"Solvent, Coordinating and Hydrogen-Bond Effects on the Chromic Luminescence of the Cationic Complex $[(phen)(H_2O)Re(CO)_3]^+$"

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Table S1. Crystal data and structure refinement for $\mathbf{1}^+(CF_3SO_3)^- \cdot (THF)_{0.5}$. and $\mathbf{1}^+(CF_3SO_3)^- \cdot (DCM)$.

	$\mathbf{1}^+(CF_3SO_3)^- \cdot (THF)_{0.5}$	$\mathbf{1}^+(CF_3SO_3)^- \cdot (DCM)$
FW/uma	1307.16	702.46
Crystal System	Triclinic	Triclinic
Space Group	$P\bar{1}$	$P\bar{1}$
a (Å)	10.8439(11)	8.9613(15)
b (Å)	10.9199(11)	10.9689(19)
c (Å)	12.5692(12)	11.7044(19)
α (°)	79.521(6)	94.367(4)
β (°)	65.587(6)	97.337(4)
γ (°)	62.424(6)	94.165(4)
V (Å^3)	1201.3(2)	1133.8(3)
Z	2	2
d (g cm^{-3})	1.807	2.058
μ (mm^{-1})	5.21	5.75
F000	628	672
θ range	2.4° to 26.0°	1.8° to 26.0°
hkl range	h = -13→13	h = -11→11
	k = -13→13	k = -13→13
	l = -15→15	l = -14→14
N_{tot}, N_{uniq} (R_{int}), N_{obs}	9223, 4702 (0.040), 4121	8865, 4436 (0.047), 3763
Refinement Parameters	324	306
GOF	1.04	1.03
R1, wR2 (obs)	0.051,0.145	0.039,0.088
Max. and min Δρ / e Å^{-3}	1.72 and -2.04	1.43 and -1.51

Table S2. Selected bond distances and angles (Å, º) $\mathbf{1}^{+}(CF_3SO_3)^{-}\cdot(THF)_{0.5}$. and $\mathbf{1}^{+}(CF_3SO_3)^{-}\cdot(DCM)$.

$\mathbf{1}^{+}(CF_3SO_3)^{-}\cdot(THF)_{0.5}$			
Re1—N1	2.156(7)	Re1—C13	1.886(11)
Re1—N2	2.165(7)	Re1—C14	1.884(10)
Re1—O1	2.176(7)	Re1—C15	1.935(11)
C13—Re1—N1	95.7(3)	C13—Re1—N2	95.7(3)
C14—Re1—N1	97.3(4)	C14—Re1—N2	172.0(3)
C15—Re1—N1	172.4(4)	C15—Re1—N2	97.8(4)
N1—Re1—N2	75.8(3)	C13—Re1—C15	88.9(4)
N1—Re1—O1	80.7(3)	C14—Re1—C13	89.0(4)
N2—Re1—O1	80.2(3)	C14—Re1—C15	88.7(5)
C13—Re1—O1	175.1(3)	C14—Re1—O1	94.8(4)
C15—Re1—O1	94.3(4)		

$\mathbf{1}^{+}(CF_3SO_3)^{-}\cdot(DCM)$			
Re1—N1	2.173(5)	Re1—C13	1.879(8)
Re1—N2	2.178(5)	Re1—C14	1.911(7)
Re1—O1	2.191(5)	Re1—C15	1.921(7)
C13—Re1—N1	94.9(3)	C13—Re1—N2	97.6(3)
C14—Re1—N1	171.5(2)	C14—Re1—N2	96.2(2)
C15—Re1—N1	99.2(2)	C15—Re1—N2	172.3(2)
N1—Re1—N2	76.00(18)	C13—Re1—C14	89.5(3)
N1—Re1—O1	81.41(19)	C13—Re1—C15	88.7(3)
N2—Re1—O1	80.57(19)	C14—Re1—C15	88.2(3)
C13—Re1—O1	176.2(3)	C14—Re1—O1	94.0(3)
C15—Re1—O1	92.9(3)		

