PLATON(V-311206)-Run for: char344a TIME: Apr 1 11:45:40 2011

Crystal Data

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

a =	30.43700	Angstrom	alpha =	90	Degree	a =	19.448	alpha =	120.00	V =	15603.0
b =	30.43700		beta =	90		b =	30.437	beta =	90.00		
c =	19.44800		gamma =	120		c =	30.437	gamma =	90.00		
V =	15603.04	Cubic-Angstrom	d(100) =	26.3592	Angstrom						
			d(010) =	26.3592							
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	19.4480							

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

Niggli Values		
378.225	926.411	926.411
-463.206	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)

$$(XO) = \begin{pmatrix} 30.43700 & -15.21850 & 0 \\ 0 & 26.35921 & 0 \\ 0 & 0 & 19.44800 \end{pmatrix} (X) \quad , \quad (X) = \begin{pmatrix} 0.03285 & 0.01897 & 0 \\ 0 & 0.03794 & 0 \\ 0 & 0 & 0.05142 \end{pmatrix} (XO)$$

$$(YO) = \begin{pmatrix} 0 & 26.35921 & 0 \end{pmatrix} (Y) \quad , \quad (Y) = \begin{pmatrix} 0 & 0.03794 & 0 \end{pmatrix} (YO)$$

$$(ZO) = \begin{pmatrix} 0 & 0 & 19.44800 \end{pmatrix} (Z) \quad , \quad (Z) = \begin{pmatrix} 0 & 0 & 0.05142 \end{pmatrix} (ZO)$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: char344a
================================================================================
:: Reflection Data are READ from File : latt.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 : latt.hkl - ( OBS-Data)

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

Intensity Distribution
================================================================================

sh st/l  Ang     #  0.25   1.0   2.0  0 Percent  Distr. for I gt 2.0 s(I)  100
================================================================================
 1 0.30 1.66  8404  94.3  91.8  90.0  **********************************....
 2 0.38 1.32  8239  97.3  95.5  91.9  **********************************...
 3 0.44 1.15  7332  96.2  92.5  87.1  *********************************.....
 4 0.48 1.04  6665  95.6  90.6  81.3  *********************************.......
 5 0.52 0.97  6262  94.9  89.6  80.9  *********************************........
 6 0.55 0.91  5735  95.6  91.8  82.9  *********************************.......
 7 0.58 0.87  5331  94.1  90.1  81.8  *********************************.......
 8 0.60 0.83  5089  92.7  88.4  80.0  *********************************........
 9 0.63 0.80  4704  90.3  84.5  74.1  ********************************.........
10 0.65 0.77  4478  87.6  81.0  70.0  ********************************.........
                                    I                   I                   I
                                    0%                 50%                100%
```

Analysis of General Reflections for Bravais Centering

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	7.95	8.06	32786	32697	56.77	-3	-4	-2	1.0
2		HKL:H+L=2N	8.06	7.94	32779	32704	56.77	-3	-4	-2	1.0
3		HKL:K+L=2N	8.06	7.95	32778	32705	55.12	-1	-3	-4	1.0
4		HKL:H+K+L=2N	8.08	7.93	32801	32682	56.77	-3	-4	-2	1.0
5	E oR	HKL:-H+K+L=3N	8.00	0.00	65483	0	0.00	0	0	0	99.0
6		HKL:H-K+L=3N	7.98	8.02	21874	43609	57.54	-4	0	-4	1.0
41		HKL:H=2N	7.96	8.05	32756	32727	56.77	-3	-4	-2	1.0
42		HKL:K=2N	7.94	8.07	32733	32750	55.12	-1	-3	-4	1.0
43		HKL:L=2N	9.64	6.37	32688	32795	49.23	2	-8	1	1.5
44		HKL:H=3N	7.88	8.06	21810	43673	57.54	-4	0	-4	1.0
45		HKL:K=3N	7.88	8.06	21817	43666	57.10	4	-4	-4	1.0
46		HKL:L=3N	7.98	8.02	21874	43609	57.54	-4	0	-4	1.0
47	E twR	-HKL, H-KL=3N	8.00	0.00	65483	0	0.00	0	0	0	99.0
48		-HKL:K2,KL4P2	7.93	9.29	61775	3708	57.08	8	0	2	0.9
49		-HKL:H2,HL4P2	7.88	9.69	61018	4465	57.08	8	0	2	0.8
50		-HKL:H2,HK4P2	8.02	7.68	61916	3567	56.63	4	-2	0	1.0
51		HKL:H+2L=3N	7.88	8.06	21817	43666	57.10	4	-4	-4	1.0

Possible 2-Fold Axes - 2-Axis Crit = 0.20, Exp. Error = 0.20 Deg., LATT = R

Nr	D	N	Rows Direct	Rows Recip	Products Dot	Products Delta	Angle Between Two Direct Axes 1	2	3	4	5	6	7	8	9
1	30.437	0	0 1-1	0 1-1	2	0.005	0.	120.	120.						
2	30.437	0	1 0-1	1 0-1	2	0.005	120.	0.	120.						
3	30.437	0	1-1 0	1-1 0	2	0.009	120.	120.	0.						

==== Transformation Matrix: Input (a,b,c) to Conventional Cell(a’, b’, c’) ====

(a’)	(1.000	0.000	0.000)	(a)	(x’)	(1.000	0.000	0.000) (x) Metrically
(b’) =	(0.000	1.000	0.000)	(b).	(y’) =	(0.000	1.000	0.000) (y) Hexagonal
(c’)	(0.000	0.000	1.000)	(c)	(z’)	(0.000	0.000	1.000) (z) FOM: 0.009

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	R	30.437	30.437	19.448	90.00	90.00	120.00	15603.04
Reduc Cell	P	18.730	18.730	18.730	108.68	108.68	108.68	5201.02
Conv. Cell	hR	30.437	30.437	19.448	90.00	90.00	120.00	15603.04

Possible 2-Fold Axes - 2-Axis Crit = 0.20, Exp. Error = 0.20 Deg., LATT = R

			Rows		Products		Angle Between Two Direct Axes							
Nr	D	N	Direct	Recip	Dot	Delta	1	2	3	4	5	6	7	8	9
1	30.437	0	0 1-1	0 1-1	2	0.005	0.								

==== Transformation Matrix: Input (a,b,c) to Conventional Cell(a', b', c') ====

