PLATON(V-311206)-Run for: jmca013 in P2(1) TIME: Nov 23 16:50:29 2010

Crystal Data

Input Cell (Lattice Type: P) - Temp = 200K

a =	9.120(4)	Angstrom	alpha =	90	Degree	a = 9.120	alpha = 90.00	V =	3113.0
b =	15.478(7)		beta =	95.424(7)		b = 15.478	beta = 95.42		
c =	22.156(11)		gamma =	90		c = 22.156	gamma = 90.00		
V =	3113(2)	Cubic-Angstrom	d(100) =	9.0788	Angstrom				
			d(010) =	15.4781					
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	22.0569					

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

Niggli Values

83.167	239.572	490.893
0.000	-19.100	0.000

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 9.12000 & 0 & -2.09430 \\ 0 & 15.47800 & 0 \\ 0 & 0 & 22.05680 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.10965 & 0 & 0.01041 \\ 0 & 0.06461 & 0 \\ 0 & 0 & 0.04534 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group P21 No: 4, Laue: 2/m [Hall: P 2yb]

Lattice Type mP, Acentric, Monoclinic, Order 2(2) [Schoenflies: C2^2]

CHIRAL - See P.G. Jones, Acta Cryst. (1986), A42, 57.

Nr	***** Symmetry Operation(s) *****		
1	X ,	Y ,	Z
2	- X ,	1/2 + Y ,	- Z

ADDSYM - CHECK (cf. MISSYM (C): Le Page, Y., J. Appl. Cryst. (1987), 20, 264-269; J. Appl. Cryst. (1988), 21, 983-984)

- ADDSYM Search on ALL NON-H Chemical Types [Max NonFit 20 Perc]
- Number of Input Atoms Included in Search 67 (Unitcell 134)
- Density based on Input Atom Set = 1.234 g.cm-3 - Vol / Non-H atom = 23.2 Ang+3
- The Structure Implies the Following Symmetry Elements Subject to the Criteria:

Criteria: 1.00 Deg (Metric), 0.25 Ang (Rot.), 0.45 Ang (Inv), 0.45 Ang (Transl)

Symm. Elem	Input Cell_Row	Reduced Cell_Row	(Ang) d	Typ	(Deg) Dot	Angle	(%) Fit	(Ang) MaxDev.		Input Cell x	y	z
c *	[0 1 0]	[0-1 0]	15.48	2	1	0.00	98	0.175	through	0	0.372	0
							C56	-C58	Glide =	0	0	1/2
-1 *	==========						98	0.175	at	1/2	0.122	1/4
							C58	-C56				

:: NonFits (i.e. Atoms with no symmetry related counterpart):

C13

T.R.A.N.S.F.O.R.M.A.T.I.O.N M.A.T.R.I.X for CELL and HKL DATA

Reduced->Convent	Input->Reduced	T = Input->Convent:	a' = T a
(-1 0 0)	(-1 0 0)	(1 0 0)	Det(T)
(0 1 0) X	(0 1 0) =	(0 1 0)	=
(0 0 -1)	(0 0 -1)	(0 0 1)	1.000

Cell	Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input	mP	9.120	15.478	22.156	90.00	95.42	90.00	3113	Monoclinic	2/m
Reduced	P	9.120	15.478	22.156	90.00	95.42	90.00	3113		
Convent	mP	9.120	15.478	22.156	90.00	95.42	90.00	3113	Monoclinic	2/m

Conventional, New or Pseudo Symmetry

Space Group P21/c No: 14, Laue: 2/m [Hall: -P 2ybc]

Lattice Type mP, Centric, Monoclinic, Order 4(2) [Schoenflies: C2h^5]

Nr	***** Symmetry Operation(s) *****		
1	X ,	Y ,	Z
2	- X ,	1/2 + Y ,	1/2 - Z
3	- X ,	- Y ,	- Z
4	X ,	1/2 - Y ,	1/2 + Z

:: Origin Shifted to: 0.4996, 0.1216, 0.2498 after Transformation

:: (1.0000 0.0000 0.0000) (-0.4996)
:: R/t for Coordinates (0.0000 1.0000 0.0000) (-0.1216)
:: (0.0000 0.0000 1.0000) (-0.2498)

:: * Symmetry Elements Preceded by an Asterisk are New and Indicate
:: Missed/Pseudosymmetry. Proposed Inversion or (Glide) Planes do NOT Apply
:: for Chiral Molecules.
:: Note: Glide Plane Codes are with Reference to the Input Cell !!

P! jmca013 in P2(1) mP=>mP 0.0 0 0 0.000 0.00 0.500 98% P21/c

:: An SPF-style file is written to be used for the cell transformation.

(Not-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

```
         Site    = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
*******  Move    = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
SYMBOLS: Type    = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
*******  El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
         ARU     = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
         RESIDUE = collection of ARU's constituting an isolated unit (= molecule, ion).
         FLAGS   : d = determined, c = calculated, R = riding G = group
```

Atom Types :	C	H	Fe	O	P	Pd
Cov.Rad(Ang):	0.68	0.35	1.35	0.68	1.05	1.50
Atom Volume :	13.87	5.08	30.40	11.39	29.50	35.00
Atom Number :	6	1	26	8	15	46
Atom Weight :	12.010	1.008	55.85	16.00	30.97	106.42
Scat.Fact.f0:	5.999	1.000	25.990	7.999	14.999	46.001
Scat.Fact.f':	0.003	0.000	0.346	0.011	0.102	-0.999
Scat.Fact.f":	0.002	0.000	0.844	0.006	0.094	1.007
Mu/Rho(MoKa):	0.58	0.37	37.63	1.22	7.97	24.67
Elem. Type :	--	--	TR	--	--	TR

