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X-ray crystal structure analysis of *N*'-acetyl-*N*'-phenyl-2-naphthohydrazide

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RESEARCH ARTICLE

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ABSTRACT

N'-Acetyl-*N*'-phenyl-2-naphthohydrazide, a biologically relevant organic molecule, was synthesized following a reported method and characterized based on its single X-ray crystallographic studies. The present manuscript deals with its detailed molecular interactions and X-ray crystal structure. Its space group is *P*-1 with the following unit cell parameters: a = 8.9164(7), b = 9.7058(9), c = 17.7384(12) Å, α = 88.308(7)°, β = 89.744(6)°, γ = 86.744(7)° and Z = 2. Crystal structure was solved by direct method and refined by full matrix least squares procedure to a final R value of 0.0580 and to a GOOF value of 1.066. The X-ray diffraction analyses showed that the asymmetric unit contains two crystallographically independent molecules. The crystal structure is stabilized by elaborate network of N-H···O and C-H···O hydrogen bonds along with C-H···π and π···π interactions to form supramolecular structures.

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1. Introduction

Hydrazones are important class of biologically potent and pharmaceutically useful organic compounds [1-3]. They find many applications in fluorescent chemosensors [4,5], as auxiliaries in asymmetric synthesis [6], photo switches in photopharmacology [7], and linkers in preparing bifunctional molecules [8-10] and as ligands or directing groups in organic synthesis [11-13].

N,*N*'-Diacylhydrazones are functionalized hydrazone derivatives which are reported to exhibit various biological activities, including antitumor, antidiabetic, anti-inflammation, and anti-infection [14-20]. The title compound, *N*'-acetyl-*N*'-phenyl-2-naphthohydrazide (**1**) was synthesized following a reported method [21] as shown in Scheme 1, and characterized based on its single X-ray crystallographic studies.

2. Experimental

2.1. General

For crystallization, 50 mg of compound *N*'-acetyl-*N*'-phenyl-2-naphthohydrazide (**1**) was dissolved in 5 mL DMSO and left for several days at ambient temperature which yielded yellowish block shaped crystals which was suitable for X-ray diffraction analysis, were synthesized following the reported method as described in literature [21].

2.2. Crystal structure determination and refinement

The cell dimensions were determined by least-squares fit of angular settings of 3226 reflections in the θ range 2.27 to 27.97°. The value of R_{int} = 0.0187 and R_{sigma} =0.0381 shows satisfactory quality of the data. The molecular structure solution was obtained by direct method procedure as using SHELXT [22]. Six cycles of full-matrix least-squares refinement was carried out and it brought the final *R*-factor to 0.0580 and to GOOF value of 1.066.

All non-hydrogen atoms of the molecule were located in the best *E*-map and refined in anisotropic approximation using SHELXL [22]. The position of all the Hydrogen atoms bonded to carbon atoms were geometrically fixed and allowed to ride on the corresponding non-H atoms (C-H = 0.93-0.96 Å, and U_{iso}(H) = 1.5 U_{eq} of the attached C atoms for methyl groups and 1.2 U_{eq}(C) for other H atoms) except for H12, H35 and H35' atoms attached to nitrogen atoms N12, N35 and N35'. The residual electron density in the final difference Fourier map between -0.27 < Δρ < 0.61. The geometry of the title molecule was calculated using WinGX [23], PARST [24] and PLATON [25] software. Crystallographic data are summarized in Table 1.

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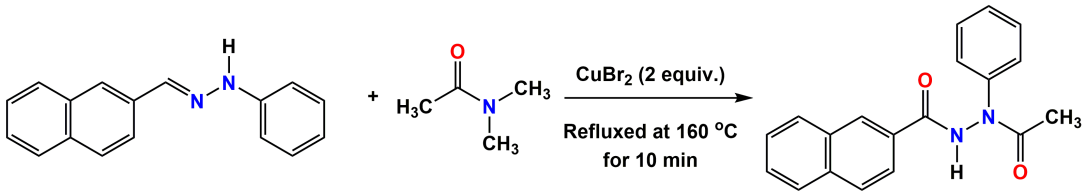
Table 1. Crystallographic characteristics, details of X-ray data collection, and structure refinement parameters for compound **1**.

