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Molecular Parity Violation.

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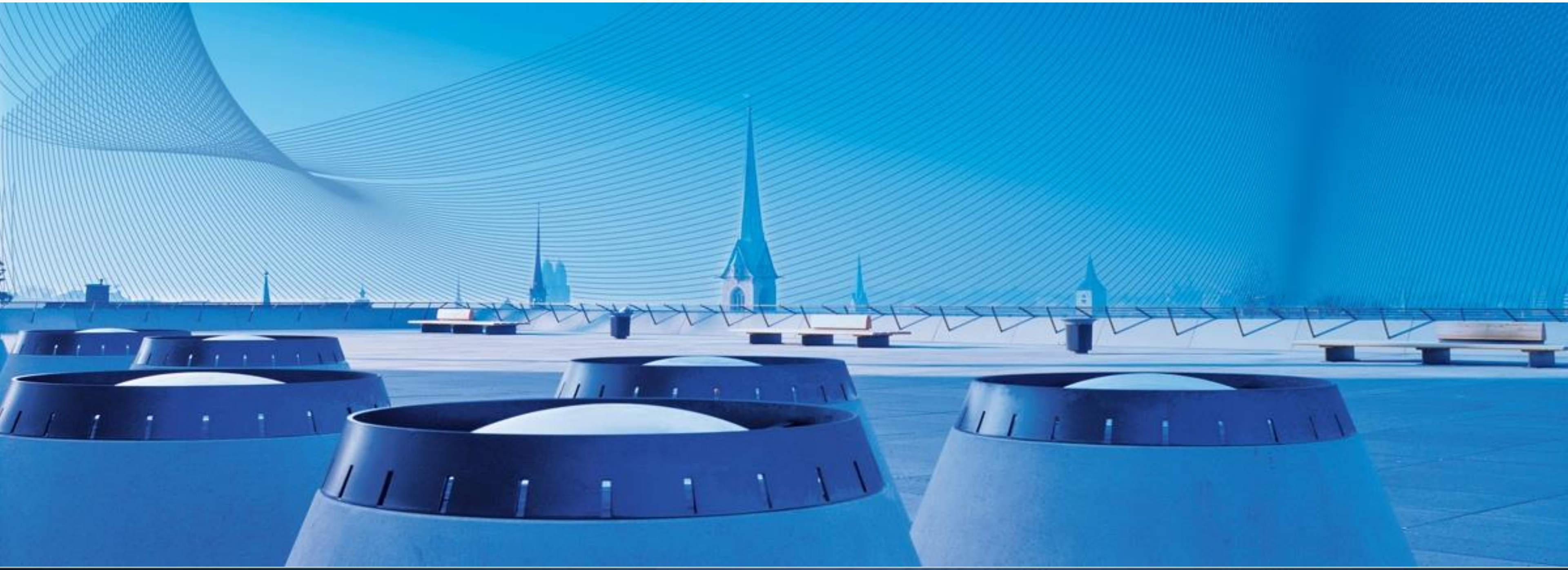
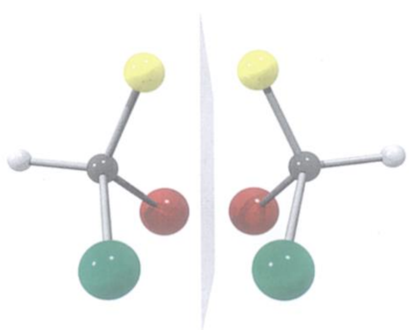


Parity violation: ***i)*** **arises when parity operator P does not commute any more with the Hamiltonian of the system**

