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Crystal structure of (DL)-trithioureatartrato-O^1,O^2,O^3-cadmium, $C_{28}H_{64}Cd_4N_{24}O_{24}S_{12}$

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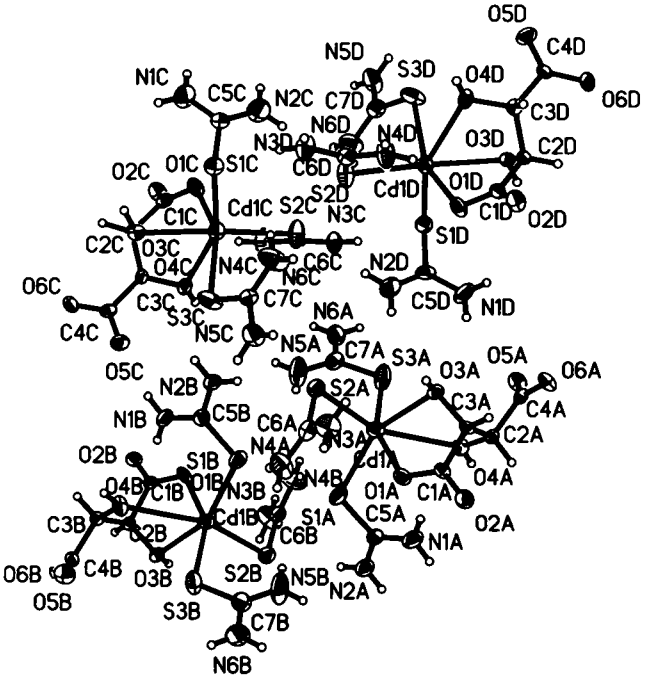

Abstract

$C_{28}H_{64}Cd_4N_{24}O_{24}S_{12}$, monoclinic, $Clc1$ (No. 9), a = 17.732(2) Å, b = 17.905(2) Å, c = 20.699(2) Å, β = 94.111(9)°, V = 6555.1 Å^3, Z = 1, $R_{gt}(F)$ = 0.028, $wR_{ref}(F^2)$ = 0.070, T = 295 K.

Source of material

The title compound was obtained by the reacting of cadmium hydroxide, tartaric acid and thiourea (molar ratio 1:1:3) in water. The crystals used for the X-ray structure analysis were obtained from a more dilute resulting aqueous solution by using temperature-lowering method.

Experimental details

The systematic absences were consistent with two possible space group *Cc* and *C2/c*, the non-centrosymmetric space group *Cc* was suggested by the intensity statistics (mean $|E^2-1|$ = 0.738) and confirmed by successful structure solution and refinement performed by SHELXTL program [1]. The solution in the space group *C2/c* was also attempted, but failed, neither direct nor patterson methods could solve the structure in the space group. The refinement was also failed by putting known molecule structure into *C2/c* space group.

Discussion

Considerable research has been done on finding organic materials, which are efficient and practical for second harmonic generate (SHG). Because materials with nonlinear optical (NLO) properties are important for many technological applications, such as optical switching, wave guides for optical transmission [2-4]. In order to explore novel NLO materials, our laboratory have done some work and found a set of new NLO crystal, urea-(D)tartaric acid (abbreviated as UDT) and urea-(DL)tartaric acid (UDLT) [5, 6]. On the basic of this work and combining the character of tartaric acid molecule with that of thiourea, we synthesized the title complex.

In the structure, the neighboring cadmium atoms are bridged by tartrate ions, which are interconnected by strong hydrogen bonds. As three thiourea molecules are also coordinated to each cadmium atom, the last is totally six-coordinated. The tartrate combines with Cd as a bidentate ligand to form a five-membered chelate ring. The length of C(3A)—O(4A) (1.432 Å) and of C(4A)—O(6A) (1.242 Å) bonds is larger than the corresponding lengths in UDLT. The bond angles of C(4A)–C(3A)–O(4A) (110.9(6)°) and O(6A)–C(4A)–C(3A) (119.2(8)°) is smaller than these of UDLT. The 171.9° of C–C–C–C torsion angle, compared with 175° in tartaric acid, shows that the chain is slightly distorted in the TUDLTC compound. The bond lengths and bond angles of the thiourea molecule in the title compound were compared to those found in a thiourea crystal [7]. No significant differences were found, as the molecule is fairly rigid because of the multiple character of C—N and C—S bonds. At the same time, the central Cd(II) atom has a distorted coordinative polyhedron. It may be the five-membered chelate ring and distorted polyhedron that make TUDLTC crystal have good nonlinear optical property.

