

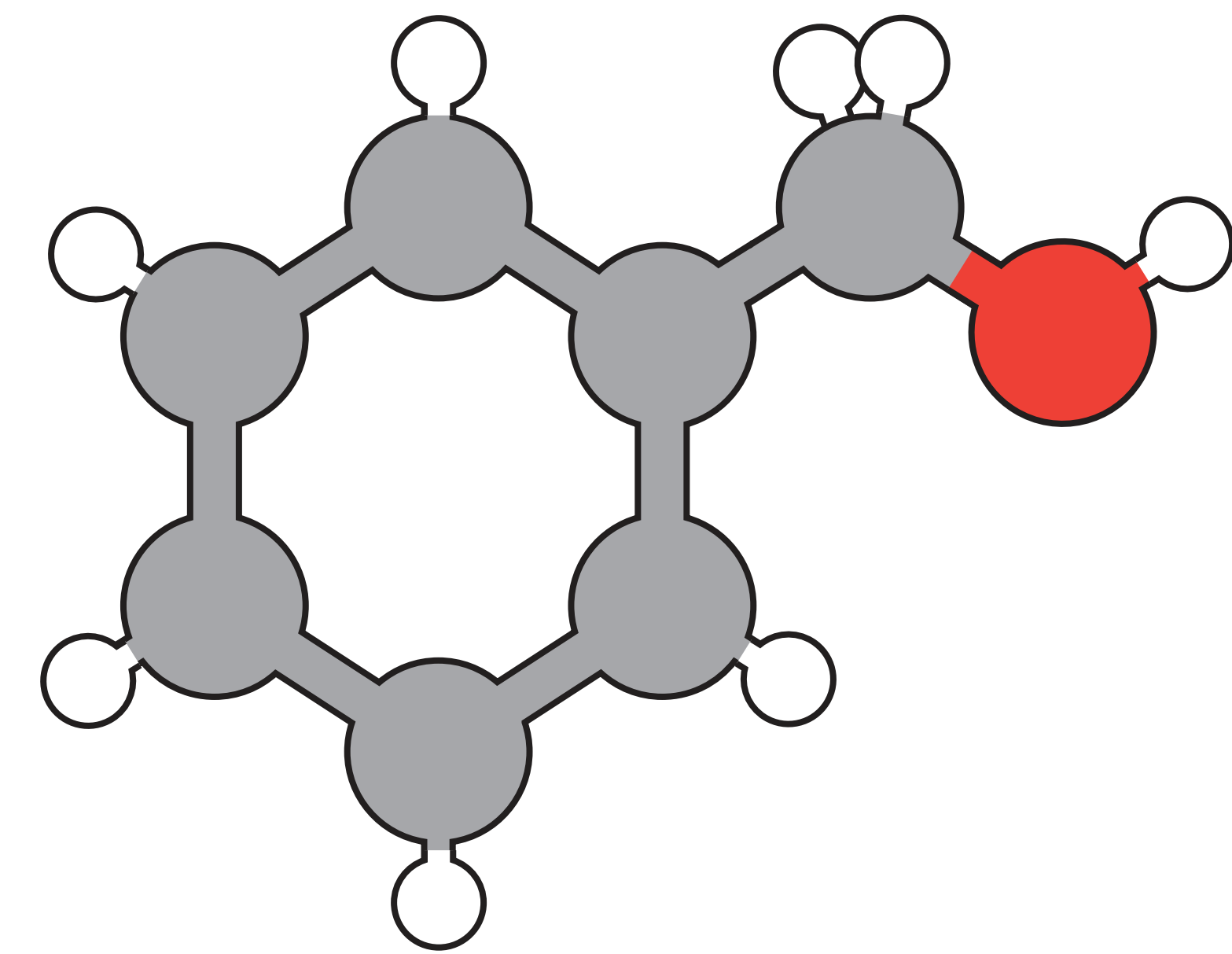
Ligand A

Intermediate 1

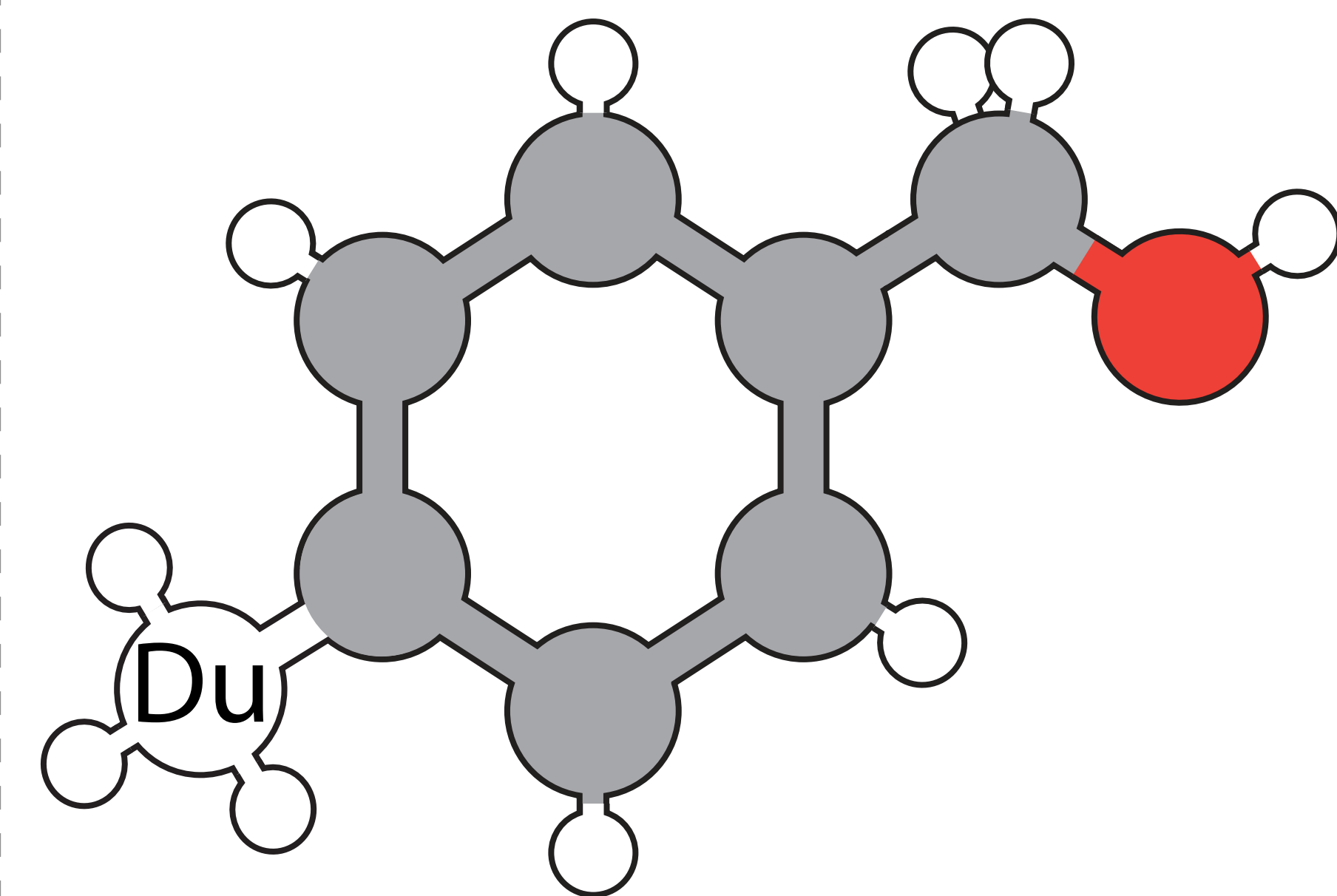
Intermediate 2

Intermediate 3

