PLATON(V-311206)-Run for: kla0150 TIME: Nov 7 13:07:54 2011

Crystal Data

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

a =	9.83300 Angstrom	alpha =	90 Degree		
b =	31.94200	beta =	90		
c =	10.55700	gamma =	90		
V =	3315.80 Cubic-Angstrom	d(100) =	9.8330 Angstrom		
		d(010) =	31.9420		
Lambda(MoKa) =	0.71070 Angstrom	d(001) =	10.5570		

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

a =	9.833	alpha =	90.00	V =	3315.8
b =	10.557	beta =	90.00		
c =	31.942	gamma =	90.00		

Niggli Values

96.688	111.450	1020.291
0.000	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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 9.83300 & 0 & 0 \\ 0 & 31.94200 & 0 \\ 0 & 0 & 10.55700 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.10170 & 0 & 0 \\ 0 & 0.03131 & 0 \\ 0 & 0 & 0.09472 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: kla0150
==========================================================================
:: 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 14.53 27.34 34.41 41.43 45.95 51.89 55.92 58.52 61.71 66.08  2037 1000.0
Shell 2 10.83 21.40 26.47 33.78 39.49 45.55 50.28 56.08 60.68 64.37  2327  287.4
Shell 3 13.01 25.46 36.71 44.74 48.60 53.20 57.15 61.14 63.89 66.38  2329  218.3
Shell 4 10.44 20.77 30.60 39.82 44.86 48.52 52.85 55.30 58.30 62.02  1964  114.8
Shell 5 10.72 21.29 31.18 39.72 47.11 52.89 57.16 60.80 65.07 68.77  1921   77.8
Shell 6 14.33 24.97 35.29 44.68 51.52 56.62 60.21 63.30 66.07 67.86  1842   55.8
Shell 7 16.25 28.86 37.77 45.11 50.00 54.08 57.59 61.29 64.49 67.50  1594   38.5
Shell 8 17.83 29.17 38.57 45.06 50.94 56.16 60.40 64.46 67.31 68.95  1649   31.1
Shell 9 17.42 27.62 36.19 42.61 48.21 53.95 58.74 62.66 66.24 69.82  1481   30.8
Shell10 22.96 29.64 38.42 45.71 52.13 56.45 60.77 64.48 68.06 70.36  1481   21.6

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  12.13 23.12 33.45 42.24 48.02 52.81 56.84 60.13 63.33 66.26
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 ( 31 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   2.31  4.39  6.61  8.05  7.15  5.86  4.37  2.63  1.25  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	E C	HKL:H+K=2N	6.45	0.00	22511	0	0.00	0	0	0	99.0
2		HKL:H+L=2N	6.54	6.37	11271	11240	16.72	4	-6	1	1.0
3		HKL:K+L=2N	6.54	6.37	11271	11240	16.72	4	-6	1	1.0
4		HKL:H+K+L=2N	6.28	6.62	11221	11290	16.72	4	-6	1	0.9
5		HKL:-H+K+L=3N	6.43	6.47	7480	15031	16.49	-2	-4	4	1.0
6		HKL:H-K+L=3N	6.43	6.47	7514	14997	16.72	4	-6	1	1.0
7	E bx	0KL:K=2N	8.34	0.00	1371	0	0.00	0	0	0	99.0
8		0KL:L=2N	8.30	8.37	682	689	15.45	0	-2	3	1.0
9		0KL:K+L=2N	8.30	8.37	682	689	15.45	0	-2	3	1.0
10	E ay	H0L:H=2N	7.89	0.00	418	0	0.00	0	0	0	99.0
11		H0L:L=2N	7.62	8.15	205	213	16.14	4	0	1	0.9
12		H0L:H+L=2N	7.62	8.15	205	213	16.14	4	0	1	0.9
13	E az	HK0:H=2N	9.06	0.31	539	643	2.29	1	25	0	29.5
14	E bz	HK0:K=2N	9.36	0.31	622	643	2.29	1	25	0	30.5
15	E nz	HK0:H+K=2N	4.68	0.00	1247	0	0.00	0	0	0	99.0
16	E 21x	H00:H=2N	10.17	0.00	18	0	0.00	0	0	0	99.0
17	E 21y	0K0:K=2N	11.61	0.00	65	0	0.00	0	0	0	99.0
18		00L:L=2N	9.08	8.71	22	19	13.61	0	0	3	1.0
19		0KL:K+L=4N	7.80	8.51	341	1030	15.45	0	-2	3	0.9
20		H0L:H+L=4N	7.72	7.94	102	316	16.14	4	0	1	1.0
21		HK0:H+K=4N	4.69	4.67	625	622	15.69	-2	20	0	1.0
22		H00:H=4N	9.68	10.65	9	9	14.99	2	0	0	0.9
23		0K0:K=4N	11.23	12.01	33	32	14.61	0	18	0	0.9
24		00L:L=4N	10.02	8.59	9	32	14.30	0	0	2	1.2
25		HHL:L=2N	8.10	7.49	351	394	15.81	-2	-2	1	1.1
26		HHL:H=2N	7.44	8.08	351	394	15.65	3	3	1	0.9
27		HHL:H+L=2N	7.72	7.83	377	368	15.81	-2	-2	1	1.0
28		HHL:2H+L=4N	7.64	7.82	177	568	15.81	-2	-2	1	1.0
29		H-HL:H+L=3N	7.29	8.16	246	481	16.46	-2	2	1	0.9
30		H-HL:-H+L=3N	7.21	8.20	243	484	15.73	2	-2	4	0.9
31		00L:L=6N	7.54	9.14	6	35	14.30	0	0	2	0.8
32	E	HH0:H=2N	8.95	0.53	18	15	1.93	11	11	0	16.9
33		H-HL:L=2N	8.12	7.65	343	384	16.46	-2	2	1	1.1
34		HHL:L=3N	7.88	7.73	226	519	15.81	-2	-2	1	1.0
35		H-2HL:L=2N	7.39	7.70	145	169	15.21	-2	4	3	1.0
36		-2HHL:L=2N	6.83	7.38	74	85	13.34	4	-2	3	0.9
37		H-2HL:L=3N	7.83	7.44	95	219	15.47	2	-4	4	1.1
38		-2HHL:L=3N	7.43	7.00	47	112	15.09	-4	2	4	1.1
39		00L:L=3N	7.56	9.53	13	28	14.30	0	0	2	0.8
40		H-HL:H=2N	7.48	8.22	345	382	15.02	1	-1	7	0.9
41		HKL:H=2N	6.46	6.45	11297	11214	16.37	3	-7	1	1.0
42		HKL:K=2N	6.46	6.45	11297	11214	16.37	3	-7	1	1.0

43	HKL:L=2N	6.28	6.62	11221	11290	16.72	4	-6	1	0.9
44	HKL:H=3N	6.37	6.50	7525	14986	16.72	4	-6	1	1.0
45	HKL:K=3N	6.43	6.47	7494	15017	16.49	-2	-4	4	1.0
46	HKL:L=3N	6.10	6.63	7522	14989	16.72	4	-6	1	0.9

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
Cm2a	39	8	Abm2	:BCA	4.94	1610	69	A
C2mb	39	8	Abm2	:-CBA	4.94	1610	69	A
Cmma	67	4	Cmma	:ABC	4.94	1610	31	C
Cmmb	67	4	Cmma	:BA-C	4.94	1610	31	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