Structure solution in *Cc* space group indicated two pseudo inversion center in the asymmetric unit: molecule A and B were related by the inversion center at about $x = 0$, $y = 0.375$, $z = 0$ and molecule C and D by that at $x = -0.5$, $y = 0.375$, $z = 0$, these position did not change during the structure refinement. Except those, we determined the powder SHG efficiencies by the powder technique of Kurtz and Perry. The incident radiation(1.064um) came from a Q-switched and mode-locked Nd:YAG laser and the results indicate that the powder SHG efficiency of TUDLTC is 2~3 times stronger than that of KDP.

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Table 1. Data collection and handling.

Crystal:	colourless, prism, size 0.3 × 0.3 × 0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	17.52 cm^{-1}
Diffractometer, scan mode:	Bruker P4, θ/2θ
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6639, 6190
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 5869
$N(param)_{refined}$:	829
Programs:	SHELXTL [1]

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

Atom	Site	x	y	z	U_{iso}
H(2AA)	4a	–0.1625	0.4786	0.2884	0.022
H(3AA)	4a	–0.0671	0.5722	0.2789	0.022
H(1AA)	4a	0.1257	0.5058	0.1954	0.053
H(1AB)	4a	0.0454	0.4812	0.1857	0.053
H(2AB)	4a	0.2022	0.4990	0.1144	0.042
H(2AC)	4a	0.1740	0.4698	0.0498	0.042
H(3AB)	4a	–0.1281	0.2100	0.1936	0.052
H(3AC)	4a	–0.1944	0.2609	0.1840	0.052
H(4AA)	4a	–0.0412	0.2052	0.1171	0.056
H(4AB)	4a	–0.0512	0.2529	0.0581	0.056
H(5AA)	4a	–0.1738	0.4398	–0.1075	0.073
H(5AB)	4a	–0.1416	0.4187	–0.0416	0.073
H(6AA)	4a	–0.2247	0.5526	–0.1265	0.049
H(6AB)	4a	–0.2269	0.6083	–0.0732	0.049
H(3AE)	4a	–0.2115	0.4330	0.1993	0.025
H(4AC)	4a	–0.0365	0.5990	0.1876	0.040
H(2BA)	4a	0.1711	0.2723	–0.2857	0.021
