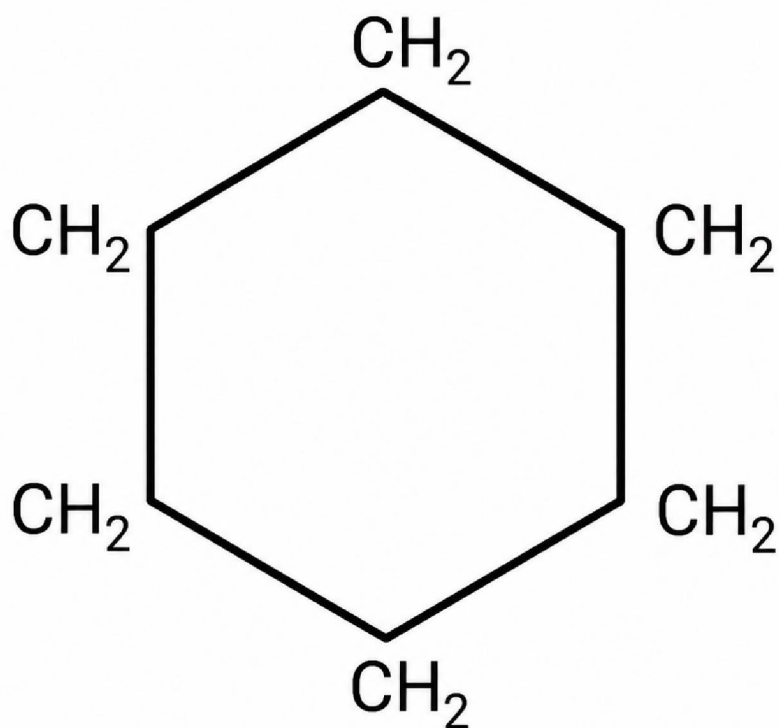
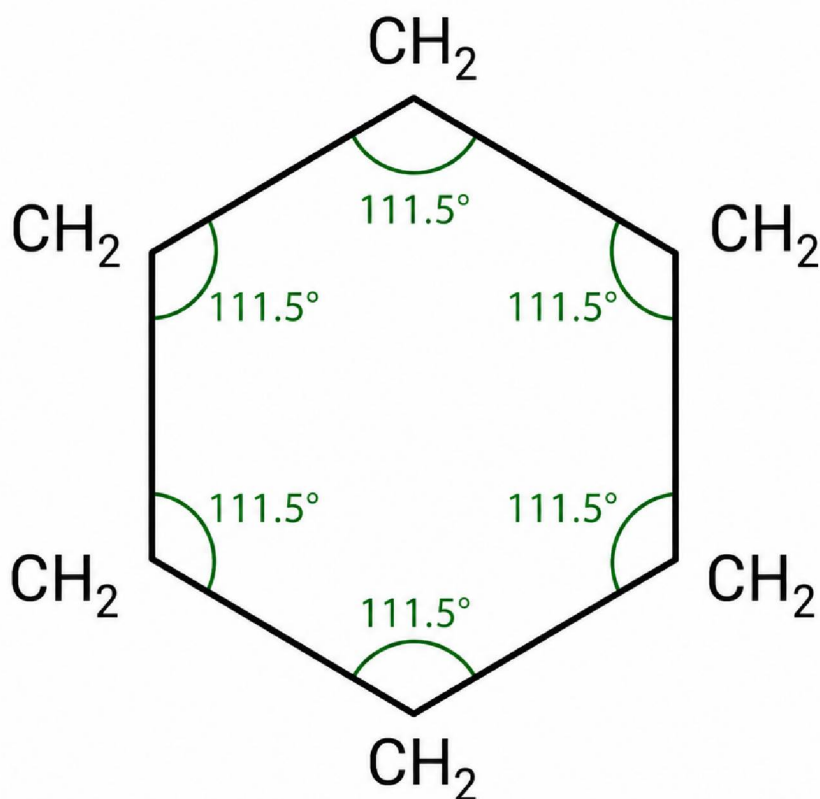


Cyclohexane Structure Drawing

draw me a picture of cyclohexane



Can you show that to me with bond angles indicated?



Bond angle: 111.5°
(approximate tetrahedral angle)

What are the bond angles in cyclohexane in the boat conformation?

Unlike the flat hexagon often drawn on paper (which has 120° internal angles), the **boat conformation** of cyclohexane is a three-dimensional shape in which the carbon atoms remain approximately sp^3 hybridized.

