Crystal structure of *tert*-butylammonium trifluoroacetyl-*N*-(*tert*-butylamino)dioxophosphate acetonitrile solvate hydrate (1 : 0.333 : 0.333), $(C_4H_9NH_3)[(F_3C_2ONH)(C_4H_9NH)PO_2)] \cdot 0.333\,CH_3CN \cdot 0.333\,H_2O$

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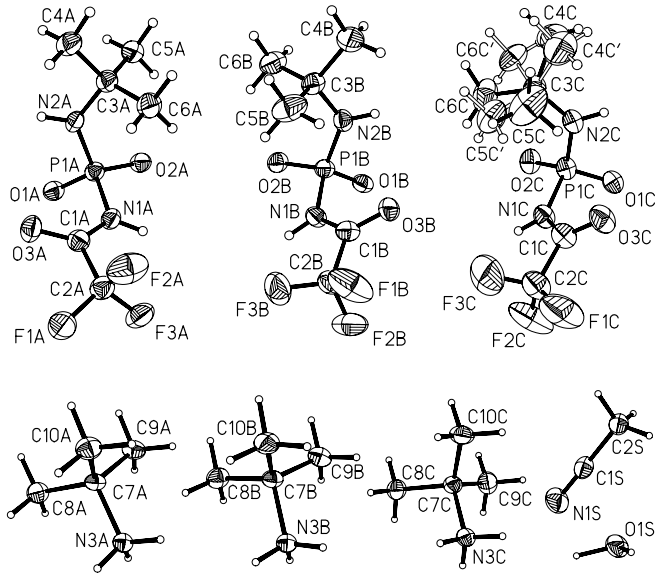

Abstract

$C_{10.667}H_{24.667}F_3N_{3.333}O_{3.333}P$, triclinic, $P\bar{1}$ (no. 2),
a = 10.523(3) Å, b = 16.082(5) Å, c = 17.382(5) Å,
α = 65.120(5)°, β = 86.867(5)°, γ = 78.073(5)°, V = 2609.2 Å^3,
Z = 6, $R_{gt}(F)$ = 0.062, $wR_{ref}(F^2)$ = 0.149, T = 120 K.

Source of material

The title compound was synthesized by the reaction of N-trifluoroacetyl phosphoramidic dichloride (1 mmol) with *tert*-butylamine (4 mmol) in CH_3CN under 4 hours stirring at 0 °C. The solvent was removed and the residue was washed with distilled water. Single crystals of product were obtained from a mixture of methanol and acetonitrile after slow evaporation at room temperature.

Experimental details

Because of the strong correlation, it was impossible to refine both thermal parameters (U_{eq}) and site occupancy factor (*s.o.f.*) simultaneously for the disordered atoms. Therefore, the refinement was done step by step: first thermal parameters, then *s.o.f.*, then again thermal parameters and so on. Final refinement was carried out with fixed site occupancy factor. The refinement with restrained C—C bond distances revealed that the *s.o.f.* values are 0.63 and 0.37. The U_{eq} values for C atoms are 0.062 Å^2 – 0.078 Å^2 for the major part and 0.076 Å^2 – 0.072 Å^2 for the minor part.

Discussion

In a previous study, we have reported the crystal structure of $(C_{10}H_{20}NH_2)PCl_2O_2$ which consists of two symmetrically independent dichlorophosphate anions as well as cyclohexyl-*tert*-butylammonium cations linked by four different kinds of intermolecular hydrogen bonds [1].