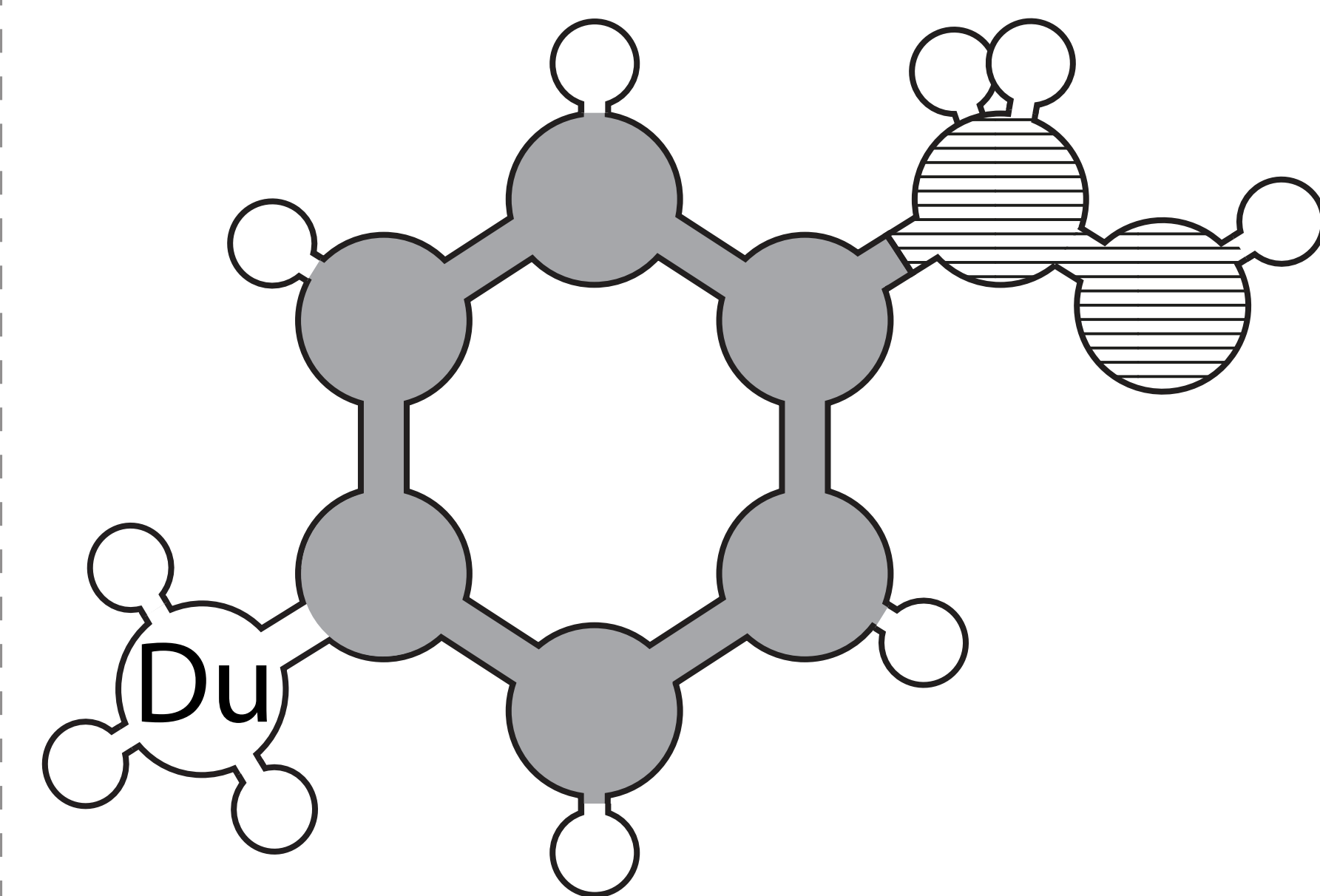
Intermediate 4



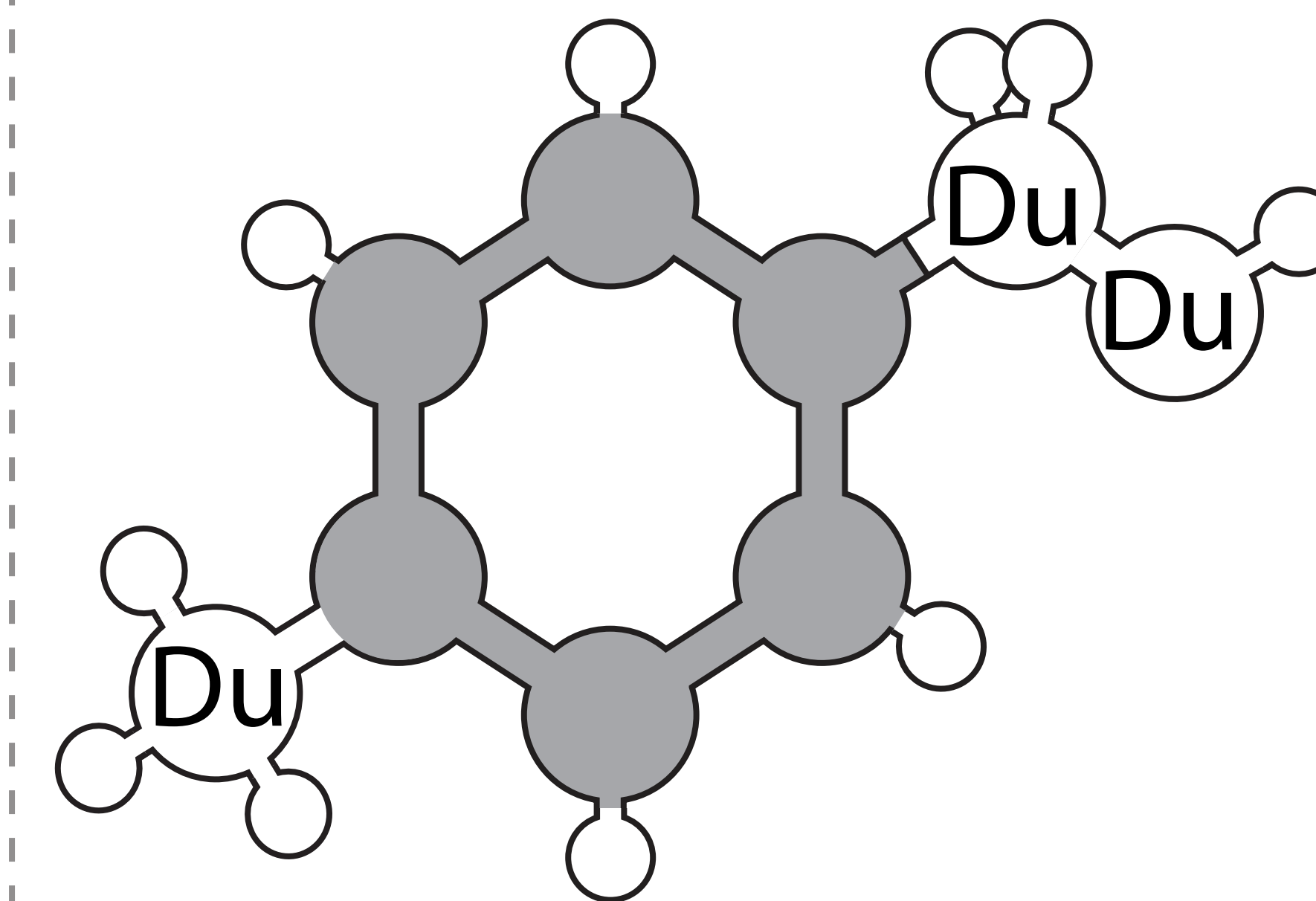
=



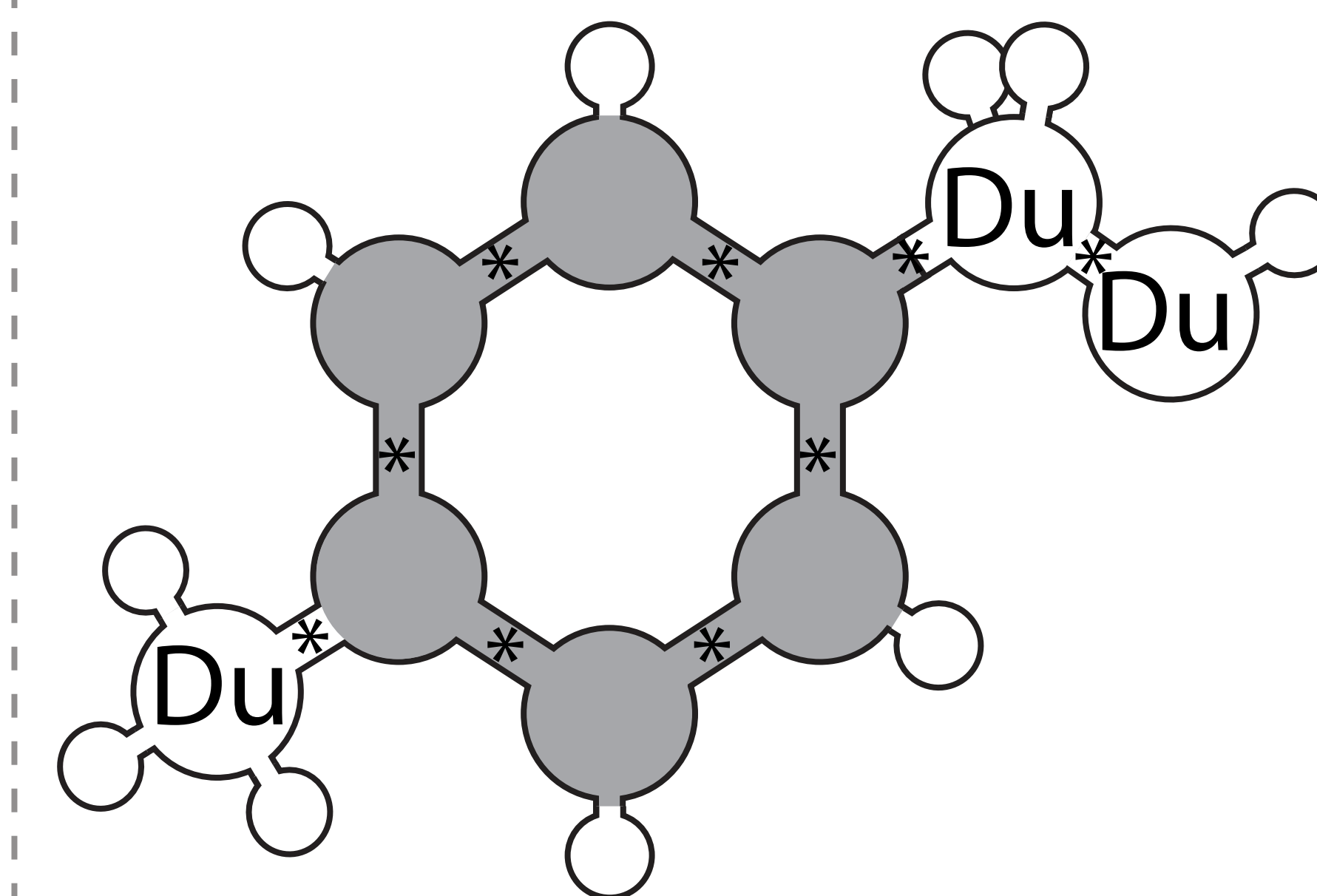