Empirical formula	$C_{19}H_{16}N_2O_2$
Formula weight	304.34
Temperature (K)	150.01(10)
Crystal system	Triclinic
Space group	*P*-1
a, (Å)	8.9164(7)
b, (Å)	9.7058(9)
c, (Å)	17.7384(12)
α (°)	88.308(7)
β (°)	89.744(6)
γ (°)	86.744(7)
Volume (Å^3)	1531.9(2)
Z	4
ρ_{calc} (g/cm^3)	1.320
μ (mm^{-1})	0.087
F(000)	640.0
Crystal size (mm^3)	0.3 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection (°)	4.206 to 51.996
Index ranges	$-10 \le h \le 10$, $-11 \le k \le 11$, $-21 \le l \le 12$
Reflections collected	8450
Independent reflections	5935 [R_{int} = 0.0187, R_{sigma} = 0.0381]
Data/restraints/parameters	5935/936/547
Goodness-of-fit on F^2	1.060
Final R indexes [I≥2σ (I)]	R_1 = 0.0580, wR_2 = 0.1421
Final R indexes [all data]	R_1 = 0.0743, wR_2 = 0.1579
Largest diff. peak/hole (e.Å^{-3})	0.61/-0.27



Scheme 1. Synthesis of *N*'-acetyl-*N*'-phenyl-2-naphthohydrazide (**1**).

3. Results and discussion

The molecular structure containing the atomic labeling of the asymmetric unit of the crystal *N*'-acetyl-*N*'-phenyl-2-naphthohydrazide is shown in Figure 2 [26]. The X-ray diffraction analyses showed that the asymmetric unit of compound **1** contains two crystallographically independent molecules *A* and *B*. The molecule consists of a naphthalene ring and a benzene ring connected through a *N*'-acetylformo hydrazide bridge. In molecule *B*, the *N*'-methyl-*N*-phenylaceto hydrazide moiety is disordered over two sites with an occupancy ratio of 0.7531:0.2469.

The geometric parameters, including bond distances and bond angles, show normal geometry [27] and are in close relation to the related structure *N*-(4-nitrobenzoyl)-*N*'-phenylhydrazine [28]. The length of the N-N single bond between nitrogen atoms is 1.388(2) Å in molecule *A* and the average value of 1.384 Å in molecule *B*; this is close to the respective bond length of 1.390(4) Å present in $C_{13}H_{11}N_3O_3$. Here, the N-N-C bond angles deviate slightly from the ideal value of 120° by 1.1°, which is due to the presence of substitutions of acetyl groups and carbonyl groups at its ends. In molecule *A,* the acetyl group is *–sc* to the hydrazine moiety as evident from the C11-N12-N13-C14 torsion angle value of -90.0(3)°. The substituent carbonyl groups have an average value of C=O bond length of 1.217 Å, which is very close to its standard value (1.210 Å, [26]). Whereas, the N-N-C bond angle value of 118.7(3)°, the torsion angle value of N2-N1-C7-O7 of -3.3(5)° signifies that carbonyl group is *–sp* to hydrazine moiety for molecule reported in literature [28]. In both title molecule **1** and the molecule of literature, nearly orthogonal values of torsion angle C-N-N-C signifies tendency of the lone-pair orbitals on nitrogen atoms to reduce the corresponding overlap and resonance integrals [28].

In the naphthalene ring systems, the endocyclic angles at C1, C3, C8 and C8' are narrowed, while those at C2, C6, C26, C27, C29, C32', C31', C29', C26', C26', C27' and C24' are expanded from 120°, respectively. This would appear to be a real effect caused by the fusion of the smaller benzene ring systems by which the strain is taken up by the angular distortion [29]. All the benzene rings are individually planar which is evident from smaller values of torsion angles. In molecule *A*, the benzene ring is twisted with respect to the naphthalene ring at a dihedral angle of 87.01(6)°. Some of the important bond lengths and bond angles are listed in Table 2. The dihedral angle value of 79.86(0)° shows that both the rings of the compound of the literature are also nearly orthogonal to each other [28].

