

PLATON(V-311206)-Run for: kla0139

TIME: Oct 15 12:42:39 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 =	13.45100	Angstrom	alpha =	101.1400 Degree	a =	13.451	alpha =	101.14 V = 4060.2
b =	14.13400		beta =	97.0600	b =	14.134	beta =	97.06
c =	22.00500		gamma =	93.1600	c =	22.005	gamma =	93.16
V =	4060.18	Cubic-Angstrom	d(100) =	13.3052 Angstrom	Niggli Values			
			d(010) =	13.8221	180.929	199.770	484.220	
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	21.3888	-60.091	-36.380	-10.480	

Orthogonalization Matrices

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

(X0) (13.45100 -0.77913 -2.70460) (X) , (X) (0.07434 0.00410 0.01025) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 14.11251 -4.40731)*(Y) , (Y) = (0 0.07086 0.01460)*(Y0) are defined as:
 (Z0) (0 0 21.38880) (Z) , (Z) (0 0 0.04675) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

=====

SPGR - Determine SpaceGroup from Observed Extinctions for: kla0139

=====

:: 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	28.51	38.18	45.29	50.75	55.34	58.53	61.44	64.77	67.24	69.35	5387	1000.0
Shell 2	26.37	38.31	46.27	51.83	56.17	60.44	63.99	66.63	69.10	71.59	5829	331.9
Shell 3	22.42	33.76	41.98	48.06	53.51	57.39	61.06	63.82	66.54	68.82	5362	231.2
Shell 4	22.39	31.78	38.74	44.33	49.57	54.11	58.44	61.81	64.80	67.10	4918	177.6
Shell 5	23.07	30.37	37.27	43.10	48.76	53.53	57.44	60.97	64.02	67.00	4594	113.9
Shell 6	28.39	33.50	39.10	43.49	47.85	52.24	56.35	60.13	64.14	67.36	4286	69.0
Shell 7	32.67	36.58	40.63	44.93	48.91	53.08	57.16	60.65	63.96	66.76	4071	56.0
Shell 8	32.71	36.18	40.51	44.64	48.55	52.08	55.39	58.46	61.80	64.71	3806	51.9
Shell 9	35.33	38.24	41.52	45.37	48.74	51.89	55.14	57.99	60.62	63.61	3685	46.0
Shell10	36.49	39.58	42.64	45.24	48.27	51.24	54.48	57.45	59.99	62.63	3497	43.0

z ->	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Av3: 6	24.07	32.35	39.27	44.74	49.92	54.31	58.32	61.68	64.88	67.57
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 (54 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	14.12	13.35	12.05	10.03	8.40	6.58	4.93	3.13	1.61	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	2.70	2.70	27097	27079	70.28	-2	-3	7	1.0
2	HKL:H+L=2N	2.67	2.72	27092	27084	70.28	-2	-3	7	1.0
3	HKL:K+L=2N	2.72	2.68	27069	27107	69.79	-1	-3	2	1.0
4	HKL:H+K+L=2N	2.73	2.66	27124	27052	66.78	-2	-2	3	1.0
5	HKL:-H+K+L=3N	2.68	2.71	18069	36107	79.91	-2	-2	2	1.0
6	HKL:H-K+L=3N	2.66	2.72	18022	36154	79.91	-2	-2	2	1.0
7	OKL:K=2N	4.53	4.59	1220	1209	54.82	0	-1	3	1.0
8	OKL:L=2N	4.72	4.40	1218	1211	54.82	0	-1	3	1.1
9	OKL:K+L=2N	5.45	3.68	1211	1218	35.31	0	-3	6	1.5
10	H0L:H=2N	4.85	4.58	1171	1171	49.87	1	0	2	1.1
11	H0L:L=2N	4.77	4.66	1177	1165	45.78	-2	0	3	1.0
12	H0L:H+L=2N	4.58	4.85	1168	1174	49.87	1	0	2	0.9
13	HK0:H=2N	3.15	3.56	665	728	42.78	1	2	0	0.9
14	HK0:K=2N	3.77	3.34	760	750	27.99	3	3	0	1.1
15	HK0:H+K=2N	3.41	3.56	727	726	42.78	1	2	0	1.0
16	H00:H=2N	5.79	5.13	30	27	11.03	9	0	0	1.1
17 > 21y	OK0:K=2N	8.82	3.50	31	29	12.33	0	7	0	2.5
18 > 21z	00L:L=2N	11.66	2.75	36	36	19.32	0	0	3	4.2
19	OKL:K+L=4N	5.75	4.17	597	1832	59.36	0	2	0	1.4
20	H0L:H+L=4N	4.76	4.70	580	1762	49.87	1	0	2	1.0
21	HK0:H+K=4N	3.10	3.62	370	1083	59.36	0	2	0	0.9
22	H00:H=4N	1.40	6.81	14	43	35.61	2	0	0	0.2
23	OK0:K=4N	2.34	7.55	15	45	59.36	0	2	0	0.3
24 > 41z	00L:L=4N	15.68	4.17	19	53	29.08	0	0	10	3.8
25 > cxy	HHL:L=2N	6.19	2.82	747	788	66.78	-2	-2	3	2.2
26	HHL:H=2N	4.17	4.72	727	808	57.76	-1	-1	2	0.9
27	HHL:H+L=2N	4.12	4.80	765	770	66.78	-2	-2	3	0.9
28	HHL:2H+L=4N	6.06	3.95	374	1161	79.91	-2	-2	2	1.5
29	H-HL:H+L=3N	3.01	3.81	487	989	54.64	-1	1	2	0.8
30	H-HL:-H+L=3N	3.33	3.66	494	982	49.96	-1	1	3	0.9
31	00L:L=6N	6.94	7.26	12	60	59.43	0	0	4	1.0
32	HH0:H=2N	10.16	12.43	18	16	27.99	3	3	0	0.8
33	H-HL:L=2N	3.02	4.05	723	753	49.96	-1	1	3	0.7
34	HHL:L=3N	4.16	4.60	488	1047	79.91	-2	-2	2	0.9
35	H-2HL:L=2N	3.48	3.79	487	515	60.35	2	-4	3	0.9
36	-2HHL:L=2N	3.07	3.27	430	445	31.84	-4	2	1	0.9
37	H-2HL:L=3N	3.56	3.67	318	684	51.45	1	-2	1	1.0
38	-2HHL:L=3N	2.75	3.36	271	604	31.84	-4	2	1	0.8
39	00L:L=3N	6.10	7.79	25	47	59.43	0	0	4	0.8
40	H-HL:H=2N	2.55	4.43	694	782	54.64	-1	1	2	0.6
41	HKL:H=2N	2.70	2.70	27079	27097	69.79	-1	-3	2	1.0
42	HKL:K=2N	2.67	2.72	27134	27042	70.28	-2	-3	7	1.0

43	HKL:L=2N	2.69	2.71	27105	27071	70.28	-2	-3	7	1.0
44	HKL:H=3N	2.66	2.72	18034	36142	79.91	-2	-2	2	1.0
45	HKL:K=3N	2.67	2.71	18053	36123	79.91	-2	-2	2	1.0
46	HKL:L=3N	2.70	2.70	18065	36111	79.91	-2	-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

P1	1	799	P1	:ABC	4.33	3898	46 Chiral A
P-1	2	15327	P-1	:ABC	4.33	3898	54 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