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ORIGINAL RESEARCH

Crystallographic and conformational analysis of two novel *trans*-azo benzene compounds

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Abstract The molecular and crystal structure of (*E*)-2-Acetyl-4-(2-bromophenyldiazenyl)phenol (**1**) and (*E*)-2-Methyl-4-(*o*-tolyldiazenyl)phenol (**2**) were characterized and determined by single crystal X-ray diffraction method besides spectroscopic means. The periodic organization of **1** is stabilized by C–H···O type weak H-bond and Br···O type weak halogen bonding and thus, a two dimensional puckered network is established almost parallel to $(10\bar{1})$ the plane. Molecules of **2** are linked into *C*(7) chains generated by translation along the [1 0 1] direction with the aid of O–H···N type H-bonds, and these chains are strengthened by C–H···π interactions involving *o*-tolylphenol ring. Quantum chemical studies at B3LYP/6-311 ++G(d,p) level reveal that potential barrier of the compounds around Ar–N torsions is of double minimum character unless it is defected by the presence of *o*-substituent groups in the vicinity of the azo bridge. The results from crystallographic and quantum chemical studies suggest that azo benzene compounds may adapt non-planar geometry apart from the most stable planar conformation, which is located on the secondary minima of double potential barrier regarding rotational motion around Ar–N bonds.

Keywords Azo benzene · DFT/B3LYP · Conformational analysis · Crystal structure

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Introduction

Azo compounds have found widespread application in many different areas such as polyester fiber [1], disperse dyes [2], biological reactions, and in analytical chemistry [3]. On the other hand, azo benzene is one of the most representative classes of photochromic molecules with two geometric isomers, *trans* and *cis* [4–6]. The *cis–trans* isomerization occurs by photoirradiation with UV light or by heating. It is generally accepted that their *trans* forms are more stable than their *cis* forms [7, 8]. In addition, molecular azo dyes are still one of the active research topics in the area of molecular engineering of optoelectronic materials [9] and photoswitchable molecules [10] due to their enhanced chemical stability and photostability. In structural sense, azo benzene compounds exhibit unusual molecular motion referred to as pedal motion in solid state leading to orientational disorder in azo bridge at either one of the lattice sites [11] or both crystal lattice sites [12]. Therefore, better understanding of such processes regarding azo compounds is of great importance in their structural control and device applications related to them.

In a continuation of our interest regarding azo-dyes, here we report the details of *trans* stereochemistry of (*E*)-2-Acetyl-4-(2-bromophenyldiazenyl)phenol (**1**) and (*E*)-2-Methyl-4-(*o*-tolyldiazenyl)phenol (**2**) by using single crystal X-ray diffraction technique and quantum chemical calculations at B3LYP/6-311 ++G(d,p) level as a part of general

study of the crystal chemistry of dyes. The results from both the methods were compared and thus, crystal packing effects on the exact *trans* configurations and possible reasons for the observed molecular conformations of the compounds, in particular *o*-substituent group in vicinity of azo bridge, are comprehensively discussed.

Experimental

Synthesis and spectral characterization of **1**

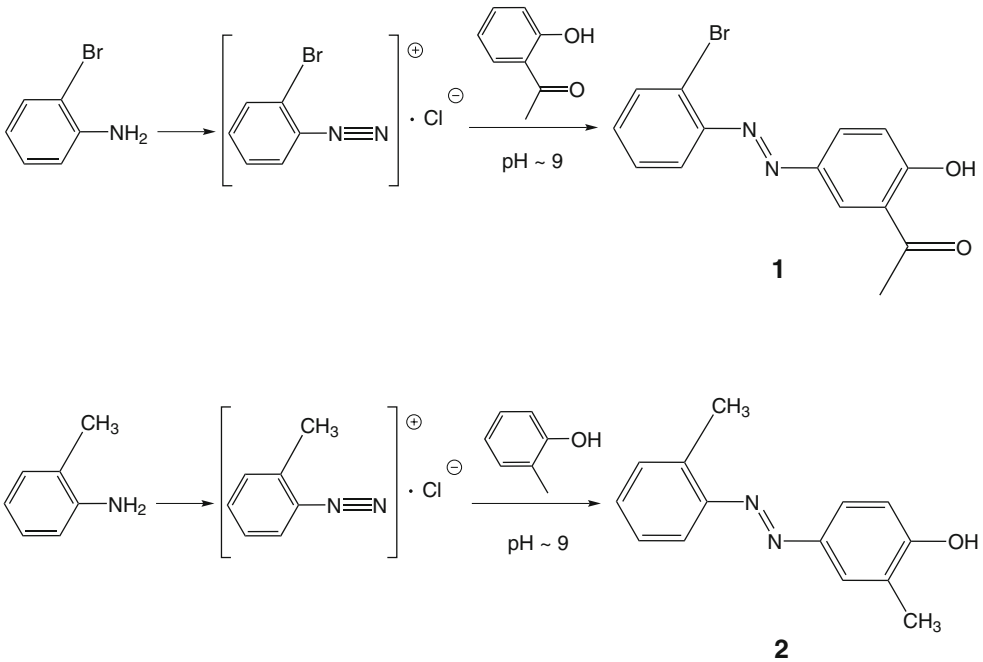
A mixture of 2-bromoaniline (1.34 g, 7.8 mmol), water (20 mL), and concentrated hydrochloric acid (1.97 mL, 23.4 mmol) was stirred until a clear solution was obtained. This solution was cooled to 273–278 K and a solution of sodium nitrite (0.75 g, 7.8 mmol) in water was added dropwise while the temperature was maintained below 278 K. The resulting mixture was stirred for 30 min in an ice bath. 2-hydroxyacetophenone (1.067 g, 7.8 mmol) solution (pH ~ 9) was gradually added to a cooled solution of 2-bromobenzenediazonium chloride, prepared as described earlier, and the resulting mixture was stirred at 273–278 K for 60 min in an ice bath. The product was recrystallized from ethyl alcohol to obtain solid (*E*)-2-Acetyl-4-(2-bromophenyldiazenyl)phenol (**1**) as shown in Scheme 1. Crystals of **1** were obtained after 2 days by slow evaporation from acetic acid (yield 52%, m.p. 423–425 K). Elemental analysis calculated for $C_{14}H_{11}BrN_2O_2$; C: 52.68, H: 3.47, O: 10.02, and N: 8.77%, found C: 52.36, H: 3.54, O: 10.28, and N: 8.59%.

