

Table 1. Data collection and crystal parameters

For all structures: $\text{CoH}_{15}\text{N}_6\text{O}_2\cdot\text{NO}_3\cdot\text{Cl}$, $M_r = 287.57$, orthorhombic, $Pnma$, $Z = 4$. Experiments were carried out with Mo $K\alpha$ radiation using a STOE IPDS 2 diffractometer. Crystal size - $0.30 \times 0.20 \times 0.15$ (mm^3). Absorption was corrected for by numerical methods, implemented in *X-RED* software.

Crystal data			
Temperature (K)	100	113	133
a, b, c (Å)	14.7021 (11), 7.1057 (8), 9.6760 (7)	14.7044 (11), 7.1209 (8), 9.6716 (7)	14.7115 (11), 7.1415 (8), 9.6639 (7)
V (Å ³)	1010.84 (15)	1012.70 (15)	1015.31 (15)
D_x (Mg m ⁻³)	1.890	1.886	1.881
μ (mm ⁻¹)	1.98	1.97	1.97
Crystal size (mm)	$0.30 \times 0.20 \times 0.15$	$0.30 \times 0.20 \times 0.15$	$0.30 \times 0.20 \times 0.15$
Data collection			
T_{\min}, T_{\max}	0.651, 0.771	0.646, 0.778	0.652, 0.771
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6811, 1119, 960	6815, 1121, 970	6849, 1123, 966
R_{int}	0.044	0.046	0.045
θ values (°)	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$
Range of h, k, l	$h = -18 \rightarrow 18, k = -8 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -8 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -8 \rightarrow 8, l = -12 \rightarrow 12$
Refinement			
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.019, 0.048, 1.02	0.020, 0.049, 1.02	0.020, 0.052, 1.02
No. of reflections	1119	1121	1123
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.23, -0.38	0.28, -0.40	0.27, -0.40

Crystal data			
Temperature (K)	153	173	193
a, b, c (Å)	14.7211 (11), 7.1625 (8), 9.6562 (7)	14.7279 (11), 7.1809 (8), 9.6504 (7)	14.7390 (11), 7.2001 (8), 9.6461 (7)
V (Å ³)	1018.15 (15)	1020.62 (16)	1023.67 (16)
D_x (Mg m ⁻³)	1.876	1.871	1.866
μ (mm ⁻¹)	1.96	1.96	1.95
Crystal size (mm)	$0.30 \times 0.20 \times 0.15$	$0.30 \times 0.20 \times 0.15$	$0.30 \times 0.20 \times 0.15$

Data collection			
T_{\min}, T_{\max}	0.653, 0.773	0.653, 0.772	0.655, 0.773
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6847, 1123, 962	6877, 1124, 958	6889, 1129, 971
R_{int}	0.045	0.045	0.047
θ values ($^{\circ}$)	$\theta_{\max} = 26.3, \theta_{\min} = 2.5$	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$
Range of h, k, l	$h = -18 \rightarrow 18, k = -8 \rightarrow 8, l = -11 \rightarrow 12$	$h = -18 \rightarrow 18, k = -8 \rightarrow 8, l = -11 \rightarrow 12$	$h = -18 \rightarrow 18, k = -8 \rightarrow 8, l = -11 \rightarrow 12$
Refinement			
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.021, 0.052, 1.03	0.021, 0.053, 1.04	0.022, 0.054, 1.07
No. of reflections	1123	1124	1129
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ($\text{e } \text{\AA}^{-3}$)	0.28, -0.36	0.30, -0.37	0.31, -0.40

Crystal data			
Temperature (K)	213	233	253
a, b, c (\AA)	14.736 (2), 7.2220 (11), 9.6239 (13)	14.755 (2), 7.2394 (11), 9.6181 (13)	14.770 (2), 7.2540 (11), 9.6152 (13)
V (\AA^3)	1024.2 (3)	1027.4 (3)	1030.2 (3)
D_x (Mg m^{-3})	1.865	1.859	1.854
μ (mm^{-1})	1.95	1.95	1.94
Crystal size (mm)	$0.30 \times 0.20 \times 0.15$	$0.30 \times 0.20 \times 0.15$	$0.30 \times 0.20 \times 0.15$
Data collection			
T_{\min}, T_{\max}	0.667, 0.773	0.660, 0.782	0.660, 0.782
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6888, 1126, 981	6950, 1133, 983	6969, 1139, 978
R_{int}	0.066	0.048	0.048
θ values ($^{\circ}$)	$\theta_{\max} = 26.3, \theta_{\min} = 2.5$	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$
Range of h, k, l	$h = -18 \rightarrow 18, k = -8 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$
Refinement			
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.026, 0.063, 1.10	0.027, 0.064, 1.10	0.027, 0.066, 1.08
No. of reflections	1126	1133	1139
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ($\text{e } \text{\AA}^{-3}$)	0.36, -0.42	0.27, -0.53	0.29, -0.56

