

Supplementary Information

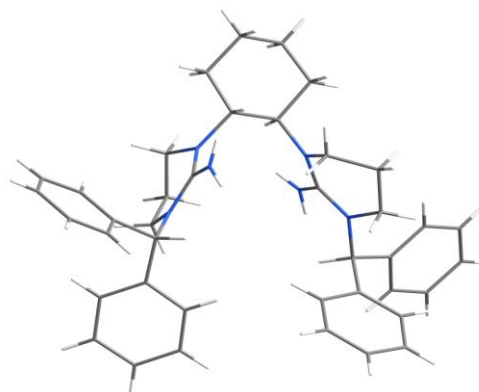
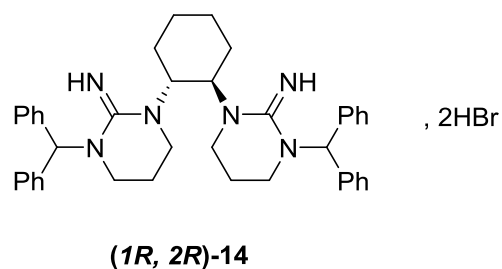
3-Bromo *N*-Alkyl Cyanamides as Versatile Building Blocks.

Wright, K. , Drouillat, B. , Menguy, L. , Marrot, J. and Couty, F.

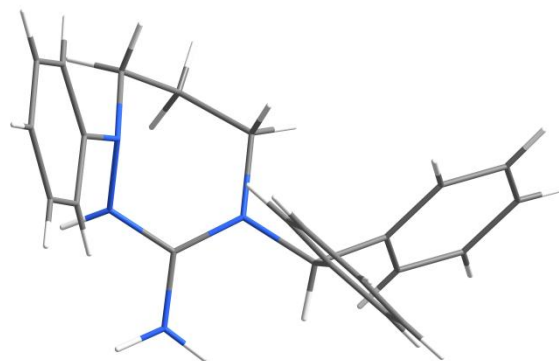
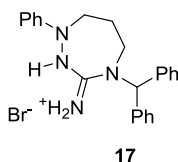
Eur. J. Org. Chem., 2019: 112-117. doi:[10.1002/ejoc.201801439](https://doi.org/10.1002/ejoc.201801439) ,

Contents:

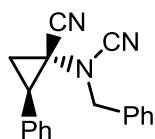
1. X-ray data for **14**, **17** and **26**
2. Copies of ^1H and ^{13}C NMR spectra for all new compounds



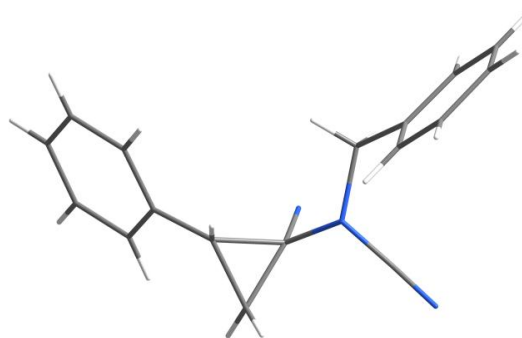
Empirical formula	C ₄₀ H ₄₈ Br ₂ N ₆
Formula weight	772.66
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
Unit cell dimensions	a = 7.7645(3) Å α = 90°. b = 22.0759(6) Å β = 90°. c = 22.8524(6) Å γ = 90°.
Volume	3917.1(2) Å ³
Z	4
Density (calculated)	1.310 Mg/m ³
Absorption coefficient	2.104 mm ⁻¹
F(000)	1600
Crystal size	0.300 x 0.080 x 0.040 mm ³
Theta range for data collection	1.782 to 25.052°.
Index ranges	-9 ≤ h ≤ 9, -26 ≤ k ≤ 26, -27 ≤ l ≤ 27
Reflections collected	46066
Independent reflections	6892 [R(int) = 0.0644]
Completeness to theta = 25.052°	99.6 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6892 / 0 / 433
Goodness-of-fit on F ²	1.044
Final R indices [I > 2σ(I)]	R1 = 0.0460, wR2 = 0.1063
R indices (all data)	R1 = 0.0613, wR2 = 0.1119
Absolute structure parameter	0.037(5)
Extinction coefficient	n/a
Largest diff. peak and hole	0.418 and -0.473 e.Å ⁻³



Empirical formula	C ₂₃ H ₂₅ Br N ₄
Formula weight	437.38
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 8.2818(5) Å α = 101.306(3)° b = 11.6418(6) Å β = 93.417(3)° c = 11.8747(7) Å γ = 108.729(3)°
Volume	1053.93(11) Å ³
Z	2
Density (calculated)	1.378 Mg/m ³
Absorption coefficient	1.966 mm ⁻¹
F(000)	452
Crystal size	0.300 x 0.180 x 0.100 mm ³
Theta range for data collection	2.278 to 25.051°
Index ranges	-9 ≤ h ≤ 9, -13 ≤ k ≤ 13, -14 ≤ l ≤ 14
Reflections collected	16145
Independent reflections	3696 [R(int) = 0.0746]
Completeness to theta = 25.051°	98.8 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3696 / 0 / 253
Goodness-of-fit on F ²	1.158
Final R indices [I > 2σ(I)]	R1 = 0.0632, wR2 = 0.1249
R indices (all data)	R1 = 0.0822, wR2 = 0.1358
Extinction coefficient	n/a
Largest diff. peak and hole	0.919 and -0.766 e.Å ⁻³



26



Empirical formula	C ₁₈ H ₁₅ N ₃
Formula weight	273.33
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
Unit cell dimensions	a = 6.0229(4) Å α = 90° b = 10.9007(6) Å β = 90° c = 22.3630(14) Å γ = 90°
Volume	1468.22(16) Å ³
Z	4
Density (calculated)	1.237 Mg/m ³
Absorption coefficient	0.075 mm ⁻¹
F(000)	576
Crystal size	0.300 x 0.080 x 0.020 mm ³
Theta range for data collection	2.609 to 30.100°
Index ranges	-8 ≤ h ≤ 8, -15 ≤ k ≤ 15, -31 ≤ l ≤ 31
Reflections collected	84562
Independent reflections	4312 [R(int) = 0.0794]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4312 / 0 / 190
Goodness-of-fit on F ²	1.075
Final R indices [I > 2σ(I)]	R1 = 0.0397, wR2 = 0.0992
R indices (all data)	R1 = 0.0445, wR2 = 0.1024
Absolute structure parameter	0.3(6)
Extinction coefficient	n/a
Largest diff. peak and hole	0.235 and -0.246 e.Å ⁻³