Sources - Cov. Radii : Manual Cambridge Crystallographic Data Base
- Atom Volume: D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493
- Atomic Wt. : SHELXL97
- Scat. Fact.: SHELXL97 (International Tables)
- mu/rho : International Tables C, table 4.2.4.2, p193-199

Residue = 1

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
-	Pd(1)	0.74255	0.54192	0.00590	6.7597	8.3879	0.1300	1	1	1	-	Met
-	Fe(4)	0.74612	0.27568	0.06899	6.6601	4.2670	1.5216	1	1	1	-	Met
-	P(6)	0.77274	0.49062	0.10449	6.8285	7.5938	2.3048	1	1	1	-	-
-	P(7)	0.72184	0.41951	-0.05237	6.6929	6.4932	-1.1550	1	1	1	-	-
-	C(6)	0.73480	0.38157	0.12504	6.4395	5.9059	2.7580	1	1	1	-	-
-	C(7)	0.74106	0.62701	-0.06323	6.8909	9.7049	-1.3947	1	1	1	-	-
-	C(10)	0.74806	0.67555	0.02997	6.7596	10.4561	0.6609	1	1	1	-	-
-	C(12)	0.75920	0.30762	-0.01982	6.9654	4.7613	-0.4372	1	1	1	-	-
-	C(13)	0.73655	0.69267	-0.03096	6.7822	10.7211	-0.6829	1	1	1	-	-
-	C(16)	0.66259	0.23671	-0.01543	6.0751	3.6637	-0.3402	1	1	1	-	-
-	C(17)	0.73690	0.77051	-0.05556	6.8368	11.9259	-1.2254	1	1	1	-	-
-	C(20)	0.64402	0.54909	0.15375	5.5515	8.4988	3.3913	1	1	1	-	-
-	C(23)	0.88027	0.19518	0.02801	7.9694	3.0210	0.6178	1	1	1	-	-
-	C(24)	0.74839	0.16845	0.01819	6.7872	2.6073	0.4012	1	1	1	-	-

-	C(25)	0.86505	0.41788	-0.10957	8.1187	6.4679	-2.4168	1	1	1	- -
-	C(28)	0.59006	0.34020	0.10792	5.1553	5.2656	2.3805	1	1	1	- -
-	C(29)	0.90171	0.28353	0.01235	8.1977	4.3885	0.2725	1	1	1	- -
-	C(31)	0.52879	0.41431	-0.08952	5.0101	6.4127	-1.9746	1	1	1	- -
-	C(35)	0.79177	0.47435	-0.16935	7.5756	7.3420	-3.7354	1	1	1	- -
-	C(36)	0.48157	0.51169	-0.11422	4.6311	7.9200	-2.5193	1	1	1	- -
-	C(37)	0.99468	0.49343	0.20581	8.6405	7.6373	4.5395	1	1	1	- -
-	C(40)	0.58505	0.25716	0.12715	5.0693	3.9803	2.8046	1	1	1	- -
-	C(42)	0.74354	0.24064	0.16115	6.4436	3.7246	3.5545	1	1	1	- -
-	C(45)	0.97731	0.51735	0.13193	8.6368	8.0075	2.9100	1	1	1	- -
-	C(47)	0.68687	0.64486	0.16556	5.9175	9.9812	3.6516	1	1	1	- -
-	C(50)	1.01947	0.60065	0.12086	9.0445	9.2968	2.6657	1	1	1	- -
-	C(51)	0.82297	0.31475	0.15447	7.1819	4.8717	3.4072	1	1	1	- -
-	C(52)	0.64567	0.50718	0.21598	5.4362	7.8501	4.7638	1	1	1	- -
-	C(54)	0.50189	0.56359	0.11835	4.3294	8.7232	2.6103	1	1	1	- -
-	C(56)	0.51613	0.34399	-0.14083	5.0020	5.3243	-3.1062	1	1	1	- -
-	C(57)	0.86794	0.32822	-0.13771	8.2040	5.0802	-3.0375	1	1	1	- -
-	C(59)	0.99844	0.46088	-0.08363	9.2810	7.1334	-1.8446	1	1	1	- -
-	C(60)	1.06843	0.44924	0.10141	9.5317	6.9533	2.2367	1	1	1	- -
-	C(97)	0.42208	0.39407	-0.04194	3.9372	6.0994	-0.9250	1	1	1	- -

