Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting Information

Inorganic Ba-Sn Nanocomposite Materials for Sulfate Sequestration from Complex Aqueous Solutions

Isaac E. Johnson, [†] Sayandev Chatterjee, [†] Gabriel B. Hall, [†] Sarah D. Burton, [‡] Emily L. Campbell, [†] Michele A. Conroy, [†] Yingge Du, [‡] Meghan S. Fujimoto, [†] Tamas Varga, [‡] Albert A. Kruger, [§] Tatiana G. Levitskaia[*†]

Organizations

[†]Energy and Environment Directorate, Pacific Northwest National Laboratory, Richland, WA 99354, USA. E-mail: Tatiana.Levitskaia@pnnl.gov

[‡]Environmental and Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99354, USA

[§] U.S. Department of Energy, Office of River Protection, Richland, WA 99352, USA

Table S1. AN-102 Low Activity Waste (LAW) Simulant composition. Metal ion concentration was analyzed by ICP after precipitate was settled and filtered out.

Component	Target Molarity (moles/L)	ICP-OES Molarity [a] (moles/L)
Na^+	5.1	5.37±0.09
Al^{3+}	0.235	0.15±0.03
K^+	0.13	0.14±0.01
CrO_4^{2-}	0.012	0.0118±0.0004
SO_4^{2-}	0.085	0.094±0.003
PO_4^{3-}	0.020	0.0205±0.0008
Cl^-	0.064	
F^-	0.047	
NO_2^-	0.94	
NO_3^-	1.11	
CO_3^{2-}	0.46	
HCO_2^- (formate)	0.37	
$C_2O_4^{2-}$ (oxalate)	0.011	
$C_2H_3O_3^-$ (glycolate)	0.28	
$C_6H_5O_7^{3-}$ (citrate)	0.047	
OH^-	0.4	0.47±0.01 [b]

[a] Standard deviation across sample measurements from six different batches of AN-102 simulant.

[b] Determined by potentiometric titration

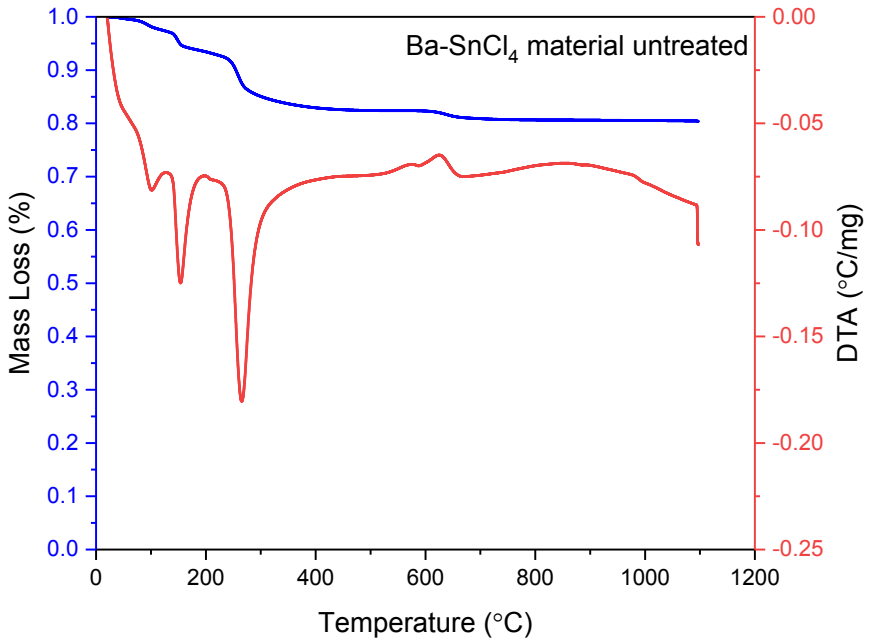

Figure S1. Thermogravimetric analysis and differential thermal analysis of the as synthesized **Ba-$SnCl_4$** material.

