

PLATON(V-311206)-Run for: joer051

TIME: Jul 25 14:02:42 2011

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Crystal Data

| Input Cell (Lattice Type: P)    |                           | Temp = 0K | Reduced Cell (Acta Cryst.(1976), A32, 297-298) |                           |
|---------------------------------|---------------------------|-----------|------------------------------------------------|---------------------------|
| a = 15.40500 Angstrom           | alpha = 90 Degree         |           | a = 9.363                                      | alpha = 116.85 V = 2006.4 |
| b = 9.36300                     | beta = 116.8500           |           | b = 15.405                                     | beta = 90.00              |
| c = 15.59100                    | gamma = 90                |           | c = 15.591                                     | gamma = 90.00             |
| V = 2006.36 Cubic-Angstrom      | d(100) = 13.7442 Angstrom |           | Niggli Values                                  |                           |
|                                 | d(010) = 9.3630           |           | 87.666                                         | 237.314 243.079           |
| Lambda(MoKa) = 0.71070 Angstrom | d(001) = 13.9102          |           | -108.479                                       | 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)

(X0) ( 15.40500 0 -7.04177 ) (X) , (X) ( 0.06491 0 0.03286 ) (X0) Orthogonal Axes A0, B0 and C0  
 (Y0) = ( 0 9.36300 0 )\*(Y) , (Y) = ( 0 0.10680 0 )\*(Y0) are defined as:  
 (Z0) ( 0 0 13.91016 ) (Z) , (Z) ( 0 0 0.07189 ) (Z0) A0 // A, C0 // C\*, B0 // C0 X A0

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SPGR - Determine SpaceGroup from Observed Extinctions for: joer051

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:: 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

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

Nz-Test Statistics

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|         |       |       |       |       |       |       |       |       |       |       |      |        |
|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|--------|
| Shell 1 | 20.50 | 31.03 | 40.85 | 47.05 | 53.61 | 58.25 | 62.96 | 65.83 | 69.05 | 70.97 | 2546 | 1000.0 |
| Shell 2 | 10.47 | 20.79 | 31.19 | 38.68 | 44.42 | 48.58 | 52.82 | 56.00 | 58.84 | 61.64 | 2857 | 160.0  |
| Shell 3 | 9.47  | 21.05 | 29.68 | 36.52 | 42.32 | 47.56 | 52.37 | 55.61 | 59.05 | 62.30 | 2618 | 121.6  |
| Shell 4 | 9.38  | 17.70 | 24.77 | 31.07 | 38.02 | 44.65 | 49.71 | 53.91 | 57.90 | 61.56 | 2430 | 89.3   |
| Shell 5 | 10.65 | 20.94 | 29.83 | 37.22 | 43.73 | 48.88 | 53.37 | 58.12 | 62.43 | 66.87 | 2273 | 45.9   |
| Shell 6 | 11.43 | 18.30 | 25.41 | 32.71 | 39.53 | 45.68 | 51.97 | 56.82 | 60.42 | 64.22 | 2082 | 28.6   |
| Shell 7 | 15.07 | 20.80 | 28.16 | 34.43 | 40.80 | 46.52 | 52.39 | 58.01 | 62.59 | 66.12 | 2010 | 17.8   |
| Shell 8 | 18.22 | 23.46 | 29.74 | 35.29 | 41.26 | 46.49 | 51.78 | 56.34 | 60.37 | 64.29 | 1910 | 11.6   |
| Shell 9 | 22.04 | 26.36 | 30.68 | 35.38 | 39.81 | 44.85 | 49.56 | 53.82 | 57.92 | 61.79 | 1806 | 9.7    |
| Shell10 | 28.20 | 32.04 | 35.51 | 39.22 | 43.53 | 47.78 | 51.68 | 54.91 | 58.86 | 62.10 | 1670 | 8.0    |

|         | z -> | 0.1   | 0.2   | 0.3   | 0.4   | 0.5   | 0.6   | 0.7   | 0.8   | 0.9   | 1.0   |
|---------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Av3: 6  |      | 10.23 | 19.50 | 27.42 | 34.38 | 40.90 | 46.69 | 51.85 | 56.12 | 59.95 | 63.74 |
| 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 ( 6 Percent Centric)