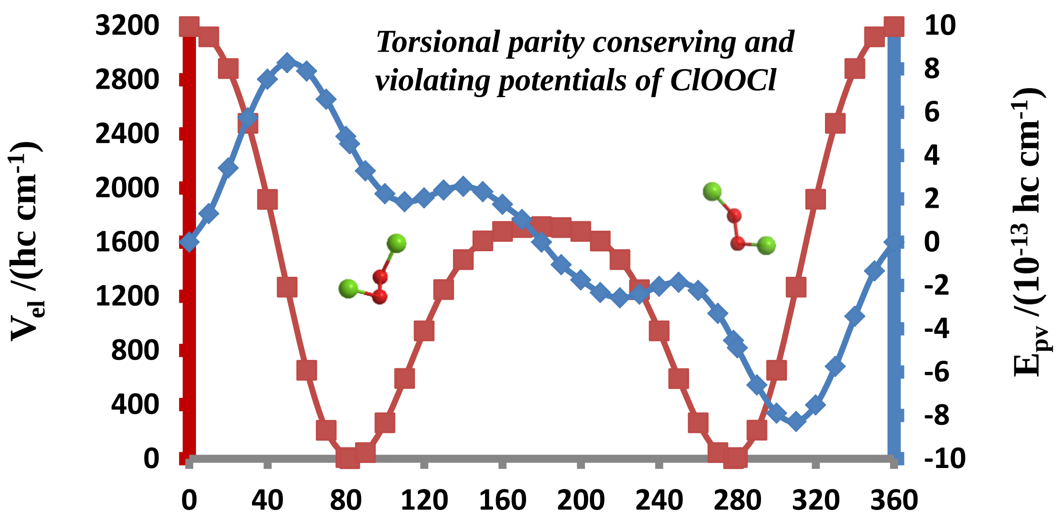
ii) **electroweak interaction does not conserve symmetry – this** ***parity violationg*** **effect has been measured and calculated very accurately for forbidden atomic transitions confirming the Standard model in particle physics to high precision.**

iii) **From the Standard model, it is also accepted that parity violation leads to small energy difference and different spectra between enatiomers of chiral molecules.**



$N_A \cdot \Delta_{PV}E \approx 10^{-11\pm3}$ J mol^{-1}

$\Delta_{PV}E \approx 10^{-16}$ eV



Molecular parity violating Hamiltonian (nonrelativistic limit).

$$\hat{H}_{pv}^{e-nucl} = \frac{G_F \alpha}{2\sqrt{2}} \sum_{i=1}^{n} \sum_{A=1}^{N} \Big[Q_W(A) \{ \hat{\vec{p}}_i \, \hat{\vec{s}}_i, \delta^3(\vec{r}_i - \vec{r}_A) \}_+$$

$$+ (-\lambda_A) \left(1 - 4\sin^2\theta_W\right) \{ \hat{\vec{p}}_i \, \hat{\vec{I}}_A, \delta^3(\vec{r}_i - \vec{r}_A) \}_+$$

$$+ 2i\lambda_A (1 - 4\sin^2\theta_W) \times (\hat{\vec{s}}_i \times \hat{\vec{I}}_A) \, [\hat{\vec{p}}_i, \delta^3(\vec{r}_i - \vec{r}_A)] \Big]$$

i) **Major contribution comes from nuclear spin independent part.**
ii**) It is purely imaginary operator and gives zero expectation value for nonrelativistic real wavefunction.**
iii) **The parity violating energy is calculated as a static linear response function.**

$G_F = 2.222\ 54 \times 10^{-14}\ E_h$ Fermi constant
α fine structure constant
$Q_w(A) = Z_A(1 - 4\sin^2\theta_w) - N_A$
Z_A number of protons in nucleus A
N_A number of neutrons in nucleus A
$\sin^2\theta_w = 0.2319$ Weinberg angle

Parity violating potential E_{pv} as a static response function.

Parity-violating operator
$$\hat{H}_{pv}^{e-nucl} = \frac{G_F \alpha}{2\sqrt{2}} \sum_{i=1}^{n} \sum_{i=1}^{A} Q_w(A) \{ \hat{\vec{p}}_i \, \hat{\vec{s}}_i , \delta^3(\vec{r}_i - \vec{r}_A) \}_+$$

Effective Spin-orbit
coupling operator
$$\hat{H}_{SO} = \frac{\alpha^2}{2} \left[\sum_{i=1}^{n} \sum_{A=1}^{N} \eta_A Z_A \frac{\hat{\vec{l}}_{i,A} \, \hat{\vec{s}}_i}{\left| \vec{r}_A - \vec{r}_i \right|^3} \right]$$

$$\longrightarrow \quad E_{pv} = \langle\langle \hat{H}_{pv} ; \hat{H}_{SO} \rangle\rangle$$

Thank you !