

Solns to Prob set 12; Chem 131a (231a)

1. $E_{Lu}(\text{---})$ 0.445 (β) — energy warts of Hückel MO
 $E_{Lu}(\text{---})$ 0.347 (β)

$\therefore$, --- is easier to reduce.

2. Will illustrate later (in class).

3. $\frac{E(Lumo)(\beta)}{+1}$ dienophile $C_{H_2}=C_{H_2}$ rel. to C_{H_2}
- | | | |
|--------|----------------|-----------------------|
| +1.414 | ---OR | E_{Lumo} is larger |
| +0.618 | --- | E_{Lumo} is smaller |

4. $E(HOMO)[C_{H_2}=C_{H_2}-C_{H_2}=C_{H_2}] = -0.618|\beta|$

- (a) $\Delta E (HOMO/LU)$ $\text{---} / \text{---}$ $\text{---} / \text{---OR}$ $\text{---} / \text{---}$
- | | | | |
|------------|--------------|-----------------------|--------------|
| $\swarrow$ | --- | --- | --- |
| | 1.618 | 0.618 + 1.414 = 2.032 | 1.236 |

- (b) Smallest gap

- (c) Fastest $\text{---} + \text{---}$, which, of course, is in accord w/ expt.

5. (a) $\text{---} + N_2 + Al_3SnBr + \text{---}$ ("via" Δ)

- (b) SOMO --- $\leftarrow -0.707 = C_c$ $C_b = \phi$ $\therefore a_h(C_b/SOMO) = \phi$
 $C_a = +0.707$
 (c) $23(0.707)^2 \approx 11.5$ Gauss
 (d) triplet