Step 1
Discharge
soft



Step 2
Vanish
soft



Step 3
Change
bonds



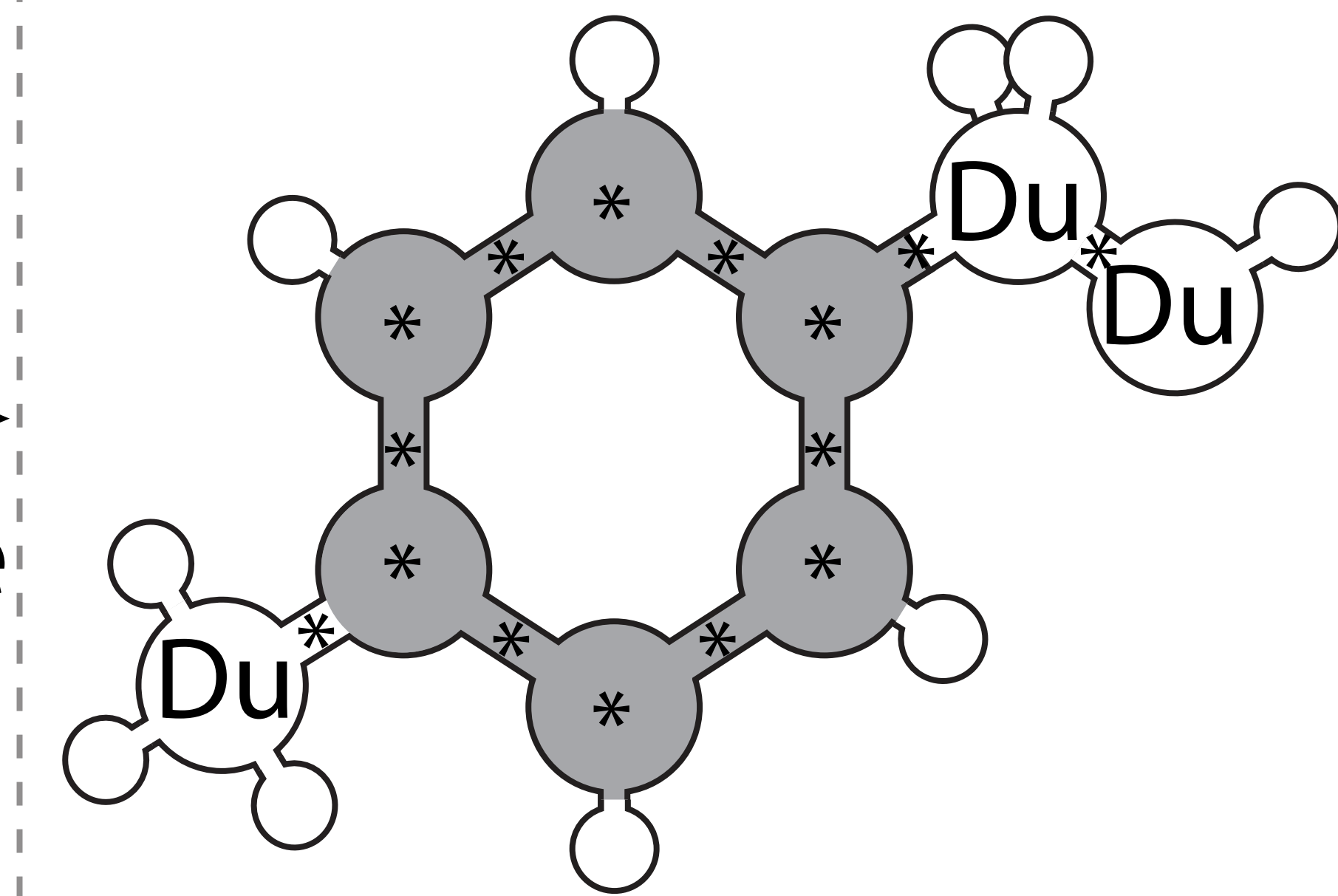