==========
********** Residue = 2 **********
==========

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
-	Pd(2)	0.74335	0.20131	0.50632	5.7189	3.1158	11.1678	1	1	1	-	Met
-	Fe(3)	0.74644	0.47013	0.56839	5.6171	7.2767	12.5368	1	1	1	-	Met
-	P(5)	0.72032	0.32670	0.44932	5.6283	5.0567	9.9106	1	1	1	-	-
-	P(8)	0.77364	0.25035	0.60454	5.7896	3.8749	13.3341	1	1	1	-	-
-	C(5)	0.72924	0.07455	0.52552	5.5501	1.1539	11.5913	1	1	1	-	-
-	C(8)	0.73090	0.36543	0.61859	5.3703	5.6561	13.6441	1	1	1	-	-
-	C(9)	0.73638	0.12200	0.42963	5.8160	1.8883	9.4762	1	1	1	-	-
-	C(11)	0.75599	0.42685	0.48310	5.8829	6.6068	10.6556	1	1	1	-	-
-	C(18)	0.64813	0.19042	0.65302	4.5434	2.9474	14.4035	1	1	1	-	-
-	C(19)	0.90455	0.54133	0.52815	7.1434	8.3788	11.6493	1	1	1	-	-
-	C(22)	0.74954	0.57424	0.50730	5.7734	8.8881	11.1895	1	1	1	-	-
-	C(26)	0.84814	0.31988	0.38597	6.9267	4.9512	8.5133	1	1	1	-	-
-	C(27)	0.89929	0.45146	0.50355	7.1470	6.9877	11.1067	1	1	1	-	-
-	C(30)	0.51548	0.32530	0.41553	3.8310	5.0350	9.1652	1	1	1	-	-
-	C(32)	0.67068	0.50668	0.48071	5.1098	7.8425	10.6030	1	1	1	-	-
-	C(33)	0.58876	0.39976	0.60538	4.1017	6.1875	13.3528	1	1	1	-	-
-	C(34)	0.81485	0.25997	0.33705	6.7256	4.0238	7.4343	1	1	1	-	-
-	C(38)	1.01298	0.24031	0.69946	7.7735	3.7195	15.4277	1	1	1	-	-
-	C(39)	0.81944	0.42951	0.65394	6.1038	6.6480	14.4238	1	1	1	-	-
-	C(41)	0.73661	0.50620	0.65458	5.3470	7.8350	14.4380	1	1	1	-	-

-	C(43)	0.47260	0.24446	0.38441	3.5050	3.7837	8.4788	1	1	1	- -
-	C(44)	0.60358	0.49182	0.63356	4.1778	7.6125	13.9744	1	1	1	- -
-	C(46)	0.71198	0.09978	0.67008	5.0899	1.5444	14.7798	1	1	1	- -
-	C(48)	0.96620	0.23528	0.63505	7.4817	3.6416	14.0072	1	1	1	- -
-	C(49)	0.48441	0.19594	0.61507	3.1297	3.0328	13.5665	1	1	1	- -
-	C(53)	1.01598	0.13928	0.61722	7.9731	2.1558	13.6138	1	1	1	- -
-	C(55)	0.61534	0.24179	0.71083	4.1232	3.7424	15.6786	1	1	1	- -
-	C(58)	0.48397	0.40084	0.36637	3.6465	6.2041	8.0810	1	1	1	- -
-	C(61)	0.90508	0.41233	0.36395	7.4921	6.3821	8.0276	1	1	1	- -
-	C(62)	1.06687	0.29258	0.59914	8.4751	4.5286	13.2152	1	1	1	- -
-	C(64)	1.01264	0.29572	0.41745	8.3610	4.5772	9.2076	1	1	1	- -
-	C(99)	0.42099	0.33826	0.46864	2.8580	5.2356	10.3368	1	1	1	- -

********** Residue = 3 **********

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move Type
-	C(3)	0.25516	0.47668	0.54781	1.1797	7.3780	12.0830	1	1	1	2.656 -

Ordered Structure — Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)

Resd	Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	H	Fe	O	P	Pd
1	1	0.746	0.444	0.029	584.51	1	2	30	-	1	-	2	1
2	1	0.746	0.312	0.532	560.49	1	2	28	-	1	-	2	1
3	1	0.255	0.477	0.548	12.01	1	2	1	-	-	-	-	-
					Unit Cell Weight =			2314.02	118	0	4	0	8	4

Calculated Analysis (Percent) = 61.2 0.0 9.7 0.0 10.7 18.4

Moiety_Formula = C30 Fe P2 Pd, C28 Fe P2 Pd, C

Sum_Formula = C59 Fe2 P4 Pd2

Formula_Weight = 1157.01 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 2

SpaceGroup_Z = 2 ===> Z' = 2 / 2 = 1.000

Calculated Density = 1.2344(8) g cm-3 [= Mg m-3]

F(000) = 1116.0 [1114.49]

mu(MoKa) = 11.58 cm-1 = 1.158 mm-1

** WARNING **
Please Check the Derived Crystal Data.
They may be Incorrect for Disordered,
Incomplete or Polymeric Structures.

Resonant Scattering = 2.87 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 2134.3[2114.4] Ang**3, 298[200]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f,f' & f"

(An)isotropic, Equivalent and Main Axes Displacement Parameters - Unusual Values Marked with a # - [Optional Coordinate Split-up]

Residue = 1

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Pd1	0.02017						0.02017				
2	Fe4	0.02350						0.02350				
3	P6	0.02031						0.02031				
4	P7	0.02422						0.02422				
5	C6	0.02654						0.02654				
6	C7	0.01942						0.01942				
7	C10	0.01535						0.01535				
8	C12	0.02739						0.02739				
9	C13	0.00078						0.00078				
10	C16	0.01694						0.01694				
11	C17	0.02826						0.02826				
12	C20	0.03761						0.03761				
13	C23	0.04154						0.04154				
14	C24	0.03007						0.03007				
15	C25	0.04293						0.04293				
16	C28	0.02279						0.02279				
17	C29	0.01905						0.01905				
18	C31	0.03642						0.03642				
19	C35	0.04552						0.04552				
20	C36	0.03655						0.03655				
21	C37	0.04012						0.04012				
22	C40	0.02456						0.02456				
23	C42	0.04757						0.04757				
24	C45	0.02944						0.02944				
25	C47	0.03316						0.03316				
26	C50	0.06008						0.06008				
27	C51	0.02873						0.02873				
28	C52	0.04256						0.04256				
29	C54	0.02822						0.02822				
30	C56	0.04195						0.04195				
31	C57	0.04211						0.04211				
32	C59	0.02392						0.02392				
33	C60	0.04988						0.04988				
34	C97	0.04687						0.04687				