Proton NMR spectra (200 MHz) were recorded with an AC-200 Bruker FT-NMR spectrometer at 297 K. ^{1}H NMR (δ, DMSO-d_6): 9.14 [s, 1H, OH]; 7.28–7.96 [m, 7H, Ar–H]; 2.60 [s, 3H, Ar–C(=O)–CH_3]. The FT-IR spectrum of the compound was recorded from KBr pellets with an IASCO FT-IR 430 spectrophotometer. IR spectroscopic data (ν, cm^{-1}): 3,240–3,400 (*br*, Ar–OH), 3,080 (aromatic CH), 2,920–2,870 (aliphatic C–H), 1,720 (C=O), 1,505–1,620 (aromatic C=C), 1,426 (N=N), 1,170 (C–N), 495 (Ar–Br).

Synthesis and spectral characterization of **2**

A mixture of 2-methylaniline (2 g, 18.7 mmol), water (50 mL), and concentrated hydrochloric acid (4.7 mL, 56 mmol) was stirred until a clear solution was obtained. This solution was cooled to 273–278 K and a solution of sodium nitrite (1.8 g, 26 mmol) in water was added dropwise while the temperature was maintained below 278 K. The resulting mixture was stirred for 30 min in an ice bath. 2-methylphenol (2.02 g, 18.7 mmol) solution (pH ~ 9) was gradually added to a cooled solution of 2-methylbenzenediazonium chloride, prepared as described earlier, and the resulting mixture was stirred at 273–278 K for 60 min in an ice bath. The product was recrystallized from ethyl alcohol to obtain solid (*E*)-2-Methyl-4-(*o*-tolyldiazenyl)phenol (**2**) as shown in Scheme 1. Crystals of **2** were obtained after 1 day by slow evaporation from acetic acid (yield 60%, m.p. 410–412 K). Elemental analysis calculated for $C_{14}H_{14}N_2O$; C: 74.31, H: 6.24, O: 7.07, and N: 12.38%, found C: 74.48, H: 6.05, O: 6.88, and N: 12.56%.

Scheme 1 Synthesis routes for the compounds



Proton NMR spectra (200 MHz) were recorded with an AC-200 Bruker FT-NMR spectrometer at 297 K. ^{1}H NMR (δ, DMSO-d_6): 8.94 [s, 1H, OH]; 7.18–7.84 [m, 7H, Ar–H]; 2.44 [s, 3H, Ar–CH_3]; 2.24 [s, 3H, Ar(OH)–CH_3]. The FT-IR spectrum of the compound was recorded from KBr pellets with an IASCO FT-IR 430 spectrophotometer. IR spectroscopic data (ν, cm^{-1}): 3,250–3,460 (*br*, Ar–OH), 3,064–3,120 (aromatic CH), 2,965–2,940 (Ar–CH_3), 2,860–2,890 (aliphatic C–H), 1,490–1,600 (aromatic C=C), and 1,430 (N=N).

X-ray crystallography

Suitable samples of size 0.390 × 0.267 × 0.150 mm and of 0.570 × 0.440 × 0.220 mm were chosen for the crystallographic study regarding **1** and **2**, and then mounted on goniometer of a STOE IPDS II diffractometer. All diffraction measurements were performed at room temperature (296 K) using graphite-monochromated MoK_α radiation ($\lambda = 0.71073$ Å). The systematic absences and intensity symmetries indicated that **1** and **2** crystallize in the monoclinic *C 2/c* and *P* $2_1/n$ space group, respectively. While a total of 8,785 reflections (2,562 unique) within the θ range of $[1.62 < \theta < 26.00]$ were collected for **1**, a total of 21,599 reflections (2,890 unique) within the θ range of $[2.62 < \theta < 27.92]$ for **2** were collected in the rotation mode. The diffraction intensities were corrected for Lorentz-polarization factors, and absorption correction was made by integration method via X-RED software [13] and cell parameters were determined by using X-AREA software [13]. The structure was solved by direct methods using SHELXS-97 [14]. The refinement was carried out by full-matrix least-squares method on the positional and anisotropic temperature parameters of the nonhydrogen atoms. H atoms except for aromatic H3, H12, and those of methyl group of **1** were located on the final difference-Fourier map and refined freely. All H atoms of **2** were located in the final difference-Fourier synthesis cycle and refined freely. The scattering factors were taken from SHELXL-97 [14]. Other details of the data collection conditions and details of refinement process are summarized in Table 1.

