PLATON(V-311206)-Run for: kla0131a TIME: Sep 17 11:26:38 2011

Crystal Data

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

a =	17.90400	Angstrom	alpha =	78.0800	Degree	a =	17.904	alpha =	78.08	V =	6747.1
b =	17.93700		beta =	77.9900		b =	17.937	beta =	77.99		
c =	22.91100		gamma =	71.5300		c =	22.911	gamma =	71.53		
V =	6747.10	Cubic-Angstrom	d(100) =	16.7800	Angstrom	Niggli Values					
			d(010) =	16.8165		320.553	321.736	524.914			
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	22.1506		84.881	85.355	101.741			

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

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 17.90400 & 5.68259 & 4.76738 \\ 0 & 17.01306 & 3.39680 \\ 0 & 0 & 22.15057 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.05585 & -0.01866 & -0.00916 \\ 0 & 0.05878 & -0.00901 \\ 0 & 0 & 0.04515 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

Orthogonal Axes AO, BO and CO are defined as:
AO // A, CO // C*, BO // CO X AO

```
SPGR - Determine SpaceGroup from Observed Extinctions for: kla0131a
================================================================================
:: 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 26.14 36.74 44.20 50.45 55.62 60.16 63.86 66.86 69.52 71.91  8868 1000.0
Shell 2 22.48 32.59 40.59 47.29 52.61 56.39 59.76 63.16 66.07 68.88  9315  423.6
Shell 3 24.92 31.07 37.08 42.90 48.40 53.41 57.83 61.83 65.32 68.45  8412  216.9
Shell 4 28.69 33.74 38.17 42.98 47.37 51.74 56.11 59.88 63.10 66.15  7682  167.7
Shell 5 31.47 35.97 40.28 44.36 48.08 51.82 55.31 58.32 61.68 64.77  7159  151.4
Shell 6 35.17 39.46 43.04 46.69 50.34 53.73 56.55 59.68 62.58 65.43  6531  135.2
Shell 7 40.72 44.31 47.21 50.69 53.79 56.66 59.60 62.26 64.38 66.60  6272  108.7
Shell 8 45.98 49.24 52.47 55.20 58.33 61.04 63.93 66.30 68.79 70.92  6024  100.1
Shell 9 54.50 58.25 61.12 64.03 66.68 68.92 71.09 73.04 74.62 76.09  5646   89.0
Shell10 47.30 52.29 57.37 60.92 64.22 67.47 70.11 72.48 74.50 76.29  5330  112.4

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  30.06 35.06 39.64 44.23 48.55 52.68 56.45 59.93 63.17 66.20
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 ( 59 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  20.25 16.34 12.83 10.07  7.71  5.76  4.02  2.47  1.14  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.	.False.	Number of Refl .True.	.False.	I/sigI Max.F	H	K	L	.T/F. Ratio
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
7		0KL:K=2N	2.15	2.31	1556	1553	55.17	0	3	2	0.9
8		0KL:L=2N	2.58	1.88	1552	1557	31.06	0	3	1	1.4
9		0KL:K+L=2N	2.34	2.12	1559	1550	55.17	0	3	2	1.1
10		H0L:H=2N	2.18	2.37	1417	1415	54.73	3	0	2	0.9
11		H0L:L=2N	2.57	1.99	1403	1429	39.71	3	0	1	1.3
12		H0L:H+L=2N	2.39	2.16	1414	1418	54.73	3	0	2	1.1
13		HK0:H=2N	2.46	2.50	986	1051	64.89	3	2	0	1.0
14		HK0:K=2N	2.65	2.66	1076	1079	63.91	2	3	0	1.0
15		HK0:H+K=2N	2.54	2.59	1048	1058	64.89	3	2	0	1.0
16		H00:H=2N	3.62	8.96	24	25	40.84	3	0	0	0.4
17		0K0:K=2N	3.32	6.86	33	36	31.21	0	3	0	0.5
18	E 21z	00L:L=2N	5.24	0.41	42	45	2.14	0	0	21	12.7
19		0KL:K+L=4N	2.27	2.22	782	2327	55.17	0	3	2	1.0
20		H0L:H+L=4N	2.26	2.28	706	2126	54.73	3	0	2	1.0
21		HK0:H+K=4N	2.42	2.62	532	1574	64.89	3	2	0	0.9
22		H00:H=4N	3.42	7.29	12	37	40.84	3	0	0	0.5
23		0K0:K=4N	3.25	5.80	17	52	31.21	0	3	0	0.6
24	> 41z	00L:L=4N	4.81	2.00	23	64	16.25	0	0	6	2.4
25	E cxy	HHL:L=2N	3.13	0.47	1101	1120	4.91	18	18	17	6.6
26		HHL:H=2N	1.65	1.92	1061	1160	43.26	3	3	2	0.9
27		HHL:H+L=2N	1.59	1.99	1105	1116	43.26	3	3	2	0.8
28	>	HHL:2H+L=4N	3.33	1.29	547	1674	42.14	1	1	4	2.6
29		H-HL:H+L=3N	2.32	2.32	563	1139	44.98	1	-1	4	1.0
30		H-HL:-H+L=3N	2.31	2.33	573	1129	60.25	-1	1	4	1.0
31	> 61z	00L:L=6N	5.94	2.18	13	74	19.93	0	0	4	2.7
32		HH0:H=2N	2.66	2.25	25	24	12.31	7	7	0	1.2
33		H-HL:L=2N	2.40	2.25	833	869	27.61	2	-2	1	1.1
34		HHL:L=3N	1.49	1.94	718	1503	43.26	3	3	2	0.8
35		H-2HL:L=2N	2.17	1.98	531	575	32.96	-1	2	3	1.1
36		-2HHL:L=2N	2.20	1.91	512	561	25.74	6	-3	1	1.2
37		H-2HL:L=3N	1.90	2.15	346	760	49.87	-1	2	2	0.9
38		-2HHL:L=3N	1.73	2.19	334	739	47.24	2	-1	2	0.8
39		00L:L=3N	3.00	2.61	29	58	19.93	0	0	4	1.1
40		H-HL:H=2N	2.11	2.52	811	891	60.25	-1	1	4	0.8
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

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
P1	1	799	P1	:ABC	6.75	2758	41 Chiral	A
P-1	2	15327	P-1	:ABC	6.75	2758	59	C

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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