Analysis of the crystal packing showed that there exists a network of N-H···O and C-H···O intermolecular hydrogen bonds. O38 acts as an acceptor atom for two types of hydrogen bonds, by interactions with N12 and C26 through H12 and H26 hydrogen atoms resulting in a relatively stronger C-H···O hydrogen bond. The hydrogen H35 on atom N35 of molecule *B* forms an intermolecular strong hydrogen bond with the carbonyl atom O15 of molecule *A*. In addition to this, there exists a wide array of C-H···π and π···π interactions for crystal structure stabilization and to form supramolecular structures. The alkyl-aromatic hydrogen bond connects the parent molecules to their centrosymmetrically related molecules. The 90° angle for stacking rings is observed for 1-1, 1-2, 1-4, 1-5, 2-1, 2-4, 4-1, 4-2, 4-4, 4-5, 5-1, 5-4, and 6-7 molecular pairs. The geometry of these interactions is presented in Tables 3 and 4, respectively. Here Cg*I*···Cg*J* represents the distance between the ring centroids; Cg*I*···P represents the perpendicular distance of the centroid of one ring from the plane of the other; α is the dihedral angle between the planes of rings *I* and *J*; β is the angle between the normal to the centroid of ring *I* and the line joining ring centroids; Δ is the displacement of the centroid of rings *J*

Table 2. Selected bond lengths and bond angles for non-hydrogen atoms (e.s.d.'s are given in parentheses) for compound **1**.

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
C1	C2	1.362(3)	C29	C30	1.403(6)
C1	C10	1.412(4)	C30	C31	1.352(5)
C1	C11	1.493(3)	C31	C32	1.425(8)
C2	C3	1.431(3)	C32	C33	1.412(7)
C3	C4	1.408(3)	C34	O40	1.216(6)
C3	C8	1.406(4)	C34	N35	1.363(6)
C4	C5	1.355(4)	N35	N36	1.408(12)
C5	C6	1.409(4)	C24'	C25'	1.331(15)
C6	C7	1.341(4)	C24'	C33'	1.446(15)
C7	C8	1.441(4)	C24'	C34'	1.45(3)
C8	C9	1.392(4)	C25'	C26'	1.465(17)
C9	C10	1.370(4)	C26'	C27'	1.374(15)
C11	N12	1.364(3)	C26'	C31'	1.47(3)
C11	O17	1.210(3)	C27'	C28'	1.354(15)
C14	C16	1.488(3)	C28'	C29'	1.405(16)
C14	N13	1.356(3)	C29'	C30'	1.346(17)
C14	O15	1.223(3)	C30'	C31'	1.42(3)
C18	C19	1.373(3)	C31'	C32'	1.36(3)
C18	C23	1.375(3)	C32'	C33'	1.364(13)
C18	N13	1.434(3)	C34'	O40'	1.210(16)
C19	C20	1.385(3)	C34'	N35'	1.367(16)
C20	C21	1.369(4)	N35'	N36	1.36(4)
C21	C22	1.375(4)	C37	C39	1.490(3)
C22	C23	1.380(3)	C37	N36	1.342(3)
N12	N13	1.388(2)	C37	O38	1.228(3)
C24	C25	1.415(5)	C41	C42	1.373(3)
C24	C33	1.367(5)	C41	C46	1.376(3)
C24	C34	1.499(8)	C41	N36	1.435(3)
C25	C26	1.356(5)	C42	C43	1.379(3)
C26	C27	1.419(5)	C43	C44	1.374(4)
C27	C28	1.418(6)	C44	C45	1.374(4)
C27	C32	1.401(10)	C45	C46	1.382(3)
C28	C29	1.363(6)			

