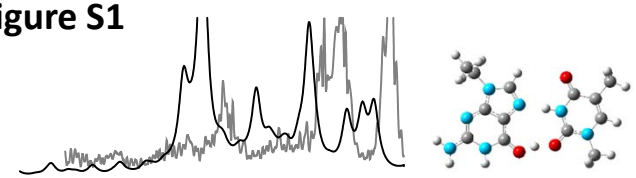
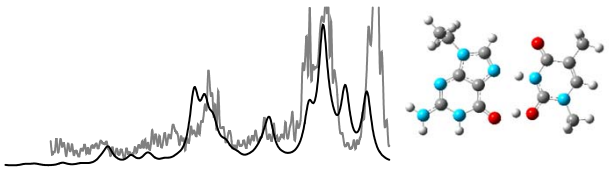
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Figure S1



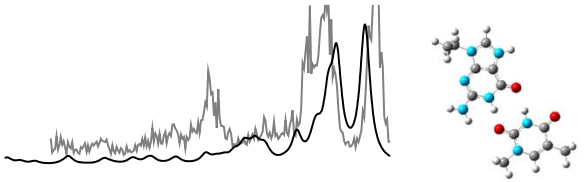
$\Delta_{rel}H$ = 20.4
$\Delta_{rel}G$ = *20.0*

GO6_TN3-GN7_GO6-TO2



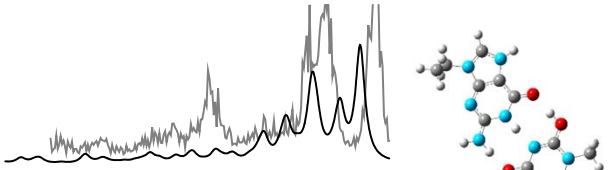
$\Delta_{rel}H$ = 17.4
$\Delta_{rel}G$ = *20.7*

TO2_TO2-GO6_TN3-GN7



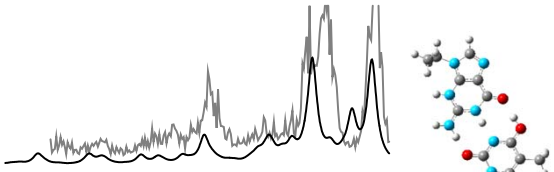
$\Delta_{rel}H$ = 21.6
$\Delta_{rel}G$ = *22.1*

GN7_GN1-TO2_TN3-GO6



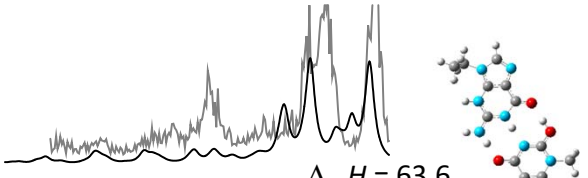
$\Delta_{rel}H$ = 23.0
$\Delta_{rel}G$ = *32.3*

GN7_GN1-TN3_GN2-TO4_TO2-GO6



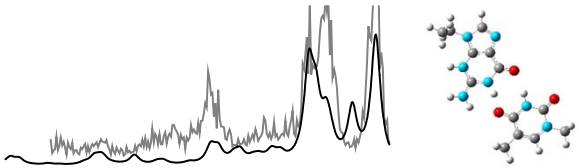
$\Delta_{rel}H$ = 51.9
$\Delta_{rel}G$ = *59.8*

GN3_GN1-TN3_GN2-TO2_TO4-GO6



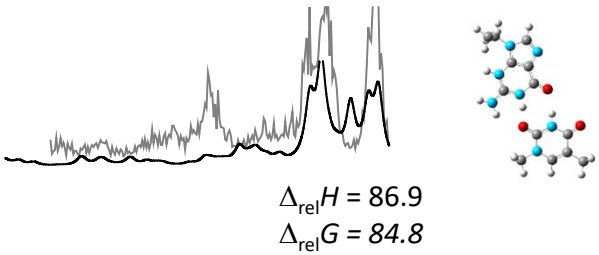
$\Delta_{rel}H$ = 63.6
$\Delta_{rel}G$ = *71.6*

GN3_GN1-TN3_GN2-TO4_TO2-GO6



$\Delta_{rel}H$ = 73.1
$\Delta_{rel}G$ = *72.1*

GN3_GN1-TO4_TN3-GO6

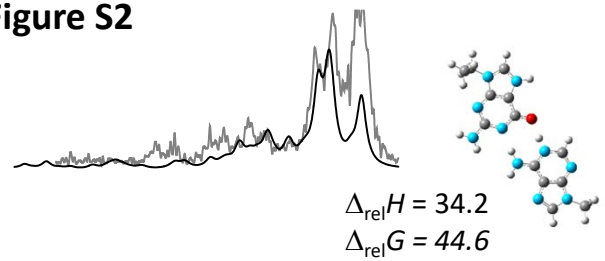


$\Delta_{rel}H$ = 86.9
$\Delta_{rel}G$ = *84.8*

GN3_GN1-TO2_TN3-GO6

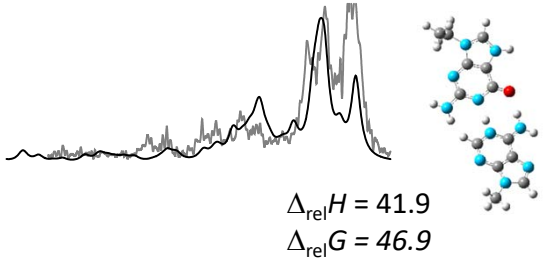
Some other higher energy structures of **(9eG:1mT)H$^+$** along with their enthalpies and 298 K Gibbs energies relative to **GN7_GN7-TO4_TN3-GO6** and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace). All energies are presented in kJ mol^{-1}

