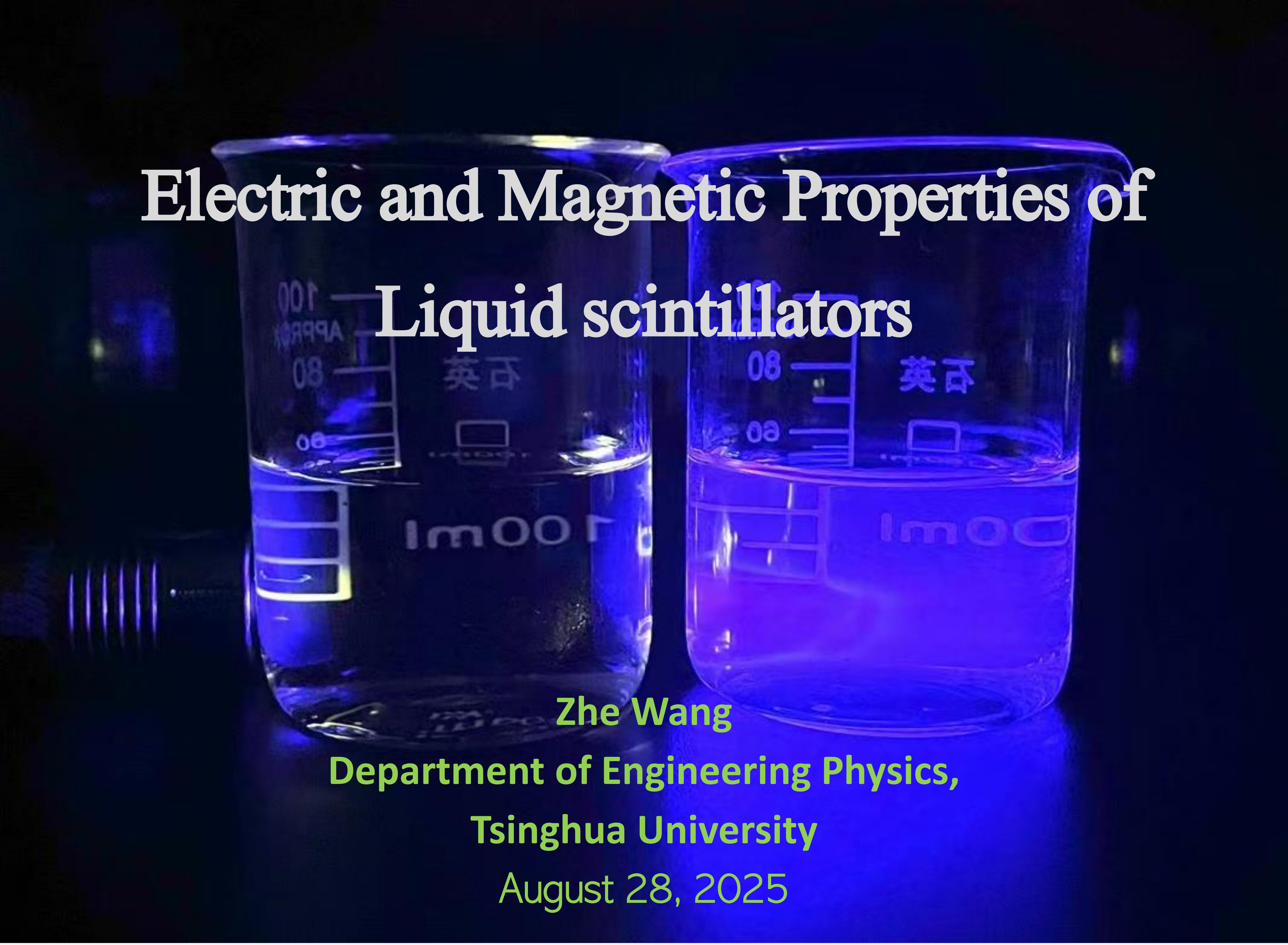

Electric and Magnetic Properties of Liquid scintillators

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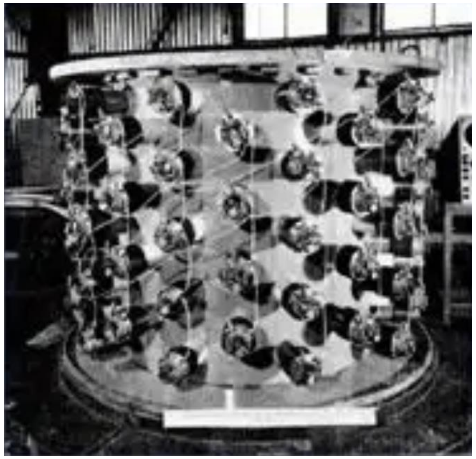
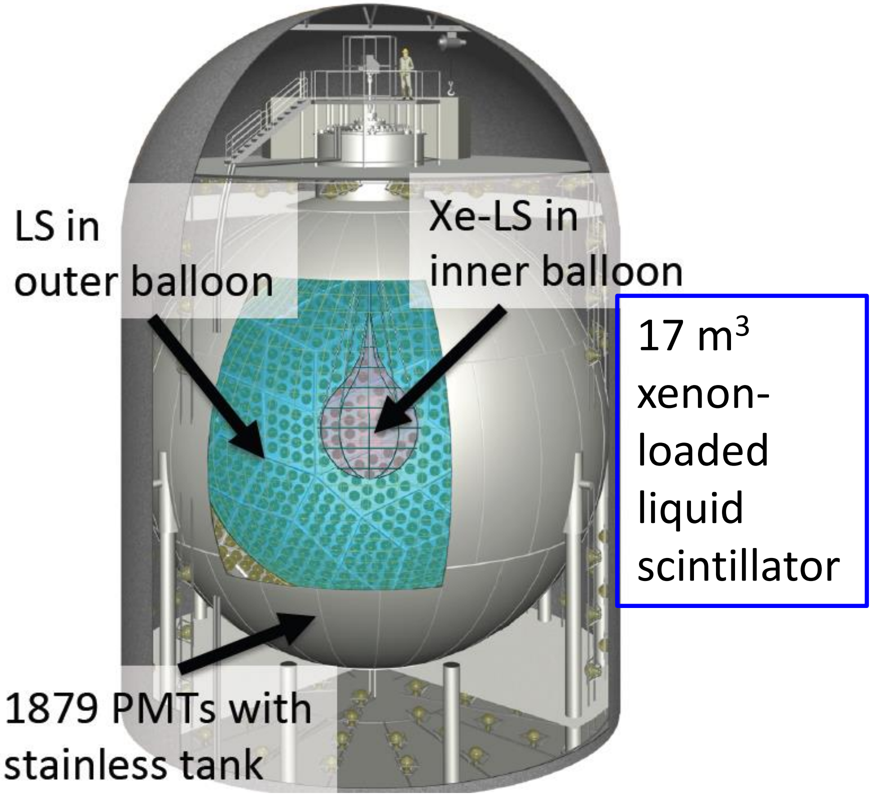
Motivation

