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**Crystal structure of (R,R)-N,N',-(2,2'-bipyridine-6,6'-dimethylenediyl)-bis-(2,2'-dimethoxy-1,1'-binaphthalene-3-carboxamide) tetratoluene solvate, (C<sub>58</sub>H<sub>46</sub>O<sub>6</sub>N<sub>4</sub>)<sub>2</sub> · 4C<sub>7</sub>H<sub>8</sub>**

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# Crystal structure of (*R,R*)-*N,N'*-(2,2'-bipyridine-6,6'-dimethylenediyl)-bis-(2,2'-dimethoxy-1,1'-binaphthalene-3-carboxamide) tetratoluene solvate, (C<sub>58</sub>H<sub>46</sub>O<sub>6</sub>N<sub>4</sub>)<sub>2</sub> · 4C<sub>7</sub>H<sub>8</sub>

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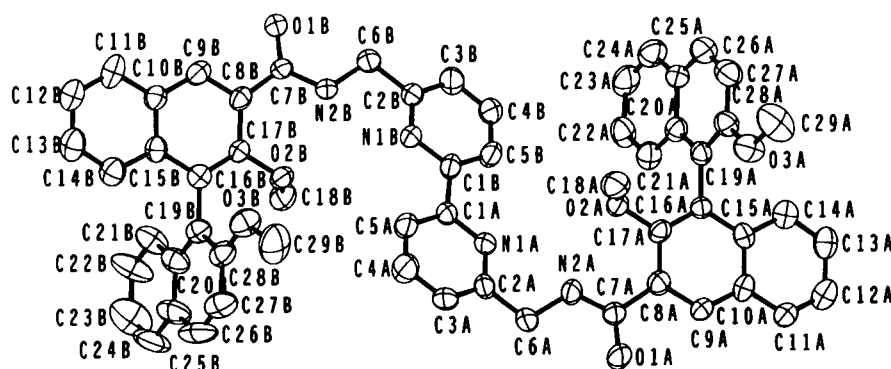
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C<sub>144</sub>H<sub>124</sub>N<sub>8</sub>O<sub>12</sub>, triclinic, *P*1 (No. 1),  
 $a = 11.397(3)$  Å,  $b = 15.785(2)$  Å,  
 $c = 18.429(5)$  Å,  $\alpha = 71.36(2)^\circ$ ,  $\beta = 73.55(1)^\circ$ ,  
 $\gamma = 72.02(3)^\circ$ ,  $V = 2924.7$  Å<sup>3</sup>,  $Z = 1$ ,  
 $R(F) = 0.071$ ,  $R_w(F^2) = 0.208$ .

Source of material: The title compound was prepared from 6,6'-bis(aminomethyl)-2,2'-bipyridine (see ref. 1) and (*R*)-2,2'-dimethoxy-1,1'-binaphthalene-3-carboxylchloride (see ref. 2 and 3) (using dichloromethane as a solvent and 7.4 equivalents of triethylamine as a base) in 75% yield. Crystals suitable for X-ray analysis were grown in the toluene-acetone 9:1 mixture. Clathrate with toluene (formed during crystallization) can be decomposed by heating in high vacuum. Pure product has  $[\alpha]_D^{20} = +189^\circ$  ( $c = 0.214$ ; THF).

The structure was refined with a low ratio of observations to parameter due to poor quality of the crystal and significantly big number of atoms in the asymmetric unit (a center of symmetry is lacking in the structure). There are two independent molecules (only one is shown in the figure) in the asymmetric unit which are mainly associated via  $\pi \cdots \pi$  interactions. The N2–H groups are

intramolecularly hydrogen bonded to the O2 atoms ( $d(N2A \cdots O2A) = 2.709(11)$  Å,  $d(N2B \cdots O2B) = 2.730(10)$  Å,  $d(N2C \cdots O2C) = 2.743(10)$  Å and  $d(N2D \cdots O2D) = 2.719(8)$  Å). The bipyridyl units are planar, the dihedral angles between adjacent naphthalene rings are near  $90^\circ$  ( $75.8(1)^\circ$ ,  $78.9(2)^\circ$ ,  $82.4(2)^\circ$  and  $76.8(1)^\circ$  for the A, B, C, D parts, respectively) like in other binaphthalene derivatives. Because of the disorder, three of four toluene molecules are isotropically refined assuming ideal phenyl ring geometry.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless, block-shaped, size 0.14 x 0.25 x 0.28 mm
Wavelength:	Cu $K_\alpha$ radiation (1.54056 Å)
$\mu$ :	6.17 cm <sup>-1</sup>
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	2 $\theta$ / $\omega$
$T_{\text{measurement}}$ :	293 K
$2\theta_{\text{max}}$ :	100°
$N(hkl)_{\text{unique}}$ :	7603
Criterion for $I_o$ :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$ :	1352
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å<sup>2</sup>)

