

Supplementary Information for the article

pH-Induced Conformational Changes of Histamine in the Solid State

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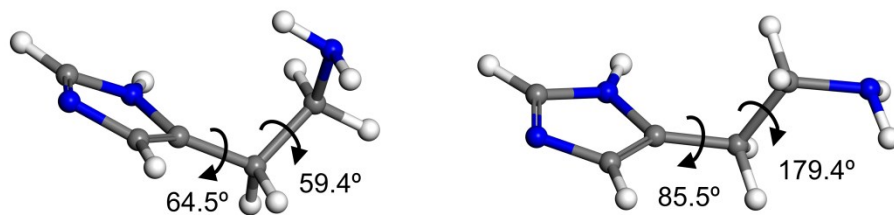
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Table S1. Comparison between the observed and calculated vibrational frequencies (in cm^{-1}) for the various histamine forms.

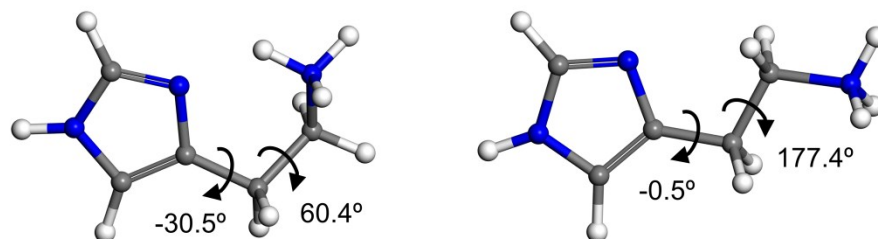
Free base (H1)			Monocation (H2)			Dication (H3)		
Observed	Calculated	Assignments	Observed	Calculated	Assignments	Observed	Calculated	Assignments
3298	3301	Am $\nu(\text{NH})$	3107	3091	Am $\nu(\text{NH}_3^+)$		3188	Am $\nu(\text{NH}_3^+)$
3251	3176	Am $\nu(\text{NH})$					3145	Im $\nu(\text{CH})$
3165	3160	Im $\nu(\text{CH})$	2987	2978	$\nu(\text{CH}_2)$		3109	Im $\nu(\text{CH})$
3105	3151	Im $\nu(\text{CH})$	2948	2939	Am $\nu(\text{NH}_3^+)$	3084	3064	Am $\nu(\text{NH}_3^+)$
2967	2996	$\nu(\text{CH}_2)$	2896		$\nu(\text{CH}_2)$	3014	3022	Im $\nu(\text{NH})$
2955	2953	$\nu(\text{CH}_2)$	2669	2663	Am $\nu(\text{NH}_3^+)$	2949	2954	Im $\nu(\text{NH})$
2581	2567	Im $\nu(\text{NH})$	1626	1631	Am $\delta(\text{NH}_3^+)$	1597	1611	Im $\nu(\text{C}=\text{C})$
1614	1615	Am $\delta(\text{NH})$	1567	1550	Im $\nu(\text{C}=\text{C})$	1526	1530	Am $\delta(\text{NH}_3^+)$
1592	1587	Im $\nu(\text{C}=\text{C})/\text{Im } \delta(\text{NH})$	1477	1465	Im $\delta(\text{ring})$			
1468	1468	Im $\nu(\text{C}=\text{C})/\text{Im } \delta(\text{NH})$	1441	1445	Im $\delta(\text{ring})$	1474	1496	Im $\nu(\text{ring})$
1453	1452	Im $\delta(\text{ring})$	1388	1372	$\omega(\text{CH}_2)$	1454	1459	Im $\delta(\text{ring})$
1429	1423	$\delta(\text{CH}_2)$	1319	1332	$t(\text{CH}_2)$	1437	1444	$\delta(\text{CH}_2)$
1355	1335	$\omega(\text{CH}_2)$	1247	1240	$\omega(\text{CH}_2)$	1347	1337	$\omega(\text{CH}_2)$
1291	1275	$\omega(\text{CH}_2)$				1237	1244	$\omega(\text{CH}_2)$
1177	1177	Im $\delta(\text{CH})$				1178	1172	Im $\delta(\text{ring})$
1124	1123	Am $t(\text{NH})$	1155	1158	Am $r(\text{NH}_3^+)$	1149	1143	Am $r(\text{NH}_3^+)$
1092	1090	Im $\delta(\text{CH})$	1094	1086	Im $\delta(\text{CH})$	1090	1099	Im $\delta(\text{CH})$
1031	1015	$\nu(\text{skel})$	1026	1014	$\nu(\text{skel})$	1030	1020	$\nu(\text{skel})$
923	906	Im $\delta(\text{ring})$	989	980	Im $\delta(\text{ring})$	957	949	$\nu(\text{skel})$
830	798	Im $\gamma(\text{CH})$	848	845	Im $\gamma(\text{ring})$	852	866	Im $\gamma(\text{ring})$
811	793	Im $\gamma(\text{CH})$	803	808	Im $\gamma(\text{ring})$	804	794	Im $\gamma(\text{CH})$
665	658	Im $\gamma(\text{ring})$	681	674	Im $\gamma(\text{ring})$			
628	643	Im $\gamma(\text{ring})$	623	626	Im $\gamma(\text{ring})$	618	611	Im $\gamma(\text{ring})$