Figure S2



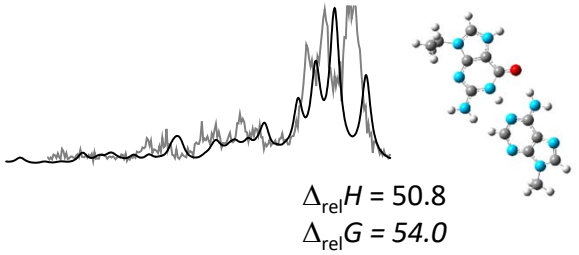
$\Delta_{rel}H$ = 34.2
$\Delta_{rel}G$ = *44.6*

AN1_AN1-GO6_AN6-GN1



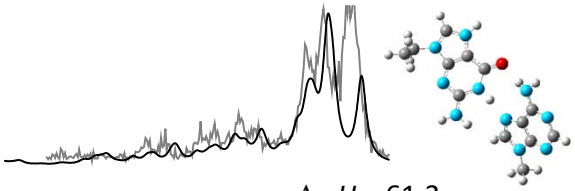
$\Delta_{rel}H$ = 41.9
$\Delta_{rel}G$ = *46.9*

AN1_AN1-GN1_AN6-GO6



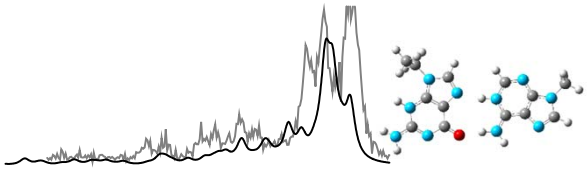
$\Delta_{rel}H$ = 50.8
$\Delta_{rel}G$ = *54.0*

GN7_GN1-AN1_GO6-AN6



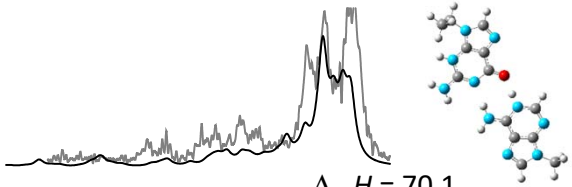
$\Delta_{rel}H$ = 61.3
$\Delta_{rel}G$ = *64.7*

GN7_GN1-AN7_AN6-GO6



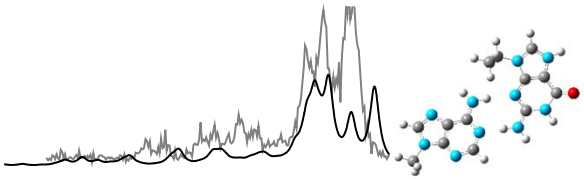
$\Delta_{rel}H$ = 65.2
$\Delta_{rel}G$ = *72.1*

AN1_AN6-GO6_AN1-GN7



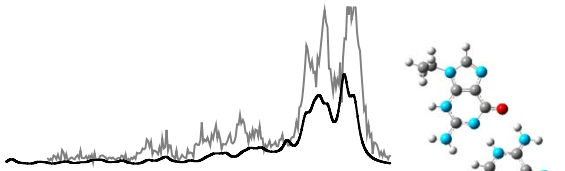
$\Delta_{rel}H$ = 70.1
$\Delta_{rel}G$ = *75.4*

AN1_AN1-GO6_AN6-GN1



$\Delta_{rel}H$ = 78.3
$\Delta_{rel}G$ = *76.0*

GN7_GN2-AN1_AN6-GN3

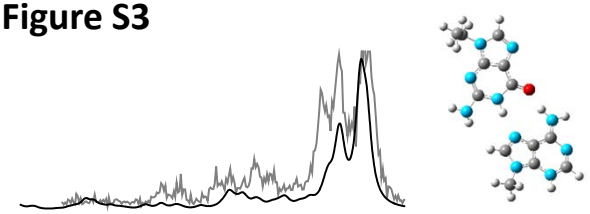


$\Delta_{rel}H$ = 85.4
$\Delta_{rel}G$ = *84.8*

AN1_AN1-GN1_AN6-GO6

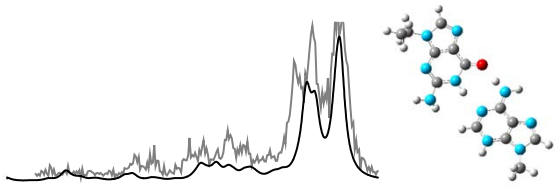
Some other higher energy structures of **(9eG:9mA)H$^+$** along with their enthalpies and 298 K Gibbs energies relative to **AN1_AN1-GO6_AN6-GN7** and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace). All energies are presented in kJ mol^{-1}

Figure S3



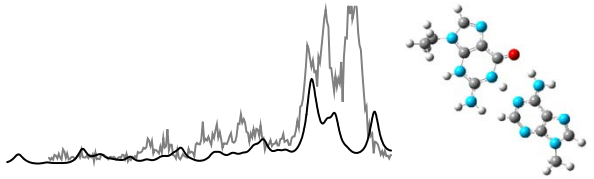
$\Delta_{rel}H$ = 92.8
$\Delta_{rel}G$ = *97.2*

AN3_GN1-AN7_AN6-GO6



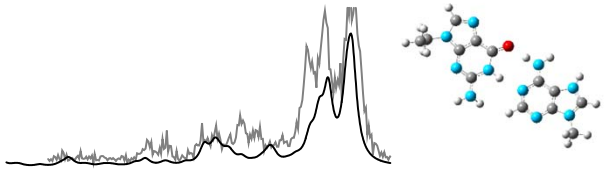
$\Delta_{rel}H$ = 103.2
$\Delta_{rel}G$ = *105.9*

