

PLATON(V-311206)-Run for: kla0167t

TIME: Dec 13 13:28:29 2011

(C) 1980-2007 A.L.Spek

Crystal Data

| Input Cell (Lattice Type: P)    |          |          |         | Temp = 0K                 | Reduced Cell  |         | (Acta Cryst.(1976),A32,297-298) |                  |
|---------------------------------|----------|----------|---------|---------------------------|---------------|---------|---------------------------------|------------------|
| a =                             | 11.22400 | Angstrom | alpha = | 69.6100 Degree            | a =           | 11.224  | alpha =                         | 69.61 V = 1875.5 |
| b =                             | 12.65900 |          | beta =  | 85.6700                   | b =           | 12.659  | beta =                          | 85.67            |
| c =                             | 15.68700 |          | gamma = | 64.3300                   | c =           | 15.687  | gamma =                         | 64.33            |
| V = 1875.51 Cubic-Angstrom      |          |          |         | d(100) = 10.0758 Angstrom | Niggli Values |         |                                 |                  |
|                                 |          |          |         | d(010) = 10.6825          | 125.978       | 160.250 | 246.082                         |                  |
| Lambda(MoKa) = 0.71070 Angstrom |          |          |         | d(001) = 14.6454          | 69.188        | 13.293  | 61.549                          |                  |

Orthogonalization Matrices

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

(X0) ( 11.22400 5.48372 1.18438 ) (X) , (X) ( 0.08909 -0.04282 0.00886 ) (X0) Orthogonal Axes A0, B0 and C0  
 (Y0) = ( 0 11.40961 5.49473 )\*(Y) , (Y) = ( 0 0.08765 -0.03288 )\*(Y0) are defined as:  
 (Z0) ( 0 0 14.64538 ) (Z) , (Z) ( 0 0 0.06828 ) (Z0) A0 // A, C0 // C\*, B0 // C0 X A0

=====

SPGR - Determine SpaceGroup from Observed Extinctions for: kla0167t

=====

:: 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 | 28.19 | 39.62 | 46.48 | 52.95 | 57.14 | 60.57 | 63.43 | 67.43 | 69.33 | 72.19 | 525 | 1000.0 |
| Shell 2 | 21.19 | 30.30 | 38.00 | 45.71 | 50.09 | 54.12 | 57.97 | 61.82 | 64.10 | 65.85 | 571 | 378.5  |
| Shell 3 | 23.31 | 32.37 | 38.92 | 45.66 | 49.71 | 53.56 | 57.03 | 59.54 | 62.43 | 64.93 | 519 | 173.1  |
| Shell 4 | 22.70 | 32.52 | 40.29 | 44.79 | 49.28 | 53.58 | 56.03 | 59.51 | 63.39 | 65.64 | 489 | 130.3  |
| Shell 5 | 22.10 | 29.91 | 38.39 | 44.87 | 50.00 | 54.69 | 59.38 | 61.61 | 64.06 | 66.96 | 448 | 97.1   |
| Shell 6 | 21.29 | 33.42 | 41.09 | 48.02 | 54.21 | 58.17 | 62.13 | 65.59 | 67.82 | 69.55 | 404 | 88.0   |
| Shell 7 | 26.09 | 31.40 | 36.71 | 42.51 | 46.86 | 50.48 | 55.56 | 58.70 | 62.56 | 64.73 | 414 | 57.5   |
| Shell 8 | 32.46 | 37.17 | 41.36 | 46.86 | 51.31 | 54.45 | 57.33 | 60.99 | 63.87 | 65.97 | 382 | 47.8   |
| Shell 9 | 32.68 | 36.06 | 40.56 | 43.94 | 48.17 | 50.70 | 53.52 | 57.18 | 60.00 | 62.25 | 355 | 36.3   |
| Shell10 | 34.38 | 39.83 | 42.12 | 45.56 | 48.71 | 50.72 | 55.30 | 59.60 | 61.60 | 65.62 | 349 | 33.5   |

