

Chapter 2.2

SUMMARY

Summary of current model

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This program displays the current state of refinement of the crystallographic model. The information is obtained from three files :

- the name.INS file.
- the STRUCT.CIF file
- the name.CIF file written by SHELXL using the ACTA command

If these files are not found, then default information is displayed.

Model Summary for RUCO12							
Unit Cell Information				Reflection data			
Cell axes(Å)	8.1028(0)	14.8436(0)	14.5820(0)	No. meas.	3881		
Cell angles (deg)	90.000(0)	100.653(0)	90.000(0)	No. uniq.	3031		
				No. obs.	2840		
Cell volume(Å ³)	1723.62(0)	Density (g cm ⁻¹)	2.46	R merge	0.019		
Crystal system	Monoclinic	Formula weight	2557.3	Av. I/sig(I)	65.79		
Space group	P 21/n	No. form. units Z	1	H min,max	-9 9		
F(000)	1199.9	Abs. coeff. (mm ⁻¹)	2.657	K min,max	-2 17		
				L min,max	-2 17		
Atomic species	Ru	O	C	Theta min	2.7		
No. in unit cell	12	48	48	Theta max	25.0		
Current refinement							
No. refln.	3031	Ext. coef.	0.0047	R _{all}	0.023	wR2 _{all}	0.060
No. param.	245	GOOF	1.203	R _{obs}	0.021	wR2 _{obs}	0.059
Shift/esd max	0.002	Delta-rho (eÅ ⁻³) max	0.530				
Shift/esd mean	0.000	Delta-rho (eÅ ⁻³) min	-0.389				
OK							

This window is also displayed when moving from one structure directory to a new one.