Supporting information

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 730357 and 730358. Copies of the data can be obtained free of charge on application to CCDC 12 Union Road, Cambridge CB21 EZ, UK (Fax: (+44) 1223 336-033; e-mail: data_request@ccdc.cam.ac.uk).

Computational procedures

The geometry optimizations of **1** and **2** leading to energy minima in vacuo were performed by using DFT calculations with the use of Becke's three-parameters hybrid exchange-correlation functional (B3LYP) [15] incorporating B88 gradient-corrected exchange [16] and Lee-Yang-Parr nonlocal correlation functional [17] by means of 6-311 ++G(d,p) basis set [18–20] implemented in Gaussian 03 W program package [21]. Geometry optimizations of the molecules were achieved by the application of Berny optimization algorithm [22]. The values of the convergence criteria in the optimization procedures for both **1** and **2** are below 4.5×10^{-4} hartree/bohr for maximum force, 3.0×10^{-4} hartree/bohr for RMS force, 1.8×10^{-3} Å for maximum displacement, and 1.2×10^{-3} Å for RMS displacement. To understand conformational behavior of the molecules and crystal packing effects on the molecular geometries, formally single C–N bonds at opposite sides around azo bridge were selected and varied from -180° to $+180^\circ$ in every 10°. Total energy of pseudo-conformer in each step was calculated by single-point calculation on the computed potential energy surface at the same level of theory. To be able to compare quantitatively, the X-ray molecular structures with their optimized counterparts and the root-mean-square (r.m.s.) fits of the relevant atomic positions were calculated.

Results and discussion

Structure determination of **1** and **2**

Molecular geometries of **1** and **2** of which thermal ellipsoid views [23] are shown in Figs. 1 and 2 have slight angular deviation from their exact *trans* configuration around azo bridges with the angles of 1.3(3)° and 1.87(9)°, respectively. While molecular geometry of **1** is almost planar, that of **2** deviates evidently from planarity and molecular fragment apart from 2-methyl phenyl ring is nearly planar. The respective dihedral angles between the aromatic rings of **1** and **2** are 3.5(2)° and 32.51(4)°. Some selected geometrical parameters experimentally obtained and their calculated values are listed in Table 2. The N=N bond distances in both compounds (Table 2) are in agreement with the corresponding values of similar compounds [24–29] and reflect their double bond character. The bond lengths of pairs of formally single C–N bonds at opposite sides around azo bridges are not sensitive to substituent effects and thus, they are almost equal in both compounds (Table 2). C_{ar}–N(=N) bond lengths reported by Allen et al. [30] is about 1.431 Å. The values of C_{ar}–N bonds in **1** and **2** are comparable with this value. The calculated values of

Table 1 Crystal data and details of the structure refinement for **1** and **2**

	1	**2**
Crystal data		
Chemical formula	$C_{14}H_{11}BrN_2O_2$	$C_{14}H_{14}N_2O$
Color/shape	Yellow/prism	Orange/prism
Formula weight	319.16	226.27
Cell setting	Monoclinic	Monoclinic
Space group	*C 2/c*	*P 21/n*
Unit cell parameters	a = 11.011(1) Å	a = 10.0359(7) Å
	b = 9.4617(8) Å	b = 11.5408(7) Å
	c = 25.310(3) Å	c = 10.6040(7) Å
	β = 95.033(9)°	β = 97.723(6)°
Volume	2626.6 (5) $Å^3$	1217.0(1) $Å^3$
Formula Z	8	4
Density (calculated)	1.614 Mgm^{-3}	1.235 Mgm^{-3}
Abs. coeff. (μ)	3.13 mm^{-1}	0.08 mm^{-1}
Data collection		
Diffractometer/meas. meth.	STOE IPDS 2/ω-scan	
T_{min}, T_{max}	0.415, 0.581	0.966, 0.972
F(000)	1,280	480
h_{min}, h_{max}	−12, 13	−13, 13
k_{min}, k_{max}	−11, 11	−15, 15
l_{min}, l_{max}	−31, 31	−13, 13
R_{int}	0.041	0.037
Refinement		
Refinement method	Full-matrix least-squares on F^2	
Measured reflections	8,785	21,599
Independent reflections	2,562	2,890
Observed reflections	1,551	1,962
Data/parameters	2,562/198	2,890/211
Goodness of fit on F^2	1.013	0.998
R indices [$I > 2\sigma(I)$]	$R_1 = 0.040$, $wR_2 = 0.097$	$R_1 = 0.034$, $wR_2 = 0.091$
R indices [all]	$R_1 = 0.076$, $wR_2 = 0.110$	$R_1 = 0.054$, $wR_2 = 0.096$
Weighting scheme	$w = 1/[\sigma (F_0^2) + (0.0566P)^2 + 0.1745P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma (F_0^2) + (0.0566P)^2]$ where $P = (F_0^2 + 2F_c^2)/3$
$\Delta\rho$max, $\Delta\rho$min ($eÅ^{-3}$)	0.47, −0.63	0.15, −0.10

single C–N bonds at opposite sides around azo bridges in both compounds are slightly different from each other due to a possible through-resonance effect between the electron-donating O atom and the two-electron accepting N atom.