H(3BA)	4a	0.0812	0.1742	–0.2816	0.023
H(1BA)	4a	–0.1219	0.2256	–0.1883	0.041
H(1BB)	4a	–0.0406	0.2464	–0.1785	0.041
H(2BB)	4a	–0.2013	0.2455	–0.1111	0.035
H(2BC)	4a	–0.1740	0.2800	–0.0483	0.035
H(3BB)	4a	0.1258	0.5600	–0.1780	0.064
H(3BC)	4a	0.1973	0.5164	–0.1686	0.064
H(4BA)	4a	0.0297	0.5379	–0.1149	0.055
	4a	0.0363	0.4798	–0.0633	0.055
H(5BA)	4a	0.1849	0.3103	0.1048	0.081
H(5BB)	4a	0.1515	0.3313	0.0392	0.081
H(6BA)	4a	0.2366	0.1980	0.1236	0.059
H(6BB)	4a	0.2381	0.1426	0.0700	0.059
H(3BD)	4a	0.2141	0.3178	–0.1958	0.024
H(4BC)	4a	0.0439	0.1444	–0.1905	0.044
H(2CA)	4a	–0.4172	0.1898	–0.2885	0.020
H(3CA)	4a	–0.3186	0.2801	–0.2800	0.021
H(1CA)	4a	–0.6854	0.2436	–0.1790	0.064
H(1CB)	4a	–0.6402	0.1740	–0.1683	0.064
H(2CB)	4a	–0.6665	0.3419	–0.1126	0.062
H(2CC)	4a	–0.6085	0.3386	–0.0570	0.062
H(3CB)	4a	–0.3790	0.5641	–0.1100	0.039
H(3CC)	4a	–0.3985	0.5403	–0.0444	0.039
H(4CA)	4a	–0.3721	0.4814	–0.1893	0.054
H(4CB)	4a	–0.3868	0.4005	–0.1790	0.054
H(5CA)	4a	–0.3055	0.1522	0.1234	0.049
H(5CB)	4a	–0.2543	0.1406	0.0703	0.049
H(6CA)	4a	–0.4198	0.2036	0.1031	0.069
H(6CB)	4a	–0.4459	0.2268	0.0361	0.069
H(3CE)	4a	–0.4558	0.1486	–0.1993	0.025
H(4CC)	4a	–0.2815	0.3189	–0.1889	0.039
H(2DA)	4a	–0.5807	0.5677	0.2916	0.020
H(3DA)	4a	–0.6782	0.4748	0.2800	0.024
H(1DA)	4a	–0.3087	0.5259	0.1932	0.052
H(1DB)	4a	–0.3596	0.5907	0.1781	0.052
H(2DB)	4a	–0.3155	0.4241	0.1259	0.058
H(2DC)	4a	–0.3707	0.4240	0.0681	0.058
H(3DA)	4a	–0.6147	0.1851	0.1175	0.042
H(3DB)	4a	–0.5885	0.2082	0.0537	0.042
H(4DB)	4a	–0.6123	0.2649	0.2001	0.049
H(4DC)	4a	–0.5844	0.3427	0.1928	0.049
H(5DA)	4a	–0.6658	0.5874	–0.1226	0.054
H(5DB)	4a	–0.7189	0.6037	–0.0718	0.054
H(6DA)	4a	–0.5607	0.5204	–0.0990	0.057
H(6DB)	4a	–0.5427	0.4914	–0.0322	0.057
H(3DD)	4a	–0.5361	0.6020	0.2026	0.023
H(4DC)	4a	–0.7068	0.4310	0.1902	0.038

