SUPPORTING INFORMATION

Unligated Diruthenium(II,II) Tetra(trifluoroacetate): The First X-Ray Structural Study, Thermal Compressibility, Lewis Acidity, and Magnetism

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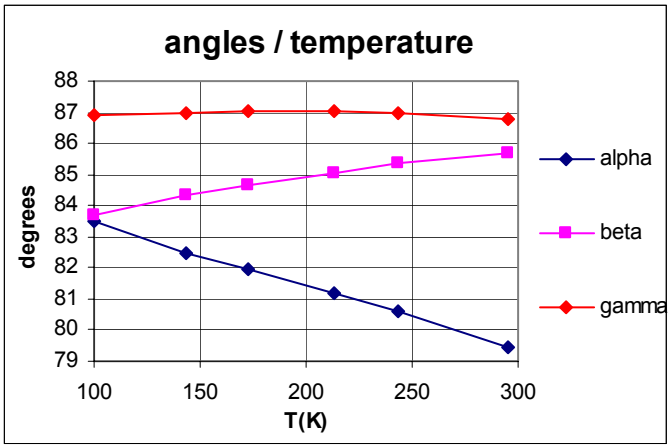
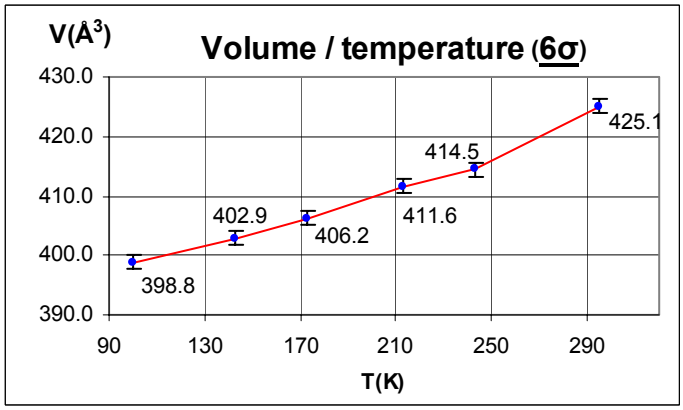
Table 1. Crystallographic Data and Structural Refinement Parameters for $[Ru_2(O_2CCF_3)_4]$ (**1**) at different temperatures (K).

	100	**143**	**173**	**213**	**243**	**295**
formula	$C_8F_{12}O_8Ru_2$	$C_8F_{12}O_8Ru_2$	$C_8F_{12}O_8Ru_2$	$C_8F_{12}O_8Ru_2$	$C_8F_{12}O_8Ru_2$	$C_8F_{12}O_8Ru_2$
fw	654.22	654.22	654.22	654.22	654.22	654.22
cryst system	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic
space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	5.2485(6)	5.2447(5)	5.2457(5)	5.2505(6)	5.2519(5)	5.2779(15)
B (Å)	8.6377(10)	8.6097(8)	8.6067(8)	8.6127(10)	8.6122(8)	8.667(3)
C (Å)	8.9147(10)	9.0518(8)	9.1343(8)	9.2508(10)	9.3269(9)	9.489(3)
α (º)	83.493(2)	82.4740(10)	81.9370(10)	81.203(2)	80.6060(10)	79.456(5)
β (º)	83.698(2)	84.3120(10)	84.6310(10)	85.057(2)	85.3370(10)	85.705(5)
γ (º)	86.921(2)	87.0010(10)	87.0310(10)	87.036(2)	86.985(2)	86.776(5)
V (Å^3)	398.77(8)	402.90(6)	406.22(6)	411.56(8)	414.49(7)	425.1(2)
Z	1	1	1	1	1	1
T (K)	100(2)	143(2)	173(2)	213(2)	243(2)	295(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
D_{calc} (g · cm^{-3})	2.724	2.696	2.674	2.640	2.621	2.555
μ (mm^{-1})	2.069	2.048	2.031	2.005	1.990	1.941
data/restr/parameters	1743 / 0 / 136	1792 / 0 / 136	1815 / 0 / 136	1813 / 36/166	1841 / 18/145	1734 / 0 / 136
$R1$[b], $wR2$[c] [$I > 2\sigma(I)$]	0.0282, 0.0725	0.0275, 0.0698	0.0277, 0.0717	0.0369, 0.0914	0.0320, 0.0798	0.1187, 0.2177
$R1$[b], $wR2$[c] (all data)	0.0313, 0.0743	0.0304, 0.0715	0.0303, 0.0733	0.0405, 0.0936	0.0355, 0.0817	0.2058, 0.2447
quality-of-fit[a] on F^2	1.087	1.077	1.077	1.073	1.075	1.100