Intermediate 5

Intermediate 6

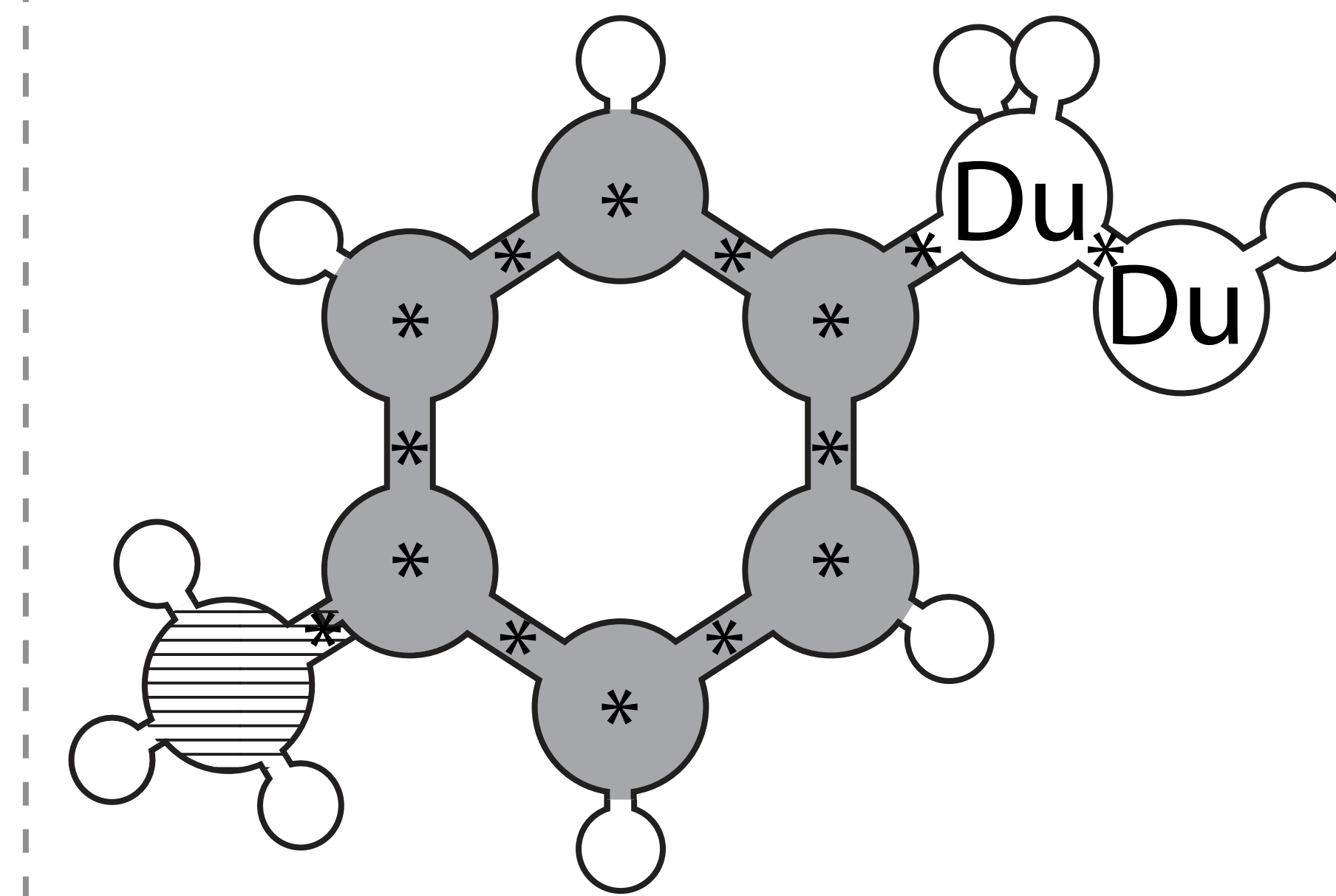
Intermediate 7

Ligand B

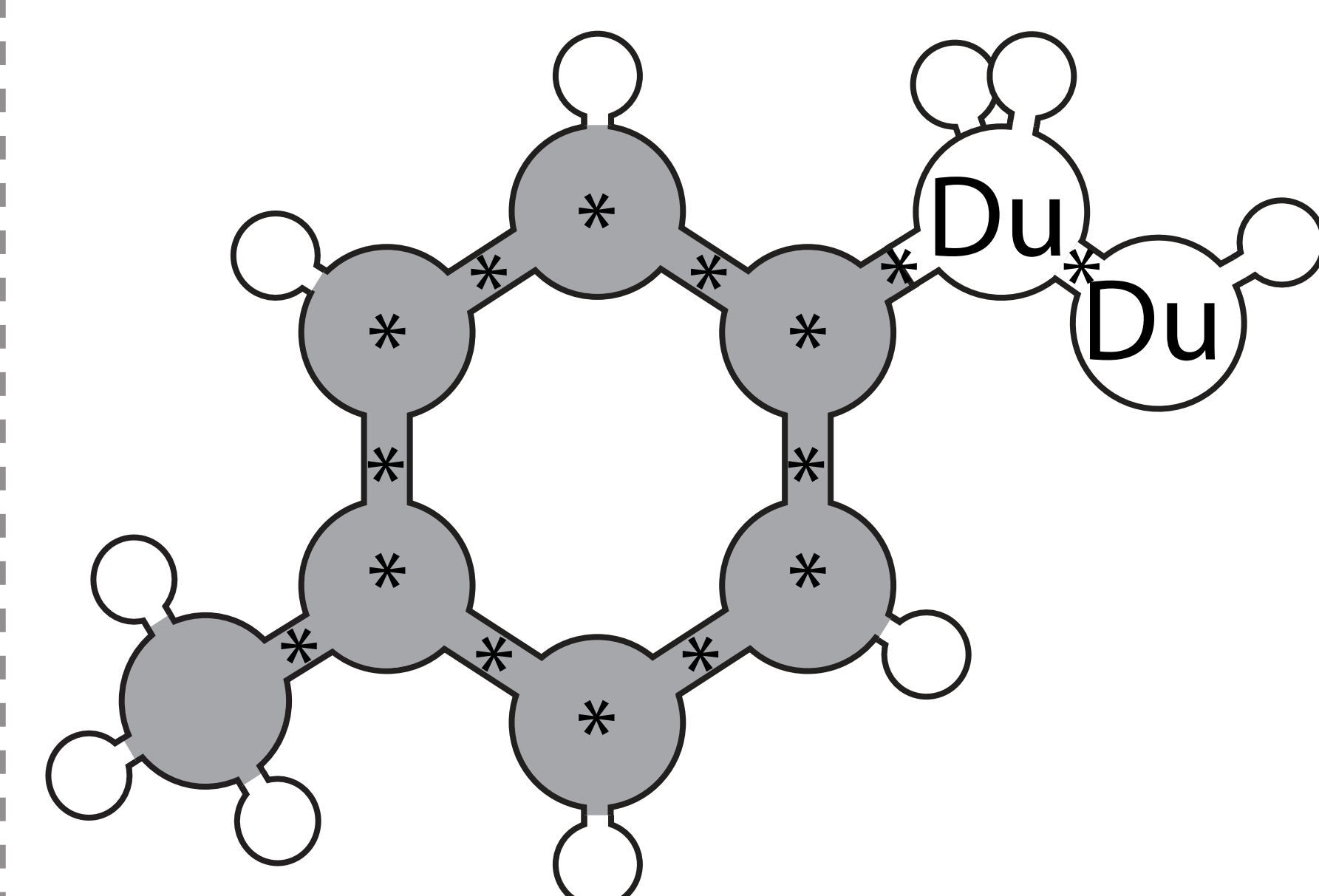
