

# ポテンシャル曲面の化学(4)

あとで、クイズが出ます。  
できるだけ、メモしておくことを、  
オススメします。



7月22(金)9:00~

担当: 大野 公一

1. 化学とポテンシャル曲面

2. 化学結合ができる仕組み

3. 分子内ポテンシャルと分子振動

## 4. 分子間ポテンシャル

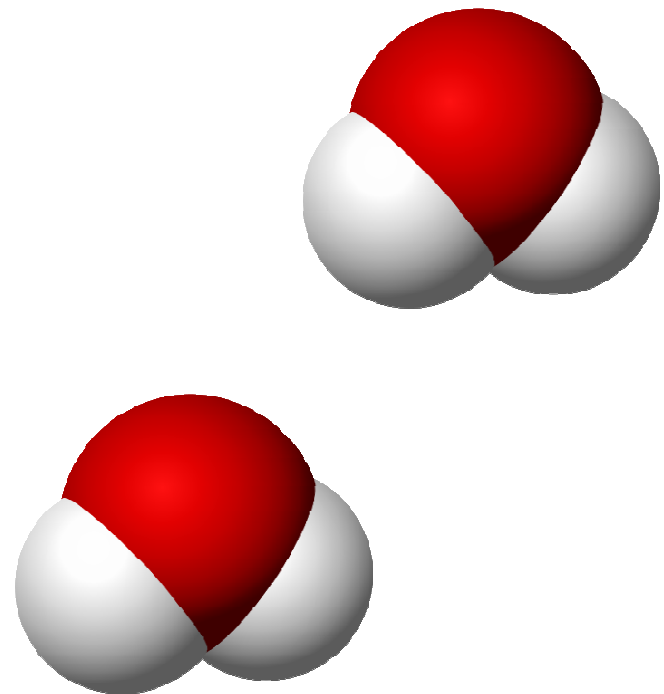
5. 原子と分子のポテンシャル

6. 化学反応とポテンシャル

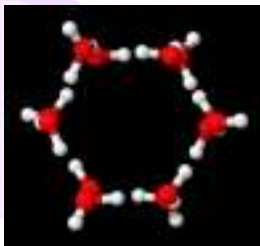
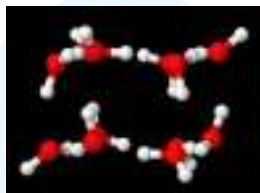
# 分子間力

- イオン間相互作用
- 水素結合
- 双極子相互作用
- London分散力  
(van der Waals力)
- 分子間の万有引力

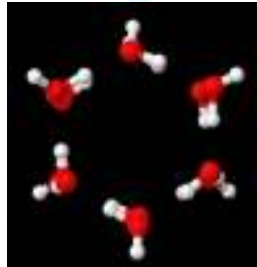
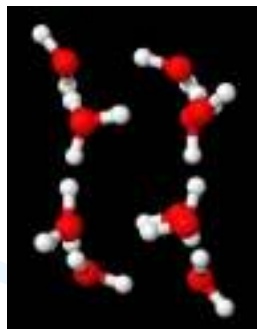
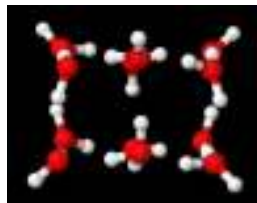
H<sub>2</sub>O分子どうしは、  
どのような構造をとるか？



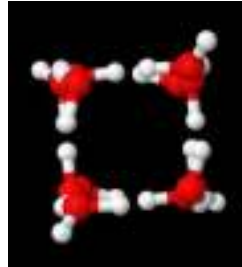
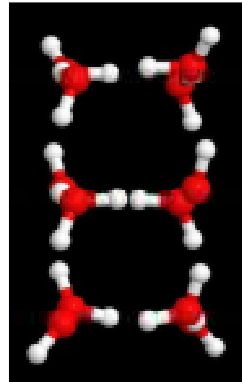
# 水の12量体クラスター $(\text{H}_2\text{O})_{12}$ の構造の 理論計算



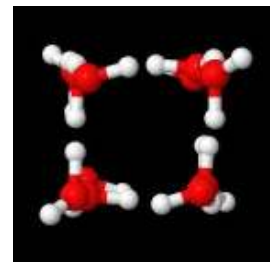
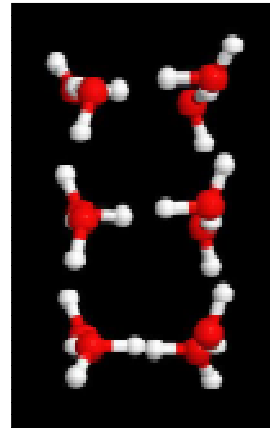
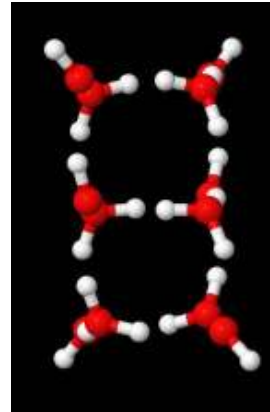
0.0 kJ/mol



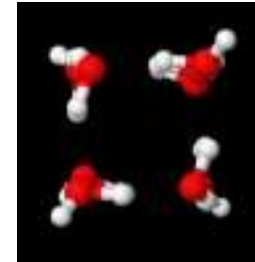
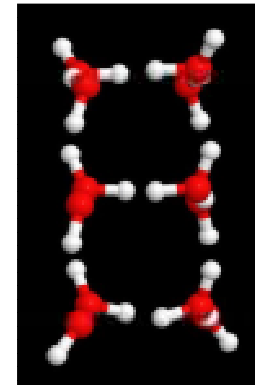
1.3 kJ/mol



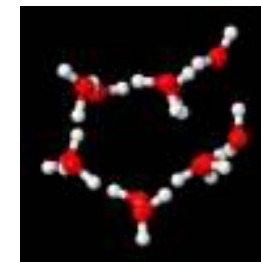
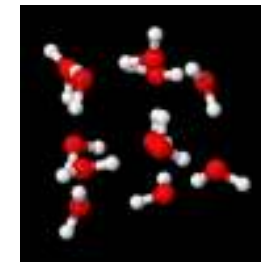
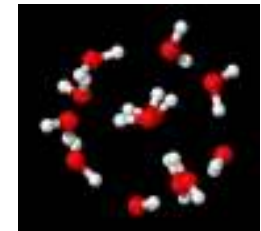
3.0 kJ/mol



