# Safety Data Sheet

According to 29 CFR 1910.1200 (OSHA Hazard Communication Standard, 2024)

Version 2 · Date of preparation 2026-10-07

## Section 1. Identification

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| Product identifier used on the label | HCTU (product number 31003) |
| Other means of identification | Product number: 31003<br>Abbreviation: HCTU<br>Molecular formula: C11H15ClF6N5OP (molecular weight 413.69) |
| Recommended use of the chemical and restrictions on use | Recommended use: laboratory chemical; peptide coupling (amide bond-forming) reagent for research and for the manufacture of substances.<br>Restrictions on use: not for use in food, drugs, pesticides or biocidal products. |
| Name, U.S. address, and U.S. telephone number of the chemical manufacturer, importer, or other responsible party | P3 BioSystems<br>270 Haven Hill Rd, Shelbyville, KY 40065<br>Telephone: +1 888-737-5598<br>Email: info@p3bio.com |
| Emergency phone number | +1 888-737-5598 (P3 BioSystems office line, business hours) |

## Section 2. Hazard identification

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| Classification of the chemical in accordance with paragraph (d)(1) of § 1910.1200, except for classification under paragraph (d)(1)(ii) | • Skin corrosion/irritation, category 2<br>• Eye damage/irritation, category 2A<br>• Specific target organ toxicity (single exposure), category 3<br>• Sensitization - skin, category 1 (including both sub-categories 1A and 1B) (sub-category 1A) |

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| Signal word, hazard statement(s), symbol(s) and precautionary statement(s) in accordance with paragraph (f) of § 1910.1200 | **Signal word: Warning**<br>Hazard pictograms: Exclamation Mark<br>Hazard statements:<br>• H315 Causes skin irritation.<br>• H319 Causes serious eye irritation.<br>• H335 May cause respiratory irritation.<br>• H317 May cause an allergic skin reaction.<br>Precautionary statements:<br>• P261 Avoid breathing dust.<br>• P264 Wash hands thoroughly after handling.<br>• P271 Use only outdoors or in a well-ventilated area.<br>• P272 Contaminated work clothing must not be allowed out of the workplace.<br>• P280 Wear protective gloves/eye protection/face protection.<br>• P302+P352 If on skin: Wash with plenty of soap and water.<br>• P304+P340 If inhaled: Remove person to fresh air and keep comfortable for breathing.<br>• P305+P351+P338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.<br>• P312 Call a poison center or doctor if you feel unwell.<br>• P321 Specific treatment (see Section 4 of this SDS).<br>• P333+P313 If skin irritation or rash occurs: Get medical advice/attention.<br>• P337+P313 If eye irritation persists: Get medical advice/attention.<br>• P362+P364 Take off contaminated clothing and wash it before reuse.<br>• P405 Store locked up.<br>• P501 Dispose of contents/container in accordance with local, state and federal regulations. |
| Hazards classified under paragraph (d)(1)(ii) of § 1910.1200 | In use as a peptide coupling reagent, HCTU releases 1,1,3,3-tetramethylurea (TMU, CAS 632-22-4) and 6-chloro-1-hydroxybenzotriazole (6-Cl-HOBt) as by-products. In a published study of peptide coupling reagents and their hydrolysis products, tetramethylurea was classified as a skin irritant (Category 2) and as causing serious eye damage (Category 1). Handle reaction mixtures and wastes with the precautions given in Sections 7 and 8. |
| Hazards not otherwise classified that have been identified during the classification process | None identified. |
| Where an ingredient with unknown acute toxicity is used in a mixture at a concentration ≥ 1% and the mixture is not classified based on testing of the mixture as a whole, a statement that X% of the mixture consists of ingredient(s) of unknown acute toxicity | Not applicable: the product is a substance, not a mixture. |

