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Synthesis, spectral analysis, X-ray structure characterization and biological evaluation of *N*, *N'*-bis (*p*-nitrophenylmethylene) Hexane 1,6-diamine as potential antioxidant Schiff base compound

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Abstract
The title compound have been synthesized and characterized by routine MS, IR and NMR spectrometry methods. Single crystal X-ray diffraction analysis showed that *N*,*N'*-bis(4-nitrophenylmethylene)hexane-1,6-diamine compound crystallized in monoclinic $P2_1/c$ space group with a = 6,1569(7)Å, b = 5,0751(5)Å, c = 30,631(4) Å, β = 94,509(7)° and z = 2. Crystal data were collected using Enraf-Nonius CAD4 X-ray diffractometer with monochromatic Kα radiation of Cu (λ = 1.54187Å). The structure was solved by direct methods and refined on F^2 by full-matrix least-squares procedures to the final R1 of 0,152, using SHELXL programs. Crystalline network cohesion of this compound was essentially assured by C-H···O hydrogen bounds and dipole-dipole type interactions. Biological investigation carried out according DPPH and ABTS methods, revealed that this compound had antioxidant activity.

Keywords: Schiff base, spectrometry, DFT, X-ray diffraction, C-H···O hydrogen bound, antioxidant activity

1. Introduction
In the last years, Schiff base ligands and complexes [1] have been studied extensively and have received considerable attention because of their variety of applications in physical, biochemical, analytical and industrial fields. Schiff base compounds played an important role in the development of coordination chemistry [2–3], and were currently attracting the attention of medicinal chemist [4]. Indeed, many studies have been reported regarding the biological activities of Schiff bases, including their anticancer, antibacterial, antifungal, antimalaria, antiproliferative, antiinflammatory, antiviral, antipyretic and herbicidal activities [5-9].
It is well known now that oxidative stress is the main cause of several diseases such as cancer, cataract, amyotrophic lateral sclerosis, acute pulmonary distress syndrome, pulmonary edema and accelerated aging [10], or is the factor that increases the occurrence of multifactorial diseases such as, Alzheimer's disease, rheumatism, cardiovascular disease and diabetes [11].This alarming situation of the devastating effects of oxidative stress requires the scientific community to intensively search for new highly effective antioxidant molecules.
Versatile Schiff bases, in addition to their wide range well known biological activities, can be a source of new molecules that possess excellent antioxidant properties. As several authors [12-13], our systematic structural and biological activities research on this kind of compound led us to synthesize many Schiff bases. The present work dealed with spectral analysis, X-ray diffraction characterization and antioxidant activity of *N*,*N'*-bis(*p*-nitrophenylmethylene) hexane-1,6-diamine compound.

2. Materiel and methods
2.1. Experimental
Synthesis
Para-nitrobenzaldehyde (0.4 mmol) and hexane-1,6-diamine (0.2 mmol) were dissolved in ether (30 ml). At room temperature, the mixture was stirred for three days to give a white

precipitate. The precipitate obtained was filtered and washed several times in methanol. Recrystallization in methanol was done several time to get pure *N, N'*-bis (phenylmethylene) hexane-1,6-diamine product showed in Figure 1 (Rf: 0.57 in hexane/acetone (50;50), yield: 60%, mp 198.6 °C). Colorless single crystals were obtained by slow evaporation of acetone solution after 7 days.

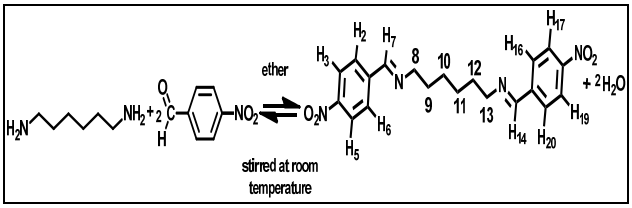

Fig 1: Way of title compound synthesis

2.2. X-ray crystal determination

Three dimensional intensity data were collected on Enraf-Nonius CAD4 diffractometer using graphite monochromatized Cu-Kα radiation (λ= 1.54187 Å). The structure showed in Figure 2, was solved by direct methods and refined on F^2 by full-matrix least-squares procedures using the SHELXL [14] programs. All the non-hydrogen atoms were refined using isotropic and later anisotropic thermal parameters. The hydrogen atoms were included in the structure factor calculation at idealized positions by using a riding model, but not refined. Images were created with ORTEP [15]. The Crystallographic data are listed in Table **1**.