- Widely used in high energy physics experiments



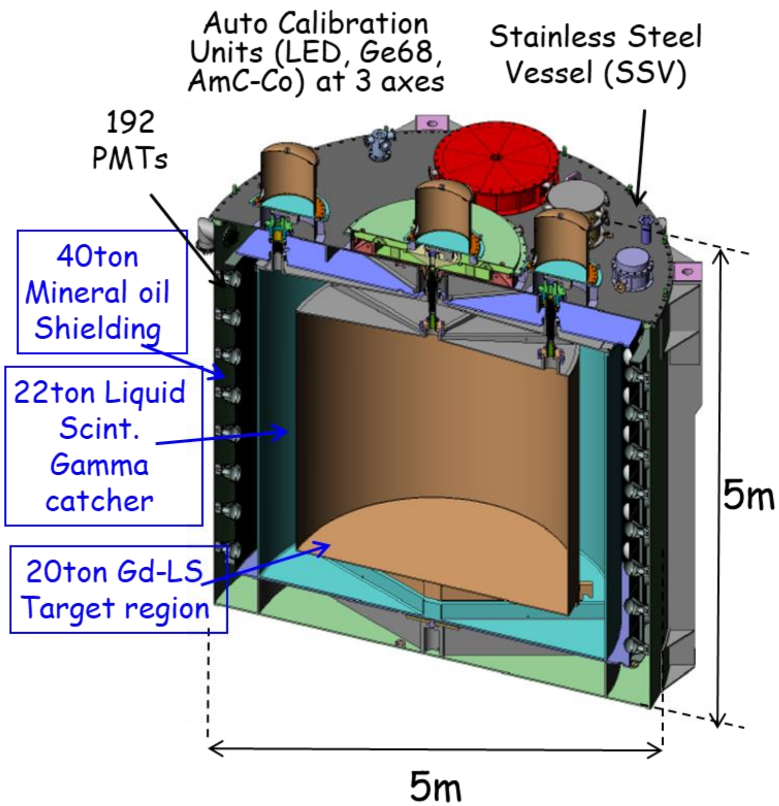
Reines and Cowan 1956 Liquid scintillator for neutrino detection



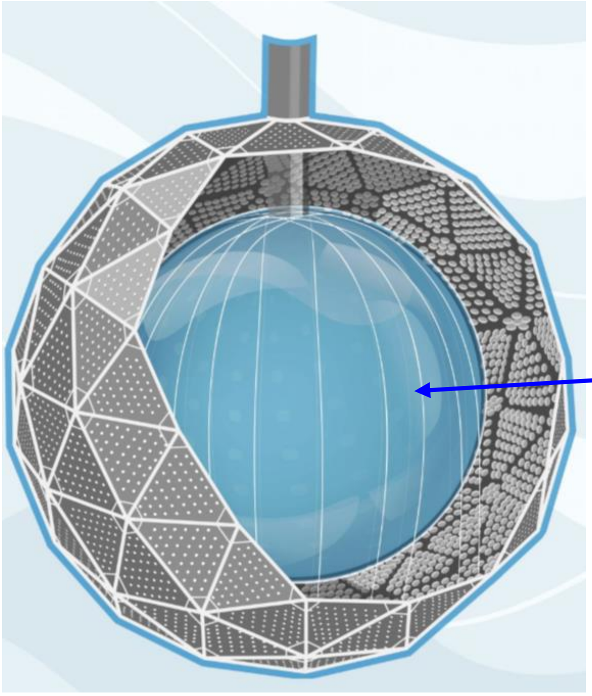
KamLAND-Zen

Motivation

- Widely used in high energy physics experiments



Daya Bay Experiment



SNO+

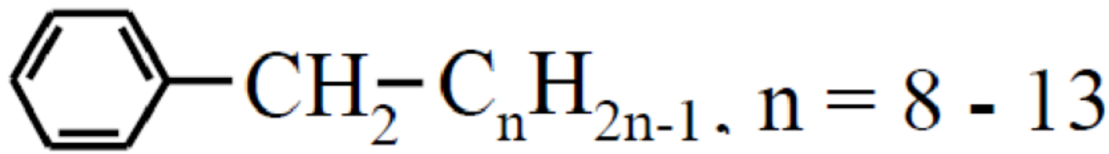
Scope: two-component liquid scintillator

- Two component liquid scintillator
  - The 1st component: solvent, absorb radiation energy, give short-wavelength scintillation light, dominant in mass and volume, Donor
  - The 2nd component: solute, wavelength shifter (absorb the short-wavelength emission from the 1st component and emit long-wavelength scintillation light), minor in mass and volume, Acceptor

LAB	PPO
Linear alkylbenzene	2,5-diphenyloxazole
Dominant in mass	3 g/L
Emission around 380 nm	Absorb at 380 nm; Emission at 430 nm
1st component	2nd component

