

Iodoform

Iodoform (also known as **triiodomethane** and, inaccurately, as **carbon triiodide**) is the organoiodine compound with the formula CHI_3 . A pale yellow, crystalline, volatile substance, it has a penetrating and distinctive odor (in older chemistry texts, the smell is sometimes referred to as that of hospitals, where the compound is still commonly used) and, analogous to chloroform, sweetish taste. It is occasionally used as a disinfectant.

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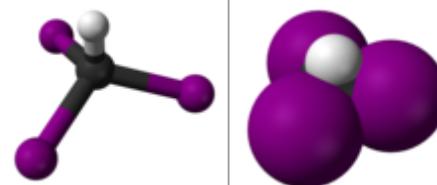
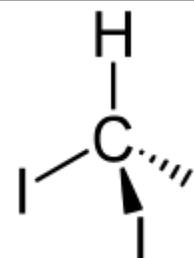
Structure

The molecule adopts tetrahedral molecular geometry with C_{3v} symmetry.

Synthesis and reactions

The synthesis of iodoform was first described by Georges-Simon Serullas in 1822, by reactions of iodine vapour with steam over red-hot coals, and also by reaction of potassium with ethanolic iodine in the presence of water;^[5] and at much the same time independently by John Thomas Cooper.^[6] It is synthesized in the haloform reaction by the reaction of iodine and sodium hydroxide with any one of these four kinds of organic compounds: a methyl ketone (CH_3COR), acetaldehyde (CH_3CHO), ethanol ($\text{CH}_3\text{CH}_2\text{OH}$), and certain secondary alcohols (CH_3CHROH , where R is an alkyl or aryl group).

Iodoform



Names

Preferred IUPAC name

Triiodomethane

Other names

Iodoform;^[1]

Carbon triiodide

Identifiers

CAS Number	75-47-8 (http://www.commonchemistry.org/ChemicalDetail.aspx?ref=75-47-8) [✓]
3D model (JSmol)	Interactive image (https://chemapps.stolaf.edu/jmol/mol.php?model=I%20C%28I%29)
Beilstein Reference	1697010
ChEBI	CHEBI:37758 (https://www.ebi.ac.uk/chebi/searchId.do?chebiId=37758) [✓]
ChEMBL	ChEMBL1451116 (https://www.ebi

	ac.uk/chembl/db/index.php/compound/inspect/ChEMBL/1451116 ✖
ChemSpider	6134 (http://www.chemspider.com/Chemical-Structure.6134.html) ✓
ECHA InfoCard	100.000.795 (https://echa.europa.eu/substance-information/-/substanceinfo/100.000.795)
EC Number	200-874-5
KEGG	D01910 (https://www.kegg.jp/entry/D01910) ✓
MeSH	iodoform (https://www.nlm.nih.gov/cgi/mesh/2014/MB_cgi?mode=&term=iodoform)
PubChem CID	6374 (https://pubchem.ncbi.nlm.nih.gov/compound/6374)
RTECS number	PB7000000
UNII	KXI2J76489 (https://fdasis.nlm.nih.gov/srs/srsdirect.jsp?regno=KXI2J76489) ✓
CompTox Dashboard (EPA)	DTXSID4020743 (https://comptox.epa.gov/dashboard/DTXSID4020743) ✎
InChI	InChI=1S/CHI3/c2-1(3)4/h1H ✓ Key: OKJPEAGHQZHRQV-UHFFFAOYSA-N ✓
SMILES	

