Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

The role of weak hydrogen bonds in chiral recognition

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Supplementary information

Figure S1

Comparison between the IRMPD spectra of QnH^+ (triangles) and its pseudo enantiomer QdH^+ (squares) in the region of the ν(OH) stretch.

Figure S2

IRMPD spectrum of $(CdQn)H^+$ in the 2800-3800 cm^{-1} energy range.

Figure S3

Most stable calculated structures of $(CdQn)H^+$ obtained at the b3-lyp/6-31+G* level of the theory.

Figure S4

Most stable calculated structures of $(CdQd)H^+$ obtained at the b3-lyp/6-31+G* level of the theory.

Figure S5

IRMPD spectrum of $(CdQd)H^+$ in the 2800-3800 cm^{-1} energy range.

Figure S1

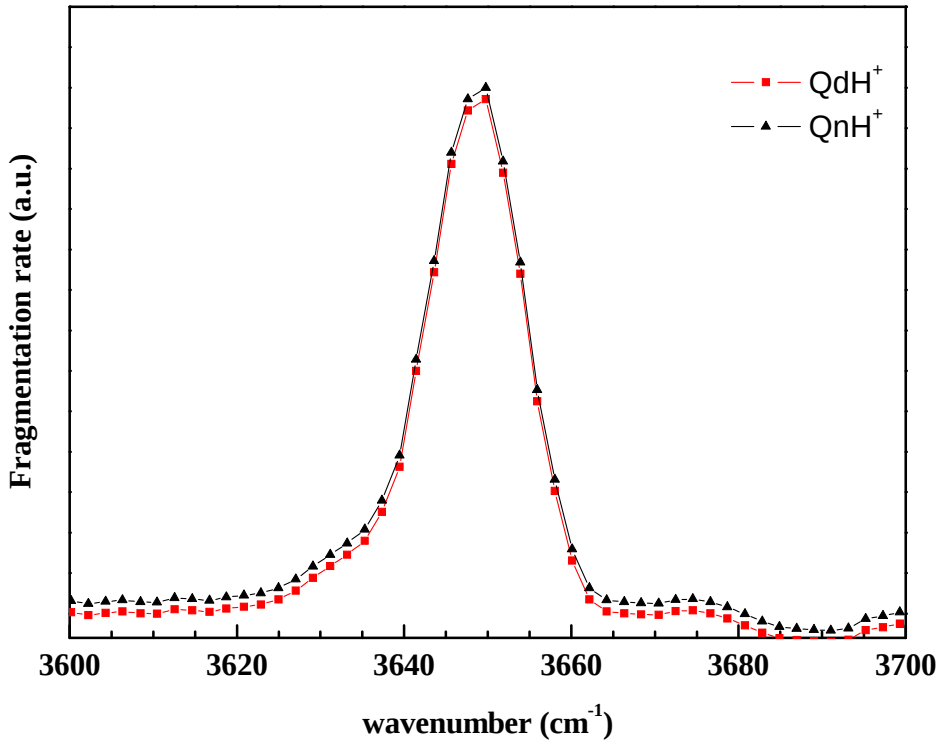

QdH+
QnH+
Fragmentation rate (a.u.)
3600
3620
3640
3660
3680
3700
wavenumber (cm-1)

