Supporting Information

Fabrication of Anion Complexes from 5,6-Dihydrodiindolo[3,2-a:2',3'-c]phenazine as a Building Block

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X-Ray Crystallographic Studies of Complexes

Single crystals of **DIPZ**·EtOAc were obtained by slow evaporation of a solution of **DIPZ** in EtOAc/MeCN at room temperature. Single crystals of **DIPZ**·TBAF, **DIPZ**·TBABr, **DIPZ**·TBAOAc, **DIPZ**·TBABzO, **DIPZ**·$TBANO_3$**,** **DIPZ**·$TBAHSO_4$ and **DIPZ**·$TBAH_2PO_4$ complexes were obtained by slow evaporation of a solution of **DIPZ** in EtOAc/MeCN in the presence of slight excess corresponding anions at room temperature within several days. Single crystals of **DIPZ**·$(TBA)_2SiF_6$ complex were obtained by slow diffusion of n-hexane into a chloroform solution of **DIPZ** and fluoride anion at room temperature. The X-ray single crystal diffraction data for them were collected on a Rigaku MicroMAX007 with Mo Kα radiation (λ = 0.71073 Å) in the ω-2θ scanning mode. The structures were solved by direct methods using the SHELXS-97 program and refined by full-matrix least-squares techniques (SHELXL-97) on F^2 (Sheldrick, G. M. *SHELXS97*, *A Program for Crystal Structure Solution*; University of Göttingen: Germany, 1997; Sheldrick, G. M. *SHELXL97*, *A Program for Crystal Structure Refinement*; University of Göttingen: Germany, 1997). Anisotropic thermal parameters were assigned to all non-hydrogen atoms.. Details of crystal data, data collections, and structure refinements are summarized in Tables S1 to S9. The structures of **DIPZ**·$TBANO_3$ and **DIPZ**·$TBAH_2PO_4$ complexes are reported as partial determinations. Restraints are made to fix the bonds at proper

length, including the N-H bond in indole group and the bonds in the disorder of tetrabutylammonium.

Table S1. Crystal data and structure refinement for **DIPZ**·EtOAc

Empirical formula	$C_{28}H_{22}N_4O_2$	
Formula weight	446.50	
Temperature	113(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P-1	
Unit cell dimensions	a = 7.9968(16) Å	α = 74.18(3)°
	b = 11.764(2) Å	β= 88.87(3)°
	c = 11.929(2) Å	γ = 89.89(3)°
Volume	1079.5(4) $Å^3$	
Z, Calculated density	2, 1.374 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	468	
Crystal size	0.18 × 0.16 × 0.08 mm	
Theta range for data collection	1.77 to 25.02°	
Limiting indices	-9<=h<=5, -14<=k<=14, -13<=l<=14	
Reflections collected / unique	6832 / 3779 [R (int) = 0.0612]	
Completeness to theta = 25.02	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9929 and 0.9842	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3779 / 2 / 317	
Goodness-of-fit on F^2	0.971	
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1147	
R indices (all data)	R1 = 0.0969, wR2 = 0.1328	
Largest diff. peak and hole	0.191 and -0.232 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for **DIPZ**·TBAF

Empirical formula	$C_{40}\ H_{50}\ F\ N_5$	
Formula weight	619.85	
Temperature	113(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, Cc	
Unit cell dimensions	a = 22.428(6) Å	α = 90°
	b = 8.4214(17) Å	β = 113.21(3)°
	c= 19.787(8) Å	γ = 90°
Volume	3434.8(18) $Å^3$	
Z, Calculated density	4, 1.199 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	1336	
Crystal size	0.26 × 0.18 × 0.10 mm	
Theta range for data collection	2.24 to 25.02°	
Limiting indices	-26<=h<=26, -6<=k<=10, -23<=l<=23	
Reflections collected / unique	11141 / 5863 [R (int) = 0.1137]	
Completeness to theta = 25.02	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9926 and 0.9809	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5863 / 4 / 427	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	R1 = 0.0626, wR2 = 0.1297	
R indices (all data)	R1 = 0.0972, wR2 = 0.1400	
Largest diff. peak and hole	0.595 and -0.205 e.$Å^{-3}$	

Table S3 Crystal data and structure refinement for **DIPZ**·TBABr

Empirical formula	$C_{40}\ H_{50}\ Br\ N_5$
Formula weight	680.76
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 13.188(3) Å α = 90°
	b = 14.799(3) Å β = 90°
	c = 18.574(4) Å γ = 90°
Volume	3625.2(13) $Å^3$
Z, Calculated density	4, 1.247 Mg/m^3
Absorption coefficient	1.168 mm^{-1}
F(000)	1440
Crystal size	0.18 × 0.12 × 0.10 mm
Theta range for data collection	3.02 to 25.02°
Limiting indices	-10<=h<=15, -17<=k<=17, -20<=l<=21
Reflections collected / unique	22179 / 6360 [R (int) = 0.1426]
Completeness to theta = 25.02	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8925 and 0.8179
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6360 / 312 / 515
Goodness-of-fit on F^2	0.986
Final R indices [I>2sigma(I)]	R1 = 0.0752, wR2 = 0.1594
R indices (all data)	R1 = 0.1193, wR2 = 0.1833
Largest diff. peak and hole	0.601 and -0.653 $e.Å^{-3}$

Table S4 Crystal data and structure refinement for **DIPZ**·TBAAcO

Empirical formula	$C_{42}\ H_{53}\ N_5\ O_2$
Formula weight	659.89
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 21.802(4) Å α = 90°
	b = 8.4417(17) Å β = 118.82(3)°
	c = 22.560(5) Å γ = 90°
Volume	3637.9(13) $Å^3$
Z, Calculated density	4, 1.205 Mg/m^3
Absorption coefficient	0.075 mm^{-1}
F(000)	1424
Crystal size	0.28 × 0.22 × 0.12 mm
Theta range for data collection	3.01 to 25.01°
Limiting indices	-24<=h<=25, -9<=k<=10, -26<=l<=24
Reflections collected / unique	23862 / 6398 [R (int) = 0.0485]
Completeness to theta = 25.01	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9911 and 0.9794
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6398 / 2 / 455
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0521, wR2 = 0.1266
R indices (all data)	R1 = 0.0715, wR2 = 0.1389
Largest diff. peak and hole	0.170 and -0.262 $e.Å^{-3}$

Table S5 Crystal data and structure refinement for **DIPZ**·TBABzO

Empirical formula	$C_{51}\ H_{63}\ N_5\ O_4$
Formula weight	810.08
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 13.965(3) Å α = 90°
	b = 20.364(4) Å β = 94.42(3)°
	c = 15.881(3) Å γ = 90°
Volume	4502.8(16) $Å^3$
Z, Calculated density	4, 1.192 Mg/m^3
Absorption coefficient	0.076 mm^{-1}
F(000)	1736
Crystal size	0.16 × 0.12 × 0.06 mm
Theta range for data collection	1.63 to 25.02°
Limiting indices	-16<=h<=15, -24<=k<=24, -16<=l<=18
Reflections collected / unique	30429 / 7943 [R (int) = 0.1483]
Completeness to theta = 25.02	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9955 and 0.9880
Refinement method	Full-matrix least-squares on F F^2
Data / restraints / parameters	7943 / 266 / 613
Goodness-of-fit on F^2	1.002
Final R indices [I>2sigma(I)]	R1 = 0.0969, wR2 = 0.2470
R indices (all data)	R1 = 0.1777, wR2 = 0.2948
Largest diff. peak and hole	0.455 and -0.582 e.$Å^{-3}$

Table S6 Crystal data and structure refinement for partially determined structure **DIPZ**·$TBANO_3$

Empirical formula	$C_{40}\ H_{50}\ N_6\ O_3$	
Formula weight	662.86	
Temperature	113(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Tetragonal, P4(1)	
Unit cell dimensions	a = 11.2848(16) Å	$\alpha = 90^\circ$
	b = 11.2848(16) Å	$\beta = 90^\circ$
	c = 27.542(6) Å	$\gamma = 90^\circ$

Table S7 Crystal data and structure refinement for **DIPZ**·$TBAHSO_4$

Empirical formula	$C_{40}\ H_{51}\ N_5\ O_4\ S$	
Formula weight	697.92	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, C2/c	
Unit cell dimensions	a = 41.692(8) Å	α = 90°
	b = 8.3351(17) Å	β = 95.70(3)°
	c = 22.227(4) Å	γ = 90°
Volume	7686(3) $Å^3$	
Z, Calculated density	8, 1.206 Mg/m^3	
Absorption coefficient	0.130 mm^{-1}	
F(000)	2992	
Crystal size	0.20 × 0.16 × 0.10 mm	
Theta range for data collection	3.04 to 25.02°	
Limiting indices	-49<=h<=49, -9<=k<=9, -23<=l<=26	
Reflections collected / unique	29260 / 6768 [R (int) = 0.0503]	
Completeness to theta = 25.02	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9871 and 0.9744	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6768 / 3 / 516	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0686, wR2 = 0.1930	
R indices (all data)	R1 = 0.1007, wR2 = 0.2171	
Largest diff. peak and hole	0.739 and -0.426 e.$Å^{-3}$	

Table S8 Crystal data and structure refinement for partially determined structure **DIPZ**·$TBAH_2PO_4$

Empirical formula	$C_{117}\ H_{139.50}\ N_{17}\ O_{10}\ P_{2.50}$	
Formula weight	2021.38	
Temperature	113(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P1	
Unit cell dimensions	a = 17.937(4) Å	α= 84.16(3)°
	b = 17.994(4) Å	β = 67.95(3)°
	c = 20.503(4) Å	γ = 63.22(3)°

Table S9 Crystal data and structure refinement for **DIPZ**·$(TBA)_2SiF_6$

Empirical formula	$C_{80}\ H_{100}\ F_6\ N_{10}\ Si$
Formula weight	1343.79
Temperature	294(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 9.5475(19) Å $\alpha = 90^\circ$
	b = 21.996(5) Å $\beta = 96.892(4)^\circ$
	c = 17.778(4) Å $\gamma = 90^\circ$
Volume	3706.5(13) $Å^3$
Z, Calculated density	2, 1.204 Mg/m^3
Absorption coefficient	0.097 mm^{-1}
F(000)	1436
Crystal size	0.22 × 0.18 × 0.16 mm
Theta range for data collection	1.48 to 25.02°
Limiting indices	-11<=h<=10, -26<=k<=26, -9<=l<=21
Reflections collected / unique	18786 / 6538 [R (int) = 0.0536]
Completeness to theta = 25.02	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9846 and 0.9790
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6538 / 2 / 451
Goodness-of-fit on F^2	1.003
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1108
R indices (all data)	R1 = 0.1230, wR2 = 0.1446
Largest diff. peak and hole	0.227 and -0.267 $e.Å^{-3}$

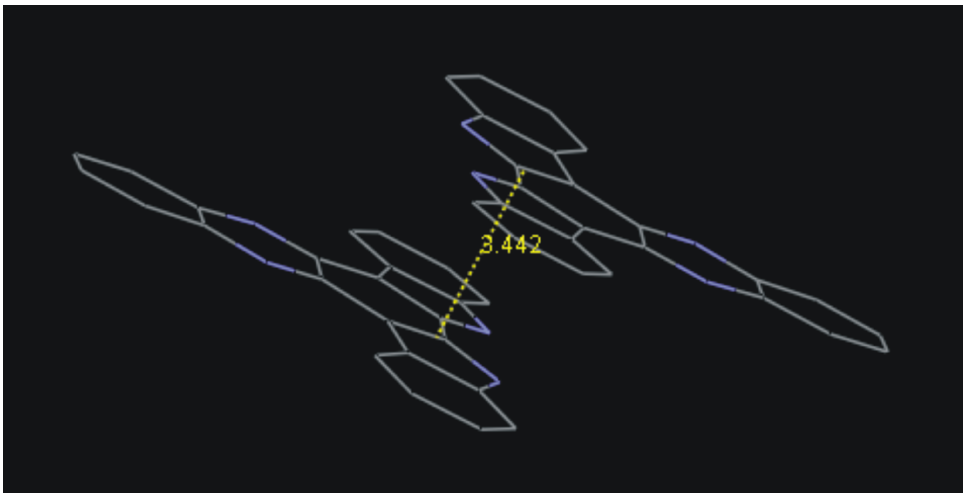

Fig. S1. View of the π–π stacking in **DIPZ**·EtOAc. Hydrogen atoms and solvent molecules have been removed for clarity. Dashed yellow line indicates the vertical distance of the two **DIPZ** planes at the side of indolocarbazole moiety.

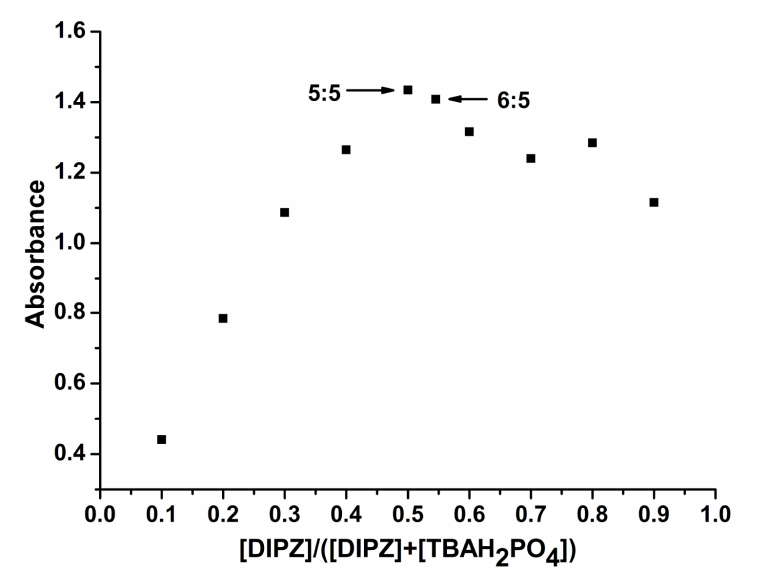

Fig. S2. Job's plot for receptor **DIPZ** with dihydrogen phosphate anion, indicating 1:1 binding stoichimetry in solution. [**DIPZ**] + [$TBAH_2PO_4$] = 1.5 × 10^{-4} M.

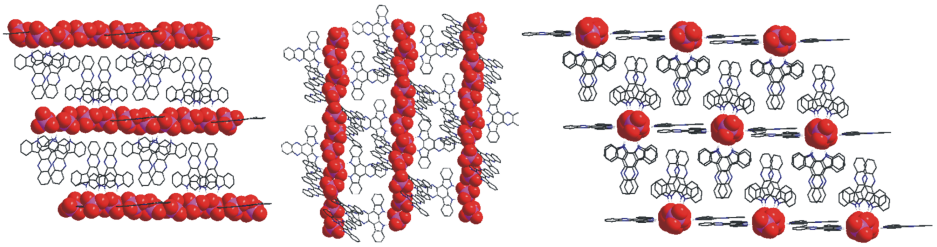

Fig. S3. View showing the infinite phosphate chains viewed along from *a* (left), *b* (middle) and *c* (left) axises. Non-acidic hydrogen atoms, counter cations and free solvent molecules have been removed for clarity.