AN3_GN1-AN1_AN6-GO6



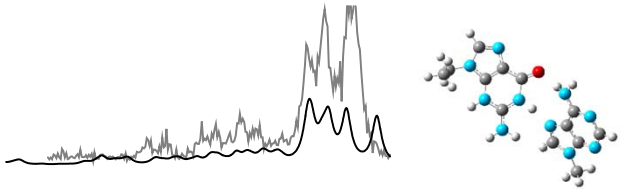
$\Delta_{rel}H$ = 111.9
$\Delta_{rel}G$ = *111.4*

GN3_GN1-AN1_AN6-GO6



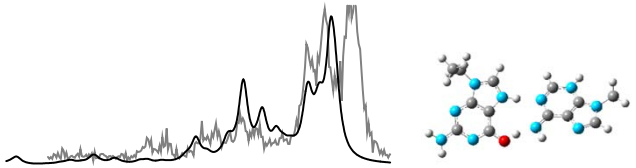
$\Delta_{rel}H$ = 113.1
$\Delta_{rel}G$ = *115.8*

AN7_GN1-AN1_AN6-GO6



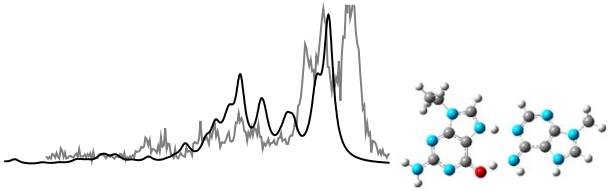
$\Delta_{rel}H$ = 113.1
$\Delta_{rel}G$ = *115.8*

GN3_GN1-AN7_AN6-GO6



$\Delta_{rel}H$ = 133.2
$\Delta_{rel}G$ = *138.0*

AN3_GN7-AN1_GO6-AN6

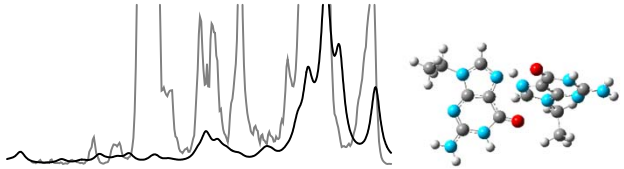


$\Delta_{rel}H$ = 138.2
$\Delta_{rel}G$ = *142.8*

AN7_GO6-AN6_GN7-AN1

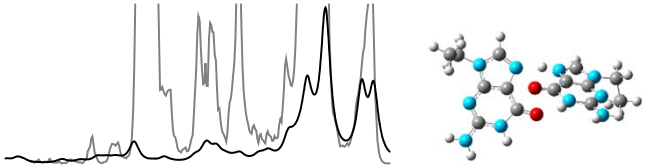
Some other higher energy structures of **(9eG:9mA)H$^+$** along with their enthalpies and 298 K Gibbs energies relative to **AN1_AN1-GO6_AN6-GN7** and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace). All energies are presented in kJ mol^{-1}

Figure S4



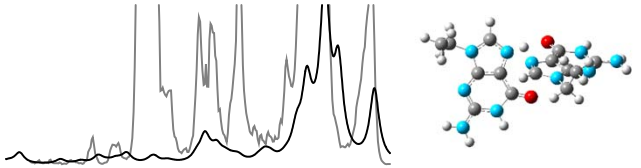
GN7_GN7-GO6

$\Delta_{rel}H$ = 22.4
$\Delta_{rel}G$ = *22.8*



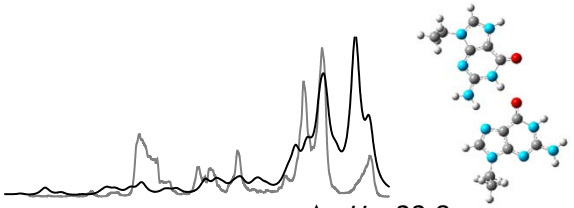
GN7_GN7-GN7

$\Delta_{rel}H$ = 21.9
$\Delta_{rel}G$ = *22.9*



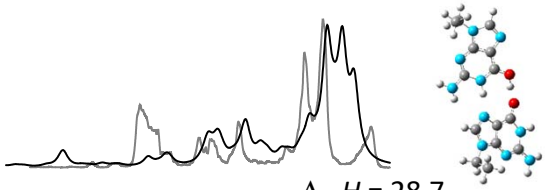
GN7_GN7-GO6_2

$\Delta_{rel}H$ = 22.3
$\Delta_{rel}G$ = *23.2*



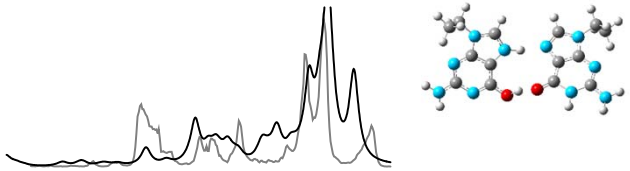
$\Delta_{rel}H$ = 23.8
$\Delta_{rel}G$ = *24.4*

GN7_GN1-GO6_GN2-GN7



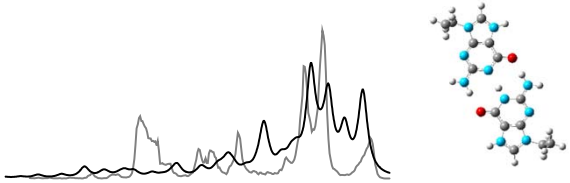
$\Delta_{rel}H$ = 28.7
$\Delta_{rel}G$ = *31.7*

GO6_GN1-GN7_GO6-GO6



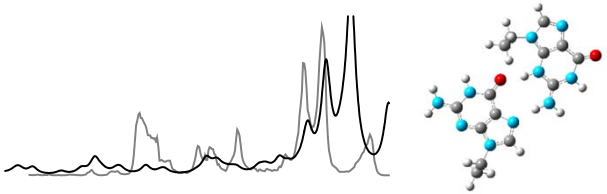
$\Delta_{rel}H$ = 35.1
$\Delta_{rel}G$ = *37.2*

