AETHERMOORE RESEARCH PACKET

Chemistry-Native CLI and Space Chemistry Systems

A governed command-line evidence room for chemistry, space chemistry, and external scientific engine bridges.

space chemistry cli nasa-cea pahdb receipts

Abstract. SCBE should not claim to replace established chemistry engines. The stronger claim is a governed chemistry-native CLI lane that can route scientific tools, preserve receipts, and separate private proof from public evidence.

Claim boundary. Does not claim official NASA, RDKit, Open Babel, ASE, or DeepChem compatibility until bridges are implemented and verified.

Status: Research brief and product-scoping note.

Research grade: Research Brief

Review model: Initial source mapping and claim-boundary pass.

PDF | Source note

Source Text

Chemistry-Native CLI and Space Chemistry Systems Research

Generated: 2026-05-31

Executive Takeaway

SCBE should not claim to be the only AI CLI that can touch chemistry. Strong chemistry tools already exist. The defensible claim is narrower and stronger:

> SCBE has a governed chemistry-native CLI lane that combines symbolic chemistry, STISTA atomic-token flow, GeoSeed orbital invariants, private-proof hashes, and future bridges to established scientific chemistry engines.

The moat is not replacing RDKit, Open Babel, ASE, DeepChem, NASA CEA, or PAHdb. The moat is a governed agentic shell that can route them, audit them, preserve receipts, and keep private proof separate from public evidence.

Existing External Chemistry Tools Worth Bridging

Tool	What It Is	SCBE Bridge Target
RDKit	Open-source cheminformatics toolkit with Python/C++ core, descriptors, 2D/3D molecular operations, ML descriptors, and database integration.	`scbe chem rdkit canonicalize`, descriptors, substructure search, fingerprints, molecule validation.
Open Babel / `obabel`	Command-line chemistry toolbox for converting, filtering, and manipulating chemical data across many molecular formats.	`scbe chem convert`, format detection, file normalization, pipeline receipts.
ASE	Atomic Simulation Environment for setting up, manipulating, running, visualizing, and analyzing atomistic simulations.	`scbe chem atoms`, simulation setup wrappers, calculator receipts, structure export.
DeepChem	Open-source Python library for deep learning in drug discovery, materials science, quantum chemistry, and biology.	`scbe chem ml`, dataset featurization, model cards, benchmark routing.

NASA / Space Chemistry Systems Worth Bridging

System	What It Does	SCBE Bridge Target
NASA CEA / CEA2022	Chemical Equilibrium with Applications solves equilibrium product concentrations and thermodynamic/transport properties for complex mixtures; used for rocket performance, shocks, detonations, and combustion.	`scbe space-chem cea` wrapper for input decks, output parsing, provenance, and comparison reports.
CEARUN	Web/online interface that facilitates use of NASA CEA; CEA remains a gold-standard combustion/rocket thermochemistry code.	Local input-template generator and browser/API adapter where allowed.
NASA Ames PAHdb	Database and analysis tools for laboratory and computed PAH infrared spectra used to interpret astronomical observations, including JWST spectra.	`scbe astrochem pahdb` fetch/cache/fit pipeline with source receipts.
SAM / Curiosity	Mars rover instrument suite using gas chromatography, mass spectrometry, tunable laser spectroscopy, ovens, and wet chemistry for Martian samples and atmosphere.	Not direct control; use as design pattern for `sample -> instrument -> spectral evidence -> claim boundary`.
CheMin / Curiosity	Chemistry and Mineralogy X-ray diffraction instrument for identifying and quantifying minerals in Martian rocks and soils.	Benchmark-style data interpretation lane for mineral/spectral classification, not rover control.
Spacecraft Materials Selector	NASA software catalog item for spacecraft material selection expert support.	Future `scbe materials` advisory adapter with export-control and provenance boundaries.

Safe Claim Boundary

Current SCBE evidence supports:

- symbolic chemistry and molecule-like scoring,
- STISTA/atomic-tokenizer flow,
- chemical-fusion reconstruction,
- ternary chemistry proxy tests,
- GeoSeed hyperbolic orbital invariants,
- private-proof hash inventory.

Current SCBE evidence does not yet support:

- validated wet-lab synthesis planning,
- validated hazardous chemistry instructions,
- official NASA CEA compatibility,
- official NASA, RDKit, Open Babel, ASE, or DeepChem certification,
- autonomous spacecraft or rover instrument operation.

Recommended CLI Branches

1. `feat/chem-cli-core`

`- scbe chem atomize "text" - scbe chem fuse "tokens" - scbe chem bonds --coords ... - scbe chem orbitals --json - scbe chem prove`

1. `feat/chem-interop-bridges`

- Detect optional tools: RDKit, Open Babel, ASE, DeepChem. - Expose wrappers only when installed. - Emit receipts with versions, command, input hash, output hash, and claim boundary.

