PLATON(V-311206)-Run for: kla0144 TIME: Oct 22 16:39:44 2011

Crystal Data

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

a =	12.78300	Angstrom	alpha =	87.8900	Degree	a =	12.783	alpha =	87.89	V =	3283.4
b =	13.90300		beta =	77.3200		b =	13.903	beta =	77.32		
c =	20.83400		gamma =	65.5900		c =	20.834	gamma =	65.59		
V =	3283.40	Cubic-Angstrom	d(100) =	11.3432	Angstrom	Niggli Values					
			d(010) =	12.6369		163.405	193.293	434.056			
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	20.2884		10.665	58.459	73.446			

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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 12.78300 & 5.74560 & 4.57318 \\ 0 & 12.66023 & -1.23308 \\ 0 & 0 & 20.28845 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.07823 & -0.03550 & -0.01979 \\ 0 & 0.07899 & 0.00480 \\ 0 & 0 & 0.04929 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: kla0144
==========================================================================
:: 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 27.53 37.16 45.98 52.16 57.72 62.18 64.91 68.04 71.25 73.67  3673 1000.0
Shell 2 24.62 34.72 41.60 46.93 51.24 54.90 58.81 62.06 64.62 66.85  3940  341.8
Shell 3 25.47 36.03 43.67 49.67 55.06 58.66 62.21 65.26 67.46 69.86  3636  195.1
Shell 4 22.74 31.83 39.74 46.28 51.17 55.82 59.41 62.91 65.55 68.38  3289  110.3
Shell 5 25.15 33.08 40.49 46.13 51.55 55.96 59.80 62.73 64.89 67.57  3102   88.7
Shell 6 23.71 30.03 36.33 42.55 48.29 52.31 56.15 59.02 61.50 64.16  2860   79.3
Shell 7 26.79 32.37 37.83 43.12 48.01 52.10 56.12 59.85 62.93 65.57  2762   56.1
Shell 8 30.15 34.31 38.33 42.09 46.15 50.02 53.52 56.61 59.51 62.71  2687   44.0
Shell 9 34.47 37.99 41.34 44.33 46.75 49.94 53.34 56.49 59.35 62.34  2443   34.9
Shell10 35.51 38.11 40.90 43.85 46.50 49.41 52.80 55.54 58.45 60.80  2301   31.7

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  24.27 32.74 40.06 46.16 51.52 55.69 59.39 62.48 64.85 67.49
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 ( 60 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  14.32 13.76 12.86 11.48 10.03  8.00  6.06  3.99  1.66  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	3.02	3.03	18212	18170	12.11	6	3	10	1.0
2	HKL:H+L=2N	3.01	3.05	18173	18209	11.97	-4	-2	7	1.0
3	HKL:K+L=2N	3.00	3.05	18203	18179	12.11	6	3	10	1.0
4	HKL:H+K+L=2N	3.05	3.01	18207	18175	12.11	6	3	10	1.0
5	HKL:-H+K+L=3N	3.02	3.03	12147	24235	12.11	6	3	10	1.0
6	HKL:H-K+L=3N	3.04	3.02	12121	24261	12.11	6	3	10	1.0
7	0KL:K=2N	4.05	4.05	874	869	11.53	0	-5	2	1.0
8	0KL:L=2N	4.07	4.03	868	875	11.54	0	8	3	1.0
9	0KL:K+L=2N	4.06	4.03	875	868	11.54	0	8	3	1.0
10	H0L:H=2N	4.26	4.32	751	765	11.54	-5	0	3	1.0
11	H0L:L=2N	4.19	4.40	765	751	11.54	-5	0	3	1.0
12	H0L:H+L=2N	4.21	4.38	758	758	11.42	-2	0	3	1.0
13	HK0:H=2N	3.57	3.94	483	525	11.46	-1	4	0	0.9
14	HK0:K=2N	4.38	3.44	554	538	11.15	6	1	0	1.3
15	HK0:H+K=2N	3.71	4.01	532	523	11.46	-1	4	0	0.9
16	H00:H=2N	5.34	5.63	19	18	11.06	3	0	0	0.9
17	0K0:K=2N	6.87	4.82	25	22	11.07	0	3	0	1.4
18	00L:L=2N	5.28	5.93	28	29	11.36	0	0	9	0.9
19	0KL:K+L=4N	4.09	4.04	437	1306	11.54	0	8	3	1.0
20	H0L:H+L=4N	4.20	4.32	380	1136	11.54	-5	0	3	1.0
21	HK0:H+K=4N	3.96	3.83	270	785	11.46	-1	4	0	1.0
22	H00:H=4N	5.39	5.50	8	29	11.06	3	0	0	1.0
23	0K0:K=4N	5.86	5.92	12	35	11.18	0	2	0	1.0
24	00L:L=4N	5.40	5.69	15	42	11.36	0	0	9	0.9
25	HHL:L=2N	4.06	4.21	628	653	11.81	-2	-2	7	1.0
26	HHL:H=2N	3.86	4.40	613	668	11.67	1	1	6	0.9
27	HHL:H+L=2N	3.89	4.39	646	635	11.81	-2	-2	7	0.9
28	HHL:2H+L=4N	4.14	4.14	319	962	11.81	-2	-2	7	1.0
29	H-HL:H+L=3N	3.47	3.53	291	580	11.62	-1	1	11	1.0
30	H-HL:-H+L=3N	3.39	3.57	289	582	11.50	1	-1	2	1.0
31	00L:L=6N	5.06	5.72	9	48	11.45	0	0	4	0.9
32	HH0:H=2N	5.36	2.69	17	14	5.00	9	9	0	2.0
33	H-HL:L=2N	3.39	3.62	426	445	11.62	-1	1	11	0.9
34	HHL:L=3N	4.37	4.03	407	874	11.81	-2	-2	7	1.1
35	H-2HL:L=2N	3.78	3.85	271	293	11.85	-1	2	7	1.0
36	-2HHL:L=2N	3.80	3.78	270	282	11.45	-4	2	7	1.0
37	H-2HL:L=3N	3.94	3.76	176	388	11.85	-1	2	7	1.0
38	-2HHL:L=3N	3.99	3.70	172	380	11.56	2	-1	8	1.1
39	00L:L=3N	5.23	5.82	20	37	11.45	0	0	4	0.9
40	H-HL:H=2N	3.39	3.61	396	475	11.62	-1	1	11	0.9
41	HKL:H=2N	3.01	3.05	18246	18136	11.85	-1	2	7	1.0
42	HKL:K=2N	3.01	3.05	18200	18182	12.11	6	3	10	1.0

```
43       HKL:L=2N         3.04    3.02  18221  18161    11.97   -4 -2  7   1.0
44       HKL:H=3N         3.03    3.03  12095  24287    11.97   -4 -2  7   1.0
45       HKL:K=3N         3.00    3.04  12114  24268    11.97   -4 -2  7   1.0
46       HKL:L=3N         3.03    3.03  12136  24246    12.11    6  3 10   1.0
:: No Extinction Conditions Found
```

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	4.43	3980	40 Chiral	A
P-1	2	15327	P-1	:ABC	4.43	3980	60	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