Assignments: Am; amine, Im; imidazole ring, ν ; stretching, δ ; in-plane bending, γ ; out-of-plane bending, r ; rocking, t ; twisting, ω ; wagging, skel; skeletal side-chain.

(a) H1 (*GG* and *GT* model)



(b) H2 (*GG* and *GT* model)



(c) H3 (*GT* and *TT* model)

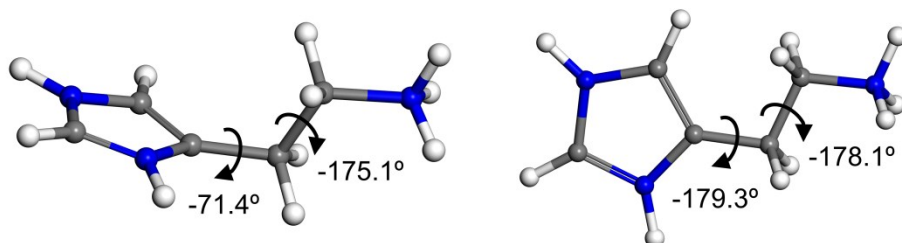


Fig. S1. Molecular conformations (*GG*, *GT* and *TT*) and the corresponding torsional angles (τ_1 and τ_2) predicted for (a) free base (H1), (b) monocation (H2), and (c) dication (H3) by the conformational analysis.