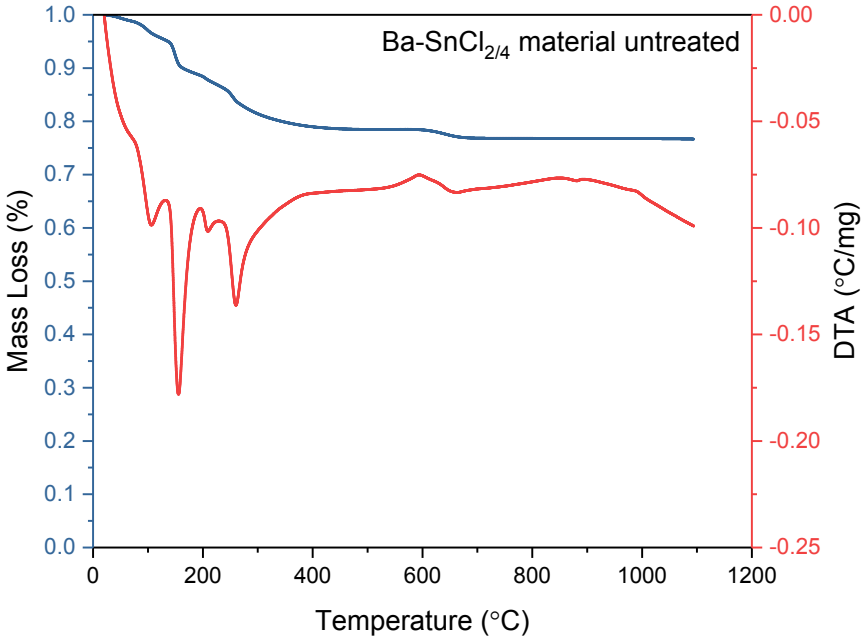

Figure S2. Thermogravimetric analysis and differential thermal analysis of the as synthesized **Ba-$SnCl_{2/4}$** material.

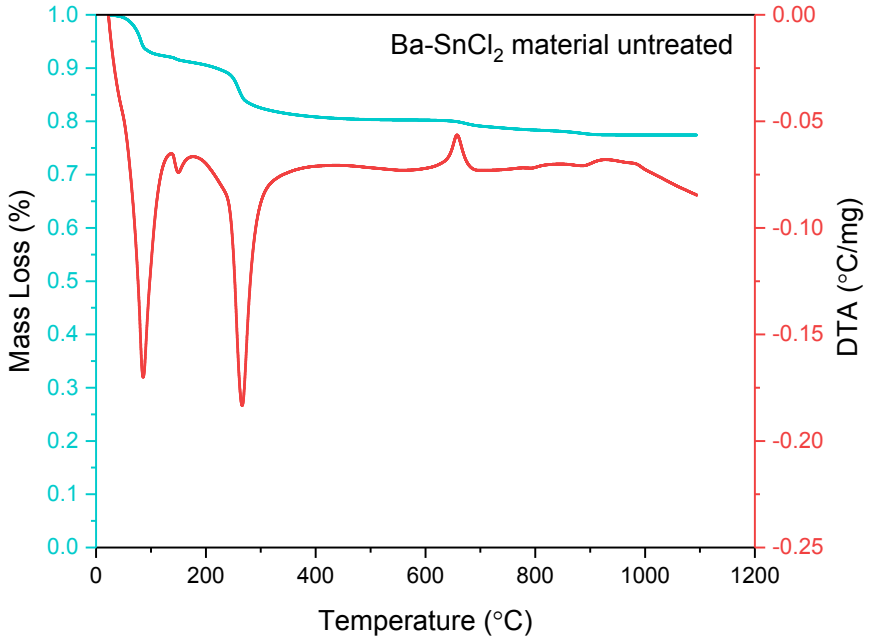

Figure S3. Thermogravimetric analysis and differential thermal analysis of the as synthesized **Ba-$SnCl_2$** material.

