PLATON(V-311206)-Run for: char278a in Pna2(1) TIME: Mar 18 12:41:19 2010

Crystal Data

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

a =	16.613(2)	Angstrom	alpha =	90	Degree	a =	10.390	alpha =	90.00
b =	10.3901(13)		beta =	90		b =	16.613	beta =	90.00
c =	18.150(2)		gamma =	90		c =	18.150	gamma =	90.00
V =	3133.0(6)	Cubic-Angstrom	d(100) =	16.6133	Angstrom				
			d(010) =	10.3901					
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	18.1502					

Reduced Cell (Acta Cryst.(1976),A32,297-298) V = 3133.0

Niggli Values

107.954	276.002	329.430
0.000	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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 16.61300 & 0 & 0 \\ 0 & 10.39010 & 0 \\ 0 & 0 & 18.15000 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.06019 & 0 & 0 \\ 0 & 0.09625 & 0 \\ 0 & 0 & 0.05510 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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 Pna21 No: 33, Laue: mmm [Hall: P 2c -2n]

Lattice Type oP, Acentric, Orthorhombic, Order 4(4) [Schoenflies: C2v^9]

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

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

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

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         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	N	O	P
Cov.Rad(Ang):	0.68	0.35	0.68	0.68	1.05
Atom Volume :	13.87	5.08	11.80	11.39	29.50
Atom Number :	6	1	7	8	15
Atom Weight :	12.010	1.008	14.01	16.00	30.97
Scat.Fact.f0:	5.999	1.000	6.995	7.999	14.999
Scat.Fact.f':	0.003	0.000	0.006	0.011	0.102
Scat.Fact.f":	0.002	0.000	0.003	0.006	0.094
Mu/Rho(MoKa):	0.58	0.37	0.84	1.22	7.97
Elem. Type :	--	--	--	--	--

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
-	P(1)	0.04712	-0.06974	0.37716	0.7828	-0.7246	6.8455	1	1	1	-	-
-	O(1)	0.00280	-0.12557	0.31191	0.0465	-1.3047	5.6611	1	1	1	-	D/A
-	N(1)	-0.01135	0.34029	0.29956	-0.1886	3.5357	5.4370	1	1	1	-	D/A
-	C(1)	0.18905	-0.14514	0.31256	3.1407	-1.5080	5.6730	1	1	1	-	-
-	C(2)	0.26869	-0.18165	0.31208	4.4637	-1.8874	5.6643	1	1	1	-	-
-	C(3)	0.31021	-0.19214	0.37783	5.1536	-1.9964	6.8575	1	1	1	-	-
-	C(4)	0.27343	-0.16631	0.44252	4.5424	-1.7280	8.0317	1	1	1	-	-
-	C(5)	0.19363	-0.12851	0.44424	3.2168	-1.3353	8.0629	1	1	1	-	-
-	C(6)	0.15065	-0.11881	0.37955	2.5027	-1.2344	6.8889	1	1	1	-	-
-	C(7)	-0.02755	-0.02731	0.51377	-0.4577	-0.2837	9.3249	1	1	1	-	-
-	C(8)	-0.06371	-0.07084	0.57739	-1.0583	-0.7360	10.4797	1	1	1	-	-
-	C(9)	-0.06863	-0.19663	0.59460	-1.1401	-2.0431	10.7919	1	1	1	-	-
-	C(10)	-0.03517	-0.28169	0.54615	-0.5843	-2.9268	9.9125	1	1	1	-	-
-	C(11)	0.00200	-0.24575	0.48127	0.0333	-2.5533	8.7351	1	1	1	-	-