Atom	Site	x	y	z	$U_{\text{iso}}$
H(2A)	1a	0.531(7)	0.092(5)	0.197(5)	0.099
H(3A)	1a	0.5946(7)	-0.0347(5)	0.4509(5)	0.105
H(4A)	1a	0.541(1)	-0.1748(6)	0.5107(5)	0.138
H(5A)	1a	0.4903(8)	-0.2458(5)	0.4358(5)	0.113
H(61A)	1a	0.5908(8)	0.1003(4)	0.3386(6)	0.112
H(62A)	1a	0.7056(8)	0.0468(4)	0.2865(6)	0.112
H(9A)	1a	0.5964(7)	0.3390(4)	0.0902(5)	0.095
H(11A)	1a	0.5914(8)	0.4659(5)	-0.0261(5)	0.104
H(12A)	1a	0.5485(9)	0.5300(6)	-0.1469(6)	0.124
H(13A)	1a	0.4212(8)	0.4715(6)	-0.1909(5)	0.117
H(14A)	1a	0.3496(7)	0.3434(5)	-0.1116(5)	0.100
H(181A)	1a	0.2601(9)	0.0799(7)	0.2315(6)	0.136
H(182A)	1a	0.2113(9)	0.1732(7)	0.1731(6)	0.136
H(183A)	1a	0.2836(9)	0.1713(7)	0.2346(6)	0.136
H(21A)	1a	0.5232(8)	0.0979(5)	-0.0132(4)	0.103
H(22A)	1a	0.5904(9)	-0.0362(5)	-0.0570(5)	0.120
H(23A)	1a	0.443(1)	-0.0843(6)	-0.0897(6)	0.139

Table 2. (Continued)

Atom	Site	x	y	z	U <sub>iso</sub>
H(24A)	1a	0.240(1)	-0.0037(6)	-0.0833(5)	0.125
H(26A)	1a	0.075(1)	0.1241(7)	-0.0474(5)	0.126
H(27A)	1a	0.0046(8)	0.2558(6)	-0.0023(6)	0.120
H(291A)	1a	0.003(1)	0.4320(8)	0.0749(8)	0.185
H(292A)	1a	-0.043(1)	0.3430(8)	0.0894(8)	0.185
H(293A)	1a	-0.014(1)	0.4051(8)	0.0042(8)	0.185
H(2B)	1a	0.469(7)	-0.425(5)	0.413(4)	0.092
H(3B)	1a	0.3785(8)	-0.2966(5)	0.1712(5)	0.106
H(4B)	1a	0.4333(8)	-0.1596(5)	0.1122(5)	0.108
H(5B)	1a	0.4826(7)	-0.0855(5)	0.1861(5)	0.100
H(61B)	1a	0.2717(7)	-0.3811(4)	0.3368(5)	0.097
H(62B)	1a	0.3894(7)	-0.4354(4)	0.2871(5)	0.097
H(9B)	1a	0.3745(6)	-0.6669(4)	0.5382(5)	0.093
H(11B)	1a	0.3732(9)	-0.7876(5)	0.6638(6)	0.122
H(12B)	1a	0.4389(9)	-0.8561(5)	0.7799(6)	0.119
H(13B)	1a	0.570(1)	-0.7985(6)	0.8134(5)	0.122
H(14B)	1a	0.6432(8)	-0.6767(6)	0.7331(5)	0.108
H(181B)	1a	0.7143(7)	-0.4100(6)	0.3929(5)	0.117
H(182B)	1a	0.6870(7)	-0.5011(6)	0.3920(5)	0.117
H(183B)	1a	0.7609(7)	-0.5028(6)	0.4526(5)	0.117
H(21B)	1a	0.8027(8)	-0.6817(7)	0.5635(5)	0.131
H(22B)	1a	1.0114(9)	-0.744(1)	0.5337(7)	0.176
H(23B)	1a	1.151(2)	-0.696(1)	0.569(1)	0.228
H(24B)	1a	1.085(1)	-0.571(1)	0.6217(9)	0.190
H(26B)	1a	0.898(1)	-0.447(1)	0.6713(6)	0.158
H(27B)	1a	0.690(1)	-0.3753(7)	0.6880(5)	0.131
H(291B)	1a	0.372(2)	-0.3135(7)	0.6770(9)	0.196
H(292B)	1a	0.479(2)	-0.3375(7)	0.7232(9)	0.196
H(293B)	1a	0.501(2)	-0.2873(7)	0.6338(9)	0.196
H(2C)	1a	-0.274(7)	0.491(6)	0.207(5)	0.100
H(3C)	1a	-0.4086(7)	0.2881(5)	0.3897(5)	0.099
H(4C)	1a	-0.2650(8)	0.2016(5)	0.4696(6)	0.114
H(5C)	1a	-0.0627(6)	0.2254(5)	0.4354(5)	0.100
H(61C)	1a	-0.3913(7)	0.3642(5)	0.2299(5)	0.103
H(62C)	1a	-0.4548(7)	0.4352(5)	0.2811(5)	0.103
H(9C)	1a	-0.4456(8)	0.6268(6)	0.0036(5)	0.104
H(11C)	1a	-0.4345(9)	0.7238(8)	-0.1318(6)	0.139
H(12C)	1a	-0.352(1)	0.8307(9)	-0.2318(7)	0.171
H(13C)	1a	-0.191(1)	0.8782(9)	-0.2226(6)	0.160
H(14C)	1a	-0.1135(8)	0.8280(7)	-0.1111(6)	0.131
H(181C)	1a	-0.1797(9)	0.6070(6)	0.2478(5)	0.123
H(182C)	1a	-0.3113(9)	0.6385(6)	0.2243(5)	0.123
H(183C)	1a	-0.2163(9)	0.7020(6)	0.1880(5)	0.123
H(21C)	1a	-0.2860(8)	0.8516(6)	0.0665(6)	0.120
H(22C)	1a	-0.324(1)	0.9875(7)	0.0968(8)	0.167
H(23C)	1a	-0.155(2)	1.0349(9)	0.1109(8)	0.207
H(24C)	1a	0.050(2)	0.948(1)	0.0812(8)	0.200
H(26C)	1a	0.202(1)	0.805(1)	0.0428(7)	0.181
H(27C)	1a	0.231(1)	0.674(1)	0.0065(8)	0.180
H(291C)	1a	0.181(1)	0.4994(9)	-0.044(1)	0.254
H(292C)	1a	0.230(1)	0.5343(9)	0.010(1)	0.254
H(293C)	1a	0.227(1)	0.5911(9)	-0.077(1)	0.254