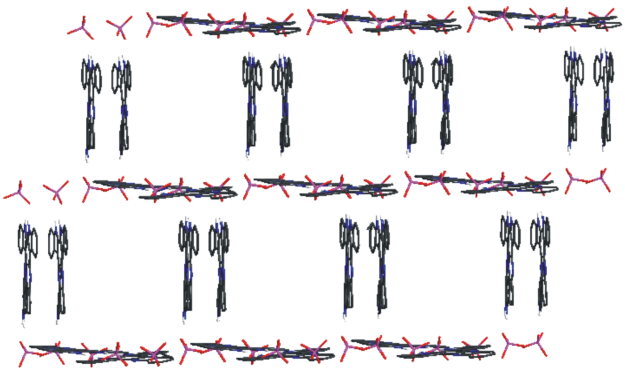

Fig. S4. View showing the cationic channels. Non-acidic hydrogen atoms, counter cations and free solvent molecules have been removed for clarity.

Anion Binding Study

Stock solutions of the host receptor **DIPZ** being studied were made up in MeCN with the final concentrations being 1.5×10^{-5} M. Stock solution of guest was prepared by dissolving 200, 400 and 800 equivalents of the TBAF, TBACl, TBABr,·TBAAcO, $TBANO_3$, $TBAH_2PO_4$ and $TBAHSO_4$ in 5 mL of a stock solution of the host, respectively. Making up the anion source solutions in this way allowed the binding studies to be carried out without having to make mathematical corrections to account for changes in host concentration as the result of dilution effects. The general procedure for the fluorescence studies involved making sequential additions of titrant (anionic guest) using Hamilton pipettes to a 2 mL aliquot of the host stock solution in the spectrometric cell.

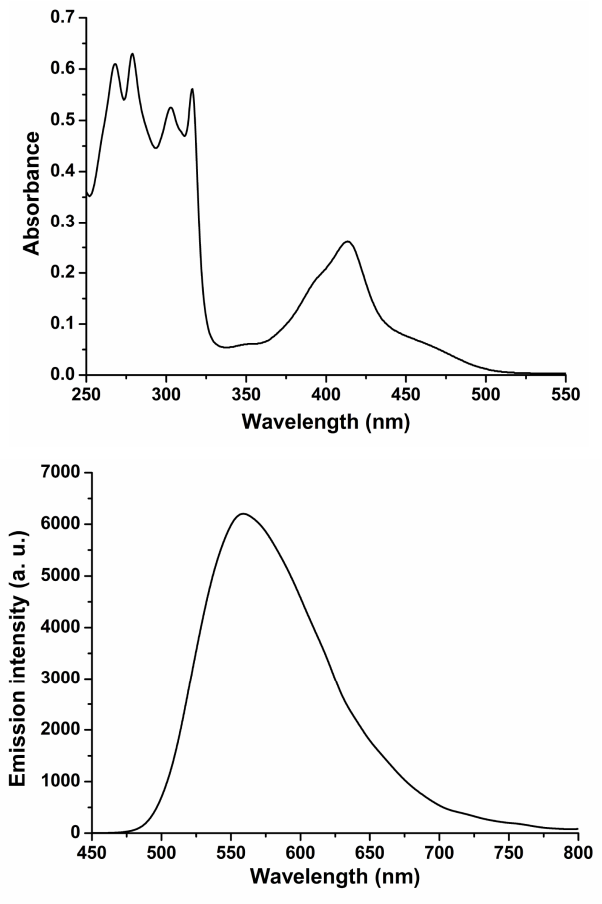

Fig. S5. UV-vis and fluorescence (λ_{exe} = 413 nm and λ_{em} = 560 nm) spectra of receptor **DIPZ** (1.5×10^{-5} M) in MeCN.

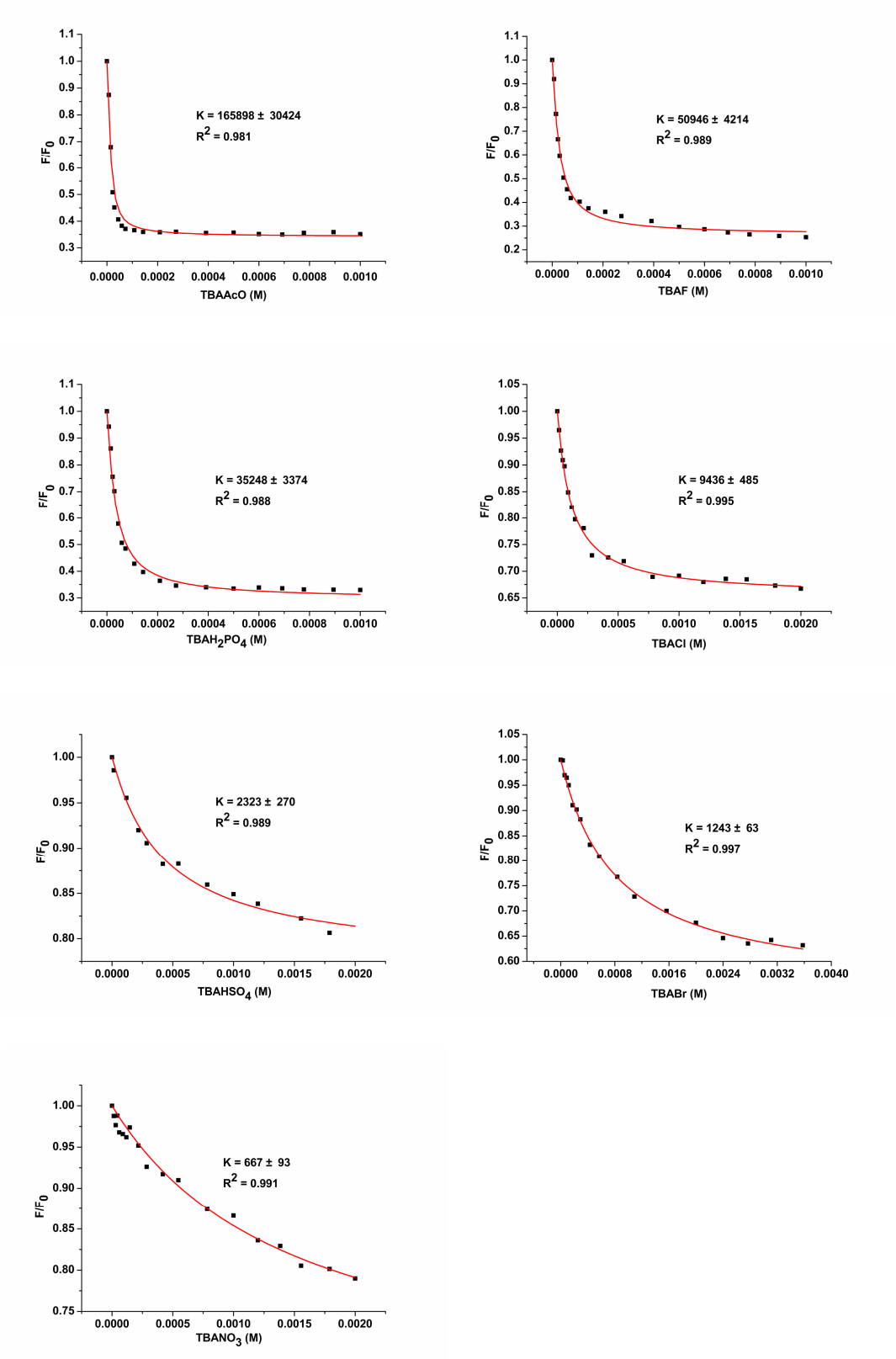

Fig. S6. Association constants of various anions determined by fluorescence titration.

Partially determined cif for **DIPZ**·$TBANO_3$

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and
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C4 C 0.2082(4) 0.8087(4) 0.36316(16) 0.0631(10) Uani 1 1 d U . .
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C5 C 0.2988(4) 0.7226(4) 0.36024(15) 0.0638(10) Uani 1 1 d U . .
H5 H 0.3284 0.6892 0.3886 0.077 Uiso 1 1 calc R . .
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C6 C 0.3438(3) 0.6873(4) 0.31627(13) 0.0478(9) Uani 1 1 d U . .
H6 H 0.4086 0.6364 0.3150 0.057 Uiso 1 1 calc R . .
C7 C 0.2933(3) 0.7270(3) 0.27500(12) 0.0376(7) Uani 1 1 d U . .
C8 C 0.3093(3) 0.7023(3) 0.22351(11) 0.0289(7) Uani 1 1 d U . .
C9 C 0.3899(2) 0.6231(3) 0.19892(12) 0.0282(7) Uani 1 1 d U . .
C10 C 0.5405(3) 0.4835(3) 0.19820(12) 0.0321(7) Uani 1 1 d U . .
C11 C 0.6250(3) 0.4226(3) 0.22176(13) 0.0416(8) Uani 1 1 d U . .
H11 H 0.6398 0.4384 0.2544 0.050 Uiso 1 1 calc R . .
C12 C 0.6894(3) 0.3380(3) 0.19837(14) 0.0398(8) Uani 1 1 d U . .
H12 H 0.7477 0.2963 0.2150 0.048 Uiso 1 1 calc R . .
C13 C 0.6672(3) 0.3135(3) 0.14821(13) 0.0375(8) Uani 1 1 d U . .
H13 H 0.7123 0.2577 0.1316 0.045 Uiso 1 1 calc R . .
C14 C 0.5802(3) 0.3724(3) 0.12578(13) 0.0378(8) Uani 1 1 d U . .
H14 H 0.5618 0.3514 0.0940 0.045 Uiso 1 1 calc R . .
C15 C 0.5143(2) 0.4655(2) 0.14780(12) 0.0246(7) Uani 1 1 d U . .
C16 C 0.3737(3) 0.6153(3) 0.14718(12) 0.0295(7) Uani 1 1 d U . .
C17 C 0.2955(3) 0.6892(3) 0.12194(11) 0.0292(7) Uani 1 1 d U . .
C18 C 0.2620(3) 0.7033(3) 0.07119(13) 0.0390(8) Uani 1 1 d U . .
C19 C 0.3126(4) 0.6563(3) 0.02795(14) 0.0535(9) Uani 1 1 d U . .
H19 H 0.3768 0.6047 0.0292 0.064 Uiso 1 1 calc R . .
C20 C 0.2643(4) 0.6891(4) -0.01498(19) 0.0752(11) Uani 1 1 d U . .
H20 H 0.2871 0.6509 -0.0434 0.090 Uiso 1 1 calc R . .
C21 C 0.1749(4) 0.7859(4) -0.01685(19) 0.0768(11) Uani 1 1 d U . .
H21 H 0.1393 0.8068 -0.0461 0.092 Uiso 1 1 calc R . .
C22 C 0.1471(4) 0.8414(4) 0.02372(17) 0.0644(10) Uani 1 1 d U . .
H22 H 0.0992 0.9083 0.0220 0.077 Uiso 1 1 calc R . .
C23 C 0.1866(3) 0.8038(3) 0.06918(13) 0.0451(8) Uani 1 1 d U . .
C24 C 0.2303(2) 0.7651(2) 0.14808(11) 0.0272(7) Uani 1 1 d U . .
C25 C 1.0631(5) 0.4339(3) 0.00130(13) 0.0691(11) Uani 0.50 1 d PDU A 1
H25A H 1.0437 0.3761 -0.0235 0.083 Uiso 0.50 1 calc PR A 1
H25B H 1.1487 0.4383 0.0037 0.083 Uiso 0.50 1 calc PR A 1
C26 C 1.0138(6) 0.5560(4) -0.01365(11) 0.0670(12) Uani 0.50 1 d PDU A 1
H26A H 1.0499 0.6178 0.0059 0.080 Uiso 0.50 1 calc PR A 1
H26B H 0.9288 0.5585 -0.0086 0.080 Uiso 0.50 1 calc PR A 1
C27 C 1.0429(5) 0.5756(4) -0.06778(11) 0.0702(13) Uani 0.50 1 d PDU A 1
H27A H 1.0353 0.6590 -0.0758 0.084 Uiso 0.50 1 calc PR A 1
H27B H 1.1238 0.5514 -0.0743 0.084 Uiso 0.50 1 calc PR A 1
C28 C 0.9575(5) 0.5029(6) -0.09882(15) 0.0751(18) Uani 0.50 1 d PDU A 1
H28A H 0.9739 0.5167 -0.1326 0.113 Uiso 0.50 1 calc PR A 1
H28B H 0.8775 0.5260 -0.0917 0.113 Uiso 0.50 1 calc PR A 1
H28C H 0.9676 0.4202 -0.0917 0.113 Uiso 0.50 1 calc PR A 1
C29 C 0.9349(5) 0.4264(3) 0.09138(14) 0.0771(11) Uani 0.50 1 d PDU A 1
H29A H 0.9437 0.3701 0.1178 0.093 Uiso 0.50 1 calc PR A 1
H29B H 0.8522 0.4293 0.0818 0.093 Uiso 0.50 1 calc PR A 1
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C30 C 0.9795(6) 0.5491(4) 0.10623(11) 0.0724(11) Uani 0.50 1 d PDU A 1
H30A H 1.0650 0.5524 0.1028 0.087 Uiso 0.50 1 calc PR A 1
H30B H 0.9452 0.6087 0.0851 0.087 Uiso 0.50 1 calc PR A 1
C31 C 0.9456(5) 0.5753(4) 0.15874(11) 0.0799(16) Uani 0.50 1 d PDU A 1
H31A H 0.8645 0.5502 0.1644 0.096 Uiso 0.50 1 calc PR A 1
H31B H 0.9501 0.6599 0.1645 0.096 Uiso 0.50 1 calc PR A 1
C32 C 1.0283(5) 0.5106(6) 0.19383(14) 0.0824(18) Uani 0.50 1 d PDU A 1
H32A H 1.0059 0.5285 0.2266 0.124 Uiso 0.50 1 calc PR A 1
H32B H 1.1084 0.5360 0.1884 0.124 Uiso 0.50 1 calc PR A 1
H32C H 1.0226 0.4267 0.1885 0.124 Uiso 0.50 1 calc PR A 1
C33 C 0.8985(3) 0.3308(5) 0.04216(17) 0.1152(13) Uani 0.50 1 d PDU A 1
H33A H 0.8412 0.3786 0.0597 0.138 Uiso 0.50 1 calc PR A 1
H33B H 0.9069 0.2585 0.0609 0.138 Uiso 0.50 1 calc PR A 1
C34 C 0.8332(3) 0.2924(5) -0.00384(12) 0.1212(11) Uani 0.50 1 d PDU A 1
H34A H 0.8242 0.3597 -0.0255 0.145 Uiso 0.50 1 calc PR A 1
H34B H 0.8788 0.2322 -0.0206 0.145 Uiso 0.50 1 calc PR A 1
C35 C 0.7112(3) 0.2432(6) 0.00933(14) 0.1269(14) Uani 0.50 1 d PDU A 1
H35A H 0.6914 0.1780 -0.0122 0.152 Uiso 0.50 1 calc PR A 1
H35B H 0.6517 0.3045 0.0054 0.152 Uiso 0.50 1 calc PR A 1
C36 C 0.7121(5) 0.1998(6) 0.06218(13) 0.155(2) Uani 0.50 1 d PDU A 1
H36A H 0.6353 0.1693 0.0704 0.233 Uiso 0.50 1 calc PR A 1
H36B H 0.7313 0.2646 0.0833 0.233 Uiso 0.50 1 calc PR A 1
H36C H 0.7702 0.1383 0.0658 0.233 Uiso 0.50 1 calc PR A 1
C37 C 1.0623(3) 0.2707(4) 0.05459(16) 0.0848(12) Uani 0.50 1 d PDU A 1
H37A H 1.1122 0.2473 0.0276 0.102 Uiso 0.50 1 calc PR A 1
H37B H 1.0015 0.2116 0.0603 0.102 Uiso 0.50 1 calc PR A 1
C38 C 1.1338(3) 0.3014(5) 0.10086(17) 0.0814(12) Uani 0.50 1 d PDU A 1
H38A H 1.1198 0.3830 0.1103 0.098 Uiso 0.50 1 calc PR A 1
H38B H 1.1104 0.2502 0.1275 0.098 Uiso 0.50 1 calc PR A 1
C39 C 1.2655(3) 0.2824(4) 0.0884(3) 0.0796(12) Uani 0.50 1 d PDU A 1
H39A H 1.3152 0.3163 0.1136 0.096 Uiso 0.50 1 calc PR A 1
H39B H 1.2845 0.3207 0.0579 0.096 Uiso 0.50 1 calc PR A 1
C40 C 1.2878(5) 0.1476(3) 0.0845(3) 0.0679(17) Uani 0.50 1 d PDU A 1
H40A H 1.3693 0.1337 0.0764 0.102 Uiso 0.50 1 calc PR A 1
H40B H 1.2378 0.1148 0.0598 0.102 Uiso 0.50 1 calc PR A 1
H40C H 1.2701 0.1107 0.1151 0.102 Uiso 0.50 1 calc PR A 1
C25' C 0.9667(6) 0.4686(5) 0.00684(10) 0.0678(12) Uani 0.50 1 d PDU A 2
H25C H 1.0002 0.5474 0.0097 0.081 Uiso 0.50 1 calc PR A 2
H25D H 0.8815 0.4761 0.0103 0.081 Uiso 0.50 1 calc PR A 2
C26' C 0.9929(6) 0.4225(5) -0.04480(10) 0.0688(12) Uani 0.50 1 d PDU A 2
H26C H 1.0778 0.4195 -0.0500 0.083 Uiso 0.50 1 calc PR A 2
H26D H 0.9616 0.3429 -0.0484 0.083 Uiso 0.50 1 calc PR A 2

