

Revolutionizing Learning General Chemistry with Dr. Lewis

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1. Introduction: Problem + Goal

Most AI tools can explain Lewis structures, but they struggle to generate **fast, free Lewis structure images and interactive 3D molecular models** for students learning **General Chemistry**.

Reliable, non-AI websites that simulate the structure of molecules, such as PhET's molecular shapes [1] and ChemicalAid's Lewis Structure Generator [2]:

- are **slower** at generating simple Lewis structures for molecules.
- **fail to account for different molecules** of the same VSEPR structure.

Goal: Build a chemistry chatbot that can generate rapidly and accurately:

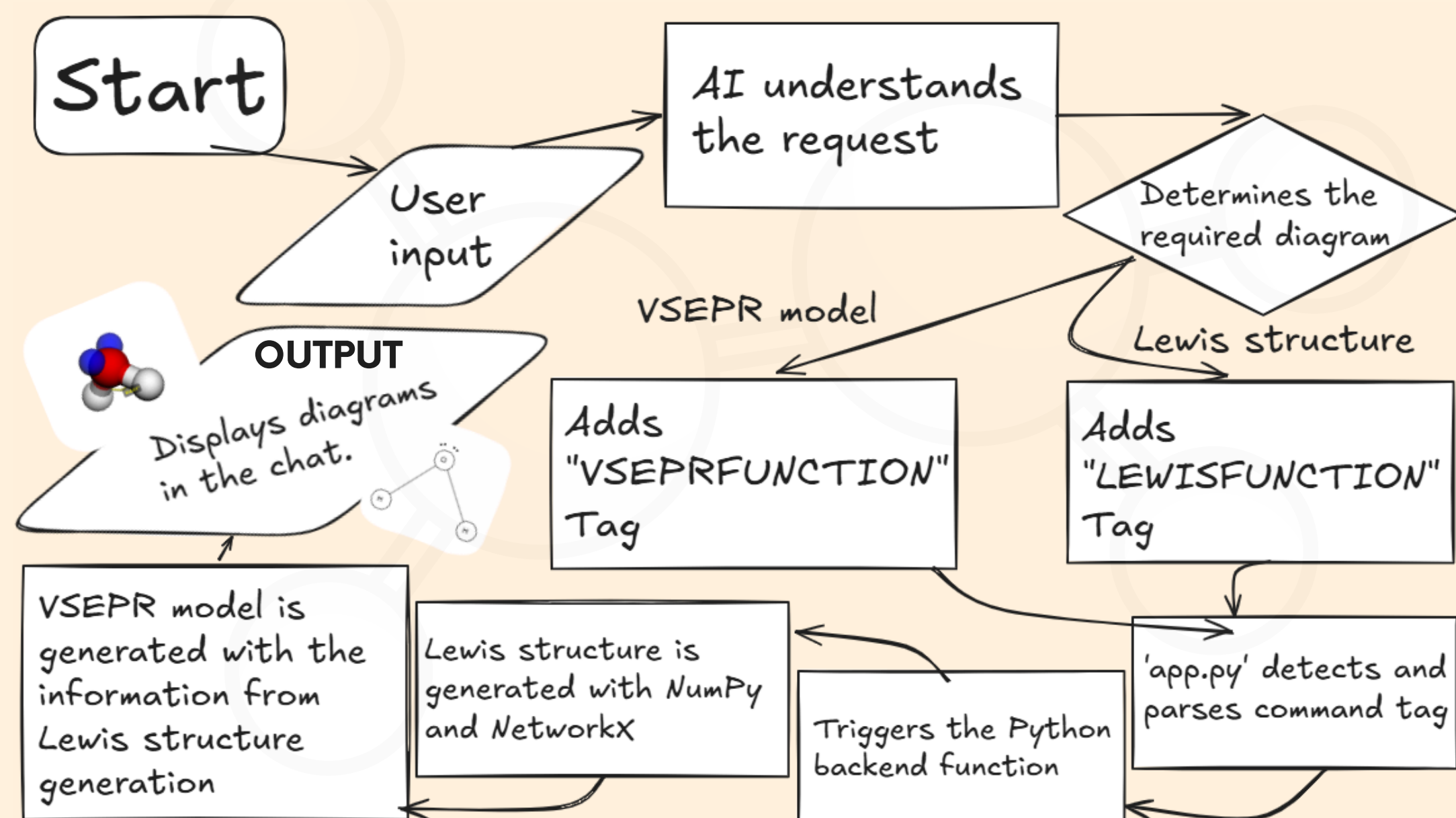
- Lewis structures
- 3D VSEPR models
- Other information about the molecule. (bond angles, hybridization)

2. Method Pipeline (How it Works)

User input examples:

"Can you give me the Lewis structure of CO₂?"