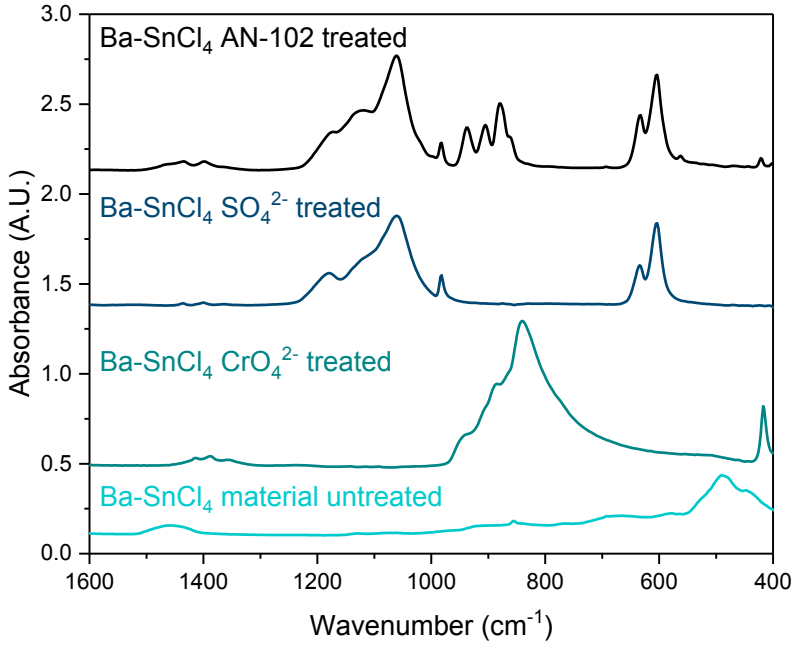

Figure S4. IR spectra of the synthesized **Ba-$SnCl_4$** material before and after being exposed to the AN-102 simulant or 0.5 M NaOH/1.11 M $NaNO_3$ solutions containing 85 mM of Na_2SO_4 or Na_2CrO_4.

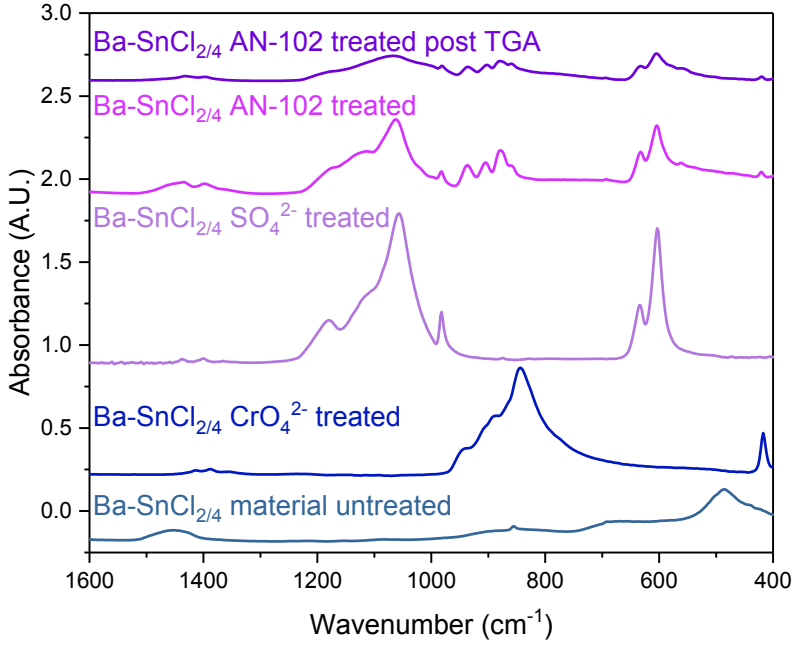

Figure S5. IR spectra of the synthesized **Ba-$SnCl_{2/4}$** material before and after being exposed to the AN-102 simulant or 0.5 M NaOH/1.11 M $NaNO_3$ solutions containing 85 mM of Na_2SO_4 or Na_2CrO_4.