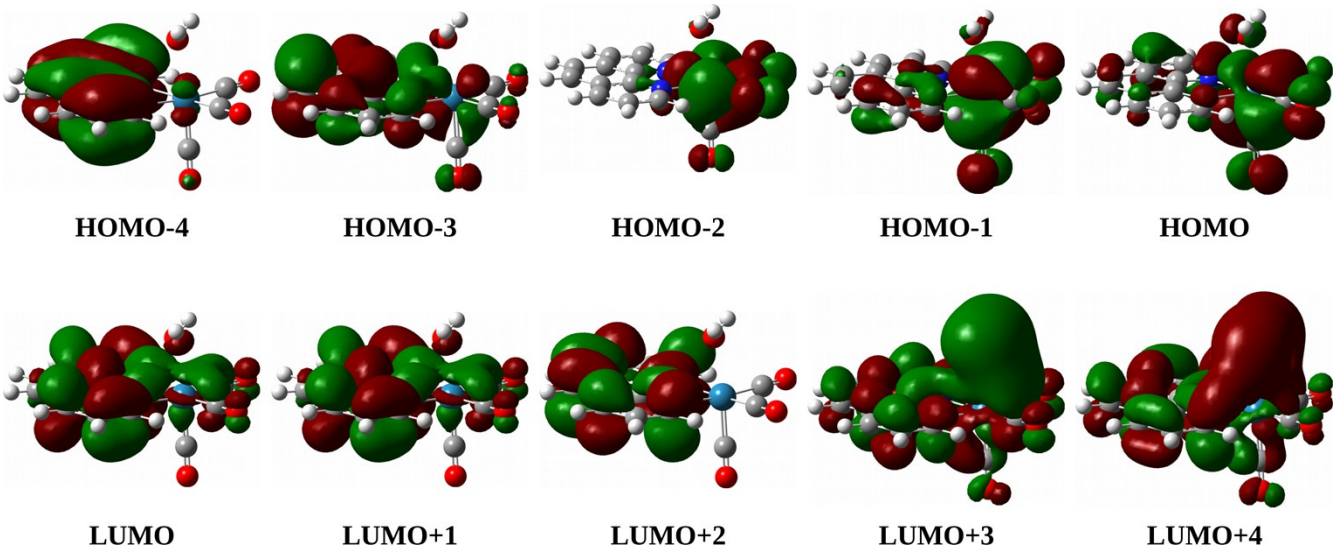

Figure S1. DFT computed frontier orbitals from HOMO − 4 to LUMO + 4 plots for $\mathbf{1}^{+}$ (gas phase).

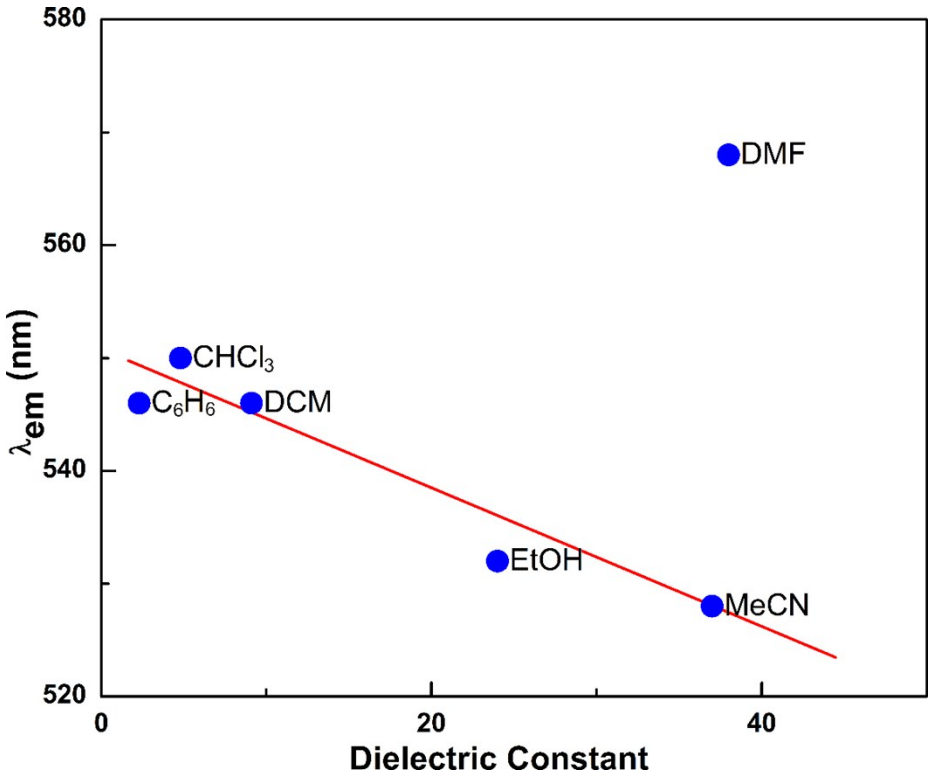

Figure S2. Emission band maxima dependence on the solvent polarity (dielectric constant) for $\mathbf{1}^{+}(CF_3SO_3)^{-}$.