4.3 kJ/mol

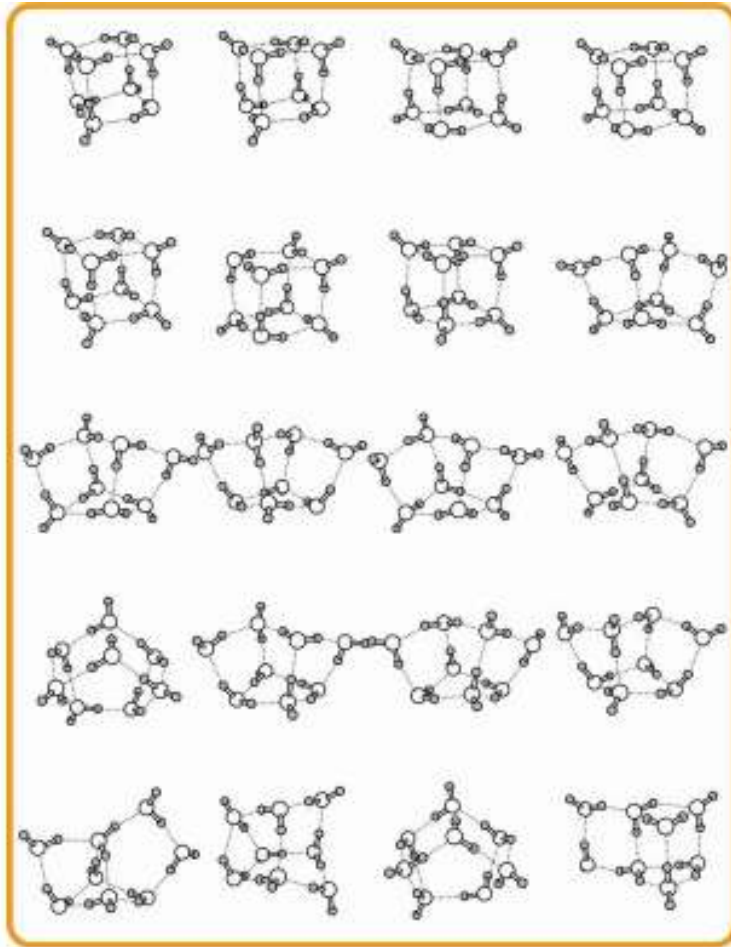


5.6 kJ/mol

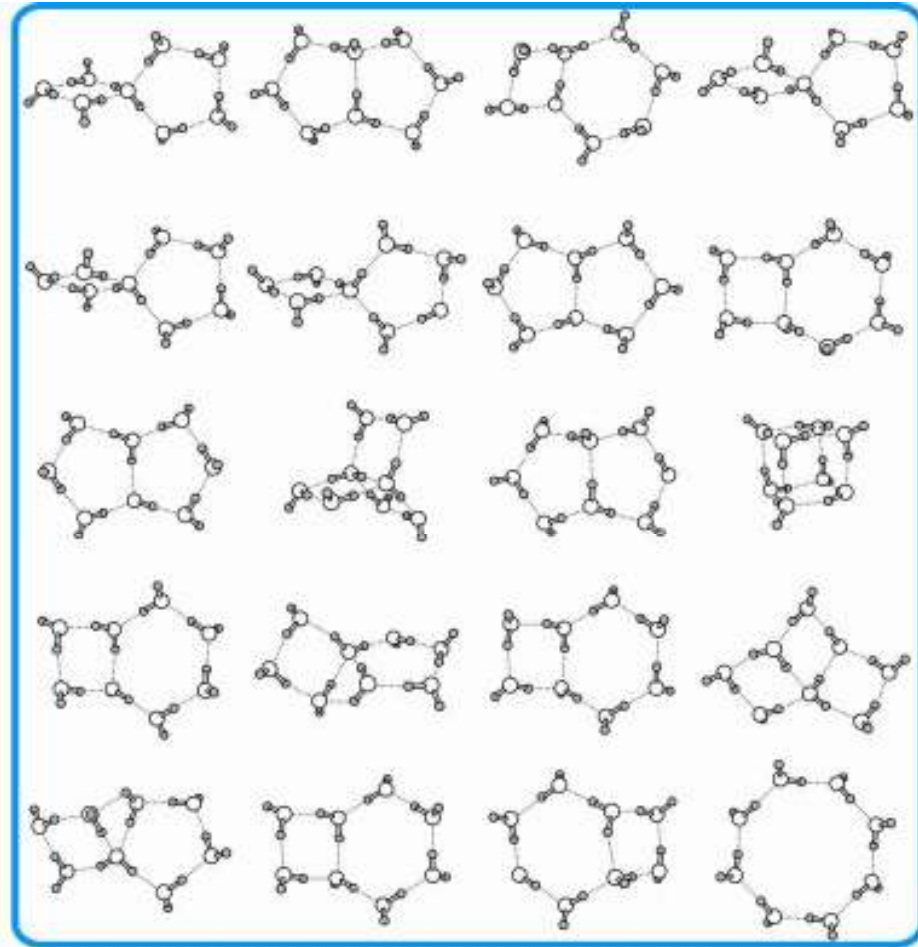


6.1 kJ/mol

# 水8量体の構造の温度依存性 (Gibbs自由エネルギーで比較)



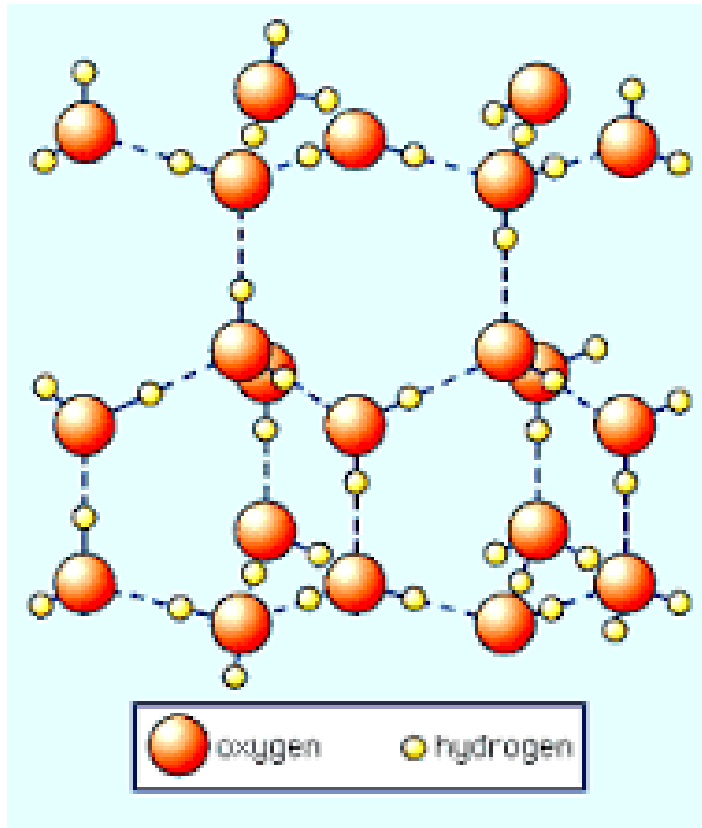
Lowest 20 minima at 0 K



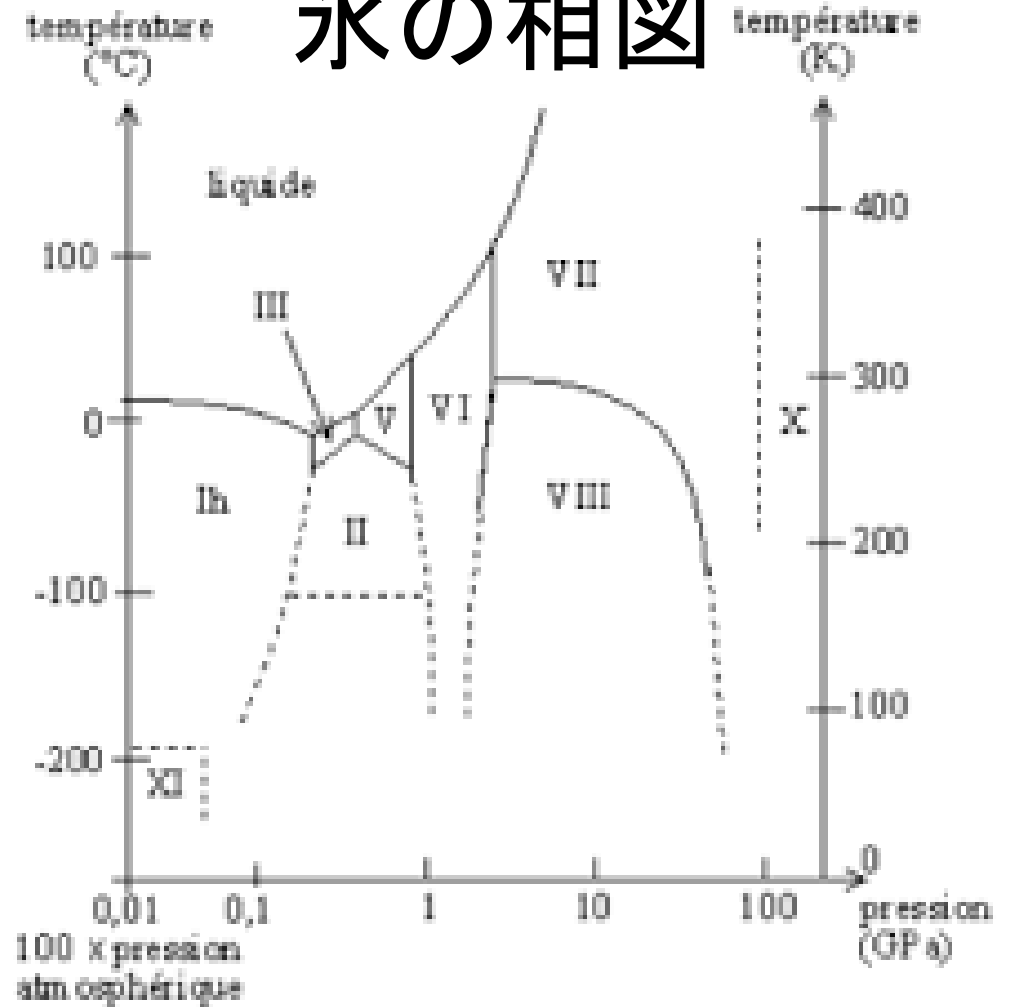
Lowest 20 minima at 400 K

# 氷の構造

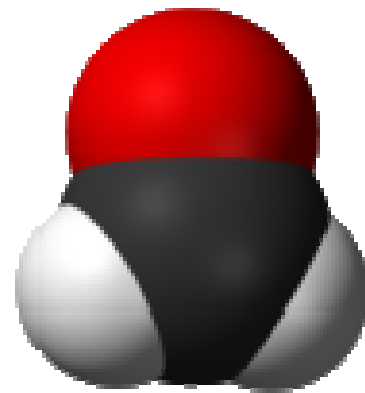
