Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Ionic liquids containing half-sandwich ruthenium complexes: in-situ interconversions via photochemical and thermal ligand exchange

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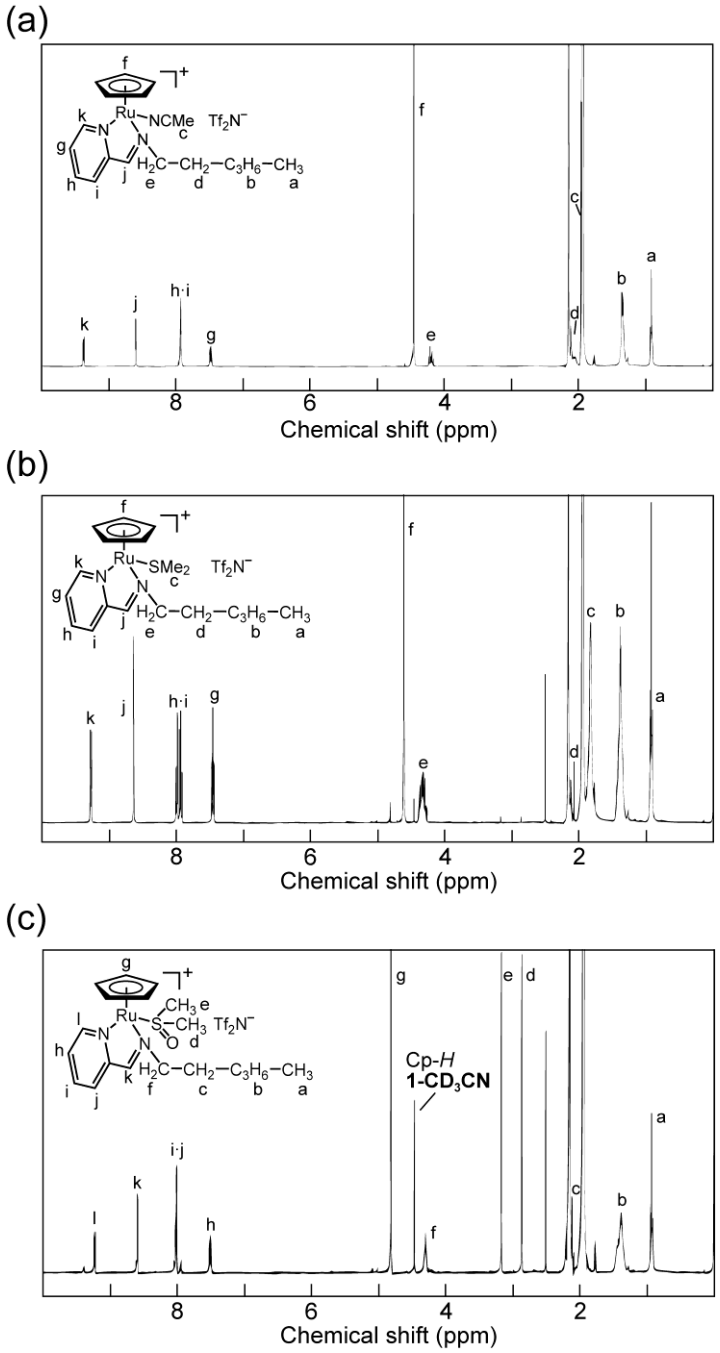

Figure S1. ^{1}H NMR spectra of (a) **1-MeCN**, (b) **1-SMe$_2$**, and (c) **1-DMSO** (in CD_3CN).