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C27' C 0.9359(6) 0.5042(5) -0.08234(10) 0.0771(13) Uani 0.50 1 d PDU A
2
H27C H 0.9697 0.5830 -0.0798 0.093 Uiso 0.50 1 calc PR A 2
H27D H 0.8514 0.5100 -0.0763 0.093 Uiso 0.50 1 calc PR A 2
C28' C 0.9578(9) 0.4544(7) -0.13373(11) 0.083(2) Uani 0.50 1 d PDU A 2
H28D H 0.9351 0.5124 -0.1575 0.125 Uiso 0.50 1 calc PR A 2
H28E H 0.9115 0.3838 -0.1382 0.125 Uiso 0.50 1 calc PR A 2
H28F H 1.0403 0.4359 -0.1375 0.125 Uiso 0.50 1 calc PR A 2
C29' C 1.0481(6) 0.4751(5) 0.09037(10) 0.0682(12) Uani 0.50 1 d PDU A 2
H29C H 1.0218 0.5549 0.0829 0.082 Uiso 0.50 1 calc PR A 2
H29D H 1.1339 0.4767 0.0927 0.082 Uiso 0.50 1 calc PR A 2
C30' C 0.9970(5) 0.4387(6) 0.13959(13) 0.0736(11) Uani 0.50 1 d PDU A 2
H30C H 0.9974 0.3531 0.1424 0.088 Uiso 0.50 1 calc PR A 2
H30D H 0.9157 0.4659 0.1422 0.088 Uiso 0.50 1 calc PR A 2
C31' C 1.0718(6) 0.4934(6) 0.18069(10) 0.0825(15) Uani 0.50 1 d PDU A 2
H31C H 1.0595 0.5785 0.1812 0.099 Uiso 0.50 1 calc PR A 2
H31D H 1.1551 0.4790 0.1742 0.099 Uiso 0.50 1 calc PR A 2
C32' C 1.0396(8) 0.4415(7) 0.23106(17) 0.086(2) Uani 0.50 1 d PDU A 2
H32D H 1.0911 0.4746 0.2553 0.129 Uiso 0.50 1 calc PR A 2
H32E H 1.0489 0.3570 0.2304 0.129 Uiso 0.50 1 calc PR A 2
H32F H 0.9589 0.4608 0.2387 0.129 Uiso 0.50 1 calc PR A 2
C33' C 0.8840(3) 0.3710(3) 0.0478(2) 0.1015(13) Uani 0.50 1 d PDU A 2
H33C H 0.8429 0.4288 0.0279 0.122 Uiso 0.50 1 calc PR A 2
H33D H 0.8500 0.3705 0.0801 0.122 Uiso 0.50 1 calc PR A 2
C34' C 0.8812(3) 0.2458(4) 0.0244(3) 0.1156(11) Uani 0.50 1 d PDU A 2
H34C H 0.9089 0.1866 0.0472 0.139 Uiso 0.50 1 calc PR A 2
H34D H 0.9313 0.2434 -0.0042 0.139 Uiso 0.50 1 calc PR A 2
C35' C 0.7493(3) 0.2223(3) 0.0104(3) 0.1260(12) Uani 0.50 1 d PDU A 2
H35C H 0.7429 0.2024 -0.0237 0.151 Uiso 0.50 1 calc PR A 2
H35D H 0.7175 0.1572 0.0294 0.151 Uiso 0.50 1 calc PR A 2
C36' C 0.6810(4) 0.3378(4) 0.0214(5) 0.144(2) Uani 0.50 1 d PDU A 2
H36D H 0.6000 0.3293 0.0113 0.216 Uiso 0.50 1 calc PR A 2
H36E H 0.7169 0.4024 0.0042 0.216 Uiso 0.50 1 calc PR A 2
H36F H 0.6835 0.3534 0.0557 0.216 Uiso 0.50 1 calc PR A 2
C37' C 1.1379(3) 0.3598(4) 0.03988(16) 0.0812(12) Uani 0.50 1 d PDU A 2
H37C H 1.1931 0.4245 0.0451 0.097 Uiso 0.50 1 calc PR A 2
H37D H 1.1498 0.3251 0.0080 0.097 Uiso 0.50 1 calc PR A 2
C38' C 1.1401(3) 0.2684(4) 0.08070(19) 0.0845(10) Uani 0.50 1 d PDU A 2
H38C H 1.0879 0.2029 0.0727 0.101 Uiso 0.50 1 calc PR A 2
H38D H 1.1121 0.3042 0.1106 0.101 Uiso 0.50 1 calc PR A 2
C39' C 1.2671(3) 0.2225(4) 0.08771(18) 0.0811(13) Uani 0.50 1 d PDU A 2
H39C H 1.3233 0.2853 0.0808 0.097 Uiso 0.50 1 calc PR A 2
H39D H 1.2783 0.1972 0.1211 0.097 Uiso 0.50 1 calc PR A 2
C40' C 1.2880(5) 0.1179(4) 0.0532(2) 0.0707(18) Uani 0.50 1 d PDU A 2
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H40D H 1.3678 0.0900 0.0568 0.106 Uiso 0.50 1 calc PR A 2
H40E H 1.2754 0.1431 0.0203 0.106 Uiso 0.50 1 calc PR A 2
H40F H 1.2338 0.0551 0.0609 0.106 Uiso 0.50 1 calc PR A 2
N1 N 0.1638(2) 0.8429(3) 0.23277(10) 0.0384(8) Uani 1 1 d . . .
H1 H 0.1105 0.8951 0.2264 0.046 Uiso 1 1 calc R . .
N2 N 0.4693(2) 0.5669(2) 0.22476(11) 0.0363(8) Uani 1 1 d . . .
N3 N 0.4382(2) 0.5297(2) 0.12279(10) 0.0354(7) Uani 1 1 d . . .
N4 N 0.1617(2) 0.8367(2) 0.11642(10) 0.0369(8) Uani 1 1 d . . .
H4A H 0.1130 0.8913 0.1251 0.044 Uiso 1 1 calc R . .
N5 N 0.0520(2) 0.0499(2) 0.92285(13) 0.0389(7) Uani 1 1 d . . .
N6 N 1.0129(2) 0.3938(2) 0.04907(9) 0.0884(13) Uani 1 1 d DU . .
O2 O -0.0217(2) 0.0412(2) 0.95971(11) 0.0565(9) Uani 1 1 d . . .
O3 O 0.0416(2) -0.0206(2) 0.88888(11) 0.0529(8) Uani 1 1 d . . .

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C2 0.0344(14) 0.0566(15) 0.0345(15) -0.0082(14) 0.0080(13) 0.0140(13)
C3 0.0613(16) 0.0722(16) 0.0382(16) -0.0147(15) 0.0024(14) 0.0402(14)
C4 0.0624(16) 0.0832(17) 0.0436(17) -0.0072(15) 0.0084(15) 0.0440(15)
C5 0.0605(17) 0.0922(19) 0.0387(17) -0.0045(16) 0.0053(15) 0.0381(15)
C6 0.0304(13) 0.0756(17) 0.0374(15) -0.0092(14) 0.0068(13) 0.0209(13)
C7 0.0268(12) 0.0522(14) 0.0337(14) -0.0076(13) 0.0074(11) 0.0118(12)
C8 0.0253(12) 0.0308(12) 0.0307(13) 0.0002(11) 0.0021(11) 0.0061(11)
C9 0.0247(12) 0.0290(13) 0.0307(13) -0.0027(11) -0.0015(11) 0.0049(10)
C10 0.0289(13) 0.0357(13) 0.0316(14) 0.0036(12) 0.0078(12) -0.0005(11)
C11 0.0397(15) 0.0488(15) 0.0364(15) 0.0076(13) 0.0041(13) 0.0014(13)
C12 0.0361(13) 0.0419(14) 0.0412(15) 0.0070(13) 0.0125(13) 0.0174(12)
C13 0.0291(13) 0.0401(14) 0.0433(15) 0.0009(13) 0.0047(12) 0.0095(12)
C14 0.0405(14) 0.0331(13) 0.0398(15) 0.0006(12) 0.0077(13) 0.0048(12)
C15 0.0177(11) 0.0248(12) 0.0312(13) -0.0002(11) -0.0015(11) 0.0027(10)
C16 0.0295(13) 0.0281(12) 0.0308(14) -0.0025(12) 0.0008(11) -0.0068(11)
C17 0.0350(12) 0.0264(12) 0.0262(13) -0.0019(11) 0.0106(11) -0.0034(11)
C18 0.0563(15) 0.0337(13) 0.0270(13) 0.0001(12) -0.0032(13) 0.0126(12)
C19 0.0734(17) 0.0498(15) 0.0373(16) 0.0005(14) -0.0074(15) 0.0312(14)
C20 0.093(2) 0.0818(19) 0.0513(18) -0.0053(17) 0.0022(18) 0.0266(17)
C21 0.0871(19) 0.089(2) 0.0544(18) 0.0089(17) -0.0140(17) 0.0331(17)
C22 0.0750(17) 0.0692(17) 0.0492(17) 0.0064(15) -0.0137(16) 0.0422(15)
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C23 0.0609(16) 0.0513(15) 0.0230(14) 0.0048(13) -0.0055(14) 0.0172(14)
C24 0.0265(12) 0.0256(12) 0.0296(13) -0.0007(12) 0.0031(11) -0.0053(11)
C25 0.0685(18) 0.0680(18) 0.0709(19) -0.0005(18) 0.0120(18) 0.0019(17)
C26 0.065(2) 0.064(2) 0.072(2) -0.0041(19) 0.0089(19) 0.0021(19)
C27 0.067(2) 0.073(2) 0.071(2) -0.002(2) -0.005(2) 0.008(2)
C28 0.084(3) 0.070(3) 0.071(3) -0.007(3) 0.001(3) 0.009(3)
C29 0.0767(19) 0.0755(19) 0.0792(19) 0.0019(18) 0.0070(18) -0.0069(18)
C30 0.0673(18) 0.0718(18) 0.0780(19) 0.0050(18) 0.0101(18) -0.0116(18)
C31 0.078(3) 0.080(3) 0.082(3) 0.009(3) 0.012(3) -0.009(2)
C32 0.082(3) 0.081(3) 0.085(3) -0.004(3) 0.005(3) -0.005(3)
C33 0.119(2) 0.117(2) 0.109(2) 0.006(2) 0.003(2) 0.002(2)
C34 0.1249(19) 0.1230(19) 0.1156(19) 0.0066(19) -0.0004(19) 0.0043(19)
C35 0.130(2) 0.129(2) 0.122(2) 0.008(2) 0.005(2) 0.012(2)
C36 0.153(4) 0.166(4) 0.148(4) 0.010(3) 0.004(3) -0.001(3)
C37 0.090(2) 0.080(2) 0.085(2) 0.002(2) 0.007(2) 0.001(2)
C38 0.084(2) 0.077(2) 0.083(2) -0.005(2) 0.008(2) -0.009(2)
C39 0.082(2) 0.077(2) 0.080(2) -0.0003(19) 0.0128(19) -0.0119(19)
C40 0.077(3) 0.053(3) 0.074(3) 0.006(3) 0.018(3) -0.002(3)
C25' 0.066(2) 0.067(2) 0.071(2) 0.0037(19) 0.0135(19) 0.0002(19)
C26' 0.067(2) 0.070(2) 0.070(2) 0.000(2) 0.0096(19) -0.0029(19)
C27' 0.080(2) 0.075(2) 0.075(2) -0.005(2) 0.004(2) 0.004(2)
C28' 0.088(3) 0.076(3) 0.086(3) 0.014(3) 0.000(3) -0.005(3)
C29' 0.068(2) 0.063(2) 0.073(2) -0.0035(19) 0.0066(19) -0.0063(19)
C30' 0.0712(19) 0.0728(19) 0.0770(19) -0.0024(18) 0.0094(18) -0.0058(18)
C31' 0.083(3) 0.078(3) 0.087(3) -0.004(2) 0.007(2) 0.002(2)
C32' 0.086(3) 0.085(3) 0.087(3) -0.008(3) 0.001(3) 0.016(3)
C33' 0.109(2) 0.097(2) 0.098(2) 0.002(2) 0.008(2) 0.001(2)
C34' 0.1201(19) 0.1175(19) 0.1092(19) 0.0046(19) 0.0054(19) 0.0040(19)
C35' 0.127(2) 0.132(2) 0.118(2) 0.006(2) 0.005(2) 0.006(2)
C36' 0.148(4) 0.145(4) 0.140(4) -0.006(3) 0.005(3) -0.004(3)
C37' 0.085(2) 0.075(2) 0.083(2) -0.006(2) 0.000(2) -0.001(2)
C38' 0.0861(17) 0.0810(17) 0.0866(17) -0.0022(17) 0.0093(17) -0.0075(17)
C39' 0.084(2) 0.081(2) 0.078(2) -0.002(2) 0.008(2) -0.011(2)
C40' 0.090(3) 0.058(3) 0.064(3) 0.016(3) -0.013(3) -0.010(3)
N1 0.0307(13) 0.0573(16) 0.0273(14) -0.0088(13) 0.0052(12) 0.0034(12)
N2 0.0197(12) 0.0456(15) 0.0434(17) -0.0062(13) -0.0026(12) 0.0031(11)
N3 0.0541(15) 0.0181(11) 0.0340(14) 0.0023(11) 0.0220(12) 0.0105(11)
N4 0.0498(15) 0.0238(12) 0.0373(16) 0.0102(11) -0.0081(13) 0.0202(11)
N5 0.0327(13) 0.0469(14) 0.0371(13) 0.0124(14) 0.0002(13) -0.0168(11)
N6 0.142(3) 0.0542(18) 0.069(2) 0.0115(19) 0.025(2) -0.002(2)
O2 0.0449(13) 0.0598(16) 0.0649(17) -0.0051(13) 0.0210(13) -0.0065(12)
O3 0.0341(12) 0.0551(14) 0.0696(19) -0.0087(14) -0.0122(12) -0.0161(11)