Step 4
Change
hard



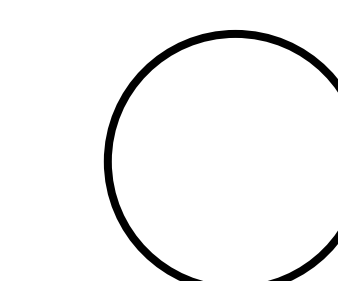
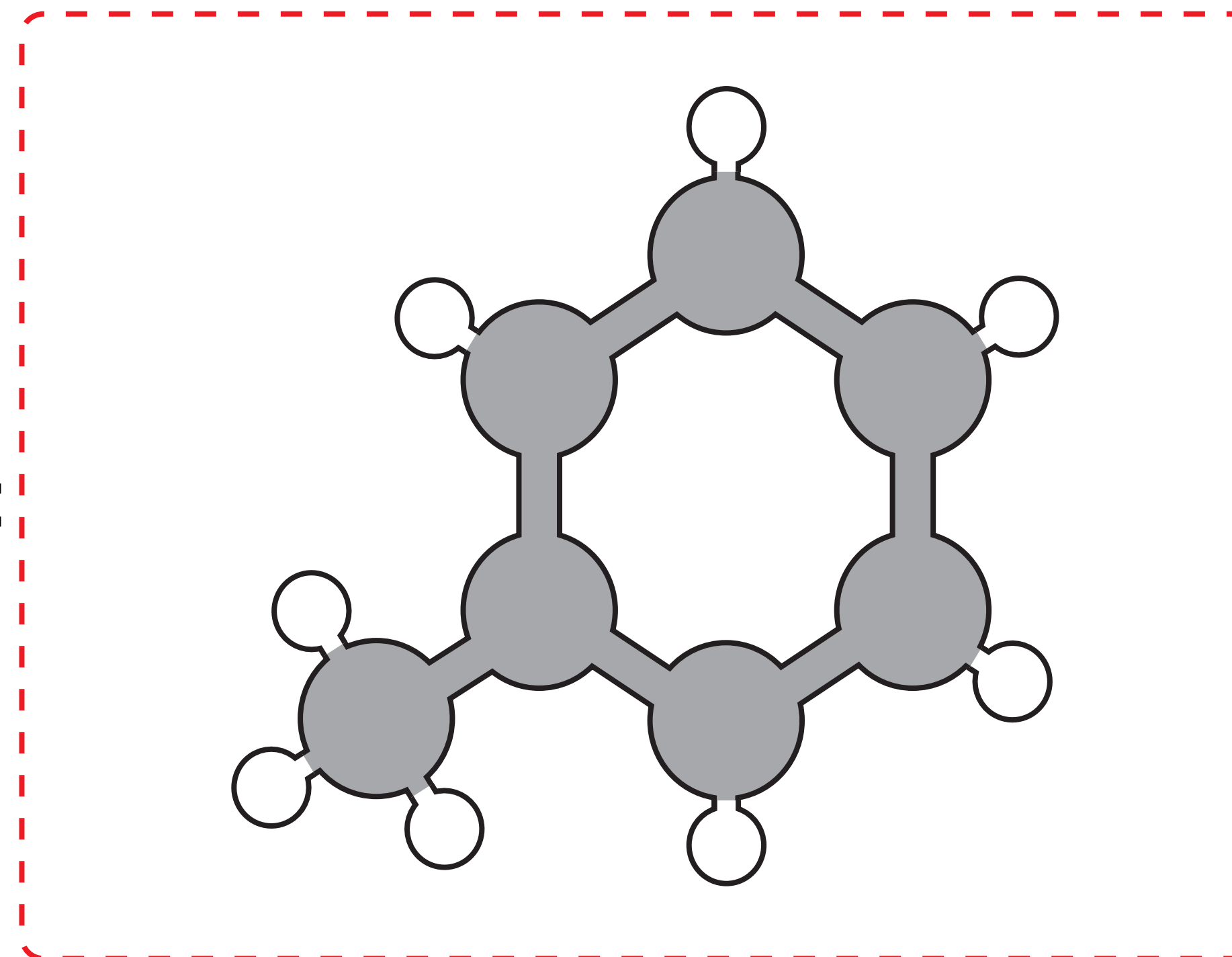
Step 5
Grow
soft