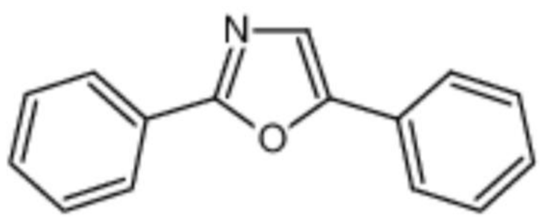
Two-component Liquid scintillator

- LAB



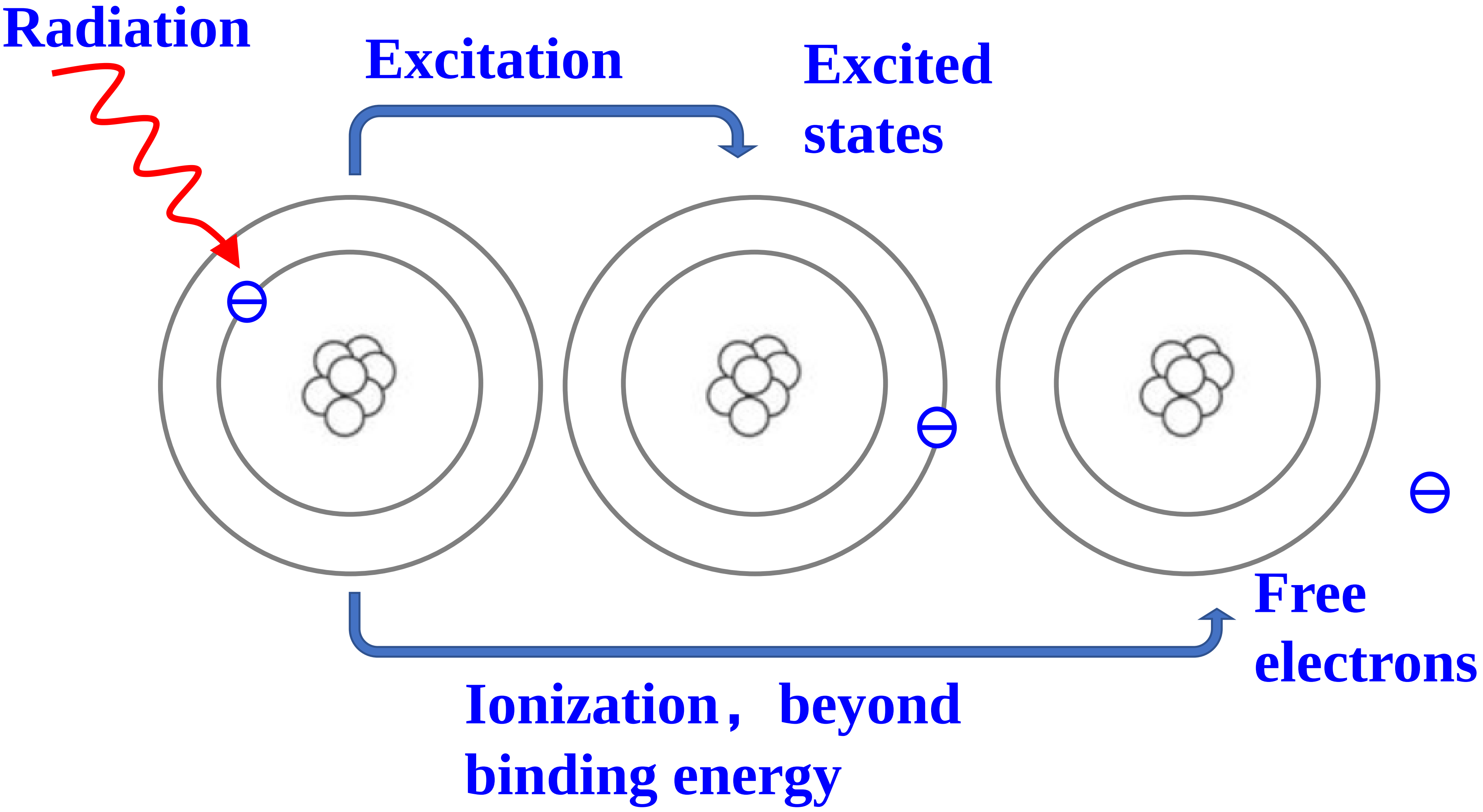
Liquid emission group, 1st component, Donor

- PPO



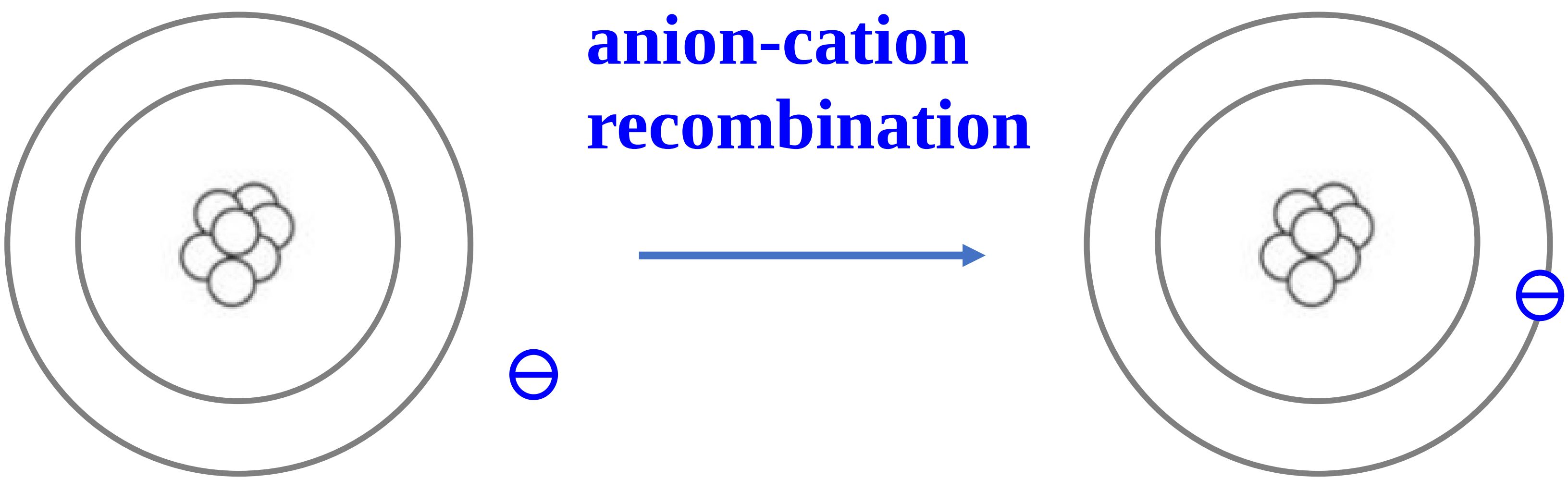
Wavelength shifter, 2nd component, Acceptor

