PLATON(V-311206)-Run for: kla0156 TIME: Nov 20 11:35:59 2011

(C) 1980-2007 A.L.Spek

Crystal Data

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

a =	13.79300	Angstrom	alpha =	90	Degree	a =	9.989	alpha =	98.90	V =	1933.2
b =	9.98900		beta =	98.9000		b =	13.793	beta =	90.00		
c =	14.20200		gamma =	90		c =	14.202	gamma =	90.00		
V =	1933.17	Cubic-Angstrom	d(100) =	13.6269	Angstrom						
			d(010) =	9.9890							
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	14.0310							

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

Niggli Values		
99.780	190.247	201.697
-30.306	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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 13.79300 & 0 & -2.19720 \\ 0 & 9.98900 & 0 \\ 0 & 0 & 14.03101 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.07250 & 0 & 0.01135 \\ 0 & 0.10011 & 0 \\ 0 & 0 & 0.07127 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: kla0156
==========================================================================
:: 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 32.52 45.19 52.36 58.01 63.01 66.82 69.65 72.95 74.03 75.49  2122 1000.0
Shell 2 28.48 39.07 45.36 50.46 56.03 59.83 63.38 67.13 70.17 72.57  2370  254.5
Shell 3 27.43 42.63 50.82 55.86 59.16 62.91 65.84 68.73 71.02 73.17  2184  232.1
Shell 4 23.99 35.36 42.09 48.52 53.21 57.37 61.03 63.90 66.77 69.24  2022  154.4
Shell 5 21.33 32.28 41.39 48.08 53.40 58.03 61.82 65.03 67.46 70.19  1899   88.5
Shell 6 22.86 30.85 39.59 47.46 54.29 59.53 64.37 68.57 71.37 73.94  1715   55.8
Shell 7 23.00 29.29 36.36 42.22 47.83 52.72 56.25 60.34 63.64 66.56  1639   47.7
Shell 8 25.34 30.49 36.48 41.89 47.04 51.14 55.37 59.41 63.52 66.45  1535   34.6
Shell 9 30.34 34.70 40.66 44.94 48.63 52.58 55.46 58.67 62.02 65.24  1493   29.3
Shell10 28.36 33.21 38.35 43.13 48.49 52.31 56.87 59.88 62.75 65.61  1361   39.0

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  23.90 35.28 43.47 49.98 55.01 59.46 63.27 66.56 69.15 71.63
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 ( 67 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  13.54 15.47 15.03 13.64 11.46  9.29  7.03  4.75  2.23  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	4.10	4.08	11284	11239	38.03	0	1	3	1.0
2		HKL:H+L=2N	4.20	3.98	11265	11258	38.03	0	1	3	1.1
3		HKL:K+L=2N	4.08	4.10	11274	11249	36.68	1	-1	4	1.0
4		HKL:H+K+L=2N	4.42	3.76	11257	11266	36.75	-1	-2	2	1.2
5		HKL:-H+K+L=3N	3.98	4.14	7504	15019	38.03	0	1	3	1.0
6		HKL:H-K+L=3N	4.14	4.06	7485	15038	38.03	0	1	3	1.0
7		0KL:K=2N	5.69	5.95	500	512	38.03	0	1	3	1.0
8		0KL:L=2N	6.15	5.49	509	503	38.03	0	1	3	1.1
9		0KL:K+L=2N	6.86	4.75	513	499	33.94	0	-1	2	1.4
10		H0L:H=2N	4.82	4.39	634	627	33.74	1	0	3	1.1
11		H0L:L=2N	4.79	4.42	637	624	33.74	1	0	3	1.1
12	E ny	H0L:H+L=2N	8.78	0.41	632	629	4.52	12	0	11	21.4
13		HK0:H=2N	4.71	5.93	404	447	36.48	-1	2	0	0.8
14		HK0:K=2N	5.51	5.34	452	467	35.48	1	1	0	1.0
15		HK0:H+K=2N	5.83	4.88	438	444	36.48	-1	2	0	1.2
16	E 21x	H00:H=2N	12.68	0.46	20	17	1.39	15	0	0	27.7
17	E 21y	0K0:K=2N	10.86	0.38	15	16	1.37	0	13	0	28.6
18	E 21z	00L:L=2N	11.96	0.38	24	22	2.56	0	0	15	31.6
19		0KL:K+L=4N	6.46	5.61	255	757	37.15	0	-1	3	1.2
20	> dy	H0L:H+L=4N	8.61	3.28	313	948	35.19	0	0	2	2.6
21		HK0:H+K=4N	6.15	5.09	221	661	36.48	-1	2	0	1.2
22		H00:H=4N	9.49	6.29	9	28	33.39	2	0	0	1.5
23		0K0:K=4N	2.51	6.47	8	23	34.59	0	2	0	0.4
24	> 41z	00L:L=4N	11.12	4.95	11	35	35.19	0	0	2	2.2
25		HHL:L=2N	5.78	5.51	331	356	31.16	-2	-2	3	1.0
26		HHL:H=2N	5.58	5.69	318	369	33.57	1	1	4	1.0
27		HHL:H+L=2N	5.33	5.97	350	337	33.57	1	1	4	0.9
28		HHL:2H+L=4N	5.51	5.68	168	519	33.57	1	1	4	1.0
29		H-HL:H+L=3N	5.44	6.15	267	550	36.68	1	-1	4	0.9
30		H-HL:-H+L=3N	6.46	5.64	273	544	31.91	-2	2	3	1.1
31		00L:L=6N	6.53	6.40	8	38	35.19	0	0	2	1.0
32		HH0:H=2N	8.84	12.13	12	13	35.48	1	1	0	0.7
33		H-HL:L=2N	6.09	5.75	396	421	31.91	-2	2	3	1.1
34		HHL:L=3N	5.39	5.76	214	473	33.57	1	1	4	0.9
35		H-2HL:L=2N	4.63	5.35	220	240	31.97	1	-2	3	0.9
36		-2HHL:L=2N	5.42	4.57	264	287	36.73	2	-1	1	1.2
37		H-2HL:L=3N	5.31	4.87	143	317	35.47	-1	2	2	1.1
38		-2HHL:L=3N	3.71	5.55	171	380	36.73	2	-1	1	0.7
39		00L:L=3N	3.53	7.97	16	30	35.19	0	0	2	0.4
40		H-HL:H=2N	5.83	6.00	392	425	36.68	1	-1	4	1.0
41		HKL:H=2N	4.09	4.09	11254	11269	36.75	-1	-2	2	1.0
42		HKL:K=2N	3.96	4.22	11213	11310	38.03	0	1	3	0.9

43	HKL:L=2N	4.13	4.05	11282	11241	38.03	0	1	3	1.0
44	HKL:H=3N	4.11	4.08	7504	15019	36.75	-1	-2	2	1.0
45	HKL:K=3N	3.78	4.25	7602	14921	38.03	0	1	3	0.9
46	HKL:L=3N	3.96	4.16	7538	14985	36.75	-1	-2	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
P21/n	14	30824	P21/c	:A-B-N	4.30	2098	67	C
P21	4	5116	P21	:ABC	4.30	2098	33 Chiral	A
Pn	7	325	Pc	:A-B-N	4.30	2098	33	A

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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