[a] Quality-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/(N_{obs} - N_{params})]^{1/2}$.
[b] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$.
[c] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

Figure 1: Temperature dependence of the unit cell angles (α, β, γ) and volume (V), as well as the calculated density in the structure of $[Ru_2(O_2CCF_3)_4]$ (**1**).





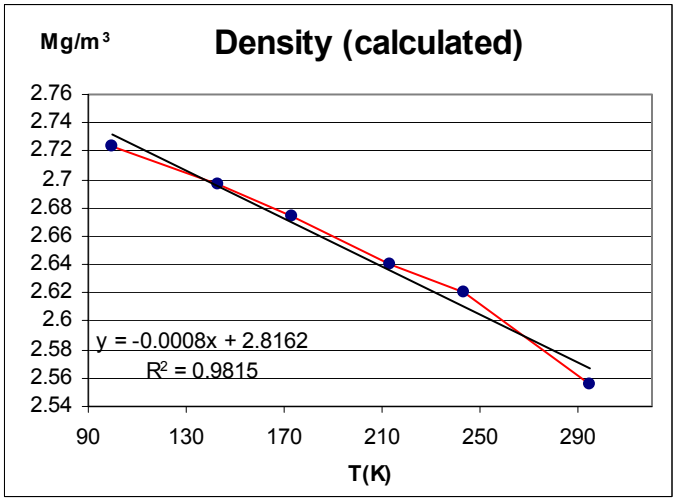


Table 2. Selected distances (Å) and angles (°) in the structures of $[Ru_2(O_2CCF_3)_4]$ (**1**) at different temperatures.

	100 K	143 K	173 K	213 K	243 K
Ru–Ru	2.2679(5)	2.2650(4)	2.2641(4)	2.2647(6)	2.2627(5)
$Ru–O_{av}$	2.066(2)	2.063(2)	2.062(2)	2.061(3)	2.061(3)
Ru(1)–O(2)[1]	2.091(2)	2.089(2)	2.090(2)	2.087(3)	2.085(3)
Ru(1)–O(2A)	2.363(2)	2.364(2)	2.366(2)	2.375(3)	2.377(3)
Ru–Ru–O(2)	167.07(6)	167.29(6)	167.43(6)	167.53(8)	167.64(7)

[1] O(2) –oxygen atom participating in intermolecular interaction

Figure 2: Perspective drawing of the $Ru_2(O_2CCF_3)_4$ (**1**) molecules with intermolecular contacts between them shown by dashed lines. Atoms are represented by thermal ellipsoids at the 50% probability level.