GN7_GO6-GO6_GN7-GN7



$\Delta_{rel}H$ = 36.4
$\Delta_{rel}G$ = *44.9*

GN7_GN1-GN1_GN2-GO6_GN2-GO6

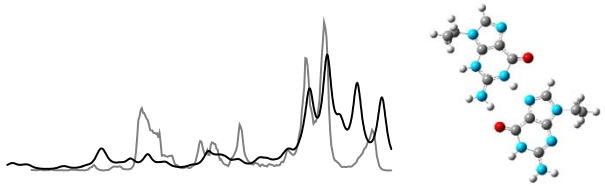


$\Delta_{rel}H$ = 47.6
$\Delta_{rel}G$ = *49.2*

GN3_GN2-GN7_GN3-GO6

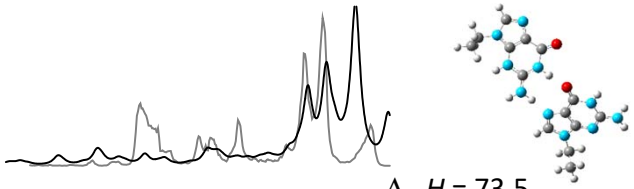
Some other higher energy structures of **(9eG:9eG)H$^+$** along with their enthalpies and 298 K Gibbs energies relative to **GN7_GN7-GN7_GC8-GO6** and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace). All energies are presented in kJ mol^{-1}

Figure S5



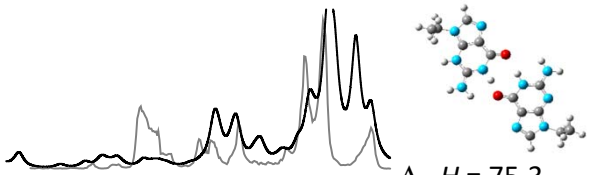
$\Delta_{rel}H$ = 49.6
$\Delta_{rel}G$ = *52.9*

GN3_GN1-GN7_GN2-GO6



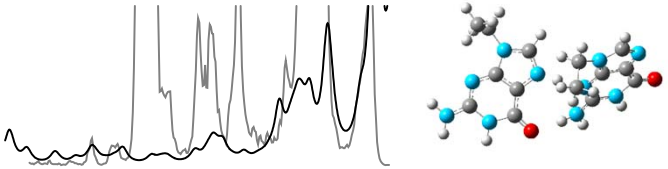
$\Delta_{rel}H$ = 73.5
$\Delta_{rel}G$ = *73.0*

GN3_GN1-GO6_GN2-GN7



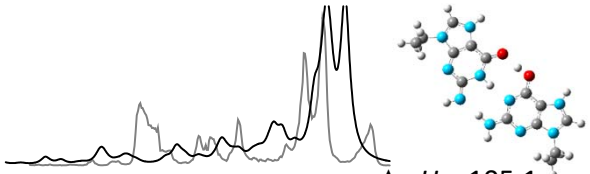
$\Delta_{rel}H$ = 75.3
$\Delta_{rel}G$ = *75.9*

GN3_GN1/GN2-GO6_GN1-GO6



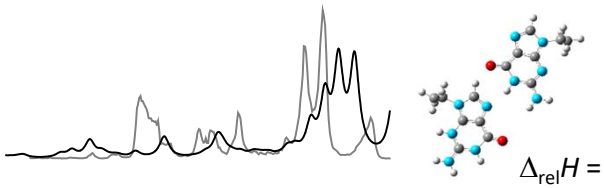
$\Delta_{rel}H$ = 74.0
$\Delta_{rel}G$ = *77.3*

GN7_GN2-GO6_GN7-GN3



$\Delta_{rel}H$ = 105.1
$\Delta_{rel}G$ = *117.1*

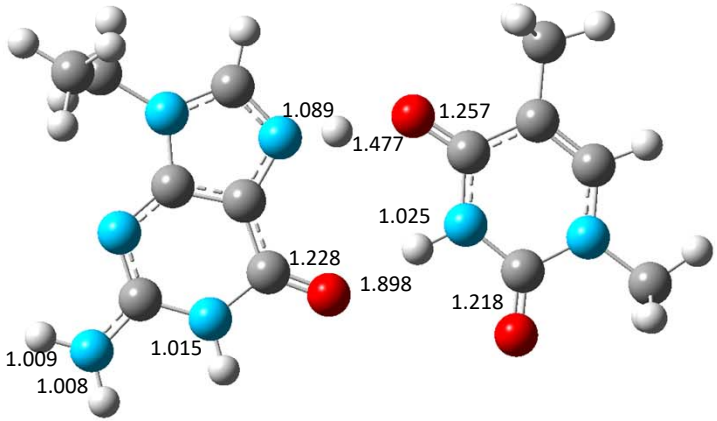
GN7_GN1-GN1_GN2-GN2_GO6-GO6



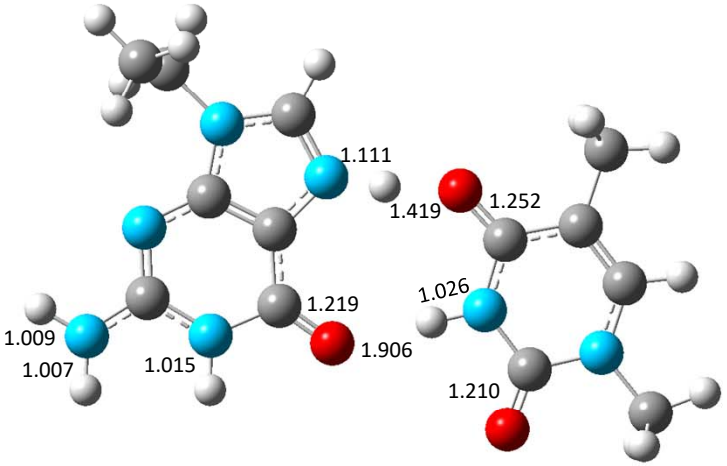
$\Delta_{rel}H$ = 177.5
$\Delta_{rel}G$ = *171.7*