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|         | z -> | 0.1   | 0.2   | 0.3   | 0.4   | 0.5   | 0.6   | 0.7   | 0.8  | 0.9  | 1.0  |
|---------|------|-------|-------|-------|-------|-------|-------|-------|------|------|------|
| Av3: 6  |      | 0.66  | 1.26  | 1.35  | 1.20  | 1.29  | 1.26  | 1.14  | 0.63 | 0.13 | 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)) |         | Number of Refl |         | I/sigI<br>Max.F |    |    |   | .T/F.<br>L Ratio |
|----|----------------|----------------|---------|----------------|---------|-----------------|----|----|---|------------------|
|    |                | .True.         | .False. | .True.         | .False. |                 | H  | K  | L |                  |
| 1  | HKL:H+K=2N     | 7.37           | 7.52    | 13625          | 13633   | 110.42          | -3 | 0  | 6 | 1.0              |
| 2  | HKL:H+L=2N     | 7.44           | 7.45    | 13633          | 13625   | 110.42          | -3 | 0  | 6 | 1.0              |
| 3  | HKL:K+L=2N     | 7.43           | 7.46    | 13618          | 13640   | 108.17          | -3 | -1 | 2 | 1.0              |
| 4  | HKL:H+K+L=2N   | 7.55           | 7.34    | 13651          | 13607   | 110.42          | -3 | 0  | 6 | 1.0              |
| 5  | HKL:-H+K+L=3N  | 7.24           | 7.54    | 9093           | 18165   | 108.17          | -3 | -1 | 2 | 1.0              |
| 6  | HKL:H-K+L=3N   | 7.29           | 7.52    | 9065           | 18193   | 106.80          | -3 | 1  | 2 | 1.0              |
| 7  | OKL:K=2N       | 11.08          | 11.04   | 544            | 546     | 90.56           | 0  | -1 | 2 | 1.0              |
| 8  | OKL:L=2N       | 10.92          | 11.20   | 549            | 541     | 82.32           | 0  | 3  | 1 | 1.0              |
| 9  | OKL:K+L=2N     | 12.16          | 9.96    | 543            | 547     | 90.56           | 0  | -1 | 2 | 1.2              |
| 10 | H0L:H=2N       | 11.84          | 11.48   | 892            | 882     | 110.42          | -3 | 0  | 6 | 1.0              |
| 11 | H0L:L=2N       | 11.36          | 11.96   | 886            | 888     | 92.84           | 1  | 0  | 1 | 1.0              |
| 12 | H0L:H+L=2N     | 12.55          | 10.78   | 886            | 888     | 110.42          | -3 | 0  | 6 | 1.2              |
| 13 | HK0:H=2N       | 10.39          | 14.47   | 470            | 511     | 102.67          | -3 | 1  | 0 | 0.7              |
| 14 | HK0:K=2N       | 13.64          | 12.27   | 538            | 539     | 102.67          | -3 | 1  | 0 | 1.1              |
| 15 | HK0:H+K=2N     | 13.58          | 11.89   | 512            | 508     | 93.55           | -4 | 1  | 0 | 1.1              |
| 16 | H00:H=2N       | 21.63          | 11.87   | 29             | 28      | 28.67           | 7  | 0  | 0 | 1.8              |
| 17 | E 21y OK0:K=2N | 33.86          | 0.27    | 21             | 18      | 1.37            | 0  | 9  | 0 | 126.8            |
| 18 | 00L:L=2N       | 15.48          | 14.31   | 29             | 29      | 26.12           | 0  | 0  | 3 | 1.1              |
| 19 | OKL:K+L=4N     | 12.12          | 10.70   | 273            | 817     | 92.19           | 0  | 2  | 0 | 1.1              |
| 20 | H0L:H+L=4N     | 10.35          | 12.11   | 449            | 1325    | 110.42          | -3 | 0  | 6 | 0.9              |
| 21 | HK0:H+K=4N     | 12.52          | 12.81   | 257            | 763     | 102.67          | -3 | 1  | 0 | 1.0              |
| 22 | H00:H=4N       | 19.68          | 15.91   | 14             | 43      | 71.20           | 2  | 0  | 0 | 1.2              |
| 23 | OK0:K=4N       | 21.69          | 17.20   | 10             | 29      | 92.19           | 0  | 2  | 0 | 1.3              |