|         | z -> | 0.1   | 0.2   | 0.3   | 0.4   | 0.5   | 0.6   | 0.7   | 0.8   | 0.9   | 1.0   |
|---------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Av3: 6  |      | 22.35 | 32.05 | 39.67 | 45.83 | 50.80 | 55.00 | 58.64 | 61.56 | 64.43 | 66.77 |
| 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 ( 57 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  |      | 12.48 | 13.21 | 12.69 | 11.44 | 9.67  | 7.74  | 5.81  | 3.65 | 1.88 | 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. |    |         |
|----|----------------|----------------|---------|----------------|---------|-----------------|-------|----|---------|
|    |                | .True.         | .False. | .True.         | .False. |                 | H     | K  | L Ratio |
| 1  | HKL:H+K=2N     | 3.36           | 3.46    | 2780           | 2773    | 118.24          | 1     | 2  | 3 1.0   |
| 2  | HKL:H+L=2N     | 3.39           | 3.43    | 2773           | 2780    | 79.95           | 1     | 2  | 2 1.0   |
| 3  | HKL:K+L=2N     | 3.52           | 3.29    | 2768           | 2785    | 118.24          | 1     | 2  | 3 1.1   |
| 4  | HKL:H+K+L=2N   | 3.40           | 3.42    | 2781           | 2772    | 100.35          | -1    | 1  | 1 1.0   |
| 5  | HKL:-H+K+L=3N  | 3.52           | 3.35    | 1861           | 3692    | 118.24          | 1     | 2  | 3 1.0   |
| 6  | HKL:H-K+L=3N   | 3.32           | 3.45    | 1855           | 3698    | 118.24          | 1     | 2  | 3 1.0   |
| 7  | OKL:K=2N       | 3.42           | 3.58    | 198            | 200     | 40.77           | 0     | -1 | 2 1.0   |
| 8  | OKL:L=2N       | 3.41           | 3.59    | 201            | 197     | 56.93           | 0     | 0  | 3 0.9   |
| 9  | OKL:K+L=2N     | 3.68           | 3.32    | 199            | 199     | 56.93           | 0     | 0  | 3 1.1   |
| 10 | H0L:H=2N       | 5.55           | 4.80    | 146            | 143     | 54.40           | -1    | 0  | 3 1.2   |
| 11 | H0L:L=2N       | 4.68           | 5.66    | 142            | 147     | 56.93           | 0     | 0  | 3 0.8   |
| 12 | H0L:H+L=2N     | 4.71           | 5.66    | 147            | 142     | 56.93           | 0     | 0  | 3 0.8   |
| 13 | HK0:H=2N       | 5.88           | 5.74    | 81             | 93      | 69.24           | 1     | 2  | 0 1.0   |
| 14 | HK0:K=2N       | 6.86           | 4.62    | 93             | 95      | 64.21           | 2     | 1  | 0 1.5   |
| 15 | HK0:H+K=2N     | 5.49           | 5.98    | 93             | 94      | 69.24           | 1     | 2  | 0 0.9   |
| 16 | E 21x H00:H=2N | 3.56           | 0.00    | 1              | 0       | 0.00            | 0     | 0  | 0 99.0  |
| 17 | OK0:K=2N       | 5.69           | 3.72    | 7              | 6       | 2.88            | 0     | 3  | 0 1.5   |
| 18 | 00L:L=2N       | 7.05           | 9.24    | 9              | 9       | 56.93           | 0     | 0  | 3 0.8   |
| 19 | OKL:K+L=4N     | 3.47           | 3.51    | 100            | 298     | 56.93           | 0     | 0  | 3 1.0   |
| 20 | H0L:H+L=4N     | 4.51           | 5.41    | 74             | 215     | 56.93           | 0     | 0  | 3 0.8   |
| 21 | HK0:H+K=4N     | 5.98           | 5.66    | 46             | 141     | 69.24           | 1     | 2  | 0 1.1   |
| 22 | E 41x H00:H=4N | 3.56           | 0.00    | 1              | 0       | 0.00            | 0     | 0  | 0 99.0  |