Table 2. (Continued)

Atom	Site	x	y	z	U <sub>iso</sub>
H(2D)	1a	0.208(6)	0.165(5)	0.450(5)	0.089
H(3D)	1a	0.3620(7)	0.3673(6)	0.2490(6)	0.113
H(4D)	1a	0.2218(8)	0.4505(7)	0.1650(6)	0.128
H(5D)	1a	0.0150(7)	0.4277(6)	0.2046(5)	0.112
H(61D)	1a	0.4100(6)	0.2311(4)	0.3566(5)	0.097
H(62D)	1a	0.3298(6)	0.2930(4)	0.4138(5)	0.097
H(9D)	1a	0.4046(6)	0.0221(5)	0.6281(5)	0.087
H(11D)	1a	0.4069(8)	-0.0880(7)	0.7599(6)	0.119
H(12D)	1a	0.3267(9)	-0.1937(7)	0.8565(6)	0.132
H(13D)	1a	0.1644(9)	-0.2483(6)	0.8457(5)	0.123
H(14D)	1a	0.0935(7)	-0.1952(5)	0.7308(4)	0.093
H(181D)	1a	0.1630(8)	0.0339(5)	0.3753(5)	0.111
H(182D)	1a	0.1997(8)	-0.0611(5)	0.4351(5)	0.111
H(183D)	1a	0.2919(8)	0.0046(5)	0.4019(5)	0.111
H(21D)	1a	-0.0486(6)	0.0531(5)	0.6323(5)	0.090
H(22E)	1a	-0.2570(7)	0.1395(6)	0.6371(6)	0.121
H(23D)	1a	-0.4073(6)	0.0777(6)	0.6217(6)	0.118
H(24D)	1a	-0.3521(6)	-0.0577(6)	0.5958(5)	0.110
H(26D)	1a	-0.1905(7)	-0.1997(5)	0.5755(5)	0.106
H(27D)	1a	0.0143(7)	-0.2807(5)	0.5582(5)	0.103
H(291D)	1a	0.3425(8)	-0.3360(5)	0.5320(6)	0.127
H(292D)	1a	0.2375(8)	-0.2932(5)	0.4822(6)	0.127
H(293D)	1a	0.2092(8)	-0.3572(5)	0.5666(6)	0.127
C(1T1)	1a	0.774(1)	0.173(1)	0.9097(8)	0.28(1)
C(2T1)	1a	0.816(1)	0.2494(8)	0.859(1)	0.218(7)
C(3T1)	1a	0.922(1)	0.2379(7)	0.7997(8)	0.210(7)
C(4T1)	1a	0.985(1)	0.150(1)	0.7907(8)	0.221(8)
C(5T1)	1a	0.944(1)	0.0739(7)	0.8413(9)	0.228(8)
C(6T1)	1a	0.838(2)	0.0854(9)	0.9008(9)	0.219(7)
C(7T1)	1a	1.105(3)	0.137(2)	0.743(2)	0.46(3)
H(1T2)	1a	0.288(1)	0.509(1)	0.6885(8)	0.182
H(2T2)	1a	0.158(2)	0.639(1)	0.715(1)	0.209
H(3T2)	1a	-0.026(1)	0.6376(8)	0.7926(7)	0.167
H(5T2)	1a	0.0435(9)	0.3692(6)	0.8358(6)	0.139
H(6T2)	1a	0.249(1)	0.3690(9)	0.7564(7)	0.157
H(7T2)	1a	-0.173(1)	0.570(1)	0.8750(9)	0.256
H(8T2)	1a	-0.129(1)	0.470(1)	0.9246(9)	0.256
H(9T2)	1a	-0.182(1)	0.487(1)	0.8497(9)	0.256
C(1T3)	1a	0.052(1)	-0.1075(6)	0.3460(7)	0.243(9)
C(2T3)	1a	0.109(1)	-0.0841(6)	0.2672(8)	0.229(8)
C(3T3)	1a	0.0683(9)	0.0035(7)	0.2208(5)	0.171(5)
C(4T3)	1a	-0.0290(8)	0.0678(5)	0.2532(5)	0.126(3)
C(5T3)	1a	-0.0856(8)	0.0445(7)	0.3319(5)	0.174(5)
C(6T3)	1a	-0.045(1)	-0.0432(8)	0.3783(5)	0.182(5)
C(7T3)	1a	-0.069(2)	0.155(1)	0.207(1)	0.256(9)
C(1T4)	1a	0.015(1)	0.5614(6)	0.4227(7)	0.217(7)
C(2T4)	1a	-0.077(1)	0.6318(8)	0.4505(4)	0.201(6)
C(3T4)	1a	-0.1215(9)	0.7136(7)	0.3983(5)	0.188(5)
C(4T4)	1a	-0.0749(8)	0.7250(5)	0.3183(5)	0.133(3)
C(5T4)	1a	0.0166(8)	0.6545(7)	0.2906(5)	0.153(4)
C(6T4)	1a	0.0616(9)	0.5727(6)	0.3428(7)	0.200(6)
C(7T4)	1a	-0.129(2)	0.803(1)	0.268(1)	0.30(1)

Table 3. Final atomic coordinates and displacement parameters (in Å<sup>2</sup>)

