Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry


# Halogenation Effects in Intramolecular Furan Diels-Alder Reactions: Broad Scope Synthetic and Computational Studies

Robert L. Rae, Justyna M. Żurek, Martin J. Paterson* and Magnus W. P. Bebbington*

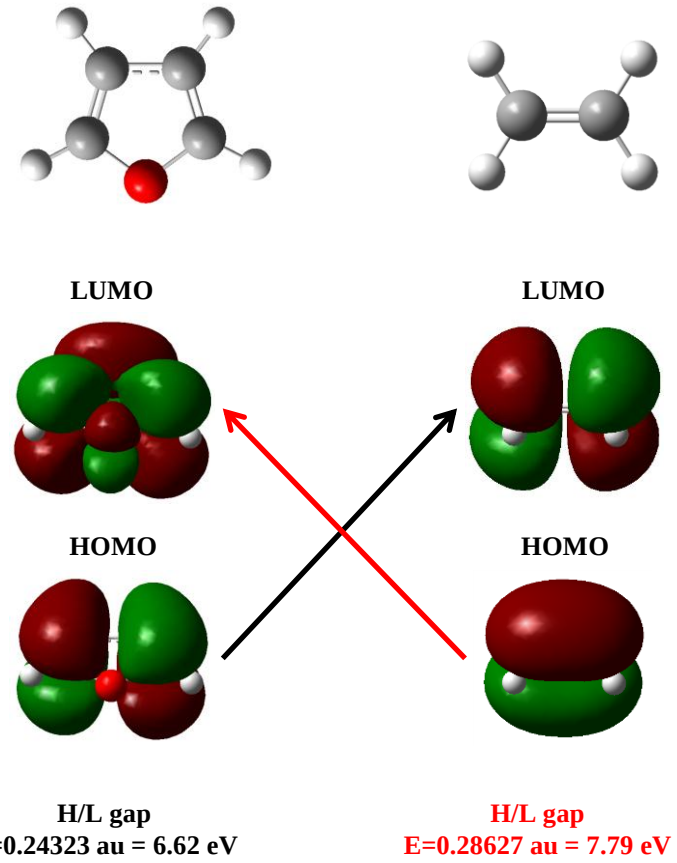
Institute of Chemical Science

Heriot-Watt University

Electronic supporting information S2

DFT-calculated (B3LYP/6-31G) pictorial representations of FMOs and HOMO-LUMO energy differences for model furan/ethylene and 2-chlorofuran/ethylene Diels-Alder reactions as well as for substrates **1a-1z.**