Residue = 2

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Pd2	0.02194						0.02194				
2	Fe3	0.02677						0.02677				
3	P5	0.02142						0.02142				
4	P8	0.02388						0.02388				
5	C5	0.01252						0.01252				
6	C8	0.02159						0.02159				
7	C9	0.01300						0.01300				
8	C11	0.01883						0.01883				
9	C18	0.02917						0.02917				
10	C19	0.02259						0.02259				
11	C22	0.02823						0.02823				
12	C26	0.01973						0.01973				
13	C27	0.03148						0.03148				
14	C30	0.03121						0.03121				
15	C32	0.06472						0.06472				
16	C33	0.04071						0.04071				
17	C34	0.03155						0.03155				
18	C38	0.03302						0.03302				
19	C39	0.03144						0.03144				
20	C41	0.03230						0.03230				
21	C43	0.04312						0.04312				
22	C44	0.05241						0.05241				
23	C46	0.04064						0.04064				
24	C48	0.03263						0.03263				
25	C49	0.04114						0.04114				
26	C53	0.02676						0.02676				
27	C55	0.03447						0.03447				
28	C58	0.03634						0.03634				
29	C61	0.03911						0.03911				
30	C62	0.03109						0.03109				
31	C64	0.06293						0.06293				
32	C99	0.02668						0.02668				

Residue = 3

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	C3	0.03347						0.03347				

The Displacement Factor has the Form of Exp(-T)

where

T = 8*(pi**2)*Uiso*sin(theta/lambda)**2, for Isotropic Atoms,

T = 2*(pi**2)*(U11*(h*as)**2+U22*(k*bs)**2+U33*(l*cs)**2+2*U23*k*l*bs*cs+2*U13*h*l*as*cs+2*U12*h*k*as*bs),for Anisotr. Atoms

Ueq = 1/3 Sum(i,j) (Uij*as(i)*as(j)*a(i).a(j))

U1, U2, U3 are the three Main Axes Components of Uij

Reference U(eq): R.X. Fischer & E. Tillmanns, Acta Cryst. (1988). C44, 775-776

Ueq [or U(iso)] Averages per Element

	Non-H	C	H	Fe	O	P	Pd
Average	0.0318	0.0330	0.0000	0.0251	0.0000	0.0225	0.0211
Minimum	0.0008	0.0008	0.0000	0.0235	0.0000	0.0203	0.0202
Maximum	0.0647	0.0647	0.0000	0.0268	0.0000	0.0242	0.0219
Ratio	9.9999	9.9999	0.0000	1.1391	0.0000	1.1925	1.0878
Number	67	59	0	2	0	4	2

Analysis of Bond Distance and Angle Values - Identification of Chiral Center(s) and Their (R/S)-Configuration (Cahn-Ingold-Prelog)

The Following Tests are done. Faults are Marked Under Note
-- V : Valency Check Fault for H, C
-- S : Bond Too Short
-- A : Unusual Bond Angle Values (PLEASE CHECK)

*** PLEASE NOTE: R/S ASSIGNMENTS ARE TENTATIVE *** (CIP Special rules NOT Implemented)
*** See Angew.Chem.Intern. Ed. Eng.,(1966),5,385 & (1982),21,567 for Authoritative Details for Special Cases

