PLATON(V-311206)-Run for: kla0077 TIME: Nov 16 15:58:54 2011

Crystal Data

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

						Reduced Cell					
a =	10.41400	Angstrom	alpha =	65.5700	Degree	a =	10.414	alpha =	65.57	V =	1231.8
b =	10.82600		beta =	71.1700		b =	10.826	beta =	71.17		
c =	12.67900		gamma =	82.0200		c =	12.679	gamma =	82.02		
V =	1231.79	Cubic-Angstrom	d(100) =	9.8565	Angstrom						
			d(010) =	9.8565							
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	11.0326							

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

Niggli Values

108.451	117.202	160.757
56.770	42.617	15.651

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 10.41400 & 1.50295 & 4.09229 \\ 0 & 10.72117 & 4.72139 \\ 0 & 0 & 11.03262 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.09602 & -0.01346 & -0.02986 \\ 0 & 0.09327 & -0.03992 \\ 0 & 0 & 0.09064 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: kla0077
==========================================================================
:: 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  9.22 15.78 25.13 34.63 42.11 47.99 53.21 57.62 62.57 67.91   748 1000.0
Shell 2  8.48 16.25 26.05 32.86 40.86 46.48 51.85 56.75 59.74 62.13   837  443.6
Shell 3 10.12 17.54 23.69 31.50 39.05 45.45 50.83 55.19 58.90 61.59   781  219.8
Shell 4  9.74 17.83 25.79 32.92 39.64 44.99 50.62 54.32 58.44 64.06   729  146.0
Shell 5 12.65 19.77 26.45 33.28 39.83 44.91 50.87 55.23 59.59 63.95   688  122.7
Shell 6 14.12 21.18 27.91 33.83 38.92 45.16 49.75 53.86 58.62 62.73   609   88.5
Shell 7 18.73 23.50 28.09 34.81 40.99 46.47 51.06 55.83 58.13 61.13   566   66.0
Shell 8 17.65 23.89 31.19 36.36 40.46 44.56 49.20 52.58 56.51 60.25   561   49.8
Shell 9 23.99 29.56 34.17 38.77 45.30 49.90 54.89 59.12 61.23 64.11   521   39.8
Shell10 27.76 30.31 35.04 38.58 44.09 48.82 53.15 57.28 60.24 63.19   508   31.9

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  11.66 19.08 25.96 32.88 39.36 45.13 50.52 54.65 58.89 63.08
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 (  2 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   2.15  0.98  0.08 -0.03  0.08  0.09  0.27 -0.31 -0.34  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	5.37	4.27	4103	4096	69.85	-1	2	0	1.3
2	HKL:H+L=2N	4.78	4.86	4114	4085	75.89	0	2	1	1.0
3	HKL:K+L=2N	4.81	4.83	4102	4097	75.89	0	2	1	1.0
4	HKL:H+K+L=2N	4.80	4.85	4079	4120	77.12	-1	-1	1	1.0
5	HKL:-H+K+L=3N	5.05	4.71	2731	5468	79.69	2	0	0	1.1
6	HKL:H-K+L=3N	4.83	4.82	2717	5482	79.69	2	0	0	1.0
7	0KL:K=2N	7.97	5.09	259	254	48.25	0	1	2	1.6
8	0KL:L=2N	6.43	6.65	260	253	75.89	0	2	1	1.0
9	0KL:K+L=2N	6.05	7.04	258	255	75.89	0	2	1	0.9
10	H0L:H=2N	10.42	7.66	192	194	65.01	1	0	3	1.4
11	H0L:L=2N	9.03	9.03	193	193	65.01	1	0	3	1.0
12	H0L:H+L=2N	8.86	9.19	189	197	58.61	2	0	1	1.0
13	HK0:H=2N	5.08	7.18	174	203	69.85	-1	2	0	0.7
14	HK0:K=2N	7.25	5.89	208	210	59.21	-1	1	0	1.2
15	HK0:H+K=2N	6.55	5.98	202	199	69.85	-1	2	0	1.1
16	E 21x H00:H=2N	23.61	2.22	9	8	2.59	7	0	0	10.6
17	> 21y 0K0:K=2N	10.71	3.71	12	12	5.01	0	3	0	2.9
18	00L:L=2N	12.06	19.80	9	9	51.42	0	0	3	0.6
19	0KL:K+L=4N	5.51	6.88	128	385	75.89	0	2	1	0.8
20	H0L:H+L=4N	9.19	8.98	95	291	79.69	2	0	0	1.0
21	HK0:H+K=4N	6.78	6.10	101	300	69.85	-1	2	0	1.1
22	H00:H=4N	10.80	14.39	4	13	79.69	2	0	0	0.8
23	0K0:K=4N	4.02	8.27	6	18	39.40	0	2	0	0.5
24	00L:L=4N	5.14	19.02	4	14	71.88	0	0	2	0.3
25	HHL:L=2N	9.87	11.01	127	139	77.12	-1	-1	1	0.9
26	HHL:H=2N	9.95	10.92	124	142	77.12	-1	-1	1	0.9
27	HHL:H+L=2N	10.70	10.22	135	131	59.90	1	1	2	1.0
28	HHL:2H+L=4N	9.76	10.70	65	201	77.12	-1	-1	1	0.9
29	H-HL:H+L=3N	8.70	7.14	93	182	59.29	-1	1	2	1.2
30	H-HL:-H+L=3N	8.78	7.11	92	183	49.62	-1	1	1	1.2
31	00L:L=6N	5.02	18.12	3	15	71.88	0	0	2	0.3
32	HH0:H=2N	13.67	14.52	5	7	41.26	1	1	0	0.9
33	H-HL:L=2N	6.90	8.39	132	143	49.62	-1	1	1	0.8
34	HHL:L=3N	10.14	10.62	83	183	77.12	-1	-1	1	1.0
35	H-2HL:L=2N	6.70	7.46	84	96	60.68	1	-2	1	0.9
36	-2HHL:L=2N	5.58	7.53	73	79	39.64	-2	1	1	0.7
37	H-2HL:L=3N	6.27	7.44	52	128	60.68	1	-2	1	0.8
38	-2HHL:L=3N	6.83	6.50	42	110	39.64	-2	1	1	1.1
39	00L:L=3N	18.61	14.59	6	12	71.88	0	0	2	1.3
40	H-HL:H=2N	6.61	8.58	127	148	59.29	-1	1	2	0.8
41	HKL:H=2N	4.75	4.90	4090	4109	77.12	-1	-1	1	1.0
42	HKL:K=2N	5.15	4.50	4100	4099	77.12	-1	-1	1	1.1

43	HKL:L=2N	4.77	4.88	4121	4078	77.12	-1	-1	1	1.0
44	HKL:H=3N	4.61	4.93	2726	5473	79.69	2	0	0	0.9
45	HKL:K=3N	4.68	4.89	2708	5491	77.12	-1	-1	1	1.0
46	HKL:L=3N	4.76	4.85	2728	5471	77.12	-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
P1	1	799	P1	:ABC	4.91	1404	98	Chiral A
P-1	2	15327	P-1	:ABC	4.91	1404	2	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