Energy deposition by radiation



Energy deposition by radiation

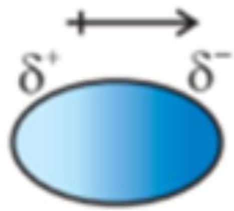
- 1st component, donor (D)
  - Absorb all the initial particle radiation
  - solvent left with excited states and electrons and cations
  - anions (electrons) and cations can recombine and contribute back to scintillation



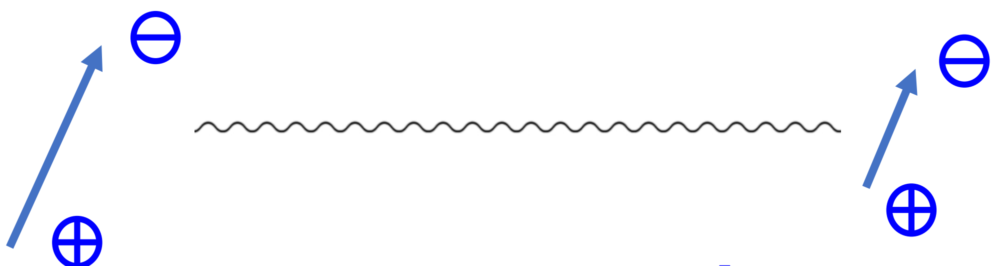
Energy transfer from donor to acceptor

- Electric dipole-dipole interaction (Forster resonance energy transfer, FRET): long-range
- Charge-exchange: short-range

Ground state non-polar molecule



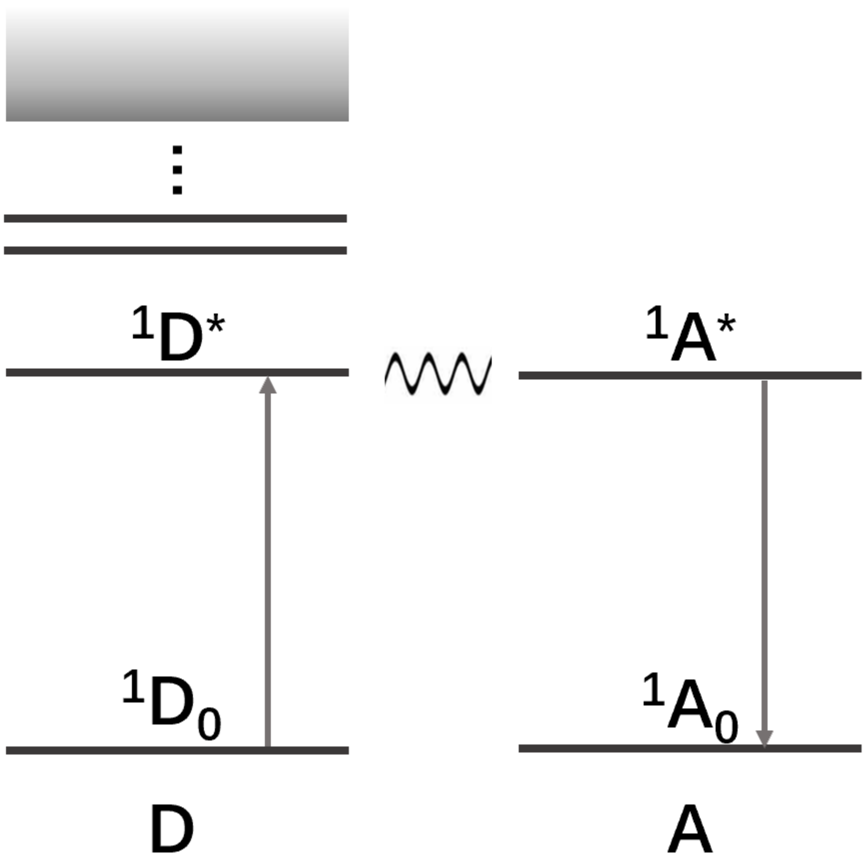
Excited state polarized Electric dipole



Donor, de-excitation, antenna

Acceptor, ground state excited, receiver

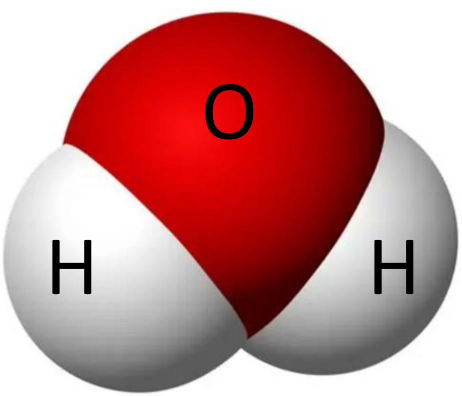
Energy deposition and energy transfer



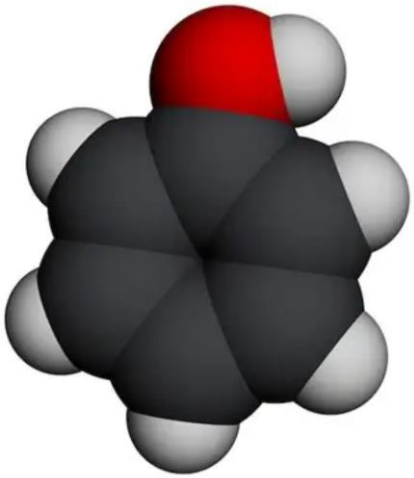
- The emission of A is at a longer wavelength, better transparency and higher quantum efficiency for PMT

