

Electronic Supplementary Information:

Preparation and Superconductivity of Intercalation Compounds of TiNCl with Aliphatic Amines

Shoji Yamanaka^{1,*}, Keita Umemoto¹, Zhanfeng Zheng¹, Yuta Suzuki², Hiroshi Matsui², Naoki Toyota², and Kei Inumaru¹

¹Department of Applied Chemistry, Graduate School of Engineering, Hiroshima University, Higashi-Hiroshima 739-8527, Japan

²Physics Department, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan

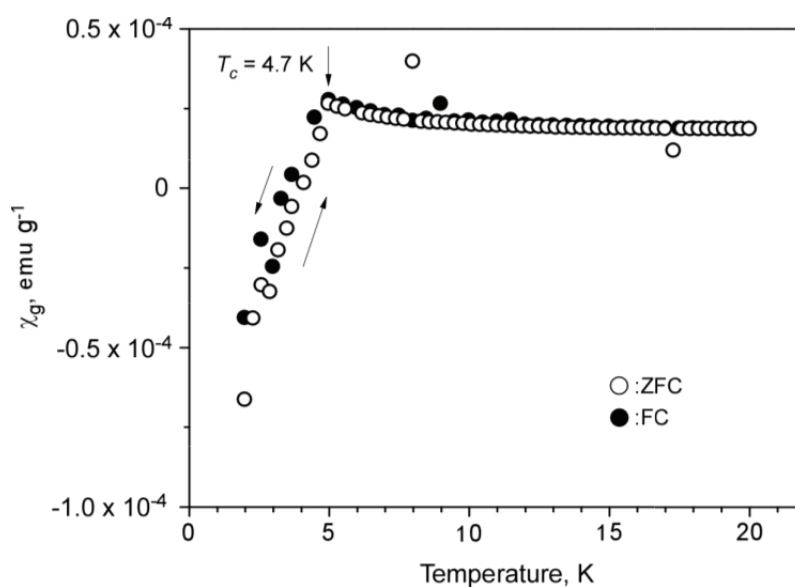


Fig. S1. Magnetic susceptibility of octylamine intercalated TiNCl as a function of temperature. A weak superconducting transition observed at 4.7 K is due to TiN contamination as impurity in the starting material.

Microwave conductivity:

Microwave conductivity measurement has been done on a cavity perturbation method utilizing the TE₀₁₁ resonant mode of a cylindrical cavity made of an oxygen-free copper in a temperature range down to 12 K. The resonance frequency f_0 was 16.3 GHz. The powder sample was filled in a glass tube of an inner diameter of 2 mm with He gas to enhance the thermal equilibrium. The resonance peak obeys a Lorentzian curve. The complex conductivity $\sigma = \sigma_1 + i\sigma_2$, can be derived from the resonance width (Γ_s, Γ_0) and resonance frequency (f_s, f_0), which were measured with the sample (Γ_s, f_s) and without sample (Γ_0, f_0) resonator. The complex conductivity can be calculated based on the observed values of $\Delta\Gamma/2f_0 = (\Gamma_s - \Gamma_0)/2f_0$ and $\Delta f/f_0 = (f_s - f_0)/f_0$. The calculation method should be changed depending on the skin depth of the microwave and size of the sample. If the skin depth is larger than the sample size, electromagnetic fields penetrate uniformly throughout the sample, where so-called a depolarization regime is applied, and the $\Delta f/f_0$ and $\Delta\Gamma/2f_0$ values are very close to zero. On the other hand, if the skin depth is shorter than the sample size, so-called a skin depth regime is applied. At the boundary between these two regimes, the $\Delta\Gamma/2f_0$ value takes a maximum, and the $\Delta f/f_0$ value exhibits a step-like change. When the metallic conductivity increases in the skin depth regime, $\Delta\Gamma/2f_0$ goes to zero, and $\Delta f/f_0$ is approaching a metallic shift $-\gamma/(n-1)$, where γ and n denote a filling factor and depolarization factor, respectively.

In depolarization regime, the complex conductivity is calculated by the following equations;

$$\sigma_1 = \frac{5c^2}{4\pi^2\gamma a^2 f_0} \frac{\Delta\Gamma}{2f_0}, \quad (1)$$

$$\sigma_2 = \frac{1}{2} f_0 \left(\frac{5c^2}{2\pi^2\gamma a^2 f_0^2} \frac{\Delta f}{f_0} + 1 \right). \quad (2)$$

where a and c stand for a sample size and the speed of light, respectively. In this study, the shape of the sample and the size is assumed to be a sphere and the radius of 1 mm, respectively. In the skin depth regime, $\Delta f/f_0$ and $\Delta\Gamma/2f_0$ are related to the surface impedance

($Z_s = R_s + iX_s$) as follows, together with resonator constant ξ and constant C , which depend on the size and shape of the sample.

$$\frac{\Delta\Gamma}{2f_0} = \xi R_s, \quad \frac{\Delta f}{f_0} = \xi X_s + C. \quad (3)$$

At the transition temperature between the depolarization and the skin depth regimes, we determined the constants ξ and C so as to achieve continuous connections in σ_1 and σ_2 .

Finally, the complex conductivity is obtained by the equations;

$$\sigma_1 = \frac{f_0 R_s X_s}{(R_s^2 + X_s^2)^2}, \quad (4)$$

$$\sigma_2 = \frac{f_0 (X_s^2 - R_s^2)}{2(R_s^2 + X_s^2)^2}. \quad (5)$$

Table S1. Intercalation compounds of TiNCl with various alkyl monoamines (melting temperature, mp , acid dissociation constant, pKa), basal spacing (d), and superconducting characteristics (T_c and superconducting volume fraction).

	Alkyl monoamine			Basal spacing	Superconducting characteristics	
	n ($C_nH_{2n+1}NH_2$)	mp , °C	pKa	d , Å	T_c , K	Volume fraction, %
Propyl	3	-83	10.6	11.96, 15.45	4.1	1.1
Butyl	4	-49	10.77	11.98, 17.28	4.5	0.4
Pentyl	5	-50	10.63	13.9		
Hexyl	6	-19	10.56	21.01	3.2	0.5
Heptyl	7	-23	10.67	16.55, 21.71	3.2	0.6
Octyl	8	-1	10.65	33.12, 21.79	3.5	0.5
Nonyl	9	-1	10.64	12.45	5.3	<0.1
Decyl	10	12	10.64	36.92	4.7	0.3
Undecyl	11	16.5	10.63	13.11	4.1	0.3
Dodecyl	12	28	10.63	16.59	3.2	0.4