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1A)	4a	–0.10009(3)	0.44704(3)	0.10539(2)	0.0245(2)	0.0319(3)	0.0222(2)	0.0024(2)	0.0005(2)	0.0039(2)
C(1A)	4a	–0.0690(4)	0.4284(4)	0.2522(3)	0.021(3)	0.018(3)	0.019(3)	0.004(3)	0.004(3)	0.005(2)
C(2A)	4a	–0.1350(4)	0.4833(4)	0.2492(3)	0.016(3)	0.020(3)	0.018(3)	0.007(3)	0.002(2)	0.003(2)
C(3A)	4a	–0.1056(4)	0.5632(3)	0.2433(3)	0.019(3)	0.020(3)	0.016(3)	–0.002(3)	0.000(2)	–0.001(2)
C(4A)	4a	–0.1708(4)	0.6195(3)	0.2494(3)	0.022(3)	0.017(3)	0.020(3)	–0.006(3)	–0.001(3)	–0.002(2)
C(5A)	4a	0.0993(4)	0.4703(4)	0.1106(3)	0.020(3)	0.022(3)	0.031(4)	–0.006(3)	0.001(3)	–0.002(3)
C(6A)	4a	–0.1291(5)	0.2653(4)	0.1150(3)	0.037(4)	0.028(4)	0.026(4)	–0.004(3)	0.000(3)	0.000(3)
C(7A)	4a	–0.1812(4)	0.5164(4)	–0.0459(3)	0.031(4)	0.033(4)	0.030(4)	–0.007(3)	0.000(3)	0.000(3)
N(1A)	4a	0.0889(4)	0.4878(4)	0.1708(3)	0.023(3)	0.072(5)	0.036(3)	–0.008(3)	0.001(3)	–0.012(3)
N(2A)	4a	0.1661(4)	0.4809(4)	0.0891(3)	0.024(3)	0.050(4)	0.032(3)	–0.007(3)	0.002(3)	–0.006(3)
N(3A)	4a	–0.1533(4)	0.2427(4)	0.1707(3)	0.047(4)	0.041(4)	0.041(4)	0.002(3)	0.004(3)	0.014(3)
N(4A)	4a	–0.0667(5)	0.2380(4)	0.0944(3)	0.062(5)	0.047(4)	0.033(3)	0.019(4)	0.014(3)	0.009(3)
N(5A)	4a	–0.1635(6)	0.4509(4)	–0.0674(3)	0.109(8)	0.042(4)	0.031(4)	0.017(5)	–0.007(4)	–0.006(3)
N(6A)	4a	–0.2148(4)	0.5647(4)	–0.0866(3)	0.050(4)	0.044(4)	0.027(3)	0.016(4)	–0.004(3)	–0.003(3)
S(1A)	4a	0.0298(1)	0.4307(1)	0.05888(9)	0.0241(9)	0.063(1)	0.0287(9)	–0.013(1)	0.0041(7)	–0.0162(9)
S(2A)	4a	–0.1819(1)	0.3312(1)	0.06990(8)	0.0286(9)	0.0288(9)	0.0256(8)	–0.0004(8)	–0.0002(7)	–0.0008(7)
S(3A)	4a	–0.1640(2)	0.5462(1)	0.0326(1)	0.086(2)	0.031(1)	0.028(1)	0.018(1)	–0.016(1)	–0.0043(8)
O(1A)	4a	–0.0497(3)	0.3993(3)	0.2008(2)	0.028(3)	0.035(3)	0.022(2)	0.013(2)	0.001(2)	0.000(2)
O(2A)	4a	–0.0377(3)	0.4148(3)	0.3068(2)	0.041(3)	0.038(3)	0.029(3)	0.019(3)	–0.007(2)	–0.003(2)
O(3A)	4a	–0.1855(3)	0.4698(2)	0.1930(2)	0.018(2)	0.017(2)	0.027(2)	–0.006(2)	–0.000(2)	0.000(2)
O(4A)	4a	–0.0709(3)	0.5683(3)	0.1841(2)	0.022(2)	0.029(2)	0.029(2)	–0.011(2)	0.011(2)	–0.003(2)
O(5A)	4a	–0.1801(3)	0.6686(3)	0.2077(2)	0.036(3)	0.022(2)	0.028(2)	0.008(2)	0.006(2)	0.009(2)
O(6A)	4a	–0.2086(3)	0.6107(3)	0.2980(2)	0.030(3)	0.026(2)	0.029(2)	0.010(2)	0.011(2)	0.004(2)
Cd(1B)	4a	0.10334(3)	0.30400(3)	–0.10680(2)	0.0226(2)	0.0305(2)	0.0207(2)	0.0024(2)	0.0008(2)	0.0024(2)

Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1B)	4*a*	0.0728(4)	0.3192(4)	–0.2546(3)	0.016(3)	0.020(3)	0.025(3)	–0.001(3)	–0.001(3)	0.000(3)
C(2B)	4*a*	0.1412(4)	0.2667(3)	–0.2480(3)	0.020(3)	0.015(3)	0.015(3)	–0.001(3)	–0.001(2)	0.001(2)
C(3B)	4*a*	0.1148(4)	0.1859(4)	–0.2433(3)	0.019(3)	0.021(3)	0.017(3)	–0.001(3)	0.004(3)	0.000(2)
C(4B)	4*a*	0.1819(4)	0.1331(4)	–0.2411(3)	0.022(3)	0.018(3)	0.022(3)	0.003(3)	0.001(3)	–0.001(2)
C(5B)	4*a*	–0.0962(4)	0.2686(4)	–0.1064(3)	0.025(4)	0.024(3)	0.026(3)	–0.002(3)	0.002(3)	0.000(3)
C(6B)	4*a*	0.1239(4)	0.4880(4)	–0.1097(3)	0.028(4)	0.036(4)	0.025(3)	–0.001(3)	–0.002(3)	–0.004(3)
C(7B)	4*a*	0.1913(5)	0.2347(4)	0.0432(3)	0.036(4)	0.041(4)	0.028(4)	0.006(4)	0.004(3)	0.001(3)
N(1B)	4*a*	–0.0850(4)	0.2441(4)	–0.1643(3)	0.026(3)	0.052(4)	0.025(3)	–0.006(3)	0.000(3)	–0.015(3)
N(2B)	4*a*	–0.1652(3)	0.2642(3)	–0.0863(3)	0.018(3)	0.037(4)	0.033(3)	–0.006(3)	0.003(3)	–0.006(3)
N(3B)	4*a*	0.1523(5)	0.5260(4)	–0.1578(3)	0.063(5)	0.048(4)	0.050(4)	0.017(4)	0.023(4)	0.025(3)
N(4B)	4*a*	0.0555(4)	0.5037(4)	–0.0942(4)	0.037(4)	0.043(4)	0.058(4)	0.009(3)	0.011(3)	0.022(4)
N(5B)	4*a*	0.1740(6)	0.2992(4)	0.0647(3)	0.127(8)	0.042(4)	0.030(3)	0.026(5)	–0.016(4)	–0.007(3)
N(6B)	4*a*	0.2261(4)	0.1861(5)	0.0837(3)	0.056(5)	0.060(5)	0.031(3)	0.018(4)	–0.008(3)	0.008(3)
S(1B)	4*a*	–0.0262(1)	0.3090(1)	–0.05586(8)	0.0244(9)	0.058(1)	0.0254(8)	–0.0103(9)	0.0048(7)	–0.0115(8)
S(2B)	4*a*	0.1797(1)	0.4217(1)	–0.07008(8)	0.0311(9)	0.0280(9)	0.0314(9)	0.0014(8)	–0.0038(7)	0.0000(7)
S(3B)	4*a*	0.1754(2)	0.2067(1)	–0.03538(9)	0.077(2)	0.034(1)	0.0247(9)	0.025(1)	–0.014(1)	–0.0049(8)
O(1B)	4*a*	0.0493(3)	0.3465(3)	–0.2036(2)	0.032(3)	0.037(3)	0.017(2)	0.019(2)	0.005(2)	–0.003(2)
O(2B)	4*a*	0.0443(3)	0.3314(3)	–0.3107(2)	0.025(2)	0.034(3)	0.019(2)	0.006(2)	–0.003(2)	0.002(2)
O(3B)	4*a*	0.1877(3)	0.2810(2)	–0.1904(2)	0.019(2)	0.017(2)	0.024(2)	–0.008(2)	–0.001(2)	0.001(2)
O(4B)	4*a*	0.0728(3)	0.1801(3)	–0.1867(2)	0.028(3)	0.025(2)	0.037(3)	–0.010(2)	0.021(2)	–0.006(2)
O(5B)	4*a*	0.1864(3)	0.0801(3)	–0.2010(2)	0.040(3)	0.030(3)	0.038(3)	0.002(2)	0.001(2)	0.011(2)
O(6B)	4*a*	0.2306(3)	0.1449(3)	–0.2822(2)	0.034(3)	0.028(3)	0.037(3)	0.015(2)	0.019(2)	0.006(2)
Cd(1C)	4*a*	–0.42754(3)	0.26169(3)	–0.10400(2)	0.0309(3)	0.0238(2)	0.0208(2)	0.0028(2)	–0.0014(2)	0.0019(2)
