PLATON(V-311206)-Run for: joer089 TIME: Dec 17 13:55:56 2011

Crystal Data

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

a =	12.98900	Angstrom	alpha =	90	Degree	a =	12.989	alpha =	90.00	V =	3401.0
b =	14.64700		beta =	92.0600		b =	14.647	beta =	92.06		
c =	17.88800		gamma =	90		c =	17.888	gamma =	90.00		

V =	3400.99	Cubic-Angstrom	d(100) =	12.9806	Angstrom	Niggli Values		
			d(010) =	14.6470		168.714	214.535	319.981
Lambda(MoKa) =	0.71070	Angstrom	d(001) =	17.8764		0.000	-8.352	0.000

Orthogonalization Matrices

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

(XO)	(	12.98900	0	-0.64300)	(X)	,	(X)	(	0.07699	0	0.00277)	(XO)
(YO) =	(	0	14.64700	0)*(Y)		,	(Y) =	(	0	0.06827	0)*(YO)	
(ZO)	(	0	0	17.87644)	(Z)	,	(Z)	(	0	0	0.05594)	(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: joer089
================================================================================
:: 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 15.36 29.45 41.76 52.42 58.75 65.39 68.56 70.95 74.63 77.64  1959 1000.0
Shell 2 15.00 24.43 31.55 37.77 43.04 48.55 53.11 57.49 60.91 64.29  3246  275.0
Shell 3 17.01 28.20 35.60 40.72 45.91 50.00 53.64 57.76 60.49 63.86  3298  225.3
Shell 4 18.94 28.45 36.29 43.28 48.97 52.88 56.81 60.60 63.51 66.50  3406  163.9
Shell 5 22.46 29.90 37.11 43.37 48.92 53.49 57.73 61.52 64.43 67.52  3371  110.3
Shell 6 29.72 34.83 39.65 45.13 50.16 54.61 58.71 62.85 65.63 68.30  3483   57.4
Shell 7 32.96 36.76 40.38 43.94 47.95 52.32 55.55 58.87 62.28 65.03  3343   44.6
Shell 8 35.19 38.82 42.52 45.51 48.75 51.56 54.52 57.51 60.72 63.35  3274   36.9
Shell 9 38.50 41.58 44.43 47.35 50.79 53.42 55.92 58.65 60.89 63.91  3117   33.5
Shell10 42.70 45.41 47.94 50.44 52.69 55.54 58.71 61.48 63.63 65.67  2843   31.5

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  22.03 30.34 37.16 43.13 48.49 52.74 56.72 60.68 63.52 66.54
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 ( 47 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  12.18 11.55 10.24  8.82  7.48  5.62  4.05  2.95  1.17  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	2.02	1.81	19159	19448	38.07	-3	0	3	1.1
2	HKL:H+L=2N	1.90	1.93	19258	19349	35.57	3	1	0	1.0
3	HKL:K+L=2N	1.95	1.88	19484	19123	38.07	-3	0	3	1.0
4	HKL:H+K+L=2N	1.96	1.87	19384	19223	35.47	-2	1	0	1.0
5	HKL:-H+K+L=3N	1.89	1.93	12920	25687	40.06	2	-2	2	1.0
6	HKL:H-K+L=3N	1.88	1.93	12849	25758	38.23	-2	-2	2	1.0
7 E bx	0KL:K=2N	4.49	0.33	761	1079	2.28	0	7	4	13.6
8	0KL:L=2N	2.17	1.93	937	903	29.99	0	0	3	1.1
9	0KL:K+L=2N	2.21	1.89	940	900	29.99	0	0	3	1.2
10	H0L:H=2N	3.81	3.53	956	947	38.07	-3	0	3	1.1
11	H0L:L=2N	3.49	3.85	949	954	38.07	-3	0	3	0.9
12	H0L:H+L=2N	3.66	3.68	952	951	29.99	0	0	3	1.0
13	HK0:H=2N	2.94	3.82	703	750	35.57	3	1	0	0.8
14	HK0:K=2N	3.93	3.04	779	780	35.57	3	1	0	1.3
15	HK0:H+K=2N	3.74	3.27	747	764	35.47	-2	1	0	1.1
16 E 21x	H00:H=2N	5.41	0.37	24	24	1.26	9	0	0	14.8
17 E 21y	0K0:K=2N	12.21	0.24	29	29	0.83	0	11	0	51.7
18	00L:L=2N	8.21	10.18	34	38	29.99	0	0	3	0.8
19	0KL:K+L=4N	2.26	1.98	479	1361	33.96	0	2	4	1.1
20	H0L:H+L=4N	3.72	3.65	480	1423	37.28	3	0	3	1.0
21	HK0:H+K=4N	3.76	3.42	374	1137	35.47	-2	1	0	1.1
22 > 41x	H00:H=4N	6.53	1.68	12	36	8.43	10	0	0	3.9
23 > 41y	0K0:K=4N	13.14	4.23	13	45	31.99	0	2	0	3.1
24	00L:L=4N	12.13	8.30	18	54	29.99	0	0	3	1.5
25	HHL:L=2N	3.16	2.28	478	510	13.15	6	6	3	1.4
26	HHL:H=2N	3.35	2.12	472	516	16.28	-3	-3	4	1.6
27	HHL:H+L=2N	2.90	2.52	488	500	16.28	-3	-3	4	1.2
28	HHL:2H+L=4N	2.96	2.62	252	736	38.23	-2	-2	2	1.1
29	H-HL:H+L=3N	2.96	2.68	324	636	40.06	2	-2	2	1.1
30	H-HL:-H+L=3N	3.16	2.58	323	637	31.63	-2	2	2	1.2
31	00L:L=6N	3.38	10.31	11	61	37.58	0	0	4	0.3
32	HH0:H=2N	5.58	4.23	21	17	5.17	3	3	0	1.3
33	H-HL:L=2N	3.18	2.36	483	477	14.73	-2	2	9	1.3
34	HHL:L=3N	2.16	2.97	319	669	38.23	-2	-2	2	0.7
35	H-2HL:L=2N	2.95	2.83	268	312	22.41	2	-4	3	1.0
36	-2HHL:L=2N	2.60	2.38	289	294	27.33	-4	2	1	1.1
37	H-2HL:L=3N	2.85	2.90	177	403	22.57	-1	2	2	1.0
38	-2HHL:L=3N	2.43	2.52	195	388	28.56	2	-1	2	1.0
39	00L:L=3N	6.93	10.49	25	47	37.58	0	0	4	0.7
40	H-HL:H=2N	3.52	2.11	449	511	15.15	3	-3	4	1.7
41	HKL:H=2N	1.92	1.91	19669	18938	38.07	-3	0	3	1.0
42	HKL:K=2N	2.32	1.53	18799	19808	35.57	3	1	0	1.5

43	HKL:L=2N	1.99	1.84	19528	19079	38.07	-3	0	3	1.1
44	HKL:H=3N	1.92	1.91	12887	25720	40.06	2	-2	2	1.0
45	HKL:K=3N	2.02	1.86	13173	25434	40.06	2	-2	2	1.1
46	HKL:L=3N	1.95	1.89	13182	25425	40.06	2	-2	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
P21	4	5116	P21	:ABC	7.93	2100	53	Chiral A
P21/m	11	596	P21/m	:ABC	7.93	2100	47	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