Electronic supplementary data (ESI) data

SUPPLEMENTARY DATA

Aluminum substituted nickel ferrite (Ni–Al–Fe): a ternary metal oxide adsorbent for arsenic adsorption in aqueous medium

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Synthesis of adsorbent

Aluminium substituted nickel ferrite [Ni-Al-Fe] crystalline adsorbents was prepared by reported procedure and the details are provided here.[1] Aluminum substituted nickel ferrite particles were prepared by self-ignition method by dissolving 0.4 M of each individual salt of aluminium nitrate [$Al(NO_3)_3 \cdot 9H_2O$], nickel nitrate [$Ni(NO_3)_2 \cdot 6H_2O$], ferric nitrate [$Fe(NO_3)_3 \cdot 9H_2O$] salts in D.D water and stir the solutions with help of a magnetic stirrer. Citric acid (1.5 M) was added to the solution as it serves as fuel source for auto/self-combustion reaction. Liquor ammonia was added to the solution to increase the pH value of the system. The temperature of the system was raised to 100 -150 ^oC, around 120 ^oC the self- ignition process starts that leads to the formation of loosely bound aluminium substituted nickel ferrite particles (i.e. Ni-Al-Fe, the composition is evaluated as $NiAl_{0.64}Fe_{0.97}O_4$ using ICP-OES).

The loose bound particles were centrifuged in D.D water at 5000 rpm for 15 mins and filtered with D.D water using normal filter. Following the filtration the powders were oven treated at 100 ºC for 18-20 h followed by heat treatment at 550 ºC in a furnace for 3-4 h in normal atmosphere conditions. These processes were given in tabular form in table S1.

Table S1. Table indicating the adsorbent name/code, precursors and heat treatment conditions.

Adsorbent name and chemical formula	**Adsorbent code**	**precursors**	**Heat treatment**
Al-substituted nickel ferrite ($NiAl_{0.64}Fe_{0.97}O_4$)	(Ni-Al-Fe)	Al $(NO_3)_3 \cdot 9H_2O$ (0.4 M) $Ni(NO_3)_2 \cdot 6H_2O$ (0.4 M) $Fe(NO_3)_3 \cdot 9H_2O$ (0.4 M) Citric acid (1.5 M)	100 ºC (oven): 18 h 550 ºC (furnace): 3-4 h

Table S2. Adsorption Kinetics data

S.No	Time (mins)	As(III) final concentration (C_f) ppm	As(V) final concentration (C_f) ppm
1.	0	12	12
2.	2	9.688	7.936
3.	5	9.534	7.779
4.	10	9.523	7.707
5.	15	9.47	7.604
6.	30	9.331	7.576
7.	60	9.277	7.36
8.	120	9.249	7.48
9.	180	9.18	7.373
10.	240	9.102	7.36
11.	360	8.841	7.323