Residue = 1

Flag	Label	- Connected to (May be Incomplete for Polymeric Structures)									=A.N.G.L.E.S= nra	min	max	Aver	=B.O.N.D.S= min	max	nrb	tnr	Hyb	RS	Note
-	Pd(1)	- P(6)	P(7)	C(7)	C(10)	C(13)	-------	-------	-------	-------10	30	160	99.9	2.019	2.471	5	21			
-	Fe(4)	- C(6) C(51)	C(12)	C(16)	C(23)	C(24)	C(28)	C(29)	C(40)	C(42)	36	37	177	99.3	1.985	2.115	10	19			
-	P(6)	- Pd(1)	C(6)	C(20)	C(45)	-------	-------	-------	-------	-------	6	99	124	109.4	1.790	2.316	4	17	sp3		
-	P(7)	- Pd(1)	C(12)	C(25)	C(31)	-------	-------	-------	-------	-------	6	98	123	109.4	1.874	2.290	4	17	sp3		
-	C(6)	- Fe(4)	P(6)	C(28)	C(51)	-------	-------	-------	-------	-------	3	105	133	120.0	1.429	2.065	3	12	sp2		
-	C(7)	- Pd(1)	C(13)	-------	-------	-------	-------	-------	-------	-------	1	95	95	95.4	1.245	2.019	2	15			
-	C(10)	- Pd(1)	C(13)	-------	-------	-------	-------	-------	-------	-------	1	87	87	86.8	1.370	2.135	2	15			
-	C(12)	- Fe(4)	P(7)	C(16)	C(29)	-------	-------	-------	-------	-------	3	107	130	119.9	1.417	2.043	3	12	sp2		
-	C(13)	- Pd(1)	C(7)	C(10)	C(17)	-------	-------	-------	-------	-------	3	114	125	119.9	1.245	2.471	3	14	sp2		
-	C(16)	- Fe(4)	C(12)	C(24)	-------	-------	-------	-------	-------	-------	1	107	107	106.6	1.417	2.043	2	11			
-	C(17)	- C(13)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.322	1.322	1	4			?
-	C(20)	- P(6)	C(47)	C(52)	C(54)	-------	-------	-------	-------	-------	6	98	119	109.4	1.468	1.905	4	6	sp3		
-	C(23)	- Fe(4)	C(24)	C(29)	-------	-------	-------	-------	-------	-------	1	115	115	114.8	1.271	2.021	2	10			
-	C(24)	- Fe(4)	C(16)	C(23)	-------	-------	-------	-------	-------	-------	1	108	108	107.6	1.271	2.007	2	10			
-	C(25)	- P(7)	C(35)	C(57)	C(59)	-------	-------	-------	-------	-------	6	100	122	109.2	1.456	1.904	4	6	sp3		
-	C(28)	- Fe(4)	C(6)	C(40)	-------	-------	-------	-------	-------	-------	1	113	113	112.6	1.356	2.000	2	11			
-	C(29)	- Fe(4)	C(12)	C(23)	-------	-------	-------	-------	-------	-------	1	103	103	103.0	1.429	1.985	2	11			
-	C(31)	- P(7)	C(36)	C(56)	C(97)	-------	-------	-------	-------	-------	6	105	113	109.4	1.533	1.874	4	6	sp3		
-	C(35)	- C(25)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.673	1.673	1	3			?
-	C(36)	- C(31)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.647	1.647	1	3			?
-	C(37)	- C(45)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.671	1.671	1	3			?
-	C(40)	- Fe(4)	C(28)	C(42)	-------	-------	-------	-------	-------	-------	1	104	104	104.2	1.356	2.064	2	10			
-	C(42)	- Fe(4)	C(40)	C(51)	-------	-------	-------	-------	-------	-------	1	106	106	106.3	1.372	2.115	2	10			
-	C(45)	- P(6)	C(37)	C(50)	C(60)	-------	-------	-------	-------	-------	6	105	115	109.3	1.374	1.951	4	6	sp3		
-	C(47)	- C(20)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.549	1.549	1	3			?
-	C(50)	- C(45)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.374	1.374	1	3			?
-	C(51)	- Fe(4)	C(6)	C(42)	-------	-------	-------	-------	-------	-------	1	112	112	112.0	1.372	2.048	2	11			
-	C(52)	- C(20)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.523	1.523	1	3			?
-	C(54)	- C(20)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.468	1.468	1	3			?
-	C(56)	- C(31)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.570	1.570	1	3			?
-	C(57)	- C(25)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.523	1.523	1	3			?
-	C(59)	- C(25)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.456	1.456	1	3			?
-	C(60)	- C(45)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.538	1.538	1	3			?
-	C(97)	- C(31)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.533	1.533	1	3			?

Residue = 2

Flag	Label	Connected to (May be Incomplete for Polymeric Structures)									=A.N.G.L.E.S= nra	min	max	Aver	=B.O.N.D.S= min	max	nrb	tnr	Hyb	RS	Note
-	Pd(2)	P(5)	P(8)	C(5)	C(9)	-------	-------	-------	-------	-------	6	67	163	113.6	2.014	2.314	4	20			
-	Fe(3)	C(8) C(44)	C(11)	C(19)	C(22)	C(27)	C(32)	C(33)	C(39)	C(41)	36	38	178	99.6	1.978	2.114	10	18			
-	P(5)	Pd(2)	C(11)	C(26)	C(30)	-------	-------	-------	-------	-------	6	104	121	109.5	1.739	2.314	4	16	sp3		
-	P(8)	Pd(2)	C(8)	C(18)	C(48)	-------	-------	-------	-------	-------	6	103	118	109.4	1.836	2.297	4	16	sp3		
-	C(5)	Pd(2)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.014	2.014	1	13			?
-	C(8)	Fe(3)	P(8)	C(33)	C(39)	-------	-------	-------	-------	-------	3	108	129	119.6	1.406	1.978	3	9	sp2		
-	C(9)	Pd(2)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.092	2.092	1	13			?
-	C(11)	Fe(3)	P(5)	C(27)	C(32)	-------	-------	-------	-------	-------	3	105	131	119.2	1.395	2.015	3	9	sp2		
-	C(18)	P(8)	C(46)	C(49)	C(55)	-------	-------	-------	-------	-------	6	99	118	109.4	1.552	1.886	4	5	sp3		
-	C(19)	Fe(3)	C(22)	C(27)	-------	-------	-------	-------	-------	-------	1	102	102	101.7	1.493	2.081	2	7			
-	C(22)	Fe(3)	C(19)	C(32)	-------	-------	-------	-------	-------	-------	1	108	108	107.9	1.370	2.106	2	7			
-	C(26)	P(5)	C(34)	C(61)	C(64)	-------	-------	-------	-------	-------	6	91	119	108.8	1.437	1.910	4	5	sp3		
-	C(27)	Fe(3)	C(11)	C(19)	-------	-------	-------	-------	-------	-------	1	112	112	111.7	1.395	2.114	2	8			
-	C(30)	P(5)	C(43)	C(58)	C(99)	-------	-------	-------	-------	-------	6	106	113	109.5	1.464	1.946	4	5	sp3		
-	C(32)	Fe(3)	C(11)	C(22)	-------	-------	-------	-------	-------	-------	1	112	112	112.0	1.370	2.078	2	8			
-	C(33)	Fe(3)	C(8)	C(44)	-------	-------	-------	-------	-------	-------	1	103	103	102.7	1.406	2.037	2	8			
-	C(34)	C(26)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.437	1.437	1	2			?
-	C(38)	C(48)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.452	1.452	1	2			?
-	C(39)	Fe(3)	C(8)	C(41)	-------	-------	-------	-------	-------	-------	1	108	108	108.0	1.408	2.048	2	8			
-	C(41)	Fe(3)	C(39)	C(44)	-------	-------	-------	-------	-------	-------	1	110	110	110.0	1.277	2.000	2	7			
-	C(43)	C(30)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.464	1.464	1	2			?
-	C(44)	Fe(3)	C(33)	C(41)	-------	-------	-------	-------	-------	-------	1	110	110	110.4	1.277	2.062	2	7			
-	C(46)	C(18)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.552	1.552	1	2			?
-	C(48)	P(8)	C(38)	C(53)	C(62)	-------	-------	-------	-------	-------	6	102	122	109.1	1.452	1.836	4	5	sp3		
-	C(49)	C(18)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.645	1.645	1	2			?
-	C(53)	C(48)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.614	1.614	1	2			?
-	C(55)	C(18)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.560	1.560	1	2			?
-	C(58)	C(30)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.605	1.605	1	2			?
-	C(61)	C(26)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.613	1.613	1	2			?
-	C(62)	C(48)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.549	1.549	1	2			?
-	C(64)	C(26)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.637	1.637	1	2			?
-	C(99)	C(30)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.536	1.536	1	2			?