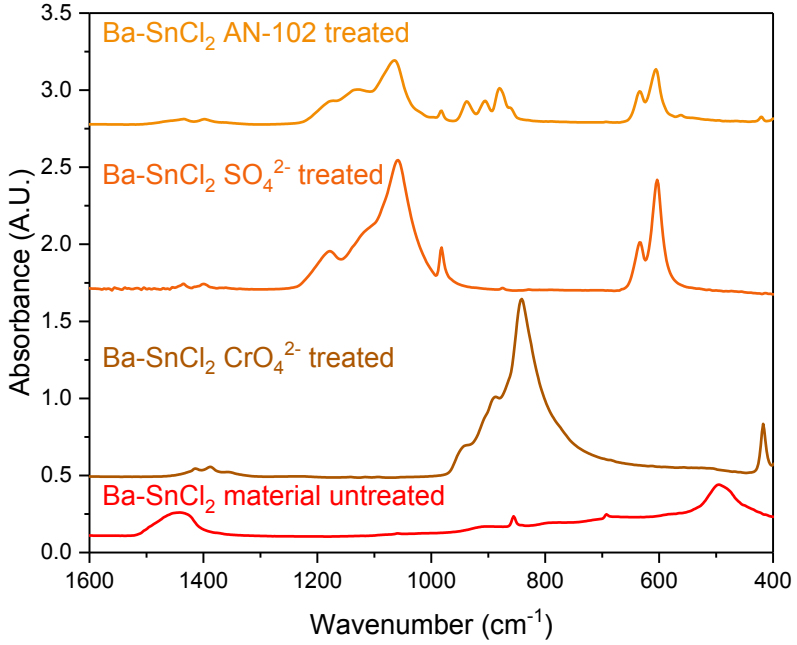

Figure S6. IR spectra of the synthesized **Ba-$SnCl_2$** material before and after being exposed to the AN-102 simulant or 0.5 M NaOH/1.11 M $NaNO_3$ solutions containing 85 mM of Na_2SO_4 or Na_2CrO_4.

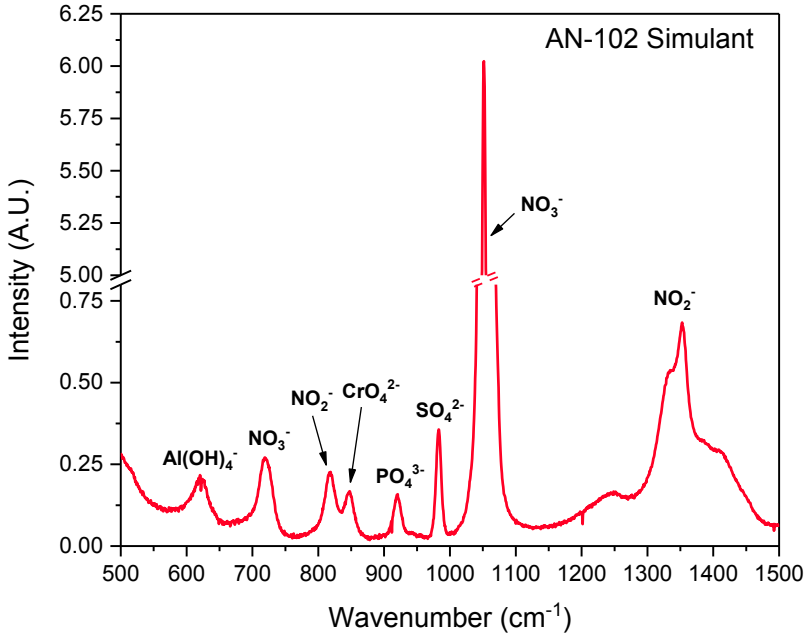

Figure S7. Raman spectrum of AN-102 simulant.

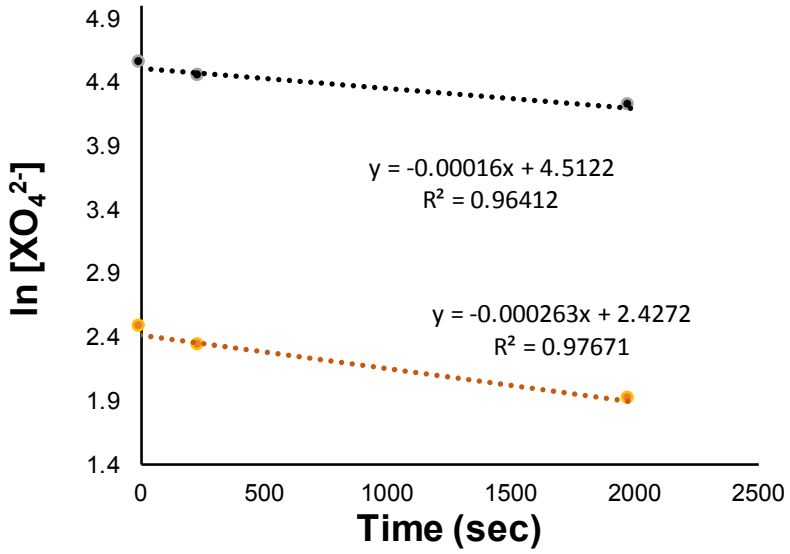

Figure S8. Kinetics of SO_4^{2-} (black symbols) and CrO_4^{2-} (orange symbols) removal by **Ba-SnO** material from the AN-102 simulant: semi-logarithmic plots of the molar concentration in the contact solutions vs time.