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
C2	C1	C10	118.9(2)	C30	C31	C32	120.4(5)
C2	C1	C11	117.6(2)	C27	C32	C31	119.2(5)
C10	C1	C11	123.4(2)	C27	C32	C33	119.6(6)
C1	C2	C3	121.3(2)	C33	C32	C31	121.2(7)
C4	C3	C2	121.1(2)	C24	C33	C32	120.7(5)
C8	C3	C2	118.4(2)	O40	C34	C24	122.4(6)
C8	C3	C4	120.5(2)	O40	C34	N35	123.7(7)
C5	C4	C3	120.3(3)	N35	C34	C24	113.9(6)
C4	C5	C6	120.0(3)	C34	N35	N36	118.6(8)
C7	C6	C5	121.3(3)	C25'	C24'	C33'	121.6(12)
C6	C7	C8	120.5(3)	C25'	C24'	C34'	126.1(14)
C3	C8	C7	117.4(3)	C33'	C24'	C34'	112.2(13)
C9	C8	C3	119.6(2)	C24'	C25'	C26'	120.5(12)
C9	C8	C7	123.0(3)	C25'	C26'	C31'	116.4(13)
C10	C9	C8	120.7(3)	C27'	C26'	C25'	122.2(12)
C9	C10	C1	121.0(2)	C27'	C26'	C31'	121.4(15)
N12	C11	C1	114.9(2)	C28'	C27'	C26'	121.0(12)
O17	C11	C1	123.6(2)	C27'	C28'	C29'	118.8(12)
O17	C11	N12	121.5(2)	C30'	C29'	C28'	122.9(13)
N13	C14	C16	117.3(2)	C29'	C30'	C31'	121.0(17)
O15	C14	C16	122.5(2)	C30'	C31'	C26'	115(2)
O15	C14	N13	120.2(2)	C32'	C31'	C26'	120.0(18)
C19	C18	C23	120.9(2)	C32'	C31'	C30'	125(2)
C19	C18	N13	118.8(2)	C33'	C32'	C31'	122.4(14)
C23	C18	N13	120.2(2)	C32'	C33'	C24'	119.1(10)
C18	C19	C20	119.1(2)	O40'	C34'	C24'	128(2)
C21	C20	C19	120.4(2)	O40'	C34'	N35'	115(2)
C20	C21	C22	120.0(2)	N35'	C34'	C24'	117(2)
C21	C22	C23	120.2(2)	N36	N35'	C34'	119(3)
C18	C23	C22	119.4(2)	N36	C37	C39	117.6(2)
C11	N12	N13	119.10(19)	O38	C37	C39	122.4(2)
C14	N13	C18	122.75(19)	O38	C37	N36	120.0(2)
C14	N13	N12	120.06(18)	C42	C41	C46	120.8(2)
N12	N13	C18	116.81(18)	C42	C41	N36	118.8(2)
C25	C24	C34	122.8(4)	C46	C41	N36	120.3(2)
C33	C24	C25	119.8(4)	C41	C42	C43	119.5(2)
C33	C24	C34	117.3(5)	C44	C43	C42	120.3(2)
C26	C25	C24	120.2(4)	C45	C44	C43	119.8(2)
C25	C26	C27	121.2(4)	C44	C45	C46	120.4(2)
C28	C27	C26	122.1(4)	C41	C46	C45	119.1(2)
C32	C27	C26	118.5(4)	N35	N36	C41	113.6(4)
C32	C27	C28	119.4(4)	N35'	N36	C41	123.8(14)
C29	C28	C27	119.4(4)	C37	N36	N35	123.3(4)
C28	C29	C30	121.5(4)	C37	N36	N35'	112.5(13)
C31	C30	C29	120.0(4)	C37	N36	C41	123.11(19)

Table 3. Geometry of inter- and intra-molecular interactions for compound **1** *.

