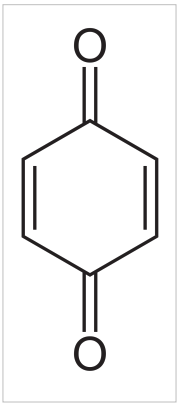
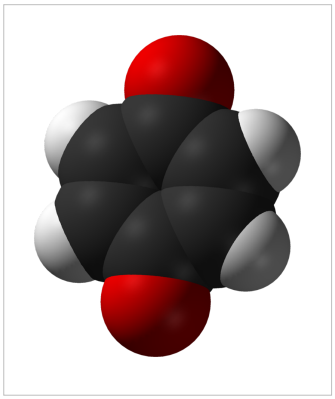
1,4-Benzoquinone

1,4-Benzoquinone	
	
Identifiers	
CAS number	106-51-4 [1] ✓
RTECS number	DK2625000
SMILES	
Properties	
Molecular formula	$C_6H_4O_2$
Molar mass	108.095 g/mol
Appearance	Yellow solid
Density	1.318 g/cm^3 at 20 °C, solid
Melting point	115 °C
Boiling point	Sublimes
Solubility in water	Slightly soluble
Solubility	Slightly soluble in petroleum ether; soluble in acetone; very soluble in ethanol, benzene, diethyl ether
Hazards	
R-phrases	R23/25 R36/37/38 R50
S-phrases	S26 S28 S45 S61
Related compounds	
Related compounds	1,2-Benzoquinone
✓ (what is this?) (verify) [2] Except where noted otherwise, data are given for materials in their standard state (at 25 °C, 100 kPa)	
Infobox references	

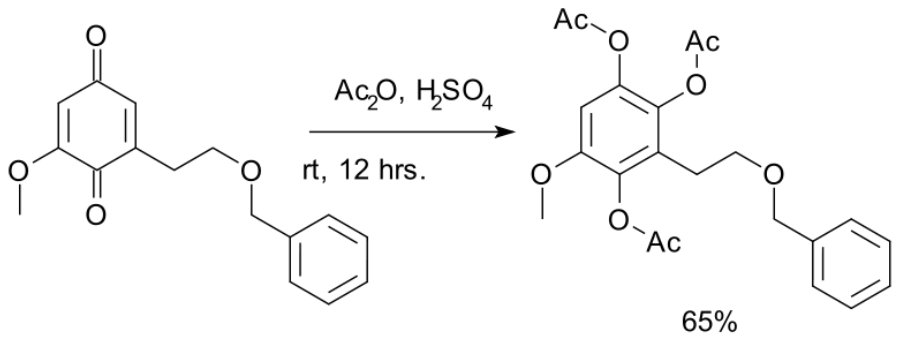
1,4-Benzoquinone, commonly known as **para-quinone**, is a chemical compound with the formula $C_6H_4O_2$. In pure state, it forms bright yellow crystals with characteristic irritating odor, resembling that of chlorine; impure samples are often dark colored due to the presence of quinhydrone (1:1 complex of quinone with hydroquinone). This six-membered ring compound is the oxidized derivative of 1,4-hydroquinone.[3] The molecule is multifunctional: it exhibits properties of a ketone, forming an oxime; an oxidant, forming the dihydroxy derivative; and an alkene,

undergoing addition reactions, especially those typical for α,β-unsaturated ketones. 1,4-Benzoquinone is sensitive towards both strong mineral acids and alkali, which cause condensation and decomposition of the compound.

Applications in organic synthesis

It is used as a hydrogen acceptor and oxidant in organic synthesis.[4] 1,4-Benzoquinone serves as a dehydrogenation reagent. It is also used as a dienophile in Diels Alder reactions.[5]

Benzoquinone reacts with acetic anhydride and sulfuric acid to the triacetate of 1,3,4-trihydroxybenzene. This reaction is called the **Thiele reaction** [6] after Johannes Thiele who first described the reaction in 1898. An application is found in total synthesis [7] :



Benzoquinone is also used to suppress double bond migration during Olefin Metathesis reactions.

An acidic potassium iodide solution reduces a solution of benzoquinone to hydroquinone, which is oxidized back with a solution of silver nitrate.

Related 1,4-benzoquinones

A variety of derivatives and analogues are known. Illustrative examples:

- 1,4-Naphthoquinone, derived by oxidation of naphthalene with chromium trioxide.[8]
- 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), a stronger oxidant and dehydrogenation agent than 1,4-benzoquinone.[9]
- Ubiquinone-1, a naturally occurring 1,4-benzoquinone.
- Chloro-p-benzoquinone, (CAS no. [695-99-8])[10]
- Chloranil, 1,4-$C_6Cl_4O_2$, a stronger oxidant and dehydrogenation agent than 1,4-benzoquinone.

See also

- Tetrahydroxybenzoquinone
- Benzoquinonetetracarboxylic acid
- 1,2-Benzoquinone
- Quinones

References

[1] http://www.commonchemistry.org/ChemicalDetail.aspx?ref=106-51-4

[2] http://en.wikipedia.org/wiki/

[3] H. W. Underwood, Jr. and W. L. Walsh (1943), "Quinone" (http://www.orgsyn.org/orgsyn/orgsyn/prepContent.asp?prep=cv2p0553), *Org. Synth.*, ; *Coll. Vol.* **2**: 553

[4] Yang, T.-K.; Shen, C.-Y. "1,4-Benzoquinone" in Encyclopedia of Reagents for Organic Synthesis (Ed: L. Paquette) 2004, J. Wiley & Sons, New York. doi:10.1002/047084289.

[5] Oda, M.; Kawase, T.; Okada, T.; Enomoto, T. (1998), "2-Cyclohexene-1,4-dione" (http://www.orgsyn.org/orgsyn/orgsyn/prepContent.asp?prep=cv9p0186), *Org. Synth.*, ; *Coll. Vol.* **9**: 186

[6] *Ueber die Einwirkung von Essigsäure-anhydrid auf Chinon und auf Dibenzoylstyrol* (pp. 1247–1249) Johannes Thiele Berichte der deutschen chemischen Gesellschaft Volume 31, Issue 1, pages 1247–1249 1898 doi:10.1002/cber.189803101226

[7] *Stereoselective Total Synthesis and Enantioselective Formal Synthesis of the Antineoplastic Sesquiterpene Quinone Metachromin A* Wanda P. Almeida, and Carlos Roque D. Correia J. Braz. Chem. Soc., Vol. 10, No. 5, 401–414, **1999** doi:10.1590/S0103-50531999000500011.

[8] E. A. Braude E. A.; Fawcett, J. S. (1963), "1,4-Naphthoquinone" (http://www.orgsyn.org/orgsyn/orgsyn/prepContent.asp?prep=cv4p0698), *Org. Synth.*, ; *Coll. Vol.* **4**: 698

[9] Vogel, E.; Klug, W.; Breuer, A. (1988), "1,6-Methano[10]annulene" (http://www.orgsyn.org/orgsyn/orgsyn/prepContent.asp?prep=cv6p0731), *Org. Synth.*, ; *Coll. Vol.* **6**: 731

[10] Harman, R. E. (1963), "Chloro-p-benzoquinone" (http://www.orgsyn.org/orgsyn/orgsyn/prepContent.asp?prep=cv4p0148), *Org. Synth.*, ; *Coll. Vol.* **4**: 148

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