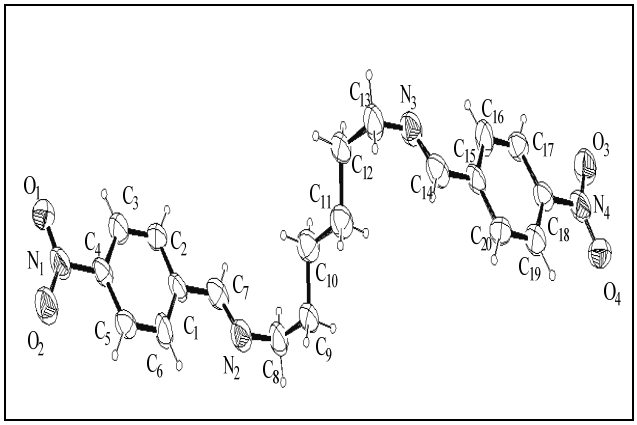

Fig 2: Molecular structure of title compound with atomic numbering scheme (Displacement ellipsoids are drawn at 30% probability level)

Table 1: Crystal data collection and structure refinement parameters

Empirical formula: $C_{20}H_{22}N_4O_4$	**2295 observed reflexions**
Formula weight: 382.41	690 independante reflexions
Temperature : 293K	128 parameters, F(0 0 0) : 360
X-ray: Cu Kα ; λ = 1.54197Å	Index ranges (h, k, l) -5~5 ; -3~4 ; -27~27
Crystal system: Monoclinic	Theta range for data collection: 2.9°-≤ θ ≤ 43°
Space group : $P2_1/c$	Absorption coefficient (μ) : 0.78 (mm-1)
a = 6.1569 (7)Å	Goodness of fit : 1.49
b =5.0751 (5)Å	Refinement on F^2
c =30.631 (4)Å	Final R indices [$I > 2\sigma(I)$]: R1 = 0.152 wR2 = 0.215
β = 94.509 (7)°	R indices (all data) : R1 = 0.427 wR2 = 0.351
V = 954.36 (17)Å^3	Maximum; minimum Δρ (eÅ^{-3}) : 0.34; -0.31
D_{calc} = 1.331 Mgm^{-3}	Enraf-Nonius CAD-4 diffractometer
Z = 2	Structure determination: SHELXS 97

Where $\boldsymbol{w = 1/[\sigma^2(F_o^2) + (0{,}1216P)^2]}$ with $\boldsymbol{P = (F_o^2 + 2F_c^2)/3}$

2.3. Protocols of antioxidant activity tests

*** Test with DiPhenyl-1-PicrylHydrazyl (DPPH)**

2,2-diphenyl-1-picrylhydrazyl was one of the first free radicals used to study structure-antioxidant activity relationship of phenolic compounds [16-18].

****Principle**

Reduction of the free radical DPPH by an antioxidant can be followed by UV-Visible spectrometry, by measuring the decrease in absorbance at 517nm caused by the antioxidants [19]. In the presence of free radical traps, purple-colored DPPH is reduced to yellow 2,2-diphenyl-1-picrylhydrazine [20].

****Dosage**

DPPH radical traping activity was measured according to the protocol described by Lopes-Lutz *et al*. [21] and Athamena *et al*. [22].100µL of each methanolic solution of the pure compound at different concentrations (0.0625-1 mg / mL) were added to 2.5mL of the methanolic solution of DPPH (0,025g/l). In parallel, a negative control is prepared by mixing 100µl of methanol with 2.5ml of the methanolic solution of DPPH. Absorbance reading was made against a blank prepared for each concentration at 517nm after 30 minutes of incubation in the dark and at room temperature. The positive control was represented by a solution of a standard antioxidant ascorbic acid, whose absorbance was measured under the same conditions as the samples and for each concentration [23].

The results were expressed in inhibition percentages (I%) of free radical using the following formula:

I% = [(Abs of con neg - Abs sample) / Abs of con neg] x 100

I%: Percentage of DPPH inhibition.