```
(a')   (-0.333 0.333-0.667) (a)   (x')   (-0.500 0.500-1.000) (x)  Metrically
(b') = ( 1.000 1.000 0.000) (b).  (y') = ( 0.500 0.500 0.000) (y)  Monoclinic
(c')   ( 0.333-0.333-0.333) (c)   (z')   ( 1.000-1.000-1.000) (z)  FOM:  0.005
```

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	R	30.437	30.437	19.448	90.00	90.00	120.00	15603.04
Reduc Cell	P	18.730	18.730	18.730	108.68	108.68	108.68	5201.02
Conv. Cell	mC	21.838	30.437	18.730	90.00	123.33	90.00	10402.02

Possible 2-Fold Axes - 2-Axis Crit = 0.20, Exp. Error = 0.20 Deg., LATT = R

			Rows		Products		Angle Between Two Direct Axes								
Nr	D	N	Direct	Recip	Dot	Delta	1	2	3	4	5	6	7	8	9
1	30.437	0	1 0-1	1 0-1	2	0.005	0.								

==== Transformation Matrix: Input (a,b,c) to Conventional Cell(a', b', c') ====

```
(a')   ( 0.667 0.333-0.667) (a)   (x')   ( 0.500 0.000-1.000) (x)  Metrically
(b') = ( 0.000-1.000 0.000) (b).  (y') = ( 0.500-1.000 0.000) (y)  Monoclinic
(c')   (-0.667-0.333-0.333) (c)   (z')   (-1.000 0.000-1.000) (z)  FOM:  0.005
```

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	R	30.437	30.437	19.448	90.00	90.00	120.00	15603.04
Reduc Cell	P	18.730	18.730	18.730	108.68	108.68	108.68	5201.02
Conv. Cell	mC	21.838	30.437	18.730	90.00	123.33	90.00	10402.02

Possible 2-Fold Axes - 2-Axis Crit = 0.20, Exp. Error = 0.20 Deg., LATT = R

Nr	D	N	Rows Direct	Rows Recip	Products Dot	Products Delta	Angle Between Two Direct Axes 1	2	3	4	5	6	7	8	9
1	30.437	0	1-1 0	1-1 0	2	0.009	0.								

==== Transformation Matrix: Input (a,b,c) to Conventional Cell(a', b', c') ====

```
(a')   (-0.333-0.667-0.667) (a)   (x')   ( 0.000-0.500-1.000) (x)  Metrically
(b') = (-1.000 0.000 0.000) (b).  (y') = (-1.000 0.500 0.000) (y)  Monoclinic
(c')   ( 0.333 0.667-0.333) (c)   (z')   ( 0.000 1.000-1.000) (z)  FOM:  0.009
```

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	R	30.437	30.437	19.448	90.00	90.00	120.00	15603.04
Reduc Cell	P	18.730	18.730	18.730	108.68	108.68	108.68	5201.02
Conv. Cell	mC	21.838	30.437	18.730	90.00	123.33	90.00	10402.02

Possible 2-Fold Axes - 2-Axis Crit = 0.20, Exp. Error = 0.20 Deg., LATT = R

==== Transformation Matrix: Input (a,b,c) to Conventional Cell(a', b', c') ====

```
(a')   ( 0.333-0.333-0.333) (a)   (x')   ( 1.000-1.000-1.000) (x)  Metrically
(b') = (-0.667-0.333-0.333) (b).  (y') = (-1.000 0.000-1.000) (y)  Anorthic
(c')   ( 0.333 0.667-0.333) (c)   (z')   ( 0.000 1.000-1.000) (z)  FOM:  0.000
```

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	R	30.437	30.437	19.448	90.00	90.00	120.00	15603.04
Reduc Cell	P	18.730	18.730	18.730	108.68	108.68	108.68	5201.02
Conv. Cell	aP	18.730	18.730	18.730	108.68	108.68	108.68	5201.01

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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 latt.ins - Data Type SPF

:: NORMAL END of PLATON : 9 Pages on:
:: latt.lis (ASCII, 132 Characters Wide)
:: latt.lps (PostScript Version of .lis)
:: latt.pdf (PDF Version of .lis)

:: SPGR.PAR on :latt.par