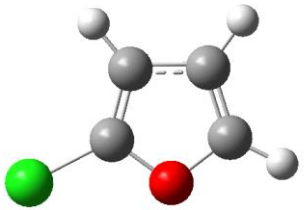
## Furan/ethylene reaction

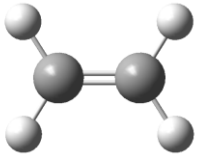



**H/L gap**
**E=0.24323 au = 6.62 eV**

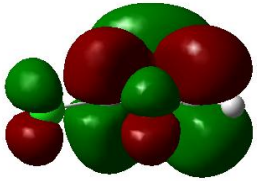
**H/L gap**
**E=0.28627 au = 7.79 eV**

**chlorofuran/ethylene reaction**

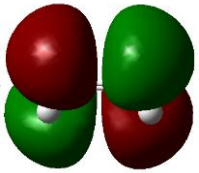




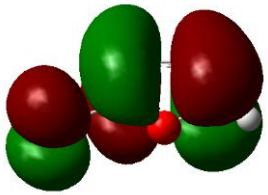
**LUMO**



**LUMO**



**HOMO**

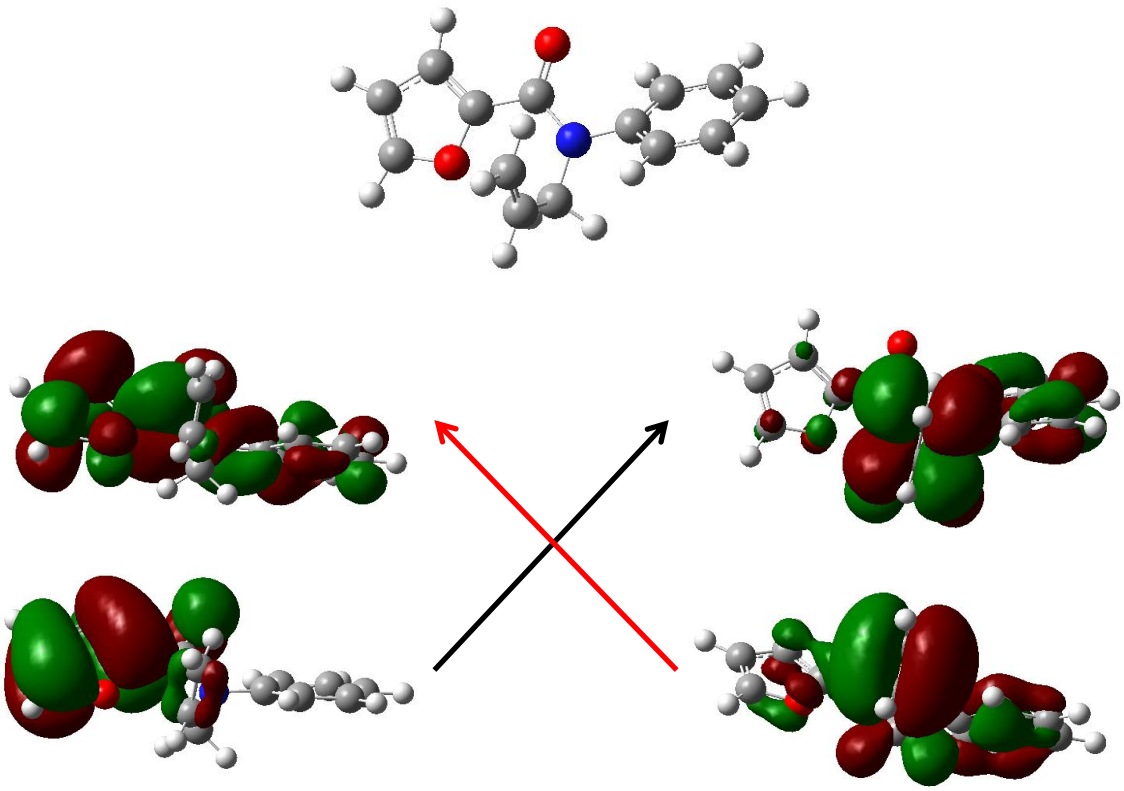


**HOMO**

**H/L gap**
**E=0.24668 au = 6.71 eV**

**H/L gap**
**E=0.2714 au = 7.39 eV**

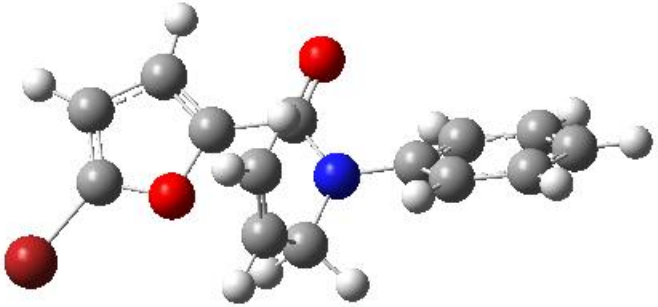
**Reaction 1a**

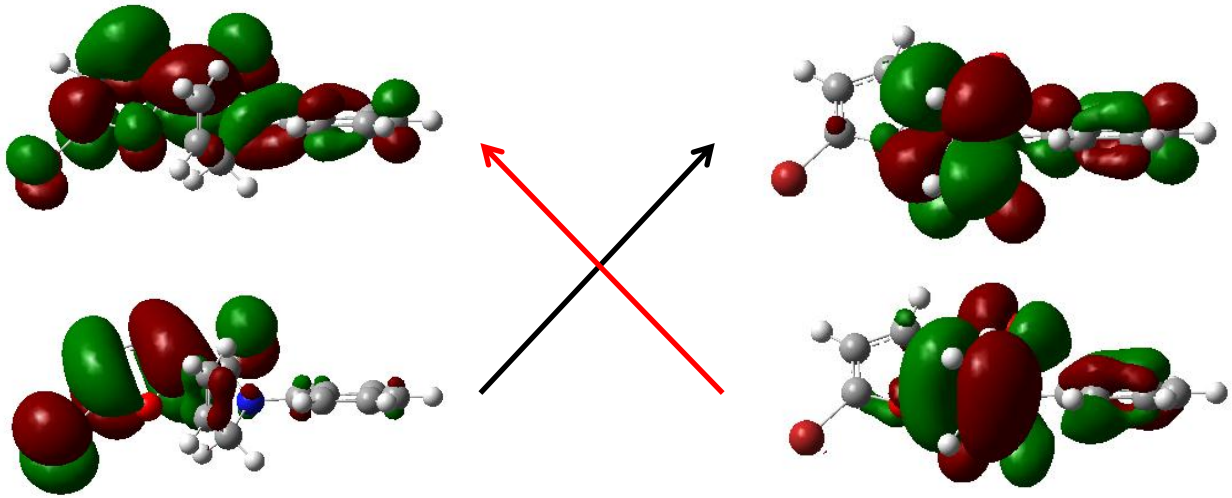


**H/L gap**
**E=0.25329 au = 6.89 eV**

**H/L gap**
**E=0.22915 au = 6.24 eV**

**Reaction 1b**

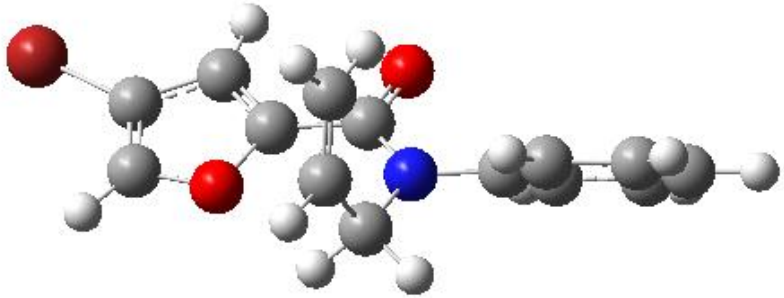