Abs Sample: Absorbance of the sample.

Abs of con neg: Absorbance of negative control

***Test with 2,2'-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid) (ABTS)**

The radical ABTS method is one of the most tests used for determining the concentration of free radicals. It is based on the neutralization of a radical - cation resulting from the monoelectronic oxidation of the 2,2'-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid) synthetic chromophore ($ABTS^{\bullet}$):

$$ABTS \longrightarrow ABTS^{\cdot+} + e^-$$

This reaction was followed spectrophotometrically by variation of the absorption spectrum [24].

****Dosage**

The radical cation ABTS was generated by mixing, at equal volume, 2.6 mM of potassium persulfate solution ($K_2S_2O_8$) and 7mM of stock solution of ABTS. The mixture was kept away from light and at room temperature for 16 hours before being used [25]. The solution obtained was diluted in methanol, 1ml of ABTS+ solution diluted in 60ml of methanol to obtain an absorbance between 1 and 1.5 at 734 nm. 2.9 ml of this freshly prepared solution were added to 0.1ml of pure compound solution and was read at 734nm after 30 min for each analyzed series. In parallel, a negative control (methanol solution of ABTS+) was carried out under the same conditions. Trolox was used as standard. The final result was expressed in micrograms of Trolox equivalents [26].

The percentage inhibition is calculated according to the following formula:

Inhibition percentage (%) = [(Abs of con neg - Abs sample)] / (Abs of con neg)] x 100

Abs of con neg: Absorbance of the negative control.

Abs sample: the absorbance of the sample [27].

3. Results and Discussion

3.1. Mass spectrometry

ESI Mass Spectrum of the title compound showed a peak at *m/z* 383.1731 $[M + H]^+$, which allowed to propose $C_{20}H_{22}N_4O_4$ as empirical formula.

3.2. IR spectroscopy

On the IR spectrum appeared a characteristic band at 1643cm^{-1}, corresponding to the elongation vibration of azomethine function($\upsilon_{C=N}$). The wide band localized between 2900-2800 cm^{-1}, corresponded to the υ_{C-H} of the cyclohexane moiety and aromatic rings. It should also be noted that the spectrum also showed a characteristic band around 1344 cm^{-1} corresponding to υ_{C-N}.

3.3. NMR spectroscopy

DFT theoretical method was used for indexing the NMR spectra. From optimised geometry of *N, N'*-bis (phenylmethylene)cyclohexane-1,2-diamine compound, calculations of the ^1H and ^{13}C chemical shifts at GIAO/B3LYP/6-31G(d,p) levels of theory were performed and reported in Table **2** with the experimental ones.

Table 2: Comparative table of theoretical / experimental chemical shifts

	^1H (δ, ppm) experimental	**^1H (δ, ppm) theoretical**	**^{13}C (δ, ppm) experimental**	**^{13}C (δ, ppm) theoretical**
atom Number				
1	-	-	146,44	140,51
2	7,98 ; *m*	7,88	126,14	130,14
3	8,30 ; *m*	8,97	121,33	123,36
4	-	-	139,27	148,17
5	8,30 ; *m*	8,95	121,33	123,48
6	7,98 ; *m*	9,03	126,14	125,98
7	8,50 ; *s*	8,80	155,92	156,70
8	3,64 ; *m*	4,20	59,33	69,13
9	1,65 ; *m*	2,29	28,12	36,65
10	1,39 ; *m*	2,12	24,65	33,36
11	1,39 ; *m*	2,02	24,65	32,84
12	1,65 ; *m*	2,31	28,12	30,94
13	3,64 ; *m*	4,60	59,33	62,21
14	8,50 ; *s*	8,88	155,92	153,46
15	-	-	146,44	141,07
16	7,98 ; *m*	9,05	126,14	125,40
17	8,30 ; *m*	8,98	121,33	123,43
18	-	-	139,27	148,07
19	8,30 ; *m*	8,99	121,33	123,31
20	7,98 ; *m*	7,89	126,14	130,08

A good agreement between the experimental NMR data and the theoretical study on chemical shifts seemed corroborated. We can therefore argue that, the title compound structure correspond to *N,N'*-bis (4-nitrophenylmethylene) hexane-1,6-diamine.

