Electronic Supplementary Information

for

Stereoselective synthesis of different cyclic tetrasiloxane isomers depending on the superacid catalyst employed

Kanako Sonoda,[a] Norimitsu Tohnai[b] and Yoshiro Kaneko*[a]

[a] Graduate School of Science and Engineering, Kagoshima University, 1-21-40, Korimoto, Kagoshima 890-0065, Japan

[b] Graduate School of Engineering, Osaka University, 2-1, Yamadaoka, Suita, Osaka 565-0871, Japan

*Correspondence Addresses (E-mail): ykaneko@eng.kagoshima-u.ac.jp

Table S1 Crystal Data, Data Collection, and Structure Refinement of Boc-CyTS-NNf_2 and Boc-CyTS-NHf_2

	Boc-CyTS-NNf_2	Boc-CyTS-NHf_2
chemical formula	$C_{36}H_{76}N_4O_{12}Si_4$	$C_{36}H_{76}N_4O_{12}Si_4$
formula weight	869.36	869.36
crystal system	monoclinic	monoclinic
space group	$P2_1/n$ (No. 14)	$P2_1/c$ (No. 14)
a (Å)	9.6119(2)	17.2917(2)
b (Å)	22.4858(4)	14.8352(2)
c (Å)	23.6228(4)	9.99670(10)
β (deg)	95.304(2)	91.5930(10)
V (Å^3)	5083.76(16)	2563.42(5)
D_{calc} (g cm^{-3})	1.136	1.126
Z	4	4
F(000)	1888	944
μ(Mo Kα) (cm^{-1})	1.535	1.522
T (°C)	−60	−60
no. of measured reflections	30731	14591
no. of unique reflections	10101	5051
R_{int}	0.0305	0.0324
$R1$[a] (w$R2$[b])	0.0557（0.1297）	0.0551（0.1342）
CCDC	2307476	2307477

[a]$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b]w$R2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma w(F_o^2)^2]^{1/2}$.

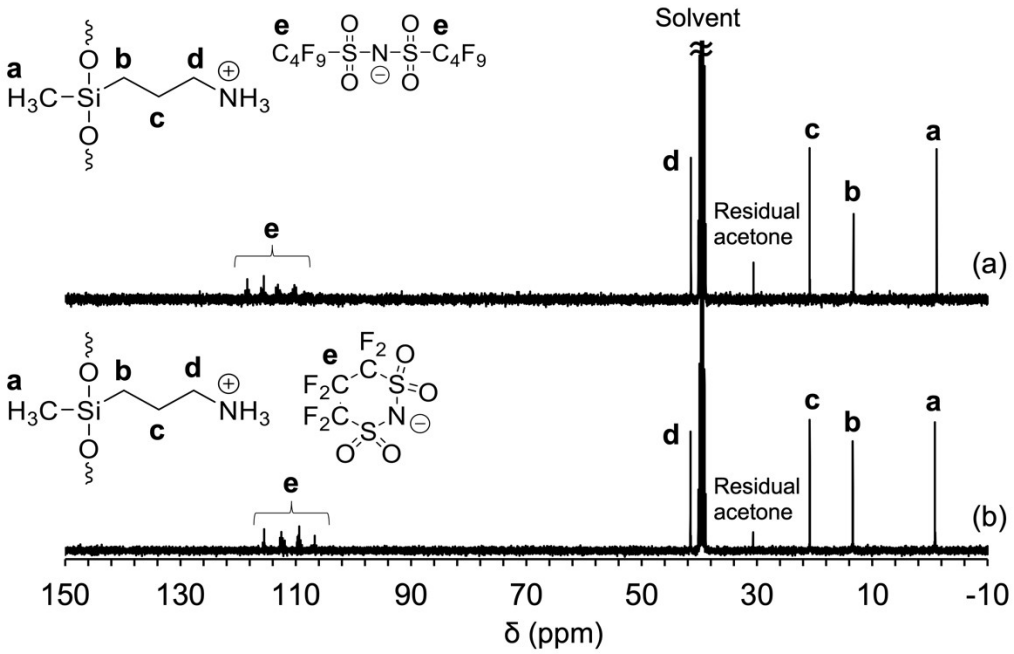

Fig. S1 ^{13}C NMR spectra of (a) Am-CyTS-NNf_2 and (b) Am-CyTS-NHf_2 in DMSO-d_6. Chemical shifts were referenced to DMSO-d_6 (δ 39.7).