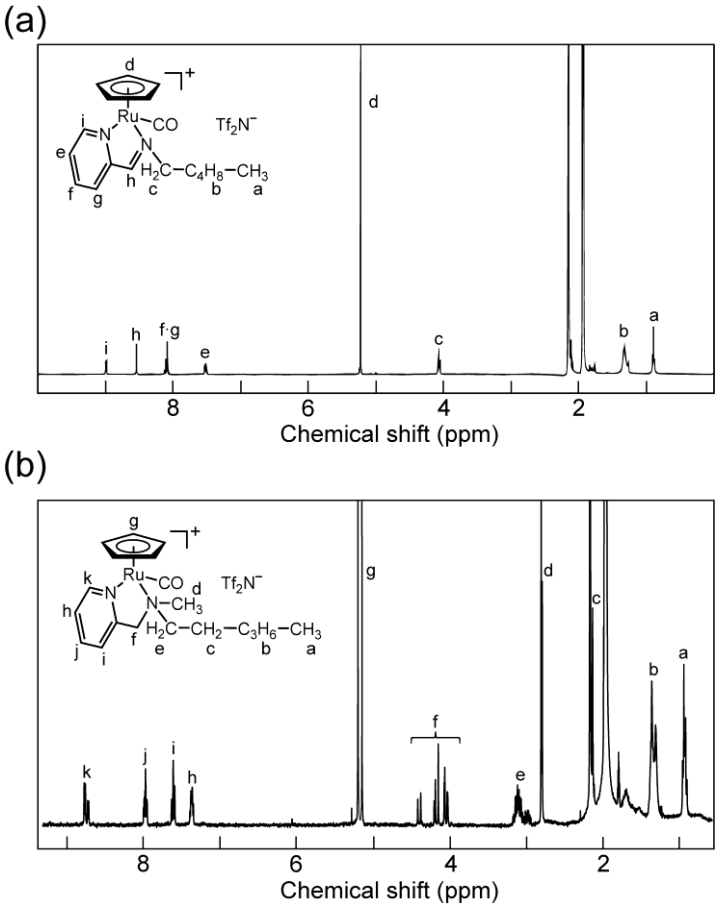

Figure S2. ^{1}H NMR spectra of (a) **1-CO** and (b) **2-CO** (in CD_3CN).

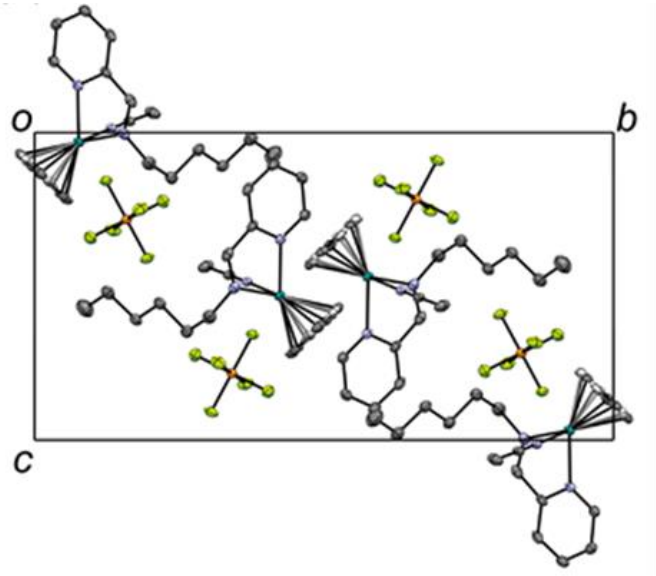

Figure S3. Packing diagram of **1-MeCN** viewed along the *a*-axis. Hydrogen atoms are omitted for clarity.

