PLATON(V-311206)-Run for: char311 TIME: Nov 1 14:41:43 2010

Crystal Data

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

a =	9.87000	Angstrom	alpha =	90	Degree	a =	9.870	alpha =	90.00
b =	19.01300		beta =	90		b =	19.013	beta =	90.00
c =	59.72200		gamma =	90		c =	59.722	gamma =	90.00
V =	11207.33	Cubic-Angstrom	d(100) =	9.8700	Angstrom				
			d(010) =	19.0130					
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	59.7220					

Reduced Cell (Acta Cryst.(1976),A32,297-298) V = 11207.3

Niggli Values: 97.417 361.494 3566.717; 0.000 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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 9.87000 & 0 & 0 \\ 0 & 19.01300 & 0 \\ 0 & 0 & 59.72200 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.10132 & 0 & 0 \\ 0 & 0.05260 & 0 \\ 0 & 0 & 0.01674 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: char311
==========================================================================
:: 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 39.20 46.75 54.09 58.85 62.49 65.43 67.92 70.07 72.64 74.12 14930 1000.0
Shell 2 37.28 47.03 52.80 57.51 61.57 64.82 67.25 69.82 72.13 73.75 16826  351.3
Shell 3 33.90 44.85 51.79 56.90 61.12 64.46 66.99 68.97 70.70 72.50 15595  247.2
Shell 4 31.86 44.51 51.54 56.22 60.32 63.46 66.08 68.19 70.18 71.65 14555  159.2
Shell 5 31.09 44.60 52.40 57.65 61.83 65.01 67.64 69.97 72.06 73.86 13311  142.9
Shell 6 27.83 41.89 50.57 56.27 60.82 63.86 66.21 68.31 70.15 72.04 12600  105.6
Shell 7 27.39 41.39 50.73 57.00 61.62 64.93 67.55 69.81 71.81 73.37 11897   82.1
Shell 8 25.98 37.58 47.50 54.37 59.14 62.87 66.08 68.76 71.05 73.17 10945   67.8
Shell 9 26.35 36.26 45.21 52.89 58.61 62.83 65.87 68.75 70.98 72.77 10872   52.1
Shell10 27.27 35.55 43.58 50.45 56.21 60.96 64.83 67.77 70.42 72.59  9896   41.8

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  31.17 43.96 51.57 56.76 61.02 64.20 66.73 68.86 70.77 72.51
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 (100 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  20.72 23.98 22.87 20.07 17.02 13.50  9.88  6.35  3.06  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	5.25	5.08	77080	77231	28.33	-2	3	0	1.0
2		HKL:H+L=2N	5.12	5.20	77113	77198	28.45	1	1	4	1.0
3		HKL:K+L=2N	5.76	4.56	76894	77417	28.45	1	1	4	1.3
4		HKL:H+K+L=2N	5.16	5.16	77425	76886	29.18	1	-1	3	1.0
5		HKL:-H+K+L=3N	5.19	5.15	51440	102871	29.62	0	0	8	1.0
6		HKL:H-K+L=3N	5.19	5.15	51436	102875	29.62	0	0	8	1.0
7	E	bx 0KL:K=2N	7.47	0.25	4440	4692	3.00	0	-15	57	29.7
8	?	cx 0KL:L=2N	6.56	0.82	4680	4452	19.15	0	0	39	8.0
9	?	nx 0KL:K+L=2N	6.55	0.83	4674	4458	19.15	0	0	39	7.8
10		H0L:H=2N	4.32	4.17	2429	2443	27.64	3	0	28	1.0
11	?	cy H0L:L=2N	7.55	0.82	2477	2395	19.15	0	0	39	9.2
12		H0L:H+L=2N	4.23	4.26	2448	2424	27.64	3	0	28	1.0
13		HK0:H=2N	8.64	9.76	693	766	26.76	-3	3	0	0.9
14		HK0:K=2N	9.15	8.99	787	787	28.33	-2	3	0	1.0
15		HK0:H+K=2N	8.74	9.21	777	761	28.33	-2	3	0	0.9
16	>	21x H00:H=2N	18.92	7.71	18	18	13.13	9	0	0	2.5
17	E	21y 0K0:K=2N	8.30	0.26	39	40	1.48	0	11	0	31.8
18	>	21z 00L:L=2N	9.75	3.04	117	84	19.15	0	0	39	3.2
19	>	dx 0KL:K+L=4N	6.73	2.74	2334	6798	28.07	0	-4	10	2.5
20		H0L:H+L=4N	4.25	4.24	1229	3643	27.64	3	0	28	1.0
21		HK0:H+K=4N	9.21	8.90	388	1150	28.33	-2	3	0	1.0
22		H00:H=4N	16.16	12.37	9	27	26.69	2	0	0	1.3
23	?	41y 0K0:K=4N	11.31	1.66	21	58	17.49	0	10	0	6.8
24	?	41z 00L:L=4N	17.28	2.65	59	142	19.15	0	0	39	6.5
25	>	cxy HHL:L=2N	10.26	3.27	2033	2056	28.20	-1	-1	3	3.1
26		HHL:H=2N	5.11	8.16	1895	2194	28.45	1	1	4	0.6
27		HHL:H+L=2N	7.47	6.03	2043	2046	28.45	1	1	4	1.2
28		HHL:2H+L=4N	10.33	5.56	1017	3072	28.45	1	1	4	1.9
29		H-HL:H+L=3N	6.79	6.81	1333	2672	29.18	1	-1	3	1.0
30		H-HL:-H+L=3N	6.78	6.81	1331	2674	29.18	1	-1	3	1.0
31		00L:L=6N	8.75	6.51	39	162	29.62	0	0	8	1.3
32		HH0:H=2N	13.39	13.95	16	16	26.51	3	3	0	1.0
33	>	H-HL:L=2N	10.19	3.44	1993	2012	29.18	1	-1	3	3.0
34		HHL:L=3N	6.60	6.82	1340	2749	28.45	1	1	4	1.0
35	?	H-2HL:L=2N	10.14	0.82	1535	1542	6.05	1	-2	25	12.3
36	>	-2HHL:L=2N	9.98	3.26	1040	1051	25.84	2	-1	1	3.1
37		H-2HL:L=3N	5.62	5.40	1001	2076	27.75	-1	2	10	1.0
38		-2HHL:L=3N	6.57	6.61	688	1403	26.68	-2	1	8	1.0
39		00L:L=3N	7.12	6.86	66	135	29.62	0	0	8	1.0
40		H-HL:H=2N	5.16	8.22	1856	2149	29.18	1	-1	3	0.6
41		HKL:H=2N	5.04	5.28	77576	76735	29.18	1	-1	3	1.0
42		HKL:K=2N	4.69	5.64	77437	76874	29.18	1	-1	3	0.8

```
43 >  2Z HKL:L=2N         8.43    1.82  77948  76363    29.18    1 -1  3   4.6
44       HKL:H=3N         4.89    5.30  51438 102873    29.18    1 -1  3   0.9
45       HKL:K=3N         5.07    5.21  51435 102876    29.18    1 -1  3   1.0
46       HKL:L=3N         5.15    5.17  51420 102891    29.62    0  0  8   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
Pnc2	30	13	Pnc2	:ABC	4.23	7579	0	A
Pncm	53	13	Pmna	:BCA	4.23	7579	100	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