C(1C)	4*a*	–0.4570(4)	0.2885(4)	–0.2485(3)	0.019(3)	0.018(3)	0.027(3)	–0.005(3)	–0.002(3)	0.003(3)
C(2C)	4*a*	–0.4064(4)	0.2186(3)	–0.2486(3)	0.022(3)	0.015(3)	0.013(3)	–0.001(3)	–0.001(2)	0.000(2)
C(3C)	4*a*	–0.3249(4)	0.2458(3)	–0.2440(3)	0.020(3)	0.016(3)	0.017(3)	–0.002(3)	0.002(2)	–0.002(2)
C(4C)	4*a*	–0.2686(4)	0.1802(4)	–0.2492(3)	0.016(3)	0.026(3)	0.021(3)	–0.003(3)	0.001(3)	0.003(3)
C(5C)	4*a*	–0.6145(4)	0.2492(4)	–0.1064(3)	0.021(3)	0.035(4)	0.034(4)	0.000(3)	0.002(3)	–0.005(3)
C(6C)	4*a*	–0.3962(4)	0.4590(4)	–0.1041(3)	0.023(3)	0.028(3)	0.028(3)	–0.002(3)	0.004(3)	–0.001(3)
C(7C)	4*a*	–0.3476(4)	0.1847(4)	0.0418(3)	0.021(3)	0.027(3)	0.019(3)	–0.002(3)	0.002(3)	0.004(2)
N(1C)	4*a*	–0.6509(4)	0.2188(4)	–0.1570(3)	0.054(5)	0.060(5)	0.042(4)	0.019(4)	–0.026(4)	–0.012(3)
N(2C)	4*a*	–0.6319(5)	0.3178(4)	–0.0901(4)	0.051(5)	0.041(4)	0.060(4)	0.012(4)	–0.016(4)	–0.001(4)
N(3C)	4*a*	–0.3906(4)	0.5294(3)	–0.0838(3)	0.044(4)	0.019(3)	0.035(3)	–0.004(3)	0.008(3)	–0.005(2)
N(4C)	4*a*	–0.3836(5)	0.4454(4)	–0.1643(3)	0.080(6)	0.027(3)	0.030(3)	–0.013(4)	0.026(4)	–0.001(3)
N(5C)	4*a*	–0.2967(4)	0.1559(4)	0.0832(3)	0.046(4)	0.045(4)	0.029(3)	0.017(4)	–0.002(3)	0.004(3)
N(6C)	4*a*	–0.4118(4)	0.2077(5)	0.0627(3)	0.044(4)	0.099(7)	0.032(4)	0.027(5)	0.013(3)	0.015(4)
S(1C)	4*a*	–0.5465(1)	0.1971(1)	–0.06298(8)	0.0273(9)	0.0294(9)	0.0244(8)	0.0013(8)	0.0006(7)	0.0048(7)
S(2C)	4*a*	–0.4214(1)	0.3916(1)	–0.05087(9)	0.074(2)	0.0241(8)	0.0264(8)	–0.009(1)	0.0130(9)	–0.0018(7)
S(3C)	4*a*	–0.3271(1)	0.1880(1)	–0.03801(9)	0.031(1)	0.065(1)	0.0225(9)	0.021(1)	0.0072(8)	0.0118(9)
O(1C)	4*a*	–0.4863(3)	0.3065(3)	–0.1983(2)	0.036(3)	0.036(3)	0.018(2)	0.016(2)	0.003(2)	0.000(2)
O(2C)	4*a*	–0.4625(3)	0.3250(3)	–0.3003(2)	0.038(3)	0.030(3)	0.023(2)	0.009(2)	0.005(2)	0.008(2)
O(3C)	4*a*	–0.4170(3)	0.1732(2)	–0.1929(2)	0.021(2)	0.016(2)	0.025(2)	–0.004(2)	0.001(2)	0.007(2)
O(4C)	4*a*	–0.3138(3)	0.2867(3)	–0.1851(2)	0.023(2)	0.025(2)	0.031(3)	–0.007(2)	0.003(2)	–0.009(2)
O(5C)	4*a*	–0.2231(3)	0.1649(3)	–0.2018(2)	0.026(3)	0.032(3)	0.034(3)	0.005(2)	–0.008(2)	0.001(2)
O(6C)	4*a*	–0.2731(3)	0.1467(3)	–0.3023(2)	0.029(3)	0.033(3)	0.030(2)	0.013(2)	–0.003(2)	–0.010(2)