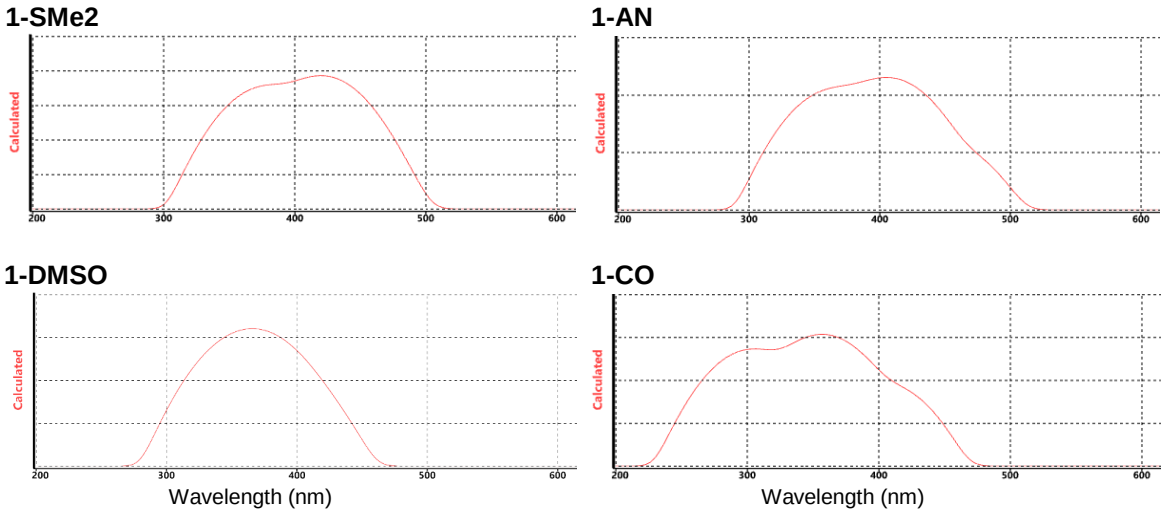

Figure S4. Simulated UV-vis spectra of **1-L** based on TD-DFT calculations.