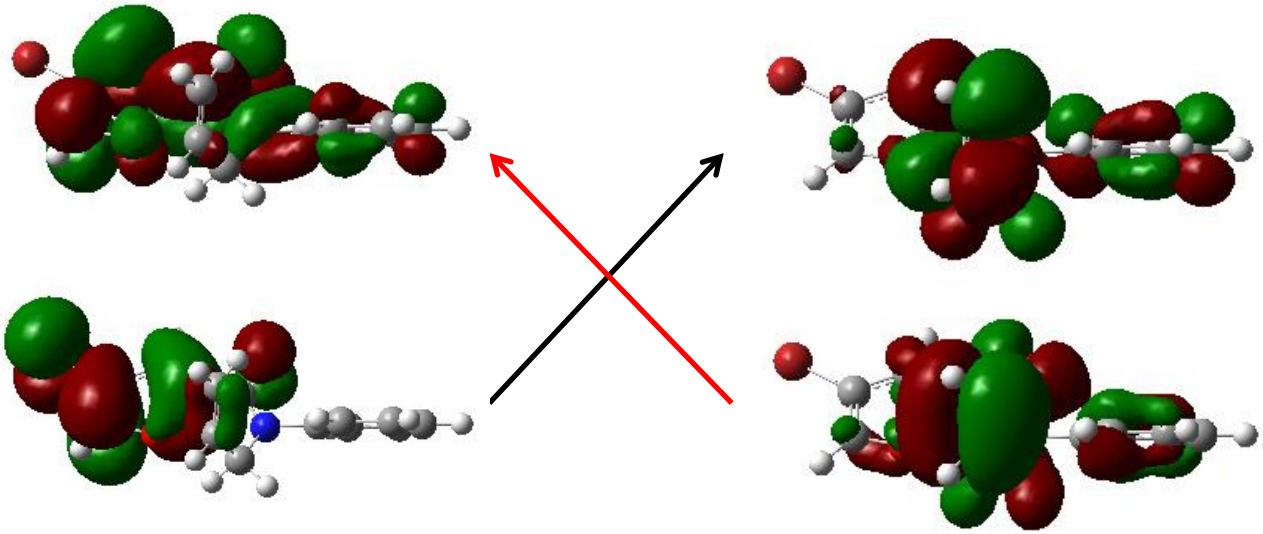


**H/L gap**
**E=0.25005 au = 6.8 eV**

**H/L gap**
**E=0.22425 au = 6.1 eV**

**Reaction 1c**

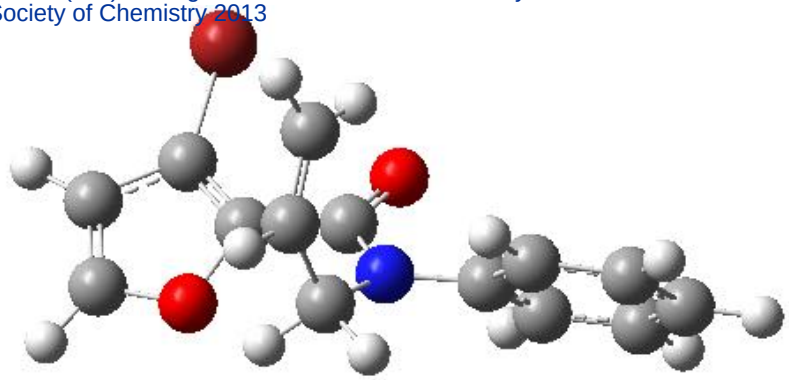


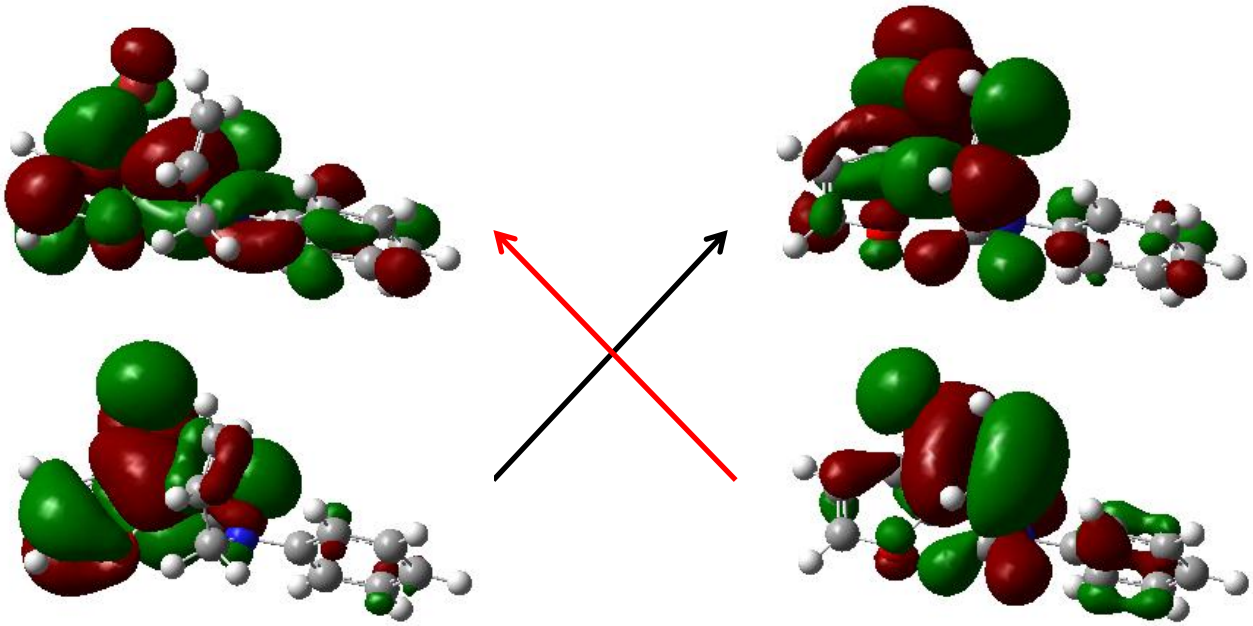


**H/L gap**
**E=0.25415 au = 6.92 eV**

**H/L gap**
**E=0.22507 au = 6.12 eV**

**Reaction 1d**

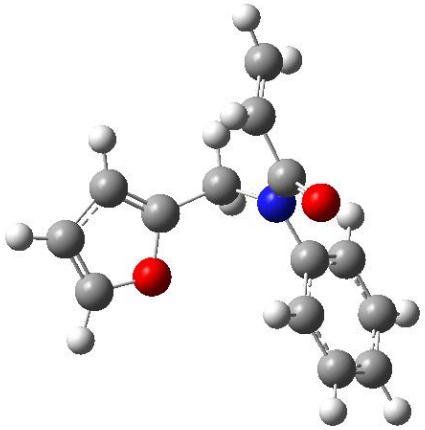


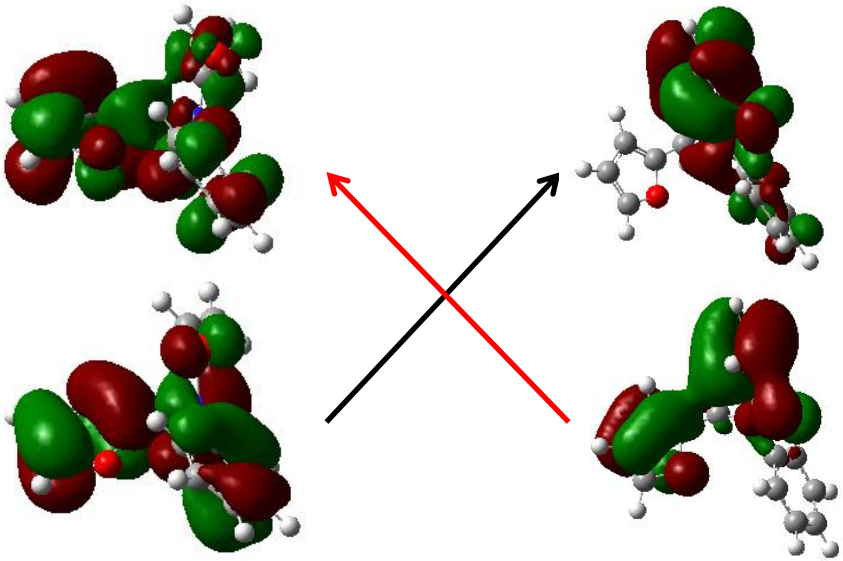


**H/L gap**
**E=0.25114 au = 6.83 eV**

**H/L gap**
**E=0.22484 au = 6.12 eV**

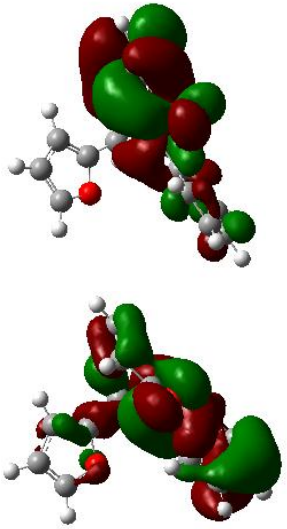
**Reaction 1e**





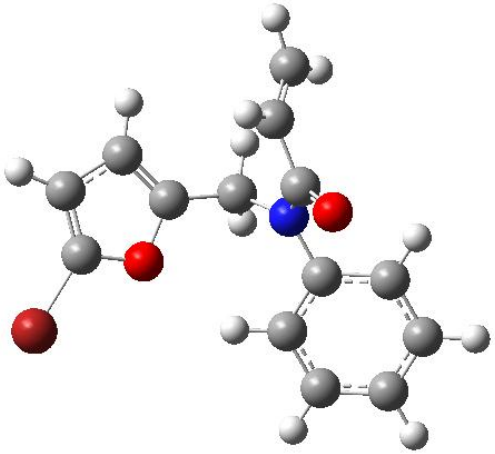
**H/L gap**
**E=0.19763 au = 5.38 eV**

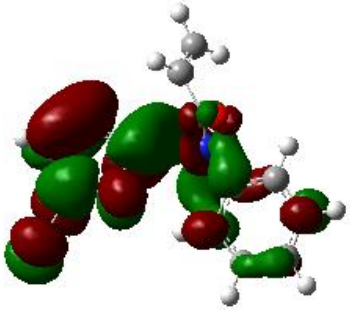
**H/L gap**
**E=0.29564 au = 7.76 eV**

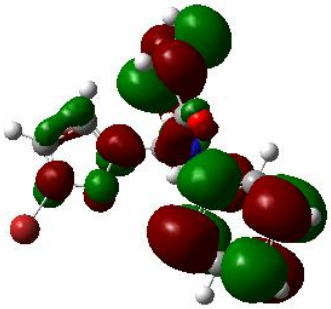


