PLATON(V-311206)-Run for: char324t TIME: Jan 3 16:28:47 2011

Crystal Data

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

a =	11.66800	Angstrom	alpha =	90.1000	Degree	a =	11.668	alpha =	90.10	V =	1930.6
b =	12.51800		beta =	95.6300		b =	12.518	beta =	95.63		
c =	13.93500		gamma =	107.5100		c =	13.935	gamma =	107.51		
V =	1930.63	Cubic-Angstrom	d(100) =	11.0677	Angstrom						
			d(010) =	11.9315							
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	13.8603							

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

Niggli Values		
136.142	156.700	194.184
-0.305	-15.951	-43.945

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 11.66800 & -3.76632 & -1.36708 \\ 0 & 11.93797 & -0.45680 \\ 0 & 0 & 13.86026 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} \quad , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.08570 & 0.02704 & 0.00934 \\ 0 & 0.08377 & 0.00276 \\ 0 & 0 & 0.07215 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: char324t
================================================================================
:: 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 24.63 32.09 38.06 47.76 56.72 59.70 63.43 65.67 66.42 67.91   134 1000.0
Shell 2 19.23 26.28 36.54 46.15 50.00 55.77 59.62 60.90 62.82 65.38   156  361.1
Shell 3 19.29 30.71 38.57 44.29 50.71 54.29 58.57 64.29 69.29 70.00   140  216.6
Shell 4 20.16 27.42 35.48 39.52 46.77 50.00 52.42 55.65 58.87 61.29   124  103.4
Shell 5 18.18 24.79 33.06 42.15 47.93 52.89 59.50 64.46 66.12 66.94   121  100.5
Shell 6 18.97 25.00 32.76 40.52 47.41 50.00 53.45 56.90 59.48 61.21   116   78.0
Shell 7 21.30 25.00 34.26 41.67 44.44 49.07 51.85 57.41 59.26 61.11   108   60.7
Shell 8 20.21 26.60 31.91 37.23 42.55 46.81 47.87 54.26 59.57 60.64    94   39.4
Shell 9 28.71 31.68 33.66 35.64 39.60 42.57 45.54 50.50 54.46 60.40   101   33.3
Shell10 22.34 25.53 27.66 31.91 34.04 37.23 44.68 47.87 51.06 55.32    94   31.2

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  19.15 26.98 34.97 41.62 48.21 51.79 55.99 60.32 63.44 64.86
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 ( 43 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   9.47  8.53  8.56  7.99  8.04  5.69  4.49  3.94  2.61  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)) .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	5.10	5.04	787	763	116.32	2	1	2	1.0
2		HKL:H+L=2N	5.24	4.89	776	774	79.21	-2	0	1	1.1
3		HKL:K+L=2N	5.02	5.11	773	777	116.32	2	1	2	1.0
4		HKL:H+K+L=2N	4.90	5.24	776	774	116.32	2	1	2	0.9
5		HKL:-H+K+L=3N	4.84	5.18	510	1040	152.68	-2	0	2	0.9
6		HKL:H-K+L=3N	5.21	5.00	516	1034	79.21	-2	0	1	1.0
7		0KL:K=2N	0.00	36.86	0	8	82.51	0	1	4	0.0
8		0KL:L=2N	39.38	34.34	4	4	62.98	0	1	3	1.1
9		0KL:K+L=2N	34.34	39.38	4	4	82.51	0	1	4	0.9
10		H0L:H=2N	7.60	6.57	106	103	69.00	-3	0	3	1.2
11		H0L:L=2N	7.18	7.01	105	104	79.21	-2	0	1	1.0
12		H0L:H+L=2N	7.06	7.14	104	105	79.21	-2	0	1	1.0
13		HK0:H=2N	5.56	3.67	37	34	18.62	-5	2	0	1.5
14		HK0:K=2N	5.93	5.15	44	40	59.53	-2	1	0	1.2
15		HK0:H+K=2N	3.32	5.95	35	36	59.53	-2	1	0	0.6
16		H00:H=2N	7.45	14.06	7	6	60.73	3	0	0	0.5
17		0K0:K=2N	0.00	0.00	0	0	0.00	0	0	0	0.0
18		00L:L=2N	0.00	0.00	0	0	0.00	0	0	0	0.0
19		0KL:K+L=4N	39.34	36.03	2	6	82.51	0	1	4	1.1
20		H0L:H+L=4N	8.57	6.59	53	156	79.21	-2	0	1	1.3
21		HK0:H+K=4N	2.93	5.20	17	54	59.53	-2	1	0	0.6
22		H00:H=4N	12.77	9.82	3	10	60.73	3	0	0	1.3
23		0K0:K=4N	0.00	0.00	0	0	0.00	0	0	0	0.0
24		00L:L=4N	0.00	0.00	0	0	0.00	0	0	0	0.0
25		HHL:L=2N	25.22	19.77	3	3	0.00	0	0	0	1.3
26		HHL:H=2N	19.15	29.19	4	2	0.00	0	0	0	0.7
27	E	HHL:H+L=2N	26.81	0.94	5	1	0.00	0	0	0	28.5
28	>	HHL:2H+L=4N	64.59	14.08	1	5	7.00	4	4	6	4.6
29		H-HL:H+L=3N	15.02	20.77	7	16	64.36	-1	1	2	0.7
30		H-HL:-H+L=3N	21.23	17.84	8	15	46.13	-2	2	3	1.2
31		00L:L=6N	0.00	0.00	0	0	0.00	0	0	0	0.0
32		HH0:H=2N	0.00	0.00	0	0	0.00	0	0	0	0.0
33		H-HL:L=2N	22.00	15.76	12	11	46.13	-2	2	3	1.4
34		HHL:L=3N	7.00	25.60	1	5	64.59	2	2	4	0.3
35		H-2HL:L=2N	21.57	11.16	2	3	8.69	-1	2	7	1.9
36		-2HHL:L=2N	8.52	8.63	21	22	39.76	-2	1	7	1.0
37		H-2HL:L=3N	18.55	13.17	2	3	13.68	-1	2	8	1.4
38		-2HHL:L=3N	6.37	9.53	13	30	63.04	-2	1	2	0.7
39		00L:L=3N	0.00	0.00	0	0	0.00	0	0	0	0.0
40		H-HL:H=2N	11.48	23.04	8	15	64.36	-1	1	2	0.5
41		HKL:H=2N	5.11	5.02	779	771	69.00	-3	0	3	1.0
42		HKL:K=2N	4.81	5.33	794	756	116.32	2	1	2	0.9

43	HKL:L=2N	5.07	5.07	773	777	79.21	-2	0	1	1.0
44	HKL:H=3N	5.72	4.74	517	1033	152.68	-2	0	2	1.2
45	HKL:K=3N	4.94	5.13	518	1032	116.32	2	1	2	1.0
46	HKL:L=3N	4.87	5.16	511	1039	152.68	-2	0	2	0.9

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	0.00	0	57	Chiral	A
P-1	2	15327	P-1	:ABC	0.00	0	43		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