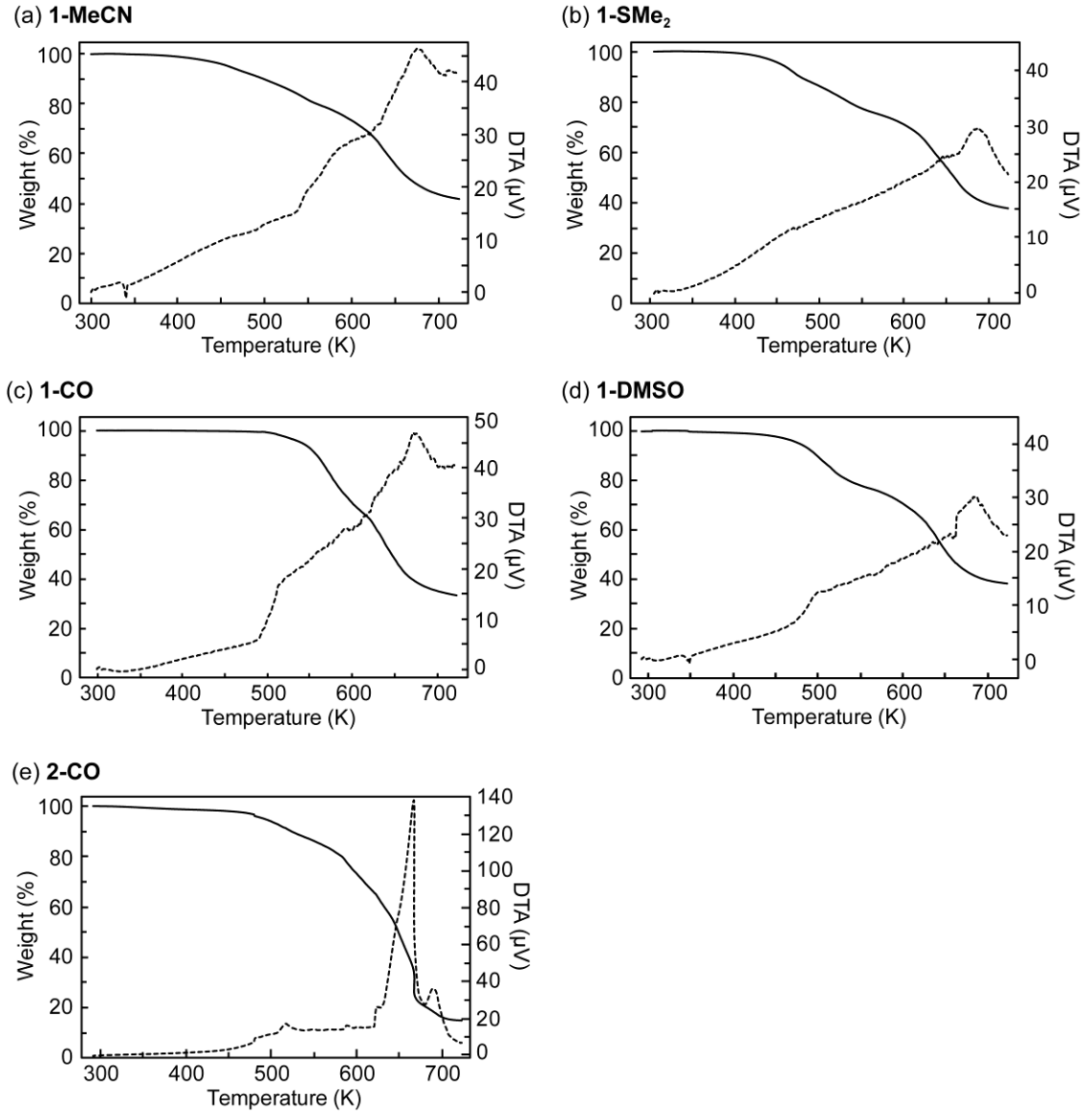

Figure S5. TG-DTA curves of **1-L** and **2-CO**.

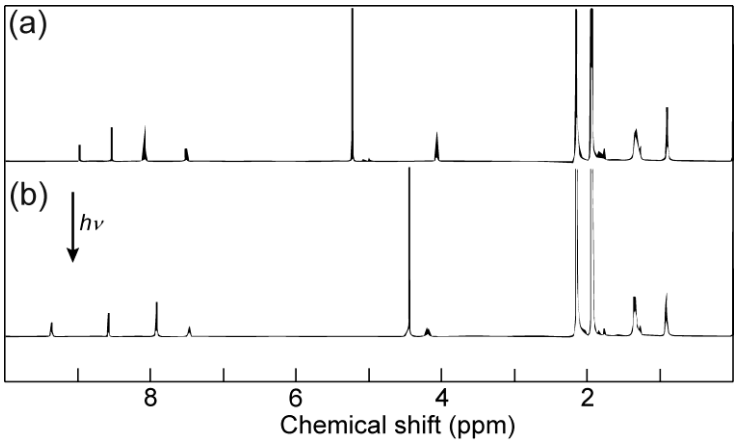

Figure S6. ^{1}H NMR spectra of **1-CO** before and after photoirradiation for 30 min (CD_3CN).