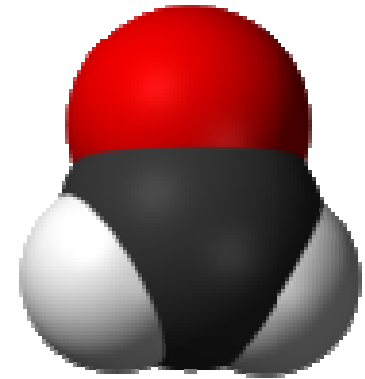
## Ih型氷の構造



## 氷の相図



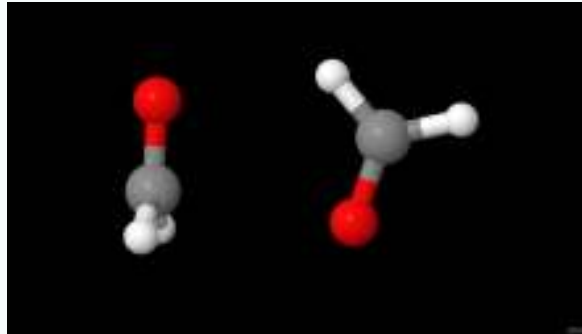
HCHO分子どうしは、  
どのような構造をとるか？





# Formaldehyde 2量体 (H<sub>2</sub>CO)<sub>2</sub>

C<sub>s</sub>



C<sub>2h</sub>



**CCSD(T)/CBS :** 0.0 kJ/mol

3.3 kJ/mol

C.A.Dolgonos, Chem.Phys.Lett. 585, 37 (2013).

