PLATON(V-311206)-Run for: test TIME: Sep 30 11:57:46 2011

Crystal Data

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

a =	12.67200	Angstrom	alpha =	90	Degree	a =	12.672	alpha =	90.00	V =	6025.7
b =	22.54600		beta =	101.5800		b =	21.529	beta =	90.00		
c =	21.52900		gamma =	90		c =	22.546	gamma =	101.58		

V =	6025.70	Cubic-Angstrom	d(100) =	12.4141	Angstrom	Niggli Values	
			d(010) =	22.5460		160.580	463.498	508.322
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	21.0908		0.000	0.000	-54.764

Orthogonalization Matrices

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

(XO)	(	12.67200	0	-4.32164)	(X)	,	(X)	(	0.07891	0	0.01617)	(XO)
(YO) =	(	0	22.54600	0)*(	(Y)	,	(Y) =	(	0	0.04435	0)*(	(YO)
(ZO)	(	0	0	21.09078)	(Z)	,	(Z)	(	0	0	0.04741)	(ZO)

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

SPGR - Determine SpaceGroup from Observed Extinctions for: test

:: Reflection Data are READ from File : spgr.hkl - (OBS-Data)

:: TRMX = -1.00 0.00 0.00 0.00 0.00 -1.00 0.00 -1.00 0.00
:: Reflection Data are READ from File : spgr.hkl - (OBS-Data)

:: TRMX = -1.00 0.00 0.00 0.00 0.00 -1.00 0.00 -1.00 0.00

Nz-Test Statistics

Shell 1	48.29	58.76	66.03	69.44	73.08	74.36	76.92	79.49	80.98	82.69	468 1000.0
Shell 2	45.33	56.76	62.29	65.33	69.14	71.81	74.48	75.62	77.52	78.67	525 694.3
Shell 3	40.58	51.07	58.06	62.14	66.60	71.07	73.79	76.89	78.64	80.58	515 399.5
Shell 4	37.50	50.20	57.38	62.30	67.01	69.06	70.70	72.34	73.16	75.41	488 301.2
Shell 5	40.52	51.20	57.08	60.35	64.05	67.32	69.93	73.42	76.03	78.00	459 320.9
Shell 6	43.02	53.38	58.33	62.39	66.67	69.82	71.17	73.42	75.00	77.25	444 279.5
Shell 7	41.90	52.14	57.14	61.19	63.57	65.48	69.52	72.38	74.05	76.19	420 220.1
Shell 8	46.27	52.99	56.72	59.45	63.18	66.17	67.66	69.65	72.39	74.38	402 178.5
Shell 9	44.89	50.27	56.45	59.95	64.52	65.59	67.47	70.16	72.58	75.00	372 125.1
Shell10	48.40	58.02	63.10	66.58	70.05	71.39	73.26	75.13	77.01	79.68	374 146.9