D–H···A	D–H, Å	H···A, Å	D···A, Å	θ(D–H···A), deg
N12-H12···O38 ^{i}	0.90(2)	1.92(2)	2.781(2)	159(2)
N35-H35···O15 ^{ii}	0.90(2)	1.88(3)	2.747(11)	161(3)
C26-H26···O38 ^{i}	0.93	2.59	3.490(4)	162
C6-H6···Cg8 ^{iii}	0.93	2.83	3.638(3)	146
C21-H21···Cg1 ^{iv}	0.93	2.76	3.617(3)	154
C29-H29···Cg3 ^{v}	0.93	2.75	3.528(5)	142
C39-H39A···Cg7 ^{vi}	0.93	2.84	3.531(3)	130

* Symmetry codes: (*i*) *x*, 1+*y*, *z*, (ii) *x*, *y*, *z*, (*iii*) –*x*, 2-*y*, 1-*z*, (*iv*) -1+*x*, *y*, *z*, (*v*) 1-*x*, 1-*y*, -*z*, (*vi*) 1-*x*, 1-*y*, 1-*z*. Cg1, Cg3, Cg7, and Cg8, and represents the center of gravity of the rings (C24A/C25A/C26A/C27A/C32A/C33A), (C41/C42/C43/C44/C45/C46), (C3/C4/C5/C6/C7/C8) and (C18/C19/C20/C21/ C22/C23), respectively.

Table 4. Geometry of π-π interactions for compound **1** *.

Cg*I*	Cg*J*	Cg*I*···Cg*J*, Å	Cg*I*···*P*, Å	α, deg	β, deg	Δ, Å
1	1^{i}	3.663	3.490	0.0	17.6	1.11
1	2^{i}	3.692	3.490	2.3	19.0	1.20
1	4^{i}	3.674	3.452	1.1	20.1	1.25
1	5^{i}	3.636	3.457	1.1	20.1	1.13
2	1^{i}	3.692	3.490	2.3	19.0	1.20
2	4^{i}	3.794	3.428	1.9	24.4	1.64
4	1^{i}	3.674	3.449	1.1	20.0	1.26
4	2^{i}	3.794	3.455	1.9	25.4	1.56
4	4^{i}	3.939	3.427	0.0	29.5	1.94
4	5^{i}	3.507	3.426	1.4	13.6	0.74
5	1^{i}	3.635	3.440	1.9	18.8	1.26
5	4^{i}	3.507	3.409	1.4	12.3	0.81
6	7^{ii}	3.7686	3.4249	1.70	26.1	1.55

* Symmetric codes: (*i*) 1-*x*, 1-*y*, -*z*, (*ii*) –*x*, 2-*y*, 1-*z*. Cg1, Cg2, Cg4, Cg5, Cg6 and Cg7 represent the center of gravity of the rings (C24A/C25A/C26A/ C32A/C33A), (C27A/C28A/C29A/C30A/C31A/C32A), (C24'/C25'/C26'/C31'/C32'/C33'), (C26'/C27'/C28'/C29'/C30'/C31'), (C1/C2/C3/C8/C9/C10) and (C3/C4/C5/C6/C7/C8), respectively.

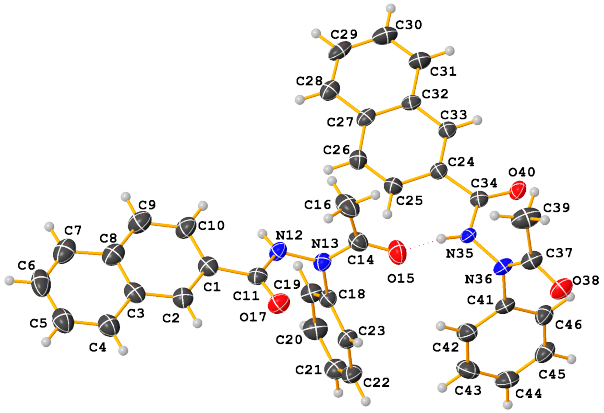


Figure 2. The molecular structure of the compound **1**.