1. `feat/space-chem-bridges`

- NASA CEA/CEARUN input deck templates. - PAHdb cache/search/fit scaffold. - SAM/CheMin-inspired evidence workflow for sample/spectrum/claim reports.

1. `feat/chem-safety-gate`

- Deny or quarantine hazardous synthesis, energetic material, toxicity, or illegal-drug requests. - Allow benign educational, file-conversion, descriptor, and public-data workflows. - Put human approval before any wet-lab actionable output.

Product Framing

SCBE should present chemistry as a command-line evidence room:

```
Human intent -> STISTA atomization -> chemistry/space tool adapte
```

That is more valuable than claiming to be a replacement chemistry package. It lets a weak or strong model use real chemistry tools safely by following explicit steps, examples, expected outputs, and audit trails.

Middle-Layer Design

We should do both: keep SCBE's symbolic chemistry/STISTA layer and bridge to real scientific chemistry systems through a governed middle layer.

```
                public/private proof packets
                         ^
                         |
Human/AI request -> SCBE Chem Middle Layer -> External engines/da
                         |
                         v
          STISTA atoms / GeoSeed orbitals / symbolic bonds
```

Layer A: SCBE Native Chemistry

This is the internal symbolic layer:

- STISTA atomic tokenization,
- chemical fusion reconstruction,
- tongue molecule/bond scoring,

- ternary chemistry proxies,
- GeoSeed orbital invariants,
- private-proof hash inventory.

This layer is useful for agent routing, semantic decomposition, claim boundaries, and safety reasoning.

Layer B: Chem Middle Layer

This is the translation and governance layer:

- canonical request schema: `intent`, `material_or_molecule`, `representation`, `operation`, `risk_class`, `allowed_engines`;
- adapter registry for RDKit, Open Babel, ASE, DeepChem, NASA CEA, PAHdb, SAM/CheMin-style data lanes;
- deterministic receipt schema: input hash, normalized input, engine, version, command, output hash, safety decision, claim boundary;
- bidirectional mapping: STISTA atoms can propose routes, external engines can return validated structures/properties that re-enter STISTA as evidence atoms;
- private/public split: public artifact gets hashes and result summaries; private artifact keeps patent/internal license material local.

Layer C: External Chemistry and Space Systems

This is where validated scientific tools live:

- RDKit for cheminformatics and descriptors,
- Open Babel for conversion and file normalization,
- ASE for atomistic structures/simulation setup,
- DeepChem for ML chemistry workflows,
- NASA CEA/CEARUN for equilibrium/rocket thermochemistry,
- PAHdb for astrochemistry spectra,
- SAM/CheMin-style workflows for sample/spectrum/mineral evidence.

Why This Is Stronger

The middle layer lets SCBE act like a governed chemistry operating shell:

- weak models can follow a tool contract without hallucinating chemistry,
- strong models get real engines and audit trails,
- hazardous or wet-lab actionable requests can be denied/quarantined,
- website claims can cite executable local receipts and external-tool provenance,
- patent/private proof remains hash-linked without exposing the private text.

First Implementation Target

Build `scbe chem bridge` as the middle-layer entrypoint:

```
scbe chem atomize "oxidizer fuel equilibrium"
scbe chem bridge --engine rdkit --operation descriptors --smiles
scbe chem bridge --engine obabel --from smi --to sdf --input mole
scbe chem bridge --engine cea --template rocket --fuel CH4 --oxic
scbe chem prove --public
```

Initial adapters should be capability-detection only unless the tools are installed. The benchmark should pass by proving graceful detection, safe denial/quarantine, STISTA fallback, and receipt generation.

Sources

- RDKit official documentation: https://www.rdkit.org/
- RDKit overview: https://www.rdkit.org/new_docs/Overview.html
- Open Babel documentation: https://openbabel.org/
- Open Babel command-line documentation: https://openbabel.org/docs/Command-line_tools/babel.html
- ASE documentation: https://docs.ase-lib.org/index.html
- DeepChem GitHub/docs: https://github.com/deepchem/deepchem
- NASA CEA software catalog: https://software.nasa.gov/software/LEW-17687-1
- NASA CEA 3.0 beta documentation: https://nasa.github.io/cea/
- NASA CEARUN introduction: https://cearun.grc.nasa.gov/intro.html
- NASA Ames PAHdb page: https://www.nasa.gov/?p=484873
- Astrochemistry databases: https://www.astrochem.org/databases.php

- NASA Laboratory Astrophysics and Astrochemistry: https://www.nasa.gov/general/laboratory-astrophysics-and-astrochemistry/
- NASA SAM overview: https://ssed.gsfc.nasa.gov/sam/samiam.html
- NASA Curiosity science instruments: https://science.nasa.gov/mission/msl-curiosity/science-instruments/
- NASA Spacecraft Materials Selector software catalog: https://software.nasa.gov/software/MFS-31328-1

Generated from `research/chemistry_cli_space_systems_2026-05-31.md` by `scripts/research/build_research_library.py`.