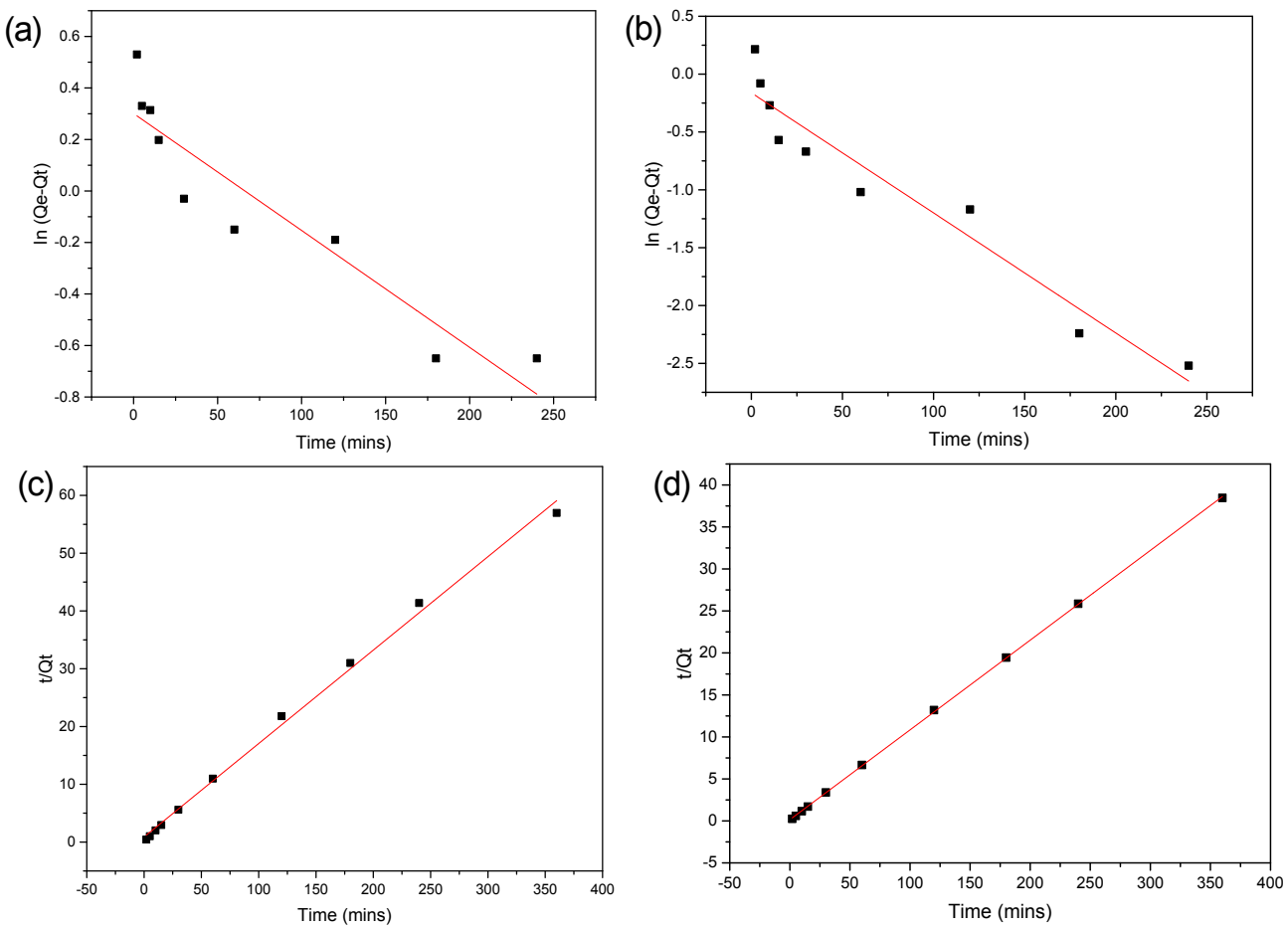

Figure S1. PFO and PSO adsorption kinetics plots of arsenic systems. (a) As(III)- pseudo first order (b) As(V) - pseudo first order (c) As(III)- pseudo second order (d) As(V)- pseudo second order.

Table S3. Adsorption isotherms data

S No.	Initial arsenic (As) concentration (C_o) ppm (mg L^{-1})	As(III) equilibrium concentration (C_e) ppm (mg L^{-1})	As(V) equilibrium concentration (C_e) ppm (mg L^{-1})
1.	0.1	0.0278	0.0059
2.	0.5	0.1837	0.0099
3.	1.0	0.3235	0.0294
4.	5.0	2.334	2.329
5.	10.0	5.286	4.84
6.	25.0	17.62	19.41
7.	50.0	35.67	39
8.	100.0	60.0	65.0
9.	150.0	93.0	98.5