"Give me the 3D model of H₂O."



3. The Science & Coding Behind the Project

A **Lewis structure** shows how valence electrons are arranged in a molecule. It helps predict:

- molecular connectivity
- bond types (single, double, triple)
- lone pairs around the central atom

Achieved with a **NetworkX graph** with nodes and vertices, the most important coding algorithms are:

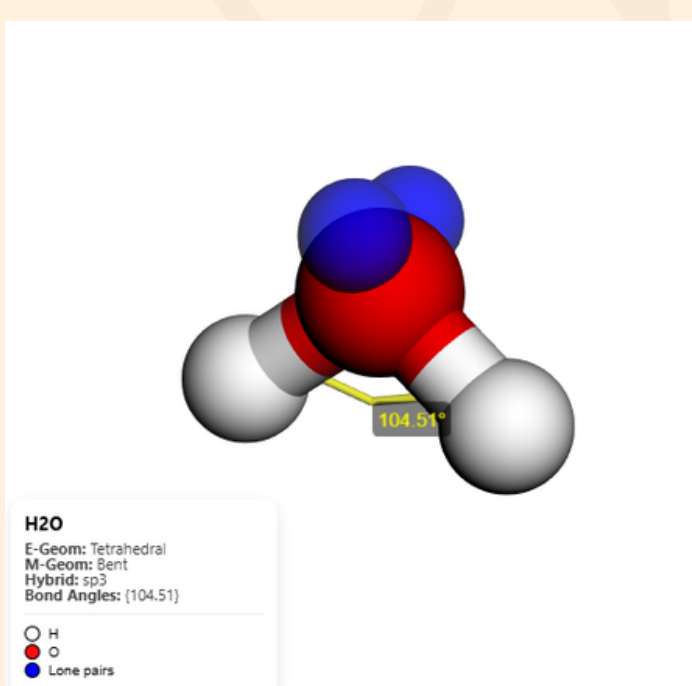
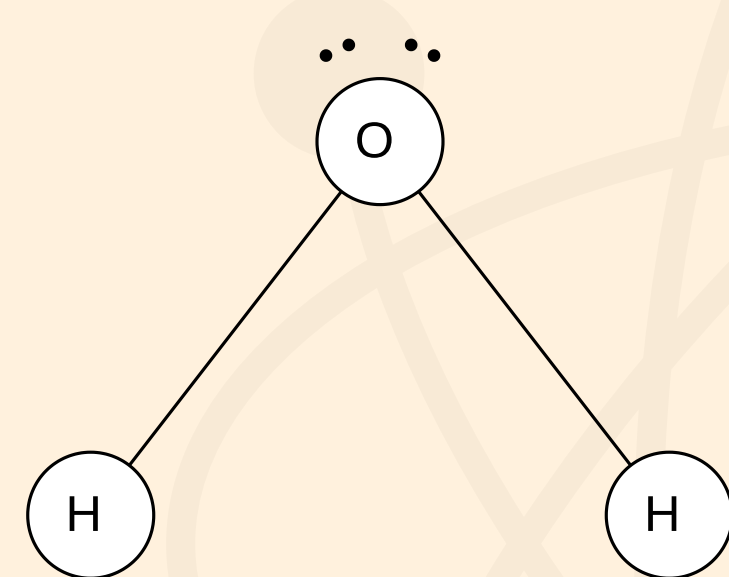
- **2D Coordinate Generation Algorithm**
- **Bond Order Optimization**

VSEPR stands for **Valence Shell Electron-Pair Repulsion**.