z ->	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Av3: 6	40.41	51.46	57.71	61.79	66.08	69.32	71.40	74.02	75.71	77.81
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 (121 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	29.43	30.42	27.41	22.98	19.44	15.44	10.84	7.27	3.23	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	4.18	3.76	2516	2504	96.39	-3	2	2	1.1
2		HKL:H+L=2N	3.90	4.03	2502	2518	111.39	-2	2	1	1.0
3		HKL:K+L=2N	3.92	4.02	2510	2510	111.39	-2	2	1	1.0
4		HKL:H+K+L=2N	3.96	3.98	2515	2505	111.39	-2	2	1	1.0
5		HKL:-H+K+L=3N	4.05	3.93	1676	3344	111.39	-2	2	1	1.0
6		HKL:H-K+L=3N	4.01	3.95	1670	3350	99.03	-1	1	4	1.0
7	>	bx 0KL:K=2N	21.50	8.10	43	39	19.40	0	-1	14	2.7
8		0KL:L=2N	18.05	12.35	40	42	72.67	0	2	3	1.5
9		0KL:K+L=2N	16.85	13.41	41	41	72.67	0	2	3	1.3
10	>	ay H0L:H=2N	5.40	2.63	100	92	39.20	-3	0	13	2.1
11	>	cy H0L:L=2N	5.62	2.52	96	96	39.20	-3	0	13	2.2
12	E	ny H0L:H+L=2N	7.81	0.33	96	96	1.85	-15	0	12	23.4
13		HK0:H=2N	10.38	11.92	12	13	29.65	-7	3	0	0.9
14		HK0:K=2N	10.25	12.04	12	13	29.65	-7	3	0	0.9
15		HK0:H+K=2N	9.76	12.72	13	12	19.25	-3	2	0	0.8
16		H00:H=2N	0.00	0.00	0	0	0.00	0	0	0	0.0
17		0K0:K=2N	0.00	0.00	0	0	0.00	0	0	0	0.0
18	E	21z 00L:L=2N	47.64	0.21	6	7	0.90	0	0	7	226.8
19		0KL:K+L=4N	13.86	15.54	20	62	150.34	0	0	6	0.9
20		H0L:H+L=4N	6.14	3.40	47	145	150.34	0	0	6	1.8
21		HK0:H+K=4N	7.91	12.00	5	20	23.95	-8	2	0	0.7
22		H00:H=4N	0.00	0.00	0	0	0.00	0	0	0	0.0
23		0K0:K=4N	0.00	0.00	0	0	0.00	0	0	0	0.0
24		00L:L=4N	21.17	22.38	3	10	150.34	0	0	6	0.9
25		HHL:L=2N	13.94	9.59	5	5	22.43	-1	-1	11	1.5
26		HHL:H=2N	7.47	13.60	3	7	39.21	-1	-1	12	0.5
27		HHL:H+L=2N	11.52	11.92	4	6	39.21	-1	-1	12	1.0
28		HHL:2H+L=4N	9.99	12.52	3	7	39.21	-1	-1	12	0.8
29		H-HL:H+L=3N	8.35	6.26	83	164	111.39	-2	2	1	1.3
30		H-HL:-H+L=3N	7.12	6.89	83	164	99.03	-1	1	4	1.0
31	?	61z 00L:L=6N	104.89	7.05	2	11	48.85	0	0	10	14.9
32		HH0:H=2N	0.00	0.00	0	0	0.00	0	0	0	0.0
33		H-HL:L=2N	7.63	6.29	124	123	111.39	-2	2	1	1.2
34		HHL:L=3N	14.73	9.78	4	6	22.43	-1	-1	11	1.5
35		H-2HL:L=2N	6.16	4.32	68	73	46.59	-2	4	7	1.4
36		-2HHL:L=2N	4.37	4.56	72	74	34.27	-6	3	7	1.0
37		H-2HL:L=3N	4.01	5.79	46	95	46.59	-2	4	7	0.7
38		-2HHL:L=3N	3.84	4.77	47	99	34.27	-6	3	7	0.8
39	>	31z 00L:L=3N	41.98	9.67	5	8	48.85	0	0	10	4.3
40		H-HL:H=2N	6.64	7.27	120	127	99.03	-1	1	4	0.9
41		HKL:H=2N	4.07	3.87	2527	2493	99.03	-1	1	4	1.1
42		HKL:K=2N	4.03	3.91	2509	2511	99.03	-1	1	4	1.0

43	HKL:L=2N	4.09	3.85	2521	2499	111.39	-2	2	1	1.1
44	HKL:H=3N	4.06	3.92	1680	3340	111.39	-2	2	1	1.0
45	HKL:K=3N	3.77	4.07	1683	3337	111.39	-2	2	1	0.9
46	HKL:L=3N	3.86	4.02	1673	3347	111.39	-2	2	1	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
Pn	7	325	Pc	:A-B-N	5.00	99	-21	A
P2/n	13	434	P2/c	:A-B-N	5.00	99	121	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