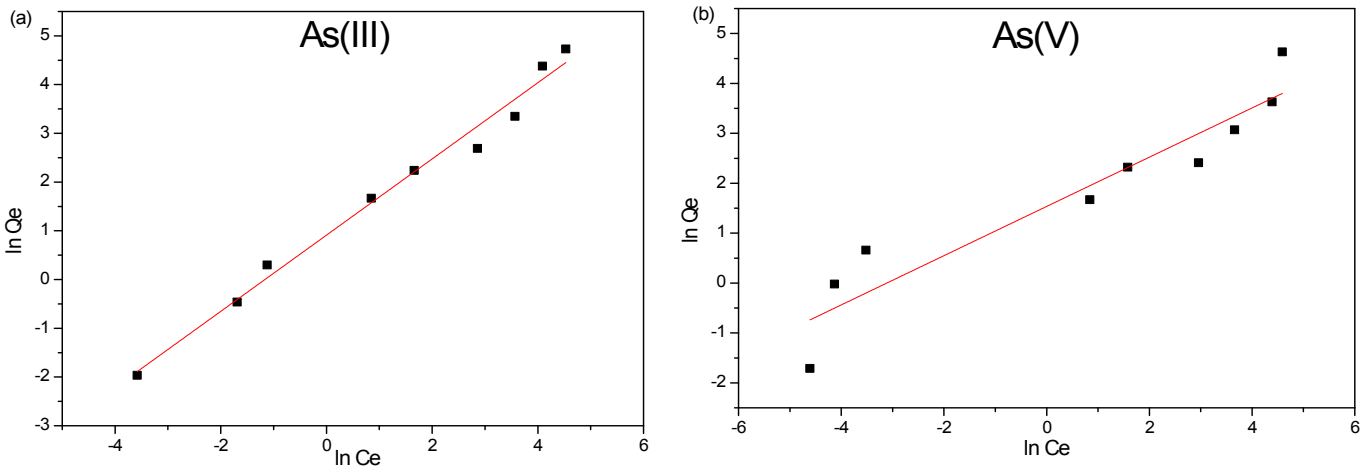

Figure S2. Freundlich adsorption isotherm plots of arsenic systems. (a) As(III) systems (b) As(V) systems.

Table S4. pH variation based studies data

S.No	pH value of the system	As(III) final concentration (C_f) ppm	As(V) Final concentration (C_f) ppm
1.	pH 2	5.77	4.45
2.	pH 5	6.36	2.69
3.	pH 7	6.92	4.87
4.	pH 9	6.58	5.42
5.	pH 12	5.53	6.35