In the crystal structure of **1**, two primary intermolecular interactions are observed. One of them is the interatomic contacts between Br1 at (x, y, z) and O1 at [(i) 3/2 − x, −1/2 − y,−z]. The distance between these atoms (3.363 Å) is slightly smaller than the sum of their noncovalent van der Waals radii [31]. For a conventional halogen bond, acceptable D···X distances between electron pair donor (D) and halogen atom (X=Br) are in the range of 2.5–3.2 Å [32]. On the basis of this consideration, it can be stated that Br1···O1 contact is referred to as a weak noncovalent halogen bonds [33]. Another interaction is also C12–H12···O2 weak H-bond whose details are given in Table 3. According to graph-set notation [34], C12–H12···O2 weak H-bond gives rise to $C(12)$ polymeric chains as shown in Fig. 3. When these chains are incorporated into Br1···O1 contacts, puckered sheets lying almost parallel to $(1\,0\,\bar{1})$ plane are formed in the crystal structure of **1** as shown in Fig. 3. Br1···O1 weak halogen bonds create a structural pattern allowing for the multipoint self-recognition property and serve to be strengthened $C(12)$ polymeric packing arrangements.

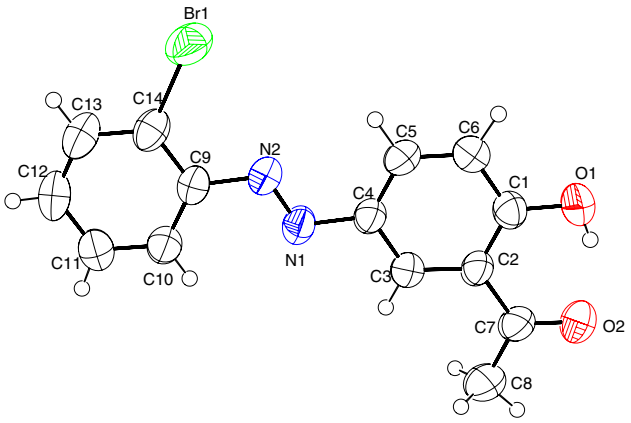


Fig. 1 Thermal ellipsoid view of (**1**) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small *spheres* of arbitrary radii

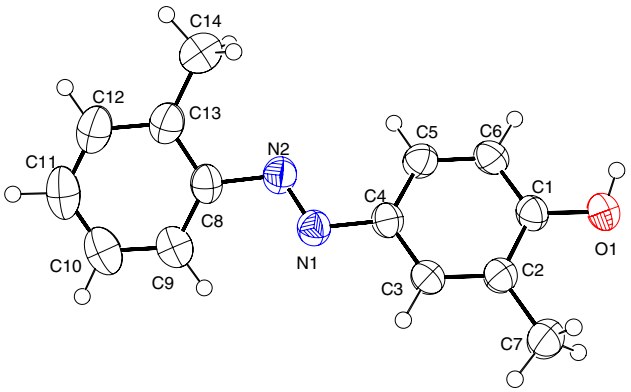


Fig. 2 Thermal ellipsoid view of (**2**) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small *spheres* of arbitrary radii

The molecules of **2** are linked into one-dimensional polymeric *C*(7) chains running along the [1 0 1] direction generated by a strong O–H···N type intermolecular H-bond (Table 3) as shown in Fig. 4, supplying primary contribution to the stabilization of periodic organization of **2** in solid state. In the crystal structure of **2**, arrangement of *C*(7) chains constructed by O–H···N type H-bonds is strengthened by C–H···π interactions involving *o*-tolylphenol ring. It can be shown that C–H···π interaction controls the stacking of the molecules of **2** in the direction of *b*-axis. As a result of O1–H1···N1 hydrogen bond on the observed molecular geometry, H1 atom deviates from the mean plane of 2-methylphenol ring by −0.20(2) Å. This hydrogen bond mediates the formation of centrosymmetric four-molecule aggregates as shown in Fig. 4 having symmetry center (½, ½, ½), which are further grouped into an extended structure by C–H···π interactions.

