Electronic Supplementary Material (ESI) for Dalton Transactions.
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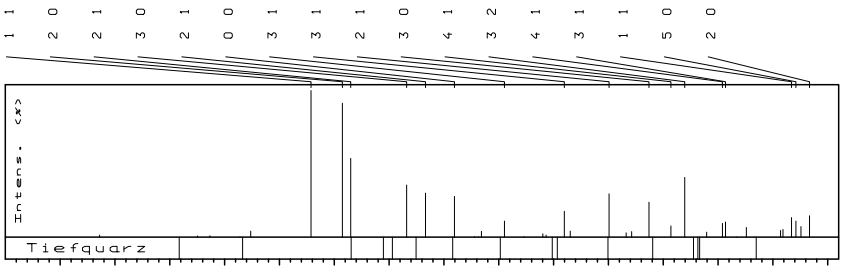
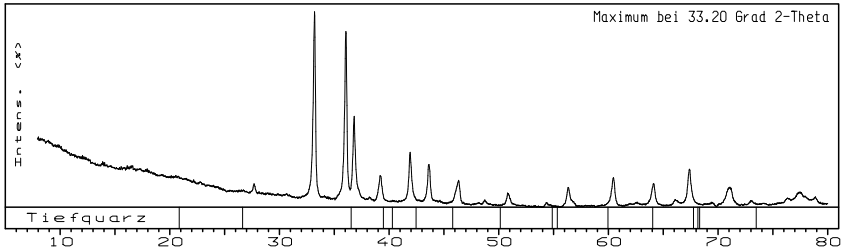
Collie2 [version10.2002] - NT-Plot vom 02-JUN-15





"Lazy-Pulverix"-Daten:

Titel: HP-CeRuSn
2-Theta-Werte: 46 (Glaettung:0.06 Grad 2-Theta)
Zellkonstanten: A = 7.51410 B = 7.51410 C = 3.94640 [A]
Al= 90.00 Be= 90.00 Ga= 120.00 [o]
V = 192.97 [A^3]
Raumgruppe: P -6 2 M

Atom	Nr	X	Y	Z	Occ	Total
SN	1	0.2505	0.0000	0.5000	1.0	3.00
CE	1	0.5925	0.0000	0.0000	1.0	3.00
RU	1	0.3333	0.6667	0.5000	1.0	2.00
RU	2	0.0000	0.0000	0.0000	1.0	1.00

"Profile"-Daten:

Datei: GH171_HP-CeRuSn.profil3.pro
Messwerte: 2989
2-Theta-Werte: Start: 7.90 Step:0.02463 Grad 2-Theta

"Asin"-Daten:

Titel: GH171_HP-CeRuSn.profil2 ..
COND: 6 1 1 1 1 1 1 1
2-Theta-Werte: 17
Zellkonstanten: A = 7.51413 B = 7.51413 C = 3.94639 [A]
0.00254 0.00000 0.00212
Al= 0.00 Be= 90.00 Ga= 120.00 [o]
0.00000 0.00000 0.00000

"2-Theta"-Werte:

h	k	l	2T c.	2T o.	I c.	I o.	h	k	l	2T c.	2T o.	I c.	I o.
1	0	0	13.60		1.4								
0	0	1	22.51		0.8								
1	1	0	23.66		1.0								
1	0	1	26.39		0.1								
2	0	0	27.39	27.40	4.1	6							
1	1	1	32.89	32.90	100.0	100							
2	0	1	35.74	35.76	91.3	88							
2	1	0	36.50	36.52	53.7	47							
3	0	0	41.60	41.62	35.5	25							
2	1	1	43.31	43.31	30.0	21							
0	0	2	45.96	45.96	27.8	12							
3	0	1	47.81		0.3								
1	0	2	48.15		0.1								
2	2	0	48.42		4.0								
3	1	0	50.53	50.50	10.9	8							
1	1	2	52.33		0.3								
2	2	1	54.02	54.01	2.3	2							
2	0	2	54.33		1.4								
3	1	1	55.98	55.98	17.7	10							
4	0	0	56.52		4.1								
2	1	2	60.06	60.00	29.5	16							
4	0	1	61.61		2.9								
3	2	0	62.12	62.13	3.8	2							
3	0	2	63.70	63.74	23.8	9							
4	1	0	65.70	65.68	7.6	2							
3	2	1	66.96	67.02	40.7	15							
2	2	2	68.96		3.4								
4	1	1	70.41		9.4								
3	1	2	70.68		10.3								
0	0	3	71.68		0.0								
5	0	0	72.58	72.58	6.6	2							
1	0	3	73.37		0.0								
4	0	2	75.71		4.5								
3	3	0	75.91		5.2								
1	1	3	76.69		13.3								
5	0	1	77.10	77.05	10.9	6							
4	2	0	77.56		7.2								
2	0	3	78.34		14.6								
3	3	1	80.38		0.2								
3	2	2	80.63		4.9								
4	2	1	82.00		8.6								
5	1	0	82.46		3.8								
2	1	3	83.22		7.5								
4	1	2	83.87		11.0								
3	0	3	86.44		0.1								
5	1	1	86.84		12.2								