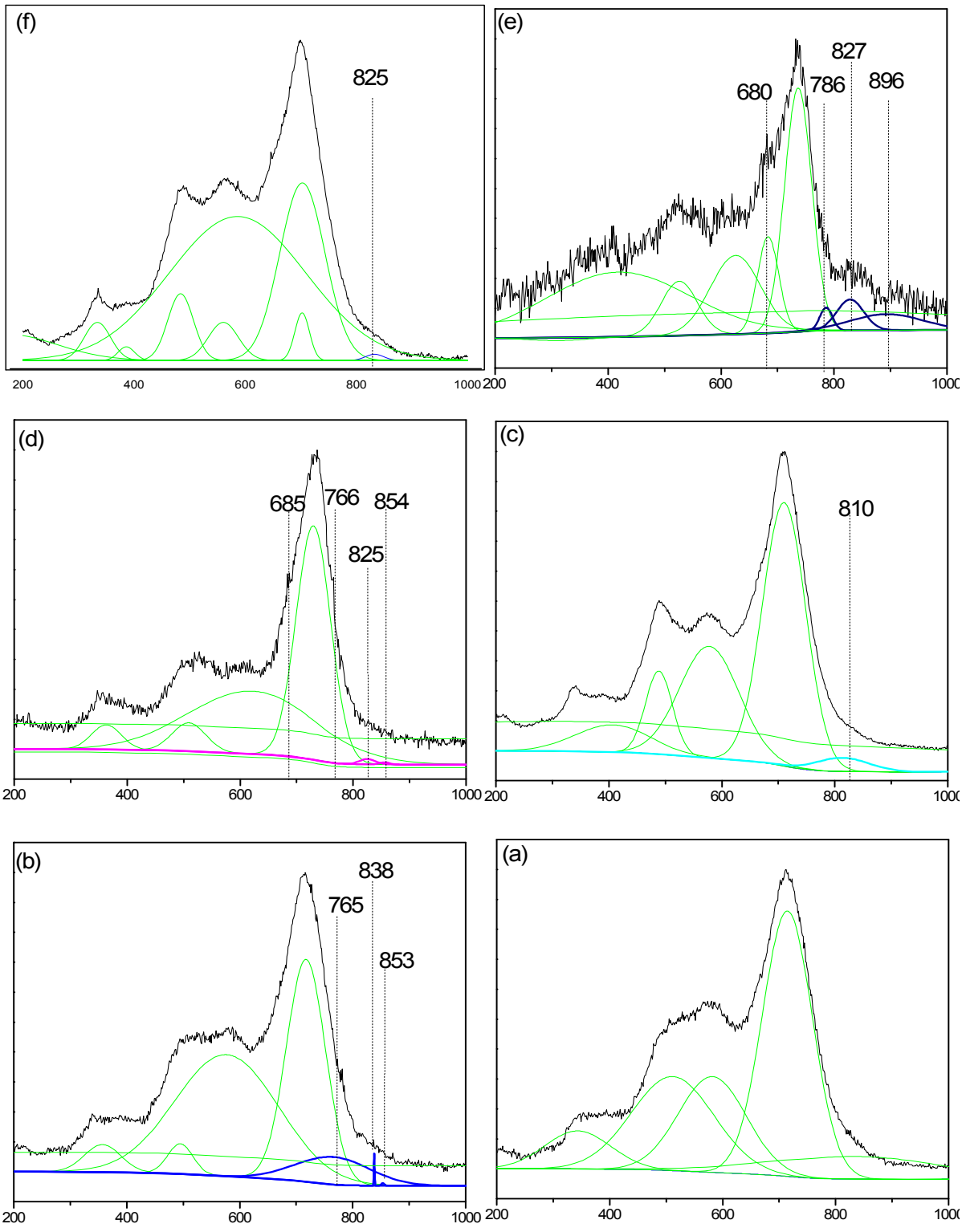

Figure S3. Raman spectra of pure and As (III) adsorbed Ni-Al-Fe ferrite particles at different pH conditions. (a) Un-adsorbed sample (b) pH 2.0 (c) pH 5.0 (d) pH 7.0 (e) pH 9.0 (f) pH 12.0.