Residue = 3

Flag	Label	- Connected to (May be Incomplete for Polymeric Structures)	=A.N.G.L.E.S= nra	min	max	Aver	=B.O.N.D.S= min	max	nrb	tnr	Hyb	RS	Note
-	C(3)	- ------- ------- ------- ------- ------- ------- ------- ------- -------	0	0	0	0.0	0.000	0.000	0	1			V?

Page - Index

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR

N: ADDSYM finds additional (pseudo)symmetry in the structure (please check!)
W: Look carefully at the approximate inversion symmetry reported by ADDSYM
N: No S.U.'s (esd) on observed/calculated parameters.
N: No-Hydrogen atoms in this structure

N: Number of Isotropic Non-H Atoms	67
N: Number of moved primary input atoms:	1
N: Number of deleted ATOMS from input stream	1
W: Number of valency check faults for H & C	1
W: Number of Carbon Atoms with missing H-atoms	27
W: Number of (Carbon) Atoms with no sp(x) assignment	26
N: Number of Ignored Lines on INPUT	4
of which blank in column 1	3

:: Input Xtal Data from File jmca013s.eld - Data Type SPF

:: NORMAL END of PLATON : 15 Pages on:
:: jmca013s.lis (ASCII, 132 Characters Wide)
:: jmca013s.lps (PostScript Version of .lis)
:: jmca013s.pdf (PDF Version of .lis)

PLATON(V-311206)-Run for: jmca013 in P2(1) New: P21/c TIME: Nov 23 16:50:29 2010

Crystal Data

Input Cell (Lattice Type: P) - Temp = 200K

a =	9.120(4)	Angstrom	alpha =	90	Degree	a = 9.120	alpha = 90.00	V =	3114.0
b =	15.478(7)		beta =	95.424(7)		b = 15.478	beta = 95.42		
c =	22.156(11)		gamma =	90		c = 22.156	gamma = 90.00		
V =	3114(2)	Cubic-Angstrom	d(100) =	9.0792	Angstrom				
			d(010) =	15.4780					
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	22.0568					

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

Niggli Values: 83.174 239.568 490.888 / 0.000 -19.100 0.000

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 9.12000 & 0 & -2.09430 \\ 0 & 15.47800 & 0 \\ 0 & 0 & 22.05680 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.10965 & 0 & 0.01041 \\ 0 & 0.06461 & 0 \\ 0 & 0 & 0.04534 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group P21/c No: 14, Laue: 2/m [Hall: -P 2ybc]

Lattice Type mP, Centric, Monoclinic, Order 4(2) [Schoenflies: C2h^5]

Nr	***** Symmetry Operation(s) *****		
1	X ,	Y ,	Z
2	- X ,	1/2 + Y ,	1/2 - Z
3	- X ,	- Y ,	- Z
4	X ,	1/2 - Y ,	1/2 + Z

-	C(36)	-0.02252	0.11638	0.13530	-0.4887	1.8014	2.9842	1	1	1	4.555	-
-	C(37)	0.50423	0.12344	0.45283	3.6502	1.9106	9.9880	1	1	1	4.555	-
-	C(40)	0.09471	0.36733	0.38056	0.0668	5.6856	8.3939	1	1	1	4.555	-
-	C(42)	0.24047	0.38278	0.40807	1.3385	5.9247	9.0007	1	1	1	4.555	-
-	C(45)	0.47215	0.10896	0.38369	3.5025	1.6865	8.4630	1	1	1	4.555	-
-	C(47)	0.19982	-0.02254	0.41802	0.9469	-0.3489	9.2201	1	1	1	4.555	-
-	C(50)	0.51813	0.01932	0.36924	3.9520	0.2990	8.1442	1	1	1	4.555	-
-	C(51)	0.32160	0.30738	0.40441	2.0861	4.7577	8.9199	1	1	1	4.555	-
-	C(52)	0.13091	0.11731	0.46361	0.2229	1.8157	10.2256	1	1	1	4.555	-
-	C(54)	-0.00645	0.06618	0.36691	-0.8272	1.0243	8.0928	1	1	1	4.555	-
-	C(56)	0.00045	0.27842	0.11297	-0.2325	4.3094	2.4918	1	1	1	4.555	-
-	C(57)	0.38691	0.29206	0.11332	3.2913	4.5205	2.4995	1	1	1	4.555	-
-	C(59)	0.50594	0.16742	0.16711	4.2642	2.5914	3.6859	1	1	1	4.555	-
-	C(60)	0.56805	0.17167	0.35048	4.4466	2.6572	7.7304	1	1	1	4.555	-
-	C(97)	-0.07806	0.22210	0.21355	-1.1592	3.4376	4.7103	1	1	1	4.555	-