Atom	Site	x	y	z	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
N(1A)	1a	0.5378(5)	-0.0651(3)	0.3018(3)	0.079(3)	0.060(3)	0.073(4)	-0.016(2)	-0.032(3)	-0.015(3)
N(2A)	1a	0.5560(6)	0.1089(4)	0.2348(4)	0.117(5)	0.051(3)	0.088(4)	-0.017(3)	-0.047(4)	-0.009(3)
O(1A)	1a	0.6279(9)	0.2304(4)	0.2125(5)	0.274(9)	0.083(4)	0.174(7)	-0.085(5)	-0.156(7)	0.019(4)
O(2A)	1a	0.3943(5)	0.1229(3)	0.1461(3)	0.100(3)	0.068(3)	0.067(3)	-0.035(2)	-0.028(3)	-0.005(2)
O(3A)	1a	0.1359(5)	0.3301(4)	0.0448(4)	0.087(3)	0.102(3)	0.134(5)	0.003(3)	-0.028(3)	-0.063(4)
C(1A)	1a	0.5076(6)	-0.1463(4)	0.3355(4)	0.083(4)	0.059(4)	0.063(5)	-0.018(3)	-0.028(4)	-0.010(4)
C(2A)	1a	0.5727(6)	-0.0249(4)	0.3437(5)	0.080(4)	0.059(4)	0.073(5)	-0.006(3)	-0.031(4)	-0.010(4)
C(3A)	1a	0.5729(7)	-0.0643(5)	0.4221(5)	0.105(5)	0.079(5)	0.098(7)	-0.027(4)	-0.045(5)	-0.025(5)
C(4A)	1a	0.541(1)	-0.1475(6)	0.4578(5)	0.182(9)	0.107(6)	0.076(6)	-0.059(6)	-0.048(6)	-0.008(5)
C(5A)	1a	0.5100(8)	-0.1888(5)	0.4134(5)	0.140(7)	0.077(4)	0.081(6)	-0.046(5)	-0.047(5)	0.000(4)
C(6A)	1a	0.6146(8)	0.0609(4)	0.3032(6)	0.112(6)	0.061(4)	0.120(7)	-0.016(4)	-0.069(5)	-0.007(4)
C(7A)	1a	0.5692(8)	0.1908(5)	0.1950(5)	0.123(6)	0.065(5)	0.087(6)	-0.032(4)	-0.051(5)	-0.012(4)
C(8A)	1a	0.5094(7)	0.2364(4)	0.1221(5)	0.091(4)	0.057(4)	0.081(5)	-0.014(3)	-0.028(4)	-0.019(4)
C(9A)	1a	0.5450(7)	0.3156(4)	0.0744(5)	0.100(5)	0.056(4)	0.092(6)	-0.028(3)	-0.034(4)	-0.012(4)

Table 3. (Continued)