**M062X/6-311+G(2d,p)**

0.0 kJ/mol

5.8 kJ/mol

**MP2/ 6-31++G(2d,2p)**

0.0 kJ/mol

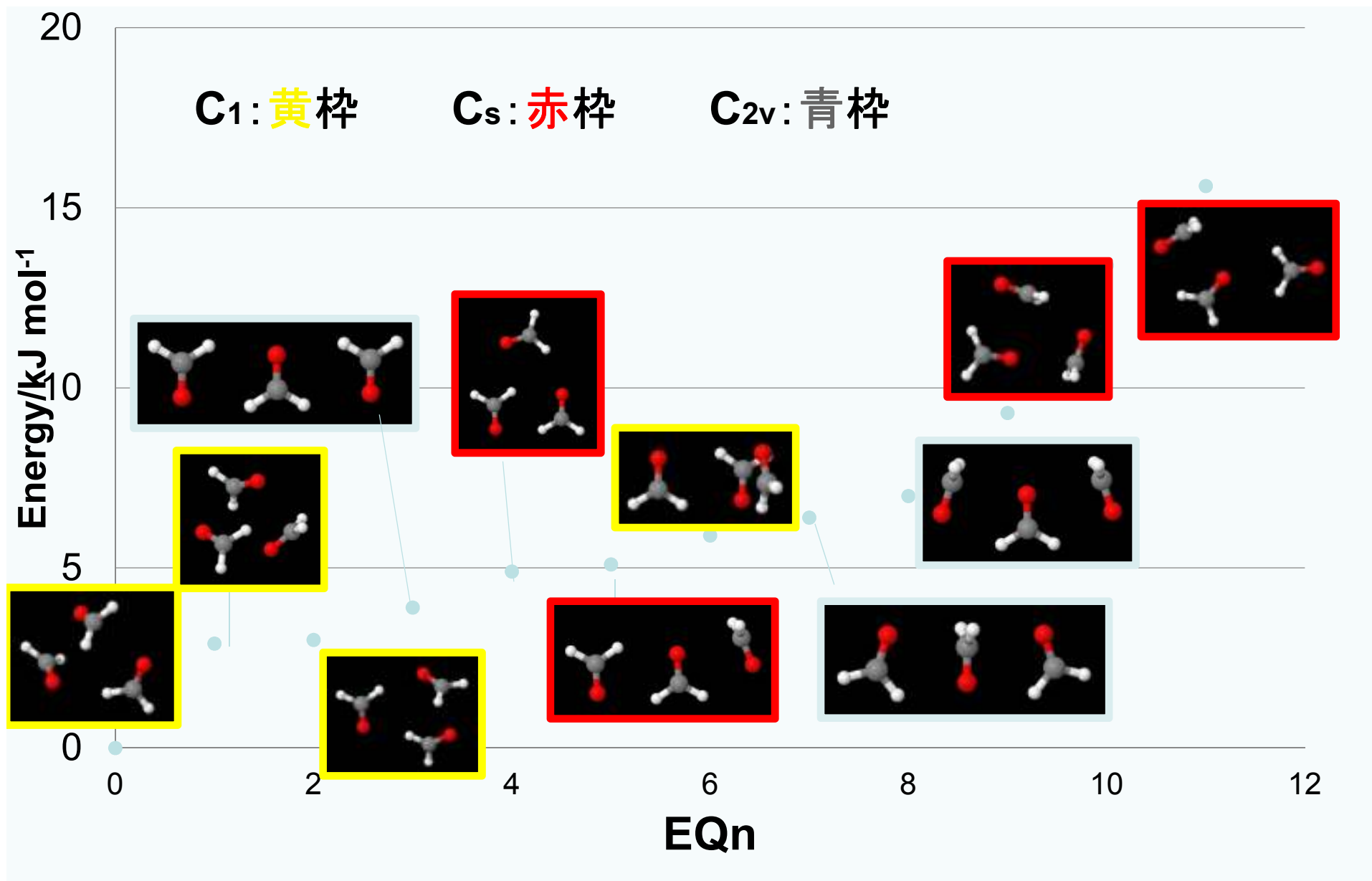
3.9 kJ/mol

**MP2/ cc-pVTZ**

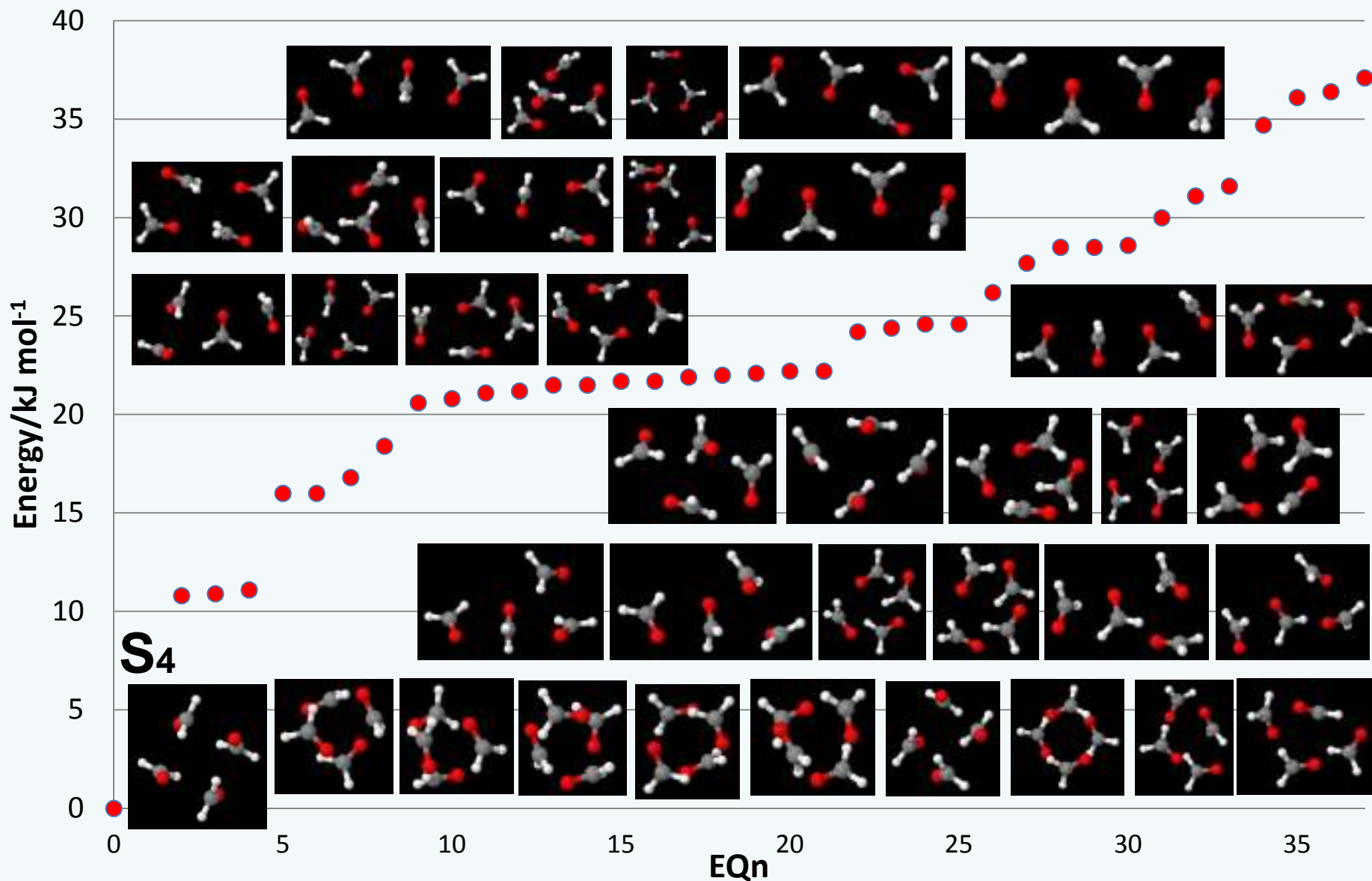
0.0 kJ/mol

1.7 kJ/mol

# Formaldehyde 3量体 (H<sub>2</sub>CO)<sub>3</sub>

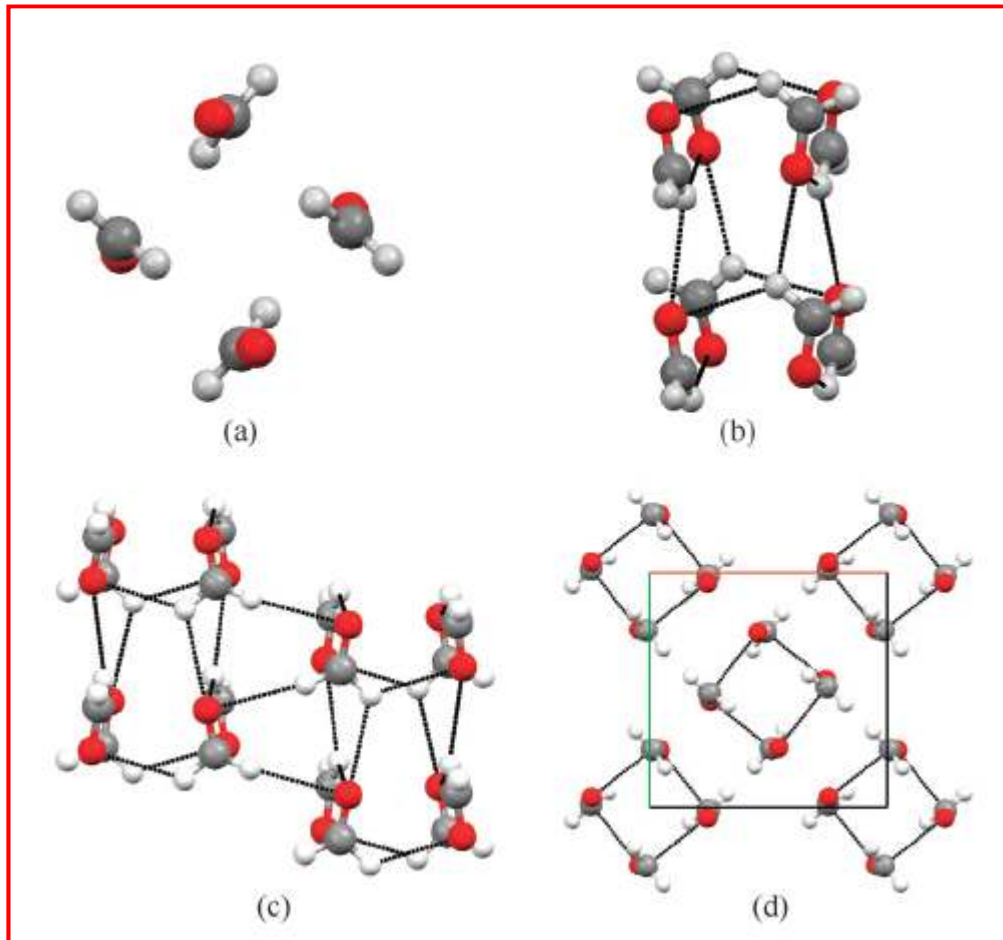