As a result:

- The **C-C-C bond angles** in the boat conformation are **very close to the tetrahedral angle of 109.5°** .
- In reality, they are **not all identical** because the boat is slightly distorted. Typical values are approximately **108° – 112°** , depending on the specific carbon atoms and the level of theory or experimental measurement.
- The boat conformation is **higher in energy** than the chair, **not because of large bond-angle strain**, but primarily because of:
 - **Eclipsing (torsional) strain** along several C-C bonds.

- **Flagpole interactions** (steric repulsion) between the two "bow" and "stern" hydrogens that point toward each other.

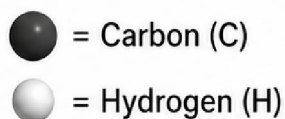
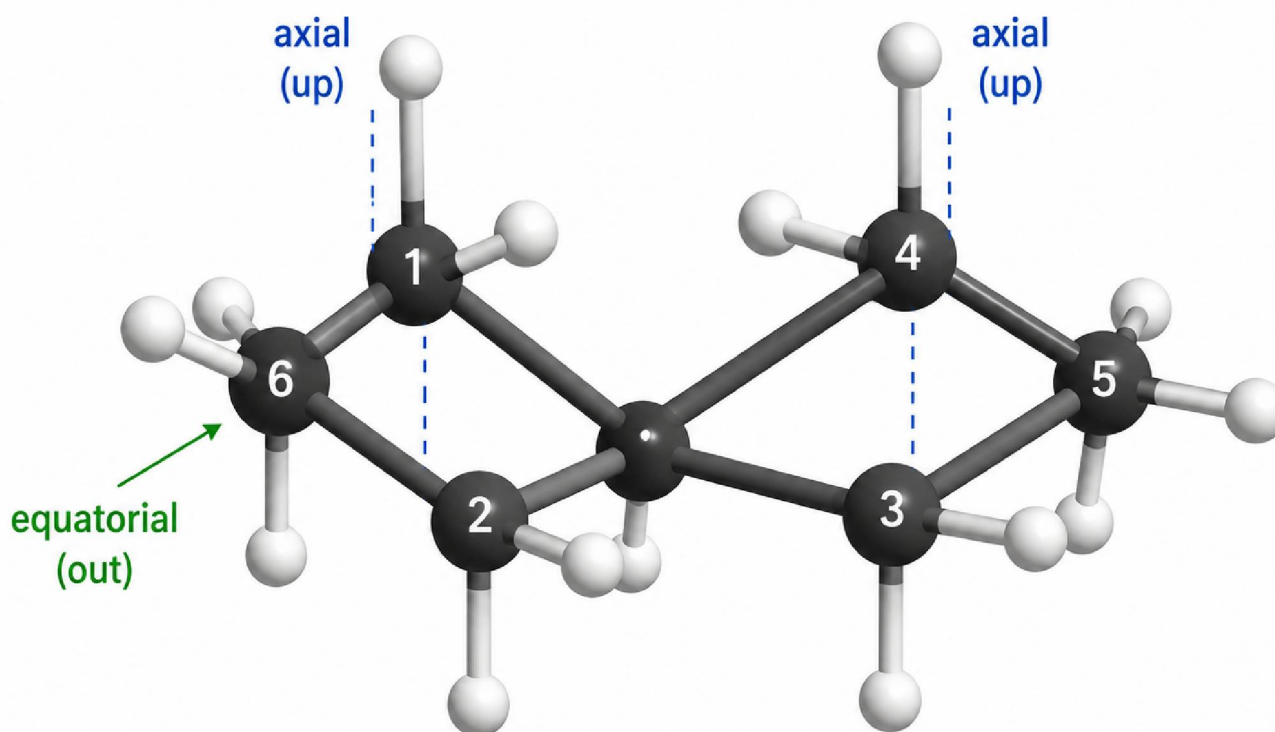
For comparison:

Conformation	Typical C-C-C bond angles	Main source of strain
Chair	$\approx 109.5^\circ$	Essentially none (minimal angle and torsional strain)
Boat	$\approx 108-112^\circ$	Torsional strain + flagpole steric interactions
Twist-boat	$\approx 108-112^\circ$	Less torsional strain than boat

So the short answer is: **the bond angles in the boat conformation are still approximately 109.5° , with only small deviations (roughly $108-112^\circ$)**. The instability of the boat comes mainly from torsional and steric effects rather than bond-angle distortion.

show me a 3d schematic of cyclohexane

Cyclohexane (Chair Conformation)



All C-C-C bond angles are approximately 109.5° (tetrahedral)

That structure has 7 carbons, and the central carbon has 5 bonds.

