Securing Autonomous Chemical Robots Through Physical and Digital Containment

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Autonomous chemical robots have the potential to revolutionize molecular discovery [1–12], yet their unprecedented power also exposes chemistry to new forms of risk. Without intrinsic containment, these systems could execute reactions beyond human oversight, posing hazards both within the laboratory and across the digital landscape. To bridge the gap between innovation and safety, we have developed the Control of Substances Hazardous to Health chemputer (CoSHHputer), a platform engineered to execute high-risk reactions while strictly isolating the chemist from danger.

The fundamental philosophy of the system is to shift the focus of automation from simple productivity to intrinsic containment. This approach allows researchers to utilize hazardous compounds and explosive reaction classes that are typically avoided in manual chemistry, thereby unlocking new pathways for discovery without compromising human safety (Fig 1).

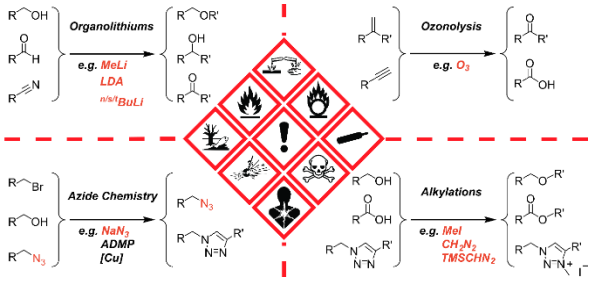

Fig. 1: Generalized reaction schemes for a range of high-value reaction classes which simultaneously represent at least one hazardous material classification according to the Globally Harmonized System (GHS) of Classification and Labelling of Chemicals.

The physical architecture of the CoSHHputer is defined by its robust measures, designed to withstand the volatile nature of high-energy chemistry. The liquid-handling backbone and reaction vessels are enclosed within a modular polycarbonate blast shield, which has been rigorously blast-tested against high explosives. Experimental validation confirmed the enclosure's ability to contain detonations equivalent to significant quantities of ammonium nitrate, effectively shielding the laboratory from shockwaves and shrapnel (Fig 2).

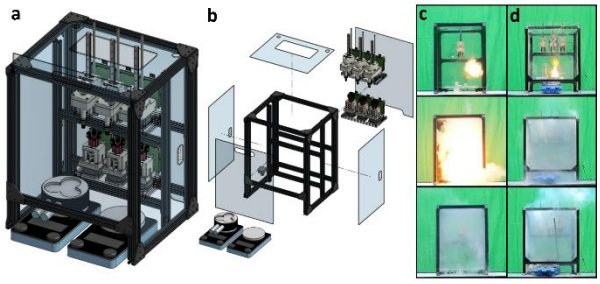

Fig. 2: Blast Shied Design & Testing. a/b – Trimetric Computer Aided Design (CAD) view of the blast-shield-enclosed ChemPU Platform CoSHHputer displaying the polycarbonate panels and aluminium V-Rails as the faces and vertices of the enclosure, respectively. c/d – Snapshots from explosive testing of different designs in collaboration with Locards Ltd demonstrating blast-shield stability and fundamental protection from unconfined low explosives (c – five grams) and high explosives (d – five grams).

To further mitigate risk, the platform moves away from the traditional model of storing solvents near the robot; instead, it utilizes a centralized waste and resource management system housed in fire-rated cabinets. These reservoirs are actively monitored by ultrasonic sensors to prevent overflows, while the system automatically identifies, neutralizes, and segregates hazardous waste streams, ensuring that volatile chemical byproducts are managed with the same precision as the synthesis itself.

Complementing this physical hardening is a sophisticated digital infrastructure driven by the Chemical Description Language (χDL), which eliminates the ambiguity of written procedures by mapping chemical operations into precise code. The platform operates as a data-rich environment, generating over thirty thousand telemetry points per hour—capturing variables such as temperature, pressure, and conductivity—to create a unique digital fingerprint for every reaction. This granular data is synchronized with low-latency video feeds, allowing researchers to monitor reactions and troubleshoot issues remotely using computer vision and real-time analytics (Fig 3).