# Formaldehyde 4量体(H<sub>2</sub>CO)<sub>4</sub> 理論探索

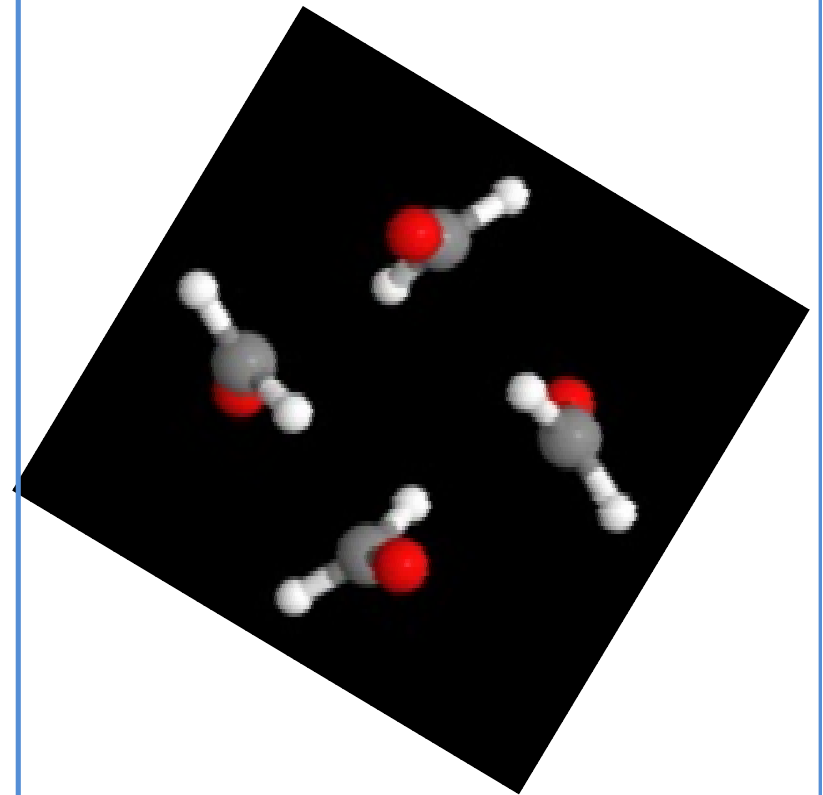


# Formaldehydeの結晶構造と4量体

T.S.Thakur et al., PCCP, 13, 14076 (2011).



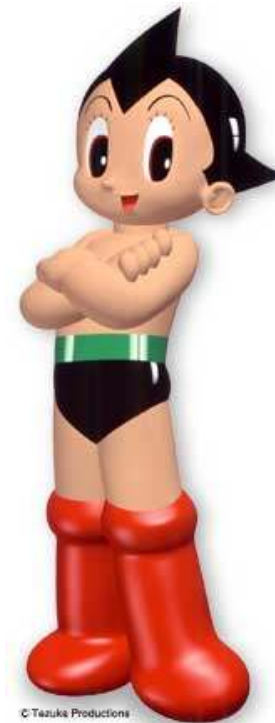
This work by GRRM :  
LADD/Bond-Condition



# 結晶構造の予測は可能か？



分子どうしが触れ合って  
反応することもある？



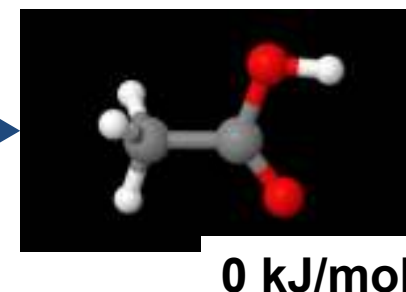
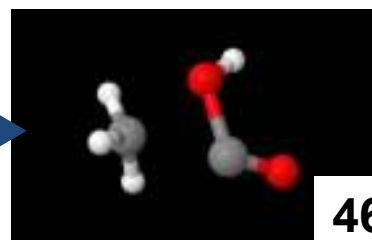
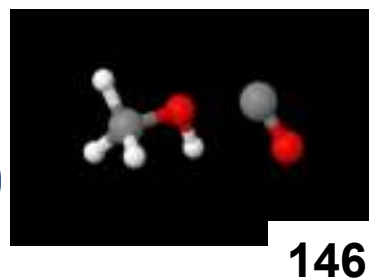
