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Dopaminium perchlorate

Davar M. Boghaei,^{a*} Sahar Baniyaghoob,^a
Mohammad Mahdi Najafpour^a and Vickie McKee^b^aDepartment of Chemistry, Sharif University of Technology, PO Box 11155-8639, Tehran, Iran, and ^bDepartment of Chemistry, Loughborough University, Leicestershire LE11 3TU, England

Correspondence e-mail: dboghaei@sharif.edu

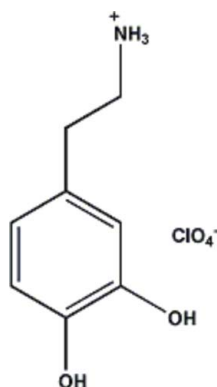
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.036; wR factor = 0.105; data-to-parameter ratio = 21.7.

In the title compound [systematic name: 2-(3,4-dihydroxyphenyl)ethanaminium perchlorate], $\text{C}_8\text{H}_{12}\text{NO}_2^+\cdot\text{ClO}_4^-$, the cations and anions are linked into three-dimensional structure *via* intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For related crystal structures, see: Bergin & Carlström (1968); Giesecke (1980). For details of the pharmacological properties of dopamine, see Salamone & Correa (2002).



Experimental

Crystal data

 $\text{C}_8\text{H}_{12}\text{NO}_2^+\cdot\text{ClO}_4^-$
 $M_r = 253.64$ Triclinic, $P\bar{1}$
 $a = 7.4925$ (3) Å $b = 8.2254$ (3) Å
 $c = 8.9524$ (4) Å
 $\alpha = 106.910$ (1)°
 $\beta = 94.186$ (1)°
 $\gamma = 101.206$ (1)°
 $V = 512.85$ (4) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 0.39$ mm⁻¹ $T = 150$ (2) K $0.30 \times 0.15 \times 0.06$ mm

Data collection

Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 2003)
 $T_{\min} = 0.893$, $T_{\max} = 0.977$ 6199 measured reflections
3146 independent reflections
2858 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.105$
 $S = 1.08$
3146 reflections145 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.49$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.45$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1O}\cdots\text{O11}$	0.85	2.16	2.9065 (14)	146
$\text{O2}-\text{H2O}\cdots\text{O11}^{\text{i}}$	0.85	1.96	2.7936 (15)	164
$\text{N1}-\text{H1A}\cdots\text{O1}^{\text{ii}}$	0.91	2.07	2.8822 (14)	148
$\text{N1}-\text{H1B}\cdots\text{O14}^{\text{iii}}$	0.91	1.93	2.8317 (16)	169
$\text{N1}-\text{H1C}\cdots\text{O12}^{\text{iv}}$	0.91	2.11	2.8002 (16)	132
$\text{N1}-\text{H1C}\cdots\text{O2}^{\text{iv}}$	0.91	2.39	3.0512 (16)	130

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x+1, -y+1, -z+2$; (iii) $x-1, y, z+1$; (iv) $x, y, z+1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINTE* (Bruker, 2005); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We are grateful to the Research Council of Sharif University of Technology and Loughborough University for their financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2470).

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supplementary materials

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Dopaminium perchlorate

D. M. Boghaei, S. Baniyaghoob, M. M. Najafpour and V. McKee

Comment

Many neuro transmitters have been discovered over the past century, such as serotonin, norepinephrine, substance P and dopamine. Dopamine is synthesized in the cenral brain from tyrosine. Dopamine has been considered as an important signal transmitter between the neurons and muscles (Salamone & Correa, 2002). Herewith we present the crystal structure of the title compound (I).

In (I) (Fig. 1), all bond lengths and angles are normal (Giesecke, 1980, Bergin & Carlström, 1968). The torsion angles C6—C1—C7—C8 and C1—C7—C8—N1 are 111.9 (1)° and 179.9 (6)°, respectively, showing that C1—C7—C8—N1 chain is almost fully extended, forming a plane that is nearly orthogonal to the plane of the ring. The crystal packing is stabilized by an extensive network of O—H···O and N—H···O hydrogen bonds (Table 1).

Experimental

The title compound was prepared by dissolving dopamine hydrochloride (2 mmol, 379 mg) and NaClO₄·H₂O (2 mmol, 280 mg) in water/HClO₄ (1mM, 10 ml). The mixture was stirred for about 2 h at room temperature. This solution yielded colourless crystals of (I) after 10 d.

