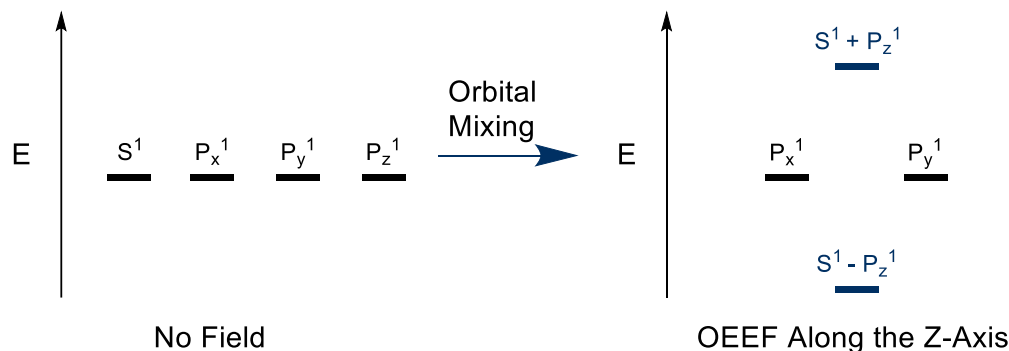


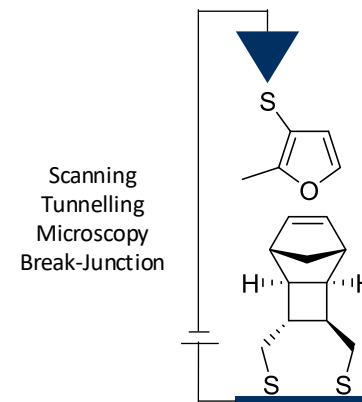
Background

- In the presence of an oriented external electric field (OEEF) **molecular symmetry is broken** which allows for orbital mixing that is forbidden in the absence of the field.¹



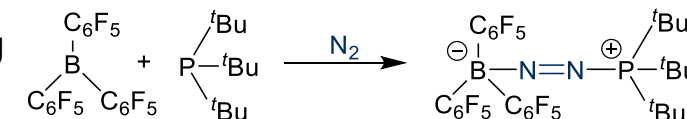
- In homopolar bonds this results in **field-dependent ionicity** and **bond elongation**. In heteropolar bonds, elongation or shortening can be observed due to the **changing covalent/ionic nature** of the bond.¹
- An OEEF applied along the direction in which electrons undergo reorganisation in the transition state (the reaction-axis) can **catalyse or inhibit** a reaction depending on the field polarity.¹
- In some cases, the orientation of the OEEF can be used **to control regioselectivity or stereoselectivity**.¹
- Many ways of inducing an electric field including the use of **STM** techniques, **interfacial-electric fields** and the inclusion of **ions** to the system.¹

Examples



An increase in the Diels-Alder reaction rate is seen when an electric field is aligned to the reaction-axis in the orientation that allows electron movement from dienophile to diene.²

Without an OEEF the N_2 activation is highly endergonic with a large barrier. In a strong OEEF the reaction becomes exergonic with a greatly reduced barrier.³



Availability

- Available in ORCA using the keyword **EField** and in Gaussian using the keyword **Field**.
- Can calculate properties such as single point energies, optimised geometries, transitions states and frequencies.