Atom	Site	x	y	z	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
C(10A)	1a	0.5073(7)	0.3613(4)	0.0041(5)	0.087(4)	0.052(4)	0.074(5)	-0.014(3)	-0.008(4)	-0.012(4)
C(11A)	1a	0.5455(8)	0.4398(5)	-0.0438(5)	0.105(5)	0.071(4)	0.092(6)	-0.033(4)	-0.031(5)	-0.009(5)
C(12A)	1a	0.5179(9)	0.4792(6)	-0.1150(6)	0.127(7)	0.077(5)	0.099(7)	-0.032(5)	-0.010(6)	-0.017(5)
C(13A)	1a	0.4418(8)	0.4436(6)	-0.1420(5)	0.109(6)	0.085(5)	0.077(6)	-0.015(5)	-0.008(5)	-0.010(5)
C(14A)	1a	0.3990(7)	0.3670(5)	-0.0943(5)	0.088(5)	0.079(5)	0.073(5)	-0.013(4)	-0.005(4)	-0.025(4)
C(15A)	1a	0.4290(6)	0.3244(4)	-0.0206(4)	0.071(4)	0.065(4)	0.057(4)	-0.003(3)	-0.017(3)	-0.017(3)
C(16A)	1a	0.3877(6)	0.2442(4)	0.0307(4)	0.074(4)	0.055(3)	0.060(4)	-0.016(3)	-0.020(3)	-0.017(3)
C(17A)	1a	0.4277(6)	0.2025(4)	0.0994(4)	0.080(4)	0.052(3)	0.071(5)	-0.017(3)	-0.015(4)	-0.021(4)
C(18A)	1a	0.2778(9)	0.1381(7)	0.2008(6)	0.116(7)	0.133(7)	0.097(7)	-0.062(6)	-0.025(6)	-0.002(6)
C(19A)	1a	0.2989(6)	0.2083(4)	0.0098(4)	0.080(4)	0.064(4)	0.058(4)	-0.015(3)	-0.021(3)	-0.010(3)
C(20A)	1a	0.3402(7)	0.1286(4)	-0.0189(4)	0.095(5)	0.066(4)	0.053(4)	-0.024(4)	-0.019(4)	-0.010(3)
C(21A)	1a	0.4652(8)	0.0777(5)	-0.0263(4)	0.110(6)	0.073(4)	0.075(5)	-0.017(4)	-0.022(4)	-0.022(4)
C(22A)	1a	0.5068(9)	-0.0028(5)	-0.0528(5)	0.122(6)	0.077(5)	0.100(6)	0.007(4)	-0.043(5)	-0.034(5)
C(23A)	1a	0.4171(1)	-0.0308(6)	-0.0726(6)	0.18(1)	0.072(5)	0.114(7)	-0.030(6)	-0.050(7)	-0.035(5)
C(24A)	1a	0.295(1)	0.0164(6)	-0.0681(5)	0.143(8)	0.095(6)	0.092(6)	-0.046(6)	-0.029(6)	-0.026(5)
C(25A)	1a	0.2536(8)	0.0956(5)	-0.0404(5)	0.102(6)	0.070(4)	0.085(5)	-0.028(4)	-0.042(4)	-0.009(4)
C(26A)	1a	0.132(1)	0.1443(7)	-0.0334(5)	0.123(7)	0.111(6)	0.093(6)	-0.046(6)	-0.041(5)	-0.006(5)
C(27A)	1a	0.0886(8)	0.2236(6)	-0.0060(6)	0.083(5)	0.112(6)	0.104(7)	-0.019(5)	-0.029(5)	-0.022(5)
C(28A)	1a	0.1720(7)	0.2538(5)	0.0157(4)	0.085(5)	0.085(5)	0.072(5)	-0.016(4)	-0.022(4)	-0.023(4)
C(29A)	1a	0.010(1)	0.3816(8)	0.0540(8)	0.124(8)	0.159(9)	0.18(1)	0.050(7)	-0.047(8)	-0.107(9)
N(1B)	1a	0.4378(5)	-0.2677(3)	0.3207(3)	0.081(3)	0.054(3)	0.075(4)	-0.019(2)	-0.026(3)	-0.012(3)
N(2B)	1a	0.4174(6)	-0.4388(4)	0.3900(4)	0.097(4)	0.063(3)	0.088(4)	-0.031(3)	-0.048(4)	-0.007(3)
O(1B)	1a	0.3559(5)	-0.5675(3)	0.4124(4)	0.127(4)	0.070(3)	0.121(4)	-0.038(3)	-0.072(4)	0.001(3)
O(2B)	1a	0.5775(4)	-0.4490(3)	0.4798(3)	0.087(3)	0.068(2)	0.073(3)	-0.035(2)	-0.017(3)	-0.013(2)
O(3B)	1a	0.5065(6)	-0.4168(4)	0.6544(4)	0.112(4)	0.093(3)	0.113(5)	-0.025(3)	-0.008(3)	-0.053(3)
C(1B)	1a	0.4692(6)	-0.1860(4)	0.2845(4)	0.073(4)	0.054(4)	0.073(5)	-0.014(3)	-0.015(3)	-0.005(4)
C(2B)	1a	0.4040(6)	-0.3063(4)	0.2785(4)	0.075(4)	0.056(4)	0.081(5)	-0.012(3)	-0.028(4)	-0.018(4)
C(3B)	1a	0.4015(8)	-0.2672(5)	0.1995(5)	0.120(6)	0.075(5)	0.078(6)	-0.016(4)	-0.035(5)	-0.023(4)
C(4B)	1a	0.4329(8)	-0.1864(5)	0.1651(5)	0.115(6)	0.089(5)	0.071(5)	-0.038(4)	-0.035(5)	-0.002(4)
C(5B)	1a	0.4647(7)	-0.1430(5)	0.2085(5)	0.112(5)	0.064(4)	0.075(6)	-0.037(4)	-0.024(4)	-0.002(4)
C(6B)	1a	0.3629(7)	-0.3944(4)	0.3214(5)	0.099(5)	0.067(4)	0.092(5)	-0.020(4)	-0.040(4)	-0.022(4)
C(7B)	1a	0.4075(6)	-0.5238(4)	0.4337(5)	0.071(4)	0.054(4)	0.095(6)	-0.018(3)	-0.031(4)	-0.019(4)
C(8B)	1a	0.4591(6)	-0.5630(4)	0.5047(4)	0.067(4)	0.051(3)	0.079(5)	-0.013(3)	-0.009(4)	-0.018(4)
C(9B)	1a	0.4257(6)	-0.6419(4)	0.5527(5)	0.072(4)	0.062(4)	0.097(6)	-0.022(3)	-0.008(4)	-0.021(4)
C(10B)	1a	0.4684(7)	-0.6868(5)	0.6251(4)	0.078(4)	0.072(4)	0.067(5)	-0.026(3)	-0.011(4)	-0.009(4)