Figure S2

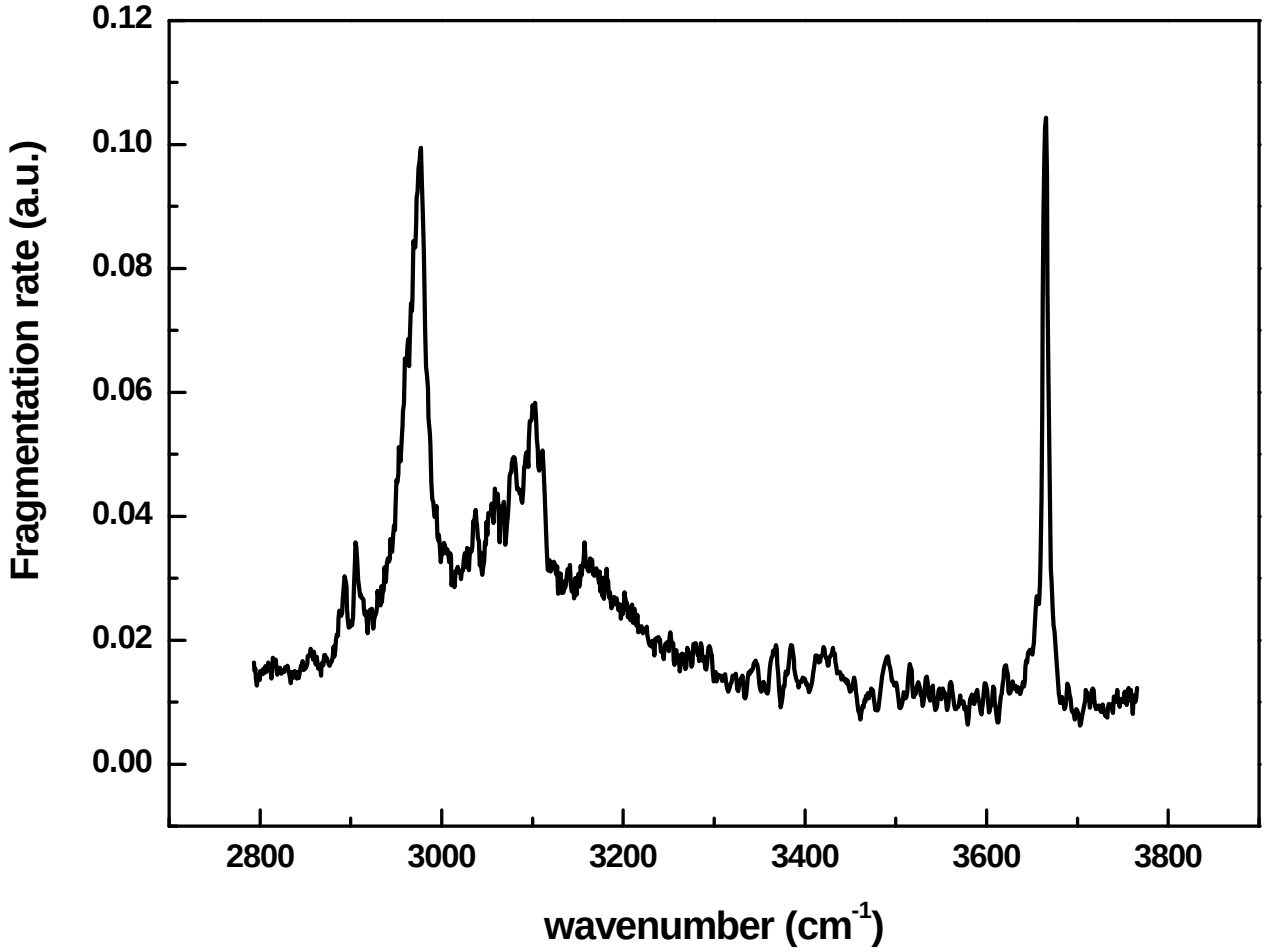
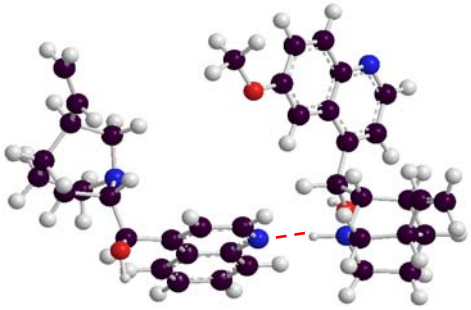
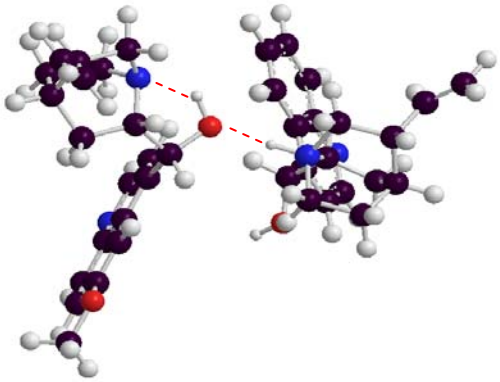

0.12
0.10
0.08
0.06
0.04
0.02
0.00
Fragmentation rate (a.u.)
2800
3000
3200
3400
3600
3800
wavenumber (cm-1)

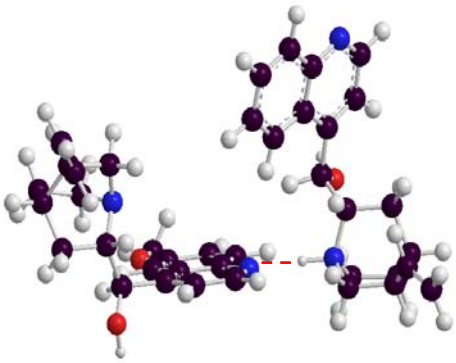
Figure S3



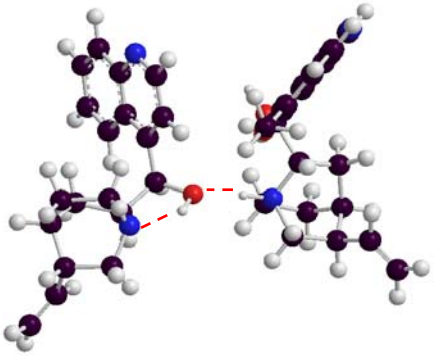
$NH_I^+ \ldots N_{IIring}$
$(Qn\ H^+Cd)$