Table 3 Geometric details of intermolecular interactions (Å, °) for **1** and **2**

	D–H···A	D–H	H···A	D···A	∠D–H···A
1	C12–H12···O2^{ii}	0.93	2.61	3.401(5)	142.9
2	O1–H1···N1^{iii}	0.85(2)	2.06(2)	2.892(1)	166(2)
3	C11–H11···Cg1^{iv}	0.97(2)	2.76(2)	3.595(2)	145.2(1)

D donor, *A* acceptor. Symmetry operation used to generate equivalent atomic positions: (ii) $x + 1/2, 1/2 - y, 1/2 + z$; (iii) $x - 1/2, 1/2 - y, z - 1/2$; (iv) $3/2 - x, 1/2 + y, 3/2 - z$. Cg1 stands for the centroid of the ring carrying O1 atom of **2**

Table 2 Some selected geometrical parameters of the compounds (Å, °) obtained from X-ray crystallographic and computational study

1	X-ray	DFT/B3LYP	**2**	X-ray	DFT/B3LYP
Bond lengths					
N1–N2	1.246(4)	1.255	N1–N2	1.253(1)	1.255
N1–C4	1.432(4)	1.409	N1–C4	1.421(1)	1.412
N2–C9	1.431(4)	1.413	N2–C8	1.422(1)	1.418
C14–Br1	1.885(4)	1.913	C13–C14	1.496(2)	1.509
C1–O1	1.344(4)	1.333	C1–O1	1.356(1)	1.367
C7–O2	1.230(5)	1.235	C2–C7	1.503(2)	1.506
Bond angles					
N1–N2–C9	113.8(3)	115.39	C8–N2–N1	114.48(9)	115.59
N2–N1–C4	113.4(3)	115.20	N2–N1–C4	114.71(9)	115.65
C2–C1–O1	122.2(3)	122.39	C2–C1–O1	116.8(1)	116.94
C2–C7–O2	120.6(4)	120.53	C8–C13–C14	121.4(1)	121.59
Torsion angles					
C9–N2–N1–C4	−178.7(3)	−179.68	C4–N1–N2–C8	178.13(9)	179.99
N2–N1–C4–C3	176.9(3)	−179.74	C13–C8–N2–N1	152.8(1)	179.99
N1–N2–C9–C14	−175.0(3)	−177.86	C3–C4–N1–N2	176.53(9)	179.98

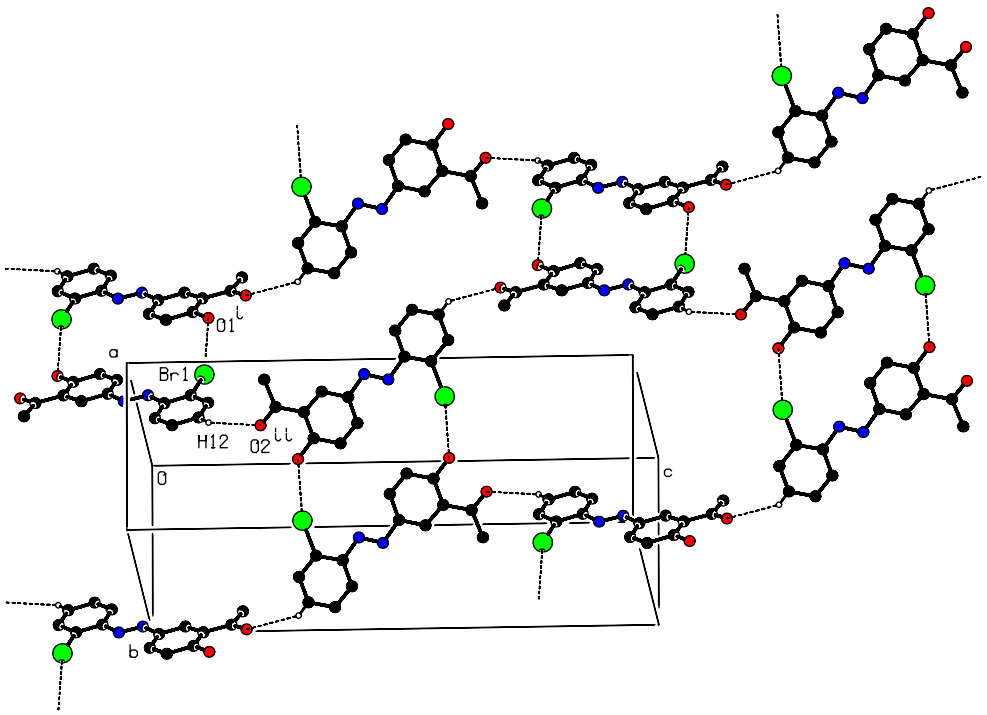


Fig. 3 Part of the puckered sheet parallel to $(10\bar{1})$ plane formed by Br1···O1 contact and C12–H12···O2 weak H-bond. H atoms not involved in the motif have been omitted for the sake of clarity

