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Dopaminium perchlorate

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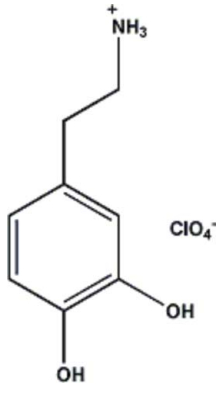
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.105; data-to-parameter ratio = 21.7.

In the title compound [systematic name: 2-(3,4-dihydroxyphenyl)ethanaminium perchlorate], $C_8H_{12}NO_2^+\cdot ClO_4^-$, the cations and anions are linked into three-dimensional structure *via* intermolecular N—H···O and O—H···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

$C_8H_{12}NO_2^+\cdot ClO_4^-$
M_r = 253.64
Triclinic, $P\overline{1}$
a = 7.4925 (3) Å
b = 8.2254 (3) Å
c = 8.9524 (4) Å
α = 106.910 (1)°
β = 94.186 (1)°
γ = 101.206 (1)°
V = 512.85 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 150 (2) K
0.30 × 0.15 × 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_{int} = 0.018

Refinement

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

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···O11	0.85	2.16	2.9065 (14)	146
O2—H2*O*···O11^{i}	0.85	1.96	2.7936 (15)	164
N1—H1*A*···O1^{ii}	0.91	2.07	2.8822 (14)	148
N1—H1*B*···O14^{iii}	0.91	1.93	2.8317 (16)	169
N1—H1*C*···O12^{iv}	0.91	2.11	2.8002 (16)	132
N1—H1*C*···O2^{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: *SAINT* (Bruker, 2005); data reduction: *SAINT*; 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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supporting information

Acta Cryst. (2008). E**64**, o2268 [doi:10.1107/S1600536808035666]

Dopaminium perchlorate

Davar M. Boghaei, Sahar Baniyaghoob, Mohammad Mahdi Najafpour and Vickie McKee

S1. 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).

S2. Experimental

The title compound was prepared by dissolving dopamine hydrochloride (2 mmol, 379 mg) and $NaClO_4.H_2O$ (2 mmol, 280 mg) in water/$HClO_4$ (1mM, 10 ml). The mixture was stirred for about 2 h at room temperature. This solution yielded colourless crystals of (I) after 10 d.

S3. 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_{iso}(H) = 1.2Ueq(C) or 1.5Ueq(N). The isotropic displacement parameter of the hydroxy H atoms were fixed to 0.04 Å^2

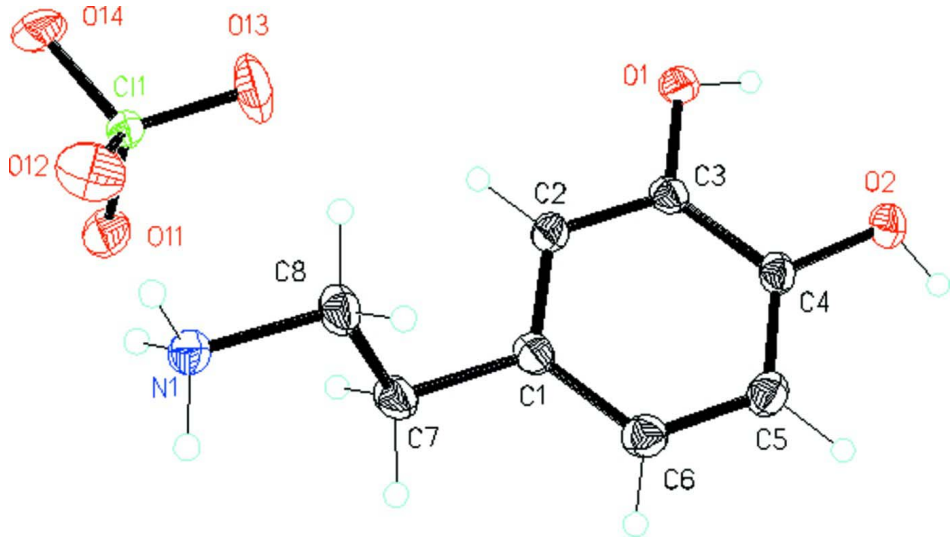

Figure 1

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

$C_8H_{12}NO_2^+\cdot ClO_4^-$
$M_r = 253.64$
Triclinic, $P\overline{1}$
Hall symbol: -P1
$a = 7.4925\ (3)$ Å
$b = 8.2254\ (3)$ Å
$c = 8.9524\ (4)$ Å
$\alpha = 106.910\ (1)°$
$\beta = 94.186\ (1)°$
$\gamma = 101.206\ (1)°$
$V = 512.85\ (4)$ Å^3
$Z = 2$
$F(000) = 264$
$D_x = 1.642$ 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}
$T = 150$ K
Plate, colourless
0.30 × 0.15 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
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 $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 31.7°$, $\theta_{min} = 2.4°$
$h = -10\rightarrow10$
$k = -12\rightarrow11$
$l = -12\rightarrow12$

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
0 restraints
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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	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 (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	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)
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, º)

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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O11	0.85	2.16	2.9065 (14)	146
O2—H2*O*···O11^{i}	0.85	1.96	2.7936 (15)	164
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