## Section 3. Composition/information on ingredients

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| Chemical name | [(5-chloro-3-oxidobenzotriazol-3-ium-1-yl)-(dimethylamino)methylidene]-dimethylazanium hexafluorophosphate |
| Common name and synonyms | HCTU<br>O-(6-Chlorobenzotriazol-1-yl)-N,N,N′,N′-tetramethyluronium hexafluorophosphate<br>O-(6-Chloro-1H-benzotriazol-1-yl)-N,N,N′,N′-tetramethyluronium hexafluorophosphate<br>2-(6-Chloro-1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate |
| CAS number and other unique identifiers | • CAS number: 330645-87-9<br>• InChIKey: AFTGMAUNHUBGAW-UHFFFAOYSA-N<br>• PubChem CID: 24179320 |
| Impurities and stabilizing additives (constituents) which are themselves classified and which contribute to the classification of the substance | None known. Purity is at least 99.0% (HPLC), per specification; no impurity or additive is known to contribute to the classification. |

## Section 4. First-aid measures

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| Description of necessary measures, subdivided according to the different routes of exposure, i.e., inhalation, skin and eye contact, and ingestion | General advice: Show this safety data sheet to the doctor in attendance.<br>Inhalation: Remove the person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Call a poison center or doctor if you feel unwell.<br>Skin contact: Take off contaminated clothing. Wash the skin with plenty of soap and water for at least 15 minutes. If skin irritation or a rash occurs, get medical advice/attention. Wash contaminated clothing before reuse.<br>Eye contact: Rinse cautiously with plenty of water for at least 15 minutes, also under the eyelids. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists, get medical advice/attention.<br>Ingestion: Rinse mouth with water. Never give anything by mouth to an unconscious person. Get medical attention if symptoms occur. |
| Most important symptoms/effects, acute and delayed | Acute: skin irritation (redness, itching); serious eye irritation (redness, pain, watering); irritation of the nose, throat and airways from dust (coughing, sneezing).<br>Delayed: allergic skin reaction (rash, itching, swelling), which can appear hours to days after contact. Once a person is sensitized, very small amounts can provoke a reaction. |
| Indication of immediate medical attention and special treatment needed, if necessary | Treat symptomatically. Get medical advice if a rash or other sign of an allergic reaction develops; a sensitized person should avoid any further contact with the product. |

## Section 5. Fire-fighting measures

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| Suitable (and unsuitable) extinguishing media | Suitable extinguishing media: water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam.<br>Unsuitable extinguishing media: no information available. |
| Specific hazards arising from the chemical (e.g., nature of any hazardous combustion products) | Not classified as flammable. Keep the product and empty containers away from heat and sources of ignition.<br>Hazardous combustion products: carbon monoxide, carbon dioxide, nitrogen oxides (NOx), hydrogen chloride, hydrogen fluoride and oxides of phosphorus. |
| Special protective equipment and precautions for fire-fighters | Wear a self-contained breathing apparatus (pressure-demand, NIOSH-approved or equivalent) and full protective gear. Avoid contact with the product and with combustion gases. |

## Section 6. Accidental release measures

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| Personal precautions, protective equipment, and emergency procedures | Wear the personal protective equipment described in Section 8, including gloves and eye protection. Avoid dust formation and avoid breathing dust. Avoid contact with skin, eyes and clothing. Ensure adequate ventilation. Keep unprotected people away. |
| Methods and materials for containment and cleaning up | Sweep up and shovel the material into a suitable, closed, labelled container for disposal, without creating dust. Clean the affected area. Do not let the product enter drains or the environment. Dispose of as described in Section 13. |

## Section 7. Handling and storage

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| Precautions for safe handling | Handle in a chemical fume hood or with adequate local exhaust ventilation. Avoid dust formation and avoid breathing dust. Avoid contact with skin, eyes and clothing. Wear protective gloves and eye/face protection (Section 8). Contaminated work clothing must not be allowed out of the workplace. Wash hands thoroughly after handling. Do not eat, drink or smoke when using this product. Keep away from heat and sources of ignition. |
| Conditions for safe storage, including any incompatibilities | Store refrigerated (2–8 °C) in a tightly closed container in a dry, well-ventilated place, protected from light (per specification). Store locked up. The product is heat- and light-sensitive.<br>Incompatible materials: strong oxidizing agents. |

