Relevant Structural Analysis to the Multi-Substituted Buckybowl of Diindeno(1,2,3,4-*defg*:1',2',3',4'-*mnop*)chrysene

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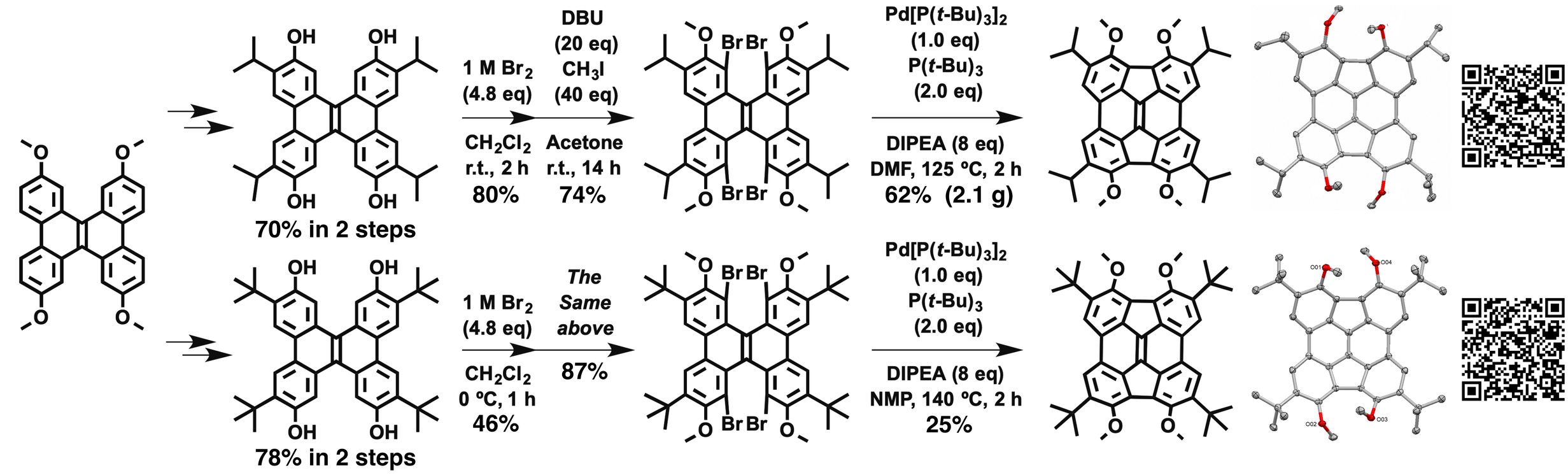
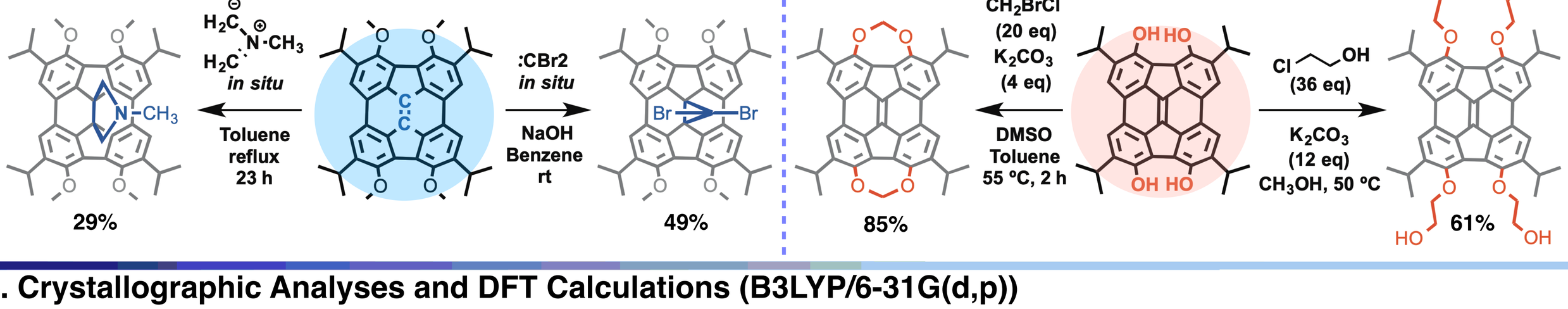
1. Summary

