

PLATON(V-311206)-Run for: xray023a

TIME: Mar 4 13:35:03 2010

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Crystal Data

Input Cell (Lattice Type: P)		Temp = 0K	Reduced Cell (Acta Cryst.(1976), A32, 297-298)	
a = 30.33300 Angstrom	alpha = 90 Degree		a = 6.101	alpha = 105.31 V = 3483.0
b = 6.10100	beta = 105.3100		b = 19.513	beta = 90.00
c = 19.51300	gamma = 90		c = 30.333	gamma = 90.00
V = 3482.95 Cubic-Angstrom	d(100) = 29.2565 Angstrom		Niggli Values	
	d(010) = 6.1010		37.222	380.757 920.091
Lambda(MoKa) = 0.71070 Angstrom	d(001) = 18.8205		-156.283	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)

(X0) (30.33300 0 -5.15224) (X) , (X) (0.03297 0 0.00903) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 6.10100 0)*(Y) , (Y) = (0 0.16391 0)*(Y0) are defined as:
 (Z0) (0 0 18.82051) (Z) , (Z) (0 0 0.05313) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

∴ Reflection Data are READ from File : spgr_hkl - (OBS-Data)

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Shell 1 59 33 65 23 68 16 70 31 72 10 73 86 75 53 76 97 78 55 79 37 4372 1000 0
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7 -> 0 1 0 2 0 3 0 4 0 5 0 6 0 7 0 8 0 9 1 0

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7 ->  0 1  0 2  0 3  0 4  0 5  0 6  0 7  0 8  0 9  1 0

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[illegible]

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.		
			.True.	.False.	.True.	.False.		H	K	L Ratio
1	?	C HKL:H+K=2N	1.77	0.49	23525	23444	7.18	-2	1	25 3.6
2		HKL:H+L=2N	1.17	1.09	23505	23464	19.14	-3	1	0 1.1
3		HKL:K+L=2N	1.17	1.09	23477	23492	19.14	-3	1	0 1.1
4		HKL:H+K+L=2N	1.27	0.99	23515	23454	19.28	3	-1	1 1.3
5		HKL:-H+K+L=3N	1.13	1.13	15650	31319	19.78	0	0	4 1.0
6		HKL:H-K+L=3N	1.13	1.13	15641	31328	19.78	0	0	4 1.0
7	E	bx OKL:K=2N	2.42	0.55	453	470	3.86	0	-3	23 4.4
8		OKL:L=2N	1.86	1.08	458	465	15.52	0	-2	3 1.7
9		OKL:K+L=2N	1.82	1.12	460	463	15.52	0	-2	3 1.6
10	?	ay H0L:H=2N	2.02	0.49	2273	2267	6.39	-3	0	25 4.1
11	?	cy H0L:L=2N	2.09	0.43	2262	2278	6.39	-3	0	25 4.9
12	?	ny H0L:H+L=2N	2.02	0.50	2269	2271	6.12	-2	0	25 4.1
13		HK0:H=2N	1.05	1.74	667	690	19.14	-3	1	0 0.6
14		HK0:K=2N	1.45	1.63	753	742	19.14	-3	1	0 0.9
15	E	nz HK0:H+K=2N	2.43	0.41	696	686	2.72	25	4	0 5.9
16	E	21x H00:H=2N	5.26	0.52	56	57	2.13	33	0	0 10.1
17	E	21y OK0:K=2N	5.48	0.17	13	12	0.75	0	3	0 31.5
18	E	21z 00L:L=2N	7.03	0.39	35	38	2.97	0	0	17 18.0
19		OKL:K+L=4N	1.60	1.42	234	689	18.71	0	2	4 1.1
20	>	dy H0L:H+L=4N	2.06	0.99	1150	3390	19.29	4	0	2 2.1
21		HK0:H+K=4N	2.22	1.16	350	1032	19.14	-3	1	0 1.9
22	>	41x H00:H=4N	6.56	1.59	29	84	12.59	6	0	0 4.1
23		OK0:K=4N	0.56	3.68	6	19	17.39	0	2	0 0.2
24	>	41z 00L:L=4N	8.57	1.82	19	54	12.31	0	0	6 4.7
25		HHL:L=2N	2.47	1.96	390	420	17.80	-1	-1	1 1.3
26		HHL:H=2N	1.83	2.49	352	458	17.84	1	1	2 0.7
27		HHL:H+L=2N	1.84	2.57	406	404	17.84	1	1	2 0.7
28		HHL:2H+L=4N	2.86	2.00	196	614	17.80	-1	-1	1 1.4
29		H-HL:H+L=3N	2.32	2.48	271	539	19.04	-1	1	2 0.9
30		H-HL:-H+L=3N	2.35	2.46	263	547	18.32	1	-1	2 1.0
31	>	61z 00L:L=6N	7.21	2.86	12	61	19.78	0	0	4 2.5
32		HH0:H=2N	1.22	4.39	12	13	12.40	1	1	0 0.3
33		H-HL:L=2N	2.69	2.18	391	419	17.00	-1	1	1 1.2
34		HHL:L=3N	2.29	2.16	254	556	17.84	1	1	2 1.1
35		H-2HL:L=2N	0.88	0.77	181	193	5.86	2	-4	1 1.1
36		-2HHL:L=2N	1.50	1.41	368	394	11.78	-4	2	1 1.1
37		H-2HL:L=3N	0.76	0.85	117	257	5.86	2	-4	1 0.9
38		-2HHL:L=3N	1.50	1.44	235	527	12.47	-4	2	4 1.0
39		00L:L=3N	3.51	3.61	26	47	19.78	0	0	4 1.0
40		H-HL:H=2N	2.03	2.73	351	459	19.04	-1	1	2 0.7
41		HKL:H=2N	1.08	1.18	23477	23492	19.28	3	-1	1 0.9
42		HKL:K=2N	1.09	1.17	23311	23658	19.28	3	-1	1 0.9

43	HKL:L=2N	1.29	0.97	23477	23492	19.28	3	-1	1	1.3
44	HKL:H=3N	1.13	1.13	15668	31301	19.29	4	0	2	1.0
45	HKL:K=3N	1.04	1.17	15541	31428	19.28	3	-1	1	0.9
46	HKL:L=3N	1.13	1.13	15674	31295	19.78	0	0	4	1.0

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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

Cc	9	844	Cc :ABC	6.89	775	13	A
C2/c	15	5965	C2/c :ABC	6.89	775	87	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