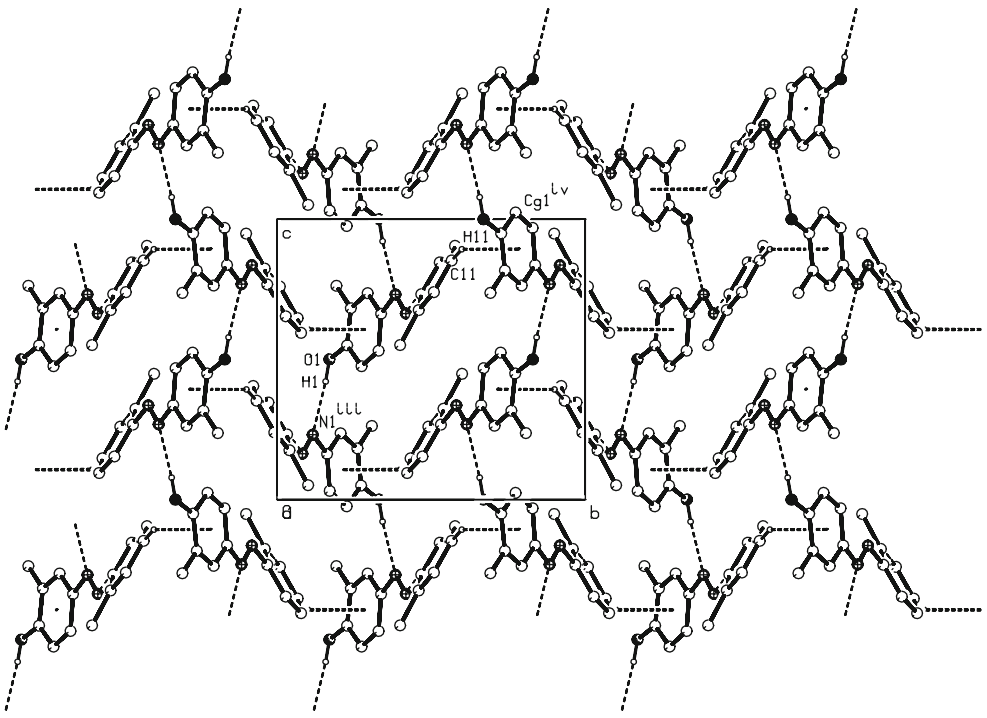


Fig. 4 Molecular stacking pattern of **2** viewed down *a*-axis. *Open*, *filled* and *shaded* spheres denote C, O and N atoms, respectively. H atoms not involved in the motif have been omitted for the sake of clarity

Computational study

Conformational discrepancies between the energy minimized molecule and the crystallographically observed geometry of the compounds were quantitatively analyzed by r.m.s. overlays, including H atoms, as shown in Fig. 5. As a guiding rule, it can be stated that the most favorable conformation of *trans*-azo benzene skeleton is planar [35].

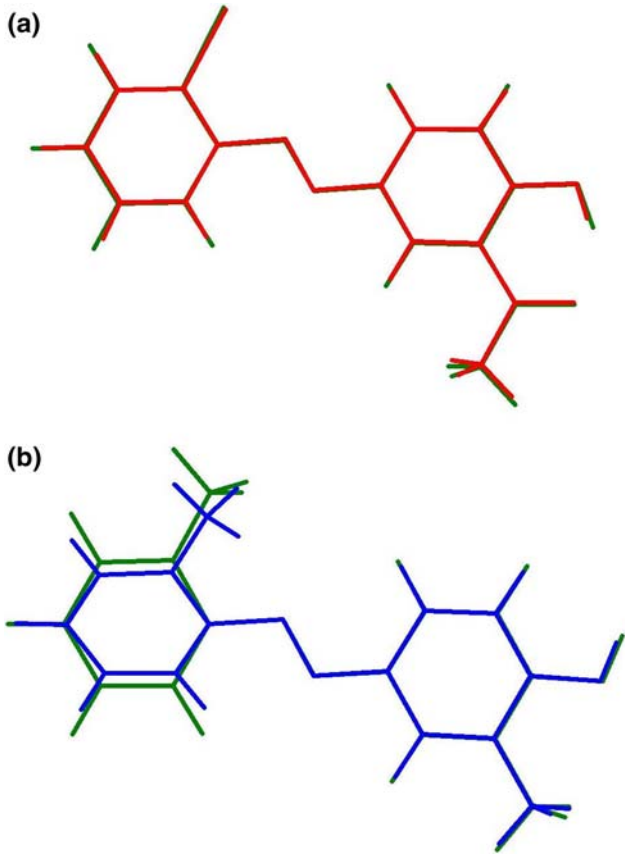


Fig. 5 Superimpositions of the X-ray structures of **1** (**a**) and **2** (**b**) with their optimized geometries

When the crystallographically observed geometries of **1** and **2** are contrasted with their optimized counterparts, it is seen that molecular geometry of **2** is far from its optimized geometry while that of **1** is very similar to its optimized counterpart. The r.m.s. fits of **1** (red) and **2** (blue) to the relevant optimized geometries (green) are 0.012 and 0.064 Å. The most important fact remains that the X-ray conformation of **2** in the absence of the crystal lattice environment is not the lowest-energy conformation of the compound. The reason for this conformational difference requires an explanation in quantum chemical sense.