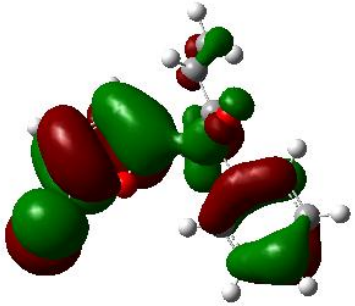
**H/L gap**
**E=0.27703 au = 7.25 eV**

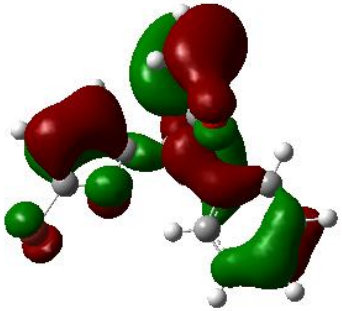
**Reaction 1f**







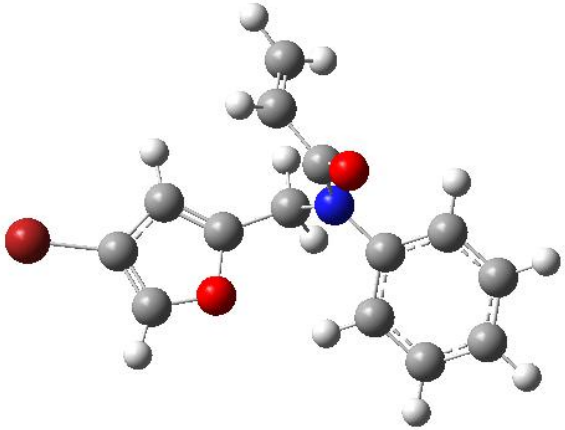


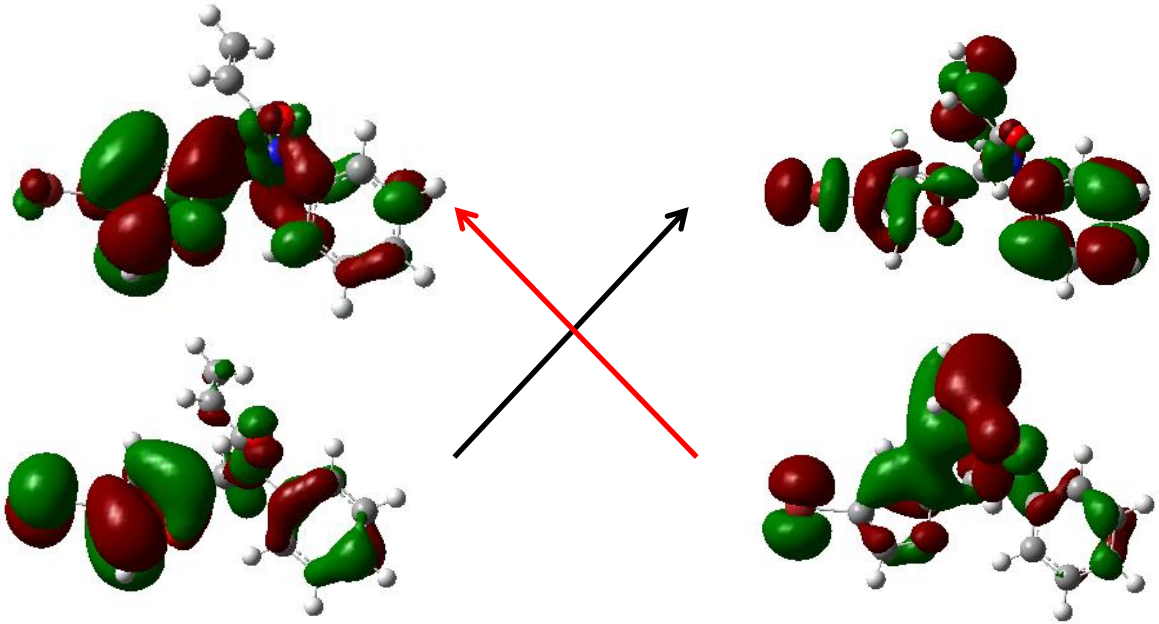


**H/L gap**
**E=0.23733 au = 6.46 eV**

**H/L gap**
**E=0.27522 au = 7.49 eV**

**Reaction 1g**

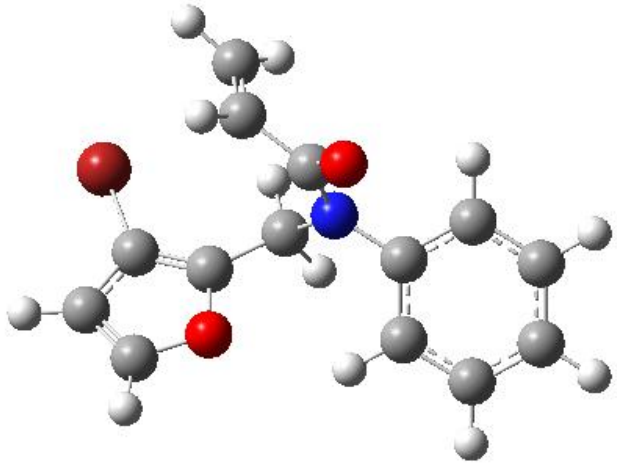


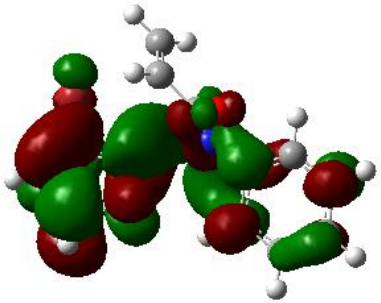


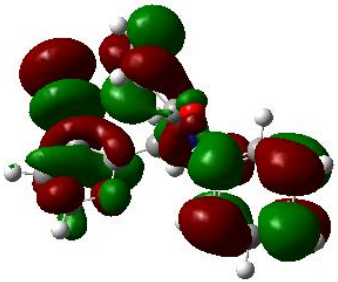
**H/L gap**
**E=0.24191 au = 6.58 eV**

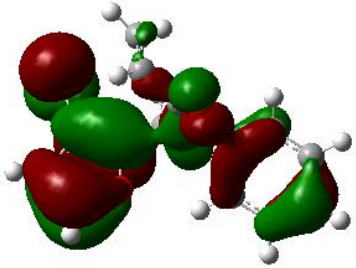
**H/L gap**
**E=0.27922 au = 7.6 eV**

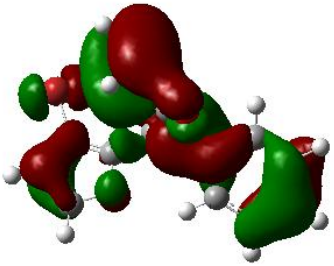
**Reaction 1h**







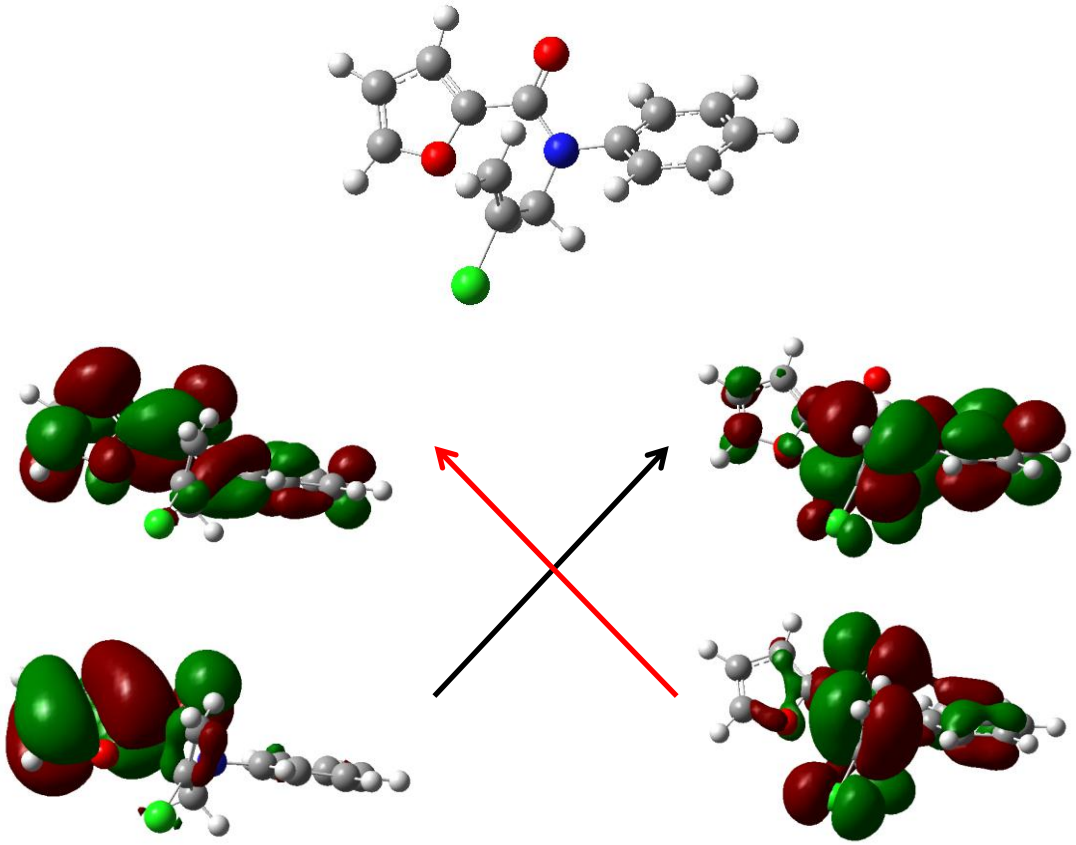




**H/L gap**
**E=0.24545 au = 6.68 eV**

**H/L gap**
**E=0.27246 au = 7.41 eV**

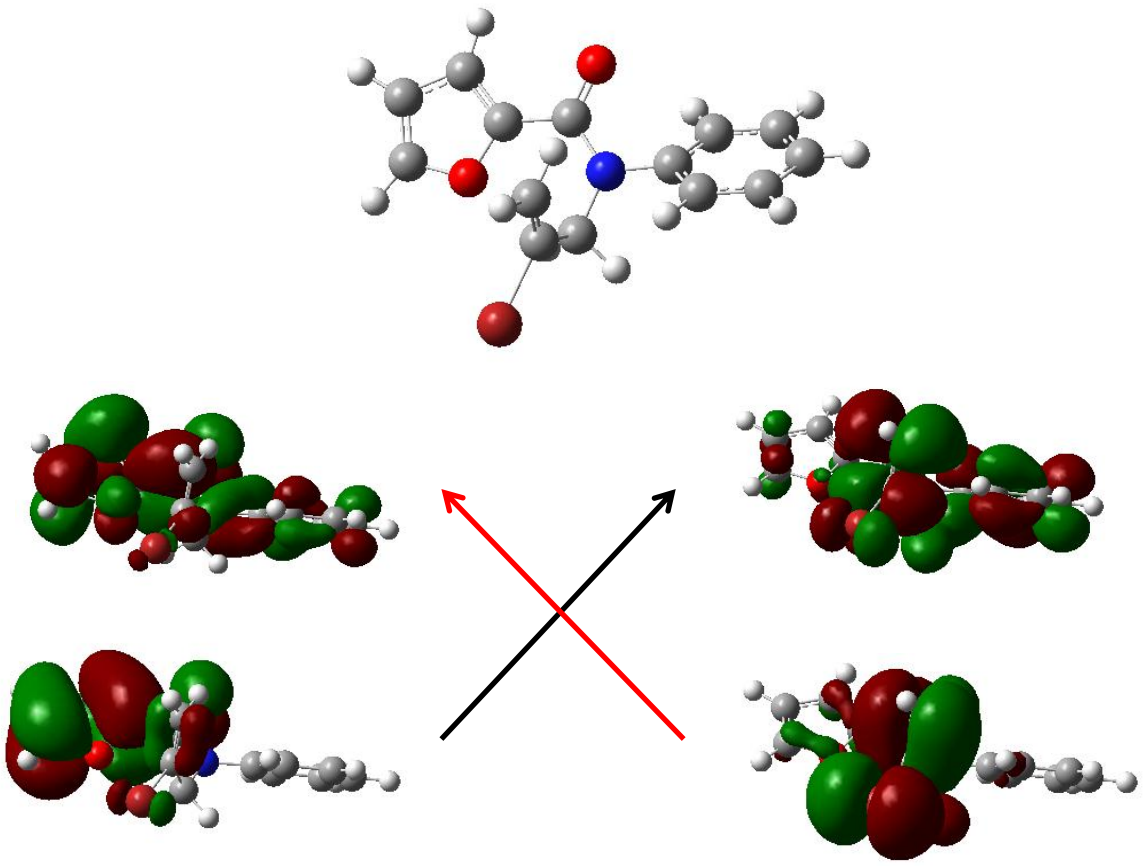