-	C(12)	0.00532	-0.11615	0.46414	0.0884	-1.2068	8.4241	1	1	1	-	-
-	C(13)	0.04764	0.10402	0.37607	0.7914	1.0807	6.8257	1	1	1	-	-
-	C(14)	0.07793	0.16027	0.30169	1.2947	1.6652	5.4757	1	1	1	-	-
-	C(15)	-0.02448	0.46597	0.30084	-0.4066	4.8415	5.4602	1	1	1	-	-
-	C(16)	0.03535	0.55821	0.30122	0.5872	5.7999	5.4671	1	1	1	-	-
-	C(17)	0.11314	0.51473	0.29983	1.8795	5.3481	5.4419	1	1	1	-	-
-	C(18)	0.12793	0.38482	0.29822	2.1253	3.9983	5.4127	1	1	1	-	-
-	C(19)	0.06573	0.30167	0.29949	1.0919	3.1343	5.4357	1	1	1	-	-
-	H(1A)	0.16022	-0.13782	0.26756	2.6617	-1.4320	4.8562	1	1	1	-	-
-	H(2A)	0.29501	-0.19958	0.26676	4.9010	-2.0736	4.8418	1	1	1	-	-
-	H(3A)	0.36511	-0.21774	0.37749	6.0656	-2.2624	6.8515	1	1	1	-	-
-	H(4A)	0.30265	-0.17418	0.48728	5.0280	-1.8098	8.8441	1	1	1	-	-
-	H(5A)	0.16850	-0.10927	0.48994	2.7993	-1.1353	8.8925	1	1	1	-	-
-	H(7A)	-0.02494	0.06230	0.50364	-0.4144	0.6473	9.1410	1	1	1	-	-
-	H(8A)	-0.08606	-0.00961	0.61045	-1.4297	-0.0999	11.0796	1	1	1	-	-
-	H(9A)	-0.09424	-0.22494	0.63850	-1.5656	-2.3372	11.5887	1	1	1	-	-
-	H(10A)	-0.03760	-0.37078	0.55772	-0.6246	-3.8524	10.1227	1	1	1	-	-
-	H(11A)	0.02469	-0.30836	0.44928	0.4101	-3.2039	8.1544	1	1	1	-	-
-	H(13A)	-0.00759	0.13570	0.38556	-0.1262	1.4099	6.9980	1	1	1	-	-
-	H(13B)	0.08265	0.13560	0.41633	1.3730	1.4089	7.5565	1	1	1	-	-
-	H(14A)	0.13586	0.14059	0.29557	2.2570	1.4607	5.3647	1	1	1	-	-
-	H(14B)	0.04830	0.11959	0.26049	0.8024	1.2426	4.7279	1	1	1	-	-
-	H(15A)	-0.07877	0.49464	0.30153	-1.3086	5.1393	5.4728	1	1	1	-	-
-	H(16A)	0.02313	0.64751	0.30239	0.3843	6.7277	5.4884	1	1	1	-	-
-	H(17A)	0.15660	0.57414	0.29997	2.6017	5.9653	5.4445	1	1	1	-	-
-	H(18A)	0.18167	0.35374	0.29623	3.0180	3.6754	5.3766	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
-	P(2)	0.30048	-0.08344	0.07329	4.9919	-0.8669	1.3303	1	1	1	3.544	-
-	O(2)	0.25789	-0.14193	0.13648	4.2844	-1.4747	2.4771	1	1	1	3.544	D/A
-	N(2)	0.24599	0.33087	0.13419	4.0866	3.4378	2.4355	1	1	1	3.544	D/A
-	C(20)	0.45083	-0.11165	0.00660	7.4897	-1.1601	0.1197	1	1	1	3.544	-
-	C(21)	0.53085	-0.14513	0.00623	8.8190	-1.5079	0.1131	1	1	1	3.544	-
-	C(22)	0.56520	-0.19780	0.06963	9.3897	-2.0551	1.2637	1	1	1	3.544	-
-	C(23)	0.51909	-0.21869	0.13173	8.6237	-2.2722	2.3909	1	1	1	3.544	-
-	C(24)	0.43940	-0.18035	0.13146	7.2998	-1.8738	2.3859	1	1	1	3.544	-
-	C(25)	0.40409	-0.13023	0.06995	6.7131	-1.3531	1.2696	1	1	1	3.544	-
-	C(26)	0.21803	-0.04746	-0.05998	3.6221	-0.4931	-1.0886	1	1	1	3.544	-
-	C(27)	0.17988	-0.09002	-0.12231	2.9884	-0.9353	-2.2200	1	1	1	3.544	-
-	C(28)	0.18078	-0.22271	-0.13870	3.0034	-2.3140	-2.5174	1	1	1	3.544	-
-	C(29)	0.22236	-0.30545	-0.09448	3.6941	-3.1736	-1.7148	1	1	1	3.544	-