Polar group, dielectric constant

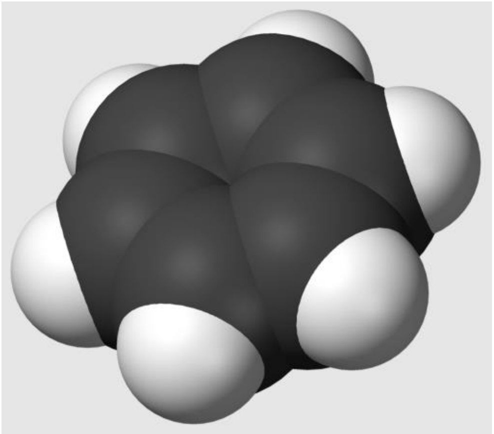
- H_2O has is a polar molecule
- Alcohol molecules also have hydroxyl groups (–OH)
- Benzene is a non-polar molecule
- Polar groups are electrophilic (attract electrons)



H_2O



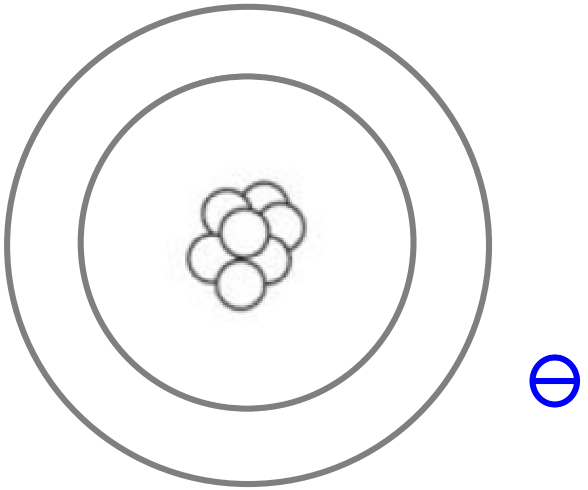
Phenol



Benzene

Polar group, dielectric constant

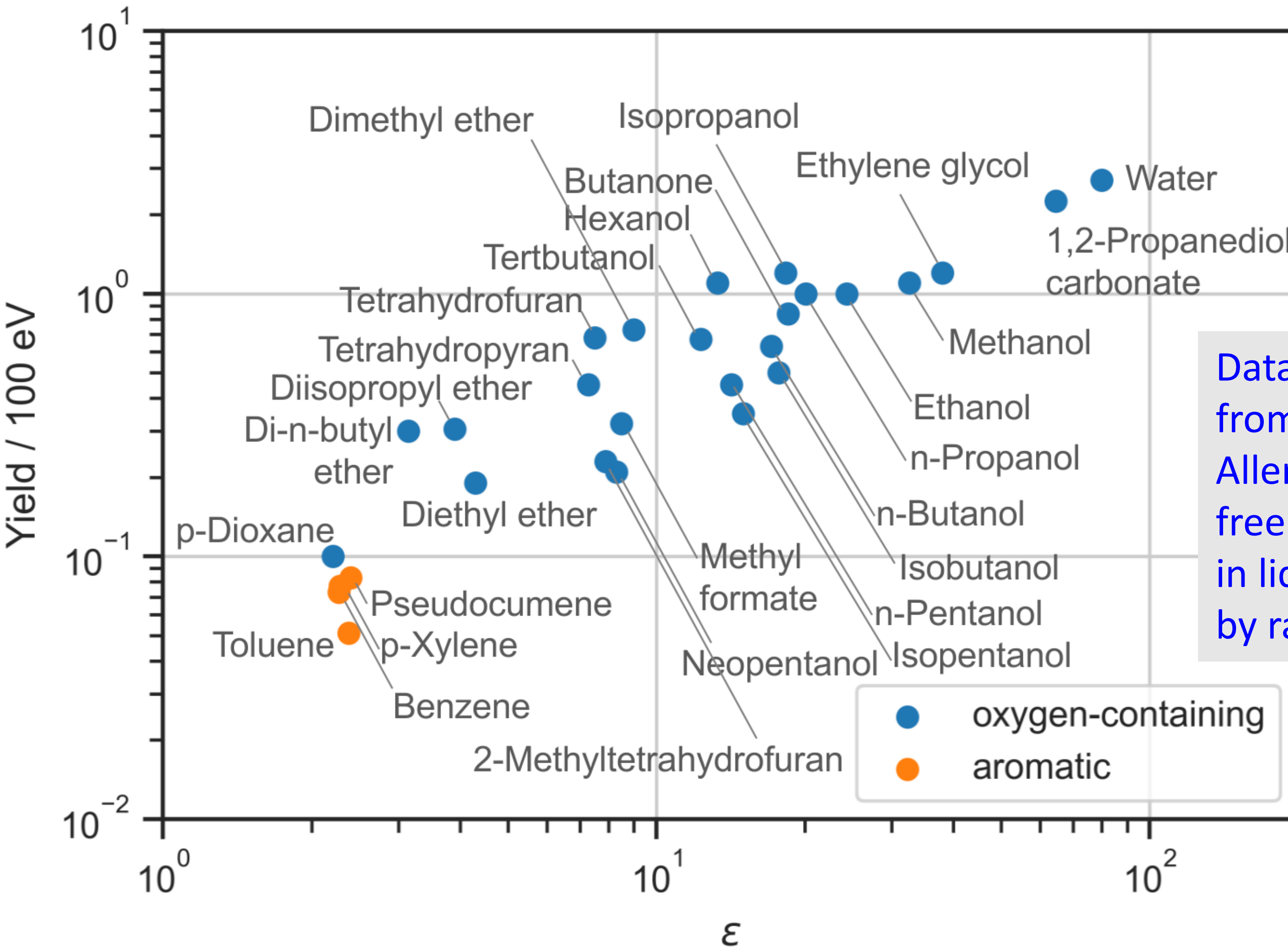
- More polar groups, higher dielectric constant
- The attraction force (Coulumb Law)
- Polar groups: slow down or prevent anion-cation recombination



$$F = \frac{1}{4\pi\epsilon_0\epsilon}\frac{q_1 q_2}{r^2}$$

F ∝ reciprocal of dielectric constant

Free ion yield vs. dielectric constant



Data collected from Augustine O. Allen. Yields of free ions formed in liquids by radiation. 1976.

