PLATON(V-311206)-Run for: feng002 TIME: May 6 14:03:26 2011

Crystal Data

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

a =	10.73400	Angstrom	alpha =	90	Degree	a =	8.708	alpha =	120.00	V =	868.9
b =	10.73400		beta =	90		b =	10.734	beta =	90.00		
c =	8.70800		gamma =	120		c =	10.734	gamma =	90.00		
V =	868.90	Cubic-Angstrom	d(100) =	9.2959	Angstrom						
			d(010) =	9.2959							
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	8.7080							

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

Niggli Values: 75.829 115.219 115.219 / -57.610 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)

$$(XO) = \begin{pmatrix} 10.73400 & -5.36700 & 0 \\ 0 & 9.29592 & 0 \\ 0 & 0 & 8.70800 \end{pmatrix} \begin{matrix}(X)\\ *(Y)\\ (Z)\end{matrix} \quad , \quad \begin{matrix}(X)\\ (Y)\\ (Z)\end{matrix} = \begin{pmatrix} 0.09316 & 0.05379 & 0 \\ 0 & 0.10757 & 0 \\ 0 & 0 & 0.11484 \end{pmatrix} \begin{matrix}(XO)\\ *(YO)\\ (ZO)\end{matrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: feng002
==========================================================================
:: 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 20.30 34.59 38.10 39.72 44.36 47.49 54.89 59.15 65.66 68.67   798 1000.0
Shell 2 17.15 31.20 39.51 50.37 54.95 60.60 64.54 69.01 70.82 72.84   939  827.5
Shell 3 23.95 36.13 44.50 51.83 53.80 57.33 61.26 64.27 67.54 70.03   764  652.7
Shell 4 14.69 24.78 32.63 37.11 42.84 49.81 57.04 62.27 64.63 66.50   803  387.0
Shell 5 12.50 26.42 38.21 45.60 52.13 56.68 61.36 65.20 69.60 73.72   704  468.7
Shell 6 12.89 26.58 39.19 49.53 54.36 59.46 62.68 65.91 68.86 71.41   745  263.3
Shell 7 17.73 29.81 37.41 43.22 48.44 55.29 59.17 62.89 65.87 67.96   671  173.9
Shell 8 12.03 19.40 29.62 37.14 44.51 50.23 55.34 62.26 68.27 72.18   665  285.8
Shell 9 18.38 30.43 35.97 43.58 50.55 54.83 59.11 64.98 68.94 72.58   631  148.5
Shell10 21.14 31.90 39.14 45.60 50.88 55.19 59.30 63.21 65.95 68.10   511  195.8

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  16.01 28.48 38.63 46.02 50.78 55.82 60.59 64.41 67.66 70.41
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 ( 44 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   5.77  8.91 10.55 10.17  7.83  6.38  5.20  3.58  1.83  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	9.01	7.63	4679	4709	27.98	3	-4	3	1.2
2		HKL:H+L=2N	9.05	7.58	4704	4684	28.84	2	0	1	1.2
3		HKL:K+L=2N	9.03	7.61	4691	4697	28.84	2	0	1	1.2
4		HKL:H+K+L=2N	8.99	7.64	4700	4688	28.84	2	0	1	1.2
5		HKL:-H+K+L=3N	8.20	8.38	3104	6284	30.13	0	0	2	1.0
6		HKL:H-K+L=3N	8.20	8.38	3114	6274	30.13	0	0	2	1.0
7		0KL:K=2N	12.58	8.13	288	287	26.56	0	-1	1	1.5
8		0KL:L=2N	11.00	9.70	291	284	27.44	0	-2	1	1.1
9		0KL:K+L=2N	11.65	8.99	296	279	27.44	0	-2	1	1.3
10		H0L:H=2N	12.47	8.66	261	273	27.08	1	0	1	1.4
11		H0L:L=2N	11.24	9.81	267	267	28.84	2	0	1	1.1
12		H0L:H+L=2N	11.87	9.10	274	260	28.84	2	0	1	1.3
13		HK0:H=2N	13.48	10.07	264	291	25.66	-1	4	0	1.3
14		HK0:K=2N	13.79	9.79	304	310	25.72	-4	3	0	1.4
15		HK0:H+K=2N	13.48	10.04	289	295	25.72	-4	3	0	1.3
16	> 21x	H00:H=2N	16.59	7.41	16	14	7.70	9	0	0	2.2
17	> 21y	0K0:K=2N	16.85	7.71	16	13	7.69	0	3	0	2.2
18	E 21z	00L:L=2N	25.49	0.26	14	15	1.51	0	0	7	96.3
19		0KL:K+L=4N	11.61	9.92	150	425	30.13	0	0	2	1.2
20		H0L:H+L=4N	11.86	10.08	133	401	30.13	0	0	2	1.2
21		HK0:H+K=4N	13.46	11.18	144	440	29.42	-2	4	0	1.2
22		H00:H=4N	11.88	12.46	8	22	28.63	6	0	0	1.0
23		0K0:K=4N	12.17	12.97	8	21	29.08	0	2	0	0.9
24	> 41z	00L:L=4N	26.05	9.61	5	24	30.13	0	0	2	2.7
25		HHL:L=2N	10.93	7.94	138	161	27.37	2	2	1	1.4
26		HHL:H=2N	10.59	8.27	135	164	23.39	3	3	1	1.3
27		HHL:H+L=2N	12.04	6.65	148	151	27.37	2	2	1	1.8
28		HHL:2H+L=4N	8.56	9.55	71	228	27.37	2	2	1	0.9
29		H-HL:H+L=3N	10.22	9.95	138	278	28.71	2	-2	2	1.0
30		H-HL:-H+L=3N	10.05	10.03	138	278	28.65	6	-6	2	1.0
31	> 61z	00L:L=6N	24.87	11.01	3	26	30.13	0	0	2	2.3
32	E	HH0:H=2N	23.89	1.25	8	12	3.01	3	3	0	19.2
33		H-HL:L=2N	9.70	10.35	199	217	28.42	2	-2	3	0.9
34		HHL:L=3N	9.12	9.40	87	212	27.37	2	2	1	1.0
35		H-2HL:L=2N	11.73	8.27	117	130	26.57	2	-4	1	1.4
36		-2HHL:L=2N	11.26	8.17	118	137	26.24	4	-2	1	1.4
37		H-2HL:L=3N	9.59	10.03	67	180	26.71	2	-4	2	1.0
38		-2HHL:L=3N	9.23	9.74	70	185	27.36	4	-2	2	0.9
39		00L:L=3N	8.41	14.25	9	20	30.13	0	0	2	0.6
40		H-HL:H=2N	12.52	7.98	189	227	26.26	1	-1	3	1.6
41		HKL:H=2N	8.94	7.70	4693	4695	28.27	1	3	3	1.2
42		HKL:K=2N	9.05	7.59	4680	4708	28.27	1	3	3	1.2

43	HKL:L=2N	7.70	8.94	4721	4667	28.84	2	0	1	0.9
44	HKL:H=3N	8.44	8.26	3132	6256	29.70	2	2	0	1.0
45	HKL:K=3N	8.35	8.30	3130	6258	29.70	2	2	0	1.0
46	HKL:L=3N	9.06	7.95	3096	6292	30.13	0	0	2	1.1

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
P63	173	59	P63	:ABC	5.74	654	56	Chiral A
P63/m	176	164	P63/m	:ABC	5.74	654	44	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