C(11B)	1a	0.4276(9)	-0.7639(5)	0.6769(6)	0.131(7)	0.065(4)	0.084(6)	-0.024(4)	0.003(5)	-0.009(5)
C(12B)	1a	0.4663(9)	-0.8048(5)	0.7461(6)	0.121(6)	0.073(5)	0.087(7)	-0.028(5)	-0.010(5)	-0.007(5)
C(13B)	1a	0.545(1)	-0.7705(6)	0.7658(5)	0.145(7)	0.087(5)	0.063(5)	-0.024(5)	-0.011(5)	-0.017(5)
C(14B)	1a	0.5873(8)	-0.6972(6)	0.7184(5)	0.104(5)	0.093(5)	0.069(5)	-0.028(4)	-0.009(4)	-0.017(5)
C(15B)	1a	0.5487(6)	-0.6505(4)	0.6463(4)	0.079(4)	0.067(4)	0.057(4)	-0.013(3)	-0.009(4)	-0.013(4)
C(16B)	1a	0.5873(6)	-0.5698(4)	0.5955(4)	0.068(4)	0.068(4)	0.065(5)	-0.013(3)	-0.006(3)	-0.024(4)
C(17B)	1a	0.5421(6)	-0.5291(4)	0.5286(4)	0.064(3)	0.050(3)	0.064(4)	-0.014(3)	-0.011(3)	-0.014(3)
C(18B)	1a	0.6947(7)	-0.4673(6)	0.4247(5)	0.092(5)	0.099(5)	0.089(6)	-0.039(4)	-0.005(5)	-0.005(5)
C(19B)	1a	0.6781(7)	-0.5352(5)	0.6160(4)	0.088(5)	0.084(4)	0.053(4)	-0.032(4)	-0.008(3)	-0.024(4)
C(20B)	1a	0.8075(8)	-0.5784(6)	0.6052(5)	0.089(5)	0.125(6)	0.066(5)	-0.029(5)	-0.021(4)	-0.024(5)
C(21B)	1a	0.8580(8)	-0.6564(7)	0.5738(5)	0.090(6)	0.150(8)	0.097(6)	-0.006(5)	-0.035(5)	-0.054(6)
C(22B)	1a	0.9825(9)	-0.696(1)	0.5582(7)	0.068(5)	0.24(1)	0.16(1)	0.002(6)	-0.045(6)	-0.10(1)
C(23B)	1a	1.066(2)	-0.666(1)	0.578(1)	0.15(1)	0.24(2)	0.19(2)	-0.01(1)	-0.06(1)	-0.09(1)
C(24B)	1a	1.027(1)	-0.592(1)	0.6100(9)	0.106(8)	0.23(1)	0.18(1)	-0.066(9)	-0.081(8)	-0.03(1)
C(25B)	1a	0.895(1)	-0.5479(9)	0.6256(6)	0.115(7)	0.18(1)	0.081(6)	-0.060(7)	-0.033(5)	-0.038(6)
C(26B)	1a	0.844(1)	-0.469(1)	0.6570(6)	0.14(1)	0.21(1)	0.096(7)	-0.116(9)	-0.020(7)	-0.050(8)
C(27B)	1a	0.719(1)	-0.4260(7)	0.6669(5)	0.134(8)	0.136(7)	0.081(6)	-0.069(7)	-0.003(6)	-0.040(5)
C(28B)	1a	0.6343(8)	-0.4567(5)	0.6456(5)	0.106(6)	0.092(5)	0.073(5)	-0.047(5)	-0.009(5)	-0.015(4)
C(29B)	1a	0.462(2)	-0.3323(7)	0.6738(9)	0.23(1)	0.098(7)	0.16(1)	-0.007(7)	-0.06(1)	-0.052(8)
N(1C)	1a	-0.1682(5)	0.3670(3)	0.2847(4)	0.063(3)	0.061(3)	0.089(4)	-0.008(2)	-0.024(3)	-0.021(3)
N(2C)	1a	-0.3261(6)	0.4771(4)	0.1891(4)	0.067(3)	0.077(4)	0.113(5)	-0.011(3)	-0.040(4)	-0.022(4)
O(1C)	1a	-0.4943(6)	0.5293(4)	0.1356(4)	0.098(4)	0.106(4)	0.138(5)	-0.022(3)	-0.069(4)	-0.020(3)
O(2C)	1a	-0.1708(4)	0.5956(3)	0.1427(3)	0.077(3)	0.096(3)	0.080(3)	-0.019(2)	-0.026(3)	-0.017(3)
O(3C)	1a	0.0638(7)	0.6018(6)	-0.0075(6)	0.117(5)	0.126(5)	0.180(8)	0.021(4)	-0.017(5)	-0.057(5)
C(1C)	1a	-0.0870(6)	0.3185(4)	0.3319(4)	0.060(4)	0.064(4)	0.086(5)	-0.005(3)	-0.024(4)	-0.027(4)
C(2C)	1a	-0.2855(6)	0.3538(4)	0.3070(5)	0.072(5)	0.060(4)	0.098(6)	-0.002(3)	-0.037(4)	-0.019(4)
C(3C)	1a	-0.3261(7)	0.2945(5)	0.3756(5)	0.067(4)	0.082(4)	0.101(6)	-0.019(4)	-0.020(4)	-0.022(5)
C(4C)	1a	-0.2409(8)	0.2441(5)	0.4235(6)	0.098(6)	0.088(5)	0.101(6)	-0.032(4)	-0.032(5)	-0.007(5)
C(5C)	1a	-0.1201(6)	0.2569(5)	0.4029(5)	0.071(4)	0.098(5)	0.081(5)	-0.037(4)	-0.031(4)	0.005(4)
C(6C)	1a	-0.3752(7)	0.4068(5)	0.2519(5)	0.090(5)	0.070(4)	0.110(6)	-0.011(4)	-0.045(5)	-0.025(4)
C(7C)	1a	-0.3890(8)	0.5331(5)	0.1362(5)	0.079(5)	0.065(4)	0.105(6)	-0.001(4)	-0.040(5)	-0.031(4)
C(8C)	1a	-0.3290(7)	0.6059(5)	0.0743(4)	0.081(5)	0.083(4)	0.071(5)	0.001(4)	-0.023(4)	-0.041(4)
C(9C)	1a	-0.3778(8)	0.6450(6)	0.0074(5)	0.091(5)	0.091(5)	0.082(6)	0.005(4)	-0.030(5)	-0.043(5)
C(10C)	1a	-0.3279(8)	0.7117(6)	-0.0555(5)	0.084(5)	0.102(5)	0.084(6)	0.005(4)	-0.039(5)	-0.036(5)
C(11C)	1a	-0.3707(9)	0.7451(8)	-0.1263(6)	0.104(6)	0.140(8)	0.079(6)	0.020(6)	-0.033(6)	-0.031(6)
C(12C)	1a	-0.321(1)	0.8074(9)	-0.1861(7)	0.130(9)	0.17(1)	0.083(8)	0.029(8)	-0.045(7)	-0.015(8)

