PLATON(V-311206)-Run for: kla0143a TIME: Oct 20 10:12:42 2011

Crystal Data

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

a =	13.45100	Angstrom	alpha =	90	Degree	a =	13.451	alpha =	90.00	V =	8394.0
b =	26.23300		beta =	103.2900		b =	24.443	beta =	90.00		
c =	24.44300		gamma =	90		c =	26.233	gamma =	103.29		
V =	8393.97	Cubic-Angstrom	d(100) =	13.0908	Angstrom						
			d(010) =	26.2330			180.929	597.460	688.170		
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	23.7884			0.000	0.000	-75.580		

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

Niggli Values

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 13.45100 & 0 & -5.61895 \\ 0 & 26.23300 & 0 \\ 0 & 0 & 23.78839 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.07434 & 0 & 0.01756 \\ 0 & 0.03812 & 0 \\ 0 & 0 & 0.04204 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

Orthogonal Axes AO, BO and CO are defined as:

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: kla0143a
================================================================================
:: Reflection Data are READ from File : spgr.hkl - ( OBS-Data)

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

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

Nz-Test Statistics
==================
Shell 1 24.59 34.68 42.00 47.07 51.89 56.38 60.78 64.25 67.09 69.49  9252 1000.0
Shell 2 23.04 33.59 40.57 46.30 51.25 55.63 58.93 62.21 64.64 67.23  9925  400.7
Shell 3 21.33 32.21 40.48 46.44 51.03 55.13 59.04 62.84 65.56 68.06  9062  295.7
Shell 4 20.40 28.87 36.55 43.38 49.03 54.01 57.64 61.40 64.50 67.46  8220  199.8
Shell 5 24.36 30.76 36.63 42.88 48.34 53.36 57.77 61.47 64.71 67.43  7685  121.1
Shell 6 26.04 30.87 35.98 41.51 46.48 51.33 55.64 59.42 62.82 65.77  7117  104.8
Shell 7 27.88 32.24 37.16 41.90 46.07 50.37 54.59 58.01 61.56 64.82  6657   92.1
Shell 8 30.24 34.34 38.27 42.26 46.26 50.09 53.50 57.28 60.52 63.64  6342   76.9
Shell 9 33.75 36.90 40.21 44.15 47.76 51.03 54.36 57.47 60.91 63.69  5946   68.9
Shell10 35.54 38.78 41.77 45.11 48.31 51.70 54.61 57.40 59.83 62.67  5810   59.4

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  23.03 30.68 37.41 43.55 48.72 53.46 57.52 61.28 64.40 67.18
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 ( 48 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  13.12 11.76 10.30  8.99  7.39  5.96  4.40  3.04  1.48  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	2.74	2.72	44048	44047	56.17	1	-6	4	1.0
2		HKL:H+L=2N	2.73	2.73	44045	44050	68.57	-3	1	2	1.0
3		HKL:K+L=2N	2.75	2.72	43988	44107	68.57	-3	1	2	1.0
4		HKL:H+K+L=2N	2.71	2.75	44054	44041	71.46	-3	-1	1	1.0
5		HKL:-H+K+L=3N	2.74	2.73	29360	58735	70.24	-3	1	1	1.0
6		HKL:H-K+L=3N	2.70	2.75	29373	58722	81.54	2	0	2	1.0
7		0KL:K=2N	3.65	3.93	1958	1947	37.07	0	-1	7	0.9
8		0KL:L=2N	3.74	3.84	1946	1959	39.70	0	10	1	1.0
9		0KL:K+L=2N	3.83	3.75	1945	1960	39.70	0	10	1	1.0
10		H0L:H=2N	2.85	3.10	1035	1052	45.72	1	0	8	0.9
11	E	cy H0L:L=2N	5.58	0.39	1041	1046	3.64	-17	0	3	14.4
12		H0L:H+L=2N	2.85	3.10	1043	1044	45.72	1	0	8	0.9
13		HK0:H=2N	3.92	4.31	894	981	55.36	1	7	0	0.9
14		HK0:K=2N	4.31	4.09	985	995	55.36	1	7	0	1.1
15		HK0:H+K=2N	4.77	3.56	978	970	34.28	3	2	0	1.3
16		H00:H=2N	5.21	6.28	16	16	9.78	3	0	0	0.8
17	E	21y 0K0:K=2N	10.48	0.22	37	36	1.03	0	25	0	47.4
18	E	21z 00L:L=2N	7.00	0.36	37	40	2.38	0	0	31	19.3
19		0KL:K+L=4N	4.01	3.72	967	2938	39.70	0	10	1	1.1
20		H0L:H+L=4N	3.13	2.92	524	1563	45.72	1	0	8	1.1
21		HK0:H+K=4N	4.75	3.98	490	1458	43.34	-2	8	0	1.2
22		H00:H=4N	4.86	6.04	8	24	12.99	2	0	0	0.8
23	?	41y 0K0:K=4N	15.64	1.82	19	54	21.85	0	10	0	8.6
24	>	41z 00L:L=4N	7.06	2.40	19	58	28.03	0	0	6	2.9
25		HHL:L=2N	3.64	4.31	831	854	46.10	-3	-3	1	0.8
26		HHL:H=2N	3.91	4.04	802	883	46.10	-3	-3	1	1.0
27		HHL:H+L=2N	3.70	4.25	842	843	44.98	-3	-3	2	0.9
28		HHL:2H+L=4N	3.77	4.05	417	1268	46.10	-3	-3	1	0.9
29		H-HL:H+L=3N	3.60	3.84	585	1162	53.63	-3	3	1	0.9
30		H-HL:-H+L=3N	3.70	3.78	577	1170	53.63	-3	3	1	1.0
31	>	61z 00L:L=6N	9.98	2.25	13	64	13.45	0	0	4	4.4
32		HH0:H=2N	8.10	4.79	16	15	10.78	7	7	0	1.7
33		H-HL:L=2N	3.43	4.06	857	890	53.63	-3	3	1	0.8
34		HHL:L=3N	3.59	4.16	537	1148	46.10	-3	-3	1	0.9
35		H-2HL:L=2N	2.98	4.10	694	721	31.35	1	-2	9	0.7
36		-2HHL:L=2N	3.84	4.05	446	467	28.68	2	-1	7	0.9
37		H-2HL:L=3N	3.37	3.63	448	967	33.60	2	-4	2	0.9
38		-2HHL:L=3N	3.38	4.22	295	618	44.37	-2	1	4	0.8
39		00L:L=3N	4.91	2.82	27	50	13.45	0	0	4	1.7
40		H-HL:H=2N	3.70	3.80	826	921	53.63	-3	3	1	1.0
41		HKL:H=2N	2.73	2.73	43965	44130	71.46	-3	-1	1	1.0
42		HKL:K=2N	2.67	2.80	44032	44063	71.46	-3	-1	1	1.0

43	HKL:L=2N	2.74	2.73	44041	44054	71.46	-3	-1	1	1.0
44	HKL:H=3N	2.73	2.74	29203	58892	81.54	2	0	2	1.0
45	HKL:K=3N	2.70	2.75	29381	58714	71.46	-3	-1	1	1.0
46	HKL:L=3N	2.71	2.75	29338	58757	81.54	2	0	2	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/c	14	30824	P21/c	:ABC	5.93	6103	48		C
P21	4	5116	P21	:ABC	5.93	6103	52	Chiral	A
Pc	7	325	Pc	:ABC	5.93	6103	52		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