**Reaction 1i**



**H/L gap**
**E=0.24051 au = 6.55 eV**

**H/L gap**
**E=0.21775 au = 5.93 eV**

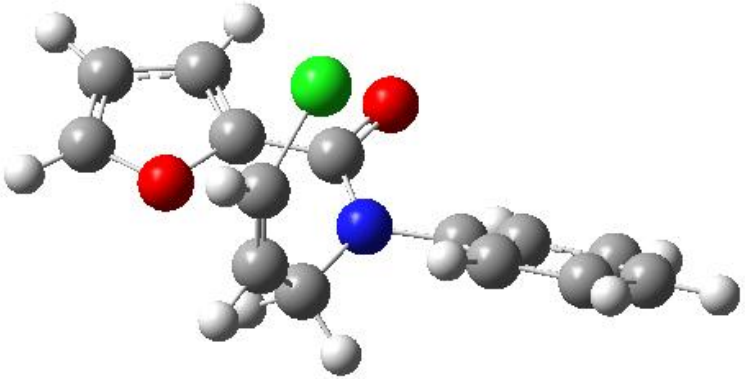
**Reaction 1j**

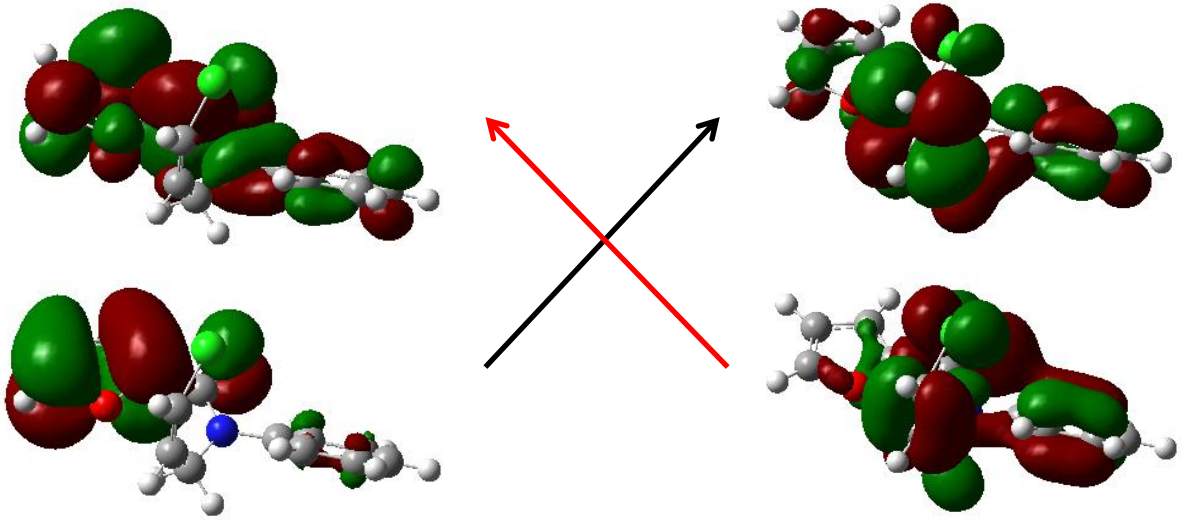


**H/L gap**
**E=0.23549 au = 6.41 eV**

**H/L gap**
**E=0.21314 au = 5.80 eV**

**Reaction 1k**

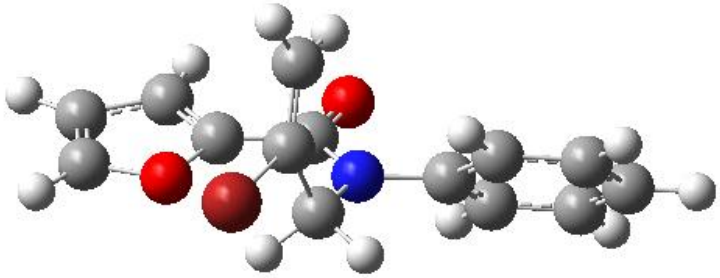


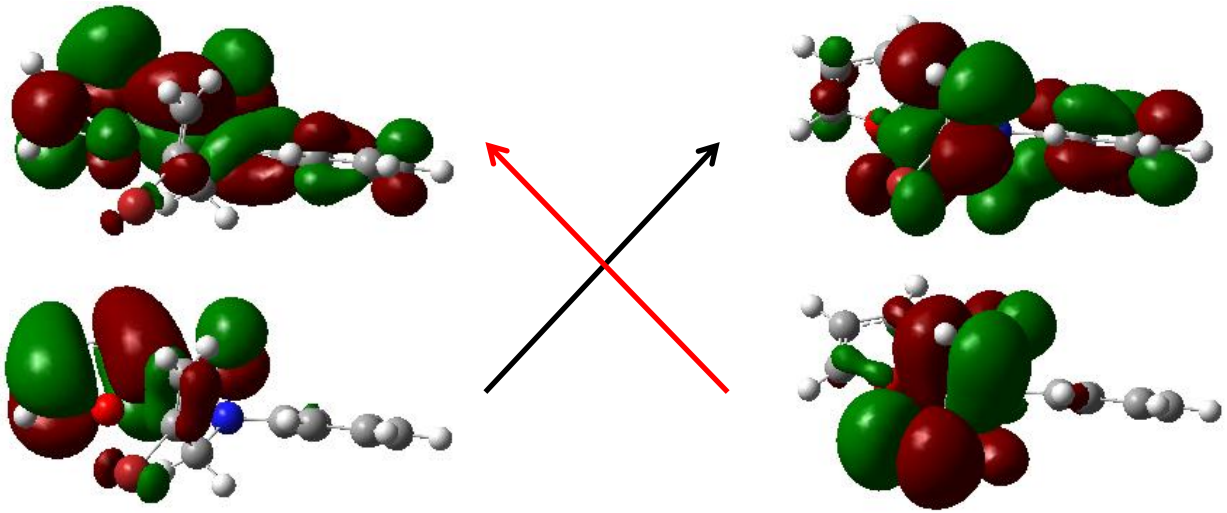


**H/L gap**
**E=0.23582 au = 6.42 eV**

**H/L gap**
**E=0.21972 au = 5.98 eV**

**Reaction 1l**

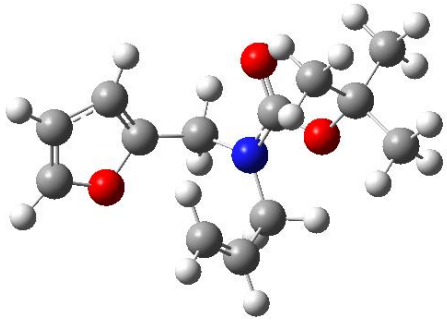


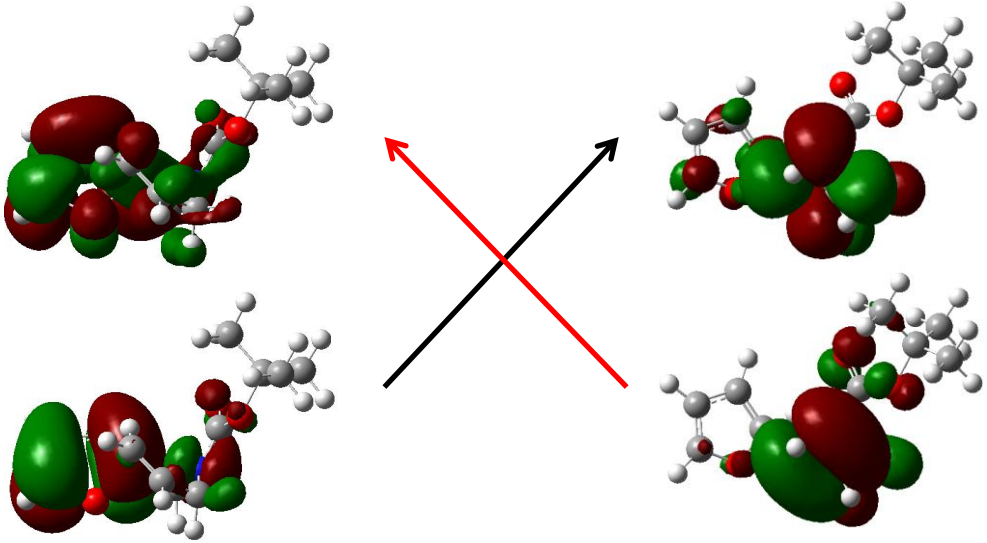


**H/L gap**
**E=0.23549 au = 6.41 eV**

**H/L gap**
**E= 0.21324 au = 5.80 eV**

**Reaction 1m**

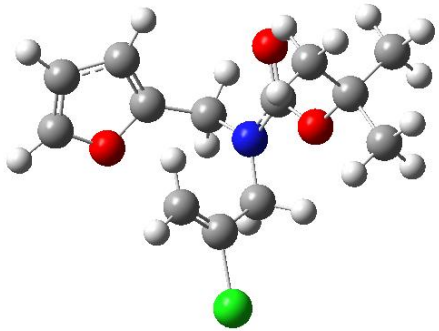