Table 3. (Continued)

Atom	Site	x	y	z	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
C(13C)	1a	-0.226(1)	0.8362(9)	-0.1801(6)	0.111(8)	0.17(1)	0.075(7)	-0.003(7)	-0.019(6)	-0.005(6)
C(14C)	1a	-0.1782(8)	0.8058(7)	-0.1139(6)	0.096(6)	0.131(7)	0.077(6)	0.005(5)	-0.020(5)	-0.024(6)
C(15C)	1a	-0.2279(8)	0.7402(5)	-0.0495(4)	0.102(6)	0.087(5)	0.051(5)	0.009(4)	-0.016(4)	-0.021(4)
C(16C)	1a	-0.1774(6)	0.7015(5)	0.0199(5)	0.075(4)	0.084(5)	0.069(5)	-0.004(4)	-0.007(4)	-0.025(4)
C(17C)	1a	-0.2253(6)	0.6351(5)	0.0792(4)	0.073(4)	0.073(4)	0.072(5)	0.009(4)	-0.035(4)	-0.027(4)
C(18C)	1a	-0.2239(9)	0.6394(6)	0.2059(5)	0.144(7)	0.108(6)	0.066(5)	-0.044(5)	-0.025(5)	-0.020(5)
C(19C)	1a	-0.0731(7)	0.7333(6)	0.0298(5)	0.084(5)	0.099(5)	0.069(5)	-0.014(4)	-0.012(4)	-0.003(4)
C(20C)	1a	-0.097(1)	0.8212(7)	0.0491(5)	0.121(7)	0.122(7)	0.065(5)	-0.058(6)	-0.001(5)	-0.010(5)
C(21C)	1a	-0.2189(8)	0.8724(6)	0.0677(6)	0.096(6)	0.100(6)	0.107(7)	-0.042(5)	0.003(5)	-0.033(5)
C(22C)	1a	-0.242(1)	0.9520(7)	0.0877(8)	0.148(8)	0.108(7)	0.18(1)	-0.053(7)	-0.014(8)	-0.057(8)
C(23C)	1a	-0.140(2)	0.9816(9)	0.0949(8)	0.25(2)	0.121(8)	0.14(1)	-0.07(1)	0.02(1)	-0.049(8)
C(24C)	1a	-0.018(2)	0.929(1)	0.0774(8)	0.22(2)	0.19(1)	0.13(1)	-0.12(1)	-0.03(1)	-0.03(1)
C(25C)	1a	0.004(1)	0.8473(9)	0.0537(6)	0.135(9)	0.17(1)	0.085(7)	-0.080(8)	-0.009(6)	-0.011(7)
C(26C)	1a	0.133(1)	0.788(1)	0.0384(7)	0.113(9)	0.23(2)	0.092(8)	-0.09(1)	-0.021(6)	0.018(9)
C(27C)	1a	0.150(1)	0.710(1)	0.0178(8)	0.089(8)	0.21(1)	0.12(1)	-0.015(9)	-0.022(6)	-0.03(1)
C(28C)	1a	0.0520(9)	0.6809(9)	0.0128(6)	0.078(6)	0.154(9)	0.105(7)	-0.019(6)	-0.018(5)	-0.003(7)
C(29C)	1a	0.185(1)	0.5530(9)	-0.031(1)	0.105(7)	0.16(1)	0.23(2)	0.059(8)	0.024(9)	-0.00(1)
N(1D)	1a	0.1240(5)	0.2869(3)	0.3520(4)	0.065(3)	0.060(3)	0.087(4)	-0.011(2)	-0.028(3)	-0.022(3)
N(2D)	1a	0.2837(6)	0.1719(4)	0.4421(4)	0.070(3)	0.060(3)	0.104(5)	-0.021(3)	-0.037(4)	-0.012(3)
O(1D)	1a	0.4438(5)	0.1309(4)	0.5043(4)	0.086(3)	0.104(3)	0.149(5)	-0.040(3)	-0.060(4)	0.008(4)
O(2D)	1a	0.1463(4)	0.0445(3)	0.4813(3)	0.063(2)	0.079(3)	0.067(3)	-0.017(2)	-0.029(2)	-0.010(2)
O(3D)	1a	0.2120(4)	-0.2325(3)	0.5658(3)	0.073(3)	0.069(3)	0.107(4)	-0.002(2)	-0.013(3)	-0.034(3)
C(1D)	1a	0.0427(6)	0.3358(4)	0.3037(5)	0.074(4)	0.067(4)	0.079(5)	-0.018(3)	-0.024(4)	-0.016(4)
C(2D)	1a	0.2397(6)	0.3012(4)	0.3311(4)	0.070(4)	0.057(3)	0.082(5)	-0.026(3)	-0.019(4)	-0.019(4)
C(3D)	1a	0.2799(7)	0.3603(6)	0.2622(6)	0.071(4)	0.100(5)	0.117(7)	-0.026(4)	-0.018(5)	-0.031(6)
C(4D)	1a	0.1972(8)	0.4098(7)	0.2122(6)	0.087(5)	0.134(7)	0.092(6)	-0.046(5)	-0.022(5)	0.002(5)
C(5D)	1a	0.0739(7)	0.3955(6)	0.2360(5)	0.090(5)	0.100(5)	0.083(6)	-0.023(4)	-0.027(5)	-0.006(5)
C(6D)	1a	0.3260(6)	0.2516(4)	0.3859(5)	0.064(4)	0.064(4)	0.119(6)	-0.025(3)	-0.018(4)	-0.018(4)
C(7D)	1a	0.3451(6)	0.1179(5)	0.4976(4)	0.059(4)	0.080(4)	0.083(5)	-0.018(3)	-0.024(4)	-0.027(4)