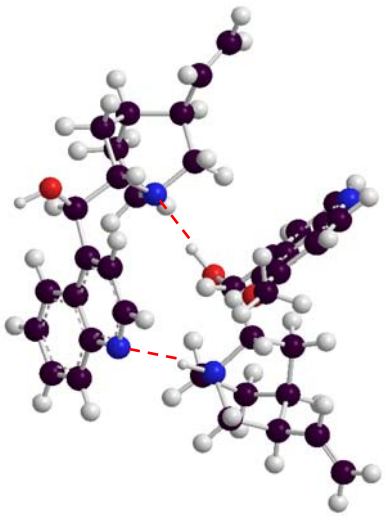
$NH_I^+ \ldots OH_{II} \ldots N_{II}$
$(QnCdH^+)$



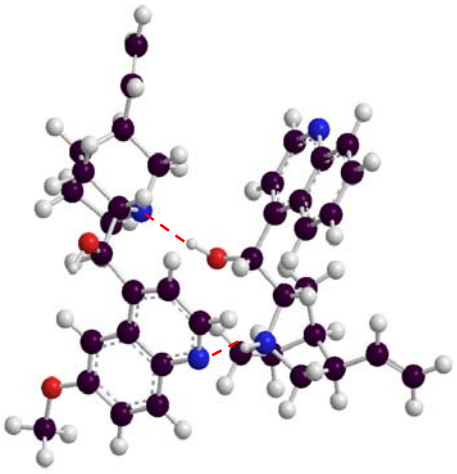
$NH_I^+ \ldots N_{IIring}$
$(QnCdH^+)$



$NH_I^+ \ldots OH_{II} \ldots N_{II}$
$(Qn\ H^+Cd)$

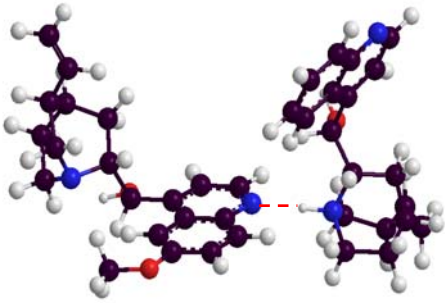


$NH_I^+ \ldots N_{IIring} / OH_I \ldots N_{II}$
$(Qn\ H^+Cd)$

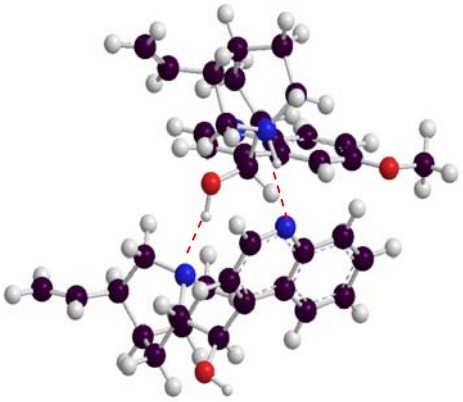


$NH_I^+ \ldots N_{IIring} / OH_I \ldots N_{II}$
$(Qn\ Cd\ H^+)$

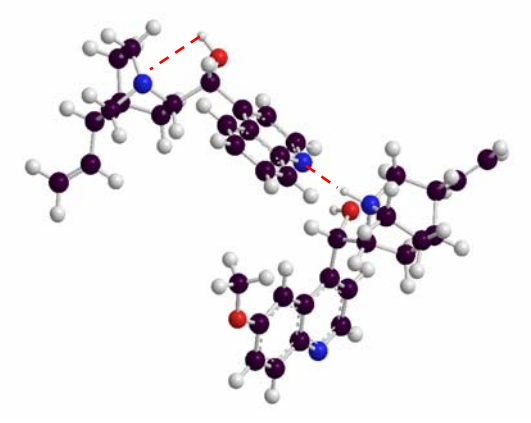
Figure S4



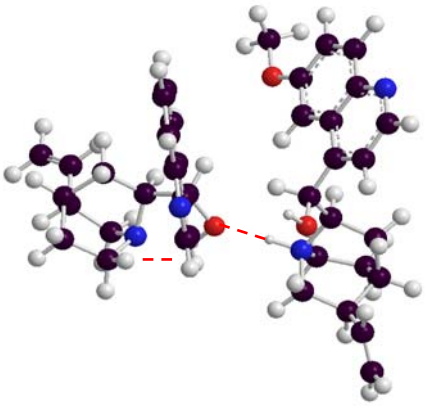
$NH_I^+ \ldots N_{IIring}$
(CdH^+Qd)