To better understand conformational flexibility of the compounds, molecular energy profiles against N–C(Ar) torsional degrees of freedom were investigated at B3LYP/6-311 ++G(d,p) level. Double minimum potential barriers throughout the rotation around N–C(2-hydroxyacetophenol) and N–C(2-methylphenol) torsional degrees of freedom as shown in Figs. 6 and 7 are peculiar to *trans*-azo benzene skeleton in the absence of substituent groups at *o*-positions in vicinity of azo bridge [27, 36]. Primary and secondary barrier height of double minimum potential barriers are found as 10.11 and 0.12 kcal/mol for **1** and as 8.68 and 0.23 kcal/mol for **2**. These values are comparable with previous studies in [27, 36]. As expected, the presence

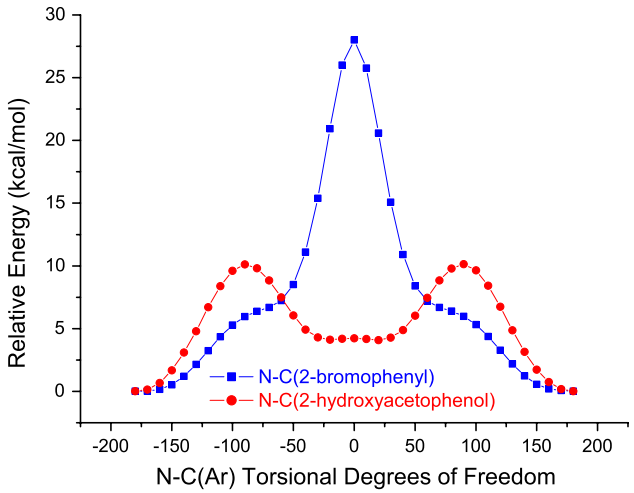


Fig. 6 Variations of the relative energies of the pseudo-conformers of **1** against N–C(Ar) torsion angles. Here relative energy values are calculated regarding the absolute minimum for which $E = -3374.398$ a.u

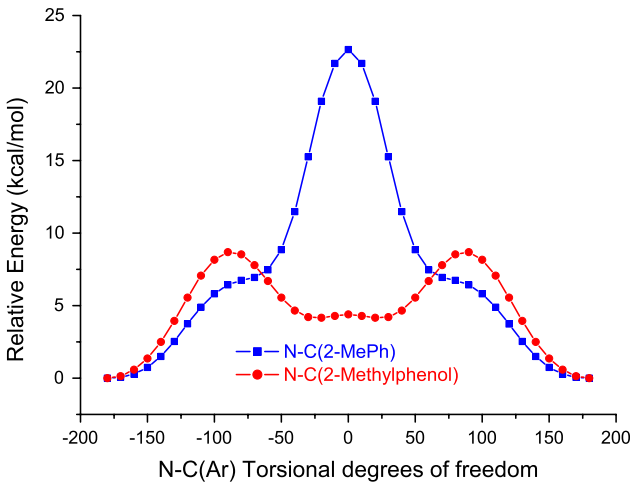


Fig. 7 Variations of the relative energies of the pseudo-conformers of **2** against N–C(Ar) torsion angles. Here relative energy values are calculated regarding the absolute minimum for which $E = -726.812$ a.u

of substituent groups at *o*-positions of the aromatic rings causes a defect in double potential barrier due to steric repulsion between *o*-substituent groups and the lone-pair electrons on the nitrogen atoms, distorting the planar geometry. The steric hindrance between *o*-substituent groups and the lone-pair electrons on the nitrogen atoms results in the appearance of evident increase in the molecular energy at 0° of the N–C(2-bromophenyl) and N–C(2-MePh) torsions as shown in Figs. 6 and 7. At 0° of the N–C(2-bromophenyl) and N–C(2-MePh), interatomic separations of bromine and methyl H atoms from the nearest nitrogen in the azo bridge are 2.391 and 2.047 Å. These distances are much smaller than the sum of their

non-covalent van der Waals radii (3.40 and 2.55 Å) [31]. Keeping in mind that dihedral angle between aromatic rings of **2** is 32.51(4)°, nonplanar conformation of **2** can be explained by secondary minimum observed at 30° of N–C(2-Methylphenol) torsional degree of freedom (Fig. 7). Another effect on the stabilities and geometries of *trans*-azo benzene skeletons is also the conjugation between the azo bridge and phenyl groups, making the molecular conformation planar. As a result of this, the bond lengths of pairs of single C–N bonds at opposite sides around azo bridges of **1** become equal (Table 2). This conjugation effect is observed in nonplanar molecular geometry of **2** as well and suggests that C–H$\cdots\pi$ interaction makes stable the molecular geometry in crystal phase.

Conclusion

Quantum chemical studies suggest that there are two possible conformational preferences for azo benzene skeleton with respect to N–C(Ar) torsional degrees of freedom. Molecular energy profiles of the compounds against two torsional degrees of freedom of N–C(Ar) in gas-phase indicate that there are two competitive factors affecting the stabilities of *trans*-azo benzene skeleton: the conjugation between the azo and phenyl groups making the molecular conformation planar, and the repulsion between *o*-substituent phenyl groups in vicinity of the azo bridge and the lone-pair electrons in the nitrogen atom distorting the planar geometry. Although planar pseudo-conformers revealing at $\pm 180°$ of both N–C(Ar) torsions is the most stable conformations of the compounds, some azo benzene compounds may adapt nonplanar molecular geometry located in one of the secondary minima (at $\pm 30°$) of the computed potential energy surface by means of interactions with surrounding molecules in solid state. Conformational discrepancies between the crystallographically observed and the energy minimized structure of the compounds cannot be explained only considering crystal packing effects.