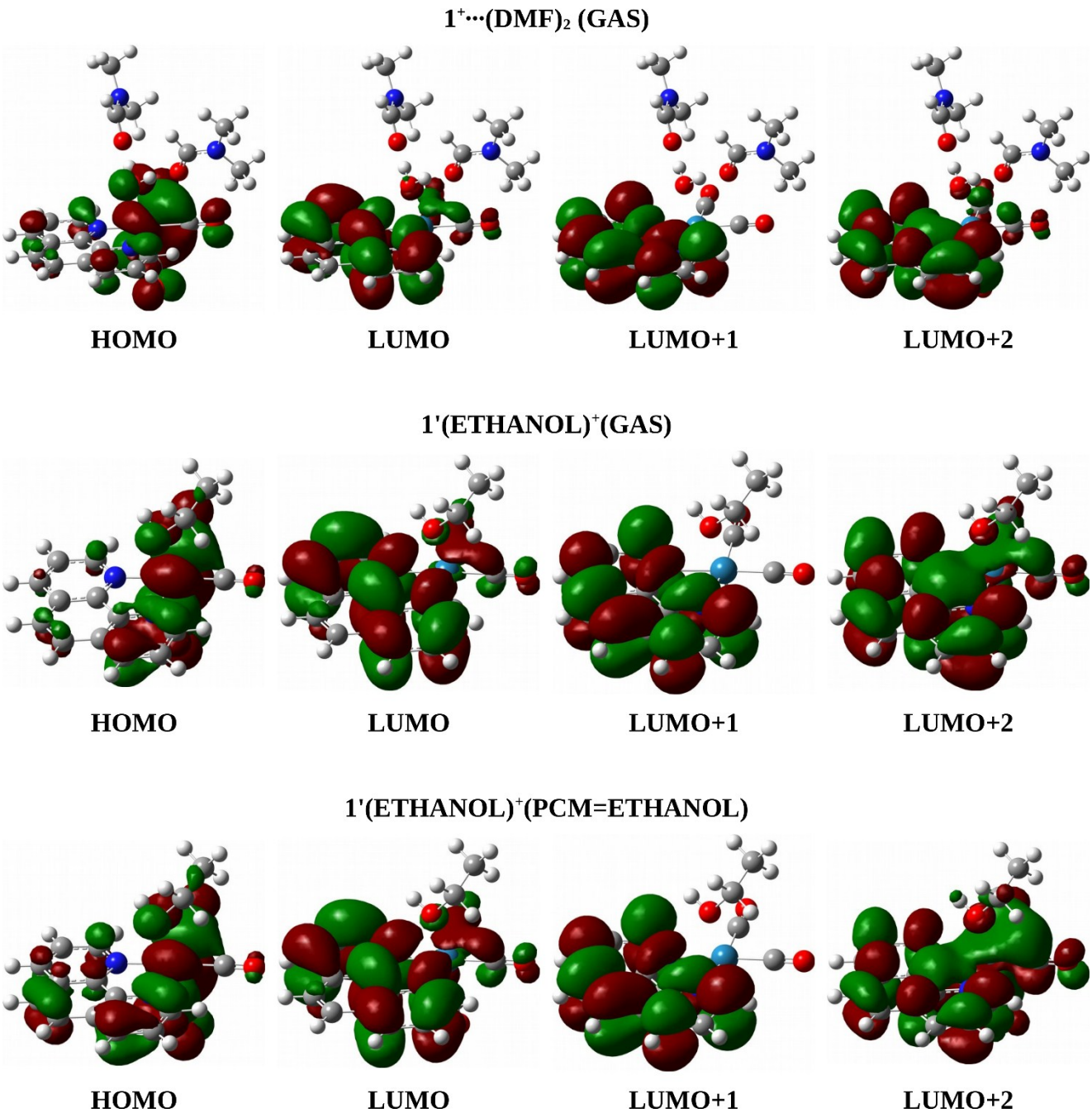

Figure S3. DFT computed frontier orbitals for the species **1a**$^+$ and **1**$^+$**(DMF)$_2$** in gas phase and in PCM (EtOH).

