A CONCEPT FOR STIMULATED PROTON TRANSFER IN 1-(PHENYLDIAZENYL)NAPHTHALEN-2-OLS

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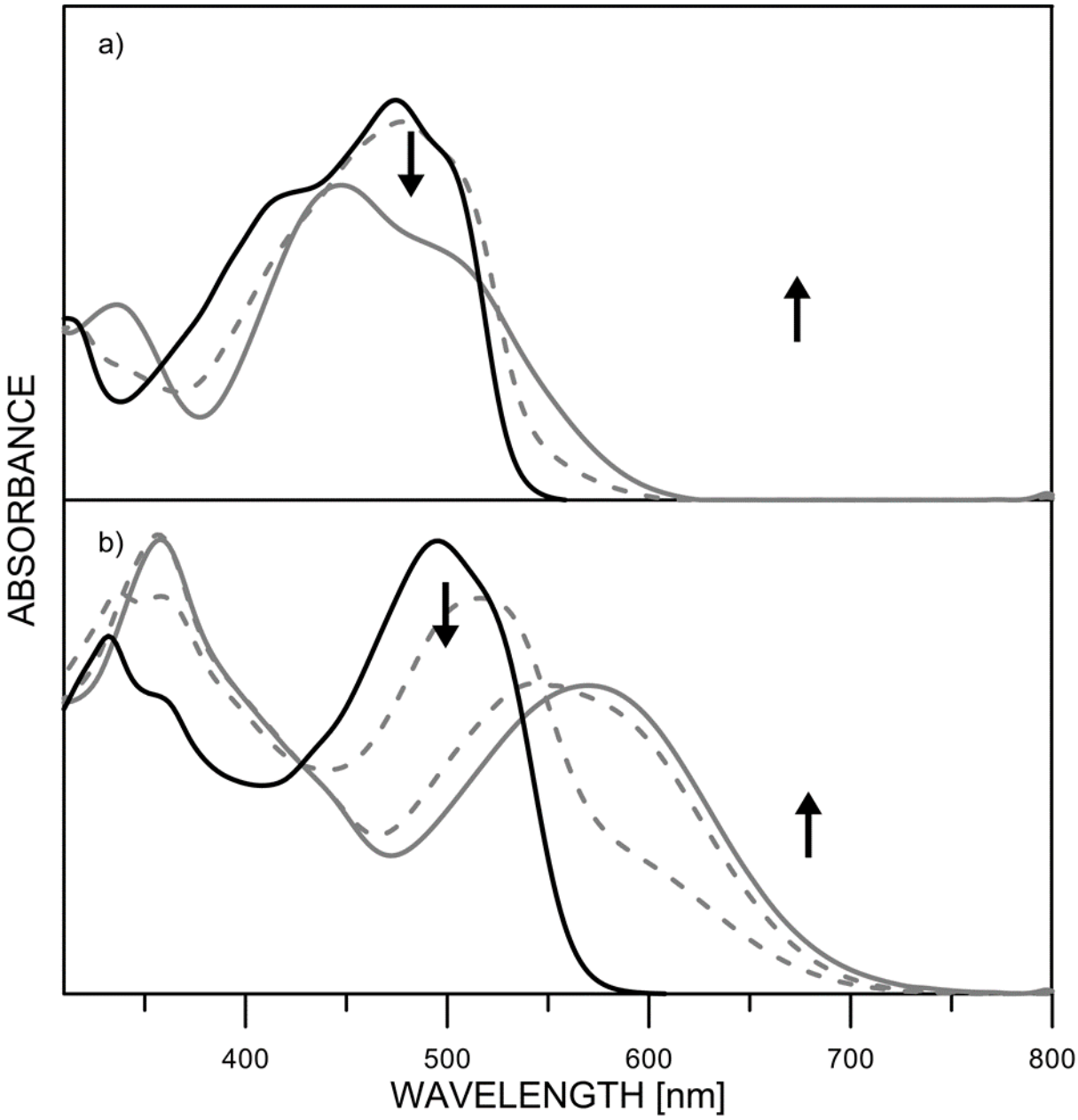


Figure S1. Absorption spectra of a) **1** and b) **2** in ACN upon base addition: (—without base addition; — final spectrum upon base addition).

Table S1 : crystallographic data of compound **3**.