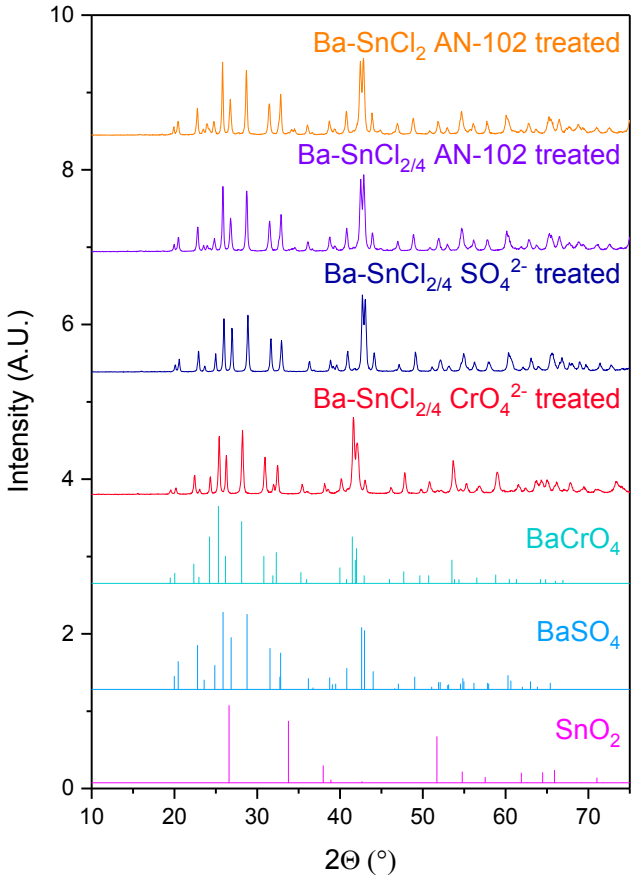

Figure S9. X-ray diffractograms of reference compounds and **Ba-$SnCl_2$, Ba-$SnCl_{2/4}$** materials exposed to the AN-102 simulant or 0.5 M NaOH/1.11 M $NaNO_3$ solutions containing 85 mM of Na_2SO_4 or Na_2CrO_4.

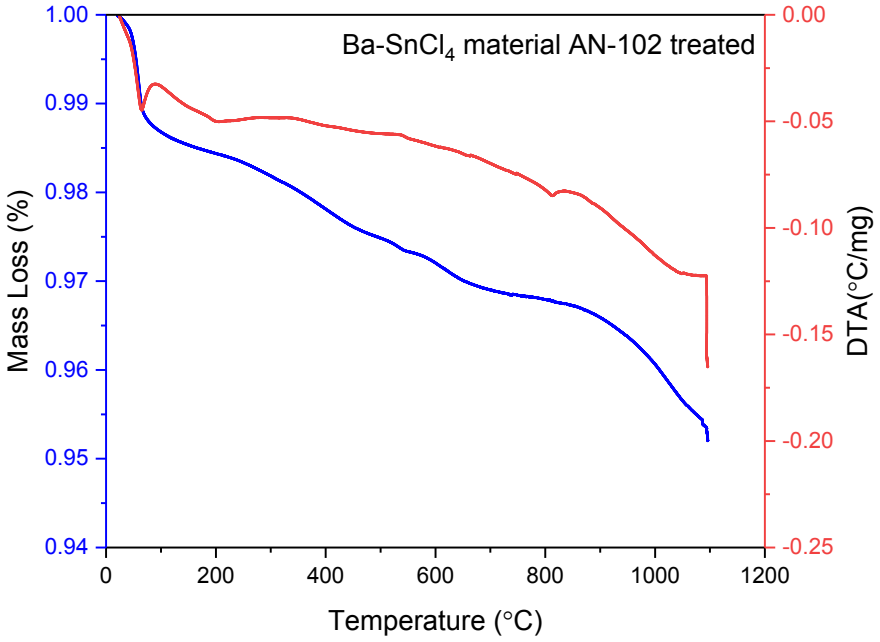

Figure S10. Thermogravimetric analysis and differential thermal analysis of the **Ba-$SnCl_4$** material after treatment with AN-102 simulant.

