



STRUCTURAL
CHEMISTRY

Volume 77 (2021)

Supporting information for article:

Co(NCS)₂(abpt)₂ and Ni(NCS)₂(abpt)₂ [abpt is 4-amino-3,5-bis-(pyridin-2-yl)-1,2,4-triazole]: structural characterization of polymorphs A and B

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Table S1 Experimental details at 300(2) K

	Co(abpt) ₂ (NCS) ₂ Polymorph A	Co(abpt) ₂ (NCS) ₂ Polymorph B
Crystal data		
Chemical formula	C ₂₆ H ₂₀ CoN ₁₄ S ₂	C ₂₆ H ₂₀ CoN ₁₄ S ₂
<i>M_r</i>	651.61	651.61
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	300	300
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.487 (5), 10.249 (6), 16.539 (10)	11.5855 (6), 9.5998 (5), 12.8411 (6)
β (°)	93.419 (13)	101.300 (1)
<i>V</i> (Å ³)	1435.9 (14)	1400.48 (12)
<i>Z</i>	2	2
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	0.79	0.81
Crystal size (mm)	0.24 × 0.16 × 0.12	0.48 × 0.22 × 0.1
Data collection		
Diffractometer	Bruker <i>SMART</i> CCD 1K area detector	Bruker <i>SMART</i> CCD 1K area detector
Absorption correction	Multi-scan <i>SADABS2008/1</i> (Bruker,2008) was used for absorption correction. <i>w</i> R2(int) was 0.1268 before and 0.0594 after correction. The Ratio of minimum to maximum transmission is 0.7415. The λ/2 correction factor is 0.0015.	Multi-scan <i>SADABS2008/1</i> (Bruker,2008) was used for absorption correction. <i>w</i> R2(int) was 0.0699 before and 0.0469 after correction. The Ratio of minimum to maximum transmission is 0.9080. The λ/2 correction factor is 0.0015.
<i>T_{min}</i> , <i>T_{max}</i>	0.683, 0.921	0.805, 0.887
No. of measured, independent and	7130, 2605, 1378	7562, 2565, 2034

observed [$I > 2\sigma(I)$] reflections

R_{int} 0.087 0.031

$(\sin \theta/\lambda)_{\text{max}}$ (\AA^{-1}) 0.602 0.602

Refinement

$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S 0.059, 0.166, 1.02 0.034, 0.079, 1.03

No. of reflections 2605 2565

No. of parameters 202 202

No. of restraints 0 0

H-atom treatment H atoms treated by a mixture of independent and constrained refinement H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e \AA^{-3}) 0.36, -0.47 0.22, -0.27

Computer programs: *SMART* v5.049 (Bruker, 1999), *SAINT* v6.45A (Bruker, 2003), *APEX2* (Bruker, 2005), *APEX2 SAINT+* V8.32B (Bruker, 2013), *SHELXS* (Sheldrick, 2008), *SHELXS1997* (Sheldrick, 2008), *SHELXL* 2018/3 (Sheldrick, 2015), *XL* (Sheldrick, 2008), *Olex2* 1.3 (Dolomanov *et al.*, 2009).