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SPGR - Determine SpaceGroup from Observed Extinctions for: kla0131a

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:: Reflection Data are READ from File : latt.hkl - (OBS-Data)

:: TRMX = 1.00 0.00 0.00 0.00 1.00 0.00 0.00 0.00 1.00

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Intensity Distribution

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sh	st/l	Ang	#	0.25	1.0	2.0	0 Percent	Distr. for I	gt 2.0 s(I)	100
1	0.30	1.66	10954	91.0	80.0	62.8	*****			
2	0.38	1.32	10481	84.7	71.8	48.1	*****			
3	0.44	1.15	9319	76.5	59.6	34.5	*****			
4	0.48	1.04	8387	69.5	50.5	28.3	*****			
5	0.52	0.97	7779	65.1	44.2	23.2	*****			
6	0.55	0.91	7086	60.1	37.8	16.9	*****			
7	0.58	0.87	6744	52.4	27.9	9.9	****			
8	0.60	0.83	6472	45.9	19.3	5.3	**			
9	0.63	0.80	6042	35.2	11.6	3.0	*			
10	0.65	0.77	5684	40.4	12.9	4.2	**			
							I	I	I	
							0%	50%	100%	

Analysis of General Reflections for Bravais Centering

Nr	Ex. Condition	Aver(I/sig(I))		Number of Refl		I/sigI Max.F				.T/F. L Ratio
		.True.	.False.	.True.	.False.		H	K	L	
1	HKL:H+K=2N	1.48	1.52	41812	41870	64.89	-3	-2	0	1.0
2	HKL:H+L=2N	1.50	1.50	41831	41851	64.89	-3	-2	0	1.0
3	HKL:K+L=2N	1.49	1.51	41819	41863	63.91	-2	-3	0	1.0
4	HKL:H+K+L=2N	1.54	1.45	41863	41819	64.89	-3	-2	0	1.1
5	HKL:-H+K+L=3N	1.49	1.50	27864	55818	64.89	-3	-2	0	1.0
6	HKL:H-K+L=3N	1.48	1.51	27911	55771	64.89	-3	-2	0	1.0
41	HKL:H=2N	1.51	1.49	41842	41840	64.89	-3	-2	0	1.0
42	HKL:K=2N	1.51	1.49	41748	41934	63.91	-2	-3	0	1.0
43	HKL:L=2N	1.62	1.38	41879	41803	39.71	-3	0	-1	1.2
44	HKL:H=3N	1.50	1.50	27860	55822	63.91	-2	-3	0	1.0
45	HKL:K=3N	1.51	1.49	27837	55845	64.89	-3	-2	0	1.0
46	HKL:L=3N	1.50	1.50	27898	55784	60.25	-1	1	4	1.0
47	-HKL, H-KL=3N	1.49	1.51	46472	37210	64.89	-3	-2	0	1.0
48	-HKL:K2,KL4P2	1.48	1.71	77888	5794	54.73	3	0	2	0.9
49	-HKL:H2,HL4P2	1.48	1.71	77693	5989	48.06	2	3	0	0.9
50	-HKL:H2,HK4P2	1.49	1.57	77733	5949	51.94	2	4	2	0.9
51	HKL:H+2L=3N	1.49	1.50	27901	55781	63.91	-2	-3	0	1.0

:: No Extinction Conditions Found

Possible 2-Fold Axes - 2-Axis Crit = 0.20, Exp. Error = 0.20 Deg., LATT = P

Nr	D	Rows		Products		Angle Between Two Direct Axes								
		N Direct	Recip	Dot	Delta	1	2	3	4	5	6	7	8	9
1	20.948	0	1-1	0	1-1	0	2	0.142	0.					

==== Transformation Matrix: Input (a,b,c) to Conventional Cell(a', b', c') ====

(a') (-1.000-1.000 0.000) (a) (x') (-0.500-0.500 0.000) (x) Metrically
 (b') = (1.000-1.000 0.000) (b). (y') = (0.500-0.500 0.000) (y) Monoclinic
 (c') (0.000 0.000 1.000) (c) (z') (0.000 0.000 1.000) (z) FOM: 0.142

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	P	17.904	17.937	22.911	78.08	77.99	71.53	6747.10
Reduc Cell	P	17.904	17.937	22.911	78.08	77.99	71.53	6747.10
Conv. Cell	mC	29.082	20.948	22.911	89.94	104.80	89.89	13494.21

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***** N O T I C E *****

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- PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13
- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow
- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)
- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.
- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.
- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@chem.uu.nl
- Recent versions of PLATON may be obtained by Anonymous FTP from xraysoft.chem.uu.nl
- More INFO can be found on <http://www.cryst.chem.uu.nl/platon/>

:: Input Xtal Data from File latt.ins - Data Type SPF

:: NORMAL END of PLATON : 5 Pages on:

:: latt.lis (ASCII, 132 Characters Wide)

:: latt.lps (PostScript Version of .lis)

:: latt.pdf (PDF Version of .lis)

:: SPGR.PAR on :latt.par