_geom_special_details

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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
;

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C2 C7 1.399(5) . ?
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C36 C35 H35B 110.0 . . ?
H35A C35 H35B 108.2 . . ?
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H36A C36 H36B 109.5 . . ?
C35 C36 H36C 109.7 . . ?
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H36B C36 H36C 109.5 . . ?
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C38 C37 H37A 112.9 . . ?
N6 C37 H37B 112.9 . . ?
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C37 C38 H38A 110.4 . . ?
C39 C38 H38B 110.4 . . ?
C37 C38 H38B 110.4 . . ?
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C39 C40 H40B 109.5 . . ?
H40A C40 H40B 109.5 . . ?
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C31' C32' H32F 109.5 . . ?
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Partially determined cif for **DIPZ**·$TBAH_2PO_4$

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'He-Fang Wang'
'Xiu-Ping Yan'
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_publ_contact_author_email       xpyan@nankai.edu.cn
_publ_contact_author_address
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Research Center for Analytical Science, College of Chemistry
Nankai University
94 Weijin Road, Tianjin 300071 (China)
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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and
is
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 not relevant to the choice of reflections for refinement.  R-factors
based
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R-
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N5 N 0.2795(6) 0.8640(6) 0.9249(6) 0.045(3) Uani 1 1 d . . .
H5 H 0.2694 0.9150 0.9180 0.053 Uiso 1 1 calc R . .
N6 N 0.4195(7) 0.5707(7) 0.9085(6) 0.044(3) Uani 1 1 d . . .
N7 N 0.5701(6) 0.5624(6) 0.7890(5) 0.036(2) Uani 1 1 d . . .
N8 N 0.4448(6) 0.8550(6) 0.7904(6) 0.039(2) Uani 1 1 d . . .
H8 H 0.4084 0.9074 0.8004 0.046 Uiso 1 1 calc R . .
N9 N 0.9953(6) 0.0952(6) 0.8469(5) 0.032(2) Uani 1 1 d . . .
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H9 H 1.0485 0.0868 0.8414 0.038 Uiso 1 1 calc R . .
N10 N 0.7023(6) 0.1225(6) 0.9429(5) 0.031(2) Uani 1 1 d . . .
N11 N 0.7010(5) 0.1185(5) 1.0837(5) 0.029(2) Uani 1 1 d . . .
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H12A H 1.0459 0.0887 0.9766 0.035 Uiso 1 1 calc R . .
N13 N 0.5027(6) 0.0560(7) 0.5005(5) 0.035(2) Uani 1 1 d . . .
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N17 N 0.4588(6) 0.8566(7) -0.0257(7) 0.048(3) Uani 1 1 d . . .
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N20 N 0.2981(6) 0.8492(6) 0.1064(6) 0.039(2) Uani 1 1 d . . .
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N21 N 0.2118(6) 0.3270(7) 0.4124(6) 0.040(2) Uani 1 1 d . . .
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N22 N 0.0935(6) 0.6164(6) 0.4379(5) 0.034(2) Uani 1 1 d . . .
N23 N -0.0448(7) 0.6241(6) 0.5719(6) 0.043(3) Uani 1 1 d . . .
N24 N 0.0629(6) 0.3327(6) 0.5582(6) 0.041(2) Uani 1 1 d . . .
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C2 C -0.0600(8) 0.2752(8) 0.4902(7) 0.045(3) Uani 1 1 d . . .
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C3 C -0.1352(12) 0.3118(13) 0.5500(9) 0.071(5) Uani 1 1 d . . .
H3 H -0.1552 0.2778 0.5817 0.085 Uiso 1 1 calc R . .
C4 C -0.1836(9) 0.3999(10) 0.5651(7) 0.049(3) Uani 1 1 d . . .
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H5A H -0.1908 0.5116 0.5279 0.055 Uiso 1 1 calc R . .
C6 C -0.0841(8) 0.4186(8) 0.4572(6) 0.038(3) Uani 1 1 d . . .
C7 C -0.0358(7) 0.4518(7) 0.3969(6) 0.038(3) Uani 1 1 d . . .
C8 C -0.0463(7) 0.5323(7) 0.3787(6) 0.033(2) Uani 1 1 d . . .
C9 C -0.1231(8) 0.6746(8) 0.4057(6) 0.039(3) Uani 1 1 d . . .
C10 C -0.1967(9) 0.7494(8) 0.4513(8) 0.048(3) Uani 1 1 d . . .
H10 H -0.2389 0.7444 0.4927 0.058 Uiso 1 1 calc R . .
C11 C -0.2027(10) 0.8256(9) 0.4328(8) 0.056(4) Uani 1 1 d . . .
H11 H -0.2487 0.8723 0.4628 0.067 Uiso 1 1 calc R . .
C12 C -0.1431(8) 0.8369(8) 0.3709(7) 0.047(3) Uani 1 1 d . . .
H12 H -0.1485 0.8903 0.3610 0.057 Uiso 1 1 calc R . .
C13 C -0.0761(8) 0.7700(8) 0.3242(7) 0.046(3) Uani 1 1 d . . .
H13A H -0.0397 0.7783 0.2808 0.056 Uiso 1 1 calc R . .
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C14 C -0.0627(7) 0.6882(7) 0.3424(7) 0.036(3) Uani 1 1 d . . .
C15 C 0.0159(8) 0.5447(7) 0.3135(7) 0.036(3) Uani 1 1 d . . .
C16 C 0.0854(7) 0.4746(7) 0.2682(6) 0.029(2) Uani 1 1 d . . .
C17 C 0.1605(7) 0.4633(7) 0.2017(6) 0.033(2) Uani 1 1 d . . .
C18 C 0.1920(8) 0.5184(9) 0.1607(7) 0.043(3) Uani 1 1 d . . .
H18 H 0.1605 0.5758 0.1721 0.051 Uiso 1 1 calc R . .
C19 C 0.2725(9) 0.4830(9) 0.1023(7) 0.048(3) Uani 1 1 d . . .
H19 H 0.2971 0.5173 0.0761 0.057 Uiso 1 1 calc R . .
C20 C 0.3171(9) 0.3974(8) 0.0823(7) 0.046(3) Uani 1 1 d . . .
H20' H 0.3663 0.3770 0.0399 0.055 Uiso 1 1 calc R . .
C21 C 0.2895(8) 0.3426(8) 0.1241(7) 0.040(3) Uani 1 1 d . . .
H21 H 0.3228 0.2852 0.1126 0.048 Uiso 1 1 calc R . .
C22 C 0.2112(8) 0.3745(8) 0.1835(7) 0.040(3) Uani 1 1 d . . .
C23 C 0.0977(7) 0.3913(7) 0.2879(6) 0.036(3) Uani 1 1 d . . .
C24 C 0.0397(7) 0.3780(7) 0.3504(6) 0.036(3) Uani 1 1 d . . .
C25 C 0.2257(8) 0.8379(8) 0.9760(6) 0.041(3) Uani 1 1 d . . .
C26 C 0.1397(7) 0.8866(8) 1.0269(8) 0.051(4) Uani 1 1 d . . .
H26 H 0.1116 0.9444 1.0272 0.062 Uiso 1 1 calc R . .
C27 C 0.0994(9) 0.8451(9) 1.0758(8) 0.052(3) Uani 1 1 d . . .
H27 H 0.0452 0.8758 1.1123 0.062 Uiso 1 1 calc R . .
C28 C 0.1389(8) 0.7546(10) 1.0721(7) 0.052(4) Uani 1 1 d . . .
H28 H 0.1082 0.7279 1.1039 0.063 Uiso 1 1 calc R . .
C29 C 0.2215(8) 0.7087(8) 1.0214(7) 0.043(3) Uani 1 1 d . . .
H29 H 0.2471 0.6507 1.0190 0.052 Uiso 1 1 calc R . .
C30 C 0.2669(7) 0.7482(9) 0.9739(7) 0.042(3) Uani 1 1 d . . .
C31 C 0.3525(7) 0.7211(7) 0.9130(6) 0.034(2) Uani 1 1 d . . .
C32 C 0.4236(7) 0.6407(7) 0.8822(7) 0.036(3) Uani 1 1 d . . .
C33 C 0.4901(8) 0.4965(8) 0.8777(7) 0.046(3) Uani 1 1 d . . .
C34 C 0.4849(9) 0.4239(8) 0.9034(8) 0.057(4) Uani 1 1 d . . .
H34 H 0.4352 0.4263 0.9419 0.068 Uiso 1 1 calc R . .
C35 C 0.5571(10) 0.3459(10) 0.8696(9) 0.071(5) Uani 1 1 d . . .
H35 H 0.5562 0.2962 0.8866 0.086 Uiso 1 1 calc R . .
C36 C 0.6309(13) 0.3446(12) 0.8094(13) 0.096(7) Uani 1 1 d . . .
H36 H 0.6783 0.2931 0.7882 0.115 Uiso 1 1 calc R . .
C37 C 0.6353(9) 0.4130(8) 0.7823(9) 0.057(4) Uani 1 1 d . . .
H37 H 0.6840 0.4087 0.7419 0.069 Uiso 1 1 calc R . .
C38 C 0.5645(7) 0.4950(7) 0.8153(7) 0.040(3) Uani 1 1 d . . .
C39 C 0.4996(7) 0.6382(6) 0.8232(6) 0.031(2) Uani 1 1 d . . .
C40 C 0.5003(7) 0.7145(8) 0.7944(6) 0.034(3) Uani 1 1 d . . .
C41 C 0.5662(8) 0.7317(8) 0.7374(7) 0.043(3) Uani 1 1 d . . .
C42 C 0.6516(8) 0.6834(8) 0.6893(7) 0.048(3) Uani 1 1 d . . .
H42 H 0.6774 0.6255 0.6896 0.058 Uiso 1 1 calc R . .
C43 C 0.6977(7) 0.7204(7) 0.6417(7) 0.040(3) Uani 1 1 d . . .
H43 H 0.7543 0.6868 0.6090 0.048 Uiso 1 1 calc R . .
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C44 C 0.6627(9) 0.8092(9) 0.6397(7) 0.051(3) Uani 1 1 d . . .
H44 H 0.6965 0.8331 0.6075 0.061 Uiso 1 1 calc R . .
C45 C 0.5750(7) 0.8598(7) 0.6884(7) 0.039(3) Uani 1 1 d . . .
H45 H 0.5492 0.9177 0.6891 0.047 Uiso 1 1 calc R . .
C46 C 0.5299(8) 0.8199(8) 0.7342(7) 0.040(3) Uani 1 1 d . . .
C47 C 0.4302(7) 0.7887(7) 0.8271(6) 0.035(3) Uani 1 1 d . . .
C48 C 0.3538(7) 0.7945(7) 0.8853(8) 0.040(3) Uani 1 1 d . . .
C49 C 0.9649(7) 0.1042(7) 0.7927(6) 0.029(2) Uani 1 1 d . . .
C50 C 1.0092(8) 0.1013(8) 0.7222(6) 0.039(3) Uani 1 1 d . . .
H50 H 1.0693 0.0907 0.7034 0.047 Uiso 1 1 calc R . .
C51 C 0.9600(7) 0.1151(8) 0.6792(6) 0.037(3) Uani 1 1 d . . .
H51 H 0.9882 0.1156 0.6308 0.044 Uiso 1 1 calc R . .
C52 C 0.8700(7) 0.1283(8) 0.7054(7) 0.042(3) Uani 1 1 d . . .
H52 H 0.8385 0.1404 0.6755 0.051 Uiso 1 1 calc R . .
C53 C 0.8285(7) 0.1228(8) 0.7783(6) 0.033(3) Uani 1 1 d . . .
H53 H 0.7712 0.1257 0.7963 0.040 Uiso 1 1 calc R . .
C54 C 0.8755(6) 0.1127(6) 0.8238(6) 0.027(2) Uani 1 1 d . . .
C55 C 0.8518(7) 0.1132(6) 0.8998(5) 0.026(2) Uani 1 1 d . . .
C56 C 0.7732(6) 0.1163(7) 0.9567(6) 0.027(2) Uani 1 1 d . . .
C57 C 0.6300(7) 0.1275(7) 0.9991(6) 0.030(2) Uani 1 1 d . . .
C58 C 0.5530(7) 0.1353(8) 0.9901(7) 0.038(3) Uani 1 1 d . . .
H58 H 0.5510 0.1399 0.9452 0.046 Uiso 1 1 calc R . .
C59 C 0.4800(7) 0.1362(8) 1.0471(7) 0.042(3) Uani 1 1 d . . .
H59 H 0.4317 0.1367 1.0398 0.050 Uiso 1 1 calc R . .
C60 C 0.4787(8) 0.1364(10) 1.1161(8) 0.053(4) Uani 1 1 d . . .
H60 H 0.4285 0.1392 1.1543 0.063 Uiso 1 1 calc R . .
C61 C 0.5515(7) 0.1326(7) 1.1277(7) 0.036(3) Uani 1 1 d . . .
H61 H 0.5495 0.1338 1.1736 0.043 Uiso 1 1 calc R . .
C62 C 0.6295(7) 0.1270(7) 1.0695(6) 0.033(2) Uani 1 1 d . . .
C63 C 0.7746(6) 0.1130(6) 1.0260(6) 0.024(2) Uani 1 1 d . . .
C64 C 0.8523(7) 0.1039(7) 1.0369(6) 0.030(2) Uani 1 1 d . . .
C65 C 0.8717(6) 0.1004(7) 1.1002(5) 0.028(2) Uani 1 1 d . . .
C66 C 0.8217(7) 0.1044(7) 1.1725(6) 0.034(3) Uani 1 1 d . . .
H66 H 0.7624 0.1129 1.1886 0.041 Uiso 1 1 calc R . .
C67 C 0.8642(7) 0.0954(8) 1.2185(6) 0.036(3) Uani 1 1 d . . .
H67 H 0.8344 0.0933 1.2663 0.043 Uiso 1 1 calc R . .
C68 C 0.9528(7) 0.0891(7) 1.1951(6) 0.032(2) Uani 1 1 d . . .
H68 H 0.9787 0.0847 1.2279 0.038 Uiso 1 1 calc R . .
C69 C 1.0001(7) 0.0896(8) 1.1248(6) 0.038(3) Uani 1 1 d . . .
H69 H 1.0577 0.0856 1.1094 0.045 Uiso 1 1 calc R . .
C70 C 0.9584(7) 0.0962(7) 1.0764(6) 0.028(2) Uani 1 1 d . . .
C71 C 0.9267(6) 0.1007(7) 0.9791(6) 0.029(2) Uani 1 1 d . . .
C72 C 0.9279(7) 0.1016(7) 0.9119(6) 0.031(2) Uani 1 1 d . . .
C73 C 0.5359(7) 0.0457(9) 0.4271(6) 0.040(3) Uani 1 1 d . . .
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C74 C 0.4959(8) 0.0442(9) 0.3790(6) 0.043(3) Uani 1 1 d . . .
H74 H 0.4391 0.0464 0.3949 0.052 Uiso 1 1 calc R . .
C75 C 0.5437(8) 0.0396(9) 0.3105(8) 0.050(3) Uani 1 1 d . . .
H75 H 0.5166 0.0429 0.2788 0.059 Uiso 1 1 calc R . .
C76 C 0.6320(8) 0.0301(9) 0.2830(7) 0.050(3) Uani 1 1 d . . .
H76 H 0.6642 0.0194 0.2345 0.060 Uiso 1 1 calc R . .
C77 C 0.6731(6) 0.0368(7) 0.3280(5) 0.031(2) Uani 1 1 d . . .
H77 H 0.7281 0.0385 0.3100 0.038 Uiso 1 1 calc R . .
C78 C 0.6261(7) 0.0406(7) 0.4016(6) 0.032(2) Uani 1 1 d . . .
C79 C 0.6423(7) 0.0492(7) 0.4614(6) 0.033(2) Uani 1 1 d . . .
C80 C 0.7174(6) 0.0508(7) 0.4709(5) 0.026(2) Uani 1 1 d . . .
C81 C 0.8605(7) 0.0422(7) 0.4282(6) 0.031(2) Uani 1 1 d . . .
C82 C 0.9395(7) 0.0262(7) 0.3701(7) 0.039(3) Uani 1 1 d . . .
H82 H 0.9452 0.0134 0.3251 0.047 Uiso 1 1 calc R . .
C83 C 1.0103(7) 0.0301(7) 0.3817(7) 0.037(3) Uani 1 1 d . . .
H83 H 1.0629 0.0215 0.3435 0.044 Uiso 1 1 calc R . .
C84 C 1.0035(8) 0.0462(7) 0.4478(8) 0.045(3) Uani 1 1 d . . .
H84 H 1.0506 0.0502 0.4536 0.054 Uiso 1 1 calc R . .
C85 C 0.9270(7) 0.0568(7) 0.5071(7) 0.038(3) Uani 1 1 d . . .
H85 H 0.9248 0.0640 0.5521 0.045 Uiso 1 1 calc R . .
C86 C 0.8515(7) 0.0563(8) 0.4976(7) 0.040(3) Uani 1 1 d . . .
C87 C 0.7108(6) 0.0613(7) 0.5428(6) 0.027(2) Uani 1 1 d . . .
C88 C 0.6326(7) 0.0703(9) 0.6017(7) 0.041(3) Uani 1 1 d . . .
C89 C 0.6082(7) 0.0775(7) 0.6763(7) 0.036(3) Uani 1 1 d . . .
C90 C 0.6517(7) 0.0826(8) 0.7203(6) 0.036(3) Uani 1 1 d . . .
H90 H 0.7089 0.0799 0.7012 0.044 Uiso 1 1 calc R . .
C91 C 0.6040(8) 0.0918(9) 0.7941(7) 0.046(3) Uani 1 1 d . . .
H91 H 0.6300 0.0963 0.8242 0.056 Uiso 1 1 calc R . .
C92 C 0.5184(8) 0.0944(8) 0.8230(7) 0.045(3) Uani 1 1 d . . .
H92 H 0.4894 0.0995 0.8718 0.054 Uiso 1 1 calc R . .
C93 C 0.4766(8) 0.0895(7) 0.7811(6) 0.032(2) Uani 1 1 d . . .
H93 H 0.4205 0.0900 0.8010 0.039 Uiso 1 1 calc R . .
C94 C 0.5191(7) 0.0838(7) 0.7085(6) 0.029(2) Uani 1 1 d . . .
C95 C 0.5592(6) 0.0678(7) 0.5922(7) 0.036(3) Uani 1 1 d . . .
C96 C 0.5674(7) 0.0553(7) 0.5216(6) 0.032(2) Uani 1 1 d . . .
C97 C 0.5367(9) 0.8306(8) -0.0793(8) 0.048(3) Uani 1 1 d . . .
C98 C 0.5768(10) 0.8738(10) -0.1292(9) 0.059(4) Uani 1 1 d . . .
H98 H 0.5465 0.9318 -0.1258 0.071 Uiso 1 1 calc R . .
C99 C 0.6543(12) 0.8365(11) -0.1802(9) 0.065(4) Uani 1 1 d . . .
H99 H 0.6784 0.8679 -0.2120 0.078 Uiso 1 1 calc R . .
C100 C 0.7053(10) 0.7430(10) -0.1880(8) 0.056(4) Uani 1 1 d . . .
H100 H 0.7617 0.7162 -0.2235 0.067 Uiso 1 1 calc R . .
C101 C 0.6667(8) 0.6968(8) -0.1411(7) 0.044(3) Uani 1 1 d . . .
H101 H 0.6945 0.6387 -0.1460 0.052 Uiso 1 1 calc R . .
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C102 C 0.5838(7) 0.7423(7) -0.0861(7) 0.036(3) Uani 1 1 d . . .
C103 C 0.5240(7) 0.7150(7) -0.0305(7) 0.034(3) Uani 1 1 d . . .
C104 C 0.5305(7) 0.6353(7) -0.0076(6) 0.032(2) Uani 1 1 d . . .
C105 C 0.6035(7) 0.4926(7) -0.0180(7) 0.040(3) Uani 1 1 d . . .
C106 C 0.6824(8) 0.4149(8) -0.0556(8) 0.054(4) Uani 1 1 d . . .
H106 H 0.7295 0.4160 -0.0949 0.065 Uiso 1 1 calc R . .
C107 C 0.6838(10) 0.3413(9) -0.0303(10) 0.067(5) Uani 1 1 d . . .
H107 H 0.7329 0.2917 -0.0539 0.080 Uiso 1 1 calc R . .
C108 C 0.6165(8) 0.3364(8) 0.0283(9) 0.062(5) Uani 1 1 d . . .
H108 H 0.6220 0.2845 0.0441 0.074 Uiso 1 1 calc R . .
C109 C 0.5398(8) 0.4089(7) 0.0641(8) 0.051(4) Uani 1 1 d . . .
H109 H 0.4939 0.4057 0.1033 0.061 Uiso 1 1 calc R . .
C110 C 0.5334(7) 0.4863(7) 0.0400(7) 0.040(3) Uani 1 1 d . . .
C111 C 0.4569(7) 0.6317(7) 0.0521(7) 0.036(3) Uani 1 1 d . . .
C112 C 0.3803(8) 0.7084(7) 0.0884(7) 0.040(3) Uani 1 1 d . . .
C113 C 0.2980(8) 0.7249(7) 0.1447(7) 0.042(3) Uani 1 1 d . . .
C114 C 0.2562(9) 0.6777(9) 0.1872(7) 0.048(3) Uani 1 1 d . . .
H114 H 0.2850 0.6197 0.1797 0.058 Uiso 1 1 calc R . .
C115 C 0.1715(8) 0.7175(8) 0.2409(8) 0.052(3) Uani 1 1 d . . .
H115 H 0.1455 0.6858 0.2702 0.063 Uiso 1 1 calc R . .
C116 C 0.1234(9) 0.8088(8) 0.2510(7) 0.048(3) Uani 1 1 d . . .
H116 H 0.0660 0.8350 0.2853 0.058 Uiso 1 1 calc R . .
C117 C 0.1627(8) 0.8552(9) 0.2105(8) 0.051(4) Uani 1 1 d . . .
H117 H 0.1328 0.9132 0.2170 0.062 Uiso 1 1 calc R . .
C118 C 0.2498(8) 0.8141(8) 0.1581(7) 0.038(3) Uani 1 1 d . . .
C119 C 0.3766(6) 0.7857(7) 0.0632(7) 0.040(3) Uani 1 1 d . . .
C120 C 0.4497(7) 0.7901(7) 0.0062(7) 0.038(3) Uani 1 1 d . . .
C121 C 0.2637(7) 0.3539(7) 0.3525(7) 0.035(3) Uani 1 1 d . . .
C122 C 0.3388(8) 0.3057(8) 0.2947(7) 0.039(3) Uani 1 1 d . . .
H122 H 0.3630 0.2478 0.2902 0.047 Uiso 1 1 calc R . .
C123 C 0.3754(9) 0.3497(9) 0.2441(9) 0.056(4) Uani 1 1 d . . .
H123 H 0.4256 0.3207 0.2040 0.067 Uiso 1 1 calc R . .
C124 C 0.3382(8) 0.4373(9) 0.2521(7) 0.045(3) Uani 1 1 d . . .
H124 H 0.3641 0.4647 0.2168 0.054 Uiso 1 1 calc R . .
C125 C 0.2641(8) 0.4843(8) 0.3110(7) 0.038(3) Uani 1 1 d . . .
H125 H 0.2406 0.5421 0.3156 0.046 Uiso 1 1 calc R . .
C126 C 0.2259(7) 0.4414(6) 0.3631(6) 0.029(2) Uani 1 1 d . . .
C127 C 0.1512(7) 0.4662(7) 0.4289(6) 0.035(2) Uani 1 1 d . . .
C128 C 0.0860(7) 0.5457(7) 0.4667(6) 0.035(3) Uani 1 1 d . . .
C129 C 0.0289(8) 0.6895(7) 0.4782(7) 0.041(3) Uani 1 1 d . . .
C130 C 0.0326(8) 0.7669(8) 0.4515(7) 0.042(3) Uani 1 1 d . . .
H130 H 0.0770 0.7651 0.4086 0.051 Uiso 1 1 calc R . .
C131 C -0.0268(9) 0.8392(8) 0.4879(8) 0.054(4) Uani 1 1 d . . .
H131 H -0.0233 0.8875 0.4696 0.065 Uiso 1 1 calc R . .
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C132 C -0.0961(9) 0.8464(8) 0.5544(8) 0.048(3) Uani 1 1 d . . .
H132 H -0.1372 0.8984 0.5787 0.058 Uiso 1 1 calc R . .
C133 C -0.1012(9) 0.7731(8) 0.5824(8) 0.049(3) Uani 1 1 d . . .
H133 H -0.1444 0.7751 0.6261 0.059 Uiso 1 1 calc R . .
C134 C -0.0376(8) 0.6960(7) 0.5413(7) 0.041(3) Uani 1 1 d . . .
C135 C 0.0150(8) 0.5541(8) 0.5329(7) 0.041(3) Uani 1 1 d . . .
C136 C 0.0130(6) 0.4758(6) 0.5604(6) 0.029(2) Uani 1 1 d . . .
C137 C -0.0476(8) 0.4584(8) 0.6221(7) 0.042(3) Uani 1 1 d . . .
C138 C -0.1257(8) 0.5087(8) 0.6792(7) 0.042(3) Uani 1 1 d . . .
H138 H -0.1478 0.5664 0.6826 0.051 Uiso 1 1 calc R . .
C139 C -0.1674(9) 0.4699(8) 0.7288(7) 0.048(3) Uani 1 1 d . . .
H139 H -0.2196 0.5023 0.7662 0.057 Uiso 1 1 calc R . .
C140 C -0.1343(9) 0.3809(9) 0.7260(8) 0.050(3) Uani 1 1 d . . .
H140 H -0.1655 0.3568 0.7606 0.061 Uiso 1 1 calc R . .
C141 C -0.0556(8) 0.3308(8) 0.6715(7) 0.043(3) Uani 1 1 d . . .
H141 H -0.0330 0.2729 0.6694 0.052 Uiso 1 1 calc R . .
C142 C -0.0110(8) 0.3697(8) 0.6196(6) 0.040(3) Uani 1 1 d . . .
C143 C 0.0787(7) 0.3977(7) 0.5227(6) 0.033(2) Uani 1 1 d . . .
C144 C 0.1453(7) 0.3934(6) 0.4590(6) 0.029(2) Uani 1 1 d . . .
N25 N 0.7737(8) 0.8427(6) 0.9844(6) 0.064(4) Uani 1 1 d D . .
N26 N 0.3227(8) 0.7755(7) 0.6592(6) 0.068(4) Uani 1 1 d D . .
N27 N 0.4817(7) 0.5668(7) 0.2898(8) 0.083(5) Uani 1 1 d D . .
N28 N 0.1963(9) 0.3768(8) 0.7005(7) 0.094(6) Uani 1 1 d D . .
N29 N 0.0226(6) 0.3714(6) 0.0829(5) 0.051(3) Uani 1 1 d D . .
N30 N 0.6774(10) 0.7869(11) 0.2099(8) 0.080(4) Uani 1 1 d . . .
N31 N 0.5054(18) 0.7526(14) 0.3734(11) 0.122(8) Uani 1 1 d . . .
N32 N 0.7728(17) 0.5032(17) 0.2679(12) 0.149(11) Uani 1 1 d . . .
N33 N 0.6034(18) 0.4213(18) 0.4590(15) 0.148(9) Uani 1 1 d . . .