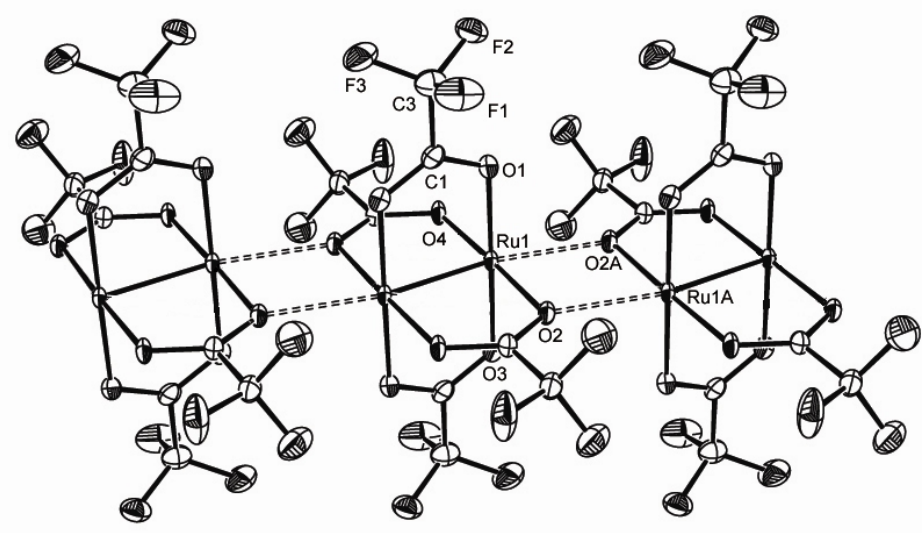


Figure 3: Temperature dependence of the selected distances (Å) and angles (°) in the structure of $[Ru_2(O_2CCF_3)_4]$ (**1**).

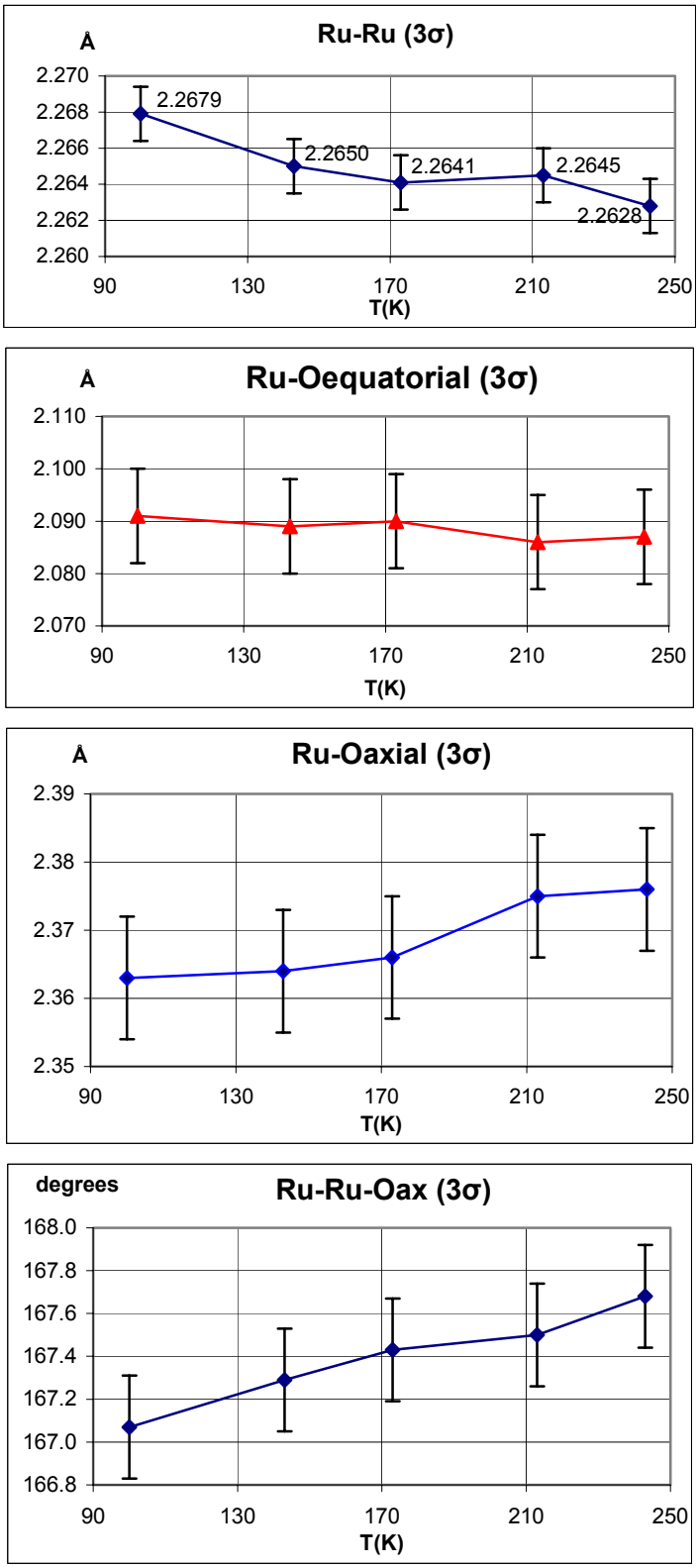


Figure 4: Fragment showing the alternating arrangement of $Ru_2(O_2CCF_3)_4$ and $C_{16}H_{16}$ in the chain structure of **2**. Atoms are represented by thermal ellipsoids at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii. Fluorine atoms are omitted for clarity.

