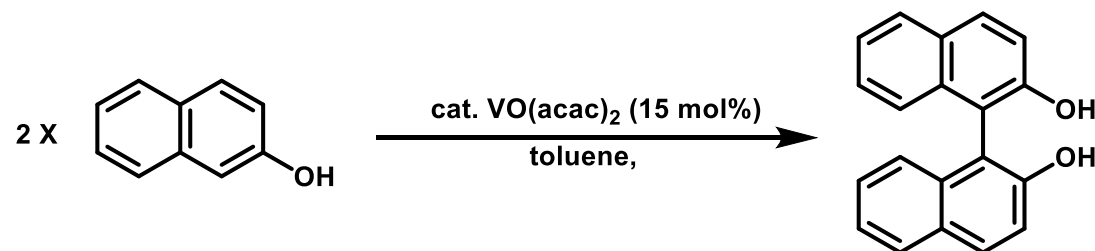


有機化学実験

3-A Catalytic Oxidative Coupling

Oxidative Coupling of 2-naphthol



Reagents

2-Naphthol (mw = 144.17) (3.0 g, 20.8 mmol)

VO(acac)₂ (mw = 265.16) (80 mg, 0.3 mmol)

Toluene (10 mL)

Preparations

1. In 25 mL egg-plant flask, 2-Naphthol and VO(acac)₂ were suspended in 10 mL of toluene at room temperature .
2. The reaction mixture was heated at over 70 °C on an oil bath. At that temperature, resulting dark red solution was swirled over 60 min.
3. After swirled over 60 min, the resulting dark green suspension was allowed to cool to room temperature.
4. Resulting residue was collected by filtration and washed with MeOH/H₂O (7/3) mixture (10 mL x 3). The residue was dried for over night.
5. The residue was dissolved into MeOH with heating on a steam bath. After almost solved the residue, activated charcoal was added to the solution. Then, the mixture was heated on a steam bath for 5 to 10 min and filtrated. The filtrate was allowed to cool to room temperature.

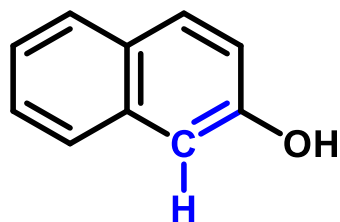
Typical Mechanism of Oxidative Coupling of 2-naphthol

○ 酸化／還元反応と酸化数

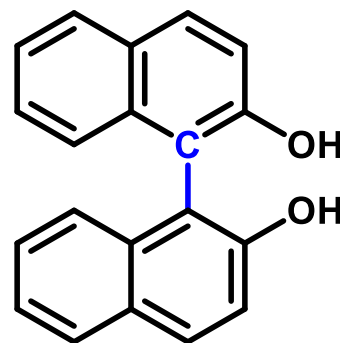
酸化数：原子の酸化状態を表す指標。反応の前後における酸化数を比較すれば、その反応でその原子が、酸化されたか、還元されたかが理解できる。

酸化数の求め方：

1. 単体の元素の酸化数は0
2. 化合物(イオン)中の酸素(O)の酸化数は-2
(過酸化水素 HOOH の酸素は-1)
3. 化合物(イオン)中の水素(H)の酸化数は+1
(ヒドリド: H^- と考えられるものは-1)
4. 化合物(イオン)中のハロゲンの酸化数は-1
5. 化合物(イオン)中のアルカリ金属の酸化数は+1
6. 化合物(イオン)中のアルカリ金属土類の酸化数は+2
7. 化合物中の全ての原子の酸化数の総和は0
8. n 価のイオン中の全ての原子の酸化数の総和は n