Total, free ion, and excited state yield comparison

	Water	Benzene
Relative dielectric constant	~80 at 0 Hz	~2 at 0 Hz
Total-ion yield (/100 eV) Geant4-DNA simulation	4.4	5.6
Excited state yield (/100 eV) Geant4-DNA simulation	2.3	6.0
Free-ion yield (/100 eV) Experimental measurement	2.7/100 eV	0.05-0.09

Water with polar structures, with a high relative dielectric constant, is poor for anion-cation recombination

Electric dipole-dipole interaction

Electric energy

$$W = \frac{1}{4\pi\epsilon_0\epsilon R^3}\left[\vec{m}_1\cdot\vec{m}_2 - 3\frac{(\vec{m}_1\cdot\vec{R})(\vec{m}_2\cdot\vec{R})}{R^2}\right]$$

Transition matrix element

$$H = \langle \Psi_{^3\mathrm{D}^*}\Psi_{^3\mathrm{A}^*}|W|\Psi_{^1\mathrm{D}^*}\Psi_{^1\mathrm{A}_0}\rangle$$

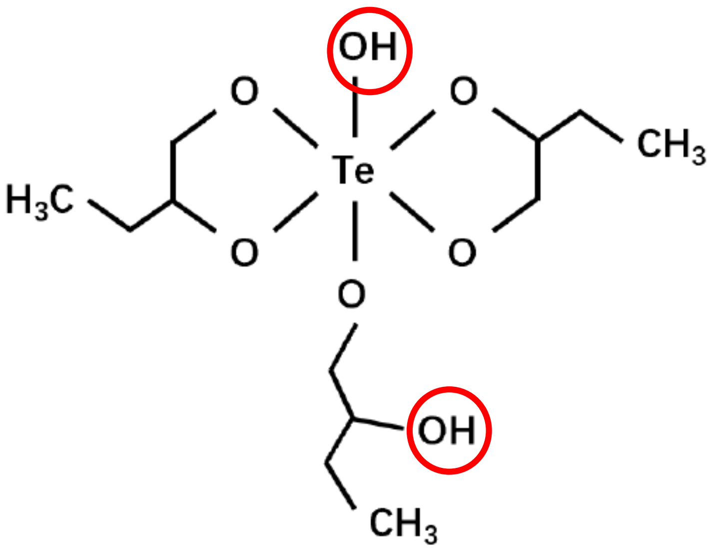
Transition rate

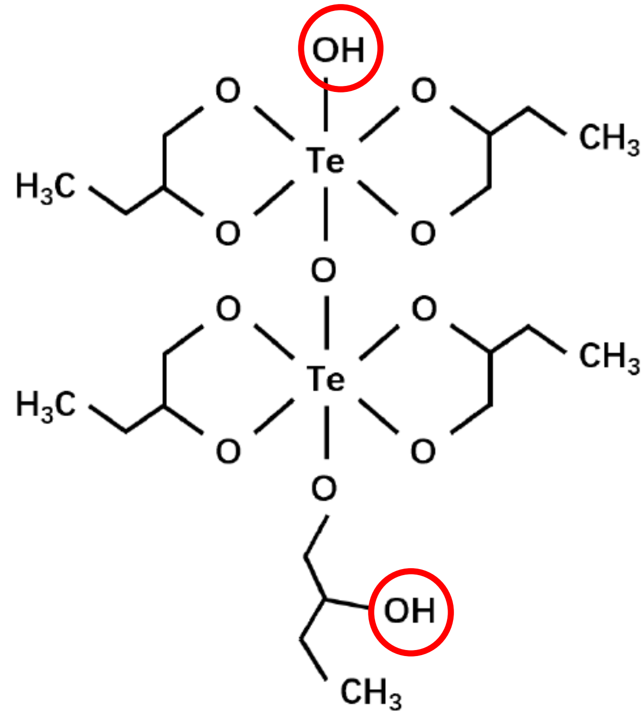
$$k = \frac{2\pi}{\hbar}|H|^2\rho$$

$$\boldsymbol{k \propto 1/\epsilon^2}$$

TeBD at SNO+ for 0νββ search

Tellurium 1,2-butanediol (TeBD) in SNO+ for 0νββ search





Electric

1. **Hydroxyl polar group –OH: electron solvation**

What causes quenching by TeBD?

