

Examining the Non-Covalent Interactions for Two Polymorphs of a 2,1,3-benzoxadiazole Derivative

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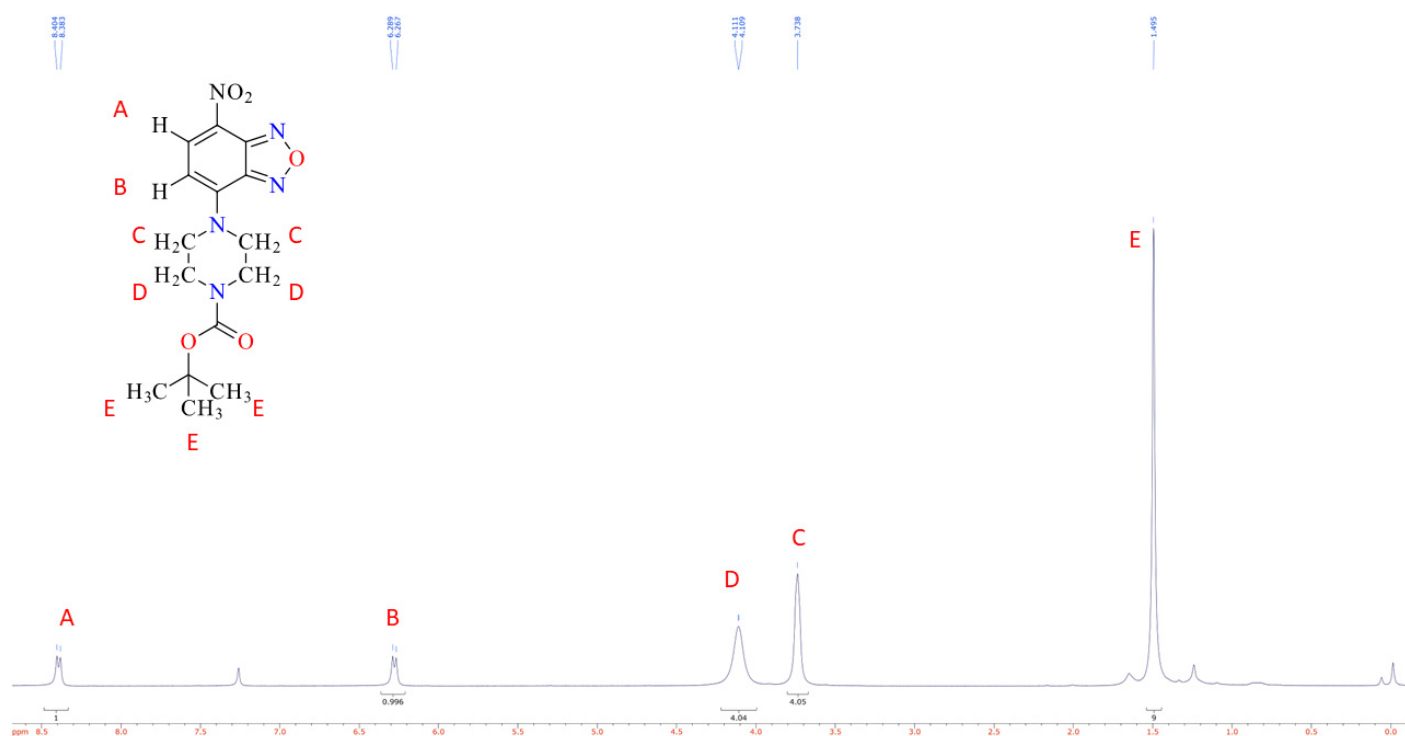


Figure S1. ¹H NMR of compound 1.