N. Yoshida, R. Akasaka, Y. Awakura, T. Amaya, T. Iwasawa, *Eur. J. Org. Chem.* **2021**, 5343-5347.

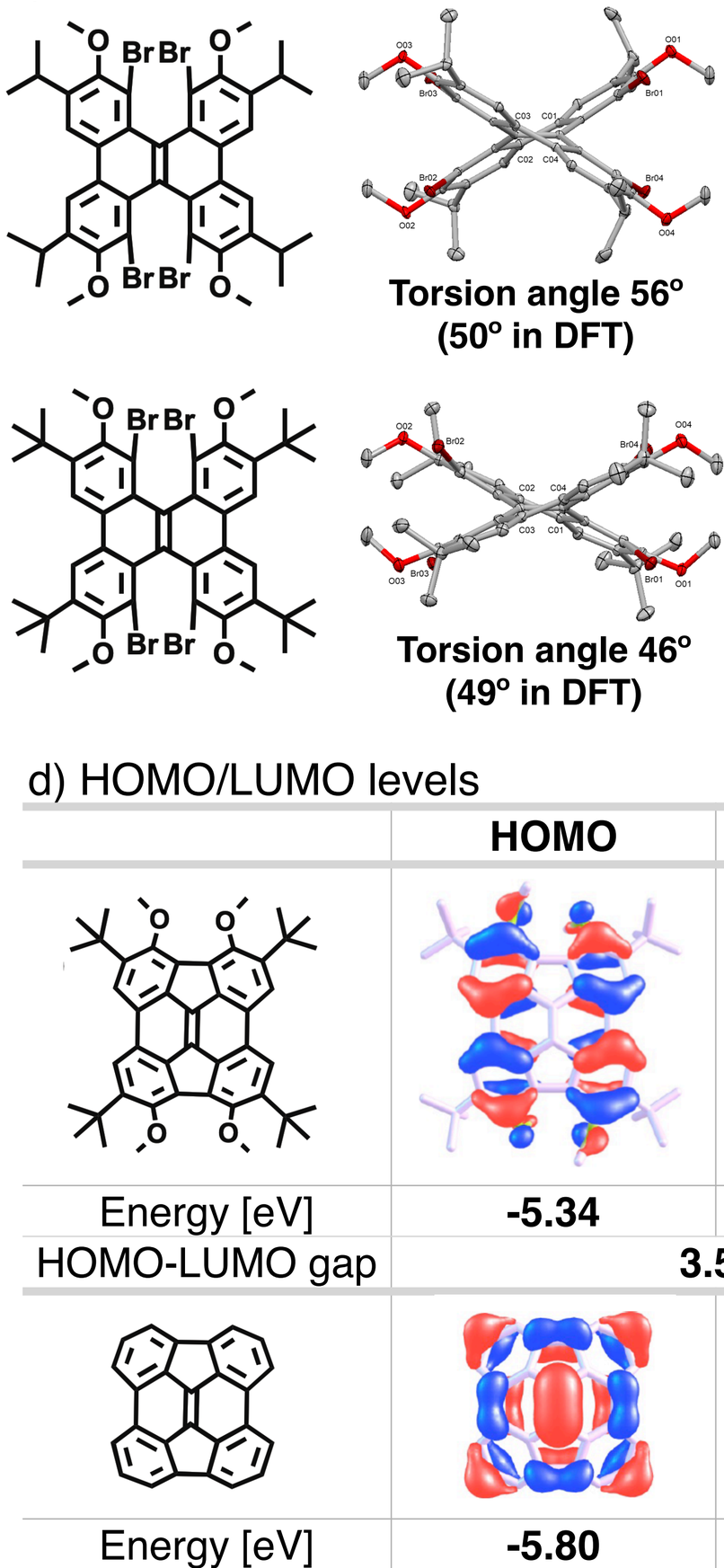


2. The Buckybowl Derivatives

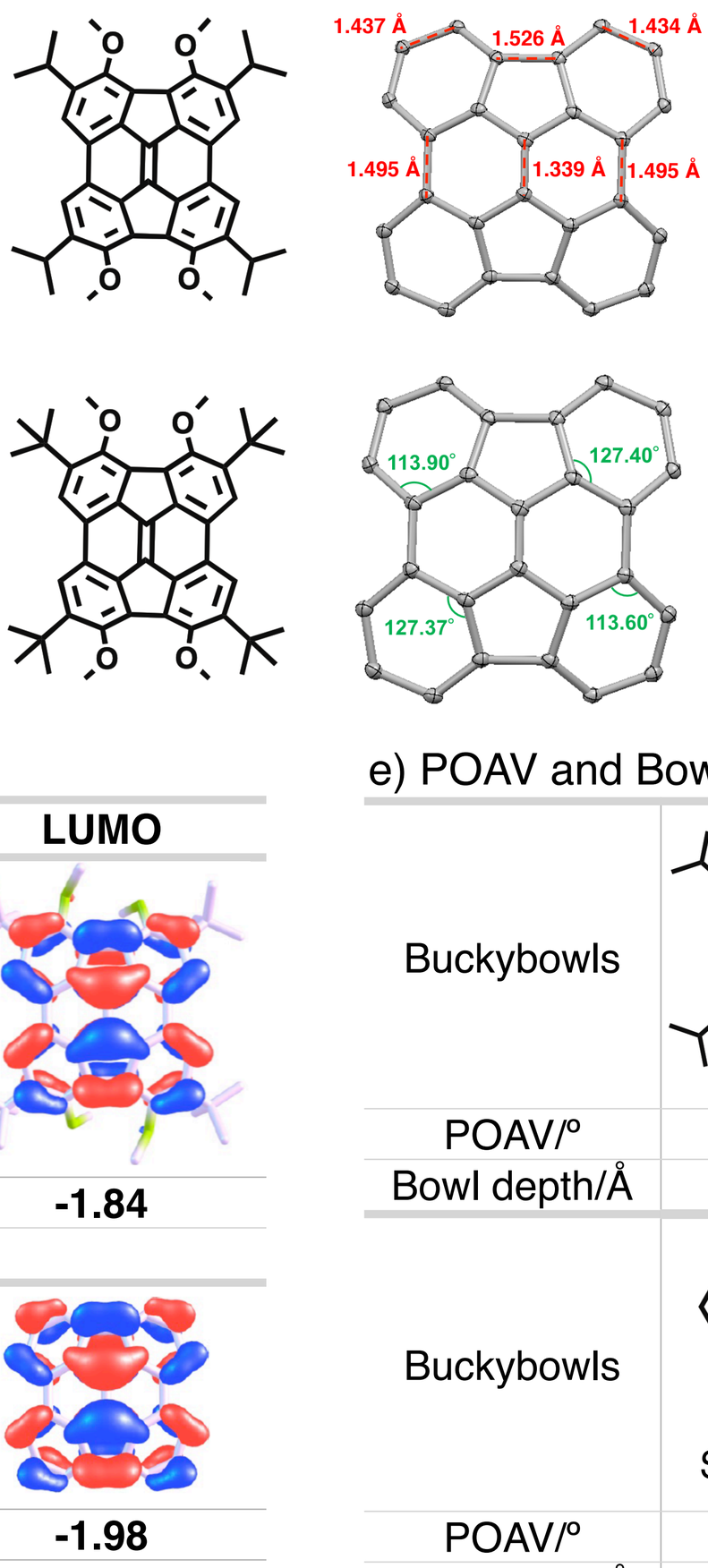