| 24 | 00L:L=4N       | 21.14          | 12.91   | 14             | 44      | 41.51           | 0  | 0  | 2 | 1.6              |
| 25 | HHL:L=2N       | 9.78           | 10.77   | 396            | 427     | 97.78           | -1 | -1 | 3 | 0.9              |
| 26 | HHL:H=2N       | 10.43          | 10.18   | 384            | 439     | 97.78           | -1 | -1 | 3 | 1.0              |
| 27 | HHL:H+L=2N     | 9.46           | 11.13   | 411            | 412     | 95.58           | 2  | 2  | 1 | 0.9              |
| 28 | HHL:2H+L=4N    | 11.90          | 9.79    | 196            | 627     | 97.78           | -1 | -1 | 3 | 1.2              |
| 29 | H-HL:H+L=3N    | 11.42          | 10.94   | 282            | 565     | 93.85           | -1 | 1  | 3 | 1.0              |
| 30 | H-HL:-H+L=3N   | 10.81          | 11.25   | 285            | 562     | 101.91          | 2  | -2 | 1 | 1.0              |
| 31 | 00L:L=6N       | 2.98           | 17.08   | 9              | 49      | 50.86           | 0  | 0  | 4 | 0.2              |
| 32 | HH0:H=2N       | 16.06          | 19.05   | 15             | 16      | 68.50           | 1  | 1  | 0 | 0.8              |
| 33 | H-HL:L=2N      | 10.77          | 11.40   | 405            | 442     | 101.91          | 2  | -2 | 1 | 0.9              |
| 34 | HHL:L=3N       | 9.60           | 10.60   | 251            | 572     | 95.58           | 2  | 2  | 1 | 0.9              |
| 35 | H-2HL:L=2N     | 11.40          | 13.39   | 205            | 222     | 94.99           | 1  | -2 | 1 | 0.9              |
| 36 | -2HHL:L=2N     | 10.39          | 10.97   | 292            | 311     | 99.87           | 2  | -1 | 1 | 0.9              |
| 37 | H-2HL:L=3N     | 10.30          | 13.34   | 127            | 300     | 98.75           | 1  | -2 | 2 | 0.8              |
| 38 | -2HHL:L=3N     | 8.17           | 11.88   | 193            | 410     | 99.87           | 2  | -1 | 1 | 0.7              |
| 39 | 00L:L=3N       | 6.77           | 19.17   | 20             | 38      | 50.86           | 0  | 0  | 4 | 0.4              |
| 40 | H-HL:H=2N      | 11.54          | 10.71   | 397            | 450     | 97.30           | 1  | -1 | 2 | 1.1              |
| 41 | HKL:H=2N       | 7.46           | 7.43    | 13621          | 13637   | 110.42          | -3 | 0  | 6 | 1.0              |
| 42 | HKL:K=2N       | 7.75           | 7.14    | 13624          | 13634   | 108.17          | -3 | -1 | 2 | 1.1              |

|    |          |      |      |       |       |        |    |    |   |     |
|----|----------|------|------|-------|-------|--------|----|----|---|-----|
| 43 | HKL:L=2N | 7.49 | 7.40 | 13630 | 13628 | 101.91 | 2  | -2 | 1 | 1.0 |
| 44 | HKL:H=3N | 7.32 | 7.50 | 9073  | 18185 | 101.91 | 2  | -2 | 1 | 1.0 |
| 45 | HKL:K=3N | 7.10 | 7.61 | 9047  | 18211 | 108.17 | -3 | -1 | 2 | 0.9 |
| 46 | HKL:L=3N | 7.46 | 7.44 | 9091  | 18167 | 108.17 | -3 | -1 | 2 | 1.0 |

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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

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Tentative Space Group Assignment - (Please Check Carefully)

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:: 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

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| Name  | #  | AbsFreq | StandSet.  | R(av)Perc. | N    | A/C-Prob    |
|-------|----|---------|------------|------------|------|-------------|
| ----- |    |         |            |            |      |             |
| P21   | 4  | 5116    | P21 :ABC   | 5.87       | 3319 | 94 Chiral A |
| P21/m | 11 | 596     | P21/m :ABC | 5.87       | 3319 | 6 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