

then, r.t., 2 h

## Solution-Compatible Synthesis of C<sub>60</sub>-Fragmentary Octacycles

Naruhiro Yoshida, Tetsuo Iwasawa\*

Department of Materials Chemistry, Ryukoku University, Seta, Otsu, Shiga 520-2194, Japan



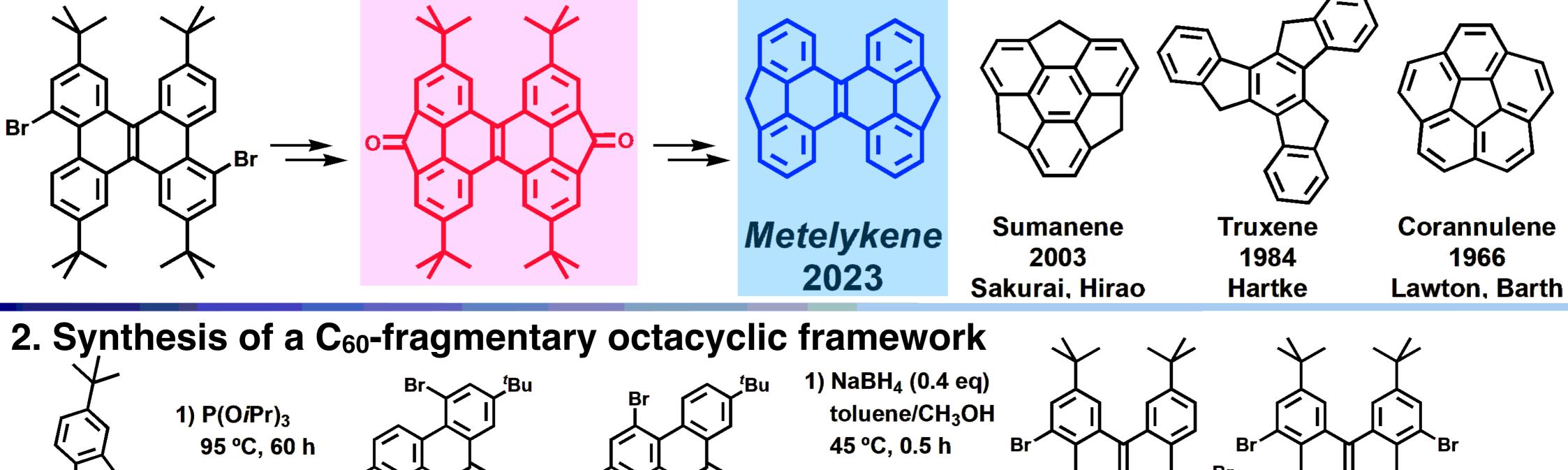
Metelykene

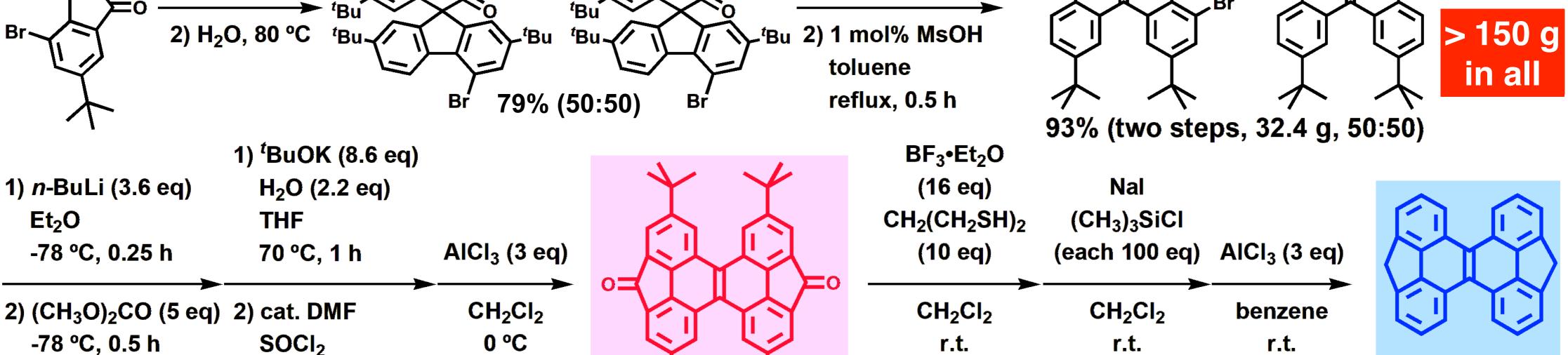
73% (624 mg)

