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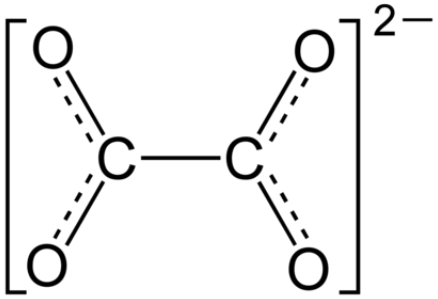
Oxalate

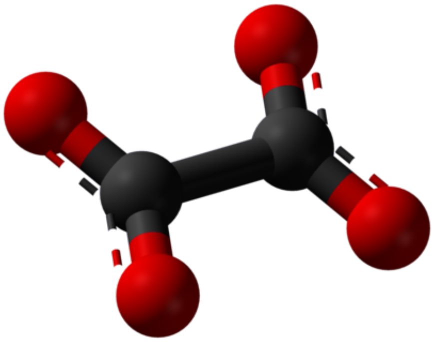
Oxalate (IUPAC: **ethanedioate**) is the dianion with the formula $C_2O_4^{2-}$, also written $(COO)_2^{2-}$. Either name is often used for derivatives, such as salts of oxalic acid, for example sodium oxalate $Na_2C_2O_4$, or dimethyl oxalate $((CH_3)_2C_2O_4)$. Oxalate also forms coordination compounds where it is sometimes abbreviated as **ox**.

Many metal ions form insoluble precipitates with oxalate, a prominent example being calcium oxalate, the primary constituent of the most common kind of kidney stones.

Oxalate



The structure of the oxalate anion



A ball-and-stick model of oxalate

Names	
IUPAC names	oxalate[1][2], ethanedioate[3]
Systematic IUPAC name	ethanedioate
Other names	oxalate ion,[1] ethanedioic acid dianion, oxalic acid dianion[2]
Identifiers	
CAS Number	338-70-5 (http://www.commonchemistry.org/ChemicalDetail.aspx?ref=338-70-5)

Contents

Relationship to oxalic acid

The dissociation of protons from oxalic acid proceeds in a stepwise manner as for other polyprotic acids. Loss of a single proton results in the monovalent hydrogenoxalate anion $HC_2O_4^-$. A salt with this anion is sometimes called an **acid oxalate**, **monobasic oxalate**, or **hydrogen oxalate**. The equilibrium constant (K_a) for loss of the first proton is 5.37×10^{-2} (pK_a = 1.27). The loss of the second proton, which yields the oxalate ion, has an equilibrium constant of 5.25×10^{-5} (pK_a = 4.28). These values imply, in solutions with neutral pH, no oxalic acid and only trace amounts of hydrogen oxalate exist.[19] The literature is often unclear on the distinction between $H_2C_2O_4$, $HC_2O_4^-$, and $C_2O_4^{2-}$, and the collection of species is referred to as oxalic acid.

Structure

X-ray crystallography of simple oxalate salts show that the oxalate anion may adopt either a planar conformation with D_{2h} molecular symmetry, or a conformation where the O–C–C–O dihedrals approach 90° with approximate D_{2d} symmetry.[20] Specifically, the oxalate moiety adopts the planar, D_{2h} conformation in the solid-state structures of $M_2C_2O_4$ (M = Li, Na, K).[21][22] However, in structure of $Cs_2C_2O_4$ the O–C–C–O dihedral angle is 81(1)°.[23][24] Therefore, $Cs_2C_2O_4$ is more closely approximated by a D_{2d} symmetry structure because the two CO_2 planes are staggered. Two forms of $Rb_2C_2O_4$ have been structurally characterized by single-crystal X-ray diffraction; one contains a planar and the other a staggered oxalate.

As the preceding examples indicate that the conformation adopted by the oxalate dianion is dependent upon the size of the alkali metal to which it is bound, some have explored the barrier to rotation about the central C–C bond. The barrier to rotation about this bond was determined computationally to be roughly 2–6 kcal/mol for the free dianion, $C_2O_4^{2-}$.[25][26][27] Such results are consistent with the interpretation that the

	[4][2]
3D model (JSmol)	Interactive image (https://chemapps.stolaf.edu/jmol/jmol.php?model=C%28%3DO%29%28C%28%3DO%29%5BO-%5D%29%5BO-%5D)
Beilstein Reference	1905970[12][13]
ChEBI	CHEBI:30623 (https://www.ebi.ac.uk/chebi/searchId.do?chebiId=30623) [1][5]
ChemSpider	64235 (http://www.chemspider.com/Chemical-Structure.64235.html) [1]
Gmelin Reference	2207[14]
KEGG	C00209 (https://www.kegg.jp/entry/C00209) [6]
PubChem CID	71081 (https://pubchem.ncbi.nlm.nih.gov/compound/71081) [2]
InChI	
SMILES	
Properties	
Chemical formula	$C_2O_4^{2-}$[18]
Molar mass	88.019 g·mol^{-1}[15][16]
Conjugate acid	Hydrogenoxalate[17]
Structure	

central carbon–carbon bond is best regarded as a single bond with only minimal pi interactions between the two CO_2^- units.[20] This barrier to rotation about the C–C bond (which formally corresponds to the difference in energy between the planar and staggered forms) may be attributed to electrostatic interactions as unfavorable O–O repulsion is maximized in the planar form.

