PLATON(V-311206)-Run for: kla0168t TIME: Dec 13 17:17:45 2011

Crystal Data

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

a =	14.89500	Angstrom	alpha =	90	Degree	a =	14.895	alpha =	90.00	V =	4623.7
b =	15.80000		beta =	96.1400		b =	15.800	beta =	96.14		
c =	19.76000		gamma =	90		c =	19.760	gamma =	90.00		
V =	4623.66	Cubic-Angstrom	d(100) =	14.8096	Angstrom						
			d(010) =	15.8000							
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	19.6466							

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

Niggli Values: 221.861 249.640 390.458 / 0.000 -31.480 0.000

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 14.89500 & 0 & -2.11349 \\ 0 & 15.80000 & 0 \\ 0 & 0 & 19.64665 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.06714 & 0 & 0.00722 \\ 0 & 0.06329 & 0 \\ 0 & 0 & 0.05090 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: kla0168t
================================================================================
:: 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 27.91 37.38 44.17 50.24 53.88 59.47 61.65 64.56 67.72 70.87   412 1000.0
Shell 2 26.61 36.14 43.24 49.45 53.22 58.31 61.20 64.08 66.52 68.07   451  230.4
Shell 3 26.97 35.56 42.96 50.12 53.46 57.28 60.38 63.25 66.83 69.21   419  171.8
Shell 4 18.97 29.49 37.95 45.13 51.03 55.38 59.49 64.10 66.92 69.74   390   88.9
Shell 5 19.66 29.21 37.08 43.26 49.44 53.93 56.74 60.67 64.61 67.70   356   73.3
Shell 6 24.93 30.56 35.31 40.95 45.40 50.15 55.19 57.86 60.53 64.69   337   48.2
Shell 7 24.84 31.37 35.71 40.99 45.34 48.76 53.73 57.76 61.49 65.53   322   36.6
Shell 8 25.82 29.08 33.33 39.22 42.81 46.08 50.33 54.58 58.50 62.75   306   32.7
Shell 9 34.53 37.41 39.93 43.17 45.68 49.64 51.80 55.76 60.43 64.39   278   29.5
Shell10 42.80 47.60 49.60 52.80 54.80 57.20 58.80 60.00 61.60 63.20   250   23.8

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  22.63 31.21 38.32 44.86 49.83 54.19 57.95 61.47 64.72 67.84
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 ( 50 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  12.65 12.15 11.02 10.05  8.17  6.29  4.37  2.71  1.22  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	5.04	4.75	2039	2038	110.74	0	3	3	1.1
2	HKL:H+L=2N	4.86	4.94	2049	2028	111.22	3	-1	2	1.0
3	HKL:K+L=2N	5.29	4.51	2025	2052	111.22	3	-1	2	1.2
4	HKL:H+K+L=2N	4.97	4.82	2050	2027	101.20	2	3	2	1.0
5	HKL:-H+K+L=3N	4.96	4.87	1361	2716	111.22	3	-1	2	1.0
6	HKL:H-K+L=3N	4.84	4.93	1353	2724	101.20	2	3	2	1.0
7	0KL:K=2N	16.77	18.61	26	27	110.74	0	3	3	0.9
8	0KL:L=2N	15.57	19.92	27	26	110.74	0	3	3	0.8
9	0KL:K+L=2N	21.92	13.65	26	27	64.18	0	4	3	1.6
10	H0L:H=2N	5.08	3.75	117	119	47.43	7	0	0	1.4
11 E cy	H0L:L=2N	8.26	0.49	119	117	4.82	7	0	23	16.8
12	H0L:H+L=2N	4.89	3.93	118	118	47.43	7	0	0	1.2
13	HK0:H=2N	9.86	10.84	49	47	51.71	-3	1	0	0.9
14	HK0:K=2N	14.41	8.68	54	53	51.71	-3	1	0	1.7
15	HK0:H+K=2N	12.08	8.74	46	50	34.66	-3	2	0	1.4
16	H00:H=2N	16.58	29.09	6	5	47.43	7	0	0	0.6
17	0K0:K=2N	0.00	0.00	0	0	0.00	0	0	0	0.0
18	00L:L=2N	0.00	0.00	0	0	0.00	0	0	0	0.0
19	0KL:K+L=4N	21.93	16.33	13	40	110.74	0	3	3	1.3
20	H0L:H+L=4N	4.82	4.28	57	179	59.08	2	0	0	1.1
21	HK0:H+K=4N	11.09	10.12	22	74	51.71	-3	1	0	1.1
22	H00:H=4N	9.07	27.21	3	8	59.08	2	0	0	0.3
23	0K0:K=4N	0.00	0.00	0	0	0.00	0	0	0	0.0
24	00L:L=4N	0.00	0.00	0	0	0.00	0	0	0	0.0
25	HHL:L=2N	6.05	7.75	71	73	70.70	3	3	1	0.8
26	HHL:H=2N	6.89	6.94	75	69	70.70	3	3	1	1.0
27	HHL:H+L=2N	7.67	6.15	72	72	65.67	3	3	2	1.2
28	HHL:2H+L=4N	5.73	7.32	37	107	70.70	3	3	1	0.8
29	H-HL:H+L=3N	10.59	16.72	11	21	61.84	-3	3	1	0.6
30	H-HL:-H+L=3N	13.29	15.31	11	21	61.84	-3	3	1	0.9
31	00L:L=6N	0.00	0.00	0	0	0.00	0	0	0	0.0
32	HH0:H=2N	0.00	0.00	0	0	0.00	0	0	0	0.0
33	H-HL:L=2N	12.63	15.97	13	19	61.84	-3	3	1	0.8
34	HHL:L=3N	6.10	7.30	47	97	70.70	3	3	1	0.8
35	H-2HL:L=2N	0.00	10.70	0	1	10.70	-3	6	7	0.0
36	-2HHL:L=2N	5.30	8.08	34	37	99.20	4	-2	1	0.7
37	H-2HL:L=3N	0.00	10.70	0	1	10.70	-3	6	7	0.0
38	-2HHL:L=3N	4.68	7.40	17	54	99.20	4	-2	1	0.6
39	00L:L=3N	0.00	0.00	0	0	0.00	0	0	0	0.0
40	H-HL:H=2N	12.59	16.64	16	16	61.84	-3	3	1	0.8
41	HKL:H=2N	4.93	4.86	2050	2027	111.22	3	-1	2	1.0
42	HKL:K=2N	4.76	5.04	2044	2033	111.22	3	-1	2	0.9

43	HKL:L=2N	4.96	4.84	2030	2047	110.74	0	3	3	1.0
44	HKL:H=3N	5.07	4.81	1364	2713	101.20	2	3	2	1.1
45	HKL:K=3N	4.82	4.94	1348	2729	111.22	3	-1	2	1.0
46	HKL:L=3N	4.88	4.91	1349	2728	111.22	3	-1	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
Pc	7	325	Pc	:ABC	6.02	314	50	A
P2/c	13	434	P2/c	:ABC	6.02	314	50	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