Refinement

All H atoms atoms were placed in calculated positions and refined using the riding model approximation, with C—H = 0.95–1.0 Å, O—H = 0.85 Å, N—H = 0.91 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{N})$. The isotropic displacement parameter of the hydroxy H atoms were fixed to 0.04 Å²

Figures

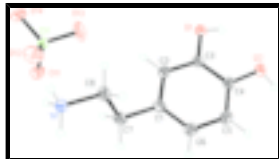


Fig. 1. The molecular structure of (I) showing the atomic labels and displacement ellipsoids for non-H atoms drawn at the 50% probability level.

2-(3,4-dihydroxyphenyl)ethanaminium perchlorate

Crystal data

C₈H₁₂NO₂⁺·ClO₄⁻

$M_r = 253.64$

$Z = 2$

$F_{000} = 264$

supplementary materials

Triclinic, *P* $\bar{1}$

Hall symbol: -P1

$a = 7.4925$ (3) Å

$b = 8.2254$ (3) Å

$c = 8.9524$ (4) Å

$\alpha = 106.910$ (1)°

$\beta = 94.186$ (1)°

$\gamma = 101.206$ (1)°

$V = 512.85$ (4) Å³

$D_x = 1.642$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3633 reflections

$\theta = 2.4$ – 31.6 °

$\mu = 0.39$ mm⁻¹

$T = 150$ (2) K

Plate, colourless

$0.30 \times 0.15 \times 0.06$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 150$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2003)

$T_{\min} = 0.893$, $T_{\max} = 0.977$

6199 measured reflections

3146 independent reflections

2858 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\text{max}} = 31.7$ °

$\theta_{\text{min}} = 2.4$ °

$h = -10 \rightarrow 10$

$k = -12 \rightarrow 11$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.105$

$S = 1.09$

3146 reflections

145 parameters

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0559P)^2 + 0.2163P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.49$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.45$ e Å⁻³

Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against all reflections. The weighted R -factor wR and

goodness of fit S are based on F^2 , conventional R -factors R are based

on F , with F set to zero for negative F^2 . The threshold expression of

$F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is

not relevant to the choice of reflections for refinement. R -factors based

on F^2 are statistically about twice as large as those based on F , and R -

factors based on all data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.78299 (4)	0.71277 (4)	0.38696 (3)	0.01882 (9)
O11	0.78911 (17)	0.88541 (14)	0.49463 (13)	0.0299 (2)
O12	0.61768 (16)	0.59722 (16)	0.39753 (16)	0.0370 (3)
O13	0.7897 (2)	0.7193 (2)	0.23036 (14)	0.0436 (3)
O14	0.93581 (16)	0.65238 (18)	0.43983 (14)	0.0373 (3)
C1	0.28726 (18)	0.78530 (16)	1.02178 (15)	0.0185 (2)
C2	0.45074 (18)	0.77363 (16)	0.95805 (14)	0.0185 (2)
H2	0.5479	0.7464	1.0135	0.022*
C3	0.47193 (17)	0.80155 (16)	0.81453 (14)	0.0177 (2)
O1	0.63545 (13)	0.79282 (13)	0.75554 (11)	0.02136 (19)
C4	0.32907 (18)	0.84083 (16)	0.73205 (14)	0.0188 (2)
O2	0.36279 (15)	0.86353 (13)	0.58877 (11)	0.0240 (2)
C5	0.16751 (18)	0.85522 (17)	0.79484 (16)	0.0212 (2)
H5	0.0713	0.8842	0.7397	0.025*
C6	0.14636 (18)	0.82696 (17)	0.93990 (16)	0.0208 (2)
H6	0.0352	0.8362	0.9829	0.025*
C7	0.2661 (2)	0.75345 (17)	1.17802 (15)	0.0215 (2)
H7A	0.1522	0.7850	1.2147	0.026*
H7B	0.3713	0.8279	1.2575	0.026*
C8	0.2576 (2)	0.56300 (17)	1.16162 (15)	0.0222 (3)
H8A	0.1526	0.4892	1.0815	0.027*
H8B	0.3714	0.5320	1.1244	0.027*
N1	0.23650 (15)	0.52615 (15)	1.31419 (13)	0.0200 (2)
H1A	0.2317	0.4112	1.2999	0.030*
H1B	0.1310	0.5528	1.3479	0.030*
H1C	0.3340	0.5921	1.3875	0.030*
H2O	0.2968	0.9273	0.5626	0.040*
H1O	0.6356	0.8281	0.6748	0.040*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.01669 (14)	0.02486 (16)	0.01828 (15)	0.00806 (11)	0.00411 (10)	0.00922 (11)
O11	0.0394 (6)	0.0222 (5)	0.0305 (5)	0.0104 (4)	0.0048 (4)	0.0096 (4)
O12	0.0253 (5)	0.0348 (6)	0.0453 (7)	-0.0014 (5)	0.0097 (5)	0.0083 (5)