3. Crystallographic Analyses and DFT Calculations (B3LYP/6-31G(d,p))

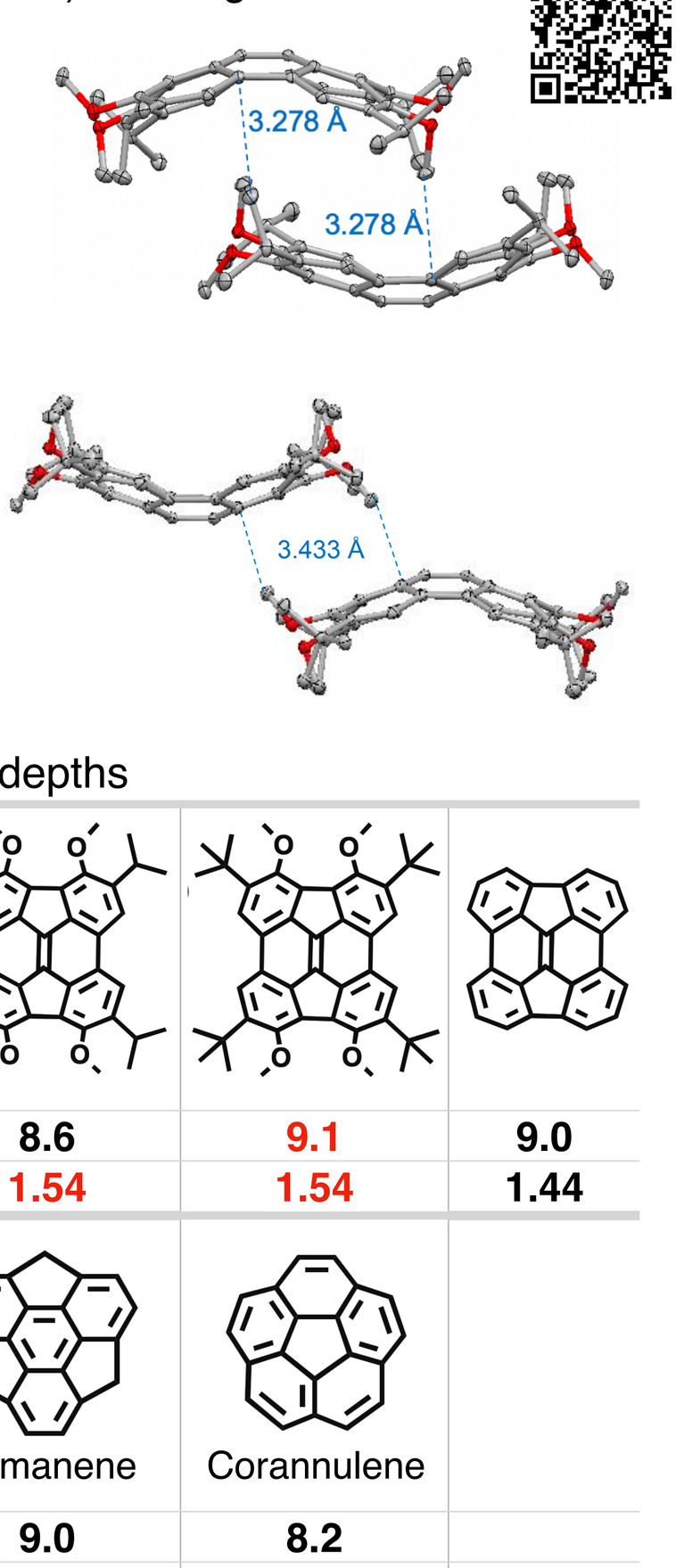
a) Twisted Precursors



b) Bond lengths and angles



c) Packing Views



d) HOMO/LUMO levels

	HOMO	LUMO
Energy [eV]	-5.34	-1.84
HOMO-LUMO gap	3.50	
Energy [eV]	-5.80	-1.98
HOMO-LUMO gap	3.82	

e) POAV and Bowl-depths

Buckybowls			
POAV/°	8.6	9.1	9.0
Bowl depth/Å	1.54	1.54	1.44
Buckybowls	Sumanene	Corannulene	
POAV/°	9.0	8.2	
Bowl depth/Å	1.11	0.87	