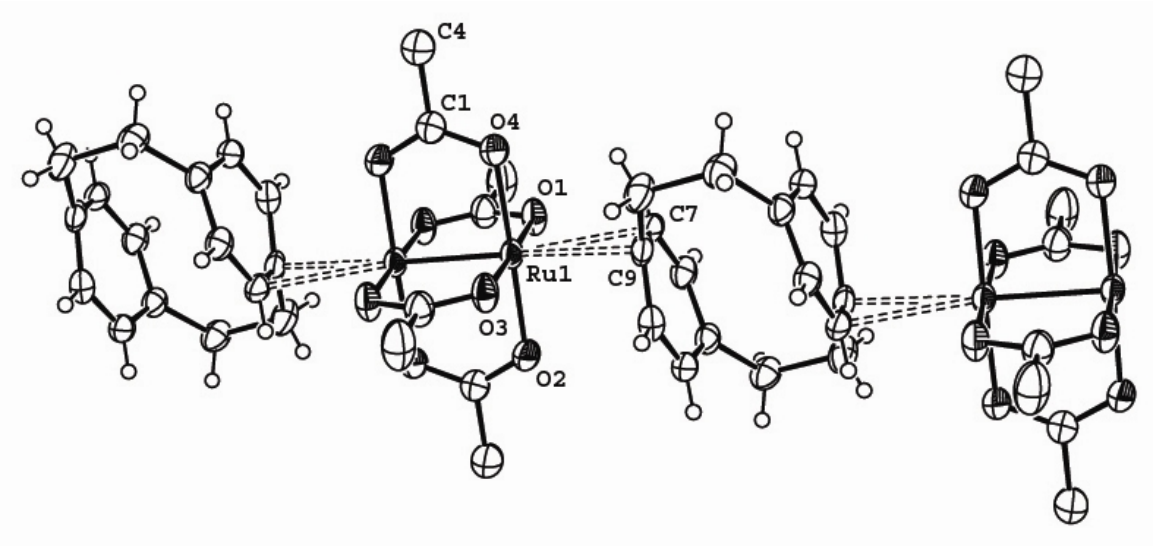


Figure 5: Perspective drawing of the $Ru_2(O_2CCF_3)_3(O_2CC_2H_5)$ (**3**) molecules with intermolecular contacts drawn as dashed lines. Atoms are represented by thermal ellipsoids at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii. Fluorine atoms are omitted for clarity.