- Electron groups around a central atom arrange themselves to minimize repulsion.
- Bonding pairs and lone pairs affect molecular shape.

Achieved with the **RDKit chemistry library** and **py3Dmol interactive viewer**, the most important coding algorithms are:

- **The molecule-to-SMILES parser algorithm**
- **Expanded-Octet 3D Positions Algorithm**



Internal Testing: Inference Latency by Model

AI Model	Lewis Structure	Interactive 3D model
Gemini 3.1 Flash	4s	N/A
Gemini 3.1 Pro (Paid)	4.5s	59s
Claude Sonnet 4.6	21s	42.8s
GPT 5.3 Instant	5.5s	N/A
GPT 5.4 Thinking (Paid)	3.6s	165s

Internal testing averaged the latency of five distinct molecule prompts

4. Results + Demo

From a sample of **100** simple molecules found in general chemistry to prove the speed of our Lewis structure and 3D molecular structure algorithms, on average:

1.66s

Lewis Structure Generation

1.58s

3D Model Generation

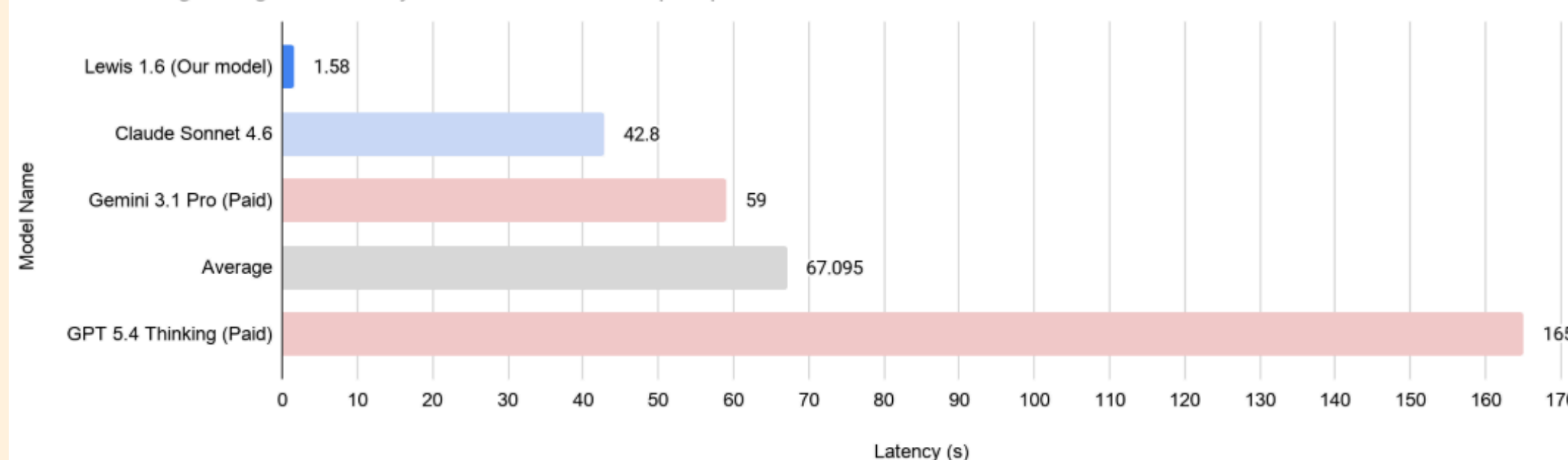
1.70s

Average Latency

Our team also ran an internal latency testing on various AI models such as Gemini 3.1 Pro and GPT 5.5 Thinking. Our AI was **6.73** times faster at generating Lewis structures and **56.29** times faster at generating VSEPR models compared to the average of industry-leading AI models. Here's the graph for 3D Model Generation:

Latency in 3D VSEPR Model Generation

Internal testing averaged the latency of five distinct molecule prompts



For accuracy of our algorithms:

82%₁

Correct structures generated out of **100** simple molecules

87.5%₂

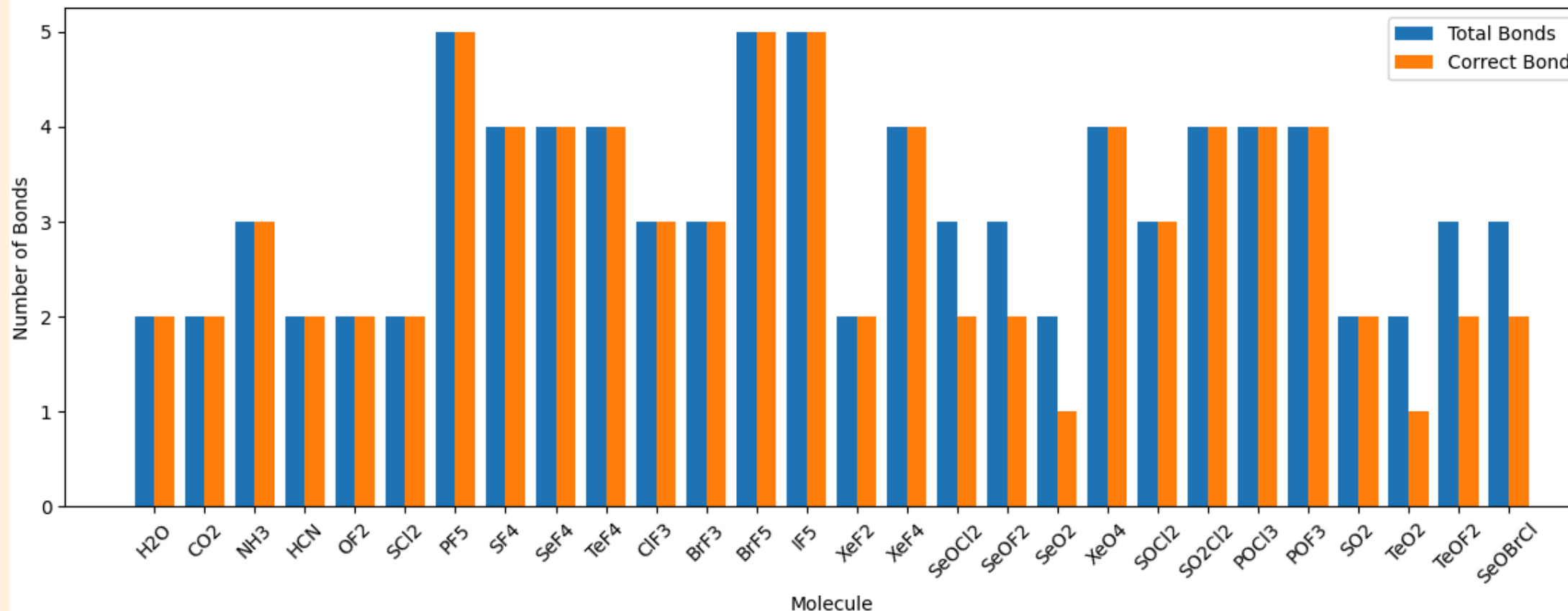
Approximately correct bond angles out of 13 molecules

78.9%₃

Correct bond orders around central atom out of 28 molecules

1. Both the correct Lewis structure and the 3D molecular structure.
2. 13 chosen molecules that take into account each and every stable molecular geometry to show the different bond angle configurations.
3. 28 selected molecules, some of which had expanded-octet central atoms or transition metals. The graph below shows where the **78.9%** comes from when building the corresponding Lewis structures. When both bars are equal, the molecule was generated correctly. Smaller orange bars show molecules where the program made mistakes, mainly in some more complex oxygen-containing compounds.

Correct Bond Orders Around the Central Atom



5. Conclusion

After 3 months of development, our team built a chemistry AI chatbot that generates Lewis structures and 3D VSEPR models faster than current AI models, achieving **82.3%** average accuracy and showing strong potential as a general chemistry learning tool.

6. References

- [1] PhET Interactive Simulations, "Molecule Shapes," University of Colorado Boulder. Accessed: May 5, 2026. [Online]. Available: https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_all.html
- [2] ChemicalAid, "Lewis Structure Generator." Accessed: May 5, 2026. [Online]. Available: <https://www.chemicalaid.com/tools/lewisstructure.php?hl=en>