GN3_GN1-GN1_GC8-GO6

Some other higher energy structures of **(9eG:9eG)H$^+$** along with their enthalpies and 298 K Gibbs energies relative to **GN7_GN7-GN7_GC8-GO6** and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace). All energies are presented in kJ mol^{-1}



B3LYPD3/6-31+G(d,p)



M06-2X/6-31+G(d,p)

Figure S6. Comparison of the geometries of the lowest energy (9eG:1mT)H^+ structure, GN7_GN7-TO4_TN3-GO6 computed using B3LYPD3 and M06-2X.

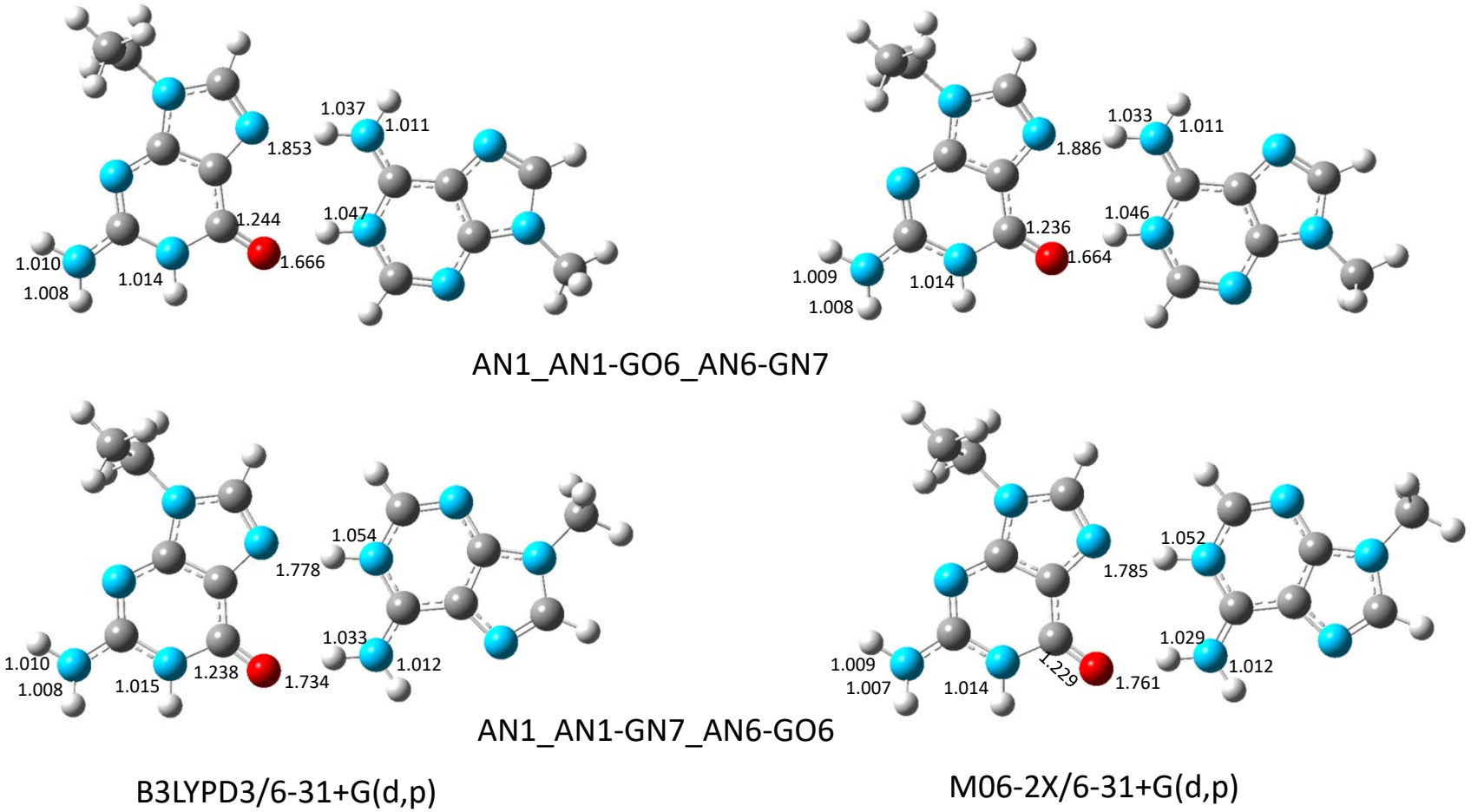
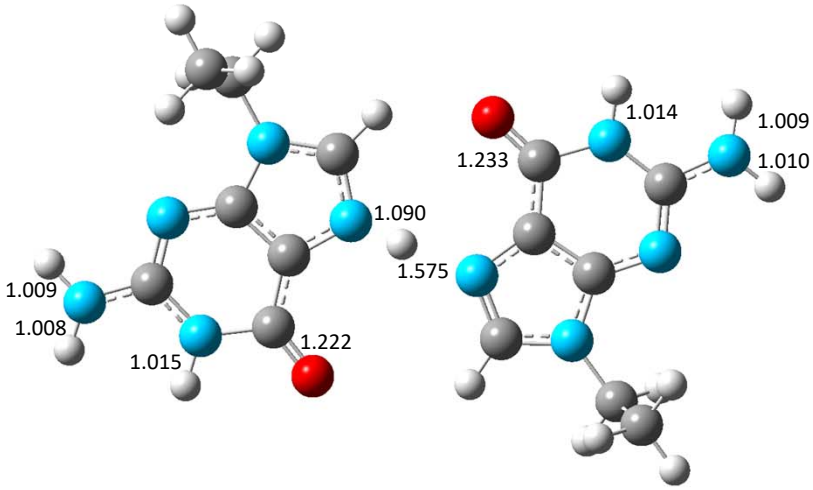
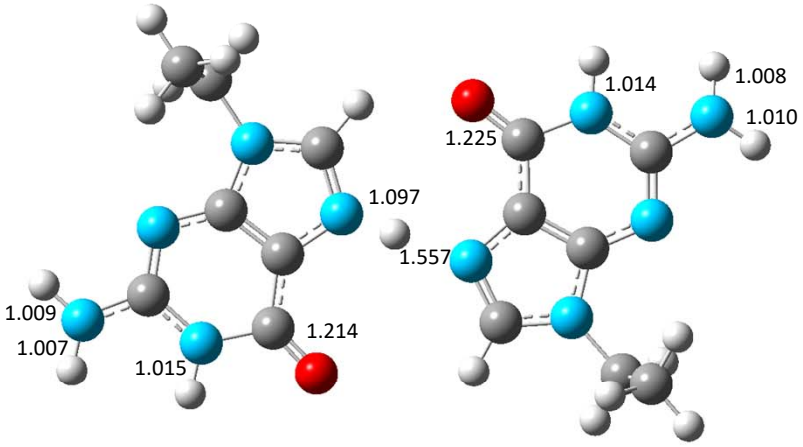