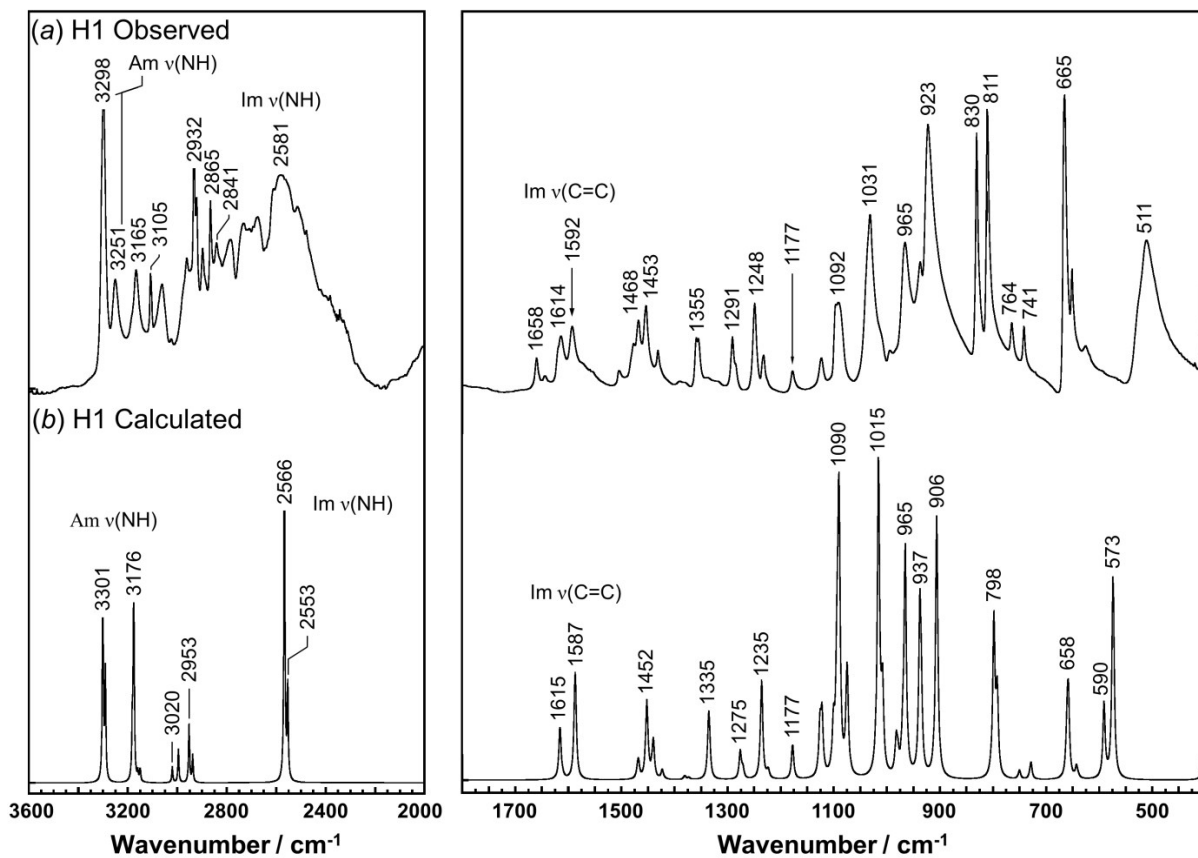


Fig. S2. Infrared spectra of histamine free base form (H1) : (a) the experimental data and (b) the calculated results.

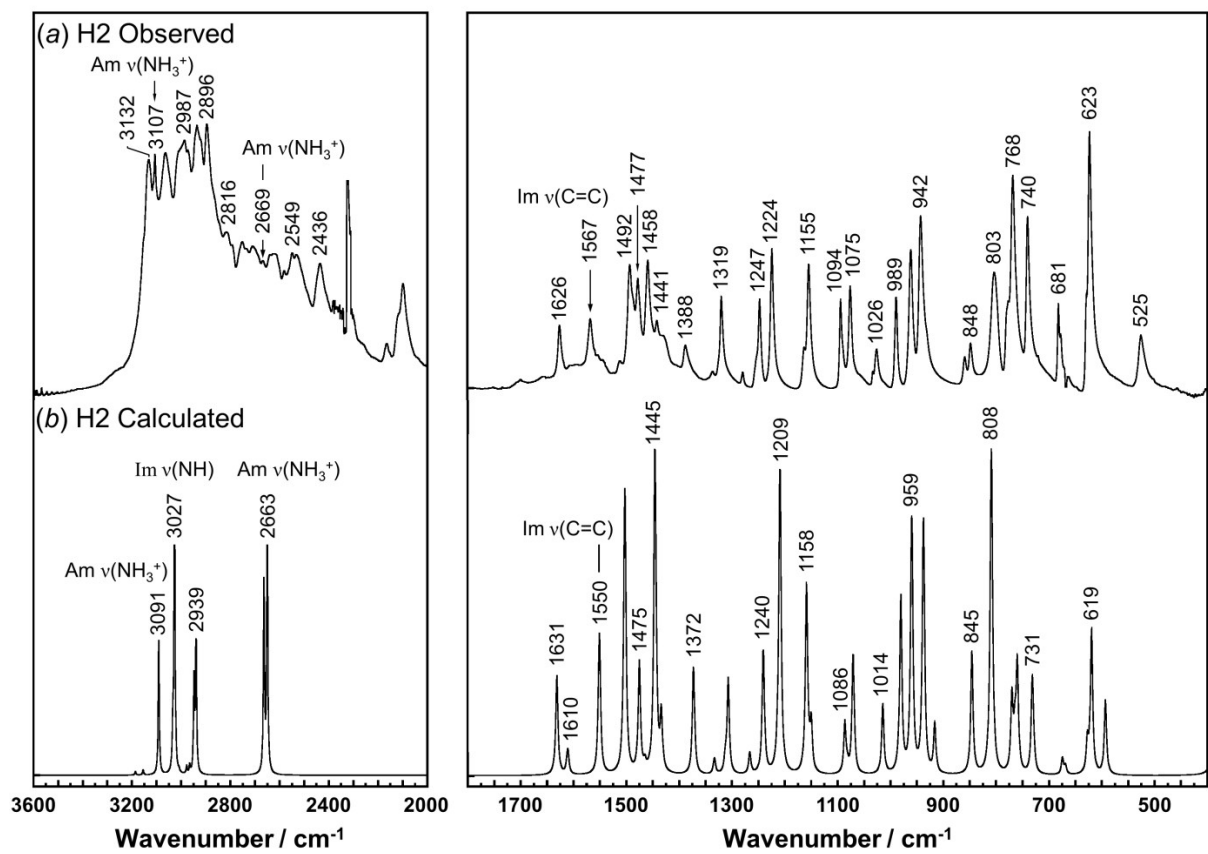


Fig. S3. Infrared spectra of histamine monocation form (H2): (a) the experimental data and (b) the calculated results.