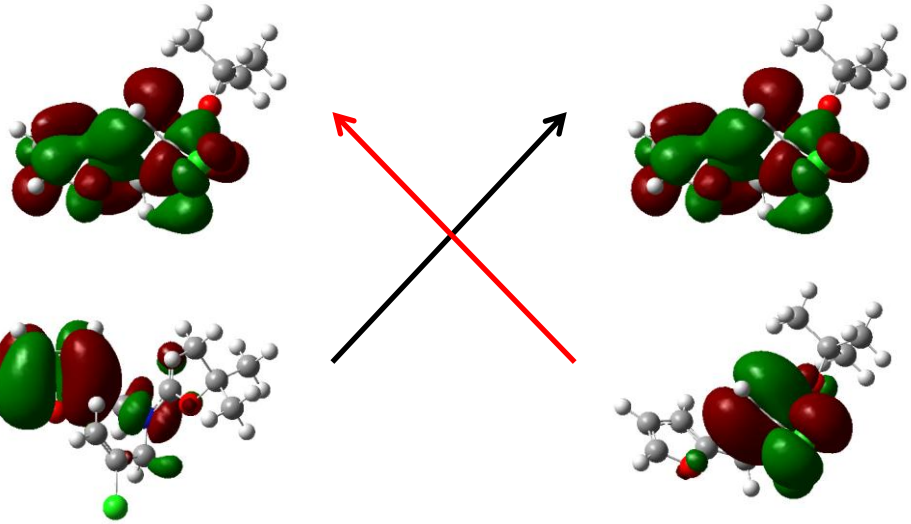


**H/L gap**
**E=0.24305 au = 6.61 eV**

**H/L gap**
**E=0.26673 au = 7.26 eV**

**Reaction 1n**

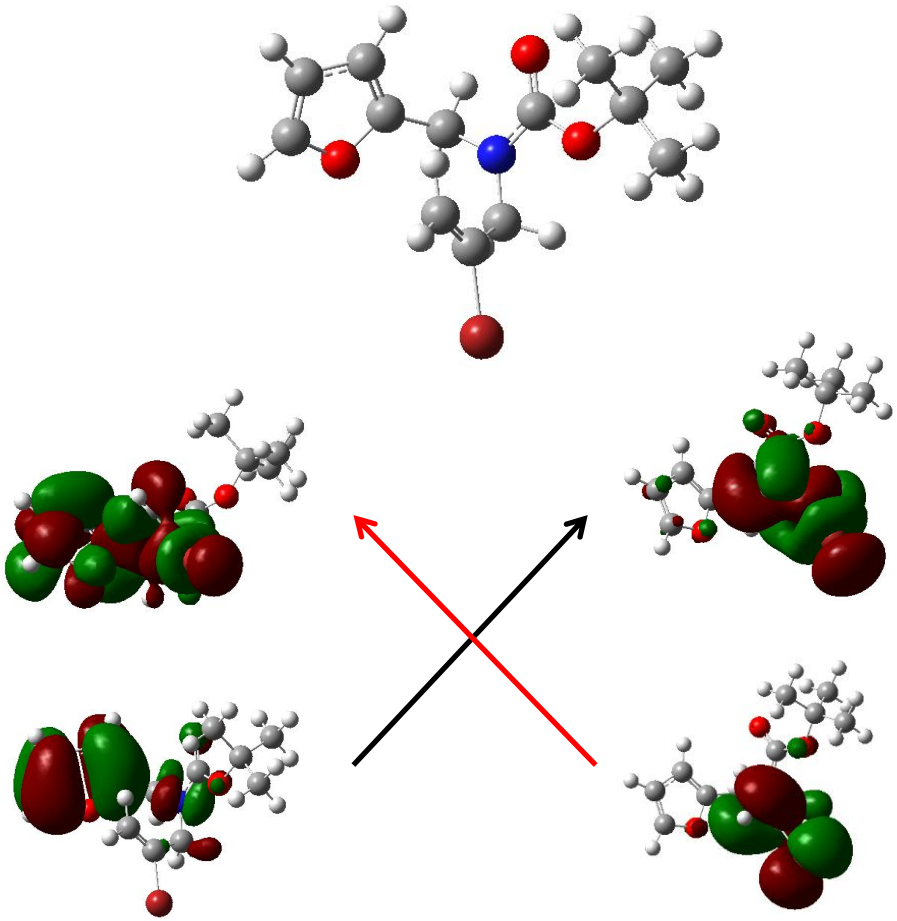




**H/L gap**
**E=0.2285 au = 6.22 eV**

**H/L gap**
**E=0.25913 au = 7.05 eV**

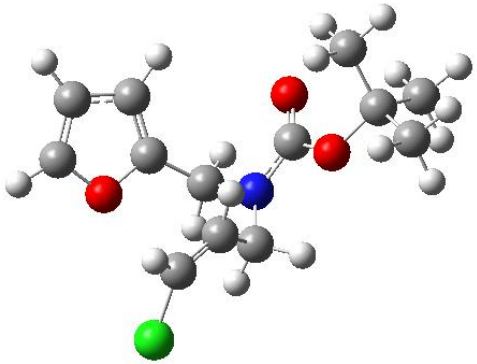
**Reaction 1o**

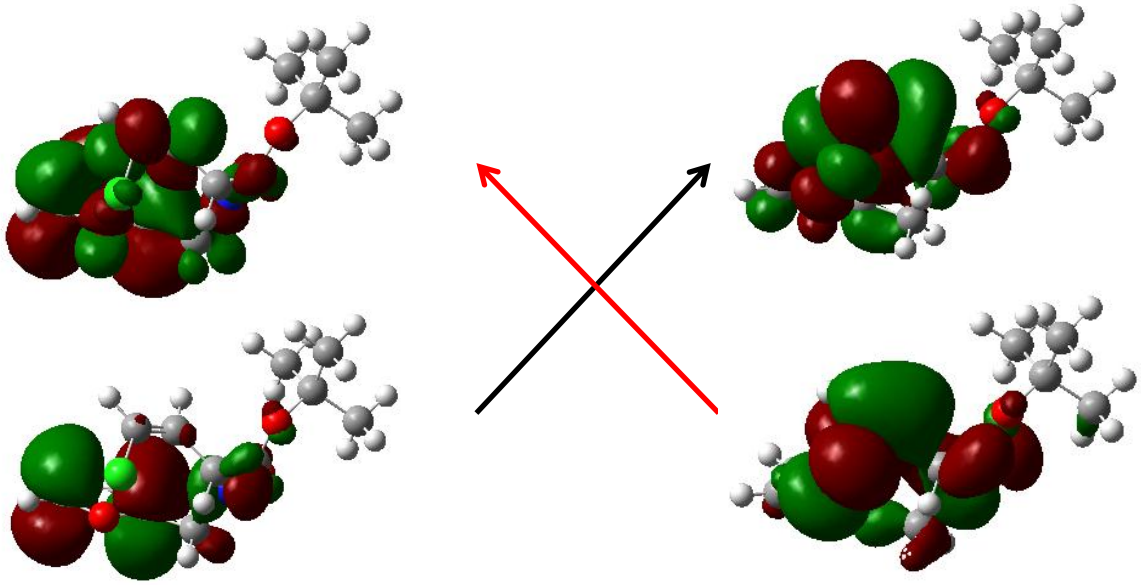


**H/L gap**
**E=0.22961 au = 6.25 eV**

**H/L gap**
**E=0.26053 au = 7.1 eV**

**Reaction 1p**

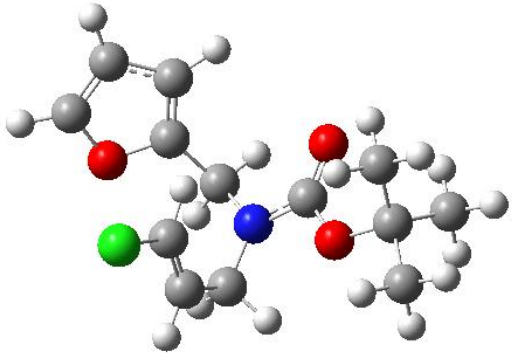


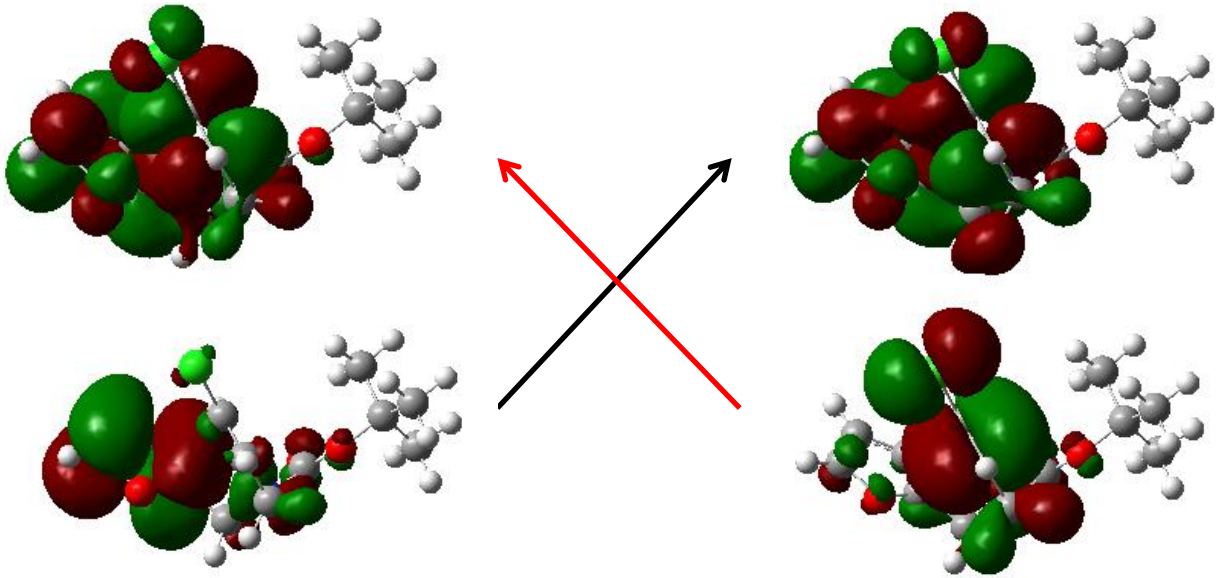


**H/L gap**
**E=0.21814 au = 5.94 eV**

**H/L gap**
**E=0.27387 au = 7.45 eV**

**Reaction 1q**

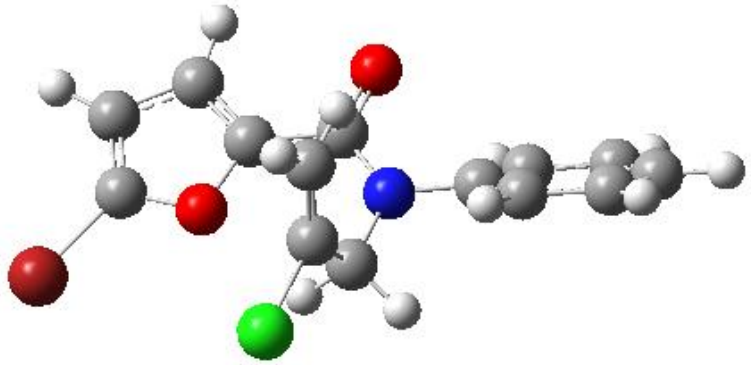


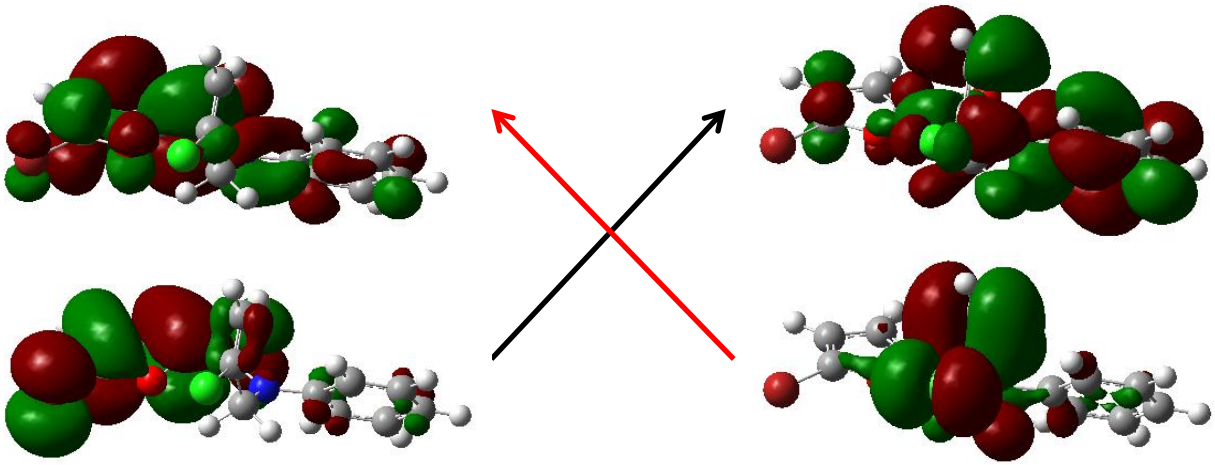