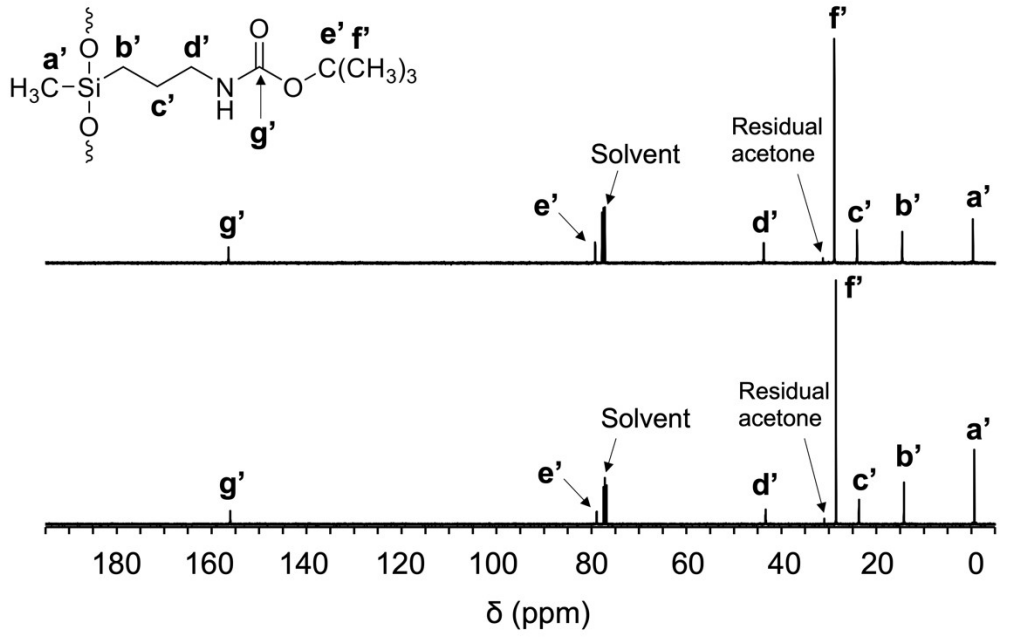

Fig. S2 ^{13}C NMR spectra of (a) Boc-CyTS-NNf_2 and (b) Boc-CyTS-NHf_2 in $CDCl_3$. Chemical shifts were referenced to $CDCl_3$ (δ 77.0).

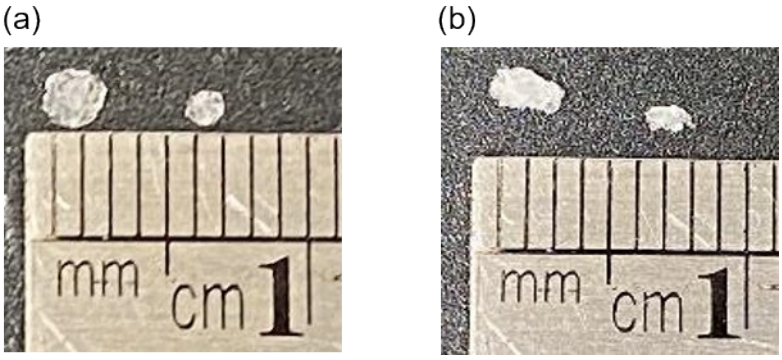

Fig. S3 Photographs of the single crystals of (a) Boc-CyTS-NNf_2 and (b) Boc-CyTS-NHf_2.

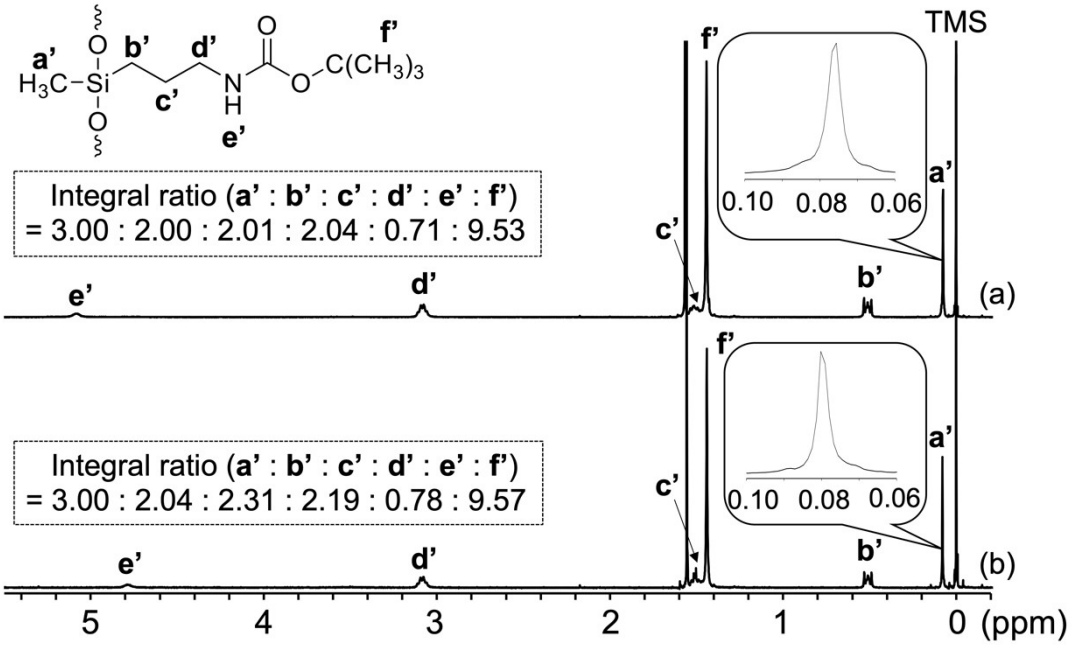

Fig. S4 ^{1}H NMR spectra of the recrystallized (a) Boc-CyTS-NNf_2 and (b) Boc-CyTS-NHf_2 in $CDCl_3$. Chemical shifts were referenced to TMS (δ 0.0).