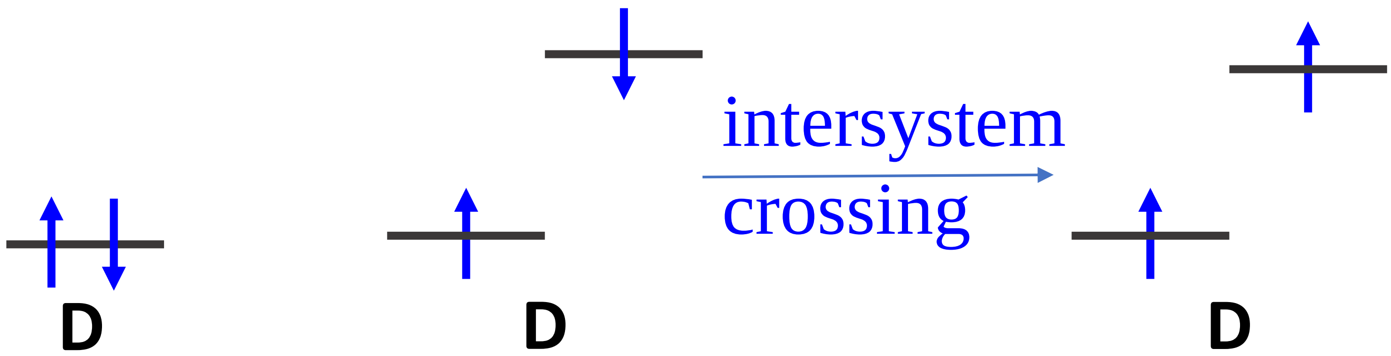
Tellurium 1,2-butanediol (TeBD) in SNO+ for 0νββ search

Electric

2. **Dielectric constant of TeBD is 17±2**
   - 7 times weaker for the Coulomb force for cation-anion recombination than LAB
   - 47 times weaker in the electric dipole-dipole energy transfer

   We measured the dielectric constant of TeBD of our sample.
   May slightly different than SNO+ product.
   Qualitative correct.

One type of quenching, intersystem crossing



Ground state

$J^P=0^-$, singlet

Pauli exclusion principle

1st singlet excited state

J=0

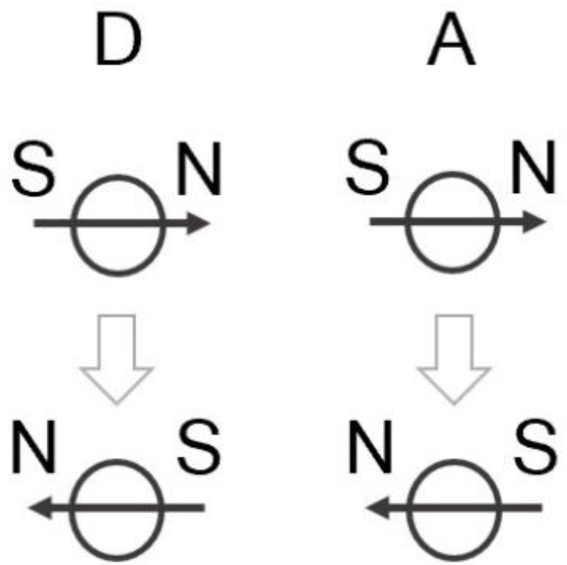
De-excitation - Electric dipole transition: fluorescence

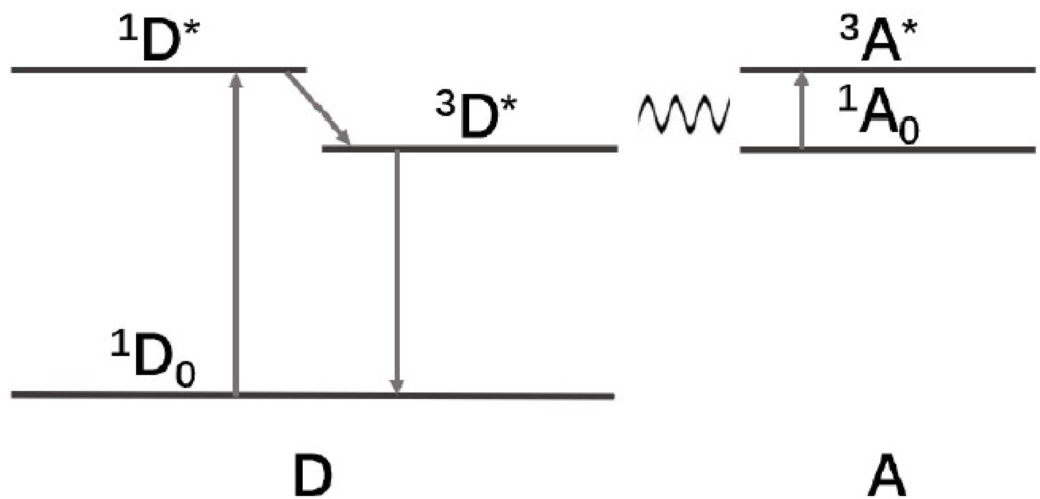
1st triplet excited state

J=1

De-excitation - Transition with one spin flipping: phosphorescence slow, SC quenched

Magnetic dipole-dipole interaction

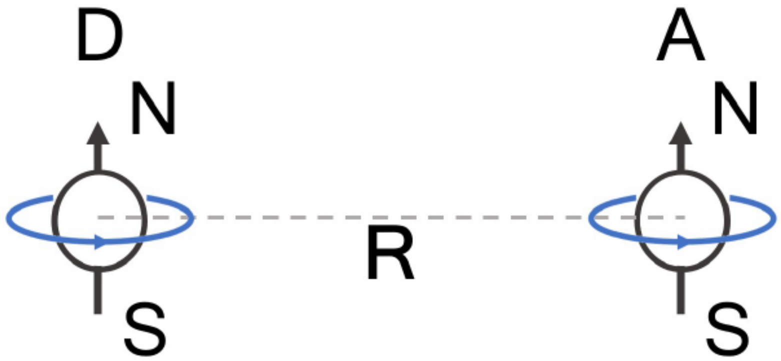




Two magnetic iron bar, one rotate the one on the left, the right one follows.