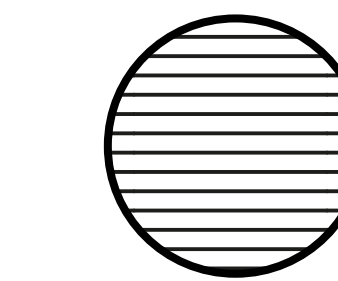
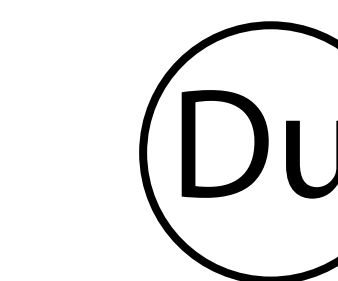
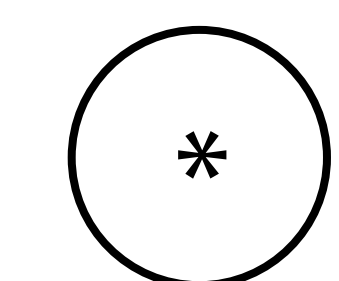
Step 6
Charge
soft



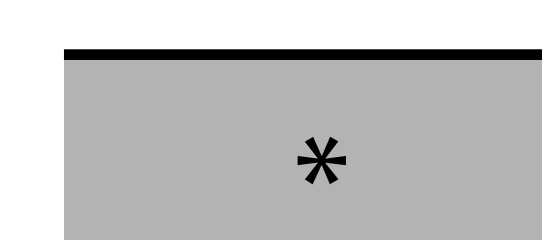
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= Heavy atom

= Heavy atom
with only VdW= Dummy atom
(No Coulomb/VdW)= Heavy atom with
ligand B Coulomb/
VdW parameters

= Covalent bond

= Covalent bond with
ligand B bond
parameters