

Supporting Information

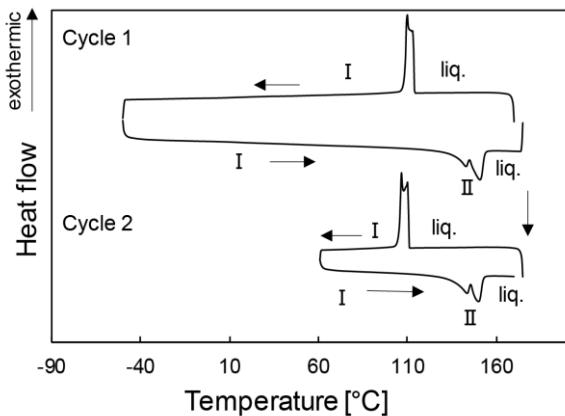
Thermal Properties and Crystal Structures of Rhenium(I) Carbonyl Complexes with Tridentate Ligands: Preparation of Rhenium-Containing Ionic Liquids

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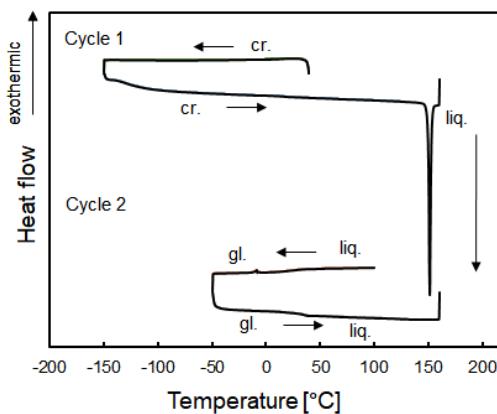
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a) [1]PF₆



b) [2]PF₆



c) [2-Cl]

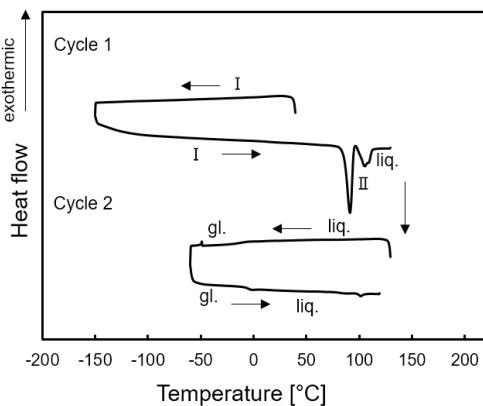
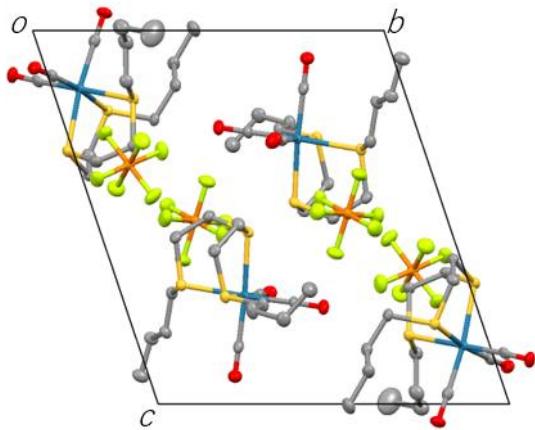
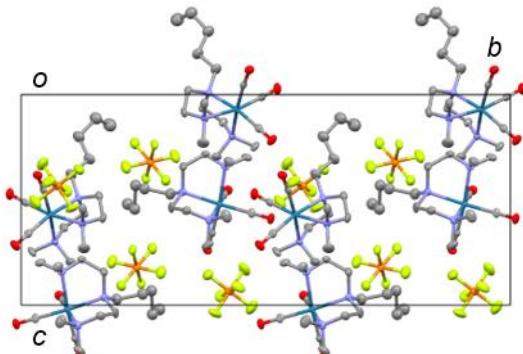


Figure S1. DSC traces.