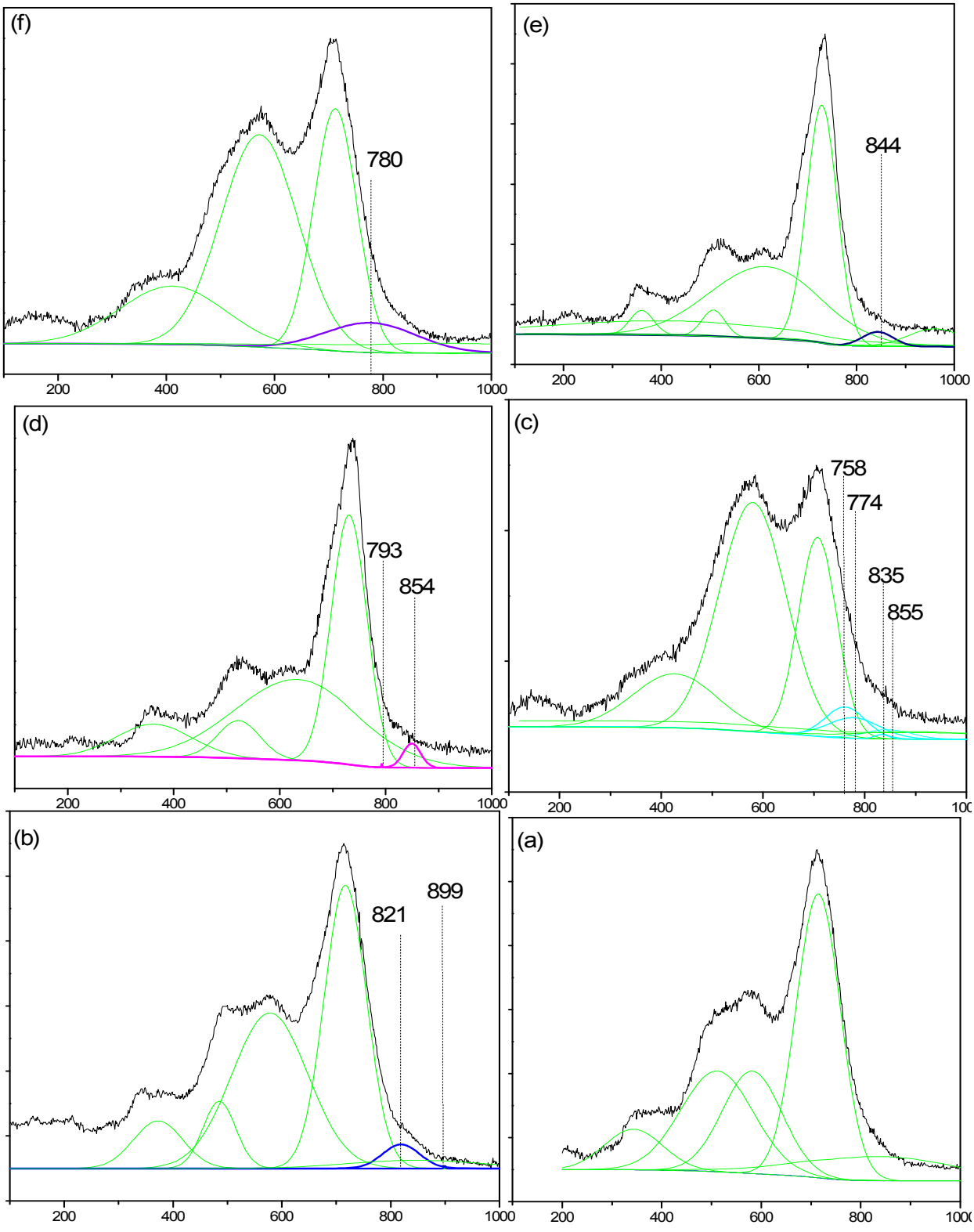

Figure S4. Raman spectra of pure and As (V) adsorbed Ni-Al-Fe ferrite particles at different pH conditions. (a) Un-adsorbed sample (b) pH 2.0 (c) pH 5.0 (d) pH 7.0 (e) pH 9.0 (f) pH 12.0.

Table S5. As-O and As-OH stretching vibrations onto different adsorbents

Adsorbent	As-O stretching vibrations -wave numbers(cm^{-1})	
	Symmetric (ν_s)	**Asymmetric (ν_{as})**
$Ca(OH)_2$ [2][*]	[+] I 798-812$_{As\text{-}OH\ [¥]}$; IR879 $_{As\text{-}O}$	I 885-905$_{As\text{-}O}$
Gibbsite [2]	I 880$_{As\text{-}O}$	N/A
Hydrous Fe-oxides[2] (freshly prepared)	I 700$_{As\text{-}OH}$; I 802$_{As\text{-}OH}$	I 875$_{As\text{-}OH}$
Goethite (α-FeOOH)[2]	I 730$_{As\text{-}OH}$; I 810$_{As\text{-}OH/}$ I 938$_{As\text{-}OH}$	I 834$_{As\text{-}OH}$
Hydrous Mn-oxide[3]	I 860-873$_{As\text{-}O}$	I 906$_{As\text{-}O}$
Granular ferric hydroxide	I 825-839$_{As\text{-}O}$	I 880-889$_{As\text{-}O}$
Feroxyhyte/ferrihydrite[5]	R840$_{As\text{-}O}$	I 880$_{As\text{-}O}$
Amorphous Fe-oxide[6]	I 817-824$_{As\text{-}OH}$; I 783$_{As\text{-}OH}$	I 854-861$_{As\text{-}O}$
Amorphous Al-oxide[6]	I 740$_{As\text{-}OH}$, R 845-853$_{As\text{-}O}$	I 887$_{As\text{-}O}$
Ag -surface[2]	R 792$_{As\text{-}OH}$; R 802$_{As\text{-}O}$	R 865$_{As\text{-}O}$
Ni-Al-Fe$^{This\ study}$	**R 810-830$_{As\text{-}O}$** **R680-690$_{As\text{-}OH}$**	**R 840-890$_{As\text{-}O}$** **R 780-790$_{As\text{-}OH}$**

{[*] Superscripts in mineral/adsorbent column represent the references. [+]Superscript prior to the wave numbers representing IR and R indicates the data collected using Infrared (FT-IR, ATR-FTIR, DRIFT) and Raman (Raman, SERS) spectroscopy tools. [¥] Subscripts followed by wave numbers represent the kind of surface complexation. I = FT-IR technique, R = Raman technique}

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