Point group	D_{2h}
Related compounds	
Related isoelectronic	dinitrogen tetroxide
Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa).	
Infobox references	

Importantly, oxalate is often encountered as a bidentate, chelating ligand, such as in potassium ferrioxalate. When the oxalate chelates to a single metal center, it always adopts the planar conformation.

Occurrence in nature

Oxalate occurs in many plants, where it is synthesized by the incomplete oxidation of carbohydrates.

Oxalate-rich plants include fat hen ("lamb's quarters"), sorrel, and several *Oxalis* species. The root and/or leaves of rhubarb and buckwheat are high in oxalic acid.[28] Other edible plants that contain significant concentrations of oxalate include, in decreasing order, star fruit (carambola), black pepper, parsley, poppy seed, amaranth, spinach, chard, beets, cocoa, chocolate, most nuts, most berries, fishtail palms, New Zealand spinach (*Tetragonia tetragonioides*), and beans. Leaves of the tea plant (*Camellia sinensis*) contain among the greatest measured concentrations of oxalic acid relative to other plants. However, the beverage derived by infusion in hot water typically contains only low to moderate amounts of oxalic acid due to the small mass of leaves used for brewing.

Common high-oxalate foods[29]

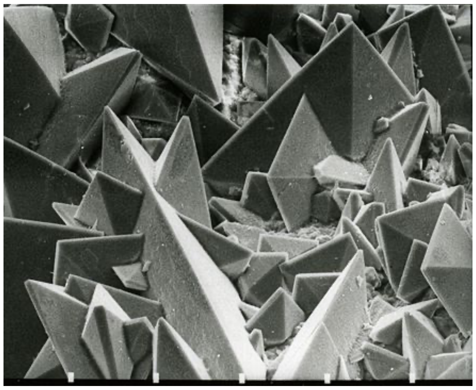
Food item	Serving	Oxalate Content (mg)
Beetroot greens, cooked	½ cup (unit)	916
Purslane, leaves, cooked	½ cup	910
Rhubarb, stewed, no sugar	½ cup	860
Spinach, cooked	½ cup	750
Beet, cooked	½ cup	675
Chard, Swiss, leaves cooked	½ cup	660

Rhubarb, canned	½ cup	600
Spinach, frozen	½ cup	600
Beet, pickled	½ cup	500
Poke greens, cooked	½ cup	476
Endive, raw	20 long leaves	273
Cocoa, dry	⅓ cup	254
Dandelion greens, cooked	½ cup	246
Okra, cooked	8–9 pods	146
Sweet potato, cooked	½ cup	141
Kale, cooked	½ cup	125
Peanuts, raw	⅓ cup (1¾ oz)	113
Turnip greens, cooked	½ cup	110
Chocolate, unsweetened	1 oz	91
Parsnips, diced, cooked	½ cup	81
Collard greens, cooked	½ cup	74
Pecans, halves, raw	⅓ cup (1¼ oz)	74
Tea, leaves (4-minute infusion)	1 level tsp in 7 fl oz water	72
Cereal germ, toasted	¼ cup	67
Gooseberries	½ cup	66
Potato, Idaho white, baked	1 medium	64
Carrots, cooked	½ cup	45
Apple, raw with skin	1 medium	41
Brussels sprouts, cooked	6–8 medium	37
Strawberries, raw	½ cup	35
Celery, raw	2 stalks	34
Milk chocolate bar	1 bar (1.02 oz)	34
Raspberries, black, raw	½ cup	33
Orange, edible portion	1 medium	24

Green beans, cooked	$^1\!/_2$ cup	23
Chives, raw, chopped	1 tablespoon	19
Leeks, raw	$^1\!/_2$ medium	15
Blackberries, raw	$^1\!/_2$ cup	13
Concord grapes	$^1\!/_2$ cup	13
Blueberries, raw	$^1\!/_2$ cup	11
Redcurrants	$^1\!/_2$ cup	11
Apricots, raw	2 medium	10
Raspberries, red, raw	$^1\!/_2$ cup	10
Broccoli, cooked	1 large stalk	6
Cranberry juice	$^1\!/_2$ cup (4 oz)	6

