PLATON(V-311206)-Run for: klat855a TIME: Nov 29 22:07:37 2011

Crystal Data

Input Cell (Lattice Type: P) - Temp = 0K

a =	14.37100	Angstrom	alpha =	90	Degree	a =	9.736	alpha =	103.77	V =	3332.0
b =	9.73600		beta =	103.7700		b =	14.371	beta =	90.00		
c =	24.51900		gamma =	90		c =	24.519	gamma =	90.00		
V =	3332.00	Cubic-Angstrom	d(100) =	13.9580	Angstrom						
			d(010) =	9.7360							
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	23.8143							

Reduced Cell (Acta Cryst.(1976),A32,297-298)

Niggli Values

94.790	206.526	601.181
-83.871	0.000	0.000

Orthogonalization Matrices

(See e.g. J.D.Dunitz, Xray Analysis and Structure Determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

$$(XO) = \begin{pmatrix} 14.37100 & 0 & -5.83613 \\ 0 & 9.73600 & 0 \\ 0 & 0 & 23.81430 \end{pmatrix} (X), \quad (X) = \begin{pmatrix} 0.06958 & 0 & 0.01705 \\ 0 & 0.10271 & 0 \\ 0 & 0 & 0.04199 \end{pmatrix} (XO)$$

$$(YO) = (Y), \quad (Y) = (YO)$$

$$(ZO) = (Z), \quad (Z) = (ZO)$$

Orthogonal Axes AO, BO and CO are defined as:

AO // A, CO // C*, BO // CO X AO

```
SPGR - Determine SpaceGroup from Observed Extinctions for: klat855a
================================================================================
:: Reflection Data are READ from File : spgr.hkl - ( OBS-Data)

:: TRMX =    0.00   1.00   0.00   1.00   0.00   0.00   0.00   0.00  -1.00
:: Reflection Data are READ from File : spgr.hkl - ( OBS-Data)

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

Nz-Test Statistics
==================
Shell 1 24.45 35.83 43.55 49.48 54.20 59.40 64.45 67.43 70.38 73.45  3288 1000.0
Shell 2 20.17 31.43 38.94 44.61 49.64 54.02 58.37 61.28 64.28 66.87  3634  306.6
Shell 3 19.38 27.63 35.52 41.98 47.84 52.34 56.06 59.57 62.85 65.56  3359  214.5
Shell 4 18.90 26.08 34.38 41.19 47.81 52.68 57.29 61.44 64.37 67.30  3037  159.7
Shell 5 23.79 29.63 35.84 41.71 47.04 52.45 56.69 60.03 62.93 65.69  2757  107.5
Shell 6 28.18 33.31 37.56 41.77 46.64 51.11 55.17 58.86 61.63 64.92  2708   75.1
Shell 7 30.34 34.53 38.15 42.05 45.51 49.04 51.85 55.43 59.58 62.38  2459   54.6
Shell 8 33.74 36.79 40.33 43.74 47.45 50.00 53.99 56.91 59.92 62.96  2430   50.2
Shell 9 37.17 40.03 43.20 46.10 48.64 51.59 54.17 56.94 59.75 62.51  2206   43.2
Shell10 38.07 40.03 42.44 45.52 48.61 51.25 54.61 57.47 59.79 61.84  2201   41.3

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  22.56 29.16 35.82 41.66 47.33 52.14 56.30 59.98 62.95 65.87
NonCent  9.52 18.13 25.92 32.97 39.35 45.12 50.34 55.07 59.34 63.21
CentroS 24.81 34.53 41.87 47.38 52.05 56.14 59.72 62.89 65.72 68.33

Normalized N(z) curves ( 44 Percent Centric)
============================================

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  12.78 10.50  9.11  7.63  6.66  5.43  4.10  2.79  1.21  0.00
NonCent  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
CentroS 17.98 20.86 21.37 20.05 17.88 15.14 11.89  8.23  4.22  0.00
```

