

PLATON(V-311206)-Run for: kla0081

TIME: Sep 21 15:14:43 2011

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Crystal Data

Input Cell (Lattice Type: P)				Temp = 0K	Reduced Cell		(Acta Cryst.(1976), A32, 297-298)		
a =	16.05900	Angstrom	alpha =	99.4400 Degree	a =	16.059	alpha =	99.44	V = 4942.7
b =	16.93100		beta =	111.6400	b =	16.931	beta =	111.64	
c =	21.18500		gamma =	105.2300	c =	21.185	gamma =	105.23	
V = 4942.68 Cubic-Angstrom					Niggli Values				
d(100) = 13.9692 Angstrom					257.891 286.659 448.804				
d(010) = 15.6299					-58.829 -125.461 -71.425				
d(001) = 18.8403									
Lambda(MoKa) = 0.71070 Angstrom									

Orthogonalization Matrices

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

(X0) (16.05900 -4.44768 -7.81247) (X) , (X) (0.06227 0.01695 0.03098) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 16.33637 -5.72812)*(Y) , (Y) = (0 0.06121 0.01861)*(Y0) are defined as:
 (Z0) (0 0 18.84033) (Z) , (Z) (0 0 0.05308) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

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SPGR - Determine SpaceGroup from Observed Extinctions for: k1a0081

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:: 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

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Shell 1	26.13	35.80	43.34	48.90	53.68	57.89	62.05	65.03	67.85	70.23	6865	1000.0
Shell 2	23.81	34.33	41.88	48.18	53.42	57.43	60.91	63.79	66.39	68.66	7242	402.3
Shell 3	24.10	33.24	40.88	46.57	51.67	55.55	59.14	62.35	65.32	67.98	6661	187.1
Shell 4	25.02	30.99	37.64	43.86	49.73	54.33	58.66	61.98	65.01	67.64	6079	114.8
Shell 5	28.87	33.61	38.66	43.39	48.55	53.13	56.98	60.61	63.91	66.76	5677	89.8
Shell 6	31.89	36.16	39.90	44.34	47.98	51.62	55.08	58.59	61.65	64.75	5296	71.4
Shell 7	34.97	38.30	41.99	45.00	48.47	51.59	54.54	57.87	60.88	63.69	4987	58.2
Shell 8	37.94	40.57	43.40	46.15	48.94	51.37	54.12	56.28	58.75	61.42	4691	47.1
Shell 9	42.73	45.07	47.45	49.64	52.36	54.64	56.76	59.30	61.42	63.74	4440	40.8
Shell10	43.32	45.56	47.95	50.13	52.26	54.79	56.59	58.69	61.11	62.69	4227	40.1

z ->	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Av3: 6	27.47	33.50	39.27	44.54	49.48	53.66	57.46	60.88	63.97	66.78
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 (57 Percent Centric)