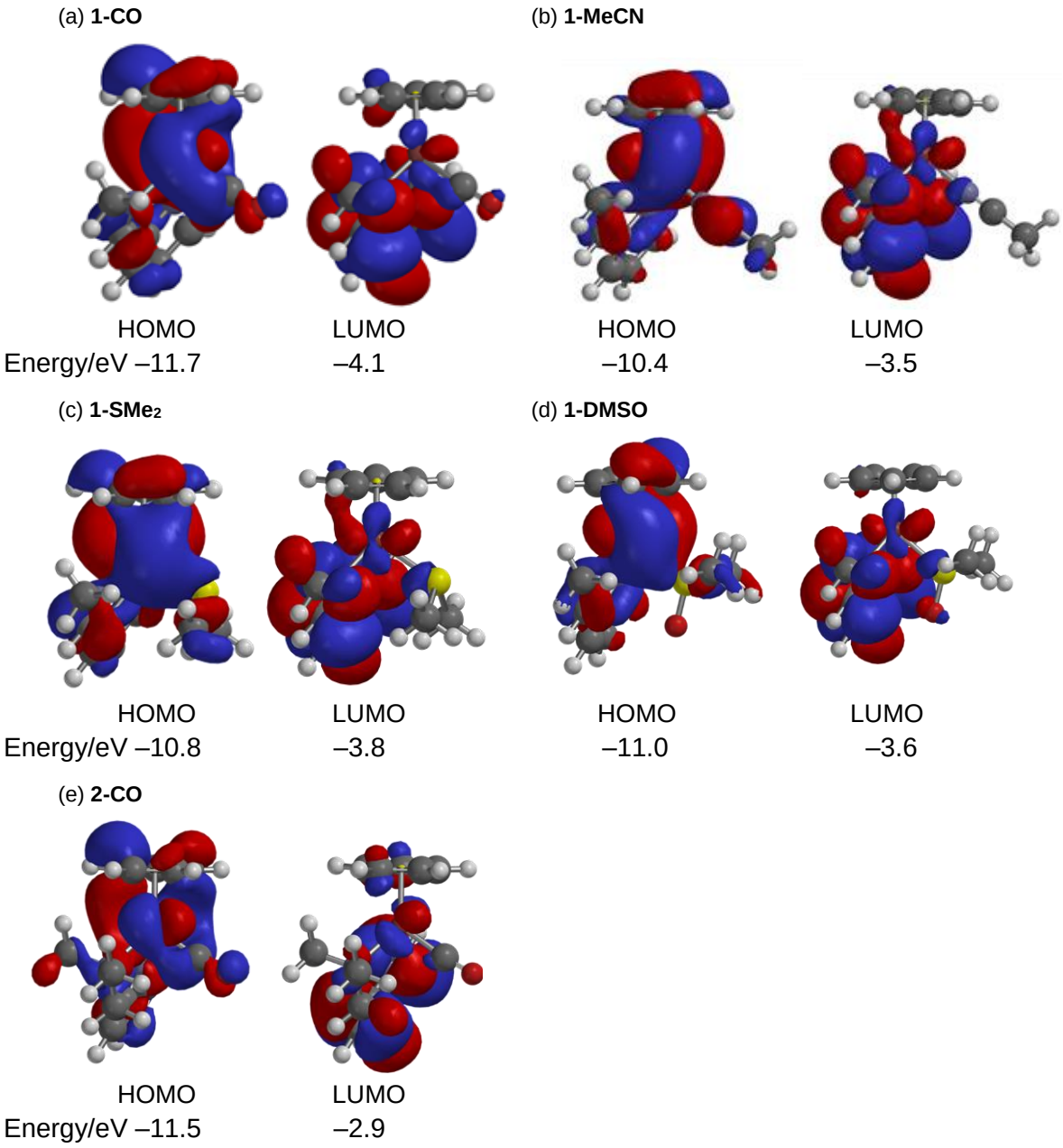

Figure S7. Molecular orbitals of the cations in **1-L** and **2-CO** obtained by DFT calculations.

Table S1. Crystallographic parameters

	[Ru(Cp)**L**^{1}(MeCN)]PF_6
Empirical formula	$C_{19}H_{26}F_6N_3PRu$
Formula weight	542.47
Crystal system	monoclinic
Space group	$P2_1/c$
a [Å]	9.4336(12)
b [Å]	21.056(3)
c [Å]	11.5841(14)
β [°]	104.669(2)
V [Å^3]	2226.0(5)
Z	4
ρ_{calcd} [g cm^{-3}]	1.619
F(000)	1096
Temperature [K]	90
Reflns collected	12833
Independent reflns	5085
Parameters	319
R_{int}	0.0446
$R_1{}^a$, $R_w{}^b$ ($I > 2\sigma(I)$)	0.0355, 0.0661
$R_1{}^a$, $R_w{}^b$ (all data)	0.0569, 0.0726
Goodness of fit	0.991
$\Delta\rho_{max,min}$ [e Å^{-3}]	0.519, –0.681
μ(Mo-Kα)	0.836

$^aR_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$. $^bR_w = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w (F_o^2)^2]^{1/2}$