



## New Features in Profex 3.3

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### **Chemical Composition**

Calculated from refined structure composition given in LST file





ieneral iranhs	Chem	istry							
3GMN		Element	Oxide	Molecular Weight	*				
Fullprof Chemistry	19	к	K2O	94.1954					
	20	Ca	CaO	56.0794	🚳 Ovide Mol	ecular Weight ? X			
	21	Sc	Sc2O3	137.91	Fe 3 ⊕ 0 <b>4</b> ⊕ Fe <sub>3</sub> O <sub>4</sub> = 231,532600 g/mol				
	22	Ti	TiO2	79.8988					
	23	v	V2O5	181.8798					
	24	Cr	Cr2O3	151.9902					
	25	Mn	MnO	70.9374					
	26	Fe	Fe2O3	159.6922					
	27	Co	CoO	74.9326					
	28	Ni	NiO	74.7094					
	29	Cu	CuO	79.5454					
	30	Zn	ZnO	81.3794		Double-click on Element to easily change your oxides without calculation			
	31	Ga	Ga2O3	187.4382					
	32	Ge	GeO2	104.5858					
	33	As	As2O3	197.89					
	34	Se							
	35	Br							
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#### **Insert Scans to Existing Project**





#### Stack Scans



#### **Context Menu to Fix/Refine Parameters**

Right-Click on Parameter in STR file



Profex

# Context Menu to open files Right-Click on file name in SAV file

Profex - 3.3.0-rc140913						
File Edit View Run	Instrument	Window Help				
🖴 🕒 🤔 🖳	<u> </u>		- ×			
1405221a.dia 🗵 140	5221a.sav 🗵	1405221a.lst 🗵				
<pre>% Theoretical instrumental function VERZERR=cubix-ads-10mm.geq % Wavelength LAMBDA=CU % Polarization (CuKa with Graphite monochromator) POL=sqr(cos(26.6*pi/180)) pi=2*acos(0) % Phases STRUC[1 alphamen attr STRUC[1 alphamen attr STRUC[1 alphamen attr</pre>						
% Mea ired da	Redo	Ctrl+Y	-			
VAL[1]=140522 % Minimum Ang % WMIN=10 % Maximum Ang % WMAX*60 % Result list	Cut Copy <b>Paste</b> Delete	Ctrl+X Ctrl+V				
LIST=1405221a	Select All	Ctrl+A				
OUTPUT=140 % Diagram out DIAGRAMM=140522 % Global parame EPS1=0	Open file 1a.dia ters for s	zero point and sample displacement				
PARAM[1]=EPS2=00.01^0.01						
	Wav	elength: 1.54183 Å Angle: 5.013° Intensity: 445.496 cts d-Spacing: 17.627 Å Line	8, Column 13			

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### Y-Axis Unit: Counts per Second

Change in «Edit  $\rightarrow$  Preferences  $\rightarrow$  Graph  $\rightarrow$  y-axis Unit» Not available for some scan file formats



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# Improved non-blocking «Spacegrp.dat» dialog Open CIF import and Spacegrp.dat dialog at the same time

Import CIF File     Files     AMCSD-0001030-Dole	STR File         CIF File         XML File           PHASE=Dolomite // Reference=amcsd_0001030 // Formula=Ca_Mg_C2_O6 // SpacegroupNo=148 Setting=1 HermannMauguin=R-3 Lattice=Trigonal UniqueAx PARAM=A=0.480690_0.475883^0.485497 PARAM=C=1.600200_1.584198^1. RP=4 k1=0 k2=0 B1=ANISO^0.01 GEWICHT=SPHAR0 // GOAL=GrainSize(1,1,1) // GOAL=my // GOAL=my //	is=c // 616202 //			
	GOAL-D0/mite=GEWICHT*fthenelse(ifdef(d),exp(my*d*3/4),1) // E=CA Wyckoff=a x=0.00000000 y=0.00000000 z=0.0000000 TDS=0.007679 E=MG Wyckoff=b x=0.00000000 y=0.00000000 z=0.24293000 TDS=0.0064042 E=O Wyckoff=c x=0.00000000 y=-0.003550000 z=0.24392000 TDS=0.0093853 	<ul> <li>Space Group Settings</li> <li>Spacegroup Number</li> <li>143</li> <li>144</li> <li>145</li> <li>146</li> <li>147</li> <li>148</li> <li>149</li> </ul>	Hermann Mauguin R-3 R-3	Wyckoff f e d c b a	Symmetry 0 0 z 0 0 -z
✓         III         ►           Warning: No Wyckoff info         Warning: No Wyckoff info           Warning: No Wyckoff info         Marning: No Wyckoff info	ormation found in atom Mg. Check manually for standard setting! ormation found in atom C. Check manually for standard setting! ormation found in atom O. Check manually for standard setting!	150 151 152 153 154 155 156 157 158 159			
		160 1c1 Trigonal SpacegroupNo=148 Herm	▼ (show all) annMauguin=R-3 Setting=1 Lat	▼ tice=Trigonal UniqueAxis=c	Close

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#### Dump Coordinates to Output Console

Profex - 3.3.0-beta140805	
<u>File Edit View Run</u> Instrument <u>W</u> indow <u>H</u> elp	
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ND-5-80-2013-HTK-0025-end.xrdml 🔀	
9000	C:\Users\Nicola Doebelin\Documents\Develop\xrd\F11_0010\ND-5-80-2013+HTK-0025-end.xrdml
10.00 20.00	30.00 40.00 50.00 60.00 70.00 80.00 Angle [°2Theta]
Refinement Protocol	e :
<pre>x=11.632036 y=200.960870 d=7.601552 x=19.189826 y=120.576522 d=4.621391 x=32.522107 y=200.960870 d=2.750928 x=50.100337 y=200.960870 d=1.819267 x=62.498509 y=281.345217 d=1.484879</pre>	Ctrl + Double Click on Scan
W	Vavelength: 1.5406 Å Angle: 47.298° Intensity: 4581.908 cts d-Spacing: 1.920 Å Line 0, Column 0