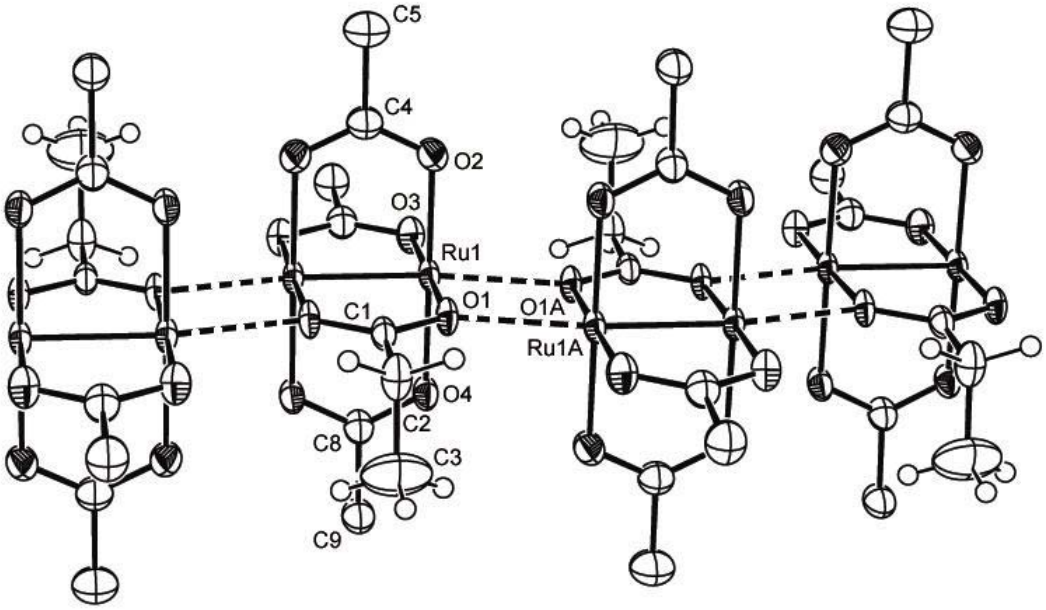


Table 3. Crystallographic Data and Structural Refinement Parameters for $[Ru_2(O_2CCF_3)_4(C_4H_{10}O)_2]$ (**4**) and $[Ru_2(O_2CCF_3)_4(C_3H_6O)_2]$ (**5**).

	4	**5**
formula	$C_{16}H_{20}F_{12}O_{10}Ru_2$	$C_{14}H_{12}F_{12}O_{10}Ru_2$
fw	802.46	770.38
cryst system	triclinic	monoclinic
space group	$P\bar{1}$	$P\,2_1/n$
a (Å)	8.5253(5)	8.7288(6)
b (Å)	8.9951(5)	8.9709(7)
c (Å)	9.7803(5)	15.1089(11)
α (º)	67.594(1)	90.00
β (º)	88.546(1)	96.752(1)
γ (º)	77.392(1)	90.00
V (Å^3)	675.28(6)	1174.9(2)
Z	1	2
T (K)	173(2)	173(2)
λ (Å)	0.71073	0.71073
D_{calc} (g · cm^{-3})	1.973	2.178
μ (mm^{-1})	1.247	1.428
data/restr/parameters	3034/0/183	2751/36/192
$R1$[b], $wR2$[c] [$I > 2\sigma(I)$]	0.0205, 0.0543	0.0399, 0.0944
$R1$[b], $wR2$[c] (all data)	0.0214, 0.0552	0.0526, 0.1006
quality-of-fit[a] on F^2	1.009	1.049

[a] Quality-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/(N_{obs} - N_{params})]^{1/2}$.
[b] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$.
[c] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

Figure 6: Perspective drawing of the $Ru_2(O_2CCF_3)_4(C_4H_{10}O)_2$ (**4**) molecule. Atoms are represented by thermal ellipsoids at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii.

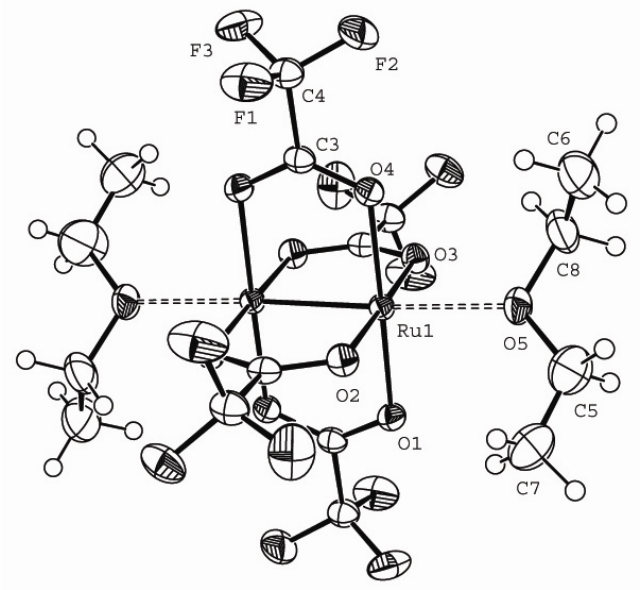


Figure 7: Perspective drawing of the $Ru_2(O_2CCF_3)_4(C_3H_6O)_2$ (**5**) molecule. Atoms are represented by thermal ellipsoids at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii. Fluorine atoms are omitted.