N34 N 0.237(3) 0.554(3) 0.923(2) 0.30(3) Uani 1 1 d . . .
C145 C 0.6872(9) 0.8438(9) 1.0329(8) 0.080(6) Uani 1 1 d D . .
H14A H 0.7002 0.8011 1.0654 0.096 Uiso 1 1 calc R . .
H14B H 0.6625 0.8280 1.0050 0.096 Uiso 1 1 calc R . .
C146 C 0.6146(9) 0.9259(10) 1.0762(10) 0.078(5) Uani 1 1 d D . .
H14C H 0.6159 0.9722 1.0479 0.093 Uiso 1 1 calc R . .
H14D H 0.6269 0.9314 1.1172 0.093 Uiso 1 1 calc R . .
C147 C 0.5202(11) 0.9296(11) 1.1006(12) 0.094(6) Uani 1 1 d D . .
H14E H 0.4786 0.9780 1.1341 0.113 Uiso 1 1 calc R . .
H14F H 0.5028 0.9397 1.0598 0.113 Uiso 1 1 calc R . .
C148 C 0.5054(13) 0.8547(11) 1.1344(12) 0.093(6) Uani 1 1 d D . .
H14G H 0.5151 0.8175 1.0985 0.139 Uiso 1 1 calc R . .
H14H H 0.4449 0.8742 1.1682 0.139 Uiso 1 1 calc R . .
H14I H 0.5468 0.8257 1.1578 0.139 Uiso 1 1 calc R . .
C149 C 0.8061(10) 0.8862(9) 1.0196(8) 0.068(4) Uani 1 1 d D . .
H14J H 0.7607 0.9438 1.0327 0.082 Uiso 1 1 calc R . .
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H14K H 0.8601 0.8870 0.9846 0.082 Uiso 1 1 calc R . .
C150 C 0.8271(12) 0.8498(9) 1.0852(9) 0.094(7) Uani 1 1 d D . .
H15A H 0.7746 0.8476 1.1213 0.112 Uiso 1 1 calc R . .
H15B H 0.8757 0.7935 1.0731 0.112 Uiso 1 1 calc R . .
C151 C 0.8540(12) 0.9056(11) 1.1127(12) 0.085(6) Uani 1 1 d D . .
H15C H 0.8060 0.9622 1.1235 0.101 Uiso 1 1 calc R . .
H15D H 0.9074 0.9067 1.0770 0.101 Uiso 1 1 calc R . .
C152 C 0.8729(14) 0.8719(12) 1.1795(10) 0.113(10) Uani 1 1 d D . .
H15E H 0.8231 0.8634 1.2122 0.170 Uiso 1 1 calc R . .
H15F H 0.8810 0.9113 1.2010 0.170 Uiso 1 1 calc R . .
H15G H 0.9265 0.8197 1.1673 0.170 Uiso 1 1 calc R . .
C153 C 0.8470(9) 0.7531(8) 0.9628(10) 0.068(4) Uani 1 1 d D . .
H15H H 0.9038 0.7546 0.9359 0.082 Uiso 1 1 calc R . .
H15I H 0.8522 0.7257 1.0053 0.082 Uiso 1 1 calc R . .
C154 C 0.8340(12) 0.7012(9) 0.9206(11) 0.085(6) Uani 1 1 d D . .
H15J H 0.8379 0.7229 0.8748 0.102 Uiso 1 1 calc R . .
H15K H 0.7746 0.7041 0.9442 0.102 Uiso 1 1 calc R . .
C155 C 0.9055(12) 0.6095(9) 0.9107(12) 0.104(8) Uani 1 1 d D . .
H15L H 0.9641 0.6058 0.8813 0.125 Uiso 1 1 calc R . .
H15M H 0.9076 0.5906 0.9563 0.125 Uiso 1 1 calc R . .
C156 C 0.8855(16) 0.5519(11) 0.8765(15) 0.115(9) Uani 1 1 d D . .
H15N H 0.8247 0.5607 0.9021 0.173 Uiso 1 1 calc R . .
H15O H 0.9261 0.4947 0.8775 0.173 Uiso 1 1 calc R . .
H15P H 0.8932 0.5644 0.8284 0.173 Uiso 1 1 calc R . .
C157 C 0.7550(9) 0.8892(9) 0.9229(7) 0.070(5) Uani 1 1 d D . .
H15Q H 0.7116 0.9469 0.9387 0.084 Uiso 1 1 calc R . .
H15R H 0.7299 0.8644 0.9024 0.084 Uiso 1 1 calc R . .
C158 C 0.8434(8) 0.8855(12) 0.8668(7) 0.089(7) Uani 1 1 d D . .
H15S H 0.8617 0.9205 0.8837 0.107 Uiso 1 1 calc R . .
H15T H 0.8907 0.8286 0.8584 0.107 Uiso 1 1 calc R . .
C159 C 0.8283(11) 0.9158(13) 0.7984(9) 0.100(8) Uani 1 1 d D . .
H15U H 0.7816 0.9730 0.8077 0.120 Uiso 1 1 calc R . .
H15V H 0.8066 0.8821 0.7839 0.120 Uiso 1 1 calc R . .
C160 C 0.9123(12) 0.9119(14) 0.7373(9) 0.092(6) Uani 1 1 d D . .
H16A H 0.9443 0.9306 0.7548 0.138 Uiso 1 1 calc R . .
H16B H 0.8948 0.9472 0.7021 0.138 Uiso 1 1 calc R . .
H16C H 0.9506 0.8554 0.7169 0.138 Uiso 1 1 calc R . .
C161 C 0.2718(14) 0.8187(13) 0.7326(8) 0.097(7) Uani 1 1 d D . .
H16D H 0.2586 0.8772 0.7297 0.117 Uiso 1 1 calc R . .
H16E H 0.3098 0.7945 0.7600 0.117 Uiso 1 1 calc R . .
C162 C 0.1832(11) 0.8123(13) 0.7712(8) 0.095(7) Uani 1 1 d D . .
H16F H 0.1422 0.8398 0.7465 0.114 Uiso 1 1 calc R . .
H16G H 0.1945 0.7542 0.7739 0.114 Uiso 1 1 calc R . .
C163 C 0.1429(12) 0.8554(12) 0.8455(7) 0.090(7) Uani 1 1 d D . .
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H16H H 0.1785 0.8213 0.8727 0.108 Uiso 1 1 calc R . .
H16I H 0.1446 0.9088 0.8422 0.108 Uiso 1 1 calc R . .
C164 C 0.0457(13) 0.8690(18) 0.8831(12) 0.123(10) Uani 1 1 d D . .
H16J H 0.0060 0.9215 0.8721 0.184 Uiso 1 1 calc R . .
H16K H 0.0313 0.8695 0.9332 0.184 Uiso 1 1 calc R . .
H16L H 0.0388 0.8246 0.8677 0.184 Uiso 1 1 calc R . .
C165 C 0.3517(12) 0.6827(7) 0.6644(10) 0.073(5) Uani 1 1 d D . .
H16M H 0.3909 0.6550 0.6175 0.088 Uiso 1 1 calc R . .
H16N H 0.2985 0.6739 0.6780 0.088 Uiso 1 1 calc R . .
C166 C 0.4002(19) 0.6382(10) 0.7152(14) 0.119(9) Uani 1 1 d D . .
H16O H 0.3583 0.6572 0.7635 0.143 Uiso 1 1 calc R . .
H16P H 0.4486 0.6529 0.7073 0.143 Uiso 1 1 calc R . .
C167 C 0.4393(15) 0.5423(10) 0.7049(15) 0.146(13) Uani 1 1 d D . .
H16Q H 0.4430 0.5164 0.7482 0.175 Uiso 1 1 calc R . .
H16R H 0.4038 0.5265 0.6886 0.175 Uiso 1 1 calc R . .
C168 C 0.5333(16) 0.519(3) 0.6480(18) 0.24(3) Uani 1 1 d D . .
H16S H 0.5580 0.5518 0.6587 0.354 Uiso 1 1 d R . .
H16T H 0.5281 0.5314 0.6028 0.354 Uiso 1 1 d R . .
H16U H 0.5722 0.4608 0.6470 0.354 Uiso 1 1 d R . .
C169 C 0.2695(13) 0.7998(9) 0.6111(10) 0.081(6) Uani 1 1 d D . .
H16V H 0.2213 0.7834 0.6309 0.097 Uiso 1 1 calc R . .
H16W H 0.3088 0.7688 0.5654 0.097 Uiso 1 1 calc R . .
C170 C 0.2286(13) 0.8943(9) 0.6004(10) 0.079(6) Uani 1 1 d D . .
H17A H 0.1858 0.9261 0.6451 0.095 Uiso 1 1 calc R . .
H17B H 0.2757 0.9123 0.5820 0.095 Uiso 1 1 calc R . .
C171 C 0.1813(15) 0.9092(16) 0.5479(11) 0.108(8) Uani 1 1 d D . .
H17C H 0.1628 0.9666 0.5356 0.129 Uiso 1 1 calc R . .
H17D H 0.2237 0.8732 0.5050 0.129 Uiso 1 1 calc R . .
C172 C 0.0986(12) 0.8921(14) 0.5775(15) 0.114(9) Uani 1 1 d D . .
H17E H 0.1178 0.8330 0.5753 0.171 Uiso 1 1 calc R . .
H17F H 0.0616 0.9177 0.5500 0.171 Uiso 1 1 calc R . .
H17G H 0.0647 0.9150 0.6257 0.171 Uiso 1 1 calc R . .
C173 C 0.3996(11) 0.7981(14) 0.6303(9) 0.090(7) Uani 1 1 d D . .
H17H H 0.4315 0.7825 0.6624 0.108 Uiso 1 1 calc R . .
H17I H 0.3759 0.8581 0.6279 0.108 Uiso 1 1 calc R . .
C174 C 0.4659(13) 0.755(2) 0.5565(9) 0.157(15) Uani 1 1 d D . .
H17J H 0.4800 0.6959 0.5567 0.188 Uiso 1 1 calc R . .
H17K H 0.4370 0.7786 0.5227 0.188 Uiso 1 1 calc R . .
C175 C 0.5536(15) 0.7629(11) 0.5321(15) 0.127(10) Uani 1 1 d D . .
H17L H 0.5953 0.7293 0.4879 0.153 Uiso 1 1 calc R . .
H17M H 0.5812 0.7427 0.5670 0.153 Uiso 1 1 calc R . .
C176 C 0.5332(10) 0.8549(8) 0.5223(11) 0.074(5) Uani 1 1 d D . .
H17N H 0.4965 0.8773 0.4943 0.111 Uiso 1 1 calc R . .
H17O H 0.5885 0.8589 0.4987 0.111 Uiso 1 1 calc R . .
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H17P H 0.5018 0.8859 0.5676 0.111 Uiso 1 1 calc R . .
C177 C 0.4040(10) 0.6252(8) 0.2686(9) 0.070(5) Uani 1 1 d D . .
H17Q H 0.3548 0.6110 0.2930 0.084 Uiso 1 1 calc R . .
H17R H 0.4222 0.6124 0.2186 0.084 Uiso 1 1 calc R . .
C178 C 0.3656(11) 0.7208(8) 0.2806(11) 0.085(6) Uani 1 1 d D . .
H17S H 0.4106 0.7335 0.2852 0.102 Uiso 1 1 calc R . .
H17T H 0.3529 0.7466 0.2397 0.102 Uiso 1 1 calc R . .
C179 C 0.2795(14) 0.7585(12) 0.3466(13) 0.20(2) Uani 1 1 d D . .
H17U H 0.2930 0.7358 0.3880 0.239 Uiso 1 1 calc R . .
H17V H 0.2358 0.7425 0.3437 0.239 Uiso 1 1 calc R . .
C180 C 0.2378(14) 0.8548(11) 0.3552(10) 0.090(6) Uani 1 1 d D . .
H18A H 0.2820 0.8711 0.3552 0.135 Uiso 1 1 calc R . .
H18B H 0.1872 0.8753 0.3991 0.135 Uiso 1 1 calc R . .
H18C H 0.2185 0.8779 0.3168 0.135 Uiso 1 1 calc R . .
C181 C 0.5619(10) 0.5846(13) 0.2536(9) 0.083(6) Uani 1 1 d D . .
H18D H 0.6132 0.5401 0.2617 0.099 Uiso 1 1 calc R . .
H18E H 0.5495 0.6359 0.2761 0.099 Uiso 1 1 calc R . .
C182 C 0.5889(11) 0.5933(12) 0.1731(8) 0.085(6) Uani 1 1 d D . .
H18F H 0.5970 0.5447 0.1496 0.101 Uiso 1 1 calc R . .
H18G H 0.5419 0.6423 0.1639 0.101 Uiso 1 1 calc R . .
C183 C 0.6771(12) 0.6013(17) 0.1449(11) 0.101(7) Uani 1 1 d D . .
H18H H 0.7225 0.5543 0.1576 0.122 Uiso 1 1 calc R . .
H18I H 0.6675 0.6520 0.1666 0.122 Uiso 1 1 calc R . .
C184 C 0.7110(18) 0.604(2) 0.0639(11) 0.133(10) Uani 1 1 d D . .
H18J H 0.7438 0.5481 0.0419 0.200 Uiso 1 1 calc R . .
H18K H 0.7497 0.6309 0.0497 0.200 Uiso 1 1 calc R . .
H18L H 0.6606 0.6348 0.0497 0.200 Uiso 1 1 calc R . .
C185 C 0.5049(15) 0.4787(9) 0.2689(15) 0.123(10) Uani 1 1 d D . .
H18M H 0.5301 0.4705 0.2177 0.148 Uiso 1 1 calc R . .
H18N H 0.4496 0.4730 0.2849 0.148 Uiso 1 1 calc R . .
C186 C 0.5714(16) 0.4084(13) 0.2976(13) 0.114(8) Uani 1 1 d D . .
H18O H 0.6288 0.4104 0.2784 0.137 Uiso 1 1 calc R . .
H18P H 0.5487 0.4180 0.3485 0.137 Uiso 1 1 calc R . .
C187 C 0.5860(15) 0.3207(15) 0.2787(14) 0.115(9) Uani 1 1 d D . .
H18Q H 0.5286 0.3192 0.2936 0.138 Uiso 1 1 calc R . .
H18R H 0.6158 0.3072 0.2280 0.138 Uiso 1 1 calc R . .
C188 C 0.645(2) 0.257(2) 0.3166(18) 0.175(14) Uani 1 1 d DU . .
H18S H 0.7054 0.2494 0.2939 0.262 Uiso 1 1 calc R . .
H18T H 0.6431 0.2048 0.3146 0.262 Uiso 1 1 calc R . .
H18U H 0.6217 0.2776 0.3650 0.262 Uiso 1 1 calc R . .
C189 C 0.465(2) 0.568(4) 0.3674(10) 0.37(5) Uani 1 1 d D . .
H18V H 0.4571 0.6209 0.3828 0.445 Uiso 1 1 calc R . .
H18W H 0.5184 0.5245 0.3741 0.445 Uiso 1 1 calc R . .
C190 C 0.3832(14) 0.5537(13) 0.4151(10) 0.099(7) Uani 1 1 d D . .
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H19A H 0.3972 0.4955 0.4091 0.119 Uiso 1 1 calc R . .
H19B H 0.3326 0.5873 0.4009 0.119 Uiso 1 1 calc R . .
C191 C 0.357(2) 0.577(3) 0.4936(12) 0.186(15) Uani 1 1 d DU . .
H19C H 0.3505 0.6334 0.4984 0.224 Uiso 1 1 calc R . .
H19D H 0.4053 0.5395 0.5089 0.224 Uiso 1 1 calc R . .
C192 C 0.269(3) 0.574(3) 0.542(2) 0.216(18) Uani 1 1 d DU . .
H19E H 0.2268 0.6278 0.5681 0.324 Uiso 1 1 calc R . .
H19F H 0.2810 0.5324 0.5749 0.324 Uiso 1 1 calc R . .
H19G H 0.2432 0.5609 0.5143 0.324 Uiso 1 1 calc R . .
C193 C 0.2311(13) 0.3155(11) 0.6398(8) 0.088(6) Uani 1 1 d D . .
H19H H 0.1808 0.3144 0.6333 0.105 Uiso 1 1 calc R . .
H19I H 0.2673 0.2602 0.6505 0.105 Uiso 1 1 calc R . .
C194 C 0.2883(18) 0.3377(18) 0.5709(9) 0.129(11) Uani 1 1 d D . .
H19J H 0.3340 0.3479 0.5771 0.155 Uiso 1 1 calc R . .
H19K H 0.2516 0.3855 0.5518 0.155 Uiso 1 1 calc R . .
C195 C 0.3294(17) 0.2558(14) 0.5250(15) 0.118(10) Uani 1 1 d D . .
H19L H 0.3606 0.2077 0.5471 0.142 Uiso 1 1 calc R . .
H19M H 0.2838 0.2485 0.5157 0.142 Uiso 1 1 calc R . .
C196 C 0.3954(14) 0.2702(13) 0.4571(13) 0.117(10) Uani 1 1 d D . .
H19N H 0.3641 0.3224 0.4403 0.176 Uiso 1 1 calc R . .
H19O H 0.4201 0.2256 0.4217 0.176 Uiso 1 1 calc R . .
H19P H 0.4431 0.2714 0.4670 0.176 Uiso 1 1 calc R . .
C197 C 0.1472(11) 0.3487(11) 0.7690(8) 0.085(6) Uani 1 1 d D . .
H19Q H 0.1254 0.3904 0.8067 0.102 Uiso 1 1 calc R . .
H19R H 0.1912 0.2973 0.7788 0.102 Uiso 1 1 calc R . .
C198 C 0.0676(10) 0.3335(10) 0.7736(9) 0.072(5) Uani 1 1 d D . .
H19S H 0.0880 0.2872 0.7405 0.086 Uiso 1 1 calc R . .
H19T H 0.0229 0.3829 0.7623 0.086 Uiso 1 1 calc R . .
C199 C 0.0269(10) 0.3133(10) 0.8498(10) 0.083(6) Uani 1 1 d D . .
H19U H 0.0708 0.2614 0.8590 0.100 Uiso 1 1 calc R . .
H19V H 0.0131 0.3572 0.8825 0.100 Uiso 1 1 calc R . .
C200 C -0.0589(13) 0.3053(15) 0.8623(13) 0.107(8) Uani 1 1 d D . .
H20A H -0.1021 0.3564 0.8525 0.161 Uiso 1 1 calc R . .
H20B H -0.0836 0.2945 0.9105 0.161 Uiso 1 1 calc R . .
H20C H -0.0449 0.2601 0.8316 0.161 Uiso 1 1 calc R . .
C201 C 0.1360(16) 0.4574(12) 0.6802(12) 0.111(8) Uani 1 1 d D . .
H20D H 0.0872 0.4501 0.6767 0.134 Uiso 1 1 calc R . .
H20E H 0.1701 0.4663 0.6332 0.134 Uiso 1 1 calc R . .
C202 C 0.094(2) 0.5374(15) 0.7274(18) 0.187(15) Uani 1 1 d DU . .
H20F H 0.1408 0.5524 0.7250 0.224 Uiso 1 1 calc R . .
H20G H 0.0655 0.5286 0.7760 0.224 Uiso 1 1 calc R . .
C203 C 0.0247(19) 0.608(2) 0.702(2) 0.173(15) Uani 1 1 d D . .
H20H H 0.0206 0.5892 0.6615 0.207 Uiso 1 1 calc R . .
H20I H -0.0343 0.6326 0.7395 0.207 Uiso 1 1 calc R . .
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C204 C 0.068(3) 0.668(3) 0.683(3) 0.23(2) Uani 1 1 d DU . .
H20J H 0.1314 0.6378 0.6582 0.344 Uiso 1 1 d R . .
H20K H 0.0560 0.6964 0.7255 0.344 Uiso 1 1 d R . .
H20L H 0.0414 0.7079 0.6537 0.344 Uiso 1 1 d R . .
C205 C 0.2692(13) 0.3903(16) 0.7085(12) 0.131(11) Uani 1 1 d D . .
H20M H 0.2420 0.4299 0.7491 0.157 Uiso 1 1 calc R . .
H20N H 0.2929 0.4163 0.6673 0.157 Uiso 1 1 calc R . .
C206 C 0.3485(17) 0.3133(13) 0.718(3) 0.30(4) Uani 1 1 d D . .
H20O H 0.3706 0.2708 0.6805 0.361 Uiso 1 1 calc R . .
H20P H 0.3260 0.2919 0.7622 0.361 Uiso 1 1 calc R . .
C207 C 0.4286(16) 0.326(2) 0.7161(15) 0.138(11) Uani 1 1 d D . .
H20Q H 0.4201 0.3754 0.6907 0.166 Uiso 1 1 calc R . .
H20R H 0.4077 0.3453 0.7649 0.166 Uiso 1 1 calc R . .
C208 C 0.5307(18) 0.285(4) 0.697(3) 0.30(3) Uani 1 1 d DU . .
H20S H 0.5578 0.3124 0.6596 0.445 Uiso 1 1 d R . .
H20T H 0.5561 0.2271 0.6820 0.445 Uiso 1 1 d R . .
H20U H 0.5420 0.2901 0.7380 0.445 Uiso 1 1 d R . .
C209 C -0.0643(7) 0.3839(7) 0.0780(8) 0.049(3) Uani 1 1 d D . .
H20V H -0.0776 0.4250 0.0443 0.059 Uiso 1 1 calc R . .
H20W H -0.1121 0.4075 0.1236 0.059 Uiso 1 1 calc R . .
C210 C -0.0673(7) 0.3060(7) 0.0563(8) 0.046(3) Uani 1 1 d D . .
H21A H -0.0213 0.2822 0.0100 0.055 Uiso 1 1 calc R . .
H21B H -0.0551 0.2642 0.0897 0.055 Uiso 1 1 calc R . .
C211 C -0.1599(8) 0.3296(11) 0.0545(9) 0.079(5) Uani 1 1 d D . .
H21C H -0.1771 0.3794 0.0292 0.094 Uiso 1 1 calc R . .
H21D H -0.1560 0.2848 0.0288 0.094 Uiso 1 1 calc R . .
C212 C -0.2330(11) 0.3460(16) 0.1282(11) 0.129(12) Uani 1 1 d D . .
H21E H -0.2341 0.2944 0.1443 0.194 Uiso 1 1 calc R . .
H21F H -0.2904 0.3843 0.1263 0.194 Uiso 1 1 calc R . .
H21G H -0.2203 0.3697 0.1603 0.194 Uiso 1 1 calc R . .
C213 C 0.0474(8) 0.3054(8) 0.1326(6) 0.055(4) Uani 1 1 d D . .
H21H H 0.0970 0.3051 0.1415 0.066 Uiso 1 1 calc R . .
H21I H 0.0689 0.2514 0.1092 0.066 Uiso 1 1 calc R . .
C214 C -0.0281(8) 0.3150(9) 0.2041(7) 0.063(4) Uani 1 1 d D . .
H21J H -0.0798 0.3193 0.1960 0.075 Uiso 1 1 calc R . .
H21K H -0.0462 0.3663 0.2301 0.075 Uiso 1 1 calc R . .
C215 C 0.0011(10) 0.2411(8) 0.2488(7) 0.061(4) Uani 1 1 d D . .
H21L H 0.0504 0.2386 0.2595 0.074 Uiso 1 1 calc R . .
H21M H 0.0223 0.1894 0.2220 0.074 Uiso 1 1 calc R . .
C216 C -0.0777(10) 0.2501(11) 0.3182(7) 0.066(4) Uani 1 1 d D . .
H21N H -0.0866 0.2907 0.3508 0.098 Uiso 1 1 calc R . .
H21O H -0.0641 0.1972 0.3384 0.098 Uiso 1 1 calc R . .
H21P H -0.1315 0.2678 0.3086 0.098 Uiso 1 1 calc R . .
C217 C 0.0100(10) 0.4504(7) 0.1143(8) 0.062(4) Uani 1 1 d D . .
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H21Q H 0.0626 0.4389 0.1245 0.074 Uiso 1 1 calc R . .
H21R H -0.0415 0.4684 0.1585 0.074 Uiso 1 1 calc R . .
C218 C -0.0046(11) 0.5213(8) 0.0648(9) 0.068(5) Uani 1 1 d D . .
H21S H -0.0612 0.5381 0.0590 0.082 Uiso 1 1 calc R . .
H21T H 0.0434 0.5020 0.0187 0.082 Uiso 1 1 calc R . .
C219 C -0.0059(12) 0.5962(9) 0.0961(12) 0.098(8) Uani 1 1 d D . .
H21U H 0.0503 0.5779 0.1029 0.117 Uiso 1 1 calc R . .
H21V H -0.0090 0.6382 0.0621 0.117 Uiso 1 1 calc R . .
C220 C -0.0835(18) 0.6365(13) 0.1661(10) 0.135(12) Uani 1 1 d D . .
H22A H -0.1351 0.6780 0.1572 0.203 Uiso 1 1 calc R . .
H22B H -0.0662 0.6624 0.1928 0.203 Uiso 1 1 calc R . .
H22C H -0.0982 0.5945 0.1925 0.203 Uiso 1 1 calc R . .
C221 C 0.0972(6) 0.3408(8) 0.0110(7) 0.052(3) Uani 1 1 d D . .
H22D H 0.0782 0.3795 -0.0226 0.062 Uiso 1 1 calc R . .
H22E H 0.1047 0.2872 -0.0029 0.062 Uiso 1 1 calc R . .
C222 C 0.1886(7) 0.3310(9) 0.0051(7) 0.056(4) Uani 1 1 d D . .
H22F H 0.2080 0.2937 0.0393 0.067 Uiso 1 1 calc R . .
H22G H 0.1832 0.3849 0.0159 0.067 Uiso 1 1 calc R . .
C223 C 0.2592(8) 0.2959(9) -0.0695(7) 0.061(4) Uani 1 1 d D . .
H22H H 0.2689 0.2397 -0.0781 0.073 Uiso 1 1 calc R . .
H22I H 0.2364 0.3299 -0.1038 0.073 Uiso 1 1 calc R . .
C224 C 0.3493(8) 0.2942(11) -0.0799(10) 0.069(5) Uani 1 1 d D . .
H22J H 0.3408 0.3503 -0.0753 0.103 Uiso 1 1 d R . .
H22K H 0.3919 0.2689 -0.1262 0.103 Uiso 1 1 d R . .
H22L H 0.3715 0.2625 -0.0450 0.103 Uiso 1 1 d R . .
C225 C 0.6836(11) 0.7961(11) 0.2647(11) 0.071(5) Uani 1 1 d . . .
C226 C 0.6906(11) 0.8046(12) 0.3287(9) 0.069(4) Uani 1 1 d . . .
H22M H 0.7484 0.7638 0.3282 0.104 Uiso 1 1 d R . .
H22N H 0.6442 0.7962 0.3664 0.104 Uiso 1 1 d R . .
H22O H 0.6840 0.8596 0.3356 0.104 Uiso 1 1 d R . .
C227 C 0.4658(16) 0.8223(18) 0.3563(9) 0.089(7) Uani 1 1 d . . .
C228 C 0.4239(12) 0.9027(12) 0.3350(12) 0.086(6) Uani 1 1 d . . .
H22P H 0.3979 0.9435 0.3738 0.129 Uiso 1 1 d R . .
H22Q H 0.3775 0.9058 0.3207 0.129 Uiso 1 1 d R . .
H22R H 0.4675 0.9136 0.2962 0.129 Uiso 1 1 d R . .
C229 C 0.7541(14) 0.5252(17) 0.3230(15) 0.106(8) Uani 1 1 d . . .
C230 C 0.719(3) 0.553(3) 0.4029(19) 0.24(3) Uani 1 1 d . . .
H23A H 0.7204 0.6041 0.4085 0.358 Uiso 1 1 d R . .
H23B H 0.7559 0.5099 0.4245 0.358 Uiso 1 1 d R . .
H23C H 0.6580 0.5600 0.4250 0.358 Uiso 1 1 d R . .
C231 C 0.652(3) 0.3620(18) 0.466(3) 0.27(3) Uani 1 1 d . . .
C232 C 0.7207(18) 0.2705(15) 0.4788(16) 0.135(10) Uani 1 1 d . . .
H23D H 0.6982 0.2606 0.5276 0.202 Uiso 1 1 d R . .
H23E H 0.7791 0.2677 0.4667 0.202 Uiso 1 1 d R . .
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H23F H 0.7249 0.2289 0.4499 0.202 Uiso 1 1 d R . .
C233 C 0.192(2) 0.542(2) 0.891(2) 0.19(2) Uani 1 1 d . . .
C234 C 0.150(2) 0.509(3) 0.877(2) 0.22(2) Uani 1 1 d . . .
H23G H 0.1886 0.4751 0.8328 0.323 Uiso 1 1 d R . .
H23H H 0.0964 0.5516 0.8725 0.323 Uiso 1 1 d R . .
H23I H 0.1355 0.4741 0.9133 0.323 Uiso 1 1 d R . .