Figure S7. Comparison of the geometries of the two lowest energy (9eG:9mA)H^+ structures computed using B3LYPD3 and M06-2X.



B3LYPD3/6-31+G(d,p)



M06-2X/6-31+G(d,p)

Figure S8. Comparison of the geometries of the lowest energy (9eG:9eG)H^+ structure, GN7_GN7-GN7_GC8-GO6, computed using B3LYPD3 and M06-2X.

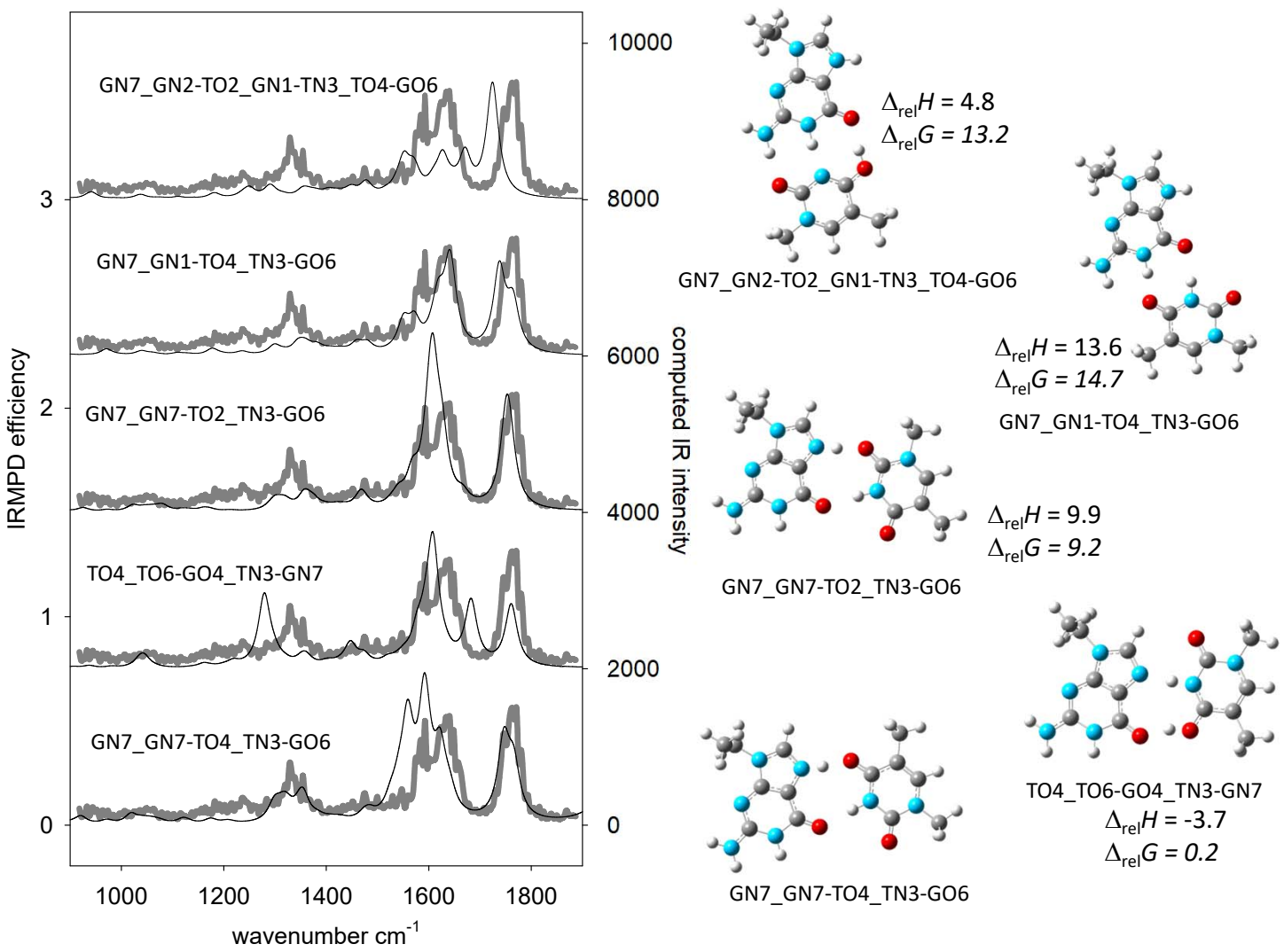


Figure S9. Comparison of the experimental IRMPD spectrum of $(9eG:1mT)H^+$ with the lowest energy computed IR spectra using M06-2x/6-31+G(d,p).

