PLATON(V-311206)-Run for: kla0202a TIME: Apr 6 15:42:07 2012



## Crystal Data

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

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| a = | 5.61700 | Angstrom | alpha = | 90 | Degree | a = | 5.617 | alpha = | 90.00 | V = | 2111.4 |
| b = | 16.00200 | | beta = | 91.6400 | | b = | 16.002 | beta = | 91.64 | | |
| c = | 23.50000 | | gamma = | 90 | | c = | 23.500 | gamma = | 90.00 | | |
| V = | 2111.39 | Cubic-Angstrom | d(100) = | 5.6147 | Angstrom | | | | | | |
| | | | d(010) = | 16.0020 | | | | | | | |
| Lambda(MoKa) = | 0.71070 | Angstrom | d(001) = | 23.4904 | | | | | | | |

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

Niggli Values: 31.551 256.064 552.250 / 0.000 -3.777 0.000

## Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 5.61700 & 0 & -0.67255 \\ 0 & 16.00200 & 0 \\ 0 & 0 & 23.49037 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.17803 & 0 & 0.00510 \\ 0 & 0.06249 & 0 \\ 0 & 0 & 0.04257 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: kla0202a
================================================================================
:: 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 32.57 40.59 45.69 50.91 55.46 59.24 63.48 66.96 70.83 73.84  2355 1000.0
Shell 2 25.93 37.22 44.80 51.75 56.61 60.03 63.45 66.08 68.39 70.47  2692  328.3
Shell 3 28.85 38.30 46.36 51.96 57.12 61.96 65.18 68.11 70.38 72.39  2731  222.8
Shell 4 31.37 40.74 48.46 56.08 61.46 65.23 68.92 71.12 73.28 75.22  2732  211.4
Shell 5 30.47 38.79 45.34 51.12 56.12 60.59 64.33 67.60 70.61 73.61  2596  167.4
Shell 6 31.65 36.92 42.53 47.64 52.78 57.38 61.90 65.53 69.03 71.69  2370  129.2
Shell 7 32.51 36.87 42.42 47.70 52.86 57.26 61.26 64.57 66.89 70.17  2501  126.7
Shell 8 33.71 38.21 43.31 48.29 52.14 56.51 59.58 62.96 66.12 69.41  2311  108.8
Shell 9 36.65 40.43 43.70 47.76 51.77 56.16 59.43 62.98 65.41 68.07  2142   92.6
Shell10 36.59 40.71 44.36 48.58 51.52 54.79 57.63 60.28 62.84 65.17  2110   83.6