3.4. X-ray analysis

With the low crystallographic parameter values a = 6.1569(7) Å and b = 5.0751(5) Å, the title compound structure in $P2_1/c$ space group accommodated with an unusual length of 30.631(4) Å for the crystallographic axis c. This feature was described by Gavezzoti *et al*. as **γ** type structural mode **[28]**. Moreover, this compound, with *Z*=2, crystallized with half-molecule in the asymmetric unit. Some selected geometric parameters such as bond lengths, valence angles and torsion angles are grouped in Table 3.

Table 3: Selected bond lengths and angles (Å, °)

O_1-N_1	1.230 (8)	N_2-C_7-C_6	121.8 (9)
N_1-O_2	1.215 (8)	C_7=N_2-C_8	116.6 (9)
N_1-C_3	1.485(10)	O_2-N_1-O_1	124.2 (9)
C_1-C_2	1.395(12)	O_2-N_1-C_3	119.3 (8)
C_3-C_2	1.342(10)	O_1-N_1-C_3	116.5 (8)
C_3-C_4	1.402(11)	C_5-C_6-C_1	120.2 (11)
C_4-C_5	1.399(12)	C_5-C_6-C_7	120.7 (10)

C_6-C_5	1.358(11)	C_1-C_6-C_7	119.1 (9)
C_6-C_1	1.391(11)	C_2-C_3-C_4	122.4 (10)
C_7-C_6	1.499(12)	C_2-C_3-N_1	121.2 (9)
C_7-N_2	1.260(9)	C_4-C_3-N_1	116.3 (9)
N_2-C_8	1.459 (9)	C_5-C_4-C_3	118.0 (9)
C_9-C_8	1.501(10)	C_6-C_5-C_4	120.3 (9)
C_9-C_{10}	1.535(12)	C_6-C_1-C_2	120.4 (9)
C_{10}-$C_{10'}$	1.524(16)	C_3-C_2-C_1	118.6 (9)
N_2- C_7-C_1-C_2	171,85 (4)	C_8-C_9-C_{10}	111.6 (7)
N_2- C_7-C_1-C_6	-9.49 (3)	N_2-C_8-C_9	111.5 (8)
C_7-N_2-C_8-C_9	116,65(3)	$C_{10'}$-C_{10}-C_9	113.7 (9)

Analysis of Table 3 showed that for the aromatic nuclei, the carbon-carbon bonds and valence angles correspond to the expected values [29]. In the other hand, azomethine C=N function length of the title compound was similar to that observed for many Schiff base compounds [30-33]. Also, for the linear central part of the title compound, the SP^3 character of carbon atoms was seen through the lengths of the carbon-carbon bonds and valence angles close to 109°.

In the table 4 below are recorded all the important intermolecular interactions that govern the cohesion of the crystalline network.

Table 4: Intermolecular interactions geometry (Å, °)

D-H···A	D-H	H···A	D···A	D-H···A
C_1-H_1…O_2^i	0.93	2.536	3.383	151.48
C_7-H_7···O_2^i	0.93	2.666	3.492	148,19
O_1···N_1^{ii}	-	-	2.928	-
N_1···O_1^{iii}	-	-	2.928	-
O_1···H_1-C_1^{iiii}	0.93	2.731	3.351	124.84
O_1···H_2-C_2^{iiii}	0.93	2.791	3.385	122.67

Codes de symétrie:(i) 1 + x,-1+ y, z ; (ii) –x, 1/2 + y, 1/2 - z; (iii) -x, y, 1/2 - z ; (iiii) 1/2-x, 1/2 + y, 1/2 - z

In the centrosymmetric dimer described in Figure 3, the oxygen atom O_2 of each molecule was engaged in chelated interactions with the hydrogen atoms H_1(2.536Å) and H_7 (2.666Å) of the other.