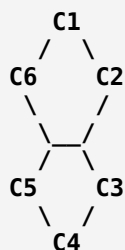
You're absolutely right—that image is chemically incorrect. Thank you for catching it.

The problems are:

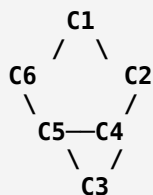
- **There are 7 carbon atoms** instead of 6.
- **The center carbon has five C-C bonds**, which violates carbon's valence of four.
- A cyclohexane ring should be a **continuous six-membered ring** with no central carbon.

Unfortunately, image-generation models often make these kinds of mistakes with chemical structures. They are good at producing illustrations that *look* scientific but are not reliable for molecular connectivity.

A correct chair conformation looks schematically like this:



A more realistic 3D line drawing is:



where alternating carbons are above and below the mean plane of the ring, giving the characteristic "chair" shape. Every carbon has exactly:

- **2 C-C bonds** (to its neighbors),
- **2 C-H bonds**,
- **tetrahedral geometry (~109.5°).**

If you're looking for a truly accurate visualization, I can also produce:

1. a **skeletal chair conformation** like you'd see in an organic chemistry textbook,
2. a **ball-and-stick model** with correct 3D geometry,
3. a **wedge-and-dash drawing** showing stereochemistry, or

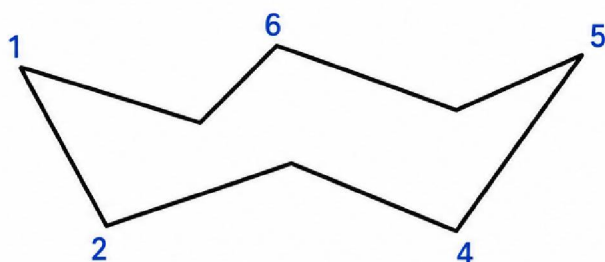
4. a **Newman-style projection** of selected bonds.

Those are much less likely to contain the kinds of valence errors that appeared in the generated image.

Let's look at both a skeletal conformation and a wedge-and-dash drawing.

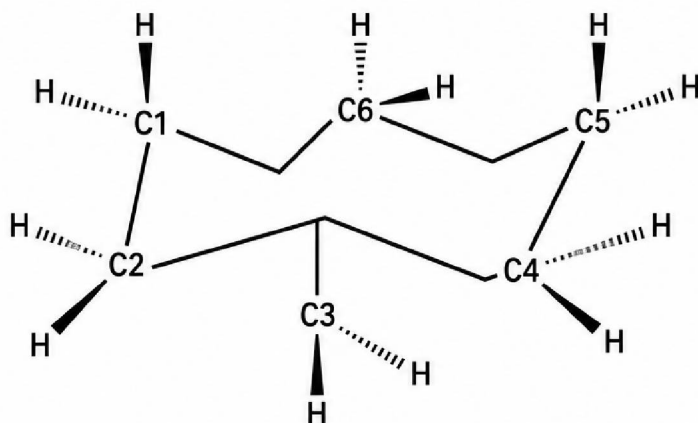
Cyclohexane (Chair Conformation)

1) Skeletal (line-angle) drawing



All C–C–C bond angles are approximately **109.5°** (tetrahedral).

2) Wedge-and-dash drawing (all hydrogens shown)

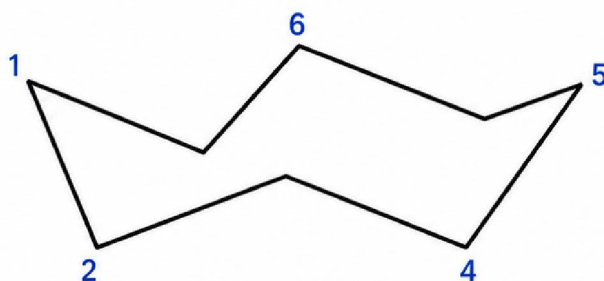


 = bond coming out of the plane (toward you)
 = bond going behind the plane (away from you)

That's um... The typical rules for skeletal drawings is that all line intersections have an implied carbon. Your skeletal structure has 8 carbons, and the wedge-and-dash has 9. Also, can you indicate the axial hydrogens with vertical lines?