Analysis of Systematic Absences

Nr	Ex.	Condition	Aver(I/sig(I)) .True.	Aver(I/sig(I)) .False.	Number of Refl .True.	Number of Refl .False.	I/sigI Max.F	H	K	L	.T/F. Ratio
1		HKL:H+K=2N	2.34	2.33	17063	16963	14.84	1	2	4	1.0
2		HKL:H+L=2N	2.45	2.22	17050	16976	14.84	1	2	4	1.1
3		HKL:K+L=2N	2.34	2.33	17037	16989	14.74	-1	1	6	1.0
4		HKL:H+K+L=2N	2.37	2.31	16994	17032	15.00	1	-1	1	1.0
5		HKL:-H+K+L=3N	2.31	2.35	11355	22671	15.00	1	-1	1	1.0
6		HKL:H-K+L=3N	2.32	2.35	11338	22688	14.74	-1	1	6	1.0
7		0KL:K=2N	3.29	3.35	640	628	13.99	0	1	3	1.0
8		0KL:L=2N	3.38	3.27	638	630	13.99	0	1	3	1.0
9		0KL:K+L=2N	3.58	3.07	636	632	13.89	0	1	2	1.2
10		H0L:H=2N	2.15	2.10	1145	1133	13.66	-5	0	1	1.0
11		H0L:L=2N	2.14	2.11	1142	1136	13.66	-5	0	1	1.0
12	E ny	H0L:H+L=2N	3.92	0.35	1131	1147	3.12	-2	0	19	11.2
13		HK0:H=2N	2.86	3.21	400	428	13.50	-3	2	0	0.9
14		HK0:K=2N	2.97	3.15	454	447	14.45	-2	1	0	0.9
15		HK0:H+K=2N	3.10	3.10	429	423	14.45	-2	1	0	1.0
16	E 21x	H00:H=2N	4.13	0.31	26	23	1.44	15	0	0	13.5
17	E 21y	0K0:K=2N	9.48	0.18	13	11	0.50	0	11	0	53.9
18	E 21z	00L:L=2N	5.37	0.26	36	38	1.17	0	0	17	21.0
19		0KL:K+L=4N	3.63	3.22	317	951	13.89	0	1	2	1.1
20	> dy	H0L:H+L=4N	4.12	1.45	572	1706	13.90	-6	0	4	2.8
21		HK0:H+K=4N	2.78	3.21	214	638	14.45	-2	1	0	0.9
22	> 41x	H00:H=4N	4.54	1.62	12	37	13.38	2	0	0	2.8
23		0K0:K=4N	7.51	4.45	6	18	13.04	0	2	0	1.7
24	> 41z	00L:L=4N	5.77	1.70	19	55	13.66	0	0	6	3.4
25		HHL:L=2N	3.13	3.48	511	537	13.34	1	1	11	0.9
26		HHL:H=2N	2.92	3.66	493	555	13.63	1	1	4	0.8
27		HHL:H+L=2N	3.50	3.12	530	518	13.63	1	1	4	1.1
28		HHL:2H+L=4N	3.49	3.25	256	792	13.63	1	1	4	1.1
29		H-HL:H+L=3N	3.60	3.62	342	678	15.00	1	-1	1	1.0
30		H-HL:-H+L=3N	3.82	3.51	334	686	14.74	-1	1	6	1.1
31	> 61z	00L:L=6N	5.05	2.25	13	61	12.31	0	0	10	2.2
32		HH0:H=2N	1.08	5.43	13	13	10.53	3	3	0	0.2
33		H-HL:L=2N	3.38	3.83	495	525	15.00	1	-1	1	0.9
34		HHL:L=3N	3.03	3.44	330	718	13.63	1	1	4	0.9
35		H-2HL:L=2N	3.29	2.81	258	263	14.18	1	-2	3	1.2
36		-2HHL:L=2N	3.15	3.50	377	396	13.20	2	-1	3	0.9
37		H-2HL:L=3N	3.06	3.05	162	359	13.76	1	-2	1	1.0
38		-2HHL:L=3N	3.01	3.48	243	530	13.96	-2	1	4	0.9
39		00L:L=3N	2.74	2.74	26	48	12.31	0	0	10	1.0
40		H-HL:H=2N	3.27	3.90	468	552	15.00	1	-1	1	0.8
41		HKL:H=2N	2.32	2.35	17037	16989	15.00	1	-1	1	1.0
42		HKL:K=2N	2.28	2.39	17030	16996	15.00	1	-1	1	1.0

43	HKL:L=2N	2.32	2.36	17003	17023	15.00	1	-1	1	1.0
44	HKL:H=3N	2.33	2.34	11368	22658	15.00	1	-1	1	1.0
45	HKL:K=3N	2.20	2.40	11347	22679	15.00	1	-1	1	0.9
46	HKL:L=3N	2.35	2.33	11369	22657	15.00	1	-1	1	1.0

NOTE: Reflections obscured by BeamStop Excluded from Statistics
5 0 0 etc. not included in Exception list (Fe?)

Extinction Conditions have been Marked with E when
<I/Sig>(.F.) < 1.0 .and. Ratio(.T./.F.) > 2.5
.or. <I/Sig>(.F.) < 1.5 .and. Ratio(.T./.F.) > 5.0
.or. <I/Sig>(.F.) < 2.5 .and. Ratio(.T./.F.) > 10.0
.or. <I/Sig>(.F.) < 10.0 .and. Ratio(.T./.F.) > 20.0
.or. <I/Sig>(.F.) < 50.0 .and. Ratio(.T./.F.) >100.0

Tentative Space Group Assignment - (Please Check Carefully)

:: NOTE: Space Group Determination Pitfalls:
- Twinning, Pseudo-Symmetry, Mult.Refl.

Candidate Space Groups in (1.00 0.00 0.00/ 0.00 1.00 0.00/ 0.00 0.00 1.00) Cell

Name	#	AbsFreq	StandSet.		R(av)	Perc.	N	A/C-Prob	
P21/n	14	30824	P21/c	:A-B-N	7.55	2113	44		C
P21	4	5116	P21	:ABC	7.55	2113	56	Chiral	A
Pn	7	325	Pc	:A-B-N	7.55	2113	56		A

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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 spgr.ins - Data Type SPF

:: NORMAL END of PLATON : 6 Pages on:
:: spgr.lis (ASCII, 132 Characters Wide)
:: spgr.lps (PostScript Version of .lis)
:: spgr.pdf (PDF Version of .lis)

:: SPGR.PAR on :spgr.par