The crystal structure of the title compound is composed of three symmetrically independent trifluoroacetyl-*N*-(*tert*-butylamino)-phosphate anions and three independent cations of *tert*-butylammonium, labeled with A, B and C. The anion labeled with ″C″ indicates disorder in the *tert*-C_4H_9 moiety (see C4C, C4C′, C5C, C5C′, C6C and C6C′ (figure, top). The P1A—O1A, P1B—O1B and P1C—O1C bond lengths (1.477(2) Å, 1.480(2) Å and 1.480(2) Å) are slightly longer than the P=O double bond length (1.45 Å) [2]. The P—N(amine) bond lengths of 1.626(3) Å, 1.628(3) Å and 1.624(3) Å for P1A—N2A, P1B—N2B and P1C—N2C, respectively, are shorter than the P—N single bond length (1.77 Å) [2] and P—N(amide) bond lengths (due to the resonance interaction of N(amide) with the C=O-π system). The phosphorus atom has slightly distorted tetrahedral configuration. The bond angles around P1A, P1B and P1C are in the range of 102.4(1)° – 120.4(1)°, 102.9(1)° – 119.0(1)° and 102.8(1)° – 118.3(2)°, respectively. The maximum and minimum values in each conformer are corresponding for the O2–P1–O1 and O2–P1–N1 angles. The environments of the nitrogen atoms are practically planar. The bond angles C1A–N1A–P1A, C3A–N2A–P1A, C1B–N1B–P1B, C3B–N2B–P1B, C1C–N1C–P1C and C3C–N2C–P1C are 124.8(2)°, 126.6(2)°, 125.6(2)°, 128.7(2)°, 124.7(2)° and 129.8(2)°, respectively. These results are in agreement with the sp^2 hybridization for nitrogen atoms, although some angles differ from the ideal values. In the network of the title structure, the organo-phosphate anions, *tert*-$C_4H_9NH_3^+$ cations, H_2O and CH_3CN molecules produce fifteen types of hydrogen bonds leading to infinite chains running along [01$\bar{1}$].

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.10 × 0.15 × 0.45 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.01 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ/ω
$2\theta_{max}$:	52.24°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	21211, 10129
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 5713
$N(param)_{refined}$:	604
Program:	SHELXTL [3]

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Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{iso}
H(1AA)	2*i*		0.5372	0.2304	–0.0049	0.037
H(2AA)	2*i*		0.7234	0.0252	0.2035	0.037
H(4AA)	2*i*		0.8115	–0.0922	0.1507	0.061
H(4AB)	2*i*		0.9132	–0.0862	0.2124	0.061
H(4AC)	2*i*		0.9591	–0.0891	0.1241	0.061
H(5AA)	2*i*		0.9386	0.1499	0.0936	0.060
H(5AB)	2*i*		1.0383	0.0645	0.0854	0.060
H(5AC)	2*i*		0.9924	0.0573	0.1769	0.060
H(6AA)	2*i*		0.7903	0.1383	–0.0108	0.062
H(6AB)	2*i*		0.7414	0.0428	0.0137	0.062
H(6AC)	2*i*		0.8892	0.0482	–0.0108	0.062
H(1BA)	2*i*		0.4411	0.4957	0.2832	0.039
H(2BA)	2*i*		0.2032	0.6280	0.0763	0.040
H(4BA)	2*i*		–0.0237	0.6882	0.0553	0.083
H(4BB)	2*i*		0.0482	0.7587	0.0706	0.083
H(4BC)	2*i*		–0.0812	0.7330	0.1196	0.083
H(5BA)	2*i*		0.1674	0.6083	0.2814	0.089
H(5BB)	2*i*		0.0353	0.6855	0.2562	0.089
H(5BC)	2*i*		0.1650	0.7102	0.2071	0.089
H(6BA)	2*i*		–0.0191	0.5313	0.1670	0.074
H(6BB)	2*i*		–0.0777	0.5764	0.2310	0.074
H(6BC)	2*i*		0.0537	0.4986	0.2566	0.074
H(1CA)	2*i*		0.5984	0.2115	0.5450	0.043
H(2CA)	2*i*		0.2676	0.3060	0.4023	0.045
H(4CA)	2*i*	0.63	0.0770	0.4014	0.4120	0.117
H(4CB)	2*i*	0.63	0.0364	0.4022	0.5018	0.117
H(4CC)	2*i*	0.63	0.0531	0.3075	0.4892	0.117
H(5CA)	2*i*	0.63	0.2698	0.4631	0.4099	0.113
H(5CB)	2*i*	0.63	0.3694	0.4148	0.4902	0.113
H(5CC)	2*i*	0.63	0.2276	0.4704	0.4970	0.113
H(6CA)	2*i*	0.63	0.3402	0.2752	0.6100	0.093
H(6CB)	2*i*	0.63	0.2132	0.2327	0.6166	0.093
H(6CC)	2*i*	0.63	0.2015	0.3310	0.6218	0.093
H(4CD)	2*i*	0.37	0.1718	0.4673	0.3993	0.114
H(4CE)	2*i*	0.37	0.0680	0.4486	0.4724	0.114
H(4CF)	2*i*	0.37	0.0776	0.3968	0.4106	0.114
H(5CD)	2*i*	0.37	0.3645	0.4054	0.5157	0.107
H(5CE)	2*i*	0.37	0.3685	0.3040	0.5912	0.107
H(5CF)	2*i*	0.37	0.2576	0.3907	0.5868	0.107
H(6CD)	2*i*	0.37	0.0801	0.2642	0.5315	0.114
H(6CE)	2*i*	0.37	0.0918	0.3109	0.5952	0.114
H(6CF)	2*i*	0.37	0.1957	0.2199	0.6020	0.114