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z ->	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Av3: 6	17.60	14.66	12.28	10.14	8.35	6.40	4.62	2.96	1.42	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	2.43	2.43	33157	33062	28.63	-3	0	1	1.0
2	HKL:H+L=2N	2.42	2.44	33116	33103	28.33	0	-3	3	1.0
3	HKL:K+L=2N	2.44	2.42	33132	33087	28.63	-3	0	1	1.0
4	HKL:H+K+L=2N	2.41	2.45	33106	33113	28.55	2	-1	2	1.0
5	HKL:-H+K+L=3N	2.42	2.44	22076	44143	28.96	-2	0	2	1.0
6	HKL:H-K+L=3N	2.40	2.45	22048	44171	28.63	-3	0	1	1.0
7	OKL:K=2N	3.76	3.70	1234	1246	28.33	0	-3	3	1.0
8	OKL:L=2N	3.64	3.82	1242	1238	28.33	0	-3	3	1.0
9	OKL:K+L=2N	3.78	3.69	1252	1228	27.73	0	-3	2	1.0
10	H0L:H=2N	4.11	3.73	1220	1206	28.63	-3	0	1	1.1
11	H0L:L=2N	4.30	3.55	1206	1220	28.63	-3	0	1	1.2
12	H0L:H+L=2N	3.75	4.10	1216	1210	27.73	-1	0	4	0.9
13	HK0:H=2N	3.22	3.65	846	915	26.39	-3	2	0	0.9
14	HK0:K=2N	3.80	3.52	930	949	25.21	-4	1	0	1.1
15	HK0:H+K=2N	3.78	3.30	908	914	26.39	-3	2	0	1.1
16	H00:H=2N	8.20	6.83	29	28	27.59	3	0	0	1.2
17	OK0:K=2N	7.67	4.79	32	29	10.08	0	3	0	1.6
18	00L:L=2N	6.62	9.26	35	38	23.31	0	0	3	0.7
19	OKL:K+L=4N	4.14	3.59	629	1851	27.73	0	-3	2	1.2
20	H0L:H+L=4N	3.88	3.94	611	1815	28.63	-3	0	1	1.0
21	HK0:H+K=4N	3.24	3.64	449	1373	28.81	-4	2	0	0.9
22	H00:H=4N	9.72	6.82	14	43	27.59	3	0	0	1.4
23	OK0:K=4N	6.67	6.17	16	45	16.72	0	6	0	1.1
24	00L:L=4N	9.83	7.35	19	54	23.31	0	0	3	1.3
25	HHL:L=2N	3.72	3.68	647	676	25.95	-2	-2	1	1.0
26	HHL:H=2N	3.62	3.77	628	695	27.26	-3	-3	4	1.0
27	HHL:H+L=2N	3.47	3.94	664	659	27.26	-3	-3	4	0.9
28	HHL:2H+L=4N	3.62	3.73	319	1004	27.42	-2	-2	2	1.0
29	H-HL:H+L=3N	3.64	3.48	639	1247	27.40	2	-2	2	1.0
30	H-HL:-H+L=3N	3.29	3.66	620	1266	28.52	-2	2	2	0.9
31	00L:L=6N	1.52	9.27	12	61	27.15	0	0	4	0.2
32	HH0:H=2N	3.72	8.27	15	15	20.03	3	3	0	0.4
33	H-HL:L=2N	3.38	3.69	917	969	26.27	-4	4	7	0.9
34	HHL:L=3N	3.56	3.77	424	899	27.42	-2	-2	2	0.9
35	H-2HL:L=2N	3.54	3.61	577	607	24.17	-1	2	1	1.0
36	-2HHL:L=2N	3.35	3.58	541	567	27.77	2	-1	1	0.9
37	H-2HL:L=3N	3.40	3.66	371	813	26.83	1	-2	2	0.9
38	-2HHL:L=3N	3.50	3.45	348	760	28.55	2	-1	2	1.0
39	00L:L=3N	5.01	9.64	26	47	27.15	0	0	4	0.5
40	H-HL:H=2N	3.53	3.55	908	978	28.06	-3	3	6	1.0
41	HKL:H=2N	2.42	2.44	33141	33078	28.63	-3	0	1	1.0
42	HKL:K=2N	2.42	2.44	33121	33098	28.55	2	-1	2	1.0

43	HKL:L=2N	2.44	2.42	33100	33119	28.63	-3	0	1	1.0
44	HKL:H=3N	2.46	2.42	22044	44175	28.96	-2	0	2	1.0
45	HKL:K=3N	2.47	2.41	22121	44098	28.81	-4	2	0	1.0
46	HKL:L=3N	2.43	2.43	22085	44134	28.96	-2	0	2	1.0

:: No Extinction Conditions Found

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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

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Tentative Space Group Assignment - (Please Check Carefully)

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:: 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

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Name	#	AbsFreq	StandSet.	R(av)	Perc.	N	A/C-Prob

P1	1	799	P1	:ABC	4.46	4248	43 Chiral A
P-1	2	15327	P-1	:ABC	4.46	4248	57 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