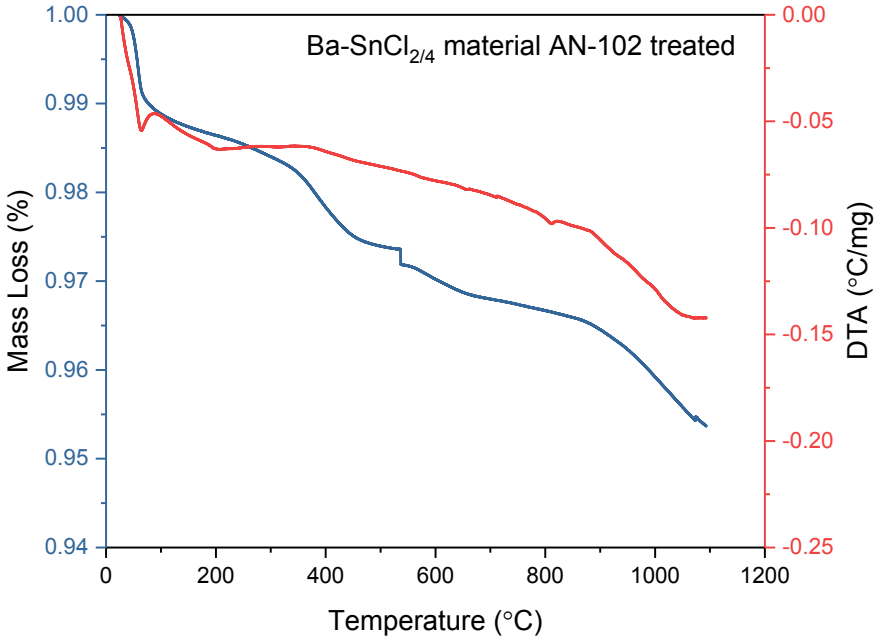

Figure S11. Thermogravimetric analysis and differential thermal analysis of the **Ba-$SnCl_{2/4}$** material after treatment with AN-102 simulant.

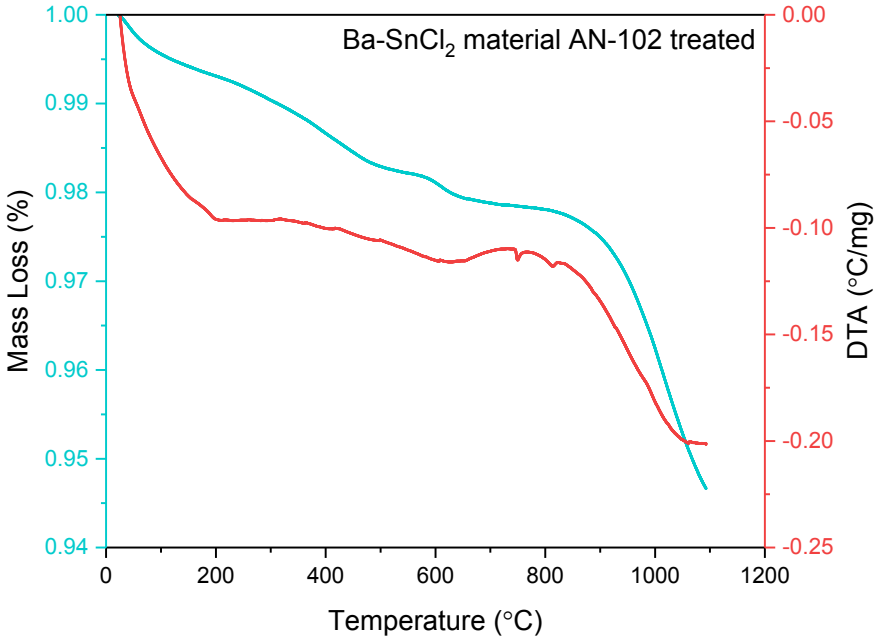

Figure S12. Thermogravimetric analysis and differential thermal analysis of the **Ba-$SnCl_2$** material after treatment with AN-102 simulant.