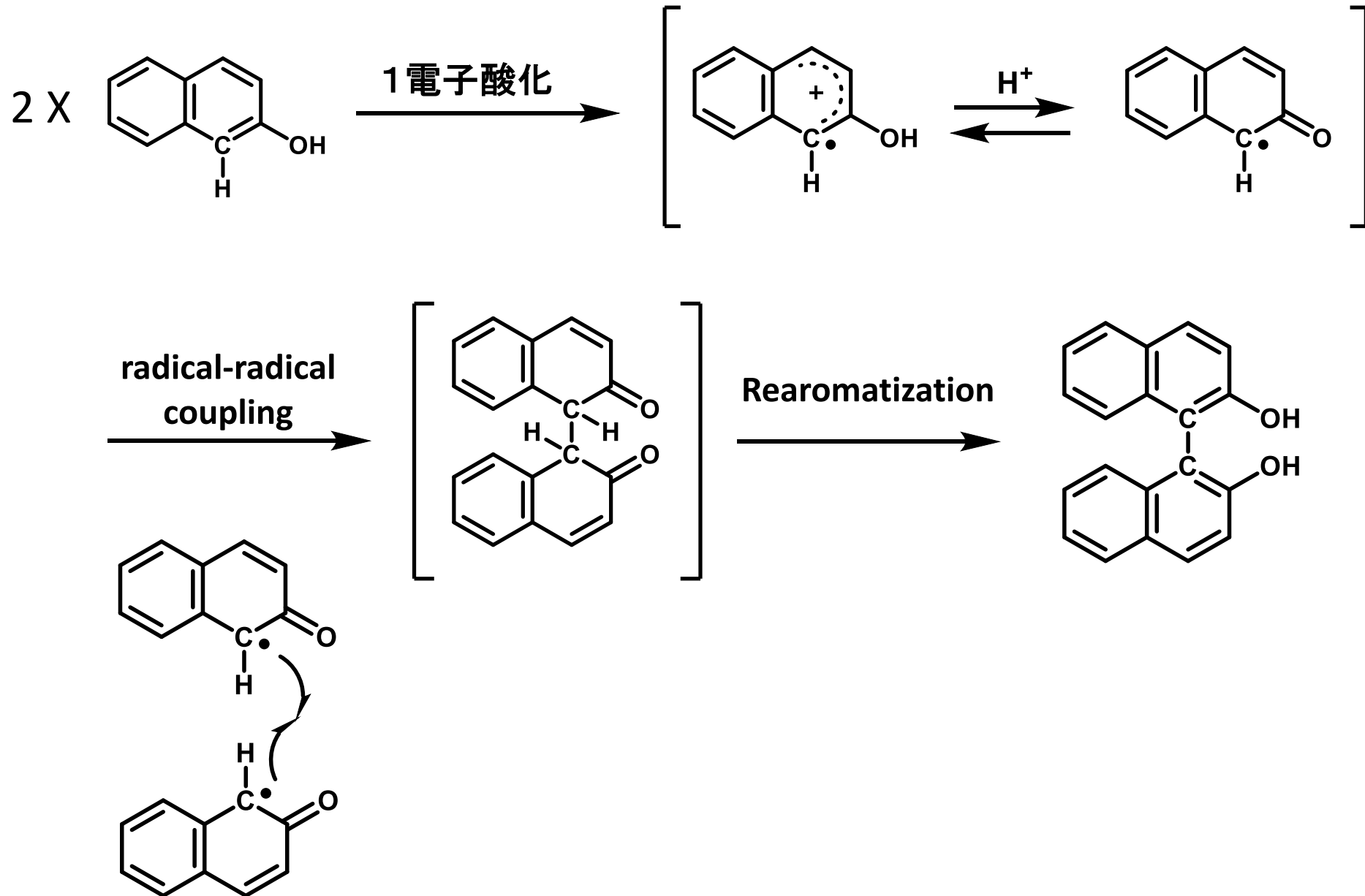
炭素原子: -1
水素原子: +1



炭素原子: 0

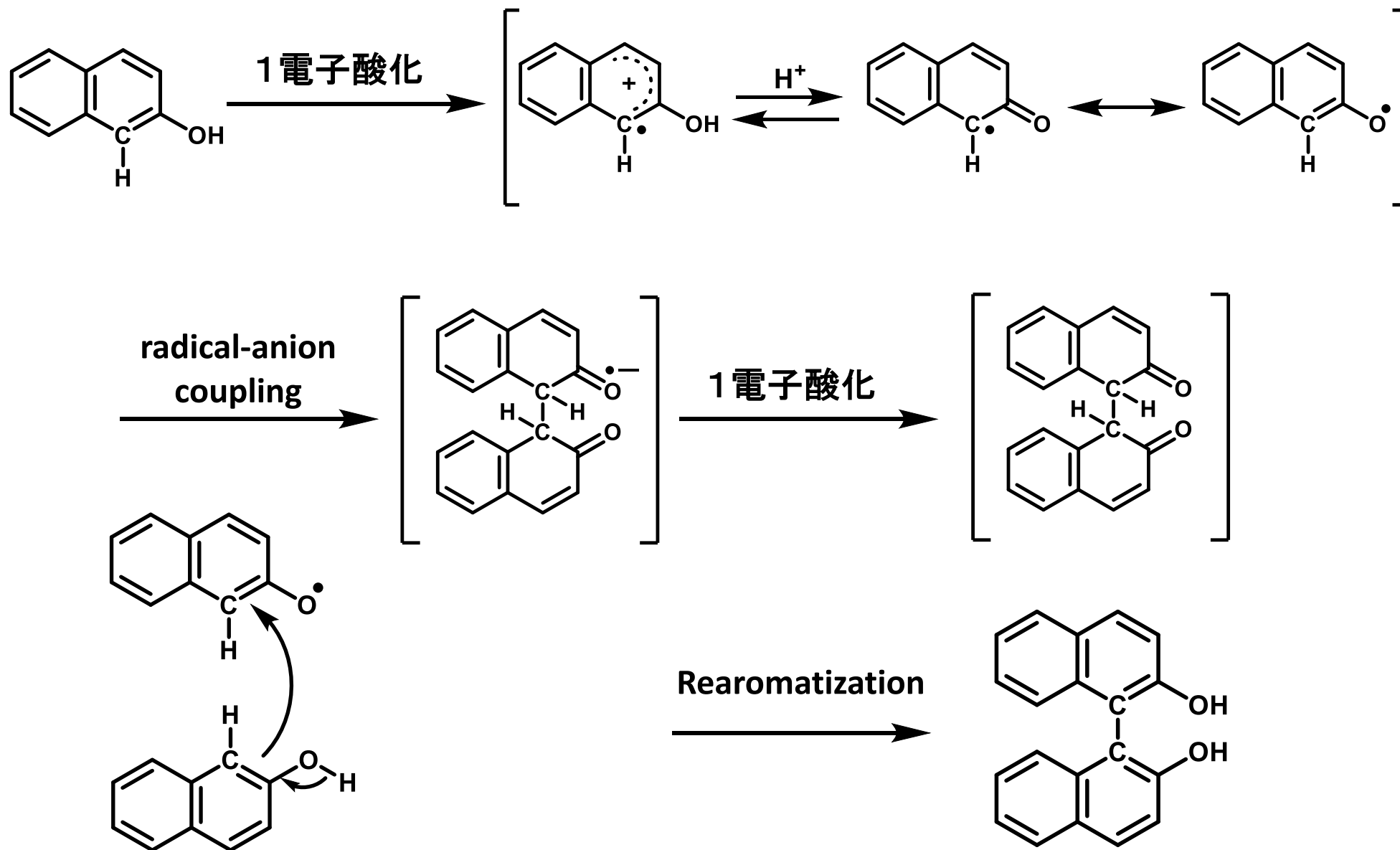
Typical Mechanism of Oxidative Coupling of 2-naphthol

▪ Radical-radical coupling



Typical Mechanism of Oxidative Coupling of 2-naphthol

▪ Radical-anion coupling



Typical Mechanism of Oxidative Coupling of 2-naphthol

▪ VO catalyzed oxidative coupling