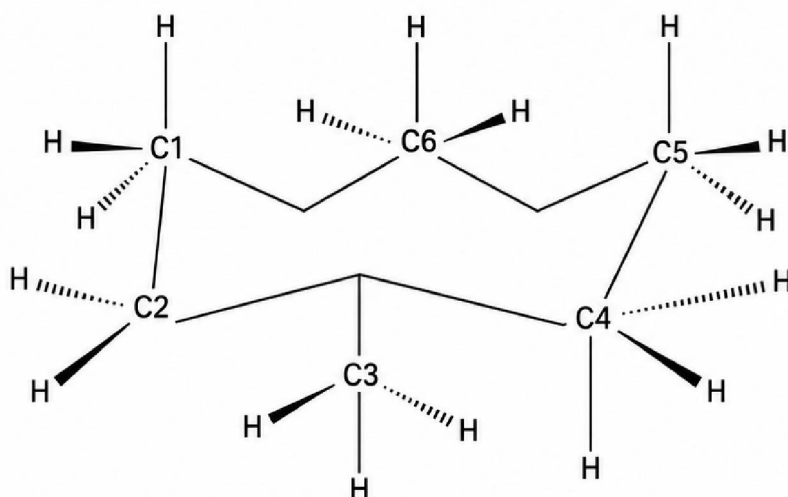
Cyclohexane (Chair Conformation)

1) Skeletal (line-angle) drawing



All C–C–C bond angles are approximately 109.5° (tetrahedral).

2) Wedge-and-dash drawing (chair conformation) (axial hydrogens shown as vertical lines)



| = axial bond (vertical)
 ▴ = bond coming out of the plane (toward you)
 ▾ = bond going behind the plane (away from you)

You're absolutely right again, and you've identified exactly the failure mode.

The image model is treating the chair as a decorative zig-zag rather than a graph with strict connectivity. It keeps introducing extra vertices because it doesn't actually count atoms the way a chemist does. Even after explicitly instructing it, it invents additional implied carbons.

Similarly, in the wedge-and-dash drawing, every **line intersection** is interpreted as a carbon in skeletal notation, so the generated drawing ends up with too many carbons. That's a fundamental limitation of current image generation models for precise chemical diagrams.

Your suggestion about **axial hydrogens being vertical** is exactly how a chemist would draw it:

- Axial bonds are drawn **straight up or straight down**.
- Equatorial bonds project approximately outward around the ring.
- Each carbon has **one axial and one equatorial hydrogen**.
- The axial positions alternate up/down around the ring.

If I wanted a publication-quality figure, I would **not** use an image model at all. I'd generate it algorithmically from molecular coordinates (the way ChemDraw, RDKit, or Avogadro do), which

guarantees:

- exactly **6 carbons**,
- exactly **12 hydrogens**,
- correct connectivity,
- proper chair geometry,
- vertical axial bonds,
- alternating up/down axial hydrogens,
- and proper wedge/dash stereochemistry.

I can produce that kind of diagram, but it needs to be drawn programmatically rather than generated artistically. The result will look like something straight out of an organic chemistry textbook instead of an AI illustration, and it will actually be chemically correct. I think that's a much better fit for what you're after.

How would you synthesize cyclohexane starting from ethane?

This is an interesting retrosynthesis problem because **ethane (C₂)** is much smaller than **cyclohexane (C₆)**. There isn't a practical one-pot conversion, so the strategy is to **build a six-carbon chain** and then **cyclize** it.

One plausible synthetic route is:

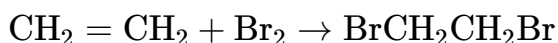
Step 1. Convert ethane to ethylene

Dehydrogenation:



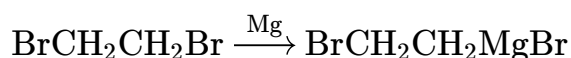
(Cr₂O₃/Al₂O₃ catalyst at elevated temperature, for example.)

Step 2. Convert ethylene to 1,2-dibromoethane



Step 3. Prepare a Grignard reagent

React with Mg:



Step 4. Extend the carbon chain

Couple with another two-carbon fragment. Repeating homologation eventually gives **1,6-dibromohexane**.

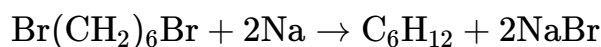
A more realistic laboratory sequence uses repeated substitution reactions or organocuprate couplings to build



from C₂ building blocks.

Step 5. Cyclize

Treat 1,6-dibromohexane with sodium metal (an intramolecular Wurtz reaction):

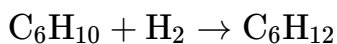


This closes the ring to give cyclohexane.

A more industrial approach

In practice, chemists would almost never start from ethane. A much more efficient route is

1. Ethane → ethylene
2. Ethylene → butadiene
3. Butadiene + ethylene → cyclohexene (via the Diels–Alder reaction)
4. Hydrogenate cyclohexene:



This is attractive because the Diels–Alder reaction forms the six-membered ring in a single step.

