$

ring1, aniline ring; ring2, aldehyde ring; ν, stretching; δ, in-plane bending; γ, out-of-plane bending; τ, torsion; s, symmetry; a, asymmetry; rock., rocking; sciss., scissoring; twist., twisting; wag., wagging. For numbering of atom refer Fig. 1.

symmetric stretching of the nitro groups, and the bands at 1604, 1645 and 1689 cm^{-1} are assigned to the stretching of C=N, and the bands above 3000 cm^{-1} (3003, 3026, 3109, and 3128 cm^{-1}) are designated to the C–H stretching.

From above analysis, we can conclude that the vibrational frequencies are identical on the whole between theoretical calculation and the experimental result, and the calculated data could offer the theoretical bases.

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