   z ->   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1.0
Av3: 6  30.58 38.69 45.67 51.70 56.87 61.29 65.08 68.09 70.82 73.23
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 ( 78 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  20.07 18.56 16.75 14.72 12.52 10.16  7.73  5.01  2.47  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 | 1.61 | 1.54 | 23474 | 23501 | 52.26 | 0 | -3 | 1 | 1.0 |
| 2 | | HKL:H+L=2N | 1.53 | 1.62 | 23512 | 23463 | 106.38 | 1 | 1 | 0 | 0.9 |
| 3 | | HKL:K+L=2N | 1.53 | 1.62 | 23523 | 23452 | 106.38 | 1 | 1 | 0 | 0.9 |
| 4 | | HKL:H+K+L=2N | 1.60 | 1.54 | 23488 | 23487 | 76.93 | -1 | 1 | 1 | 1.0 |
| 5 | | HKL:-H+K+L=3N | 1.56 | 1.58 | 15706 | 31269 | 81.71 | -1 | 3 | 0 | 1.0 |
| 6 | | HKL:H-K+L=3N | 1.55 | 1.59 | 15664 | 31311 | 81.71 | -1 | 3 | 0 | 1.0 |
| 7 | | 0KL:K=2N | 3.24 | 2.82 | 1319 | 1306 | 52.26 | 0 | -3 | 1 | 1.2 |
| 8 | | 0KL:L=2N | 2.82 | 3.25 | 1318 | 1307 | 63.57 | 0 | -2 | 1 | 0.9 |
| 9 | | 0KL:K+L=2N | 3.21 | 2.85 | 1310 | 1315 | 63.57 | 0 | -2 | 1 | 1.1 |
| 10 | | H0L:H=2N | 2.62 | 2.22 | 926 | 933 | 25.35 | -3 | 0 | 2 | 1.2 |
| 11 | | H0L:L=2N | 2.70 | 2.15 | 924 | 935 | 24.54 | -2 | 0 | 3 | 1.3 |
| 12 | | H0L:H+L=2N | 2.61 | 2.22 | 937 | 922 | 25.35 | -3 | 0 | 2 | 1.2 |
| 13 | | HK0:H=2N | 1.18 | 2.29 | 539 | 587 | 106.38 | 1 | 1 | 0 | 0.5 |
| 14 | | HK0:K=2N | 2.00 | 2.24 | 616 | 608 | 106.38 | 1 | 1 | 0 | 0.9 |
| 15 | E | nz HK0:H+K=2N | 3.85 | 0.29 | 581 | 605 | 2.74 | -6 | 13 | 0 | 13.2 |
| 16 | E | 21x H00:H=2N | 10.63 | 0.26 | 17 | 21 | 0.90 | 3 | 0 | 0 | 40.6 |
| 17 | E | 21y 0K0:K=2N | 14.04 | 0.26 | 30 | 30 | 1.24 | 0 | 9 | 0 | 53.7 |
| 18 | E | 21z 00L:L=2N | 8.34 | 0.23 | 42 | 43 | 2.02 | 0 | 0 | 15 | 36.5 |
| 19 | | 0KL:K+L=4N | 3.15 | 2.99 | 660 | 1965 | 76.12 | 0 | 2 | 0 | 1.1 |
| 20 | | H0L:H+L=4N | 2.53 | 2.38 | 471 | 1388 | 41.37 | 2 | 0 | 0 | 1.1 |
| 21 | | HK0:H+K=4N | 2.53 | 1.87 | 286 | 900 | 106.38 | 1 | 1 | 0 | 1.4 |
| 22 | | H00:H=4N | 7.04 | 4.33 | 8 | 30 | 41.37 | 2 | 0 | 0 | 1.6 |
| 23 | | 0K0:K=4N | 5.48 | 7.66 | 14 | 46 | 76.12 | 0 | 2 | 0 | 0.7 |
| 24 | > | 41z 00L:L=4N | 9.57 | 2.37 | 22 | 63 | 31.46 | 0 | 0 | 10 | 4.0 |
| 25 | | HHL:L=2N | 2.61 | 2.05 | 714 | 748 | 31.24 | -1 | -1 | 1 | 1.3 |
| 26 | | HHL:H=2N | 2.19 | 2.44 | 682 | 780 | 47.37 | -1 | -1 | 2 | 0.9 |
| 27 | | HHL:H+L=2N | 2.14 | 2.50 | 732 | 730 | 47.37 | -1 | -1 | 2 | 0.9 |
| 28 | | HHL:2H+L=4N | 2.82 | 2.16 | 357 | 1105 | 39.47 | -2 | -2 | 2 | 1.3 |
| 29 | | H-HL:H+L=3N | 2.66 | 2.39 | 462 | 905 | 78.69 | -1 | 1 | 2 | 1.1 |
| 30 | | H-HL:-H+L=3N | 2.54 | 2.45 | 462 | 905 | 76.93 | -1 | 1 | 1 | 1.0 |
| 31 | | 00L:L=6N | 2.50 | 4.55 | 13 | 72 | 66.62 | 0 | 0 | 4 | 0.5 |
| 32 | | HH0:H=2N | 2.16 | 17.85 | 15 | 18 | 106.38 | 1 | 1 | 0 | 0.1 |
| 33 | | H-HL:L=2N | 2.62 | 2.35 | 673 | 694 | 76.93 | -1 | 1 | 1 | 1.1 |
| 34 | | HHL:L=3N | 1.93 | 2.50 | 462 | 1000 | 47.37 | -1 | -1 | 2 | 0.8 |
| 35 | | H-2HL:L=2N | 1.23 | 1.92 | 482 | 498 | 22.16 | -1 | 2 | 1 | 0.6 |
| 36 | | -2HHL:L=2N | 2.43 | 2.63 | 375 | 389 | 23.73 | 2 | -1 | 7 | 0.9 |
| 37 | | H-2HL:L=3N | 1.26 | 1.72 | 307 | 673 | 22.16 | -1 | 2 | 1 | 0.7 |
| 38 | | -2HHL:L=3N | 2.23 | 2.68 | 246 | 518 | 27.48 | -2 | 1 | 4 | 0.8 |
| 39 | | 00L:L=3N | 1.25 | 5.86 | 30 | 55 | 66.62 | 0 | 0 | 4 | 0.2 |
| 40 | | H-HL:H=2N | 2.15 | 2.77 | 645 | 722 | 78.69 | -1 | 1 | 2 | 0.8 |
| 41 | | HKL:H=2N | 1.58 | 1.57 | 23464 | 23511 | 106.38 | 1 | 1 | 0 | 1.0 |
| 42 | | HKL:K=2N | 1.55 | 1.60 | 23457 | 23518 | 106.38 | 1 | 1 | 0 | 1.0 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 43 | HKL:L=2N | 1.58 | 1.57 | 23491 | 23484 | 76.93 | -1 | 1 | 1 | 1.0 |
| 44 | HKL:H=3N | 1.56 | 1.58 | 15726 | 31249 | 106.38 | 1 | 1 | 0 | 1.0 |
| 45 | HKL:K=3N | 1.53 | 1.59 | 15693 | 31282 | 106.38 | 1 | 1 | 0 | 1.0 |
| 46 | HKL:L=3N | 1.57 | 1.58 | 15663 | 31312 | 78.69 | -1 | 1 | 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 |
|---|---|---|---|---|---|---|---|---|
| P1 | 1 | 799 | P1 | :ABC | 6.26 | 1510 | 22 | Chiral A |
| P-1 | 2 | 15327 | P-1 | :ABC | 6.26 | 1510 | 78 | 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