## Section 8. Exposure controls/personal protection

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| OSHA permissible exposure limit (PEL), ACGIH Threshold Limit Value (TLV), and any other exposure limit used or recommended by the chemical manufacturer, importer, or employer preparing the safety data sheet, where available | No OSHA PEL or ACGIH TLV has been established. |
| Appropriate engineering controls | Use a chemical fume hood or local exhaust ventilation to keep airborne dust as low as possible. Eyewash stations and safety showers should be close to the workstation. |
| Individual protection measures, such as personal protective equipment | Eye/face protection: chemical safety goggles or safety glasses with side shields meeting OSHA's eye and face protection regulations (29 CFR 1910.133); add a face shield where dust or splashes are likely.<br>Skin protection: chemical-resistant protective gloves, inspected before use and removed without touching the outer surface; dispose of contaminated gloves after use. Wear a laboratory coat or other protective clothing to prevent skin contact.<br>Respiratory protection: not normally required when the product is handled in a fume hood. Where dust cannot be controlled, use a NIOSH-approved particulate respirator (N95 or better) under a respiratory protection program meeting 29 CFR 1910.134.<br>Hygiene: wash hands before breaks and at the end of work. Do not eat, drink or smoke in the work area. |

## Section 9. Physical and chemical properties

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| Physical state | Solid (crystalline powder), per specification. |
| Color | White to off-white, per specification. |
| Odor (includes odor threshold) | Odor: no information available.<br>Odor threshold: no information available. |
| Melting point/freezing point | Melting point: 185–191 °C, per specification. |
| Boiling point (or initial boiling point or boiling range) | No information available. |
| Flammability | No test data available. Not classified as a flammable solid. |
| Lower and upper explosion limit/flammability limit | No data available. |
| Flash point | No information available. |
| Auto-ignition temperature | No data available. |
| Decomposition temperature | No data available. |
| pH | No information available. |
| Kinematic viscosity | Not applicable (solid). |

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| Solubility | Water: no data available.<br>Soluble in N,N-dimethylformamide (DMF) and N-methyl-2-pyrrolidone (NMP), giving clear solutions (per specification). |
| Partition coefficient n-octanol/water (log value) | No data available. |
| Vapor pressure (includes evaporation rate) | Vapor pressure: no data available.<br>Evaporation rate: not applicable (solid). |
| Density and/or relative density | No data available. |
| Relative vapor density | Not applicable (solid). |
| Particle characteristics | No data available. |

## Section 10. Stability and reactivity

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| Reactivity | No hazardous reactivity known, based on the information available. |
| Chemical stability | Stable under the recommended storage conditions. Light-sensitive and heat-sensitive. |
| Possibility of hazardous reactions, including those associated with foreseeable emergencies | No hazardous reactions known under normal processing. Hazardous polymerization does not occur. |
| Conditions to avoid (e.g., static discharge, shock, or vibration) | Excess heat, exposure to light, dust formation and contact with incompatible materials. |
| Incompatible materials | Strong oxidizing agents. |
| Hazardous decomposition products | Thermal decomposition can release carbon monoxide, carbon dioxide, nitrogen oxides (NOx), hydrogen chloride, hydrogen fluoride and oxides of phosphorus. |

## Section 11. Toxicological information

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| Information on the likely routes of exposure (inhalation, ingestion, skin, and eye contact) | Skin contact, eye contact and inhalation of dust. Ingestion is possible but unlikely in normal laboratory use. |
| Symptoms related to the physical, chemical, and toxicological characteristics | Skin: redness, itching and irritation; in sensitized persons, allergic dermatitis (rash, itching, swelling).<br>Eyes: redness, pain, watering and irritation.<br>Inhalation: irritation of the nose, throat and airways (coughing, sneezing, shortness of breath).<br>Ingestion: no specific information available. |