# 分子間反応



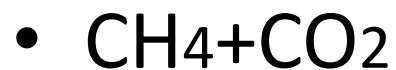
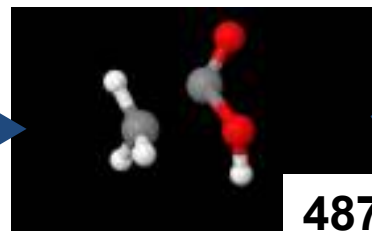
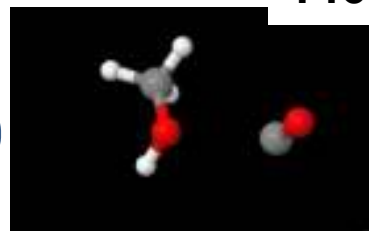
# 1-step synthesis of CH<sub>3</sub>COOH



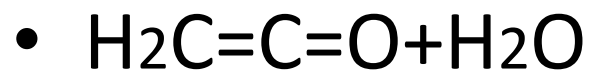
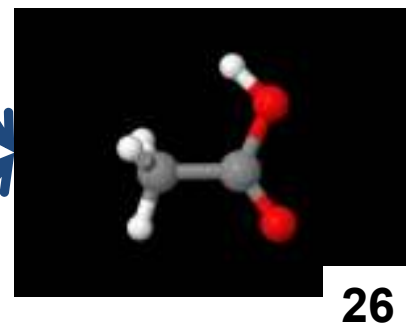
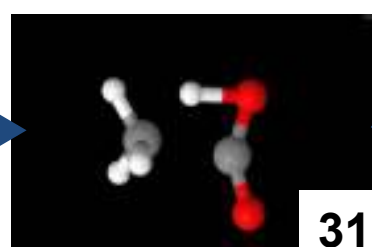
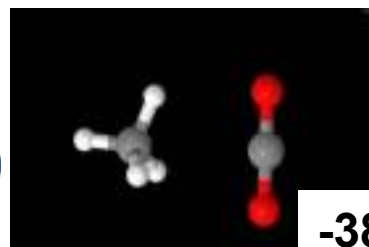
1