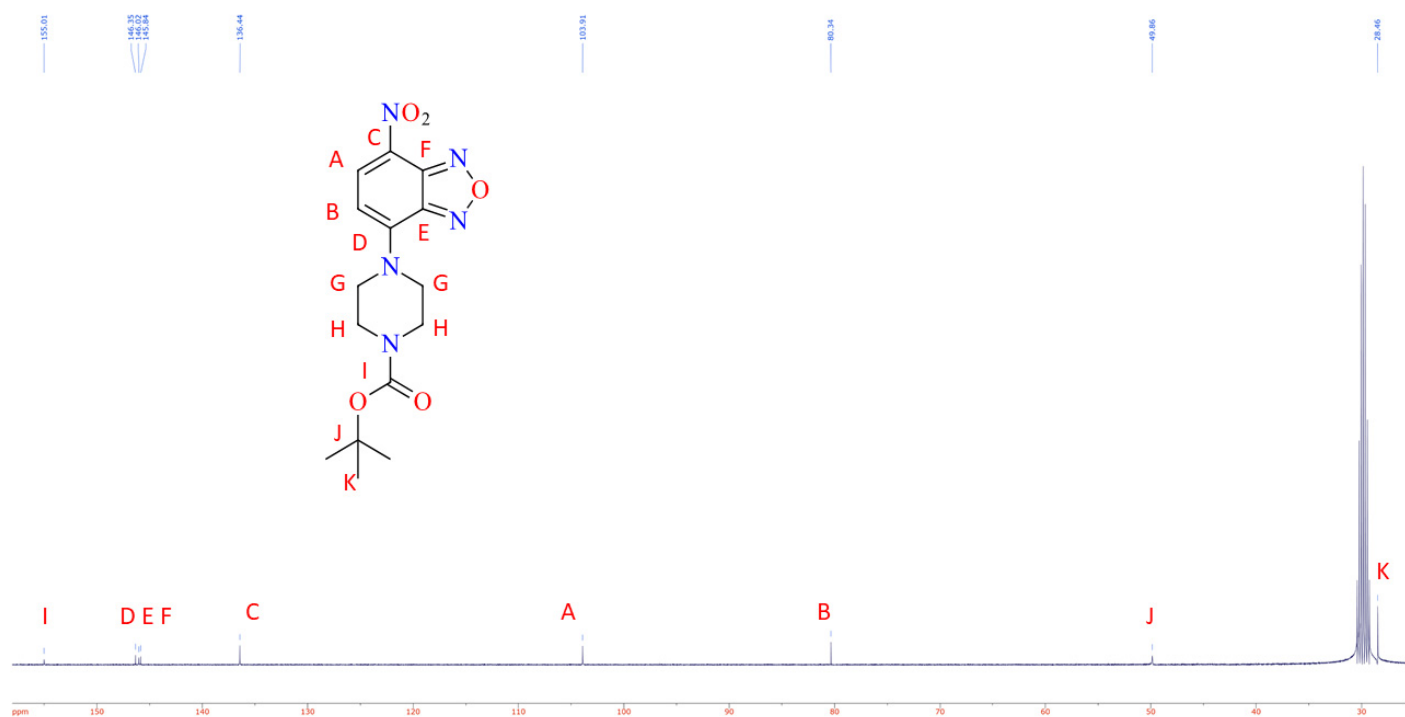


Figure S2. ¹³C NMR of compound 2.