$(9eG:1mT)H^+$ (M06-2X)

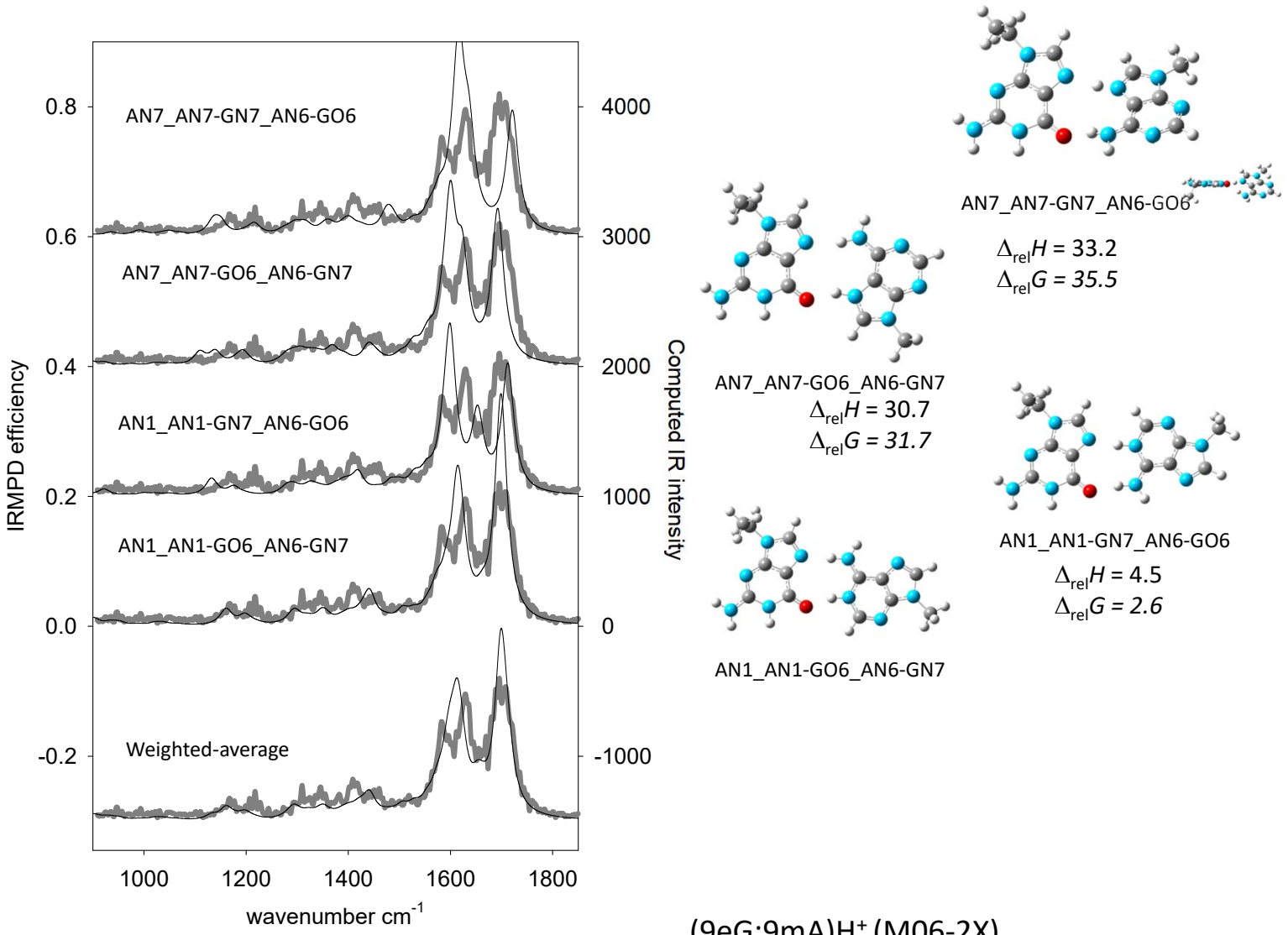


Figure S10. Comparison of the experimental IRMPD spectrum of $(9eG:9mA)H^+$ with the lowest energy computed IR spectra using M06-2x/6-31+G(d,p).

