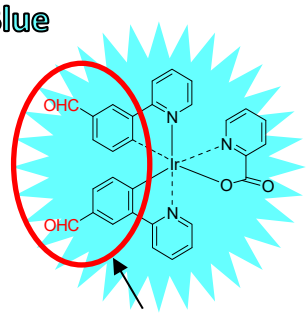
Prediction of emission wavelength in Ir complexes for organic EL materials using quantum chemical calculations

We performed quantum chemical calculations on Ir complexes for organic EL materials and accurately predicted the difference of emission wavelength between the structural isomers. From this result, it is possible to determine the ligand structure by confirming the agreement between the experimental emission wavelength and calculated one, or to predict the emission wavelength of the product denatured by deterioration etc.

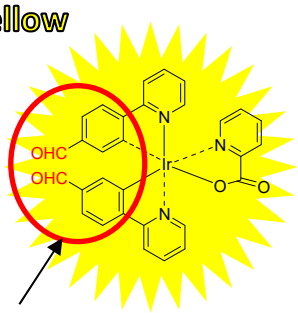
1. Change of emission wavelength in Ir complex

It has been reported that **slight differences in the ligand structure inside Ir complexes lead to changes of emission wavelength**[*a*, *b*]. Controlling the ligand structure is important in the design of organic EL devices.

Blue



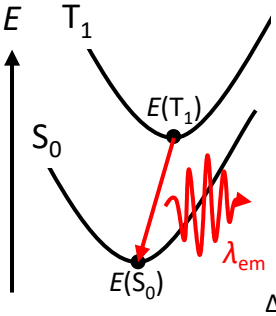
Yellow



It is difficult to determine the detailed ligand structure from instrumental analysis alone.

2. Calculation method of emission wavelength

Quantum chemical calculations allow us to **accurately predict the difference of emission wavelengths** between Ir complexes with similar ligand structures.



The emission wavelength can be evaluated approximately from the energy difference between the T_1 and S_0 states.

Emission wavelength $\lambda_{em} \approx \Delta E$

$\Delta E = E(T_1) - E(S_0) + \Delta ZPE$

ΔZPE: Zero-point energy correction

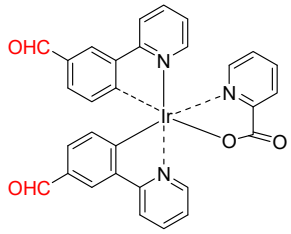
✓ Compound containing a **heavy element (Ir)**
✓ Ground state (S_0) and **triplet excited state (T_1)**

*Need to **professionally set conditions***

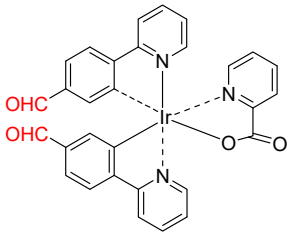
3. Emission wavelengths in structural isomers of Ir complexes

The emission wavelengths of the two structural isomers were calculated and compared with experimental values.

Different substitution sites of CHO groups

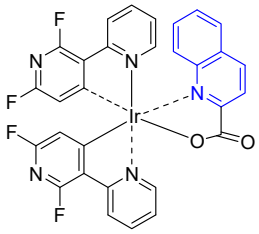


Compound A1

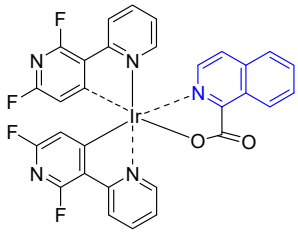


Compound A2

Different arrangements of quinoline rings



Compound B1



Compound B2

Calculated and experimental emission wavelengths

[a] D. Wang *et al.*, Org. Electron. **14**, 2233 (2013).
[b] H. Oh *et al.*, Organometallics **32**, 6427 (2013).

	Compound A1	Compound A2	Compound B1	Compound B2
Calc. (nm)	488	590	532	562
Expt. (nm)	[a]487	[a]579	[b]539	[b]555
Relative error with Expt. (%)	0.2	1.9	−1.3	1.3

The tendencies of the emission wavelengths between the isomers were reproduced **with sufficient accuracy**.

By **professionally and skillfully setting calculation conditions**, we can **determine the ligand structure**, which is **difficult with instrumental analysis**, or **predict the emission wavelengths of denatured products**.

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