PLATON(V-311206)-Run for: test TIME: May 31 15:55:02 2011

Crystal Data

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

a =	10.32200	Angstrom	alpha =	118.9600	Degree	a =	10.322	alpha =	118.96	V =	4683.7
b =	22.73500		beta =	90		b =	22.735	beta =	90.00		
c =	22.81100		gamma =	90		c =	22.811	gamma =	90.00		

V = 4683.71 Cubic-Angstrom

Lambda(MoKa) = 0.71070 Angstrom

d(100) = 10.3220 Angstrom

d(010) = 19.8922

d(001) = 19.9587

Reduced Cell (Acta Cryst.(1976),A32,297-298)

Niggli Values

106.544 516.880 520.342

-251.109 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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 10.32200 & 0 & 0 \\ 0 & 22.73500 & -11.04506 \\ 0 & 0 & 19.95867 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.09688 & 0 & 0 \\ 0 & 0.04399 & 0.02434 \\ 0 & 0 & 0.05010 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

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

Nz-Test Statistics
==================
Shell 1 22.01 33.28 41.07 48.56 52.65 57.56 61.27 64.98 68.38 71.48  1322 1000.0
Shell 2 22.02 31.86 39.23 44.86 50.05 54.59 58.09 61.48 64.10 67.21  1830  462.1
Shell 3 25.09 34.91 43.08 49.44 54.64 58.51 62.55 65.25 68.01 70.03  1885  269.6
Shell 4 26.20 35.56 42.01 49.40 54.70 58.48 62.58 65.26 67.94 70.13  1828  170.0
Shell 5 25.38 31.14 37.19 42.20 47.26 52.79 56.98 60.88 64.20 67.17  1718  134.7
Shell 6 31.74 37.19 42.89 47.73 51.47 56.43 60.05 63.17 66.24 69.36  1632  107.2
Shell 7 31.54 36.14 40.08 45.07 49.08 53.61 56.64 59.79 63.27 65.77  1522   90.0
Shell 8 33.69 37.32 41.96 45.73 49.56 53.19 56.76 59.85 62.68 65.50  1487   69.3
Shell 9 39.70 42.46 45.15 47.91 50.45 53.96 56.12 58.88 61.42 63.51  1340   57.3
Shell10 40.12 43.50 46.73 48.73 51.73 53.65 56.57 58.95 61.49 63.80  1301   54.7

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  27.10 34.70 41.29 47.19 52.02 56.56 60.54 63.64 66.60 69.17
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 ( 63 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  16.99 15.38 13.59 11.84  9.69  7.86  6.03  3.81  1.89  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	1.13	1.10	9482	9498	16.73	2	-3	1	1.0
2	HKL:H+L=2N	1.14	1.09	9483	9497	18.28	1	-3	2	1.0
3	HKL:K+L=2N	1.12	1.10	9519	9461	18.28	1	-3	2	1.0
4	HKL:H+K+L=2N	1.10	1.13	9464	9516	18.13	-2	0	1	1.0
5	HKL:-H+K+L=3N	1.11	1.12	6343	12637	18.28	1	-3	2	1.0
6	HKL:H-K+L=3N	1.11	1.12	6351	12629	18.13	-2	0	1	1.0
7	0KL:K=2N	1.15	1.06	460	486	14.62	0	1	2	1.1
8 E cx	0KL:L=2N	2.09	0.15	466	480	1.14	0	-5	23	14.4
9	0KL:K+L=2N	1.13	1.08	470	476	14.62	0	1	2	1.0
10	H0L:H=2N	1.49	1.10	256	263	8.64	-3	0	3	1.4
11	H0L:L=2N	1.38	1.19	264	255	18.13	-2	0	1	1.2
12	H0L:H+L=2N	1.56	1.03	255	264	18.13	-2	0	1	1.5
13	HK0:H=2N	1.58	1.52	189	206	16.20	-1	3	0	1.0
14	HK0:K=2N	1.69	1.61	209	212	16.20	-1	3	0	1.0
15	HK0:H+K=2N	1.69	1.48	202	204	15.75	2	3	0	1.1
16 E 21x	H00:H=2N	7.39	0.10	7	8	0.45	9	0	0	75.8
17 > 21y	0K0:K=2N	3.83	1.76	5	6	3.56	0	9	0	2.2
18 E 21z	00L:L=2N	3.11	0.13	9	12	0.83	0	0	21	24.7
19	0KL:K+L=4N	1.22	1.07	237	709	14.62	0	1	2	1.1
20	H0L:H+L=4N	1.43	1.25	128	391	18.13	-2	0	1	1.1
21	HK0:H+K=4N	1.54	1.59	100	306	16.20	-1	3	0	1.0
22	H00:H=4N	5.35	2.83	4	11	16.43	2	0	0	1.9
23 > 41y	0K0:K=4N	4.75	2.25	2	9	7.02	0	14	0	2.1
24 > 41z	00L:L=4N	3.09	1.13	3	18	13.97	0	0	6	2.7
25	HHL:L=2N	1.35	1.28	213	216	14.84	-2	-2	3	1.1
26	HHL:H=2N	1.26	1.36	207	222	15.79	-3	-3	4	0.9
27	HHL:H+L=2N	1.20	1.42	213	216	15.79	-3	-3	4	0.8
28	HHL:2H+L=4N	1.32	1.31	108	321	15.79	-3	-3	4	1.0
29	H-HL:H+L=3N	1.44	1.42	165	340	12.48	-1	1	3	1.0
30	H-HL:-H+L=3N	1.49	1.40	168	337	13.39	-2	2	2	1.1
31 ? 61z	00L:L=6N	7.84	0.73	2	19	5.56	0	0	8	10.8
32 ?	HH0:H=2N	1.33	1.11	6	5	1.18	3	3	0	1.2
33	H-HL:L=2N	1.42	1.43	246	259	12.84	6	-6	3	1.0
34	HHL:L=3N	1.30	1.32	130	299	15.79	-3	-3	4	1.0
35	H-2HL:L=2N	1.44	1.94	203	203	13.85	1	-2	1	0.7
36	-2HHL:L=2N	1.11	1.23	114	121	10.24	2	-1	3	0.9
37	H-2HL:L=3N	1.66	1.71	137	269	14.77	2	-4	2	1.0
38	-2HHL:L=3N	1.11	1.20	71	164	10.84	-2	1	2	0.9
39 ? 31z	00L:L=3N	2.75	0.87	6	15	5.56	0	0	8	3.2
40	H-HL:H=2N	1.51	1.35	244	261	13.30	1	-1	2	1.1
41	HKL:H=2N	1.11	1.12	9409	9571	18.28	1	-3	2	1.0
42	HKL:K=2N	1.14	1.09	9523	9457	18.28	1	-3	2	1.0

43	HKL:L=2N	1.14	1.08	9516	9464	18.13	-2	0	1	1.1
44	HKL:H=3N	1.03	1.15	6411	12569	18.28	1	-3	2	0.9
45	HKL:K=3N	1.31	1.02	6308	12672	15.17	3	-4	2	1.3
46	HKL:L=3N	1.12	1.11	6272	12708	18.28	1	-3	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	16.74	206	37	Chiral A
P-1	2	15327	P-1	:ABC	16.74	206	63	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