Cd(1D)	4*a*	–0.55905(3)	0.48286(3)	0.11413(2)	0.0270(2)	0.0234(2)	0.0189(2)	0.0036(2)	–0.0002(2)	–0.0001(2)
C(1D)	4*a*	–0.5368(4)	0.4660(4)	0.2613(3)	0.017(3)	0.023(3)	0.018(3)	0.003(3)	0.003(3)	0.000(3)
C(2D)	4*a*	–0.5873(3)	0.5357(3)	0.2532(3)	0.016(3)	0.020(3)	0.016(3)	0.004(3)	0.001(2)	–0.001(2)
C(3D)	4*a*	–0.6689(4)	0.5080(4)	0.2437(3)	0.022(3)	0.020(3)	0.020(3)	–0.002(3)	0.003(3)	0.001(2)
C(4D)	4*a*	–0.7251(4)	0.5726(4)	0.2443(3)	0.016(3)	0.024(3)	0.019(3)	0.005(3)	0.003(2)	–0.001(2)
C(5D)	4*a*	–0.3733(4)	0.5122(4)	0.1174(3)	0.017(3)	0.040(4)	0.026(3)	–0.001(3)	0.002(3)	0.005(3)
C(6D)	4*a*	–0.5812(4)	0.2851(4)	0.1162(3)	0.023(3)	0.023(3)	0.026(3)	0.001(3)	0.004(3)	0.001(3)
C(7D)	4*a*	–0.6342(4)	0.5463(4)	–0.0408(3)	0.032(4)	0.031(4)	0.026(3)	0.002(3)	–0.004(3)	0.004(3)
N(1D)	4*a*	–0.3438(4)	0.5469(4)	0.1688(3)	0.045(4)	0.042(4)	0.039(4)	0.002(3)	–0.023(3)	–0.009(3)
N(2D)	4*a*	–0.3506(4)	0.4460(4)	0.1021(3)	0.045(4)	0.057(5)	0.040(4)	0.016(4)	–0.018(3)	–0.010(3)
N(3D)	4*a*	–0.5965(4)	0.2186(3)	0.0932(3)	0.051(4)	0.024(3)	0.029(3)	–0.009(3)	0.008(3)	0.002(2)
N(4D)	4*a*	–0.5941(4)	0.2992(3)	0.1766(3)	0.067(5)	0.026(3)	0.031(3)	–0.007(3)	0.019(3)	–0.003(3)
N(5D)	4*a*	–0.6780(4)	0.5834(4)	–0.0833(3)	0.062(5)	0.046(4)	0.027(3)	0.027(4)	0.004(3)	0.005(3)
N(6D)	4*a*	–0.5721(4)	0.5159(5)	–0.0595(3)	0.033(3)	0.084(6)	0.025(3)	0.015(4)	0.008(3)	0.006(3)
S(1D)	4*a*	–0.4462(1)	0.5561(1)	0.07122(7)	0.0268(8)	0.0307(9)	0.0226(7)	0.0018(8)	0.0005(7)	0.0024(7)
S(2D)	4*a*	–0.5433(1)	0.3508(1)	0.06674(8)	0.062(1)	0.0217(8)	0.0260(8)	–0.0056(9)	0.0166(9)	–0.0004(7)
S(3D)	4*a*	–0.6638(1)	0.5365(1)	0.03599(9)	0.0258(9)	0.075(2)	0.0258(9)	0.018(1)	0.0066(8)	0.0146(9)
O(1D)	4*a*	–0.5052(3)	0.4428(3)	0.2124(2)	0.036(3)	0.034(3)	0.021(2)	0.019(2)	0.002(2)	–0.001(2)
O(2D)	4*a*	–0.5308(3)	0.4353(3)	0.3153(2)	0.040(3)	0.030(3)	0.022(2)	0.011(2)	0.002(2)	0.005(2)
O(3D)	4*a*	–0.5746(3)	0.5769(2)	0.1963(2)	0.016(2)	0.022(2)	0.021(2)	–0.004(2)	0.004(2)	0.000(2)
O(4D)	4*a*	–0.6768(3)	0.4653(3)	0.1857(2)	0.031(3)	0.021(2)	0.025(2)	–0.011(2)	0.006(2)	–0.007(2)
O(5D)	4*a*	–0.7790(3)	0.5761(3)	0.2030(2)	0.027(3)	0.034(3)	0.037(3)	0.003(2)	–0.013(2)	–0.003(2)
O(6D)	4*a*	–0.7125(3)	0.6188(3)	0.2908(3)	0.033(3)	0.051(3)	0.042(3)	0.025(3)	–0.011(3)	–0.029(3)

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