Compound	3
Formula	$C_{22}H_{23}N_3O$
$D_{calc.}$/ g cm^{-3}	1.268
μ/mm^{-1}	0.079
Formula Weight	345.43
Colour	red
Shape	block
Size/mm^3	0.20×0.15×0.08
T/K	250
Crystal System	triclinic
Space Group	P-1
a/Å	10.8103(10)
b/Å	11.2369(12)
c/Å	17.1688(18)
α/°	80.314(10)
β/°	75.096(7)
γ/°	64.142(7)
V/Å^3	1809.8(3)
Z	4
Z'	2
Wavelength/Å	0.71073
Radiation type	MoK$_\alpha$
Θ_{min}/°	1.230
Θ_{max}/°	25.219
Measured Refl.	23416
Independent Refl.	6462
Reflections Used	1986
R_{int}	0.1037
Parameters	469
Restraints	0
Largest Peak	0.133
Deepest Hole	-0.127
GooF	0.723
wR_2 (all data)	0.1004
wR_2	0.0729
R_1 (all data)	0.1714
R_1	0.0424

A red block-shaped crystal with dimensions 0.20×0.15×0.08 mm^3 was mounted on a MiTeGen holder in oil. X-ray diffraction data were collected using a STOE IPDS 2 diffractometer equipped with a Oxford Cryosystems low-temperature device, operating at T = 250 K.

Data were measured using rotation method scans using MoK$_\alpha$ radiation (fine-focus sealed tube). The maximum resolution achieved was Θ = 25.219°.

Cell parameters were retrieved using the X-Area (Stoe & Cie, 2009) software and refined using X-RED32(Stoe & Cie, 2009) on 5733 reflections, 24 % of the observed reflections. Data reduction was performed using the X-RED32(Stoe & Cie, 2009) software which corrects for Lorentz polarisation. The final completeness is 98.90 % out to 25.219° in Θ.

A integration absorption correction was performed using Stoe & Cie (2002). X-SHAPE. Stoe & Cie, Darmstadt, Germany The absorption coefficient μ of this material is 0.079 mm^{-1} at this wavelength (λ = 0.71073Å) and the minimum and maximum transmissions are 0.7405 and

0.9710.

The structure was solved in the space group *P*-1 (# 2) by Intrinsic Phasing using the **ShelXT** (Sheldrick, 2015) structure solution program and refined by Least Squares using version 2017/1 of **ShelXL** (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

Refinement model details :

1. Fixed Uiso, at 1.2 times of all C(H) groups, all C(H,H) groups, all N(H) groups
2.a Riding coordinates: N1(H1), N4(H4a)
2.b Secondary CH2 refined with riding coordinates: C17(H17a,H17b), C18(H18a,H18b), C19(H19a,H19b), C20(H20a,H20b), C21(H21a,H21b), C22(H22a,H22b), C39(H39a,H39b), C40(H40a,H40b), C41(H41a,H41b), C42(H42a,H42b), C43(H43a,H43b), C44(H44a,H44b)
2.c Aromatic/amide H refined with riding coordinates: C1(H1a), C2(H2), C3(H3), C4(H4), C5(H5), C10(H10), C12(H12), C13(H13), C14(H14), C15(H15), C23(H23), C24(H24), C25(H25), C26(H26), C27(H27), C32(H32), C34(H34), C35(H35), C36(H36), C37(H37)

_exptl_absorpt_process_details: Stoe & Cie (2002). X-SHAPE. Stoe & Cie, Darmstadt, Germany

Table S2: Hydrogen Bond information for **3**.

D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/deg**
N1	H1	O1	0.97	1.75	2.522(4)	133.9
N4	H4A	O2	0.91	1.75	2.500(4)	137.8

Scheme S1: labelling of crystal structure of **3**.