Simplified energy level diagram (A is quenching acceptor)

Magnetic dipole-dipole interaction



Magnetic energy

$$W = -\frac{\mu_0 \mathbf{m}_{\mathrm{A}} \cdot \mathbf{m}_{\mathrm{D}}}{4\pi R^3} + \frac{3\mu_0 (\mathbf{m}_{\mathrm{A}} \cdot \mathbf{R})(\mathbf{m}_{\mathrm{D}} \cdot \mathbf{R})}{4\pi R^5}$$

Transition matrix element

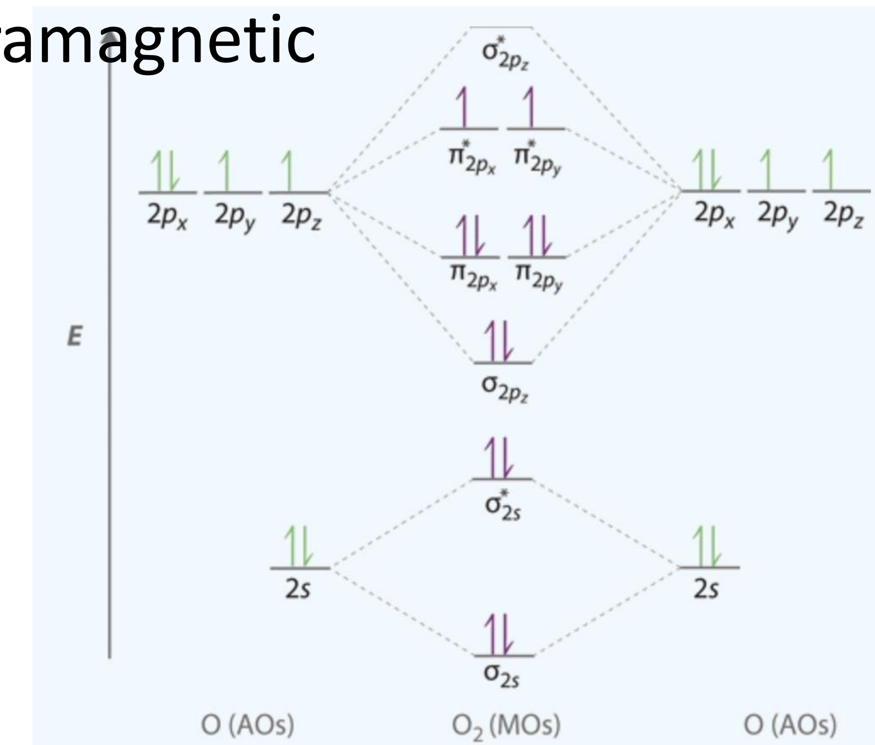
$$H = \langle \Psi_{^3\mathrm{D}^*} \Psi_{^3\mathrm{A}^*} | W | \Psi_{^1\mathrm{D}^*} \Psi_{^1\mathrm{A}_0} \rangle$$

Transition rate

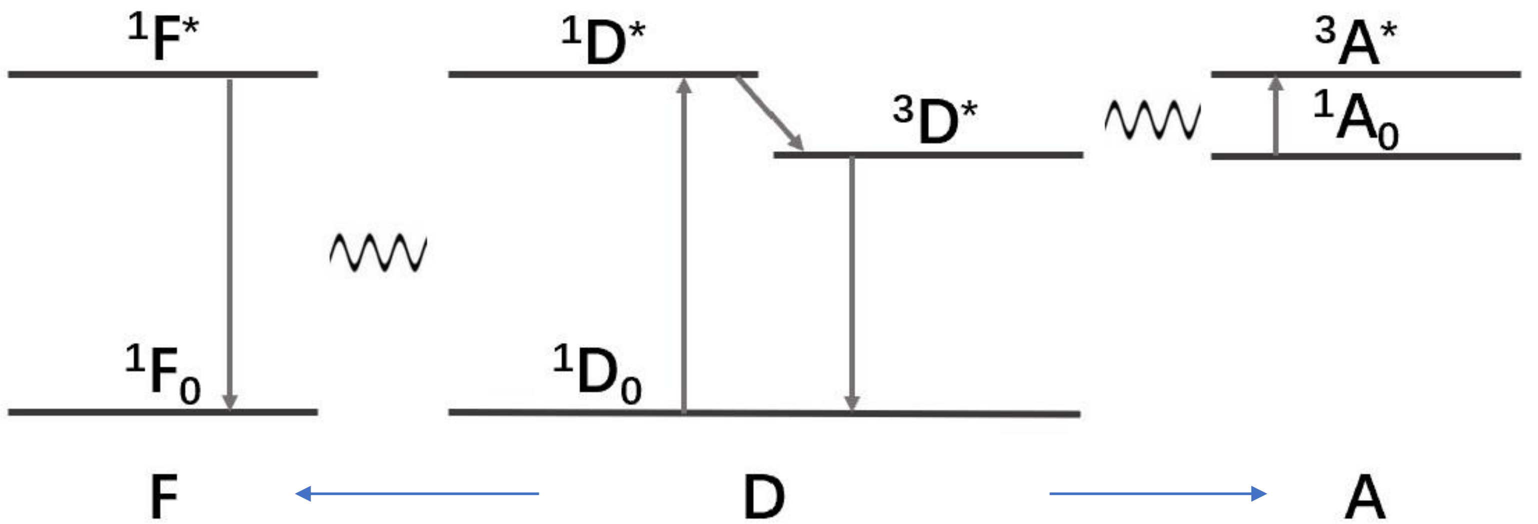
$$k = \frac{2\pi}{\hbar} |H|^2 \rho$$

Magnetic dipole-dipole interaction

- A long-range interaction (a long range quenching mechanism)
- Most chemicals diamagnetic, except for free radicals
- Possible receiver: O_2, paramagnetic



Summary



1. Radiation energy deposition, energy transfer for fluorescence: electric process
   Polar groups and dielectric constants important!
2. Quenching, intersystem cross: magnetic process
   Magnetic dipole-dipole interaction, long range

Summary

Hope to study them in the future liquid scintillator design before molecule synthesized and before measuring their yield with radiative sources!

Note that there are some aspects not mentioned. For instance

1. Transparency changing with different structure
2. Chemical interaction
3. …

Thanks.

This talk is based on these recent two publications:

1. Magnetic dipole-dipole transition for scintillation quenching

https://arxiv.org/abs/2505.11361

2. Molecular structure, electric property, and scintillation and quenching of liquid scintillators

https://arxiv.org/abs/2508.19568