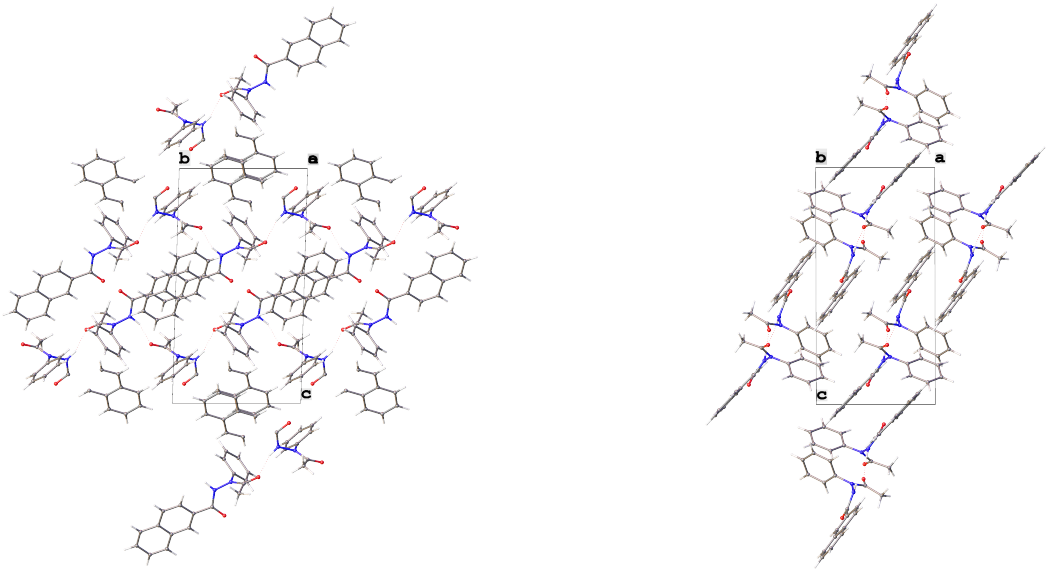


Figure 3. Packing view of molecules down to *a* and *b*-axis.

relative to the intersection point of the normal to the centroid of ring *I* and the least-squares plane of ring *J*. These π···π contacts describe the interactions present between the naphthalene ring and the benzene ring of compound **1**. The packing of the molecule within the unit cell viewed down the *a* and *b*-axis is shown in Figure 3. Molecules are packed together to form infinite layers along the (001) plane. Whereas the crystal packing arrangement for the related compound of the literature is linked to a complex three-dimensional framework structure by a combination of N-H···O, N-H···N, and C-H···O types of intermolecular H-bonds, resulting in sheet-like structure in dearth of other C-H···π and π···π contacts [28].

4. Conclusions

Single crystal X-ray diffraction studies led to unambiguous crystal structure determination of the compound which crystallizes into triclinic crystal system with space group *P*-1. Direct methods were used to solve the crystal structure and refined by full matrix least squares procedure to final *R* value of 0.0580. In molecule *B*, the moiety is disordered over two sites with an occupancy ratio of 0.7521:0.2469. A complete set of intermolecular hydrogen bonds; C-H···π and π···π interactions was observed and quantified for crystal packing analysis.

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Supporting information

CCDC-2110780 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via https://www.ccdc.cam.ac.uk/structures/, or by e-mailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033.

Disclosure statement

Conflict of interest: The authors declare that they have no conflict of interest.
Ethical approval: All ethical guidelines have been adhered.
Sample availability: Samples of the compound are available from the author.

CRediT authorship contribution statement

Conceptualization: Vivek Kumar Gupta, Goutam Brahmachari; Methodology: Varun Sharma, Indrajit Karmakar; Software: Varun Sharma, Indrajit Karmakar; Validation: Vivek Kumar Gupta, Goutam Brahmachari; Formal Analysis: Vivek Kumar Gupta, Goutam Brahmachari; Investigation: Indrajit Karmakar, Varun Sharma; Resources Vivek Kumar Gupta, Goutam Brahmachari; Data Curation: Varun Sharma, Indrajit Karmakar; Writing - Original Draft: Varun Sharma, Indrajit Karmakar; Writing - Review and Editing: Vivek Kumar Gupta, Goutam Brahmachari; Varun Sharma, Indrajit Karmakar; Visualization: Goutam Brahmachari, Vivek Kumar Gupta; Funding acquisition: none; Supervision: Vivek Kumar Gupta, Goutam Brahmachari.

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