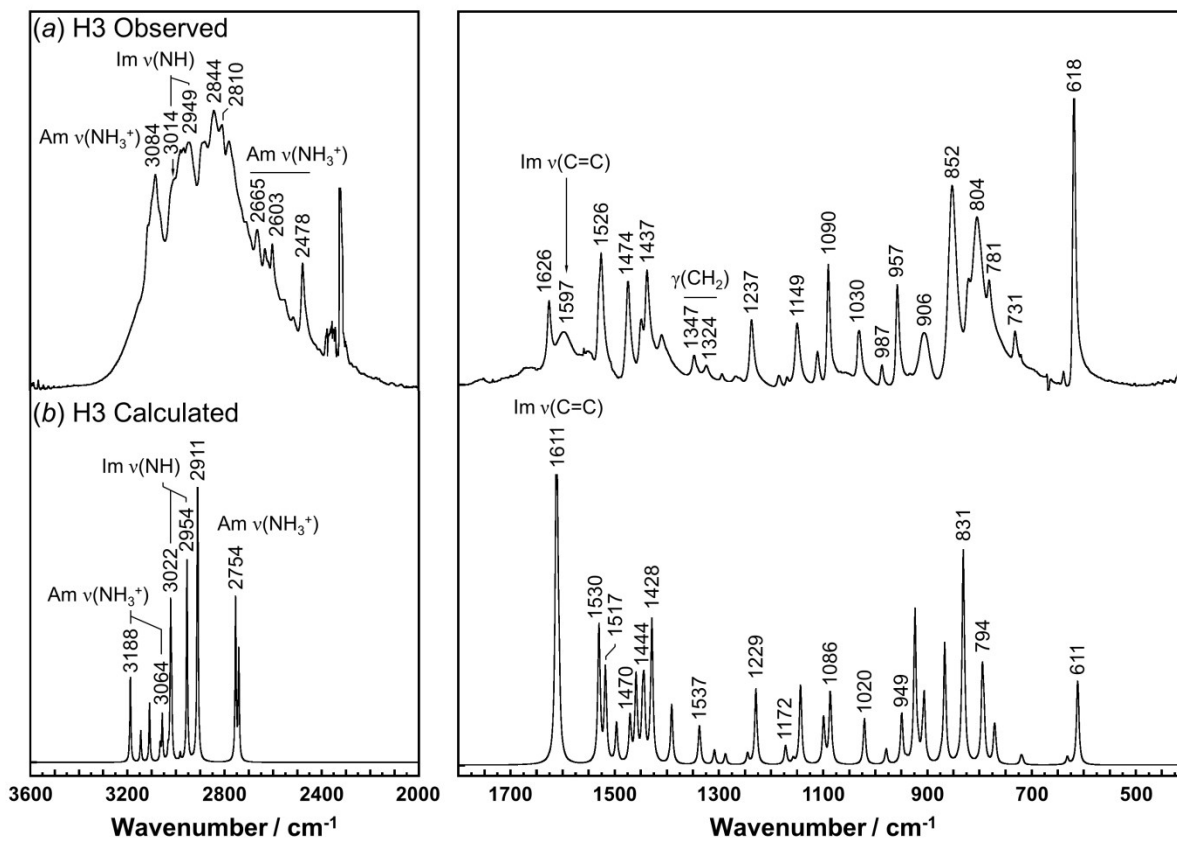


Fig. S4. Infrared spectra of histamine free base form (H3): (a) the experimental data and (b) the calculated results.