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| Delayed and immediate effects and also chronic effects from short- and long-term exposure | Immediate effects: skin irritation, serious eye irritation and respiratory tract irritation from dust.<br>Delayed effects: allergic skin reaction. HCTU was a strong skin sensitizer in the mouse local lymph node assay (Category 1A). Once sensitized, a person may react to very small amounts. A published case report describes anaphylaxis after repeated laboratory exposure to the coupling reagents HATU, HBTU and HCTU, with positive skin-prick tests to all three.<br>Chronic effects: no data available on the effects of long-term or repeated exposure. |
| Numerical measures of toxicity (such as acute toxicity estimates) | Acute oral toxicity: LD50 (rat) > 200 mg/kg; no study details are available.<br>Acute dermal and inhalation toxicity: no data available.<br>Skin sensitization: local lymph node assay (mouse) positive, EC3 0.50% (Graham et al., Chem. Res. Toxicol. 2022, 35, 1011–1022). |
| Interactive effects; information on interactions should be included if relevant and readily available | No information available. |
| Whether the hazardous chemical is listed in the National Toxicology Program (NTP) Report on Carcinogens (latest edition) or has been found to be a potential carcinogen in the International Agency for Research on Cancer (IARC) Monographs (latest edition), or by OSHA | Not listed as a carcinogen or potential carcinogen by NTP (Report on Carcinogens), IARC or OSHA. |
| When specific chemical data or information is not available, whether alternative information is used and the method used to derive the information (e.g., information from a class of chemicals rather than the exact chemical, using SAR) | No information from analogous substances or chemical classes was used. The information above is for HCTU itself. |

## Section 12. Ecological information

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| Ecotoxicity (aquatic and terrestrial, where available) | No ecotoxicity data available. Do not let the product enter drains, surface water or soil. |
| Persistence and degradability | No information available. |
| Bioaccumulative potential | No information available. |
| Mobility in soil | No information available. |
| Other adverse effects (such as hazardous to the ozone layer) | No ozone-depleting potential. No other adverse effects known. |

## Section 13. Disposal considerations

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| Description of waste residues and information on their safe handling and methods of disposal, including the disposal of any contaminated packaging | Dispose of contents and container as hazardous chemical waste through a licensed waste disposal company, in accordance with local, state and federal regulations. Waste generators must determine whether the discarded material is a hazardous waste under US EPA rules (40 CFR Part 261) and any state rules.<br>Contaminated packaging: dispose of as unused product.<br>Do not dispose of in drains or with household waste. |

## Section 14. Transport information

US DOT: not regulated.

IMDG: not offered — P3 does not ship by sea.

IATA: not regulated.

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| UN number | See above: not regulated by any mode P3 ships by. |
| UN proper shipping name | See above: not regulated by any mode P3 ships by. |
| Transport hazard class(es) | See above: not regulated by any mode P3 ships by. |
| Packing group, if applicable | See above: not regulated by any mode P3 ships by. |
| Environmental hazards (e.g., Marine pollutant (Yes/No)) | See above: not regulated by any mode P3 ships by. |
| Transport in bulk (according to IMO instruments) | Not applicable. The product is shipped only in non-bulk packages and is not shipped by sea. |
| Special precautions which a user needs to be aware of, or needs to comply with, in connection with transport or conveyance either within or outside their premises | No special precautions are required beyond those in Sections 7 and 8. |

## Section 15. Regulatory information

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| Safety, health and environmental regulations specific for the product in question | TSCA: The chemicals shipped by P3 BioSystems are not subject to TSCA.<br>SARA Title III, Sections 302 and 313: not listed.<br>SARA 311/312 hazard categories: see Section 2.<br>CERCLA: not a listed hazardous substance.<br>California Proposition 65: this product does not contain any chemicals known to the State of California to cause cancer, birth defects or other reproductive harm. |

## Section 16. Other information, including date of preparation or last revision

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| The date of preparation of the SDS or the last change to it | Date of preparation: 2026-10-07. |

The information above is believed to be accurate and represents the best information available to P3 BioSystems on the date of preparation. It is provided for the safe handling of the product by trained persons in a laboratory and is not a warranty of any kind.