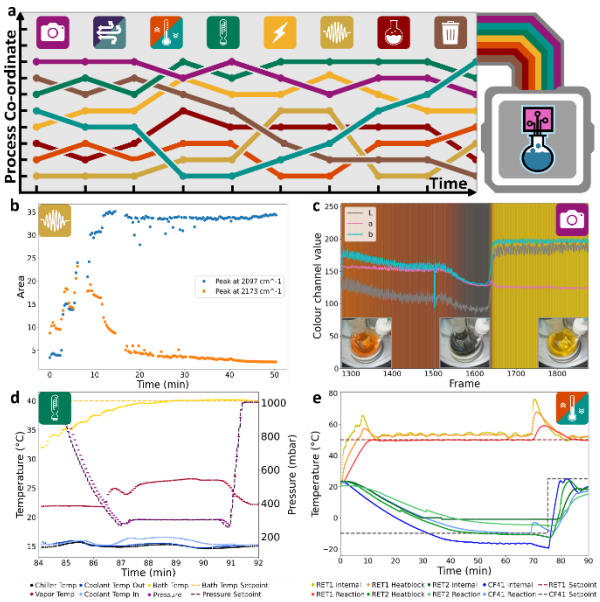

Fig. 3: Multi-dimensional, Real-Time Telemetry Data for Platform Monitoring. a – Combining multiple data streams from, for example from left to right: cameras, pressure sensors, heaters and chillers, rotary evaporators, conductivity sensors, spectrometers, chemical sensors in reactors and waste containers. b – On-line IR for reaction monitoring. c – Qualitative on-line camera monitoring during reaction and work-up. d – Utilising known sensors and functionality of rotary evaporators for automated evaporations. e – Temperature sensors across devices to accurately track temperature deviations and discrepancies across the spatial domain of reactions.

Furthermore, the automation extends beyond the synthesis; the system autonomously handles work-up procedures including extraction, filtration, and evaporation, allowing the platform to reset and propagate molecules for subsequent experiments without human intervention (Fig 4).

The CoSHHputer further addresses the ethical and security implications of automated hazardous chemistry through advanced encryption and simulation. To ensure safe knowledge transfer, the system features a mixed-reality digital twin that allows trainees to interact with the platform in virtual and augmented reality, mastering the hardware without exposure to physical risks. Simultaneously, to prevent the misuse of dangerous chemical protocols, the platform employs a tiered encryption model. This digital safeguard ensures that sensitive procedural metadata—such as reaction stoichiometry and thermal profiles—remains accessible only to authorized supervisors via secure digital keys.

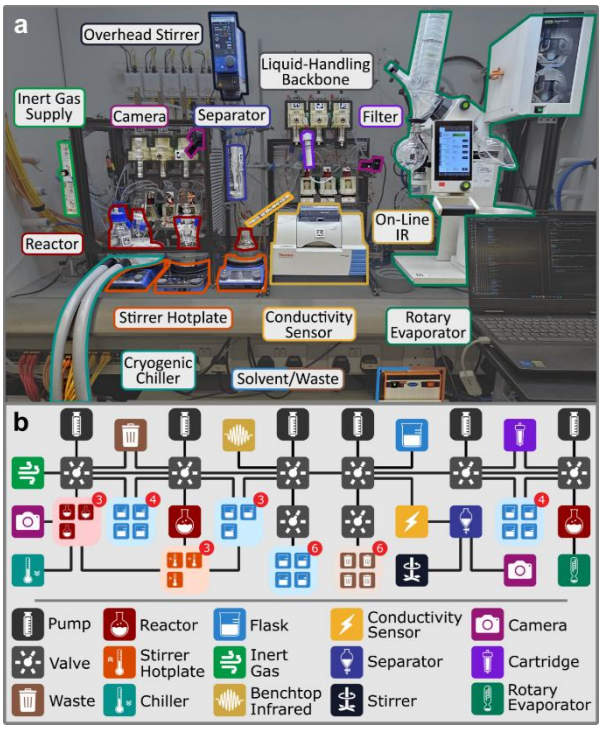

Fig. 4: Physical and Graph CoSHHputer Representations. a – Highlighted components include the hotplate stirrer/reactor (orange/red), on-line IR (yellow), online PoE cameras (pink), separator station (dark blue), purification station (purple) and rotary evaporator (dark green). b – Graphical representation of the CoSHHputer for general purpose usage.

Ultimately, the integration of industry-standard safety protocols, advanced sensing, and encrypted digital control establishes a comprehensive model for responsible chemical automation. By combining blast-proof hardware with a secure digital ecosystem, the CoSHHputer transforms automation from a mere productivity tool into a resilient infrastructure for scientific exploration. This dual emphasis on security and autonomy not only mitigates the risks associated with dangerous reactions but also lays the groundwork for the next generation of digitally controlled laboratories. In this new paradigm, verifiable automation and rigorous human oversight coexist, expanding the frontiers of safe, scalable, and intelligent chemical discovery.

Acknowledgments

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