Ordered Structure — Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)

Resd	Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	H	Fe	O	P	Pd
1	1	0.246	0.178	0.279	584.51	1	4	30	-	1	-	2	1
					Unit Cell Weight =	2338.04		120	0	4	0	8	4
					Calculated Analysis (Percent) =			61.6	0.0	9.6	0.0	10.6	18.2

Moiety_Formula = C30 Fe P2 Pd

Sum_Formula = C30 Fe P2 Pd

Formula_Weight = 584.51 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 4

SpaceGroup_Z = 4 ===> Z' = 4 / 4 = 1.000

Calculated Density = 1.2468(8) g cm-3 [= Mg m-3]

F(000) = 1128.0 [1126.50]

mu(MoKa) = 11.58 cm-1 = 1.158 mm-1

Resonant Scattering = 2.86 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

** WARNING **
Please Check the Derived Crystal Data.
They may be Incorrect for Disordered,
Incomplete or Polymeric Structures.

Predicted Volume = 2162.0[2141.9] Ang**3, 298[200]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f,f' & f"

(An)isotropic, Equivalent and Main Axes Displacement Parameters - Unusual Values Marked with a # - [Optional Coordinate Split-up]

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Pd1	0.02017						0.02017				
2	Fe4	0.02350						0.02350				
3	P6	0.02031						0.02031				
4	P7	0.02422						0.02422				
5	C6	0.02654						0.02654				
6	C7	0.01942						0.01942				
7	C10	0.01535						0.01535				
8	C12	0.02739						0.02739				
9	C13	0.00078						0.00078				
10	C16	0.01694						0.01694				
11	C17	0.02826						0.02826				
12	C20	0.03761						0.03761				
13	C23	0.04154						0.04154				
14	C24	0.03007						0.03007				
15	C25	0.04293						0.04293				
16	C28	0.02279						0.02279				
17	C29	0.01905						0.01905				
18	C31	0.03642						0.03642				
19	C35	0.04552						0.04552				
20	C36	0.03655						0.03655				
21	C37	0.04012						0.04012				
22	C40	0.02456						0.02456				
23	C42	0.04757						0.04757				
24	C45	0.02944						0.02944				
25	C47	0.03316						0.03316				
26	C50	0.06008						0.06008				
27	C51	0.02873						0.02873				
28	C52	0.04256						0.04256				
29	C54	0.02822						0.02822				
30	C56	0.04195						0.04195				
31	C57	0.04211						0.04211				
32	C59	0.02392						0.02392				
33	C60	0.04988						0.04988				
34	C97	0.04687						0.04687				

==========

The Displacement Factor has the Form of Exp(-T)

where

T = 8*(pi**2)*Uiso*sin(theta/lambda)**2, for Isotropic Atoms,

T = 2*(pi**2)*(U11*(h*as)**2+U22*(k*bs)**2+U33*(l*cs)**2+2*U23*k*l*bs*cs+2*U13*h*l*as*cs+2*U12*h*k*as*bs),for Anisotr. Atoms

Ueq = 1/3 Sum(i,j) (Uij*as(i)*as(j)*a(i).a(j))

U1, U2, U3 are the three Main Axes Components of Uij

Reference U(eq): R.X. Fischer & E. Tillmanns, Acta Cryst. (1988). C44, 775-776

Ueq [or U(iso)] Averages per Element

	Non-H	C	H	Fe	O	P	Pd
Average	0.0316	0.0329	0.0000	0.0235	0.0000	0.0223	0.0202
Minimum	0.0008	0.0008	0.0000	0.0235	0.0000	0.0203	0.0202
Maximum	0.0601	0.0601	0.0000	0.0235	0.0000	0.0242	0.0202
Ratio	9.9999	9.9999	0.0000	1.0000	0.0000	1.1925	1.0000
Number	34	30	0	1	0	2	1

Analysis of Bond Distance and Angle Values - Identification of Chiral Center(s) and Their (R/S)-Configuration (Cahn-Ingold-Prelog)

The Following Tests are done. Faults are Marked Under Note
-- V : Valency Check Fault for H, C
-- S : Bond Too Short
-- A : Unusual Bond Angle Values (PLEASE CHECK)

*** PLEASE NOTE: R/S ASSIGNMENTS ARE TENTATIVE *** (CIP Special rules NOT Implemented)
*** See Angew.Chem.Intern. Ed. Eng.,(1966),5,385 & (1982),21,567 for Authoritative Details for Special Cases