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References

1. Koh J, Greaves AJ (2001) Dyes Pigments 50:117
2. Hallas G, Choi JH (1999) Dyes Pigments 40:119
3. Kandil SS (1998) Trans Met Chem 23:461
4. Lee M-J, Yoo BW, Shin ST, Keum SR (2001) Dyes Pigments 51:15
5. Aramaki S, Atkinson GH (1992) J Am Chem Soc 114:438
6. Tamai N, Miasaka H (2000) Chem Rev 100:1875
7. Azuki M, Morihashi K, Watanabe T, Taskahashi O, Kikuchi O (2001) J Mol Struc: THEOCHEM 542:255
8. Grebenkin SY, Bolshakov BV (1999) J Photochem Photobiol A: Chemistry 122:205
9. Frampton MJ, Anderson HL (2007) Angew Chem Int Ed 46:1028
10. Browne WR, Feringa BL (2009) Annu Rev Phys Chem 60:407
11. Harada J, Ogawa K (2001) J Am Chem Soc 123:10884
12. Ocak-Iskeleli N, Karabiyik H, Albayrak C, Agar E (2008) J Chem Crystallogr 38:671
13. Stoe & Cie (2002) X-AREA (Version 1.18) and X-RED32 (Version 1.04), Darmstadt, Germany
14. Sheldrick GM (2008) Acta Cryst A 64:112
15. Hertwig RH, Koch W (1997) Chem Phys Lett 268:345
16. Becke AD (1988) Phys Rev A 38:3098
17. Lee C, Yang W, Parr RG (1988) Phys Rev B 37:785
18. Hariharan PA, Pople JA (1973) Theor Chim Acta 28:213
19. Ditchfield R, Hehre WJ, Pople JA (1971) J Chem Phys 54:724
20. Frisch MJ, Pople JA, Krishnam R, Binkley JS (1984) J Chem Phys 80:3265
21. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Montgomery JA, Vreven T Jr, Kudin KN, Burant JC, Millam JM, Iyengar SS, Tomasi J, Barone V, Mennucci B, Cossi M, Scalmani G, Rega N, Petersson GA, Nakatsuji H, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Klene M, Li X, Knox JE, Hratchian HP, Cross JB, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Ayala PY, Morokuma K, Voth GA, Salvador P, Dannenberg JJ, Zakrzewski VG, Dapprich S, Daniels AD, Strain MC, Farkas O, Malick DK, Rabuck AD, Raghavachari K, Foresman JB, Ortiz JV, Cui Q, Baboul AG, Clifford S, Cioslowski J, Stefanov BB, Liu G, Liashenko A, Piskorz P, Komaromi I, Martin RL, Fox DJ, Keith T, Al-Laham MA, Peng CY, Nanayakkara A, Challacombe M, Gill PMW, Johnson B, Chen W, Wong MW, Gonzalez C, Pople JA (2003) Gaussian 03, Revision E.01. Gaussian, Pittsburgh PA
22. Schlegel HB (1982) J Comput Chem 3:214
23. Farrugia LJ (1997) J Appl Cryst 30:565
24. Iskeleli NO, Karabiyik H, Albayrak C, Petek H, Agar E (2006) J Chem Crystallogr 36:709
25. Karabiyik H, Iskeleli NO, Albayrak C, Agar E (2007) Struct Chem 18:87
26. Iskeleli NO, Karabiyik H, Albayrak C, Petek H, Agar E (2006) Struct Chem 17:393
27. Iskeleli NO, Karabiyik H, Albayrak C, Agar E, Gumrukcuoglu IE (2008) Struct Chem 19:565
28. Soylu S, Kocaokutgen H, Gür M, Lönnecke P (2004) Acta Cryst C60:o498
29. Huang X, Kuhn GH, Nesterov VN, Averkiev BB, Penn B, Antipin MY, Timofeeva TV (2002) Acta Cryst C58:o624
30. Allen FH, Watson DG, Brammer L, Orpen AG, Taylor R (2004) In: Prince E (ed) International tables for crystallography vol C: mathematical, physical and chemical tables, 3rd edn. Kluver Academic Publishers, Dordrecht, pp 790–811
31. Bondi A (1964) J Phys Chem 68:441
32. Forni A, Metrangolo P, Pilati T, Resnati G (2004) Cryst Growth Des 4:291
33. Metrangolo P, Meyer F, Pilati T, Resnati G, Terraneo G (2008) Angew Chem Int Ed 47:6114
34. Bernstein J, Davis RE, Shimoni L, Chang N-L (1995) Angew Chem Int Ed Engl 34:1555
35. Biswas N, Umapathy S (1997) J Phys Chem A 101:5555
36. Tsuji T, Takashima H, Takeuchi H, Egawa T, Konaka S (2001) J Phys Chem A 105:9347