C(8D)	1a	0.2924(5)	0.0409(4)	0.5554(4)	0.054(3)	0.059(3)	0.081(5)	-0.007(3)	-0.031(3)	-0.016(3)
C(9D)	1a	0.3408(6)	0.0008(5)	0.6227(5)	0.053(3)	0.087(4)	0.092(6)	-0.012(3)	-0.031(4)	-0.033(4)
C(10D)	1a	0.2984(6)	-0.0708(5)	0.6833(4)	0.059(4)	0.085(4)	0.067(5)	-0.006(3)	-0.023(4)	-0.021(4)
C(11D)	1a	0.3427(8)	-0.1082(7)	0.7537(6)	0.088(5)	0.116(6)	0.090(6)	-0.010(5)	-0.037(5)	-0.021(6)
C(12D)	1a	0.2956(9)	-0.1709(7)	0.8107(6)	0.096(6)	0.136(7)	0.086(7)	-0.007(6)	-0.041(5)	-0.012(6)
C(13D)	1a	0.1984(9)	-0.2049(6)	0.8043(5)	0.105(6)	0.106(6)	0.078(6)	-0.012(5)	-0.026(5)	-0.005(5)
C(14D)	1a	0.1558(7)	-0.1723(5)	0.7360(4)	0.072(4)	0.084(4)	0.067(5)	-0.010(3)	-0.019(4)	-0.009(4)
C(15D)	1a	0.2033(6)	-0.1055(4)	0.6738(4)	0.056(3)	0.071(4)	0.076(5)	-0.001(3)	-0.017(4)	-0.026(4)
C(16D)	1a	0.1571(5)	-0.0674(4)	0.6022(4)	0.045(3)	0.063(3)	0.061(4)	-0.005(3)	-0.019(3)	-0.021(3)
C(17D)	1a	0.2005(5)	0.0032(4)	0.5470(4)	0.048(3)	0.060(3)	0.061(4)	-0.001(3)	-0.015(3)	-0.022(3)
C(18D)	1a	0.2050(8)	0.0020(5)	0.4182(5)	0.115(6)	0.100(5)	0.083(5)	-0.043(4)	-0.033(5)	-0.023(5)
C(19D)	1a	0.0568(5)	-0.1036(4)	0.5936(4)	0.058(4)	0.055(3)	0.061(4)	-0.012(3)	-0.018(3)	-0.009(3)
C(20D)	1a	-0.0723(6)	-0.0520(4)	0.6030(4)	0.063(4)	0.061(3)	0.055(4)	-0.009(3)	-0.015(3)	-0.014(3)
C(21D)	1a	-0.1077(6)	0.0309(5)	0.6225(5)	0.051(4)	0.079(4)	0.091(5)	-0.012(3)	-0.010(3)	-0.022(4)
C(22D)	1a	-0.2334(7)	0.0816(6)	0.6273(6)	0.074(5)	0.093(5)	0.128(7)	-0.002(4)	-0.022(5)	-0.037(5)
C(23D)	1a	-0.3236(6)	0.0447(6)	0.6174(6)	0.050(4)	0.116(6)	0.127(7)	-0.008(4)	-0.019(4)	-0.040(6)
C(24D)	1a	-0.2907(6)	-0.0349(6)	0.6024(5)	0.057(4)	0.118(6)	0.109(6)	-0.022(4)	-0.020(4)	-0.036(5)
C(25D)	1a	-0.1648(6)	-0.0892(5)	0.5956(4)	0.059(4)	0.088(4)	0.073(4)	-0.029(3)	-0.011(3)	-0.021(4)
C(26D)	1a	-0.1289(7)	-0.1749(5)	0.5793(5)	0.081(5)	0.093(5)	0.104(6)	-0.040(4)	-0.020(4)	-0.024(5)
C(27D)	1a	-0.0074(7)	-0.2234(5)	0.5688(5)	0.083(5)	0.083(4)	0.101(6)	-0.027(4)	-0.016(4)	-0.033(4)
C(28D)	1a	0.0857(6)	-0.1856(5)	0.5741(4)	0.067(4)	0.088(5)	0.076(5)	-0.029(4)	-0.016(3)	-0.018(4)
C(29D)	1a	0.2538(8)	-0.3112(5)	0.5340(6)	0.107(6)	0.090(5)	0.115(7)	-0.006(4)	-0.012(5)	-0.045(5)
C(1T2)	1a	0.213(1)	0.506(1)	0.7256(8)	0.16(1)	0.127(9)	0.15(1)	-0.056(9)	-0.048(9)	0.025(9)
C(2T2)	1a	0.135(2)	0.584(1)	0.739(1)	0.20(1)	0.109(9)	0.20(2)	-0.06(1)	-0.04(1)	0.01(1)
C(3T2)	1a	0.028(1)	0.5818(8)	0.7860(7)	0.21(1)	0.116(8)	0.111(9)	-0.071(9)	-0.064(9)	-0.001(7)
C(4T2)	1a	-0.0111(8)	0.5028(9)	0.8270(6)	0.105(7)	0.16(1)	0.088(6)	0.015(7)	-0.020(5)	-0.052(7)
C(5T2)	1a	0.0683(9)	0.4243(6)	0.8126(6)	0.139(8)	0.105(6)	0.102(7)	-0.024(6)	-0.031(6)	-0.022(6)
C(6T2)	1a	0.191(1)	0.4234(9)	0.7626(7)	0.121(8)	0.16(1)	0.120(8)	0.011(7)	-0.054(7)	-0.056(8)
C(7T2)	1a	-0.133(1)	0.508(1)	0.8726(9)	0.129(9)	0.31(2)	0.19(2)	0.05(1)	-0.028(9)	-0.16(2)

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