supplementary materials

O13	0.0561 (8)	0.0597 (8)	0.0200 (5)	0.0123 (7)	0.0065 (5)	0.0201 (5)
O14	0.0303 (6)	0.0537 (7)	0.0342 (6)	0.0287 (5)	0.0029 (4)	0.0113 (5)
C1	0.0249 (6)	0.0149 (5)	0.0170 (5)	0.0059 (4)	0.0049 (4)	0.0058 (4)
C2	0.0241 (6)	0.0173 (5)	0.0166 (5)	0.0079 (4)	0.0028 (4)	0.0070 (4)
C3	0.0224 (5)	0.0153 (5)	0.0168 (5)	0.0066 (4)	0.0046 (4)	0.0052 (4)
O1	0.0248 (5)	0.0250 (5)	0.0206 (4)	0.0118 (4)	0.0087 (3)	0.0114 (4)
C4	0.0256 (6)	0.0168 (5)	0.0150 (5)	0.0061 (4)	0.0016 (4)	0.0059 (4)
O2	0.0327 (5)	0.0276 (5)	0.0174 (4)	0.0132 (4)	0.0047 (4)	0.0116 (4)
C5	0.0229 (6)	0.0209 (5)	0.0213 (6)	0.0070 (5)	0.0005 (4)	0.0079 (5)
C6	0.0215 (6)	0.0199 (5)	0.0229 (6)	0.0063 (4)	0.0052 (5)	0.0079 (5)
C7	0.0301 (6)	0.0193 (5)	0.0194 (6)	0.0091 (5)	0.0094 (5)	0.0085 (4)
C8	0.0331 (7)	0.0189 (5)	0.0168 (5)	0.0077 (5)	0.0048 (5)	0.0077 (4)
N1	0.0215 (5)	0.0229 (5)	0.0208 (5)	0.0085 (4)	0.0064 (4)	0.0118 (4)

Geometric parameters (Å, °)

Cl1—O13	1.4225 (11)	O2—H2O	0.8540
Cl1—O12	1.4347 (11)	C5—C6	1.3989 (18)
Cl1—O14	1.4355 (11)	C5—H5	0.9500
Cl1—O11	1.4559 (11)	C6—H6	0.9500
C1—C6	1.3939 (18)	C7—C8	1.5185 (18)
C1—C2	1.3968 (18)	C7—H7A	0.9900
C1—C7	1.5099 (17)	C7—H7B	0.9900
C2—C3	1.3842 (16)	C8—N1	1.4954 (16)
C2—H2	0.9500	C8—H8A	0.9900
C3—O1	1.3753 (15)	C8—H8B	0.9900
C3—C4	1.3975 (18)	N1—H1A	0.9100
O1—H1O	0.8537	N1—H1B	0.9100
C4—C5	1.3826 (19)	N1—H1C	0.9100
C4—O2	1.3828 (15)		
O13—Cl1—O12	111.25 (8)	C6—C5—H5	120.2
O13—Cl1—O14	111.08 (8)	C1—C6—C5	120.47 (12)
O12—Cl1—O14	107.81 (8)	C1—C6—H6	119.8
O13—Cl1—O11	110.40 (8)	C5—C6—H6	119.8
O12—Cl1—O11	108.15 (7)	C1—C7—C8	110.27 (10)
O14—Cl1—O11	108.02 (7)	C1—C7—H7A	109.6
C6—C1—C2	119.24 (11)	C8—C7—H7A	109.6
C6—C1—C7	121.09 (11)	C1—C7—H7B	109.6
C2—C1—C7	119.67 (11)	C8—C7—H7B	109.6
C3—C2—C1	120.37 (12)	H7A—C7—H7B	108.1
C3—C2—H2	119.8	N1—C8—C7	111.89 (10)
C1—C2—H2	119.8	N1—C8—H8A	109.2
O1—C3—C2	119.37 (11)	C7—C8—H8A	109.2
O1—C3—C4	120.57 (11)	N1—C8—H8B	109.2
C2—C3—C4	120.06 (11)	C7—C8—H8B	109.2
C3—O1—H1O	109.3	H8A—C8—H8B	107.9
C5—C4—O2	124.27 (11)	C8—N1—H1A	109.5
C5—C4—C3	120.16 (11)	C8—N1—H1B	109.5
O2—C4—C3	115.56 (11)	H1A—N1—H1B	109.5

C4—O2—H2O	111.4	C8—N1—H1C	109.5
C4—C5—C6	119.69 (12)	H1A—N1—H1C	109.5
C4—C5—H5	120.2	H1B—N1—H1C	109.5

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1O \cdots O11	0.85	2.16	2.9065 (14)	146
O2—H2O \cdots O11 ⁱ	0.85	1.96	2.7936 (15)	164
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Fig. 1

