Electronic Supplementary Information

Thermodynamic parameters of the pedal motion in the crystal structures of two bromomethylated azobenzenes

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Table S1. Experimental details of x-ray structure determination for compound **1.**

Temperature (K)	90	120	150	180	210	250	270	300	330	375
Crystal data										
Chemical formula	$C_{14}H_{12}Br_2N_2$									
M_r	368.08									
Crystal system, space group	Monoclinic, $P2_1/c$									
a, b, c (Å)	13.858 (2), 4.3834 (7), 11.1513 (17)	13.8531 (19), 4.3928 (6), 11.1633 (15)	13.891 (2), 4.4024 (7), 11.1676 (17)	13.936 (2), 4.4112 (7), 11.1717 (16)	13.9822 (18), 4.4209 (6), 11.1785 (14)	14.0179 (18), 4.4297 (6), 11.1892 (14)	14.051 (2), 4.4406 (6), 11.2041 (16)	14.0837 (18), 4.4538 (6), 11.2236 (14)	14.105 (3), 4.4657 (10), 11.245 (2)	14.129 (5), 4.4805 (14), 11.264 (4)
β (°)	98.584 (2)	98.597 (2)	98.719 (2)	98.840 (2)	98.951 (2)	99.047 (2)	99.129 (2)	99.2049 (18)	99.262 (3)	99.369 (5)
V (Å^3)	669.81 (18)	671.70 (16)	675.03 (18)	678.62 (17)	682.57 (15)	686.15 (15)	690.24 (17)	694.95 (16)	699.1 (3)	703.6 (4)
Z	2									
Radiation type	Mo $K\alpha$									
μ (mm^{-1})	6.03	6.02	5.99	5.96	5.92	5.89	5.86	5.82	5.78	5.74
Crystal size (mm)	0.55 × 0.52 × 0.47									
Data collection										
Diffractometer	Bruker Smart Apex area detector diffractometer									
Absorption correction	Multi-scan, Bruker SADABS 2008-1									
T_{min}, T_{max}	0.530, 0.746									
No. of measured, independent and observed [I > 2σ(I)] reflections	6248, 2091, 1867	6638, 2111, 1839	6512, 2119, 1794	6570, 2135, 1746	7202, 2155, 1679	7107, 2174, 1588	7672, 2197, 1541	6558, 2157, 1442	6764, 2196, 1312	7885, 2250, 1275
R_{int}	0.025	0.025	0.025	0.028	0.029	0.031	0.031	0.023	0.033	0.034
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.739	0.738	0.738	0.738	0.738	0.739	0.739	0.737	0.735	0.739
Refinement										
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.055, 1.06	0.022, 0.055, 1.06	0.025, 0.062, 1.05	0.027, 0.066, 1.08	0.028, 0.071, 1.06	0.030, 0.076, 1.04	0.031, 0.080, 1.02	0.039, 0.096, 1.03	0.035, 0.088, 1.01	0.032, 0.094, 1.00
Fraction of major conformer	0.963(2)	0.969(2)	0.930(3)	0.884(3)	0.834(4)	0.782(4)	0.741(4)	0.718(5)	0.667(5)	0.639(4)
No. of reflections	2091	2111	2119	2135	2155	2174	2197	2157	2196	2250
No. of parameters	111									
No. of restraints	21									
H-atom treatment	H-atom parameters constrained									
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.95, −0.54	0.80, −0.49	0.77, −0.47	0.71, −0.40	0.53, −0.39	0.39, −0.36	0.41, −0.34	0.40, −0.47	0.33, −0.34	0.29, −0.30

Table S2. Experimental details of x-ray structure determination for compound **2**

Temperature (K)	90	140	190	240	293	340	375
Crystal data							
Chemical formula	$C_{14}H_{12}Br_2N_2$						
M_r	368.08						
Crystal system, space group	Monoclinic, $P2_1/c$						
a, b, c (Å)	12.9324 (11), 4.4704 (4), 11.5909 (10)	12.9484 (15), 4.4854 (5), 11.6092 (13)	12.9648 (11), 4.5026 (4), 11.6333 (10)	12.9974 (15), 4.5160 (5), 11.6594 (13)	13.035 (10), 4.527 (4), 11.687 (10)	13.061 (3), 4.5482 (9), 11.736 (2)	13.097 (4), 4.5652 (15), 11.779 (4)
β (°)	102.592 (1)	102.5452 (14)	102.499 (1)	102.481 (2)	102.573 (10)	102.463 (3)	102.471 (5)
V (Å^3)	653.99 (10)	658.15 (13)	663.00 (10)	668.19 (13)	673.1 (10)	680.7 (2)	687.7 (4)
Z	2						
Radiation type	Mo $K\alpha$						
μ (mm^{-1})	6.18	6.14	6.10	6.05	6.00	5.94	5.88
Crystal size (mm)	0.55 × 0.34 × 0.17						
Data collection							
Diffractometer	Bruker Smart 1000 area detector diffractometer						
Absorption correction	Multi-scan, SADABS2008/1						
T_{min}, T_{max}	0.250, 0.746	0.249, 0.746	0.253, 0.746	0.248, 0.746	0.362, 0.746	0.255, 0.746	0.273, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14059, 2062, 1933	7391, 2156, 1907	14654, 2170, 1908	7535, 2184, 1705	15300, 2211, 1684	7724, 2224, 1373	15439, 2239, 1472
R_{int}	0.040	0.041	0.043	0.043	0.044	0.045	0.046
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.722	0.744	0.746	0.745	0.714	0.744	0.741
Refinement							
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.073, 1.063	0.029, 0.078, 1.05	0.032, 0.085, 1.10	0.034, 0.089, 1.02	0.038, 0.109, 1.08	0.039, 0.112, 0.97	0.045, 0.127, 1.10
Fraction of major conformer	0.768(3)	0.771(3)	0.778(4)	0.732(4)	0.686(4)	0.645(5)	0.632(5)
No. of reflections	2062	2156	2170	2184	2211	2224	2239
No. of parameters	110						
No. of restraints	17						
H-atom treatment	H-atom parameters constrained						
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.63, −0.94	0.47, −0.93	0.47, −0.93	0.38, −0.86	0.39, −0.84	0.30, −0.63	0.30, −0.52