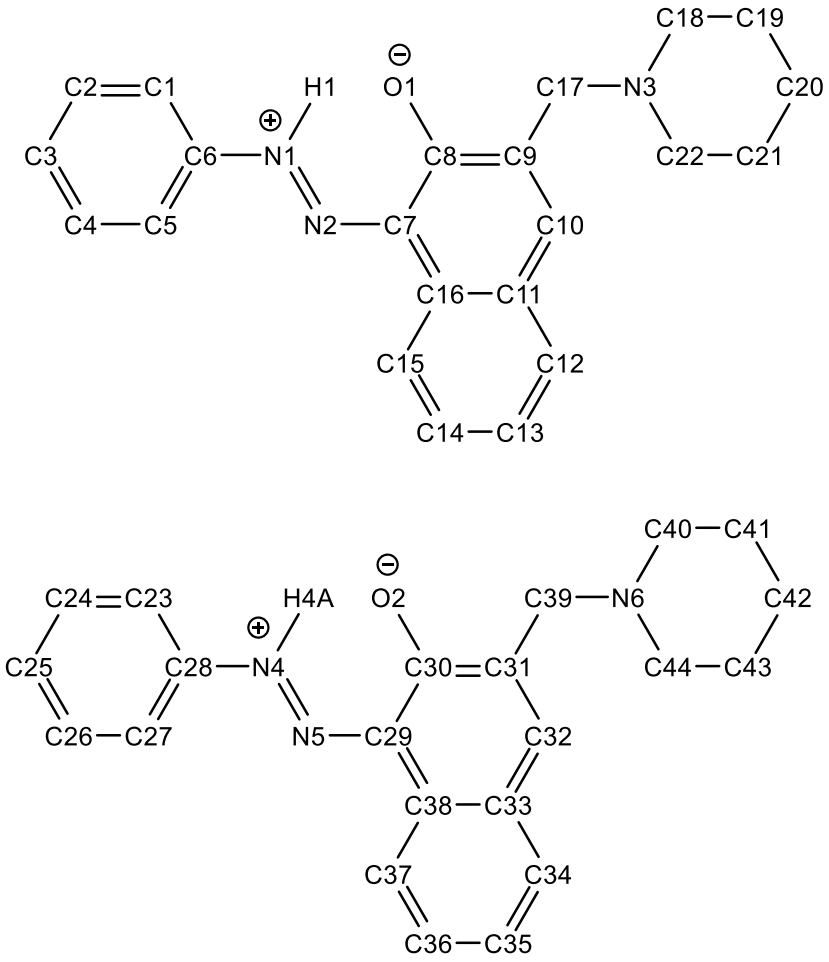


Figure S2: Statistics on N-N bonds in Ph-N-N-Ph motifs (no H atoms request). (CSD version 5.38, updates May 2017, 207 hits)

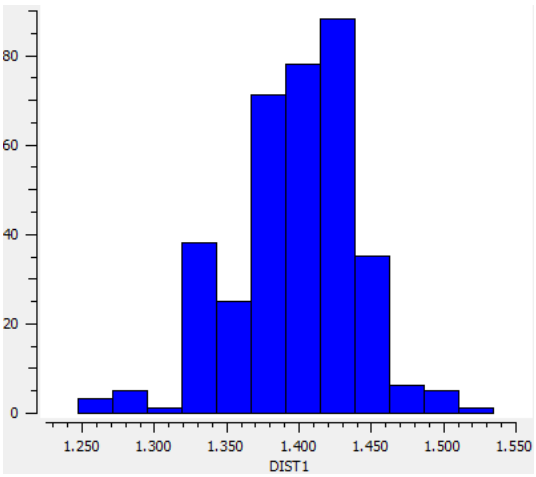
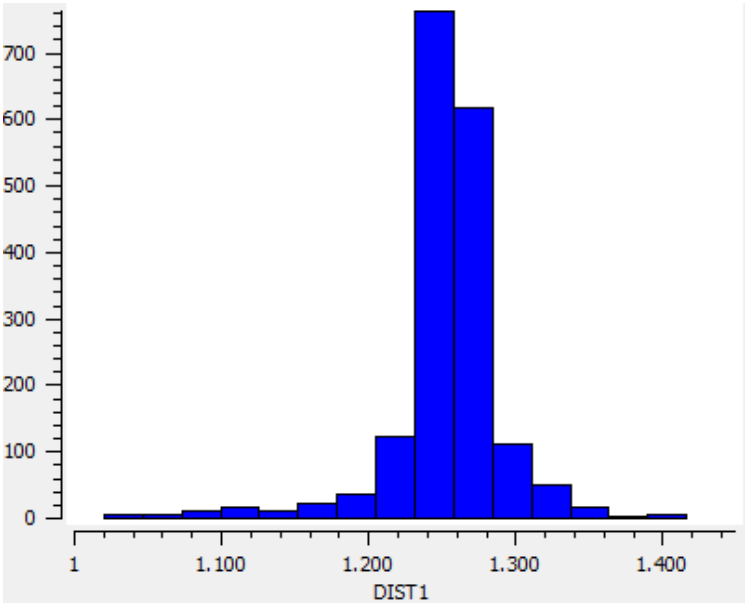


Figure S3: Statistics on N=N bonds in Ph-N=N-Ph motifs (no H atoms request). (CSD version 5.38, updates May 2017, 1377 hits)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