IC(I)I	
Properties	
Chemical formula	CHI ₃
Molar mass	393.732 g·mol ⁻¹
Appearance	Pale, light yellow, opaque crystals
Odor	Saffron-like ^[2]
Density	4.008 g cm ⁻³ ^[2]
Melting point	119 °C (246 °F; 392 K) ^[2]
Boiling point	218 °C (424 °F; 491 K) ^[2]
Solubility in water	100 mg L ⁻¹ ^[2]
Solubility in diethyl ether	136 g L ⁻¹
Solubility in acetone	120 g L ⁻¹
Solubility in ethanol	78 g L ⁻¹
log <i>P</i>	3.118
Henry's law constant (<i>k</i> _H)	3.4 μmol Pa ⁻¹ kg ⁻¹
Magnetic susceptibility (<i>χ</i>)	−117.1·10 ⁻⁶ cm ³ /mol
Structure	
Crystal structure	Hexagonal
Coordination geometry	Tetragonal
Molecular shape	Tetrahedron
Thermochemistry	
Heat capacity (<i>C</i>)	157.5 J K ⁻¹ mol ⁻¹
Std enthalpy of formation (<i>Δ</i> _f <i>H</i> [⊖] ₂₉₈)	180.1–182.1 kJ mol ⁻¹
Std enthalpy of combustion (<i>Δ</i> _c <i>H</i> [⊖] ₂₉₈)	−716.9 – −718.1 kJ mol ⁻¹
Pharmacology	
ATC code	D09AA13 (WHO (https://www.who

	cc.no/atc_ddd_in dex/?code=D09A A13))
Hazards	
GHS pictograms	
GHS Signal word	Warning
GHS hazard statements	H315, H319, H335
GHS precautionary statements	P261, P280, P305+351+338
NFPA 704 (fire diamond)	
Flash point	204 °C (399 °F; 477 K)
Lethal dose or concentration (LD, LC):	
LD ₅₀ (median dose)	355 mg/kg (oral, rat) ^[2] 1180 mg/kg (dermal, rat) ^[2] 1.6 mmol/kg(s.c., mouse) ^[4]
NIOSH (US health exposure limits):	
PEL (Permissible)	none ^[3]
REL (Recommended)	0.6 ppm (10 mg/m ³) ^[3]
IDLH (Immediate danger)	N.D. ^[3]
Related compounds	
Related haloalkanes	Methyl iodide Diiodomethane Carbon tetraiodide Chloroform Bromoform
Related	Guanidine

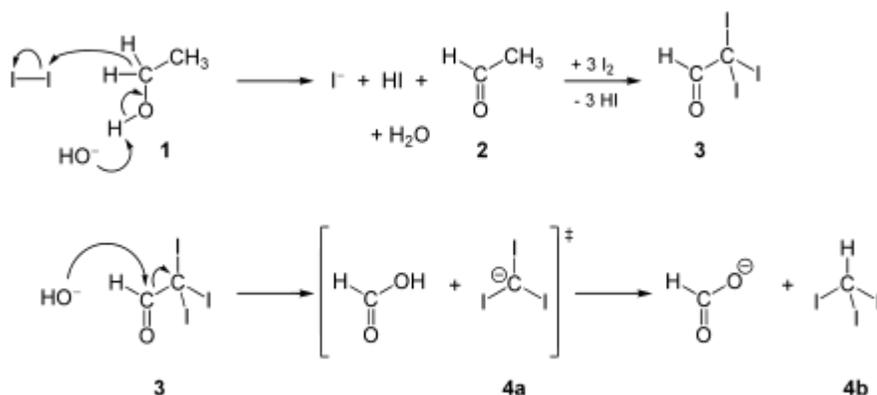
compounds

Pimagedine

Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa).

✗ verify (what is ✓✗ ?)

Infobox references



The reaction of iodine and base with methyl ketones is so reliable that the iodoform test (the appearance of a yellow precipitate) is used to probe the presence of a methyl ketone. This is also the case when testing for specific secondary alcohols containing at least one methyl group in alpha-position.

Some reagents (e.g. hydrogen iodide) convert iodoform to diiodomethane. Also conversion to carbon dioxide is possible: Iodoform reacts with aqueous silver nitrate to produce carbon monoxide. When treated with powdered elemental silver the iodoform is reduced, producing acetylene. Upon heating iodoform decomposes to produce diatomic iodine, hydrogen iodide gas, and carbon.