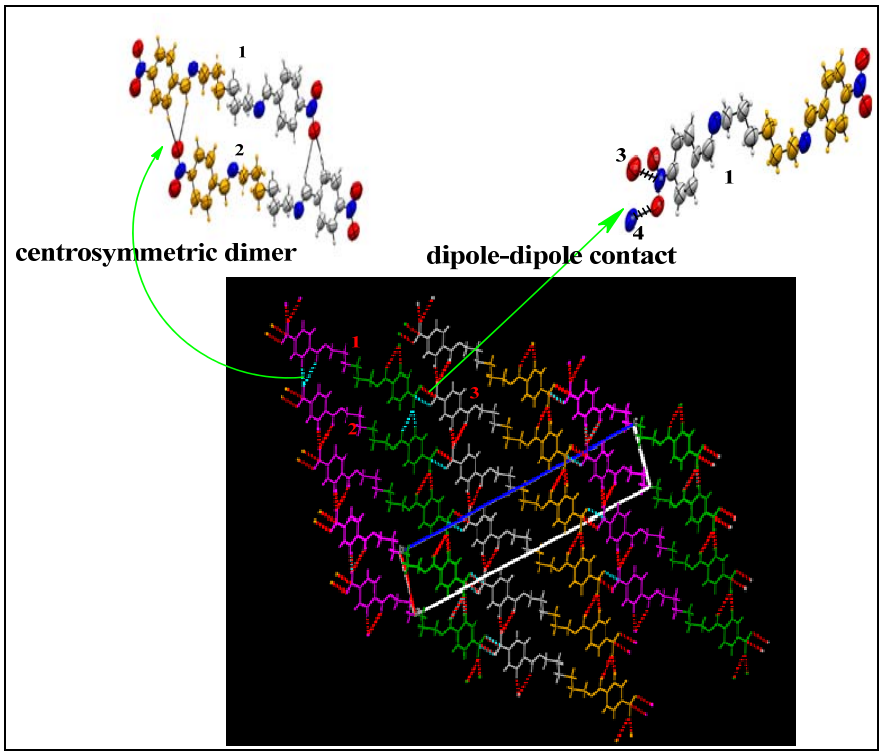

Fig 3: View of crystal packing showing C-H···O interactions in the centrosymmetric dimers and dipole-dipole contacts

While the oxygen atoms O_2 of each nitro group were engaged in double weak C-H···O type hydrogen bonds, each N_1-O_1 dipole interacts with two other N_1-O_1 dipoles of two other neighboring molecules as indicated in Table 4 and illustrated on Figure 3. Thus, the molecules within the crystal were packed in clusters in an infinite chain along the planes parallel to (104) plane. The cohesion within each cluster was essentially ensured by these kinds of dipole-dipole interactions with three molecules. Between the different clusters, the low C-H···O hydrogen bond interactions described above, act as binders and contributed effectively to the stabilization of the crystal network.

3.5. Antioxidant activity

The determination of antioxidant activity of the title compound was carried out according to two chemical techniques: Trapping of free radical DPPH and ABTS test. The results are recorded in Table 5.

Table 5: Results of DPPH and ABTS

	DPPH	ABTS
	Inhibition % ± standard deviation	
Title compound	14,507 ± 0,183	4,965 ± 1,316
Vitamin C	68,896 ± 6,007	45,039 ± 8,191

The Inhibition % values are an average of three trials

Analysis of the Table 5 showed that, the title compound exhibited antioxidant activity whatever the technique used. But, compared to vitamin C, this activity was modest.

From this molecule, we envisage structural modifications through multi substitutions, in order to improve this activity for development of a new class of Schiff bases profile antioxidant compounds.

4. Conclusion

The title compound was easily synthesized and characterized by conventional spectrometry methods (NMR, IR ESI-MS).The single crystal x-ray diffraction characterization showed that this compound, crystallized in monoclinic $P2_1/c$ space group with a = 6,1569(7)Å, b = 5,0751(5)Å, c = 30,631(4) Å, β = 94,509(7)° and z = 2. We have also examined antioxidant activity of *N, N'*-bis (*p*-nitrophenylmethylene) Hexane 1,6-diamine. Trapping of free radical DPPH and ABTS test show that, this compound exhibited modest activity compared to vitamin C IC_{50} value.

Supplementary material

Crystallographic data for the structural analysis have been deposited at the Cambridge Crystallographic Data Centre, CCDC No. 1538500. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge, CBZ1E Z, UK (Fax: +44-1223-336033; email: deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk).

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