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P2 0.0482(17) 0.0374(18) 0.0230(15) 0.0010(12) -0.0144(13) -0.0149(14)
P3 0.0289(13) 0.0323(15) 0.0226(14) 0.0035(11) -0.0092(11) -0.0166(11)
P4 0.0282(13) 0.0547(19) 0.0206(14) 0.0067(12) -0.0112(11) -0.0255(13)
P5 0.0254(13) 0.0407(16) 0.0171(13) 0.0030(11) -0.0063(10) -0.0178(12)
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O2 0.024(4) 0.059(6) 0.052(6) -0.027(5) -0.007(4) 0.002(4)
O3 0.052(5) 0.051(5) 0.029(4) -0.003(4) -0.007(4) -0.035(4)
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O7 0.032(4) 0.063(6) 0.041(5) -0.014(4) -0.013(4) -0.014(4)
O8 0.043(4) 0.078(6) 0.020(4) 0.004(4) -0.007(3) -0.045(4)
O9 0.023(3) 0.046(5) 0.038(5) 0.017(4) -0.001(3) -0.025(3)
O10 0.047(4) 0.059(5) 0.037(5) 0.021(4) -0.029(4) -0.037(4)
O11 0.035(4) 0.034(5) 0.037(5) 0.003(4) -0.009(4) -0.002(3)
O12 0.041(4) 0.025(4) 0.042(5) 0.008(3) -0.022(4) -0.018(3)
O13 0.021(3) 0.052(5) 0.014(4) 0.001(3) 0.000(3) -0.012(3)
O14 0.026(4) 0.052(5) 0.035(5) -0.014(4) -0.013(3) -0.011(3)
O15 0.044(4) 0.035(5) 0.055(6) 0.015(4) -0.021(4) -0.021(4)
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O17 0.029(4) 0.043(5) 0.025(4) 0.008(3) -0.009(3) -0.019(3)
O18 0.033(4) 0.049(5) 0.036(4) 0.002(4) -0.021(3) -0.022(4)
O19 0.019(3) 0.033(4) 0.017(4) 0.000(3) 0.004(3) -0.008(3)
O20 0.024(3) 0.026(4) 0.031(4) -0.008(3) -0.009(3) -0.007(3)
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N3 0.054(6) 0.016(5) 0.037(6) -0.003(4) -0.015(5) -0.009(4)
N4 0.028(4) 0.035(5) 0.047(6) 0.002(4) -0.009(4) -0.018(4)
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N5 0.026(5) 0.028(5) 0.069(8) -0.004(5) -0.011(5) -0.006(4)
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N7 0.029(4) 0.028(5) 0.033(5) 0.011(4) -0.005(4) -0.005(4)
N8 0.037(5) 0.027(5) 0.052(7) 0.008(4) -0.019(5) -0.012(4)
N9 0.029(4) 0.054(6) 0.021(5) 0.000(4) -0.011(4) -0.024(4)
N10 0.029(4) 0.030(5) 0.025(5) 0.002(4) 0.000(4) -0.014(4)
N11 0.028(4) 0.027(5) 0.034(5) 0.004(4) -0.017(4) -0.009(4)
N12 0.028(4) 0.039(5) 0.025(5) -0.005(4) -0.008(4) -0.017(4)
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N14 0.044(5) 0.040(6) 0.042(6) 0.007(5) -0.017(5) -0.020(5)
N15 0.022(4) 0.046(6) 0.051(6) 0.010(5) -0.014(4) -0.020(4)
N16 0.032(5) 0.040(5) 0.034(5) 0.006(4) -0.017(4) -0.024(4)
N17 0.020(4) 0.031(5) 0.087(9) 0.009(5) -0.011(5) -0.014(4)
N18 0.025(4) 0.024(5) 0.063(7) 0.008(5) -0.008(5) -0.011(4)
N19 0.036(5) 0.019(5) 0.053(7) -0.003(4) -0.010(5) -0.011(4)
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C6 0.038(6) 0.049(7) 0.036(7) 0.011(5) -0.018(5) -0.024(5)
C7 0.033(6) 0.035(6) 0.033(6) 0.014(5) -0.010(5) -0.010(5)
C8 0.032(5) 0.027(6) 0.037(6) 0.005(5) -0.013(5) -0.009(5)
C9 0.039(6) 0.034(7) 0.034(6) -0.006(5) -0.014(5) -0.007(5)
C10 0.050(7) 0.036(7) 0.050(8) -0.004(6) -0.025(6) -0.005(6)
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C63 0.019(4) 0.028(5) 0.029(5) 0.007(4) -0.012(4) -0.012(4)
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C85 0.034(6) 0.038(7) 0.053(8) -0.005(5) -0.019(5) -0.021(5)
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C87 0.025(5) 0.035(6) 0.032(6) 0.003(4) -0.016(4) -0.017(4)
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C89 0.034(6) 0.031(6) 0.043(7) 0.005(5) -0.015(5) -0.014(5)
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C98 0.055(8) 0.069(10) 0.092(12) 0.043(9) -0.053(9) -0.047(8)
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C103 0.022(5) 0.037(6) 0.047(7) 0.003(5) -0.008(5) -0.019(5)
C104 0.026(5) 0.020(5) 0.043(7) -0.001(5) -0.013(5) -0.004(4)
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C111 0.022(5) 0.033(6) 0.046(7) -0.008(5) -0.006(5) -0.009(4)
C112 0.034(6) 0.026(6) 0.063(8) 0.009(6) -0.026(6) -0.011(5)