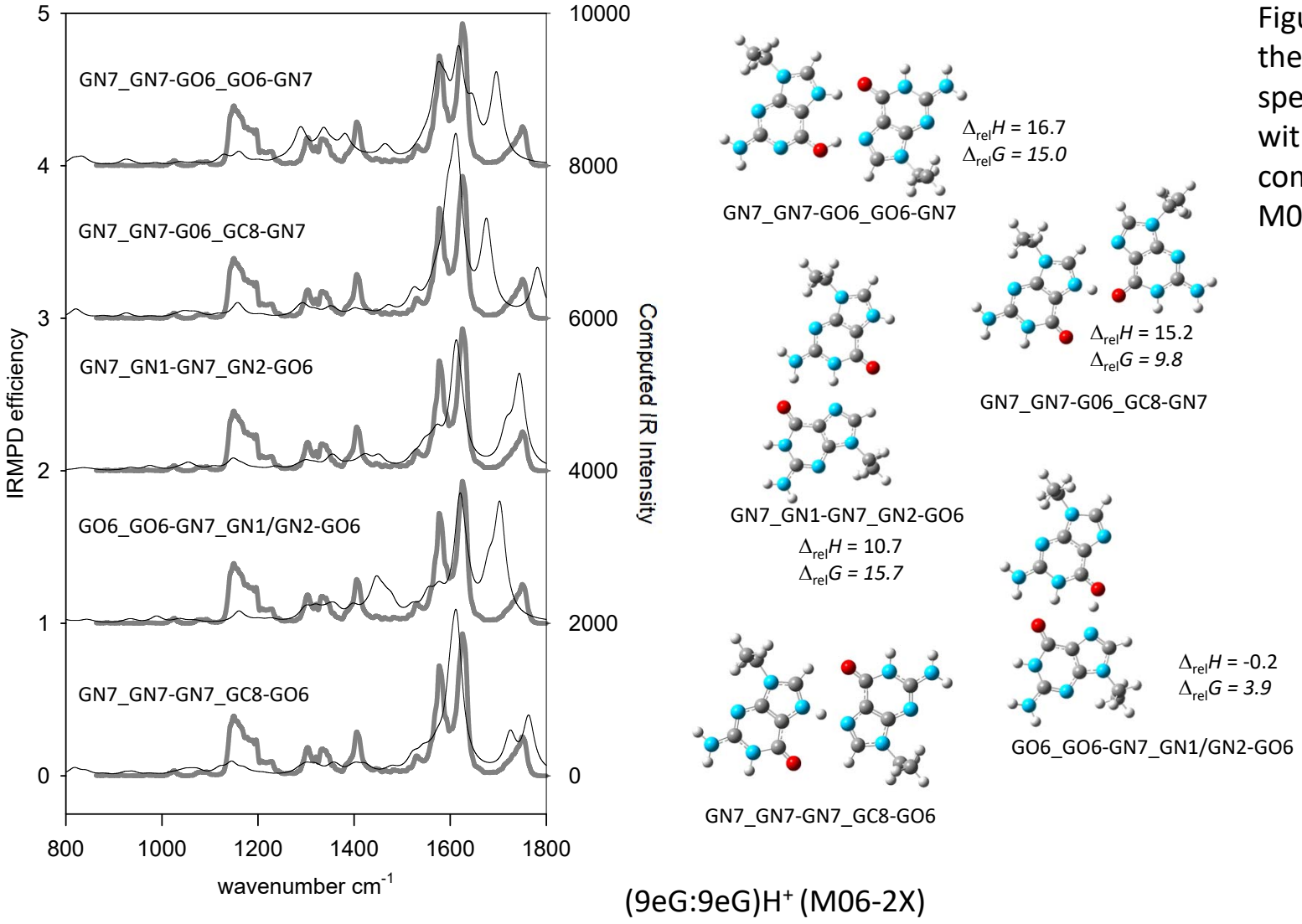


Figure S11. Comparison of the experimental IRMPD spectrum of $(9eG:9eG)H^+$ with the lowest energy computed IR spectra using M06-2x/6-31+G(d,p).

Table S1 298K relative enthalpies and Gibbs energies, in kJ mol^{-1}, of five lowest energy isomers of $(9eG:1mT)H^+$ by three different computational methods. Relative Gibbs energies are indicated in parentheses.

Structures of $(9eG:1mT)H^+$	B3LYPD3/6-31+G(d,p)	B3LYPD3/6-311+G(3df,3pd) //B3LYPD3/6-31+G(d,p)	M06-2X/6-31+G(d,p)
GN7_GN7-TO4_TN3-GO6	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
TO4_TO4-GO6_TN3-GN7	2.6 (6.8)	3.4 (7.6)	-3.7 (0.2)
GN7_GN7-TO2_TN3-GO6	10.7 (9.8)	10.2 (9.3)	9.9 (9.2)
GN7_GN1-TO4_TN3-GO6	11.6 (13.0)	11.5 (12.9)	13.6 (14.7)
GN7_GN2-TO2_GN1-TN3_TO4-GO6	7.0 (16.5)	7.9 (17.4)	4.8 (13.2)

Table S2 298K relative enthalpies and Gibbs energies, in kJ mol^{-1}, of four lowest energy isomers of $(9eG:1mA)H^+$ by three different computational methods. Relative Gibbs energies are indicated in parentheses.

Structures of $(9eG:1mA)H^+$	B3LYPD3/6-31+G(d,p)	B3LYPD3/6-311+G(3df,3pd) //B3LYPD3/6-31+G(d,p)	M06-2X/6-31+G(d,p)
AN1_AN1-GO6_AN6-GN7	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
AN1_AN1-GN7_AN6-GO6	2.1 (4.1)	3.8 (1.8)	4.5 (2.6)
AN7_AN7-GO6_AN6-GN7	28.3 (29.3)	28.8 (27.8)	30.7 (31.7)
AN7_AN7-GN7_AN6-GO6	35.6 (36.7)	34.9 (36.0)	33.2 (35.5)

Table S3 298K relative enthalpies and Gibbs energies, in kJ mol^{-1}, of five lowest energy isomers of $(9eG:9eG)H^+$ by three different computational methods. Relative Gibbs energies are indicated in parentheses.

Structures of $(9eG:9eG)H^+$	B3LYPD3/6-31+G(d,p)	B3LYPD3/6-311+G(3df,3pd) //B3LYPD3/6-31+G(d,p)	M06-2X/6-31+G(d,p)
GN7_GN7-GN7_GC8-GO6	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
GO6_GO6-GN7_GN1/GN2-GO6	4.1 (7.3)	3.2 (6.4)	-0.2 (3.9)
GN7_GN1-GN7_GN2-GO6	7.1 (12.2)	6.3 (11.5)	10.7 (15.7)
GN7_GN7-G06_GC8-GN7	15.9 (14.4)	14.4 (12.8)	15.2 (9.8)
GN7_GN7-GO6_GO6-GN7	19.5 (21.6)	17.0 (19.0)	16.7 (15.0)