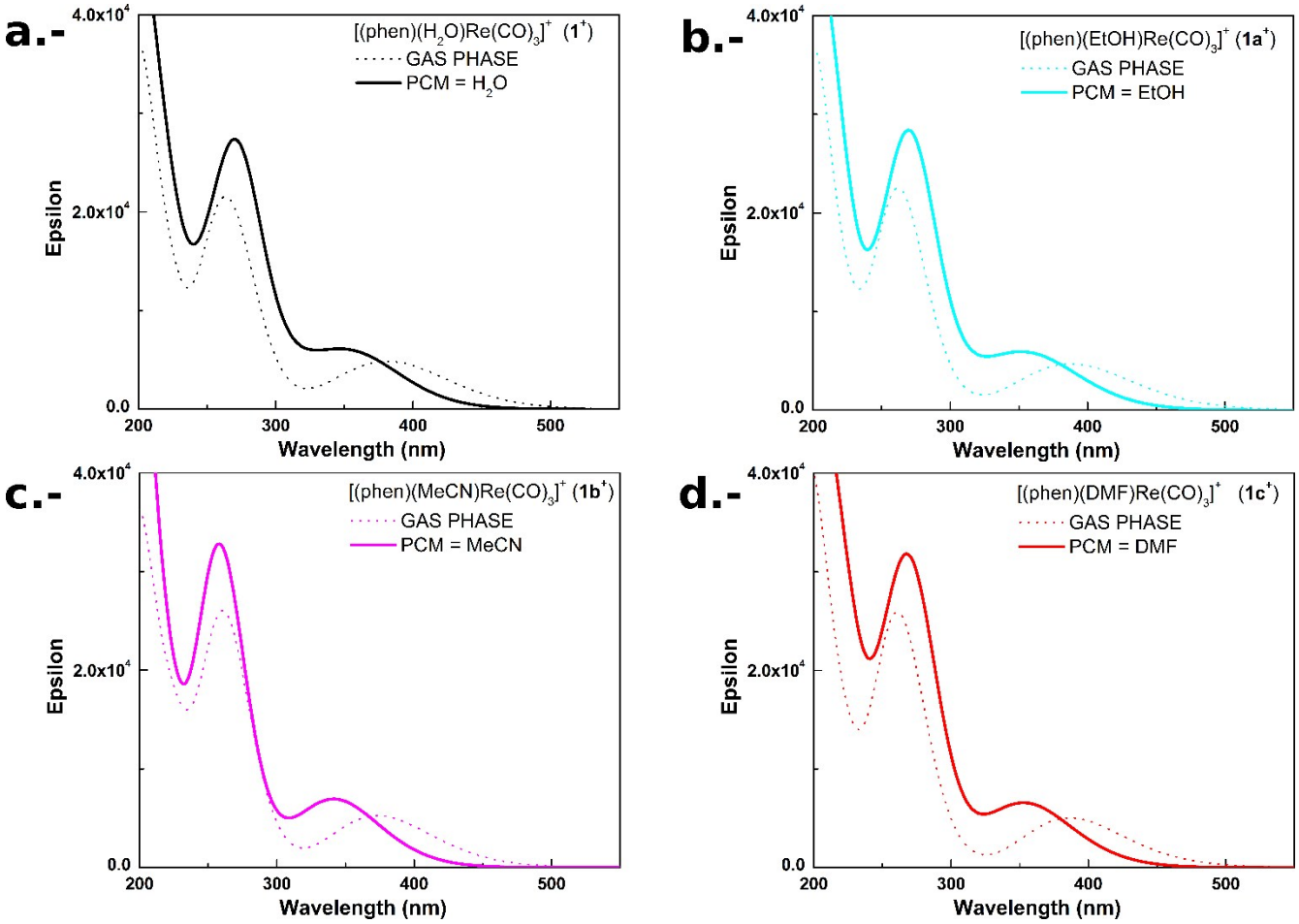

Figure S4. TD-DFT computed transitions for: **a.- 1**$^{+}$; gas phase (···), PCM = H_2O (—). **b.- 1a**$^{+}$; gas phase (···), PCM = EtOH (—). **c.- 1b**$^{+}$; gas phase (···), PCM = MeCN (—). **d.- 1c**$^{+}$; gas phase (···), PCM DMF (—).