**H/L gap**
**E=0.22908 au = 6.23 eV**

**H/L gap**
**E=0.2595 au = 7.06 eV**

**Reaction 1r**

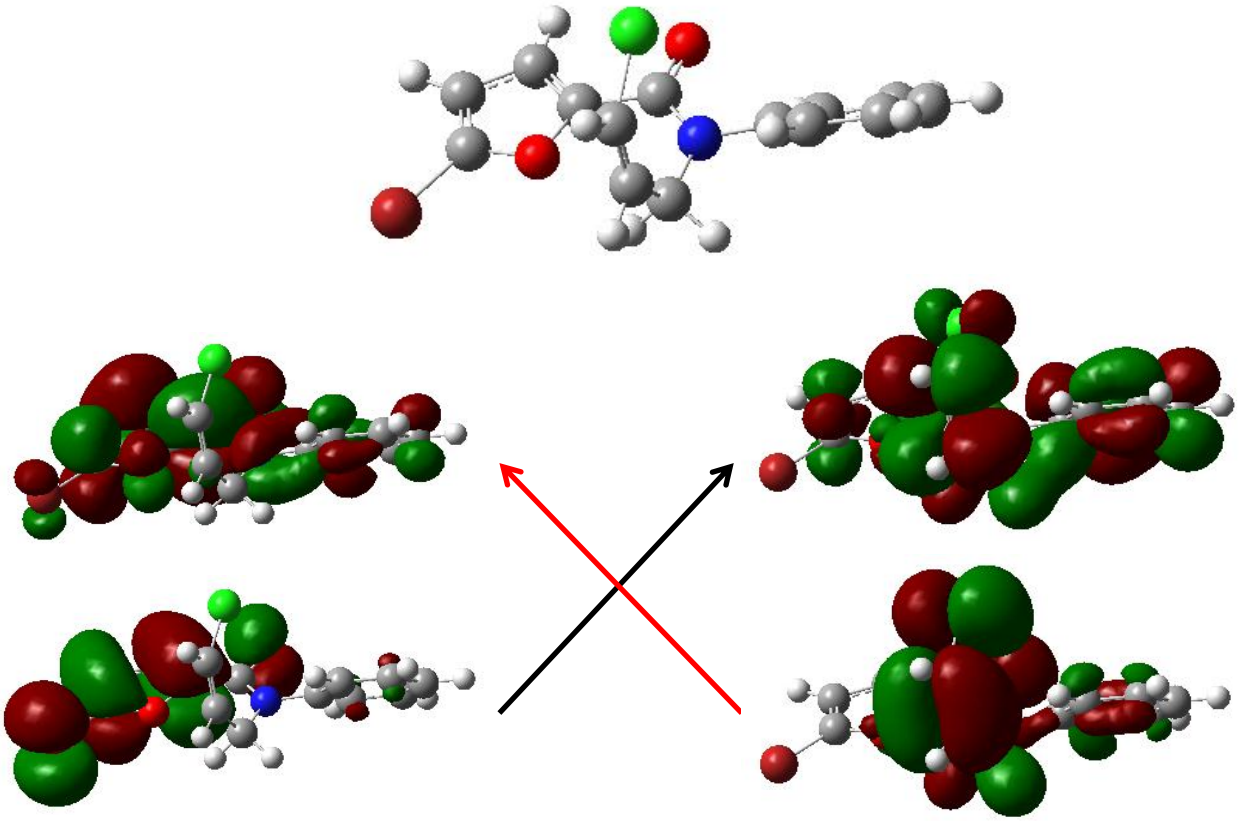




**H/L gap**
**E=0.23503 au = 6.40 eV**

**H/L gap**
**E=0.21341 au = 5.81 eV**

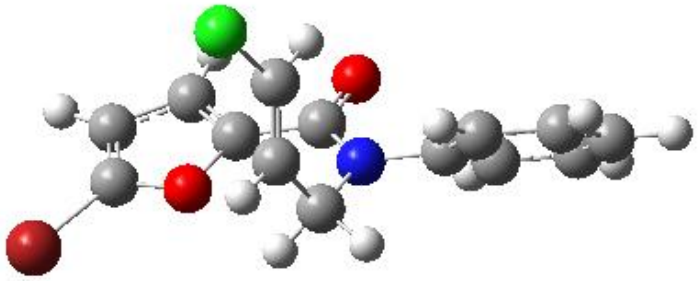
**Reaction 1s**

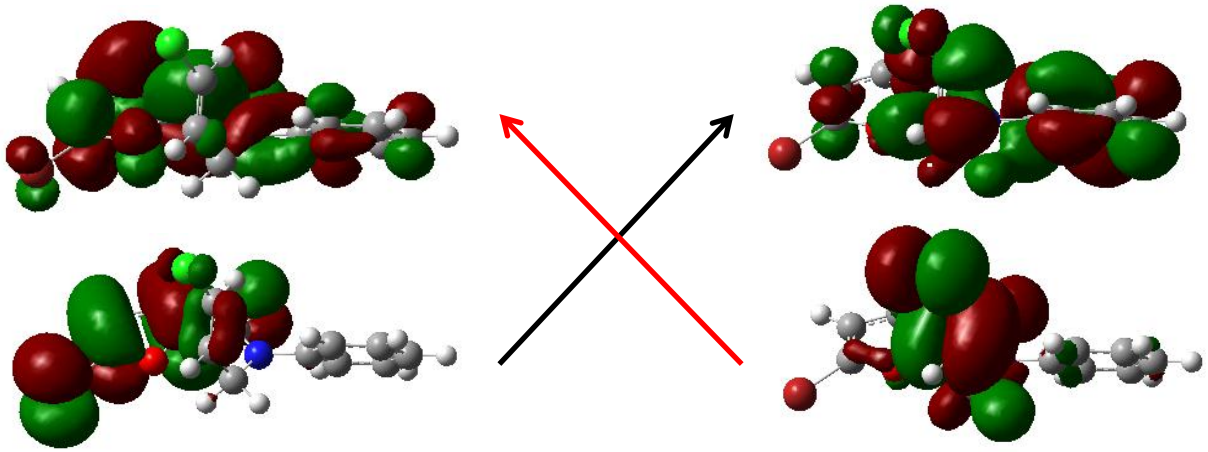


**H/L gap**
**E=0.23563 au = 6.41 eV**

**H/L gap**
**E=0.21534 au = 5.86 eV**

**Reaction 1t**

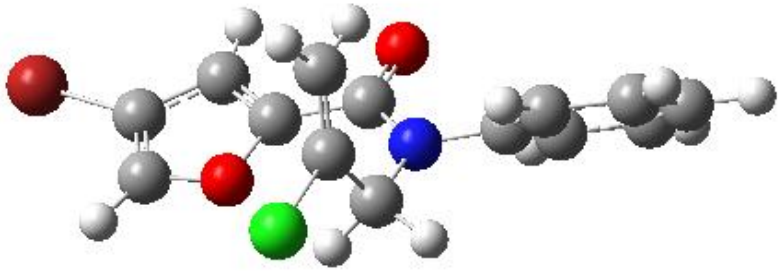


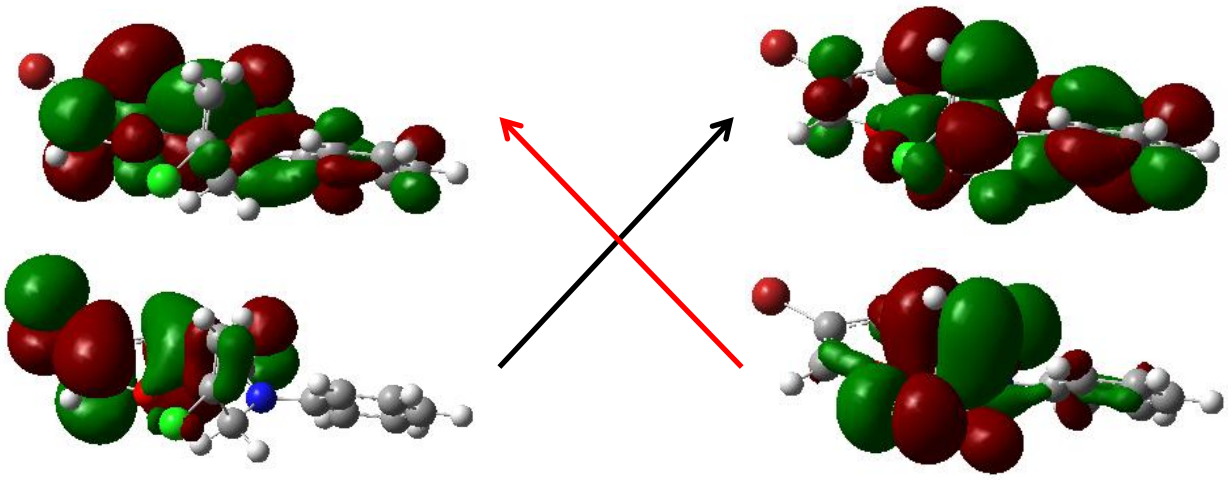


**H/L gap**
**E=0.23589 au = 6.42 eV**

**H/L gap**
**E=0.20876 au = 5.68 eV**

**Reaction 1u**

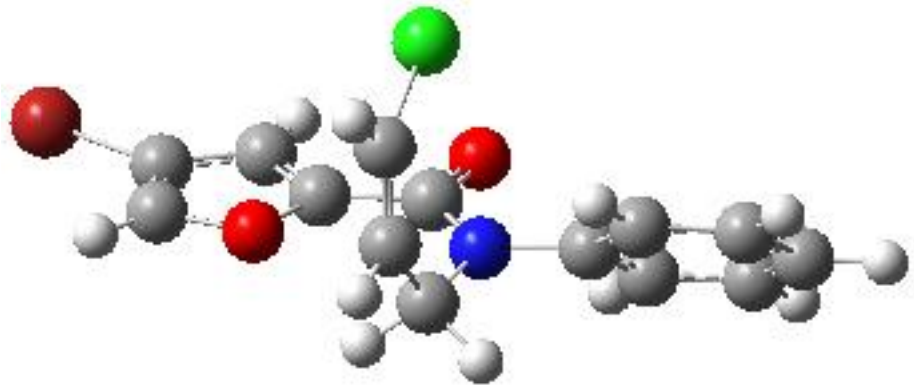


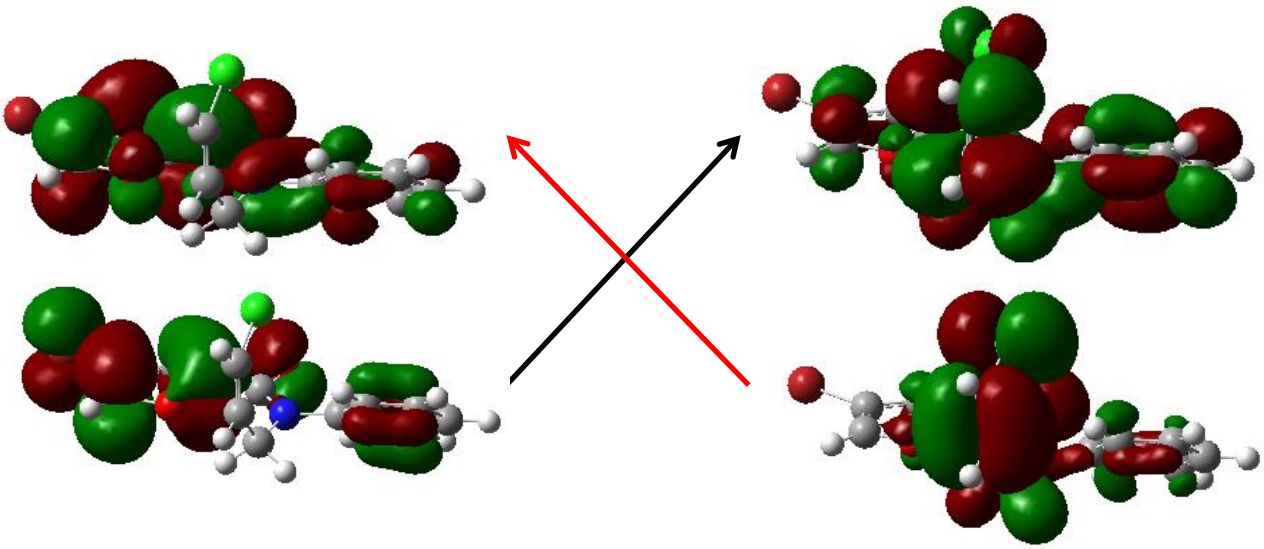


**H/L gap**
**E=0.23953 au = 6.52 eV**

**H/L gap**
**E=0.21344 au = 5.81 eV**

**Reaction 1v**

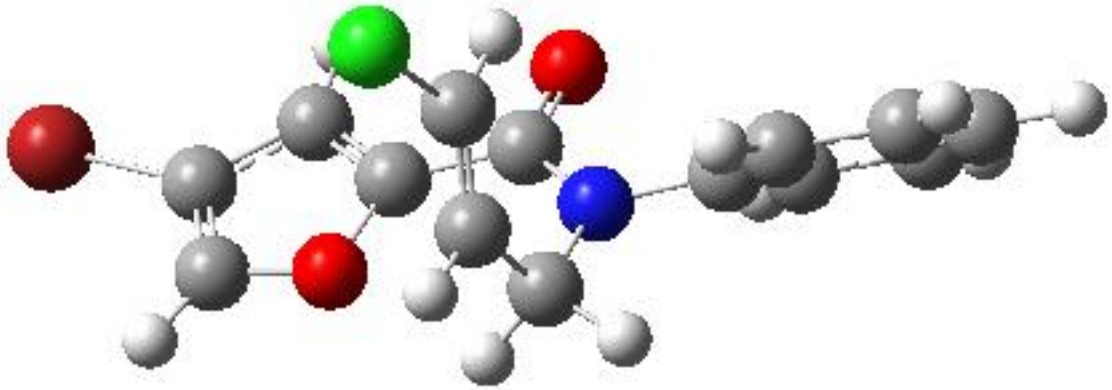