Flag	Label	- Connected to (May be Incomplete for Polymeric Structures)									=A.N.G.L.E.S= nra	min	max	Aver	=B.O.N.D.S= min	max	nrb	tnr	Hyb	RS	Note
-	Pd(1)	- P(6)	P(7)	C(7)	C(10)	C(13)	-------	-------	-------	-------10	32	161	100.2	2.054	2.473	5	11			
-	Fe(4)	- C(6) C(51)	C(12)	C(16)	C(23)	C(24)	C(28)	C(29)	C(40)	C(42) 36	40	178	99.5	2.018	2.060	10	10			
-	P(6)	- Pd(1)	C(6)	C(20)	C(45)	-------	-------	-------	-------	------- 6	101	121	109.4	1.821	2.306	4	9	sp3		
-	P(7)	- Pd(1)	C(12)	C(25)	C(31)	-------	-------	-------	-------	------- 6	101	122	109.5	1.816	2.302	4	9	sp3		
-	C(6)	- Fe(4)	P(6)	C(28)	C(51)	-------	-------	-------	-------	------- 3	106	131	120.0	1.443	2.021	3	6	sp2		
-	C(7)	- Pd(1)	C(13)	-------	-------	-------	-------	-------	-------	------- 1	91	91	91.4	1.327	2.054	2	7			
-	C(10)	- Pd(1)	C(13)	-------	-------	-------	-------	-------	-------	------- 1	90	90	90.3	1.337	2.073	2	7			
-	C(12)	- Fe(4)	P(7)	C(16)	C(29)	-------	-------	-------	-------	------- 3	107	131	119.9	1.427	2.027	3	6	sp2		
-	C(13)	- Pd(1)	C(7)	C(10)	C(17)	-------	-------	-------	-------	------- 3	113	125	120.0	1.264	2.473	3	8	sp2		
-	C(16)	- Fe(4)	C(12)	C(24)	-------	-------	-------	-------	-------	------- 1	109	109	109.2	1.421	2.060	2	5			
-	C(17)	- C(13)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.264	1.264	1	2			?
-	C(20)	- P(6)	C(47)	C(52)	C(54)	-------	-------	-------	-------	------- 6	107	112	109.5	1.531	1.896	4	3	sp3		
-	C(23)	- Fe(4)	C(24)	C(29)	-------	-------	-------	-------	-------	------- 1	108	108	108.2	1.399	2.047	2	4			
-	C(24)	- Fe(4)	C(16)	C(23)	-------	-------	-------	-------	-------	------- 1	108	108	108.1	1.399	2.054	2	4			
-	C(25)	- P(7)	C(35)	C(57)	C(59)	-------	-------	-------	-------	------- 6	106	112	109.4	1.535	1.904	4	3	sp3		
-	C(28)	- Fe(4)	C(6)	C(40)	-------	-------	-------	-------	-------	------- 1	107	107	107.3	1.444	2.018	2	5			
-	C(29)	- Fe(4)	C(12)	C(23)	-------	-------	-------	-------	-------	------- 1	108	108	107.8	1.427	2.047	2	5			
-	C(31)	- P(7)	C(36)	C(56)	C(97)	-------	-------	-------	-------	------- 6	107	111	109.5	1.532	1.908	4	3	sp3		
-	C(35)	- C(25)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.545	1.545	1	1			?
-	C(36)	- C(31)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.551	1.551	1	1			?
-	C(37)	- C(45)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.548	1.548	1	1			?
-	C(40)	- Fe(4)	C(28)	C(42)	-------	-------	-------	-------	-------	------- 1	108	108	107.8	1.429	2.060	2	4			
-	C(42)	- Fe(4)	C(40)	C(51)	-------	-------	-------	-------	-------	------- 1	108	108	108.3	1.388	2.057	2	4			
-	C(45)	- P(6)	C(37)	C(50)	C(60)	-------	-------	-------	-------	------- 6	107	113	109.4	1.493	1.891	4	3	sp3		
-	C(47)	- C(20)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.546	1.546	1	1			?
-	C(50)	- C(45)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.493	1.493	1	1			?
-	C(51)	- Fe(4)	C(6)	C(42)	-------	-------	-------	-------	-------	------- 1	110	110	110.1	1.388	2.048	2	5			
-	C(52)	- C(20)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.531	1.531	1	1			?
-	C(54)	- C(20)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.548	1.548	1	1			?
-	C(56)	- C(31)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.585	1.585	1	1			?
-	C(57)	- C(25)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.549	1.549	1	1			?
-	C(59)	- C(25)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.535	1.535	1	1			?
-	C(60)	- C(45)	-------	-------	-------	-------	-------	-------	-------	------- 0	0	0	0.0	1.540	1.540	1	1			?

-	C(97)	- C(31)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.532	1.532	1	1	?

==========

********** 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/

Page - Index

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR

N: ADDSYM finds additional (pseudo)symmetry in the structure (please check!)
N: No S.U.'s (esd) on observed/calculated parameters.
N: No-Hydrogen atoms in this structure

N: Number of Isotropic Non-H Atoms 34
N: Number of moved primary input atoms: 34
N: Input Data following TRNS [e.g. (CELL/CESD)/SPGR/COORDS/UIJ)] have been
transformed according to the specified Cell Transformation Matrix:

1.00000 0.00000 0.00000
0.00000 1.00000 0.00000
0.00000 0.00000 1.00000

N: INPUT data (COORDINATES) have been transformed
according to additive coordinate shift vector:

-0.49960 -0.12160 -0.24980

N: Number of deleted ATOMS from input stream 33
W: Number of Carbon Atoms with missing H-atoms 13
W: Number of (Carbon) Atoms with no sp(x) assignment 13
N: Number of Ignored Lines on INPUT 69
of which blank in column 1 0

:: Input Xtal Data from File jmca013s.eld - Data Type SPF

:: NORMAL END of PLATON : 25 Pages on:
:: jmca013s.lis (ASCII, 132 Characters Wide)
:: jmca013s.lps (PostScript Version of .lis)
:: jmca013s.pdf (PDF Version of .lis)

:: SHELXL Style Output on :jmca013s.res