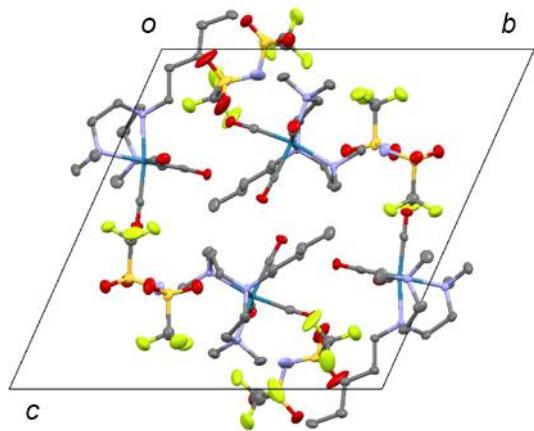
a) $[1]\text{PF}_6$



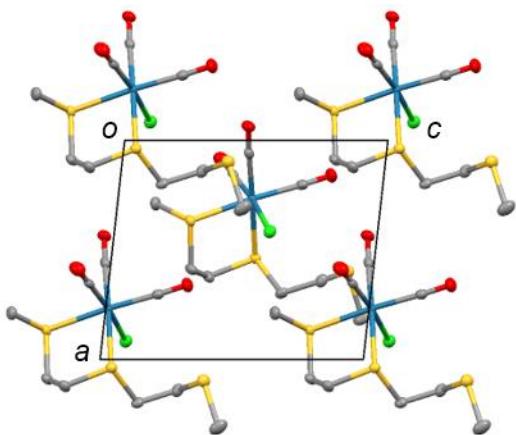
b) $[2]\text{PF}_6$



c) $[2]\text{Tf}_2\text{N}$



d) $[1'\text{-Cl}]$



e) $[2\text{-Cl}]$

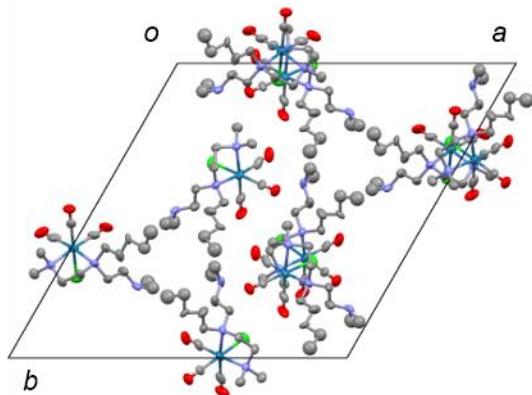


Figure S2. Packing diagrams. In the disordered part, the lower occupancy moieties have been omitted.

Table S1. Crystallographic parameters

	[1]PF ₆	[2]PF ₆	[2]Tf ₂ N
Empirical formula	C ₁₅ H ₂₆ S ₃ O ₃ ReF ₆ P	C ₁₆ H ₃₁ N ₃ O ₃ RePF ₆	C ₁₈ H ₃₁ F ₆ N ₄ O ₇ ReS ₂
Formula weight	681.71	644.61	779.79
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	<i>P</i> –1	<i>Cc</i>	<i>P</i> –1
<i>a</i> [Å]	12.101(3)	13.490(11)	9.7417(10)
<i>b</i> [Å]	13.378(3)	28.17(2)	17.7109(18)
<i>c</i> [Å]	15.687(4)	12.581(11)	18.1194(19)
α [°]	70.089(3)	90	111.7300(10)
β [°]	71.784(3)	105.98(2)	103.9650(10)
γ [°]	82.403(3)	90	96.0330(10)
<i>V</i> [Å ³]	2267.1(10)	4596.0(7)	2751.9(5)
<i>Z</i>	4	8	4
ρ_{calcd} [g cm ⁻³]	1.997	1.863	1.882
<i>F</i> (000)	1328.0	2528	1536
μ (mm ⁻¹)	5.77	5.426	4.652
Temperature [K]	100	90	90
Reflns collected	9938	12551	12907
<i>R</i> (int)	0.0204	0.0118	0.0246
<i>R</i> ₁ ^{<i>a</i>} , <i>R</i> _w ^{<i>b</i>} (<i>I</i> > 2σ)	0.0252, 0.0600	0.0220, 0.0584	0.0256, 0.0639
<i>R</i> ₁ ^{<i>a</i>} , <i>R</i> _w ^{<i>b</i>} (all data)	0.0314, 0.0663	0.0228, 0.0587	0.0290, 0.0651
Goodness of fit	1.138	1.041	1.063

^{*a*}*R*₁ = Σ||*F*_o| – |*F*_c|| / Σ|*F*_o|. ^{*b*}*R*_w = [Σ*w* (*F*_o² – *F*_c²)²/Σ*w* (*F*_o²)²]^{1/2}.

Table S2. Crystallographic parameters

	[1'-Cl]	[2-Cl]
Empirical formula	C ₉ H ₁₄ S ₃ O ₃ ReCl	C ₁₆ H ₃₁ N ₃ O ₃ ReCl
Formula weight	488.03	535.09
Crystal system	Monoclinic	Trigonal
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>R</i> 3c
<i>a</i> [Å]	7.9569(15)	22.703(4)
<i>b</i> [Å]	19.283(4)	22.703(4)
<i>c</i> [Å]	9.5161(18)	20.758(3)
α [°]	90	90
β [°]	96.405(2)	90
γ [°]	90	120
<i>V</i> [Å ³]	1451.0(5)	9266(3)
<i>Z</i>	4	18
ρ_{calcd} [g cm ⁻³]	2.234	1.726
<i>F</i> (000)	928	4752
μ (mm ⁻¹)	8.982	6.049
Temperature [K]	100	90
Reflns collected	7536	17133
<i>R</i> (int)	0.0201	0.0234
<i>R</i> ₁ ^{<i>a</i>} , <i>R</i> _w ^{<i>b</i>} (<i>I</i> > 2 σ)	0.0166, 0.0429	0.0298, 0.0674
<i>R</i> ₁ ^{<i>a</i>} , <i>R</i> _w ^{<i>b</i>} (all data)	0.0169, 0.0430	0.0367, 0.0712
Goodness of fit	1.133	1.054

^{*a*} $R_1 = \Sigma \|F_o - |F_c\| / \Sigma |F_o|$. ^{*b*} $R_w = [\sum w (F_o^2 - F_c^2)^2 / \sum w (F_o^2)^2]^{1/2}$.