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C116 0.056(8) 0.034(7) 0.041(8) 0.001(6) -0.010(6) -0.014(6)
C117 0.024(6) 0.042(8) 0.075(10) -0.006(7) -0.012(6) -0.007(5)
C118 0.044(6) 0.036(7) 0.036(7) 0.003(5) -0.016(5) -0.017(5)
C119 0.016(5) 0.036(6) 0.060(8) -0.006(6) -0.009(5) -0.008(4)
C120 0.030(5) 0.023(6) 0.060(8) -0.003(5) -0.007(5) -0.017(5)
C121 0.031(5) 0.034(6) 0.044(7) 0.010(5) -0.015(5) -0.019(5)
C122 0.039(6) 0.032(6) 0.040(7) -0.004(5) -0.008(5) -0.014(5)
C123 0.044(7) 0.053(9) 0.070(10) -0.004(7) -0.015(7) -0.024(6)
C124 0.040(6) 0.054(8) 0.039(7) 0.004(6) -0.005(5) -0.027(6)
C125 0.054(7) 0.035(6) 0.047(7) 0.018(5) -0.024(6) -0.036(6)
C126 0.034(5) 0.023(5) 0.028(6) 0.011(4) -0.006(4) -0.018(4)
C127 0.037(6) 0.034(6) 0.027(6) 0.006(5) -0.007(5) -0.016(5)
C128 0.039(6) 0.027(6) 0.036(6) 0.004(5) -0.008(5) -0.016(5)
C129 0.042(6) 0.030(6) 0.044(7) -0.003(5) -0.008(5) -0.017(5)
C130 0.052(7) 0.049(8) 0.038(7) 0.007(6) -0.021(6) -0.029(6)
C131 0.068(9) 0.022(6) 0.071(10) 0.006(6) -0.032(8) -0.014(6)
C132 0.058(8) 0.031(7) 0.059(9) 0.006(6) -0.022(7) -0.022(6)
C133 0.049(7) 0.024(6) 0.051(8) -0.003(6) -0.013(6) 0.000(5)
C134 0.054(7) 0.022(6) 0.054(8) 0.000(5) -0.022(6) -0.020(5)
C135 0.037(6) 0.035(7) 0.042(7) 0.005(5) -0.006(5) -0.017(5)
C136 0.025(5) 0.017(5) 0.033(6) -0.004(4) -0.007(4) -0.002(4)
C137 0.044(6) 0.035(7) 0.047(8) 0.021(6) -0.025(6) -0.015(5)
C138 0.050(7) 0.035(7) 0.039(7) 0.007(5) -0.019(6) -0.014(5)
C139 0.058(8) 0.037(7) 0.046(8) 0.008(6) -0.025(6) -0.016(6)
C140 0.050(7) 0.042(8) 0.053(9) 0.008(6) -0.014(6) -0.021(6)
C141 0.048(7) 0.034(7) 0.047(8) 0.019(6) -0.014(6) -0.025(5)
C142 0.043(6) 0.048(7) 0.024(6) -0.011(5) 0.008(5) -0.030(6)
C143 0.032(5) 0.031(6) 0.039(7) 0.014(5) -0.017(5) -0.016(5)
C144 0.031(5) 0.017(5) 0.035(6) -0.003(4) -0.009(5) -0.009(4)
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C148 0.086(13) 0.056(11) 0.126(19) 0.013(12) -0.055(13) -0.012(10)
C149 0.052(8) 0.059(10) 0.089(13) 0.018(9) -0.033(9) -0.017(7)
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C156 0.135(18) 0.047(11) 0.18(3) -0.005(14) -0.108(19) -0.017(12)
C157 0.062(9) 0.047(9) 0.120(15) 0.012(9) -0.050(10) -0.030(7)
C158 0.059(10) 0.076(13) 0.069(12) -0.003(9) -0.027(9) 0.025(9)
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C161 0.17(2) 0.102(16) 0.074(13) 0.031(11) -0.047(14) -0.113(16)
C162 0.125(17) 0.087(15) 0.080(14) 0.014(11) -0.072(13) -0.026(12)
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C164 0.135(19) 0.17(3) 0.066(14) 0.004(15) 0.012(13) -0.11(2)
C165 0.096(12) 0.041(9) 0.112(15) 0.020(9) -0.068(11) -0.035(8)
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C216 0.082(10) 0.070(11) 0.070(11) 0.027(8) -0.053(9) -0.039(9)
C217 0.056(8) 0.056(9) 0.089(12) -0.006(8) -0.042(8) -0.023(7)
C218 0.071(9) 0.047(9) 0.115(14) 0.042(9) -0.075(10) -0.026(7)
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C222 0.072(9) 0.049(8) 0.078(11) 0.021(7) -0.047(8) -0.041(7)
C223 0.072(9) 0.042(8) 0.063(10) -0.003(7) -0.019(8) -0.025(7)
C224 0.055(8) 0.066(11) 0.075(12) -0.021(9) -0.013(8) -0.021(8)
C225 0.071(10) 0.066(11) 0.087(14) 0.027(10) -0.034(10) -0.039(9)
C226 0.067(10) 0.085(13) 0.064(11) 0.003(9) -0.022(8) -0.041(9)
C227 0.125(17) 0.14(2) 0.043(10) -0.004(12) -0.027(11) -0.093(17)
C228 0.069(10) 0.055(11) 0.111(17) -0.033(11) -0.012(10) -0.018(9)
C229 0.074(12) 0.14(2) 0.107(19) -0.022(16) -0.022(13) -0.050(13)
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C232 0.14(2) 0.077(17) 0.15(3) 0.013(16) -0.053(19) -0.019(15)
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C234 0.15(3) 0.31(6) 0.27(5) 0.17(4) -0.17(3) -0.13(3)