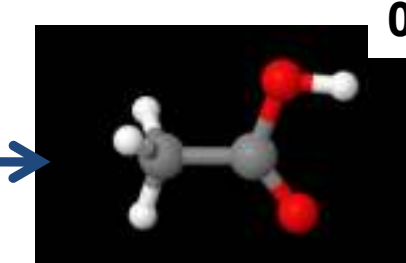
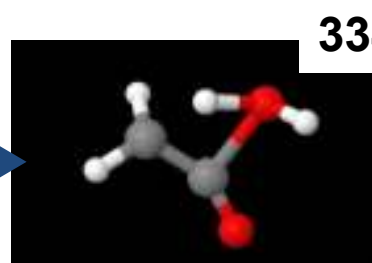
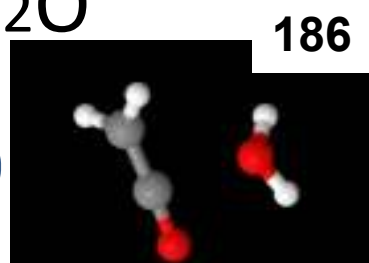
2



3



4

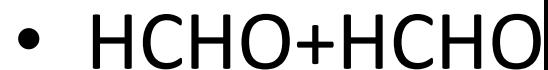
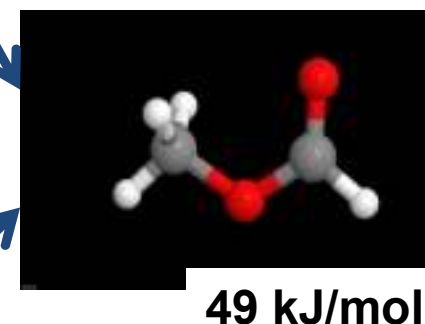
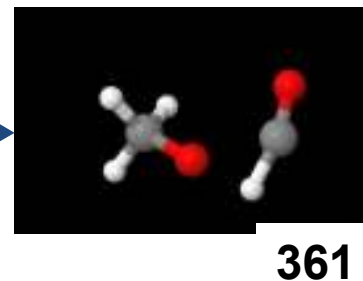
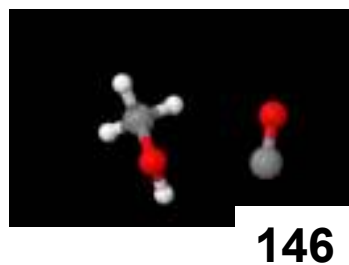




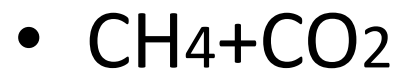
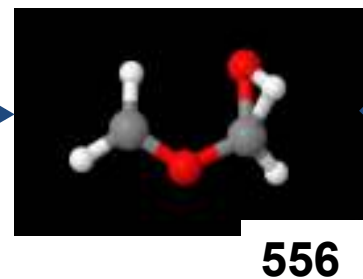
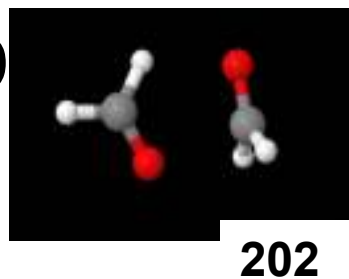
# 1-step synthesis of HCOOCH<sub>3</sub>