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(3AA)	2*i*		0.3328	0.6408	–0.0793	0.046
H(3AB)	2*i*		0.4346	0.5671	–0.0892	0.046
H(3AC)	2*i*		0.3664	0.5463	–0.0080	0.046
H(8AA)	2*i*		0.3387	0.5818	–0.2145	0.064
H(8AB)	2*i*		0.2287	0.6650	–0.2106	0.064
H(8AC)	2*i*		0.1886	0.5775	–0.2173	0.064
H(9AA)	2*i*		0.1365	0.5436	0.0004	0.065
H(9AB)	2*i*		0.0608	0.5511	–0.0805	0.065
H(9AC)	2*i*		0.1047	0.6412	–0.0817	0.065
H(10A)	2*i*		0.3836	0.4275	–0.0900	0.063
H(10B)	2*i*		0.2345	0.4192	–0.0891	0.063
H(10C)	2*i*		0.3031	0.4121	–0.0060	0.063
H(3BA)	2*i*		0.4114	0.2338	0.2243	0.047
H(3BB)	2*i*		0.3676	0.2179	0.3112	0.047
H(3BC)	2*i*		0.3237	0.3104	0.2392	0.047
H(8BA)	2*i*		0.2729	0.2458	0.1149	0.069
H(8BB)	2*i*		0.1779	0.3310	0.1265	0.069
H(8BC)	2*i*		0.1227	0.2430	0.1325	0.069
H(9BA)	2*i*		0.1394	0.2119	0.3490	0.070
H(9BB)	2*i*		0.0383	0.2306	0.2752	0.070
H(9BC)	2*i*		0.1056	0.3129	0.2712	0.070
H(10D)	2*i*		0.3391	0.0950	0.2387	0.067
H(10E)	2*i*		0.1903	0.0886	0.2588	0.067
H(10F)	2*i*		0.2863	0.0819	0.3303	0.067
H(3CA)	2*i*		0.4268	–0.0834	0.6081	0.050
H(3CB)	2*i*		0.3743	–0.0795	0.6879	0.050
H(3CC)	2*i*		0.3815	0.0085	0.6121	0.050
H(8CA)	2*i*		0.1473	–0.0043	0.4839	0.070
H(8CB)	2*i*		0.2957	–0.0572	0.4913	0.070
H(8CC)	2*i*		0.2617	0.0486	0.4812	0.070
H(9CA)	2*i*		0.1444	–0.0015	0.6890	0.083
H(9CB)	2*i*		0.0501	0.0234	0.6098	0.083
H(9CC)	2*i*		0.1596	0.0827	0.5997	0.083
H(10G)	2*i*		0.2052	–0.1630	0.7059	0.082
H(10H)	2*i*		0.2763	–0.1870	0.6318	0.082
H(10I)	2*i*		0.1233	–0.1452	0.6236	0.082
H(1SA)	2*i*		0.4643	0.0331	0.7835	0.073
H(1SB)	2*i*		0.4310	0.0862	0.6827	0.073
H(2SA)	2*i*		0.6705	0.1638	0.8260	0.070
H(2SB)	2*i*		0.8109	0.0989	0.8336	0.070
H(2SC)	2*i*		0.6842	0.0538	0.8547	0.070