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_geom_special_details
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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P1 O2 1.565(9) . ?
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P2 O8 1.514(8) . ?
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P2 O7 1.546(9) . ?
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P3 O9 1.503(7) . ?
P3 O10 1.549(8) . ?
P3 O12 1.567(8) . ?
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P4 O14 1.525(8) . ?
P4 O13 1.557(8) . ?
P4 O15 1.589(9) . ?
P5 O20 1.514(7) . ?
P5 O18 1.516(7) . ?
P5 O19 1.540(7) . ?
P5 O17 1.594(8) . ?
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N1 C1 1.371(16) . ?
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N2 C9 1.324(16) . ?
N2 C8 1.367(15) . ?
N3 C15 1.319(15) . ?
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N5 H5 0.8600 . ?
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N6 C33 1.354(17) . ?
N7 C38 1.307(15) . ?
N7 C39 1.388(14) . ?
N8 C47 1.417(15) . ?
N8 C46 1.420(15) . ?
N8 H8 0.8600 . ?
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N9 C72 1.396(14) . ?
N9 H9 0.8600 . ?
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C48 C31 C30 105.0(10) . . ?
C32 C31 C30 132.7(11) . . ?
N6 C32 C31 121.1(10) . . ?
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C44 C45 H45 121.3 . . ?
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C99 C100 H100 120.5 . . ?
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C172 C171 H17D 109.0 . . ?
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N5 C25 C30 C29 -178.7(12) . . . . ?
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N5 C25 C30 C31 -2.0(15) . . . . ?
C26 C25 C30 C31 177.8(12) . . . . ?
C29 C30 C31 C48 175.6(15) . . . . ?
C25 C30 C31 C48 -0.4(13) . . . . ?
C29 C30 C31 C32 -3(3) . . . . ?
C25 C30 C31 C32 -179.3(13) . . . . ?
C33 N6 C32 C31 -178.6(12) . . . . ?
C33 N6 C32 C39 0.3(18) . . . . ?
C48 C31 C32 N6 -177.8(11) . . . . ?
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C48 C31 C32 C39 3.3(17) . . . . ?
C30 C31 C32 C39 -178.0(12) . . . . ?
C32 N6 C33 C34 -178.1(13) . . . . ?
C32 N6 C33 C38 -3.9(19) . . . . ?
N6 C33 C34 C35 177.5(15) . . . . ?
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C33 C34 C35 C36 -2(3) . . . . ?
C34 C35 C36 C37 -1(3) . . . . ?
C35 C36 C37 C38 2(3) . . . . ?
C39 N7 C38 C33 -0.9(19) . . . . ?
C39 N7 C38 C37 179.7(12) . . . . ?
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C34 C33 C38 N7 178.4(14) . . . . ?
N6 C33 C38 C37 -176.2(13) . . . . ?
C34 C33 C38 C37 -2(2) . . . . ?
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C38 N7 C39 C40 -177.0(11) . . . . ?
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C31 C32 C39 N7 -177.8(11) . . . . ?
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N7 C39 C40 C41 -7(2) . . . . ?
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C47 C40 C41 C46 -3.8(15) . . . . ?
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C40 C41 C42 C43 -178.7(14) . . . . ?
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C42 C43 C44 C45 -2(2) . . . . ?
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C46 N8 C47 C40 -2.6(13) . . . . ?
C46 N8 C47 C48 -178.4(12) . . . . ?
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C25 N5 C48 C47 -178.4(13) . . . . ?
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C53 C54 C55 C72 -178.6(12) . . . . ?
C49 C54 C55 C56 -176.7(11) . . . . ?
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C57 N10 C56 C55 -178.2(9) . . . . ?
C72 C55 C56 N10 -175.9(9) . . . . ?
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N10 C57 C58 C59 176.7(11) . . . . ?
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C63 N11 C62 C57 2.0(15) . . . . ?
C60 C61 C62 N11 -176.2(11) . . . . ?
C60 C61 C62 C57 1.6(18) . . . . ?
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C62 N11 C63 C64 -180.0(9) . . . . ?
N10 C56 C63 N11 -2.0(16) . . . . ?
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N10 C56 C63 C64 178.1(10) . . . . ?
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N11 C63 C64 C65 -1.4(18) . . . . ?
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C63 C64 C65 C70 -176.3(11) . . . . ?
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C56 C55 C72 N9 175.8(9) . . . . ?
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C96 N13 C73 C78 -1.6(14) . . . . ?
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N13 C73 C78 C77 -174.9(11) . . . . ?
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C77 C78 C79 C96 175.7(13) . . . . ?
C73 C78 C79 C96 2.8(13) . . . . ?
C77 C78 C79 C80 -6(2) . . . . ?
C73 C78 C79 C80 -178.9(12) . . . . ?
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C81 N14 C80 C87 -1.6(16) . . . . ?
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C96 C79 C80 N14 176.2(11) . . . . ?
C78 C79 C80 C87 179.9(12) . . . . ?
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C84 C85 C86 C81 2.1(17) . . . . ?
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C86 N15 C87 C80 -3.5(16) . . . . ?
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N14 C80 C87 C88 -178.6(11) . . . . ?
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N15 C87 C88 C89 -6(2) . . . . ?
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C95 C88 C89 C90 179.6(13) . . . . ?
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C94 N16 C95 C88 -1.6(14) . . . . ?
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C108 C109 C110 C105 -2(2) . . . . ?
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C104 C111 C112 C119 2.8(18) . . . . ?
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C114 C115 C116 C117 -3(2) . . . . ?
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N22 C129 C134 C133 177.6(12) . . . . ?
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