0.5 h

89 h

## 1. Summary, Eur. J. Org. Chem. 2023, e202300407; DOI: 10.1002/ejoc.202300407





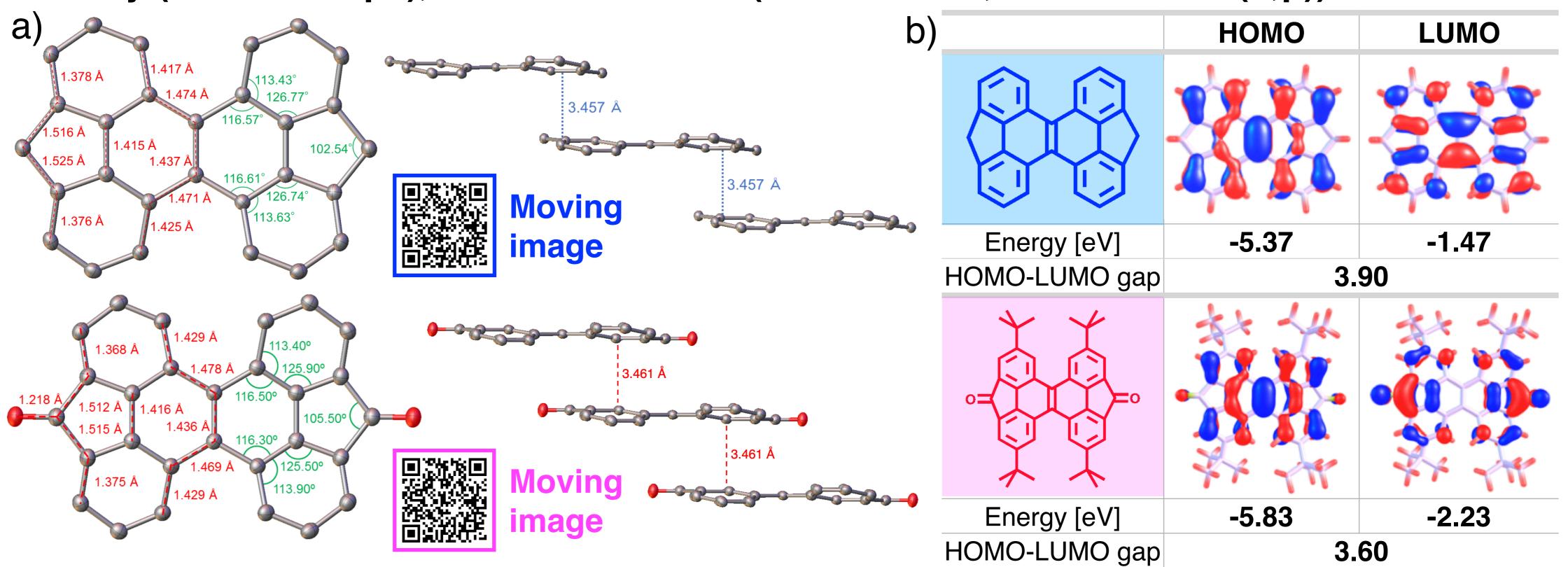
1 h

## 3. X-ray (saddle-shape), DFT calculations (twisted form, B3LYP/6-31G(d,p))

92% (3 steps, 5.2 g)

0.5 h

r.t., 0.5 h



| c) | Point           | Energy differences |                |              |                |
|----|-----------------|--------------------|----------------|--------------|----------------|
|    | group           | Metelykene         | [kcal/mol] [a] | Metelykenone | [kcal/mol] [a] |
|    | C <sub>2h</sub> | Saddle             | 0              | Saddle       | 0              |
|    | $D_2$           | Twisted            | -1.87          | Twisted      | -1.94          |