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
P(1A)	2*i*		0.64659(8)	0.17137(6)	0.12316(5)	0.0291(5)	0.0258(5)	0.0304(5)	–0.0057(4)	–0.0016(4)	–0.0101(4)
F(1A)	2*i*		0.2654(2)	0.1179(2)	0.0011(1)	0.051(1)	0.055(2)	0.055(1)	–0.028(1)	–0.014(1)	–0.004(1)
F(2A)	2*i*		0.4344(2)	0.1079(2)	–0.0689(2)	0.067(2)	0.079(2)	0.057(2)	0.010(1)	–0.018(1)	–0.044(1)
F(3A)	2*i*		0.3419(2)	0.2386(2)	–0.0706(1)	0.050(1)	0.038(1)	0.052(1)	–0.014(1)	–0.020(1)	0.001(1)
O(1A)	2*i*		0.5666(2)	0.1730(2)	0.1952(1)	0.033(1)	0.035(1)	0.033(1)	–0.004(1)	–0.003(1)	–0.013(1)
O(2A)	2*i*		0.7182(2)	0.2465(2)	0.0768(1)	0.031(1)	0.027(1)	0.040(1)	–0.006(1)	–0.003(1)	–0.011(1)
O(3A)	2*i*		0.4462(2)	0.0588(2)	0.1199(1)	0.047(2)	0.033(1)	0.032(1)	–0.016(1)	–0.001(1)	–0.006(1)
N(1A)	2*i*		0.5385(3)	0.1831(2)	0.0451(2)	0.032(2)	0.026(2)	0.029(1)	–0.007(1)	–0.002(1)	–0.006(1)
N(2A)	2*i*		0.7406(3)	0.0683(2)	0.1546(2)	0.035(2)	0.026(2)	0.024(1)	–0.004(1)	–0.001(1)	–0.004(1)
C(1A)	2*i*		0.4585(3)	0.1264(2)	0.0554(2)	0.031(2)	0.026(2)	0.036(2)	–0.005(2)	0.001(2)	–0.013(2)
C(2A)	2*i*		0.3740(3)	0.1480(2)	–0.0217(2)	0.035(2)	0.031(2)	0.036(2)	–0.008(2)	–0.005(2)	–0.010(2)
C(3A)	2*i*		0.8517(3)	0.0396(2)	0.1096(2)	0.036(2)	0.030(2)	0.033(2)	–0.004(2)	0.003(2)	–0.011(2)
C(4A)	2*i*		0.8870(4)	–0.0663(2)	0.1530(2)	0.042(2)	0.032(2)	0.042(2)	–0.001(2)	–0.001(2)	–0.012(2)
C(5A)	2*i*		0.9654(3)	0.0816(3)	0.1170(2)	0.036(2)	0.038(2)	0.042(2)	–0.006(2)	0.002(2)	–0.012(2)
C(6A)	2*i*		0.8149(4)	0.0699(3)	0.0173(2)	0.043(2)	0.044(2)	0.033(2)	–0.002(2)	0.003(2)	–0.016(2)
P(1B)	2*i*		0.31583(8)	0.50589(6)	0.17606(5)	0.0283(5)	0.0272(5)	0.0340(5)	–0.0058(4)	–0.0024(4)	–0.0106(4)
F(1B)	2*i*		0.5228(3)	0.7154(2)	0.2552(2)	0.105(2)	0.039(1)	0.090(2)	–0.005(1)	–0.051(2)	–0.028(1)
F(2B)	2*i*		0.6587(2)	0.5999(2)	0.2550(2)	0.040(1)	0.088(2)	0.076(2)	–0.010(1)	–0.012(1)	–0.041(2)
F(3B)	2*i*		0.5148(3)	0.5790(2)	0.3460(1)	0.093(2)	0.091(2)	0.039(1)	–0.054(2)	–0.002(1)	–0.020(1)
O(1B)	2*i*		0.3965(2)	0.4914(2)	0.1086(1)	0.031(1)	0.032(1)	0.036(1)	–0.002(1)	–0.006(1)	–0.011(1)
O(2B)	2*i*		0.2712(2)	0.4255(2)	0.2429(1)	0.034(1)	0.026(1)	0.043(1)	–0.010(1)	0.002(1)	–0.009(1)

Table 3. Continued.