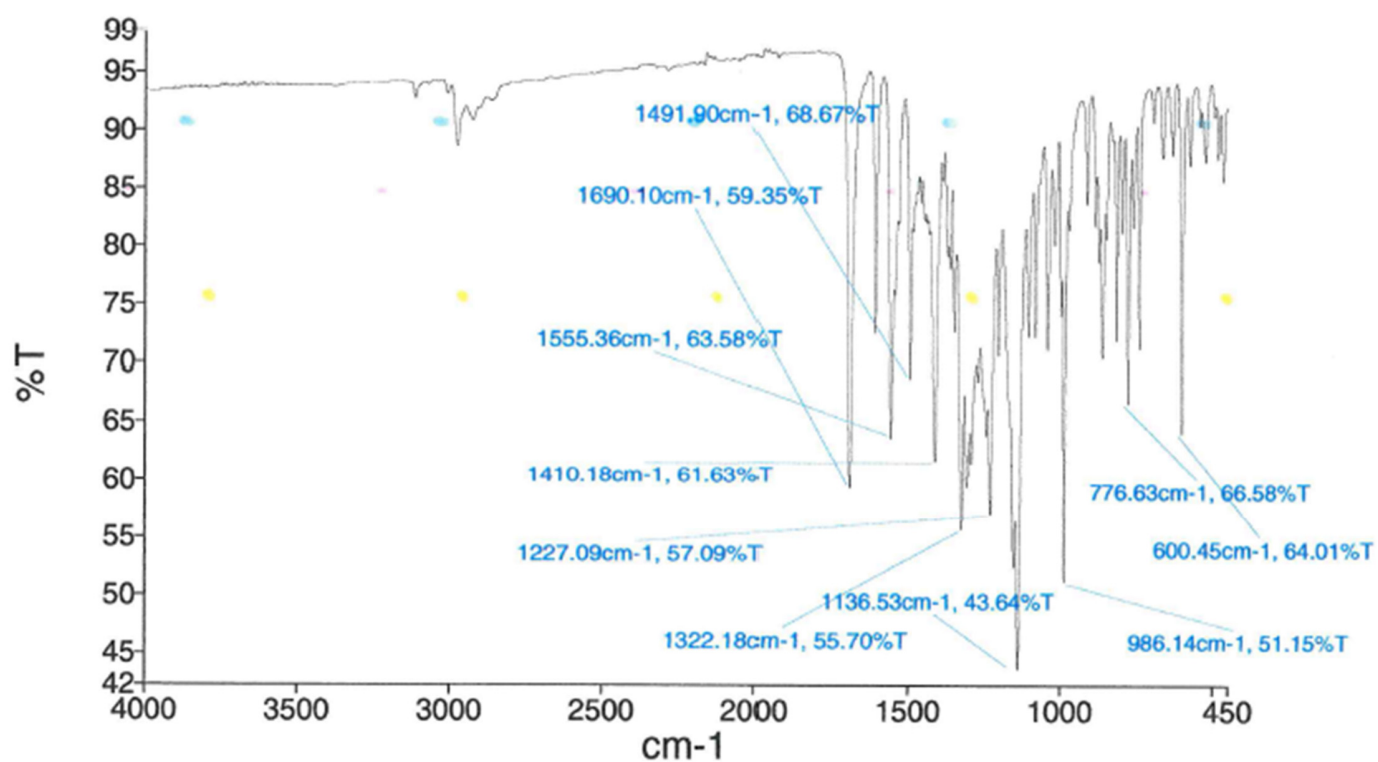


Figure S3. Infrared spectrum of Compound 1 taken from reaction.

	Compound 1-M
Crystal data	
Chemical formula	C ₁₅ H ₁₉ N ₅ O ₅
<i>M</i> _r	349.35
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.9124 (11), 8.5559 (8), 16.5519 (11)
β (°)	107.166 (3)
<i>V</i> (Å ³)	1611.8 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.11
Crystal size (mm)	0.29 × 0.27 × 0.23
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Absorption correction	Multi-scan <i>SADABS</i> 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., <i>J. Appl. Cryst.</i> 48 (2015) 3-10
<i>T</i> _{min} , <i>T</i> _{max}	0.599, 0.747
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	23605, 6121, 4546
<i>R</i> _{int}	0.041
(sin θ/λ) _{max} (Å ⁻¹)	0.770
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.044, 0.115, 1.02
No. of reflections	6121
No. of parameters	229
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.39, -0.27

Compound 1-O	
Crystal data	
Chemical formula	C ₁₅ H ₁₉ N ₅ O ₅
<i>M_r</i>	349.35
Crystal system, space group	Orthorhombic, <i>Pca</i> 2 ₁
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	33.438 (5), 6.4498 (9), 7.6136 (10)
<i>V</i> (Å ³)	1642.0 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.11
Crystal size (mm)	0.27 × 0.18 × 0.05
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Absorption correction	Multi-scan <i>SADABS</i> 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., <i>J. Appl. Cryst.</i> 48 (2015) 3-10
<i>T</i> _{min} , <i>T</i> _{max}	0.663, 0.746
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	12333, 3813, 3206
<i>R</i> _{int}	0.047
(sin θ/λ) _{max} (Å ⁻¹)	0.668
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.039, 0.089, 1.05
No. of reflections	3813
No. of parameters	229
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.28, -0.21
Absolute structure	Flack <i>x</i> determined using 1217 quotients [(<i>I</i> ⁺)-(<i>I</i> ⁻)]/[(<i>I</i> ⁺)+(<i>I</i> ⁻)] (Parsons, Flack and Wagner, <i>Acta Cryst. B</i> 69 (2013) 249-259).
Absolute structure parameter	0.0 (6)