-	C(30)	0.25876	-0.25832	-0.03222	4.2987	-2.6840	-0.5848	1	1	1	3.544 -
-	C(31)	0.25839	-0.13056	-0.01320	4.2927	-1.3565	-0.2397	1	1	1	3.544 -
-	C(32)	0.29923	0.08839	0.07606	4.9710	0.9184	1.3805	1	1	1	3.544 -
-	C(33)	0.32778	0.14309	0.14921	5.4454	1.4867	2.7083	1	1	1	3.544 -
-	C(34)	0.23664	0.45715	0.13788	3.9313	4.7499	2.5025	1	1	1	3.544 -
-	C(35)	0.29225	0.54275	0.15926	4.8552	5.6393	2.8906	1	1	1	3.544 -
-	C(36)	0.36489	0.49447	0.17977	6.0618	5.1376	3.2629	1	1	1	3.544 -
-	C(37)	0.37650	0.36526	0.17571	6.2547	3.7951	3.1891	1	1	1	3.544 -
-	C(38)	0.31682	0.28560	0.15253	5.2633	2.9674	2.7685	1	1	1	3.544 -
-	H(20A)	0.42708	-0.07572	-0.03634	7.0951	-0.7867	-0.6596	1	1	1	3.544 -
-	H(21A)	0.56251	-0.13255	-0.03676	9.3449	-1.3772	-0.6672	1	1	1	3.544 -
-	H(22A)	0.62076	-0.21943	0.07002	10.3127	-2.2799	1.2708	1	1	1	3.544 -
-	H(23A)	0.54173	-0.25876	0.17397	8.9998	-2.6885	3.1575	1	1	1	3.544 -
-	H(24A)	0.40846	-0.18912	0.17519	6.7858	-1.9649	3.1796	1	1	1	3.544 -
-	H(26A)	0.21673	0.04174	-0.04852	3.6006	0.4336	-0.8807	1	1	1	3.544 -
-	H(27A)	0.15323	-0.03105	-0.15402	2.5457	-0.3226	-2.7954	1	1	1	3.544 -
-	H(28A)	0.15251	-0.25437	-0.18043	2.5336	-2.6429	-3.2748	1	1	1	3.544 -
-	H(29A)	0.22606	-0.39420	-0.10658	3.7556	-4.0958	-1.9345	1	1	1	3.544 -
-	H(30A)	0.28561	-0.31725	-0.00063	4.7448	-3.2963	-0.0115	1	1	1	3.544 -
-	H(32A)	0.24371	0.11874	0.06653	4.0487	1.2337	1.2074	1	1	1	3.544 -
-	H(32B)	0.33407	0.12192	0.03619	5.5499	1.2668	0.6569	1	1	1	3.544 -
-	H(33A)	0.38542	0.12217	0.15614	6.4030	1.2693	2.8339	1	1	1	3.544 -
-	H(33B)	0.29720	0.10242	0.18983	4.9373	1.0642	3.4454	1	1	1	3.544 -
-	H(34A)	0.18555	0.49036	0.12403	3.0826	5.0949	2.2511	1	1	1	3.544 -
-	H(35A)	0.28147	0.63253	0.16005	4.6760	6.5721	2.9048	1	1	1	3.544 -
-	H(36A)	0.40656	0.54978	0.19656	6.7542	5.7122	3.5676	1	1	1	3.544 -
-	H(37A)	0.42714	0.33006	0.18928	7.0961	3.4293	3.4354	1	1	1	3.544 -

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	N	O	P
1	1	0.074	0.029	0.389	307.31	1	4	19	18	1	1	1
2	1	0.327	0.015	0.062	307.31	1	4	19	18	1	1	1
				Unit Cell Weight =	2458.51			152	144	8	8	8
				Calculated Analysis (Percent) =				74.3	5.9	4.6	5.2	10.1

Moiety_Formula = C19 H18 N O P

Sum_Formula = C19 H18 N O P

Formula_Weight = 307.31 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 8

SpaceGroup_Z = 4 ===> Z' = 8 / 4 = 2.000

Calculated Density = 1.3031(2) g cm-3 [= Mg m-3]

F(000) = 1296.0 [1297.27]

mu(MoKa) = 1.77 cm-1 = 0.177 mm-1

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

Resonant Scattering = 0.41 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 3261.3[3230.9] 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"

Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6

van der Waals (or ion) Radii used in the Analysis

C	H	N	O	P
1.70	1.20	1.55	1.52	1.80

:: Grid: Y-Axis Step = 0.0208 = Points 48, Angstrom Step = 0.22
:: Grid: X-Axis Step = 0.0119 = Points 84, Angstrom Step = 0.20
:: Grid: Z-Axis Step = 0.0104 = Points 96, Angstrom Step = 0.19

:: Unit cell Contains NO Residual Solvent Accessible Void.

 :: Note: use CALC VOID (not CALC SOLV) for Packing Index.

:: SQUEEZE xyz on :char278a.sqz
:: SQUEEZE CIF on :char278a.sqf