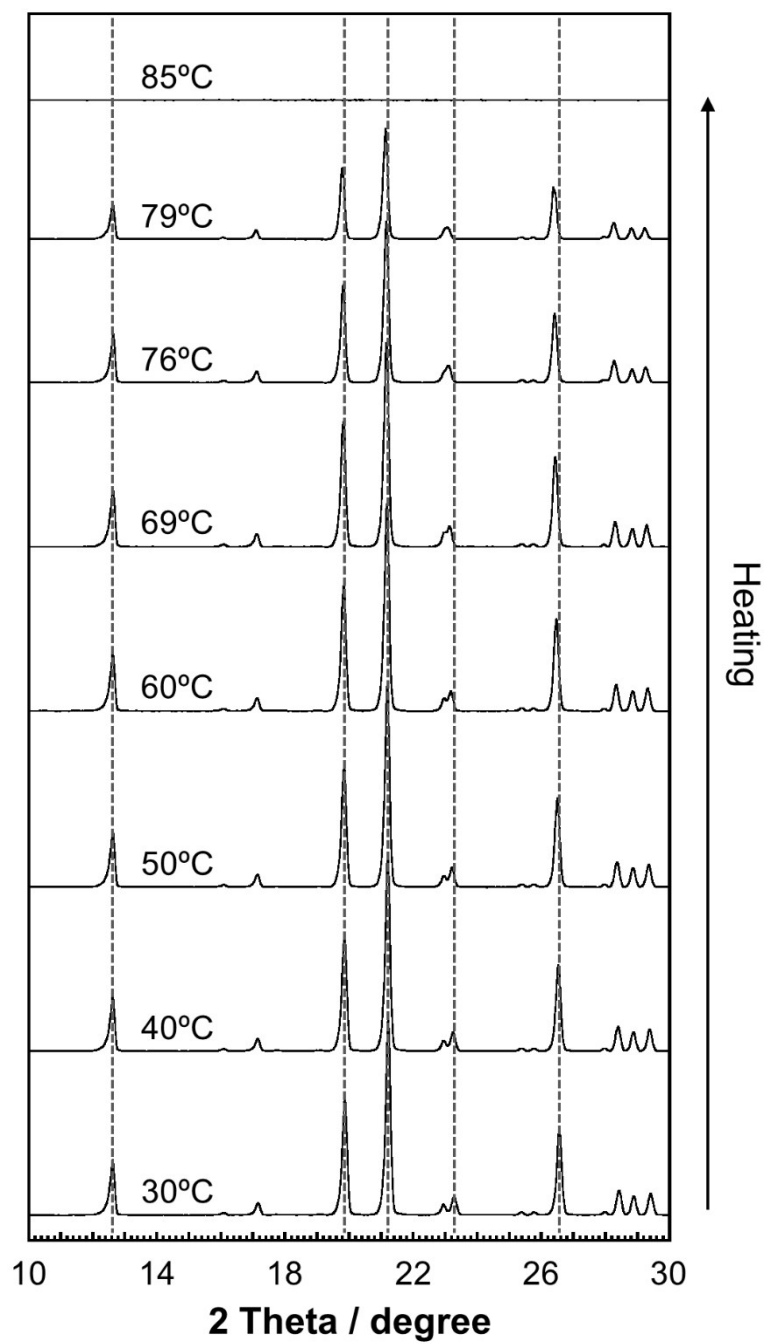


Fig. S5. X-ray diffraction profiles of histamine free base (H1) measured in the heating process. The X-ray wavelength is 1.5418 Å (Cu-K α).

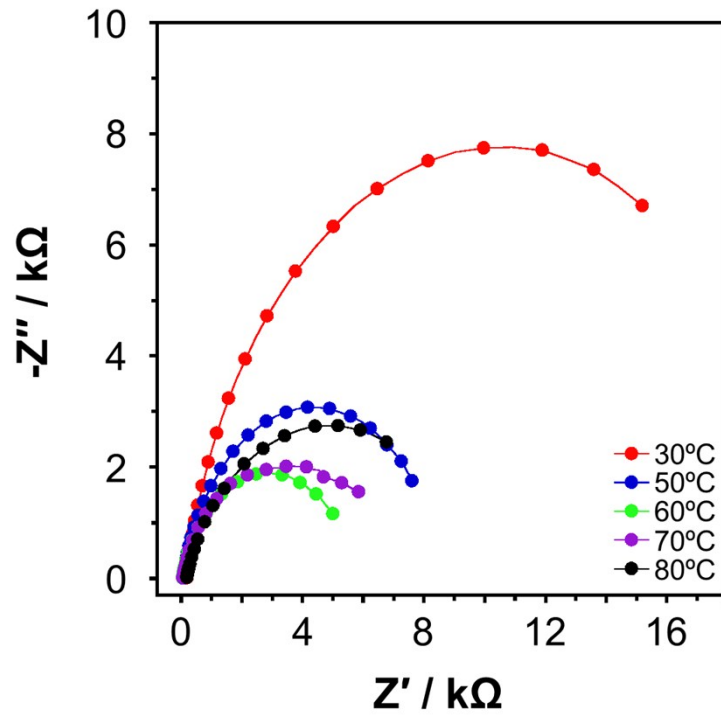


Fig. S6. Nyquist plot of histamine free base (H1) measured at the various temperature.