| 23 | OK0:K=4N       | 1.82           | 5.66    | 3              | 10      | 23.21           | 0     | 2  | 0 0.3   |
| 24 | 00L:L=4N       | 4.97           | 9.05    | 4              | 14      | 56.93           | 0     | 0  | 3 0.5   |
| 25 | HHL:L=2N       | 5.31           | 6.33    | 112            | 121     | 63.66           | -2    | -2 | 1 0.8   |
| 26 | HHL:H=2N       | 5.73           | 5.94    | 111            | 122     | 45.51           | -1    | -1 | 1 1.0   |
| 27 | HHL:H+L=2N     | 6.02           | 5.65    | 118            | 115     | 63.66           | -2    | -2 | 1 1.1   |
| 28 | HHL:2H+L=4N    | 4.96           | 6.12    | 57             | 176     | 63.66           | -2    | -2 | 1 0.8   |
| 29 | H-HL:H+L=3N    | 5.36           | 3.35    | 69             | 131     | 28.90           | -1    | 1  | 3 1.6   |
| 30 | H-HL:-H+L=3N   | 3.22           | 4.43    | 64             | 136     | 100.35          | -1    | 1  | 1 0.7   |
| 31 | 00L:L=6N       | 5.45           | 8.68    | 3              | 15      | 56.93           | 0     | 0  | 3 0.6   |
| 32 | E HH0:H=2N     | 27.80          | 3.69    | 3              | 3       | 4.56            | 7     | 7  | 0 7.5   |
| 33 | H-HL:L=2N      | 3.44           | 4.63    | 99             | 101     | 100.35          | -1    | 1  | 1 0.7   |
| 34 | HHL:L=3N       | 5.34           | 6.05    | 71             | 162     | 63.66           | -2    | -2 | 1 0.9   |
| 35 | H-2HL:L=2N     | 3.37           | 3.18    | 62             | 63      | 21.58           | -1    | 2  | 7 1.1   |
| 36 | -2HHL:L=2N     | 3.63           | 4.07    | 53             | 56      | 22.49           | 2     | -1 | 3 0.9   |
| 37 | H-2HL:L=3N     | 2.59           | 3.60    | 40             | 85      | 32.01           | -1    | 2  | 4 0.7   |
| 38 | -2HHL:L=3N     | 3.62           | 3.96    | 35             | 74      | 40.24           | -2    | 1  | 2 0.9   |
| 39 | > 31z 00L:L=3N | 13.02          | 5.70    | 6              | 12      | 23.58           | 0     | 0  | 2 2.3   |
| 40 | H-HL:H=2N      | 3.13           | 4.82    | 92             | 108     | 100.35          | -1    | 1  | 1 0.7   |
| 41 | HKL:H=2N       | 3.41           | 3.41    | 2784           | 2769    | 118.24          | 1     | 2  | 3 1.0   |
| 42 | HKL:K=2N       | 3.42           | 3.40    | 2781           | 2772    | 100.35          | -1    | 1  | 1 1.0   |

|    |          |      |      |      |      |        |    |   |   |     |
|----|----------|------|------|------|------|--------|----|---|---|-----|
| 43 | HKL:L=2N | 3.32 | 3.50 | 2784 | 2769 | 118.24 | 1  | 2 | 3 | 0.9 |
| 44 | HKL:H=3N | 3.23 | 3.50 | 1862 | 3691 | 118.24 | 1  | 2 | 3 | 0.9 |
| 45 | HKL:K=3N | 3.30 | 3.46 | 1853 | 3700 | 118.24 | 1  | 2 | 3 | 1.0 |
| 46 | HKL:L=3N | 3.46 | 3.38 | 1828 | 3725 | 100.35 | -1 | 1 | 1 | 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      |
|-------|---|---------|-----------|------------|------|---------------|
| ----- |   |         |           |            |      |               |
| P1    | 1 | 799     | P1        | :ABC       | 0.00 | 0 43 Chiral A |
| P-1   | 2 | 15327   | P-1       | :ABC       | 0.00 | 0 57 C        |

=====

\*\*\*\*\* N O T I C E \*\*\*\*\*

=====

- 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