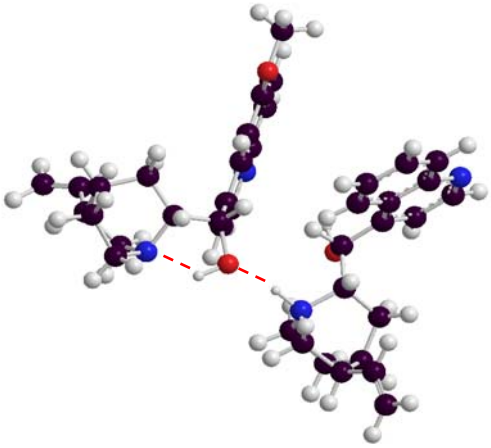
$NH_I^+ \ldots N_{IIring}/ OH_I \ldots N_{II}$
$(CdQdH^+)$



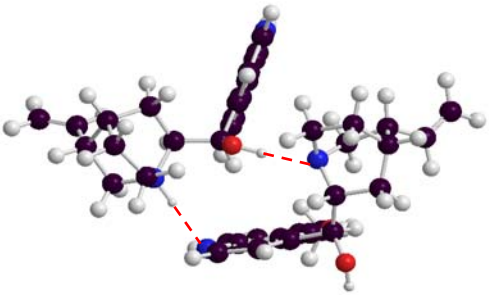
$NH_I^+ \ldots N_{IIring}$
$(CdQdH^+)$



$NH_I^+ \ldots OH_{II} \ldots N_{II}$
$(CdQdH^+)$

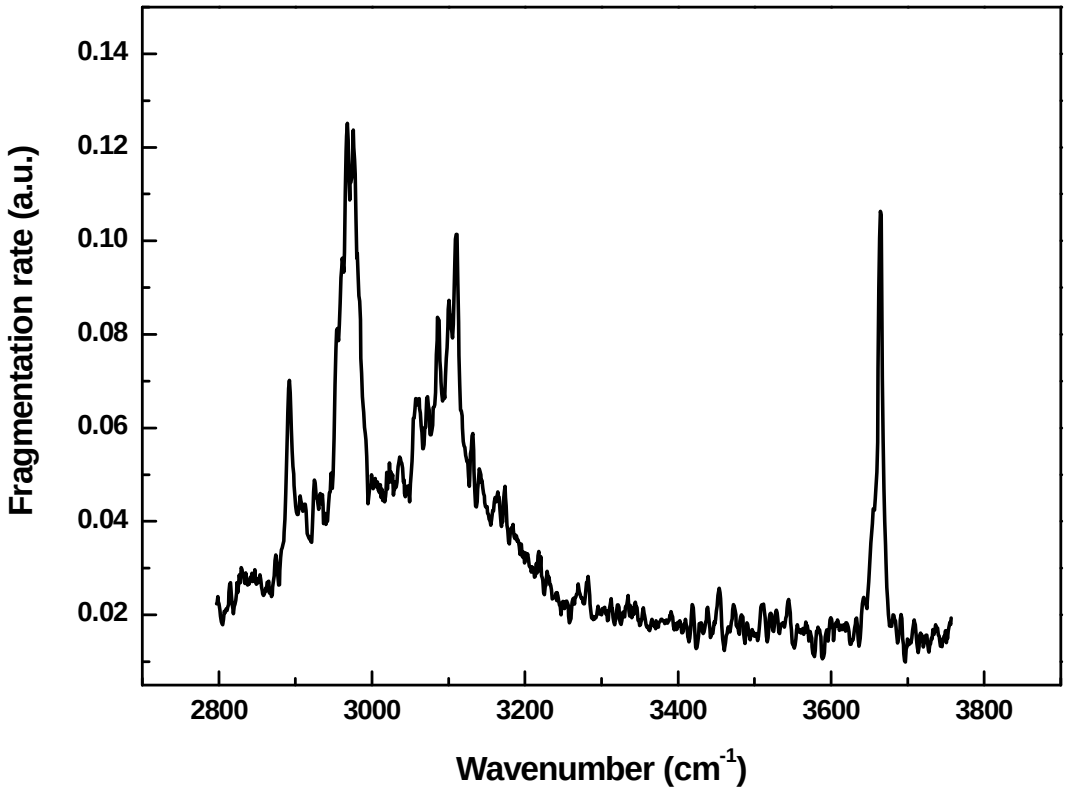


$NH_I^+ \ldots OH_{II} \ldots N_{II}$
$(Cd\ H^+Qd)$



$NH_I^+ \ldots N_{IIring}/ OH^I \ldots N^{II}$
$(Cd\ H^+Qd)$

Figure S 5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