Physiological effects

In the body, oxalic acid combines with divalent metallic cations such as calcium (Ca^{2+}) and iron(II) (Fe^{2+}) to form crystals of the corresponding oxalates which are then excreted in urine as minute crystals. These oxalates can form larger kidney stones that can obstruct the kidney tubules. An estimated 80% of kidney stones are formed from calcium oxalate.[30] Those with kidney disorders, gout, rheumatoid arthritis, or certain forms of chronic vulvar pain (vulvodynia) are typically advised to avoid foods high in oxalic acid. Methods to reduce the oxalate content in food are of current interest.[31]



Scanning electron micrograph of the surface of a kidney stone showing tetragonal crystals of weddellite (calcium oxalate dihydrate) emerging from the amorphous central part of the stone; the horizontal length of the picture represents 0.5 mm of the figured original.

Magnesium (Mg^{2+}) oxalate is 567 times more soluble than calcium oxalate, so the latter is more likely to precipitate out when magnesium levels are low and calcium and oxalate levels are high. Magnesium oxalate is a million times more soluble than mercury oxalate. Oxalate solubility for metals decreases in the order Mg > Ca > Cd > Zn > {Mn, Ni, Fe, Cu} > {As, Sb, Pb} > Hg.

The highly insoluble iron(II) oxalate appears to play a major role in gout, in the nucleation and growth of the otherwise extremely soluble sodium urate. This explains why gout usually appears after age 40, when ferritin levels in blood exceed 1 μg/L. Foods high in oxalate[32] should be avoided by people suffering from, or at risk of gout.[33]

Cadmium catalyzes the transformation of vitamin C into oxalic acid. This can be a problem for people exposed to high levels of cadmium in their diets, in the workplace, or through smoking.

In studies with rats, calcium supplements given along with foods high in oxalic acid can cause calcium oxalate to precipitate in the gut and reduce the levels of oxalate absorbed by the body (by 97% in some cases).[34][35]

Oxalic acid can also be produced by the metabolism of ethylene glycol ("antifreeze"), glyoxylic acid, or ascorbic acid (vitamin C).[36]

Powdered oxalate is used as a pesticide in beekeeping to combat the bee mite.

Some fungi of the genus *Aspergillus* produce oxalic acid.[37]

Some preliminary evidence indicates the administration of probiotics can affect oxalic acid excretion rates in a positive manner.[38]

As a ligand

Oxalate, the conjugate base of oxalic acid, is an excellent ligand for metal ions. It usually binds as a bidentate ligand forming a 5-membered MO_2C_2 ring. An illustrative complex is potassium ferrioxalate, $K_3[Fe(C_2O_4)_3]$. The drug oxaliplatin exhibits improved water solubility relative to older platinum-based drugs, avoiding the dose-limiting side-effect of nephrotoxicity. Oxalic acid and oxalates can be oxidized by permanganate in an autocatalytic reaction. One of the main applications of oxalic acid is rust-removal, which arises because oxalate forms water-soluble derivatives with the ferric ion.

Excess

An excess oxalate level in the blood is termed *hyperoxalemia*, and high levels of oxalate in the urine is termed hyperoxaluria.

Acquired

Although unusual, consumption of oxalates (for example, the grazing of animals on oxalate-containing plants such as *Bassia hyssopifolia*, or human consumption of wood sorrel or, specifically in excessive quantities, black tea) may result in kidney disease or even death due to oxalate poisoning. *The New England Journal of Medicine* reported acute oxalate nephropathy "almost certainly due to excessive consumption of iced tea" in a 56-year-old man, who drank "sixteen 8-ounce glasses of iced tea daily" (roughly 3.8 liters). The authors of the paper hypothesized that acute oxalate nephropathy is an underdiagnosed cause of kidney failure and suggested thorough examination of patient dietary history in cases of unexplained kidney failure without proteinuria (an excess of protein in the urine) and with large amounts of calcium oxalate in urine sediment.[39] *Oxalobacter formigenes* in the gut flora may help alleviate this.[40]

Congenital

Primary hyperoxaluria is a rare, inherited condition, resulting in increased excretion of oxalate, with oxalate stones being common.

See also

- Dimethyl oxalate – $(CH_3)_2C_2O_4$
- Diphenyl oxalate – $(C_6H_5)_2C_2O_4$
- Potassium ferrioxalate – $K_3[Fe(C_2O_4)_3]$, an iron complex with oxalate ligands
- Raphide
- Sodium oxalate – $Na_2C_2O_4$

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