If carbon economy is the goal

The most elegant conceptual synthesis is:

- 3 ethane → 3 ethylene
- 3 ethylene → 1,3-butadiene + ethylene
- Butadiene + ethylene → cyclohexene
- Cyclohexene → cyclohexane

This route builds the ring directly rather than assembling a six-carbon chain first, and it illustrates several fundamental reactions in organic synthesis: dehydrogenation, dimerization/homologation, cycloaddition, and hydrogenation.

If I wanted to do a molecular dynamics simulation on cyclohexane, what force field parameters should I use?

That depends on what you're trying to simulate. Cyclohexane is actually a classic benchmark for molecular mechanics because a good force field should reproduce:

- Chair as the global minimum.
- Boat ≈ 6.5 – 7 kcal/mol above chair.
- Twist-boat ≈ 5.5 kcal/mol above chair.
- Ring-flip barrier ≈ 10 – 11 kcal/mol.
- Correct C–C bond lengths (~ 1.53 Å).
- Correct C–C–C angles ($\sim 111^\circ$).
- Correct liquid density and heat of vaporization.

General-purpose force fields

For all-atom simulations, these are all good choices:

Force field	Recommendation	Comments
OPLS-AA	★★★★★	Excellent for hydrocarbons; reproduces cyclohexane conformational energetics well.
CHARMM36	★★★★★	Very reliable if using CHARMM software or biomolecular systems.
AMBER GAFF2	★★★★☆	Good for small organic molecules.
GROMOS	★★★☆☆	Often uses united atoms; less detailed.
MM3	★★★★★	Historically one of the best for hydrocarbon conformations.

If you're starting a new project involving only cyclohexane, I'd probably choose **OPLS-AA**.

Typical OPLS-AA parameters

For an sp^3 carbon (CT):

Bond stretching

- C–C

- $r_0 \approx 1.529 \text{ \AA}$
 - $k_r \approx 268 \text{ kcal mol}^{-1} \text{ \AA}^{-2}$
 - C-H
 - $r_0 \approx 1.09 \text{ \AA}$
-

Bond angles

- C-C-C
 - equilibrium angle $\approx 111^\circ$
 - force constant $\approx 58 \text{ kcal mol}^{-1} \text{ rad}^{-2}$
 - H-C-C
 - $\approx 109.5^\circ$
-

Dihedrals

These are the critical parameters.

Cyclohexane's conformational behavior is almost entirely controlled by the torsional potential

$$V(\phi) = \sum_{n=1}^4 \frac{V_n}{2} (1 + \cos(n\phi - \delta_n))$$

For OPLS,

$$V(\phi) = \frac{V_1}{2}(1 + \cos \phi) + \frac{V_2}{2}(1 - \cos 2\phi) + \frac{V_3}{2}(1 + \cos 3\phi) + \frac{V_4}{2}(1 - \cos 4\phi)$$

with parameters fitted for alkane torsions.

These torsional coefficients are what determine whether the chair is stable and what the ring-flip barrier will be.

Lennard-Jones

Typical OPLS values

Carbon

- $\sigma \approx 3.50 \text{ \AA}$
- $\epsilon \approx 0.066 \text{ kcal/mol}$

Hydrogen

- $\sigma \approx 2.50 \text{ \AA}$
- $\epsilon \approx 0.030 \text{ kcal/mol}$

Charges

Cyclohexane is essentially nonpolar.

Typical OPLS charges are

Carbon

$$q_C \approx -0.12e$$

Hydrogen

$$q_H \approx +0.06e$$

giving a net charge of zero.

If you want to study ring flips

The torsions matter much more than the bond-angle force constants.

If you artificially make the angle force constants very large, the ring still flips.

If you change the torsional coefficients by even 10–20%, the relative stability of chair, boat, and twist-boat changes dramatically.

If you're implementing your own MD code

A standard molecular mechanics potential is

$$E = \sum k_r (r - r_0)^2 + \sum k_\theta (\theta - \theta_0)^2 + \sum V_{\text{dihedral}} + \sum 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] + \sum \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$

where the torsional term is the key ingredient for reproducing cyclohexane's conformational landscape.

If your goal is educational or you're writing an MD engine from scratch, I can also provide a **minimal force field** for cyclohexane (about a dozen parameters) that reproduces the chair, boat, and ring-flip energetics surprisingly well without the full complexity of OPLS or CHARMM.

ChatGPT can make mistakes. Check important info.