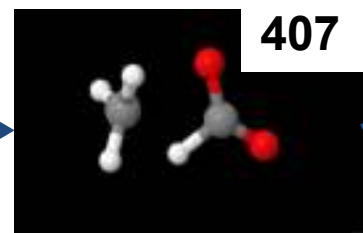
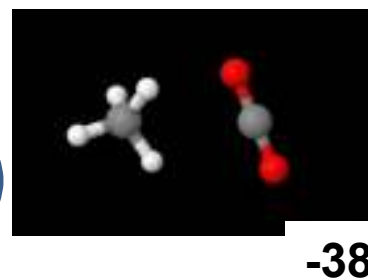
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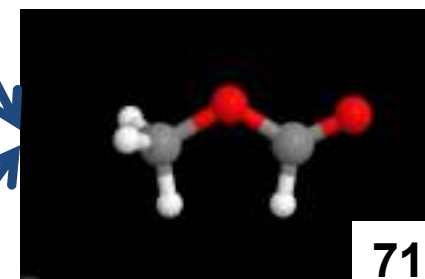
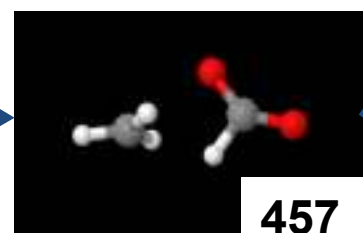
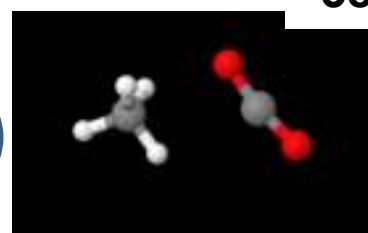
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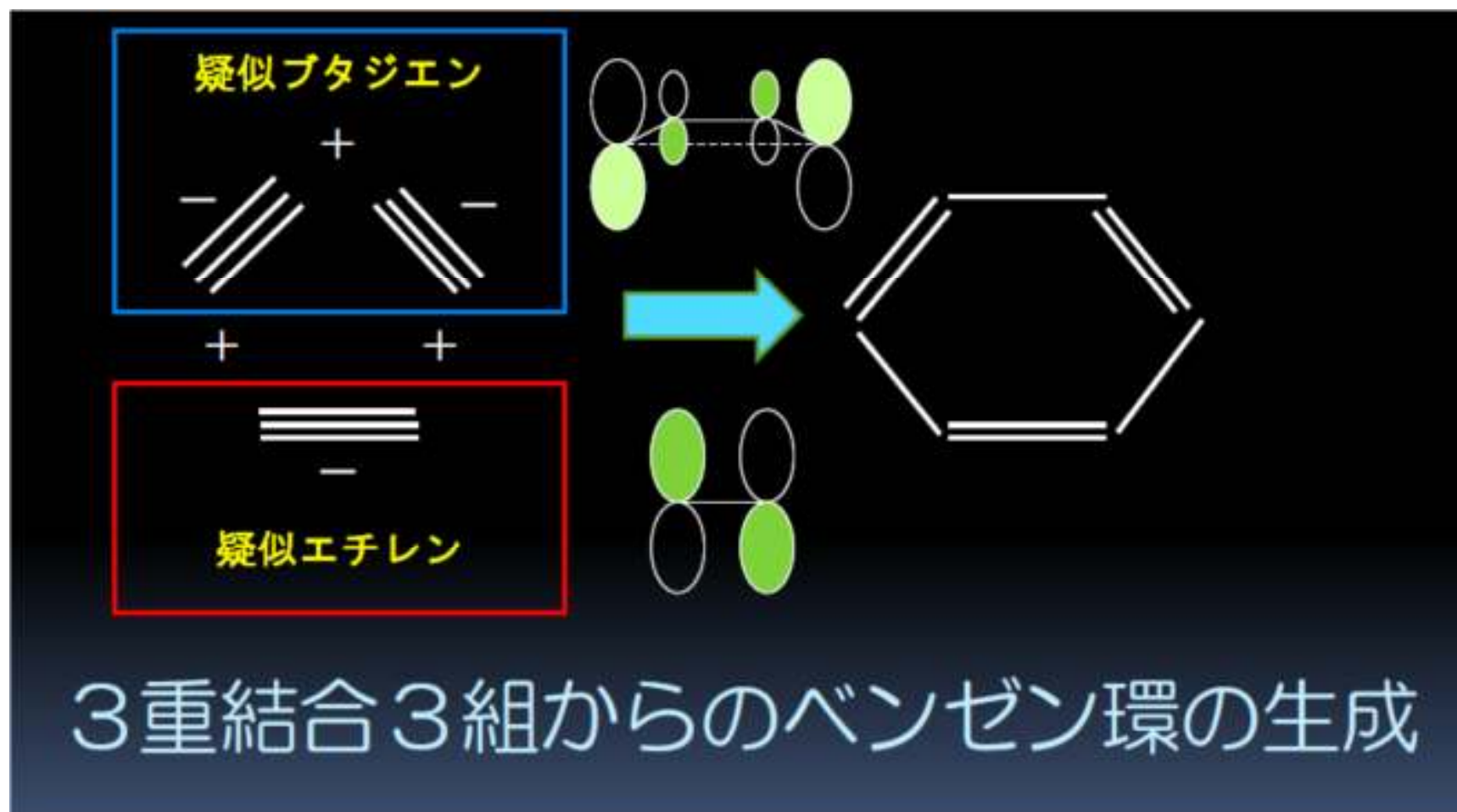
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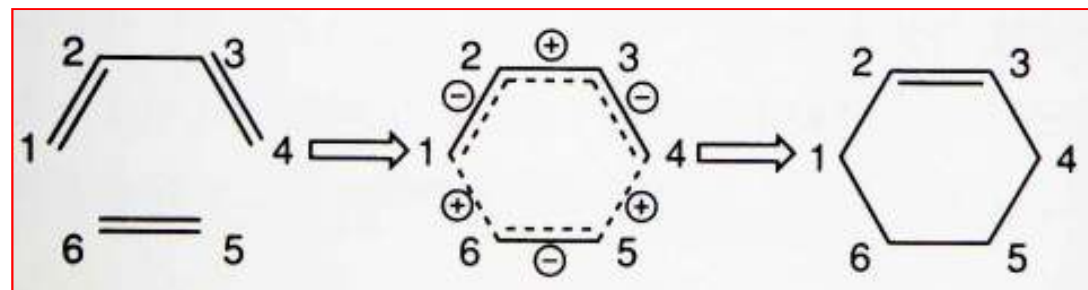
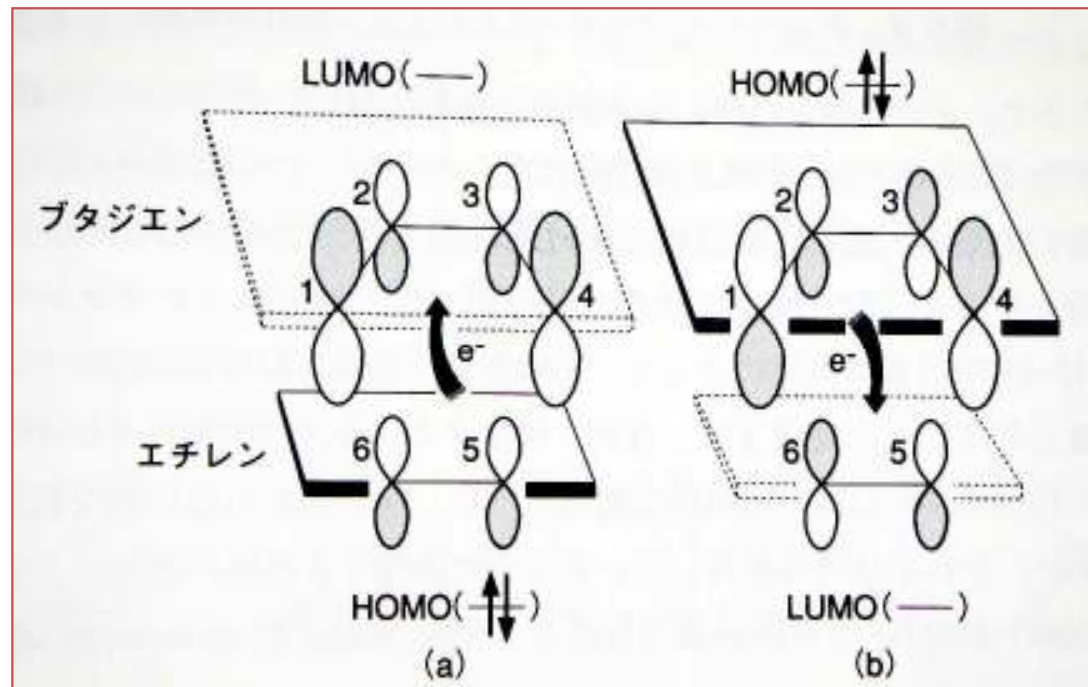
8



# ベンゼンの合成



# エチレンとブタジエンの HOMO-LUMO相互作用



アセチレン3分子から、  
ベンゼンができる反応の仕組み？



1. 化学とポテンシャル曲面
2. 化学結合ができる仕組み
3. 分子内ポテンシャルと分子振動
4. 分子間ポテンシャル

**Next** → 5. 原子と分子のポテンシャル

6. 化学反応とポテンシャル