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(3B)	2*i*		0.4193(2)	0.6855(2)	0.1363(1)	0.039(1)	0.030(1)	0.035(1)	–0.012(1)	–0.004(1)	–0.001(1)
N(1B)	2*i*		0.4130(3)	0.5376(2)	0.2320(2)	0.037(2)	0.028(2)	0.030(2)	–0.009(1)	–0.006(1)	–0.008(1)
N(2B)	2*i*		0.1969(3)	0.5948(2)	0.1311(2)	0.038(2)	0.031(2)	0.029(1)	–0.011(1)	0.001(1)	–0.009(1)
C(1B)	2*i*		0.4487(3)	0.6195(3)	0.2044(2)	0.030(2)	0.033(2)	0.039(2)	–0.006(2)	–0.003(2)	–0.016(2)
C(2B)	2*i*		0.5359(4)	0.6291(3)	0.2665(2)	0.041(2)	0.036(2)	0.042(2)	–0.008(2)	–0.006(2)	–0.015(2)
C(3B)	2*i*		0.0801(3)	0.6271(2)	0.1697(2)	0.032(2)	0.028(2)	0.045(2)	–0.008(2)	0.002(2)	–0.014(2)
C(4B)	2*i*		–0.0014(4)	0.7090(3)	0.0974(3)	0.044(2)	0.046(3)	0.058(3)	0.004(2)	0.002(2)	–0.010(2)
C(5B)	2*i*		0.1151(4)	0.6608(3)	0.2344(3)	0.041(2)	0.077(3)	0.079(3)	–0.011(2)	0.009(2)	–0.052(3)
C(6B)	2*i*		0.0025(4)	0.5518(3)	0.2095(3)	0.035(2)	0.044(2)	0.065(3)	–0.009(2)	0.004(2)	–0.020(2)
P(1C)	2*i*		0.42030(9)	0.20025(6)	0.48562(6)	0.0419(6)	0.0289(5)	0.0319(5)	–0.0094(4)	–0.0013(4)	–0.0098(4)
F(1C)	2*i*		0.7566(3)	0.4028(2)	0.3990(2)	0.081(2)	0.093(2)	0.084(2)	–0.061(2)	–0.016(2)	0.017(2)
F(2C)	2*i*		0.8089(3)	0.2646(2)	0.4888(2)	0.064(2)	0.071(2)	0.131(3)	–0.017(2)	–0.044(2)	–0.016(2)
F(3C)	2*i*		0.6947(3)	0.3629(3)	0.5235(2)	0.120(3)	0.169(3)	0.119(3)	–0.088(3)	0.020(2)	–0.097(3)
O(1C)	2*i*		0.4478(2)	0.1692(2)	0.4164(1)	0.043(1)	0.032(1)	0.038(1)	–0.005(1)	–0.005(1)	–0.013(1)
O(2C)	2*i*		0.4079(2)	0.1291(2)	0.5721(1)	0.056(2)	0.035(1)	0.035(1)	–0.017(1)	0.004(1)	–0.010(1)
O(3C)	2*i*		0.5397(2)	0.3644(2)	0.3686(2)	0.051(2)	0.037(2)	0.036(1)	–0.009(1)	–0.011(1)	0.001(1)
N(1C)	2*i*		0.5530(3)	0.2414(2)	0.4966(2)	0.041(2)	0.031(2)	0.029(2)	–0.010(1)	–0.004(1)	–0.004(1)
N(2C)	2*i*		0.2967(3)	0.2875(2)	0.4546(2)	0.041(2)	0.038(2)	0.034(2)	–0.009(2)	–0.004(1)	–0.015(1)
C(1C)	2*i*		0.5921(4)	0.3147(3)	0.4377(2)	0.042(2)	0.033(2)	0.043(2)	–0.009(2)	–0.004(2)	–0.013(2)
C(2C)	2*i*		0.7137(4)	0.3379(3)	0.4612(3)	0.054(3)	0.048(3)	0.047(2)	–0.021(2)	–0.006(2)	–0.008(2)
C(3C)	2*i*		0.2259(4)	0.3404(2)	0.5008(2)	0.054(3)	0.041(2)	0.040(2)	–0.005(2)	0.004(2)	–0.019(2)
C(4C)	2*i*	0.63	0.0861(6)	0.3650(7)	0.4736(7)	0.052(5)	0.103(8)	0.101(8)	0.004(5)	–0.004(5)	–0.072(7)
C(5C)	2*i*	0.63	0.2778(8)	0.4302(5)	0.4719(6)	0.099(6)	0.059(5)	0.096(6)	–0.033(5)	0.034(5)	–0.055(5)