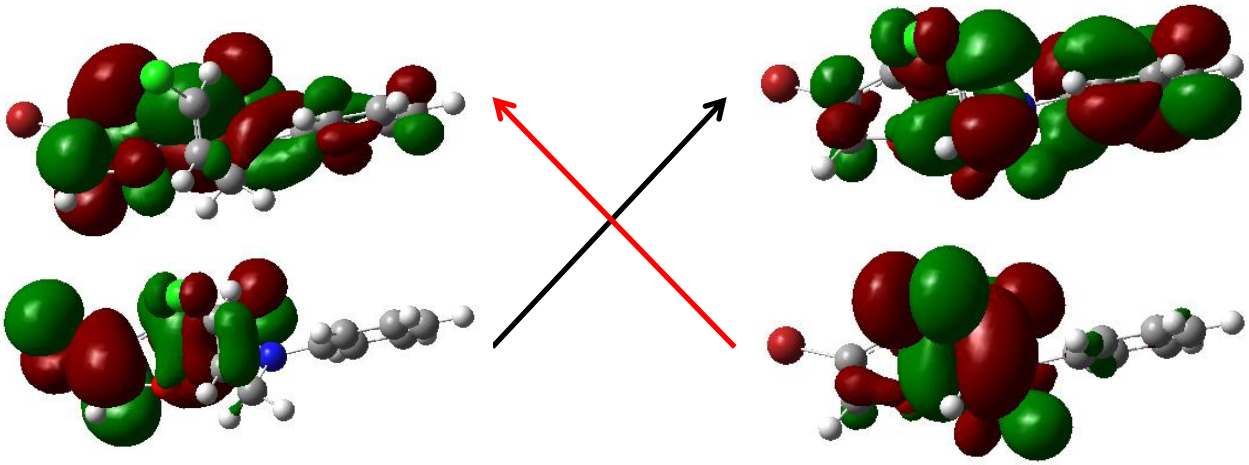


**H/L gap**
**E=0.23872 au = 6.50 eV**

**H/L gap**
**E=0.21573 au = 5.87 eV**

**Reaction 1w**

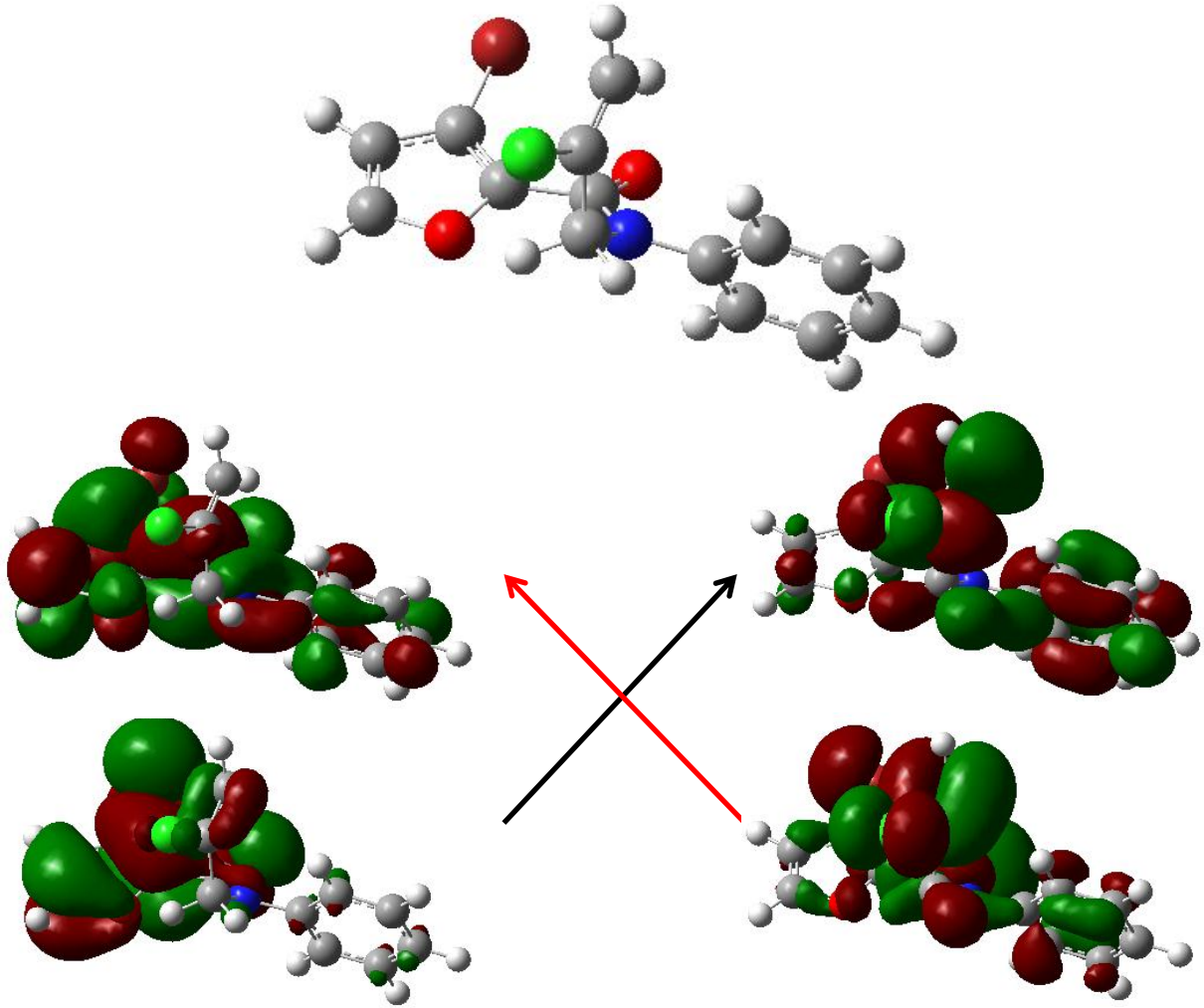




**H/L gap**
**E=0.2402 au = 6.54 eV**

**H/L gap**
**E=0.2087 au = 5.68 eV**

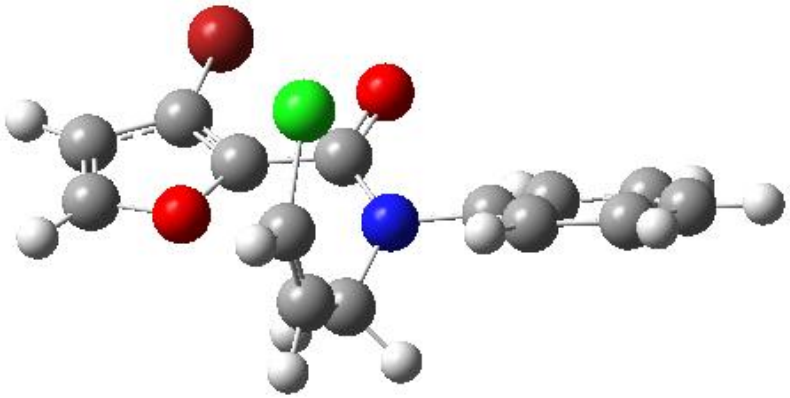
**Reaction 1x**

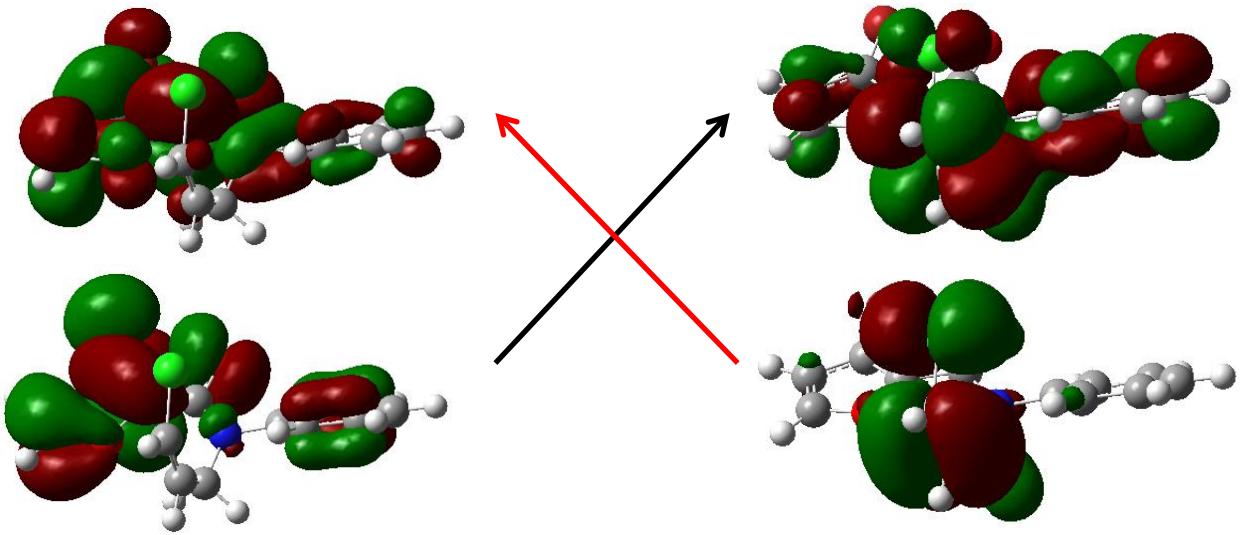


**H/L gap**
**E=0.23893 au = 6.50 eV**

**H/L gap**
**E=0.20892 au = 5.69 eV**

**Reaction 1y**

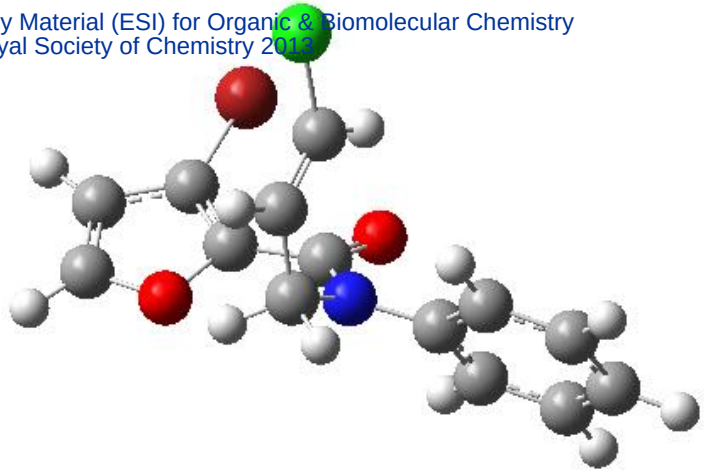


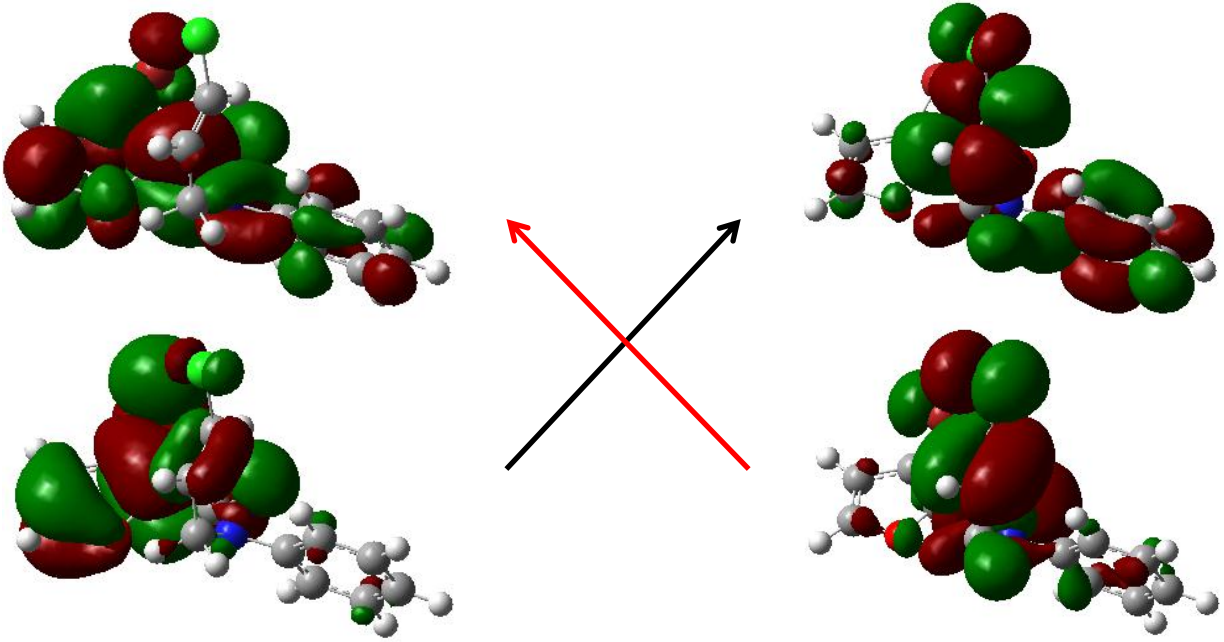


**H/L gap**
**E=0.23399 au = 6.37 eV**

**H/L gap**
**E=0.21482 au = 5.85 eV**

**Reaction 1z**





**H/L gap**
**E=0.23862 au = 6.49 eV**

**H/L gap**
**E=0.20565 au = 5.60 eV**