Natural occurrence

The angel's bonnet mushroom contains iodoform, and shows its characteristic odor.

Applications

The compound finds small-scale use as a disinfectant.^{[4][7]} Around the beginning of the 20th century, it was used in medicine as a healing and antiseptic dressing for wounds and sores, although this use is now superseded by superior antiseptics. It is the active ingredient in many ear powders for dogs and cats, along with zinc oxide and propionic acid, which are used to prevent infection and facilitate removal of ear hair.

See also

- Iodoform reaction
- Chloroform

References

1. "Front Matter". *Nomenclature of Organic Chemistry: IUPAC Recommendations and Preferred Names 2013 (Blue Book)*. Cambridge: The Royal Society of Chemistry. 2014. p. 661. doi:10.1039/9781849733069-FP001 (<https://doi.org/10.1039%2F9781849733069-FP001>). ISBN 978-0-85404-182-4. "The retained names 'bromoform' for HCB₃, 'chloroform' for HCCl₃, and 'iodoform' for HCl₃ are acceptable in general nomenclature. Preferred IUPAC names are substitutive names."
2. Record ([http://gestis-en.itrust.de/nxt/gateway.dll?f=id\\$t=default.htm\\$vid=gestiseng:sdbeng\\$id=491168](http://gestis-en.itrust.de/nxt/gateway.dll?f=id$t=default.htm$vid=gestiseng:sdbeng$id=491168)) in the GESTIS Substance Database of the Institute for Occupational Safety and Health
3. NIOSH Pocket Guide to Chemical Hazards. "#0343" (<https://www.cdc.gov/niosh/npg/npgd0343.html>). National Institute for Occupational Safety and Health (NIOSH).
4. *Merck Index*, 12 Edition, **5054**
5. Surellas, Georges-Simon (1822), *Notes sur l'Hydriodate de potasse et l'Acide hydriodique. -- Hydriodure de carbone; moyen d'obtenir, à l'instant, ce composé triple* (<http://gallica.bnf.fr/ark:/12148/bpt6k6137757n/f2.image>) [*Notes on the hydroiodide of potassium and on hydroiodic acid -- hydroiodide of carbon; means of obtaining instantly this compound of three elements*] (in French), Metz, France: Antoine, pp. 17–20, 28–29
6. James, Frank A. J. L. (2004). "Cooper, John Thomas" (<http://www.oxforddnb.com/view/article/39361>). *Oxford Dictionary of National Biography* (online ed.). Oxford University Press. doi:10.1093/ref:odnb/39361 (<https://doi.org/10.1093%2Fref%3Aodnb%2F39361>). Retrieved 26 January 2012. (Subscription or UK public library membership (<https://www.oxforddnb.com/help/subscribe#public>) required.)
7. Lyday, Phyllis A. (2005), "Iodine and Iodine Compounds", *Ullmann's Encyclopedia of Industrial Chemistry*, Wiley-VCH, Weinheim, pp. 1–13, doi:10.1002/14356007.a14_381.pub2 (https://doi.org/10.1002%2F14356007.a14_381.pub2), ISBN 9783527306732

External links

- NIOSH Pocket Guide to Chemical Hazards. "#0343" (<https://www.cdc.gov/niosh/npg/npgd0343.html>). National Institute for Occupational Safety and Health (NIOSH).
- MSDS at JT Baker (<http://hazard.com/msds/mf/baker/baker/files/i3480.htm>)
- A Method for the Specific Conversion of Iodoform to Carbon Dioxide (http://pubs.acs.org/cgi-bin/abstract.cgi/jacsat/1952/74/i09/f-pdf/f_ja01129a067.pdf?sessid=6006l3)
- Preparation (<https://www.creative-chemistry.org.uk/documents/N-ch3-16.pdf>)
- "Iodoform" (https://en.wikisource.org/wiki/1911_Encyclop%C3%A6dia_Britannica/Iodoform). *Encyclopædia Britannica*. **14** (11th ed.). 1911. p. 726.

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