C(6C)	2*i*	0.63	0.2470(8)	0.2905(5)	0.5955(3)	0.083(6)	0.051(5)	0.044(4)	0.011(4)	–0.009(4)	–0.023(3)
C(4C')	2*i*	0.37	0.127(1)	0.4202(9)	0.4405(8)	0.08(1)	0.08(1)	0.064(9)	0.010(9)	0.008(8)	–0.032(8)
C(5C')	2*i*	0.37	0.312(1)	0.362(1)	0.5531(9)	0.077(9)	0.07(1)	0.09(1)	–0.011(8)	0.012(8)	–0.063(9)
C(6C')	2*i*	0.37	0.141(1)	0.2783(8)	0.5629(8)	0.09(1)	0.064(9)	0.074(9)	0.010(8)	0.008(8)	–0.037(8)
N(3A)	2*i*		0.3574(3)	0.5784(2)	–0.0655(2)	0.031(2)	0.026(2)	0.032(2)	–0.005(1)	–0.000(1)	–0.009(1)
C(7A)	2*i*		0.2566(3)	0.5472(2)	–0.0980(2)	0.029(2)	0.029(2)	0.036(2)	–0.010(2)	–0.001(2)	–0.010(2)
C(8A)	2*i*		0.2528(4)	0.5972(3)	–0.1935(2)	0.048(2)	0.039(2)	0.035(2)	–0.012(2)	–0.005(2)	–0.007(2)
C(9A)	2*i*		0.1284(3)	0.5730(3)	–0.0618(2)	0.032(2)	0.045(2)	0.054(2)	–0.011(2)	0.004(2)	–0.020(2)
C(10A)	2*i*		0.2981(4)	0.4422(2)	–0.0681(2)	0.047(2)	0.029(2)	0.047(2)	–0.009(2)	–0.001(2)	–0.013(2)
N(3B)	2*i*		0.3441(3)	0.2475(2)	0.2551(2)	0.032(2)	0.025(2)	0.034(2)	–0.005(1)	0.000(1)	–0.011(1)
C(7B)	2*i*		0.2289(3)	0.2154(2)	0.2394(2)	0.033(2)	0.031(2)	0.036(2)	–0.011(2)	–0.002(2)	–0.009(2)
C(8B)	2*i*		0.1979(4)	0.2629(3)	0.1451(2)	0.047(2)	0.044(2)	0.042(2)	–0.011(2)	–0.008(2)	–0.011(2)
C(9B)	2*i*		0.1183(4)	0.2453(3)	0.2880(2)	0.038(2)	0.047(2)	0.053(2)	–0.012(2)	0.006(2)	–0.017(2)
C(10B)	2*i*		0.2642(4)	0.1112(2)	0.2694(2)	0.058(3)	0.030(2)	0.043(2)	–0.018(2)	0.000(2)	–0.008(2)
N(3C)	2*i*		0.3671(3)	–0.0506(2)	0.6302(2)	0.038(2)	0.028(2)	0.030(2)	–0.008(1)	–0.001(1)	–0.006(1)
C(7C)	2*i*		0.2328(3)	–0.0464(3)	0.6015(2)	0.038(2)	0.044(2)	0.034(2)	–0.015(2)	–0.002(2)	–0.012(2)
C(8C)	2*i*		0.2345(4)	–0.0118(3)	0.5061(2)	0.053(2)	0.051(3)	0.034(2)	–0.016(2)	–0.004(2)	–0.013(2)
C(9C)	2*i*		0.1386(4)	0.0203(3)	0.6273(3)	0.040(2)	0.075(3)	0.047(2)	–0.005(2)	–0.001(2)	–0.025(2)
C(10C)	2*i*		0.2072(4)	–0.1438(3)	0.6444(2)	0.057(3)	0.058(3)	0.048(2)	–0.033(2)	0.001(2)	–0.012(2)
O(1S)	2*i*		0.3893(3)	0.0814(2)	0.7419(2)	0.069(2)	0.057(2)	0.044(2)	–0.019(2)	–0.001(1)	–0.005(1)
N(1S)	2*i*		0.6966(4)	0.1356(3)	0.6629(2)	0.089(3)	0.069(3)	0.045(2)	–0.022(2)	–0.013(2)	–0.013(2)
C(1S)	2*i*		0.7061(4)	0.1247(3)	0.7311(3)	0.048(2)	0.042(2)	0.046(2)	–0.016(2)	–0.009(2)	–0.006(2)
C(2S)	2*i*		0.7189(4)	0.1091(3)	0.8183(2)	0.052(2)	0.041(2)	0.039(2)	–0.016(2)	–0.007(2)	–0.006(2)

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