

PLATON(V-311206)-Run for: kla0133

TIME: Sep 22 10:23:05 2011

(C) 1980-2007 A.L.Spek

Crystal Data

Input Cell (Lattice Type: P)				Temp = 0K	Reduced Cell (Acta Cryst.(1976), A32, 297-298)			
a =	12.77000	Angstrom	alpha =	110.2900 Degree	a =	12.770	alpha =	110.29 V = 1856.0
b =	12.94500		beta =	112.0400	b =	12.945	beta =	112.04
c =	13.70700		gamma =	99.2800	c =	13.707	gamma =	99.28
V =	1856.02	Cubic-Angstrom	d(100) =	11.1522 Angstrom	Niggli Values			
			d(010) =	11.4395	163.073	167.573	187.882	
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	11.3766	-61.530	-65.684	-26.657	

Orthogonalization Matrices

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

(X0) (12.77000 -2.08750 -5.14360) (X) , (X) (0.07831 0.01280 0.04177) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 12.77558 -5.65669)*(Y) , (Y) = (0 0.07827 0.03892)*(Y0) are defined as:
 (Z0) (0 0 11.37660) (Z) , (Z) (0 0 0.08790) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

=====

SPGR - Determine SpaceGroup from Observed Extinctions for: kla0133

=====

:: 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	24.31	34.72	41.60	47.68	52.41	56.70	60.59	63.40	65.95	67.92	2238	1000.0
Shell 2	23.38	33.48	40.89	46.67	51.43	55.82	58.72	62.32	65.17	67.99	2524	465.9
Shell 3	21.86	33.03	41.00	47.66	52.81	56.28	60.04	62.42	65.54	67.75	2310	251.4
Shell 4	25.22	33.58	39.80	44.98	50.48	53.75	57.38	61.15	64.33	66.83	2201	178.4
Shell 5	23.77	33.22	40.11	45.87	50.64	53.74	56.74	60.43	63.14	66.14	2032	145.1
Shell 6	26.67	36.85	43.73	49.23	53.23	57.33	60.53	62.88	65.07	67.89	1875	125.2
Shell 7	22.46	31.80	38.19	42.86	47.75	52.58	56.36	59.09	61.92	64.59	1799	92.2
Shell 8	25.90	33.62	39.43	44.60	48.90	52.73	56.39	59.58	62.83	65.33	1722	59.9
Shell 9	22.41	32.46	39.76	45.76	51.69	56.37	60.42	63.86	67.29	70.04	1602	49.6
Shell10	25.18	36.35	41.90	46.99	52.41	56.77	60.28	62.39	64.51	67.09	1513	40.4

	z ->	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Av3: 6		24.38	34.17	41.16	46.93	51.79	55.27	58.68	61.72	64.52	67.15
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 (62 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		14.47	15.25	14.06	12.39	10.47	7.79	5.57	3.50	1.63	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))		Number of Refl		I/sigI Max.F				.T/F. L Ratio
		.True.	.False.	.True.	.False.		H	K	L	
1	HKL:H+K=2N	10.98	11.01	11965	11979	24.49	-4	3	1	1.0
2	HKL:H+L=2N	11.01	10.97	11968	11976	24.49	-4	3	1	1.0
3	HKL:K+L=2N	11.03	10.95	11969	11975	24.38	-8	1	4	1.0
4	HKL:H+K+L=2N	10.99	10.99	11943	12001	24.38	-8	1	4	1.0
5	HKL:-H+K+L=3N	10.99	10.99	7975	15969	24.49	-4	3	1	1.0
6	HKL:H-K+L=3N	10.99	10.99	7985	15959	24.38	-8	1	4	1.0
7	OKL:K=2N	12.13	12.06	582	569	22.95	0	1	7	1.0
8	OKL:L=2N	12.28	11.91	581	570	23.72	0	-2	1	1.0
9	OKL:K+L=2N	12.10	12.09	576	575	23.72	0	-2	1	1.0
10	H0L:H=2N	12.25	12.41	514	515	23.41	1	0	2	1.0
11	H0L:L=2N	12.96	11.70	514	515	22.70	0	0	7	1.1
12	H0L:H+L=2N	12.13	12.52	509	520	23.41	1	0	2	1.0
13	HK0:H=2N	12.93	12.83	439	492	23.81	1	2	0	1.0
14	HK0:K=2N	12.85	13.07	502	505	22.82	1	1	0	1.0
15	HK0:H+K=2N	13.03	12.90	488	491	23.81	1	2	0	1.0
16	H00:H=2N	14.77	10.92	14	14	20.25	7	0	0	1.4
17	OK0:K=2N	15.72	13.57	24	24	22.07	0	3	0	1.2
18	00L:L=2N	15.41	14.32	20	21	22.70	0	0	7	1.1
19	OKL:K+L=4N	12.00	12.12	291	860	23.93	0	0	6	1.0
20	H0L:H+L=4N	11.43	12.62	252	777	23.93	0	0	6	0.9
21	HK0:H+K=4N	12.79	13.02	239	740	23.81	1	2	0	1.0
22	H00:H=4N	15.38	12.00	7	21	20.25	7	0	0	1.3
23	OK0:K=4N	17.16	13.99	10	38	23.74	0	2	0	1.2
24	00L:L=4N	14.46	14.96	9	32	23.93	0	0	6	1.0
25	HHL:L=2N	11.69	12.57	318	349	23.15	1	1	3	0.9
26	HHL:H=2N	11.67	12.58	314	353	23.15	1	1	3	0.9
27	HHL:H+L=2N	11.79	12.51	335	332	22.29	1	1	2	0.9
28	HHL:2H+L=4N	11.50	12.36	164	503	23.15	1	1	3	0.9
29	H-HL:H+L=3N	11.83	11.32	277	541	23.31	2	-2	3	1.0
30	H-HL:-H+L=3N	12.52	10.99	266	552	23.31	2	-2	3	1.1
31	00L:L=6N	14.82	14.86	6	35	23.02	0	0	2	1.0
32	HH0:H=2N	14.15	13.36	11	14	22.82	1	1	0	1.1
33	H-HL:L=2N	11.13	11.81	385	433	23.31	2	-2	3	0.9
34	HHL:L=3N	12.53	11.99	204	463	22.47	2	2	4	1.0
35	H-2HL:L=2N	12.24	12.90	225	250	22.56	-1	2	1	0.9
36	-2HHL:L=2N	11.75	11.41	221	248	22.96	4	-2	1	1.0
37	H-2HL:L=3N	11.91	12.87	139	336	22.69	3	-6	8	0.9
38	-2HHL:L=3N	11.09	11.79	146	323	22.96	4	-2	1	0.9
39	00L:L=3N	15.58	14.43	15	26	23.02	0	0	2	1.1
40	H-HL:H=2N	11.33	11.64	387	431	22.58	-3	3	3	1.0
41	HKL:H=2N	10.98	11.00	11966	11978	24.38	-1	7	3	1.0
42	HKL:K=2N	10.98	11.00	11977	11967	24.49	-4	3	1	1.0

43	HKL:L=2N	10.97	11.01	11948	11996	24.49	-4	3	1	1.0
44	HKL:H=3N	10.90	11.04	7990	15954	24.49	-4	3	1	1.0
45	HKL:K=3N	10.91	11.03	7974	15970	24.39	0	2	2	1.0
46	HKL:L=3N	10.91	11.03	7969	15975	24.49	-4	3	1	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	2.96	7139	38 Chiral A
P-1	2	15327	P-1	:ABC	2.96	7139	62 C

=====

***** N O T I C E *****

=====

- 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