Crystal data			
Temperature (K)	273	293	303
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.787 (2), 7.2696 (11), 9.6113 (13)	14.804 (2), 7.2851 (11), 9.6112 (14)	14.815 (2), 7.2951 (11), 9.6129 (13)
<i>V</i> (Å ³)	1033.1 (3)	1036.6 (3)	1039.0 (3)
<i>D_x</i> (Mg m ⁻³)	1.849	1.843	1.838
μ (mm ⁻¹)	1.94	1.93	1.92
Crystal size (mm)	0.30 × 0.20 × 0.15	0.30 × 0.20 × 0.15	0.30 × 0.20 × 0.15
Data collection			
<i>T</i> _{min} , <i>T</i> _{max}	0.662, 0.783	0.663, 0.784	0.662, 0.784
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	6985, 1141, 961	6968, 1141, 966	6985, 1143, 964
<i>R</i> _{int}	0.045	0.045	0.043
θ values (°)	θ _{max} = 26.4, θ _{min} = 2.5	θ _{max} = 26.4, θ _{min} = 2.5	θ _{max} = 26.4, θ _{min} = 2.5
Range of <i>h</i> , <i>k</i> , <i>l</i>	<i>h</i> = -18→18, <i>k</i> = -9→8, <i>l</i> = -12→12	<i>h</i> = -18→18, <i>k</i> = -9→8, <i>l</i> = -12→12	<i>h</i> = -18→18, <i>k</i> = -9→8, <i>l</i> = -12→12
Refinement			
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.027, 0.066, 1.08	0.027, 0.065, 1.08	0.027, 0.063, 1.12
No. of reflections	1141	1141	1143
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.30, -0.53	0.32, -0.42	0.31, -0.39

Crystal data			
Temperature (K)	313	323	333
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.825 (2), 7.3004 (11), 9.6126 (14)	14.832 (2), 7.3084 (11), 9.6102 (14)	14.841 (2), 7.3153 (11), 9.6100 (13)
<i>V</i> (Å ³)	1040.3 (3)	1041.7 (3)	1043.3 (3)
<i>D_x</i> (Mg m ⁻³)	1.836	1.834	1.831
μ (mm ⁻¹)	1.92	1.92	1.92
Crystal size (mm)	0.30 × 0.20 × 0.15	0.30 × 0.20 × 0.15	0.30 × 0.20 × 0.15
Data collection			
<i>T</i> _{min} , <i>T</i> _{max}	0.662, 0.784	0.662, 0.784	0.663, 0.785
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)]	6992, 1144, 960	7004, 1146, 961	7017, 1148, 974

reflections			
R_{int}	0.043	0.042	0.042
θ values ($^{\circ}$)	$\theta_{\text{max}} = 26.4, \theta_{\text{min}} = 2.5$	$\theta_{\text{max}} = 26.4, \theta_{\text{min}} = 2.5$	$\theta_{\text{max}} = 26.4, \theta_{\text{min}} = 2.5$
Range of h, k, l	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$
Refinement			
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.027, 0.065, 1.13	0.027, 0.066, 1.11	0.028, 0.067, 1.11
No. of reflections	1144	1146	1148
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ($\text{e } \text{\AA}^{-3}$)	0.31, -0.39	0.32, -0.43	0.30, -0.43

Crystal data			
Temperature (K)	343	353	363
a, b, c (\AA)	14.851 (2), 7.3236 (11), 9.6090 (13)	14.860 (2), 7.3294 (11), 9.6098 (14)	14.872 (2), 7.3394 (11), 9.6071 (14)
V (\AA^3)	1045.1 (3)	1046.7 (3)	1048.7 (3)
D_x (Mg m^{-3})	1.828	1.825	1.821
μ (mm^{-1})	1.91	1.91	1.91
Crystal size (mm)	$0.30 \times 0.20 \times 0.15$	$0.30 \times 0.20 \times 0.15$	$0.30 \times 0.20 \times 0.15$
Data collection			
$T_{\text{min}}, T_{\text{max}}$	0.663, 0.785	0.663, 0.785	0.665, 0.786
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7027, 1150, 956	7018, 1150, 963	7031, 1152, 958
R_{int}	0.042	0.041	0.042
θ values ($^{\circ}$)	$\theta_{\text{max}} = 26.4, \theta_{\text{min}} = 2.5$	$\theta_{\text{max}} = 26.3, \theta_{\text{min}} = 2.5$	$\theta_{\text{max}} = 26.4, \theta_{\text{min}} = 2.5$
Range of h, k, l	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$
Refinement			
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.028, 0.067, 1.10	0.029, 0.067, 1.09	0.028, 0.066, 1.06
No. of reflections	1150	1150	1152
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ($\text{e } \text{\AA}^{-3}$)	0.36, -0.43	0.30, -0.36	0.27, -0.39

Crystal data			
Temperature (K)	373	383	393
a, b, c (\AA)	14.877 (2), 7.3463	14.881 (2), 7.3506	14.896 (3), 7.3587

	(12), 9.6072 (14)	(12), 9.6096 (14)	(15), 9.6062 (17)
V (Å ³)	1050.0 (3)	1051.2 (3)	1053.0 (3)
D_x (Mg m ⁻³)	1.819	1.817	1.814
μ (mm ⁻¹)	1.90	1.90	1.90
Crystal size (mm)	0.30 × 0.20 × 0.15	0.30 × 0.20 × 0.15	0.30 × 0.20 × 0.15
Data collection			
T_{\min}, T_{\max}	0.665, 0.786	0.665, 0.786	0.664, 0.786
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7048, 1154, 949	7066, 1157, 948	7074, 1159, 953
R_{int}	0.040	0.041	0.041
θ values (°)	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$	$\theta_{\max} = 26.4, \theta_{\min} = 2.5$
Range of h, k, l	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$	$h = -18 \rightarrow 18, k = -9 \rightarrow 8, l = -12 \rightarrow 12$
Refinement			
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.029, 0.068, 1.06	0.029, 0.069, 1.05	0.029, 0.067, 1.07
No. of reflections	1154	1157	1159
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.27, -0.46	0.26, -0.40	0.25, -0.41