Accommodating Unwelcome Guests in Inorganic Layered Hosts: Inclusion of Chloranil in a Layered Double Hydroxide

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Supporting Information

Figure S1. TGA profiles of (a) Mg-Al LDH-AB, (b) Mg-Al LDH-(AB·*p*-chloranil) and (c) Mg-Al LDH-(AB·*o*-chloranil). The *para*-chloranil to AB molar ratio is 0.81 and *ortho*-chloranil to AB is 0.45. The weight loss below 250 °C was used to estimate the water content.

Figure S2. Calculated Mulliken charges on individual atoms of the (a) *p*-aminobenzoate anion, (b) *para*-chloranil and (c) *ortho*-chloranil molecules.

Table S1. Infrared and Raman band positions and assignments for Mg-Al LDH-AB and potassium *p*-aminobenzoate.

Table S2. Infrared and Raman band positions and assignments for Mg-Al LDH-(AB·*p*-chloranil).

Table S3. Infrared and Raman band positions and assignments for Mg-Al LDH-(AB·*o*-chloranil).

Figure S3. Variation of the interlayer spacing of Mg-Al LDH-(AB·chloranil) with increasing chloranil:AB molar ratio as obtained from MD simulations.

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Figure S2. Calculated Mulliken charges on individual atoms of the (a) *p*-aminobenzoate anion, (b) *para*-chloranil and (c) *ortho*-chloranil molecules. Color code:- dark grey : Carbon, light grey : Hydrogen, red : Oxygen, light green : Chlorine and blue : Nitrogen.

Table S1. Infrared and Raman band positions (cm^{-1}) and assignments for Mg-Al LDH-AB and potassium *p*-aminobenzoate.

Infrared		Raman		Assignment
Potassium <i>p</i> -aminobenzoate	Mg-Al LDH-AB	Potassium <i>p</i> -aminobenzoate	Mg-Al LDH-AB	
3383	3385	3337	3319	$\nu_{\text{asym}}(\text{NH}_2)$
3370	3350	----	----	$\nu(\text{OH})$
3227	3217	3228	3206	$\nu_{\text{symm}}(\text{NH}_2)$
----	----	3062	3062	$\nu(\text{Aromatic C-H})$
----	----	3015	3014	$\nu(\text{Aromatic C-H})$
1606	1611	----	----	$\nu_{\text{asym}}(\text{Aromatic C-C})$
1591	1592	1606	1607	$\delta(\text{N-H})$
1530	1528	1520	1521	$\nu_{\text{asym}}(\text{COO}^-)$ and $\nu_{\text{symm}}(\text{Aromatic C-C})$
1395	1397	1395	1391	$\nu_{\text{symm}}(\text{COO}^-)$
1285	1281	1283	1277	$\nu(\text{C-N})$
1174	1176	1179	1182	$\delta(\text{N-H})$ and $\delta(\text{C-H})$ (out-of-plane) for <i>p</i> -disubstituted benzene
1136	1139	1139	1140	$\delta(\text{C-H})$
1084	1093	----	----	$\delta(\text{C-H})$ (in-plane)
859	857	855	852	$\delta(\text{C-H})$ (out-of-plane) for <i>p</i> -disubstituted benzene
----	673	640	640	Benzene ring vibration
----	444	----	----	$\delta(\text{Layer O-H})$

Table S2. Infrared and Raman band positions (cm⁻¹) and assignments for Mg-Al LDH-(AB·*p*-chloranil).

Infrared	Raman	Assignment
3385	3335	$\nu_{\text{asym}}(\text{NH}_2)$
3350	-----	$\nu(\text{OH})$
3217	3219	$\nu_{\text{symm}}(\text{NH}_2)$
----	3063	$\nu(\text{Aromatic C-H})$
----	3015	$\nu(\text{Aromatic C-H})$
----	1643	$\nu(\text{C=O})$ of chloranil
1611	----	$\nu_{\text{asym}}(\text{Aromatic C-C})$
1592	1606	$\delta(\text{N-H})$
----	1588	$\nu(\text{C=C})$ of chloranil
1528	1517	$\nu_{\text{symm}}(\text{Aromatic C-C})$ and $\nu_{\text{asym}}(\text{COO}^-)$
1397	1391	$\nu_{\text{symm}}(\text{COO}^-)$
----	1311	$\nu(\text{C-C})$ of chloranil
1281	1278	$\nu(\text{C-N})$
----	1245	$\nu(\text{C-Cl})$ of chloranil
1176	1180	$\delta(\text{N-H})$ and $\delta(\text{C-H})$ (out-of-plane) for <i>p</i> -disubstituted benzene
1139	1140	$\delta(\text{C-H})$
1093	----	(C-H) (in-plane)
----	997	$\nu(\text{C-Cl})$ of chloranil
857	852	$\delta(\text{C-H})$ (out-of-plane) for <i>p</i> -disubstituted benzene
673	640	Benzene ring vibration

Table S3. Infrared and Raman band positions (cm^{-1}) and assignments for Mg-Al LDH-(AB·*o*-chloranil).

Infrared	Raman	Assignment
3385	3335	$\nu_{\text{asym}}(\text{NH}_2)$
3350	----	$\nu(\text{OH})$
3217	3219	$\nu_{\text{symm}}(\text{NH}_2)$
----	3063	$\nu(\text{Aromatic C-H})$
----	3015	$\nu(\text{Aromatic C-H})$
----	1637	$\nu(\text{C=O})$ of chloranil
1611	----	$\nu_{\text{asym}}(\text{Aromatic C-C})$
1592	1606	$\delta(\text{N-H})$
----	1562	$\nu(\text{C=C})$ of chloranil
1528	1519	$\nu_{\text{symm}}(\text{Aromatic C-C})$ and $\nu_{\text{asym}}(\text{COO}^-)$
1397	1391	$\nu_{\text{symm}}(\text{COO}^-)$
1281	1278	$\nu(\text{C-N})$
----	1248	$\nu(\text{C-Cl})$ of chloranil
1176	1182	$\delta(\text{C-H})$ (out-of-plane) for <i>p</i> -disubstituted benzene
1139	1142	$\delta(\text{C-H})$
1093	----	(C-H) (in-plane)
----	989	$\nu(\text{C-Cl})$ of chloranil
857	852	$\delta(\text{C-H})$ (out-of-plane) for <i>p</i> -disubstituted benzene
673	640	Benzene ring vibration
444	----	$\delta(\text{Layer O-H})$

Figure S3. Variation of the interlayer spacing of Mg-Al LDH-(AB·chloranil) with increasing chloranil:AB molar ratio as obtained from MD simulations.