Structure of Pb^{2+}/deprotonated dGMP complexes in the gas phase: a combined MS-MS/IRMPD spectroscopy/Ion Mobility study.

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6) CNRS- UMR 5280

Supporting information

1S. Low energy CID spectrum of the $[Pb(GMP)-H]^+$ complex recorded at 30 eV (laboratory frame).

2S. Structure and geometrical details of the various structures optimized for the $[Pb(dGMP)-H^+$ complex

3S. Total energy and ZPE (Hartree) of the various structures considered

4S. DFT-computed IR absorption spectra for the $[Pb(dGMP)-H]^+$ structures. The experimental IRMPD spectrum is overlayed in grey.

5S. Evolution of $[Pb(dGMP)-H]^+$ arrival time as a function of 1/E, the electric field applied across the mobility tube.

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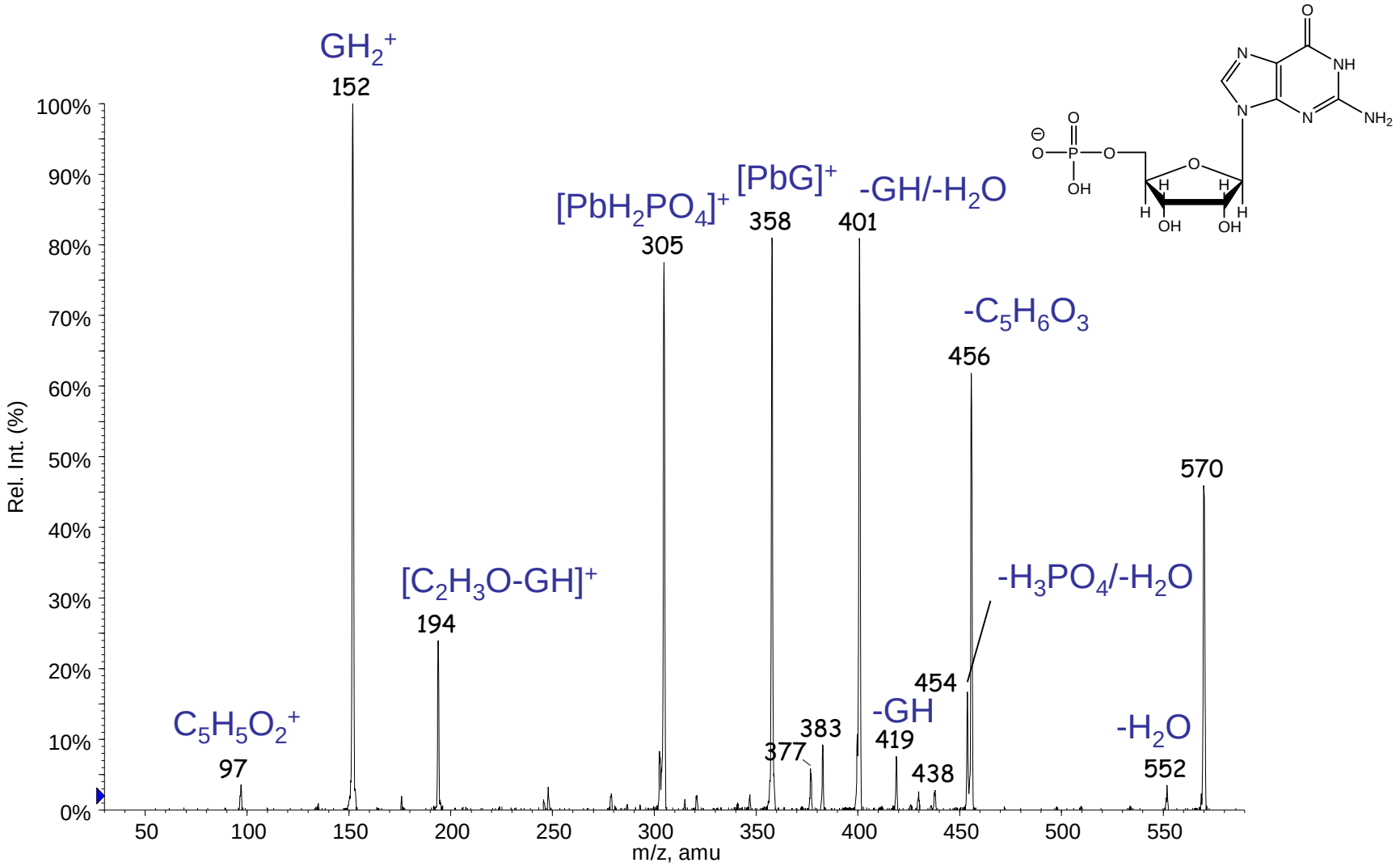
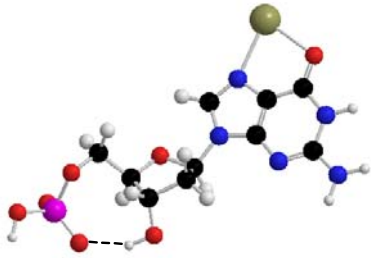
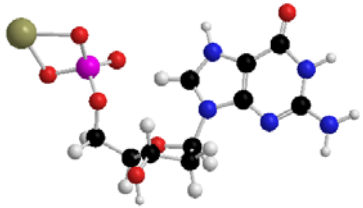


2S. Structure and geometrical details of the various structures optimized for the $[Pb(dGMP)-H]^+$ complex

2.1 *Anti* forms



dGMPA1



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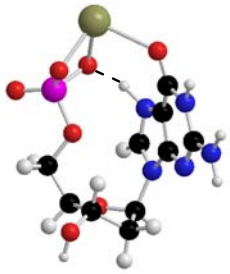

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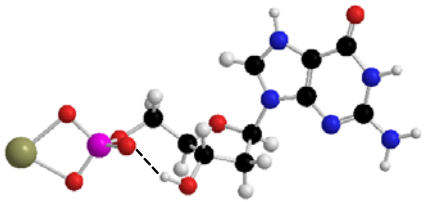
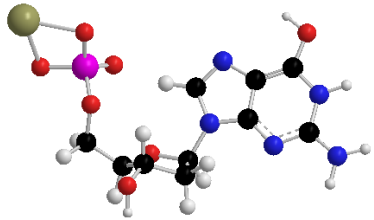


dGMPA4



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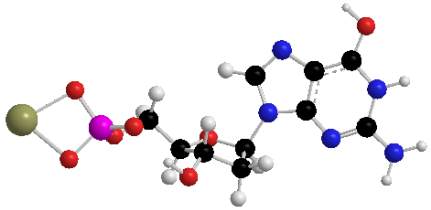

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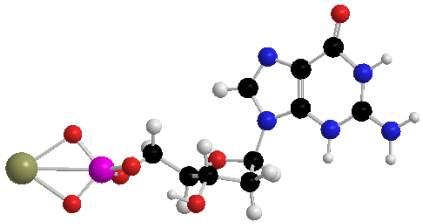

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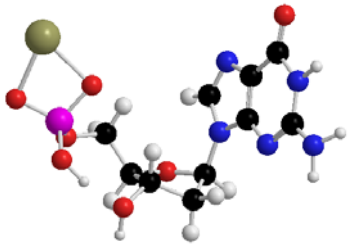

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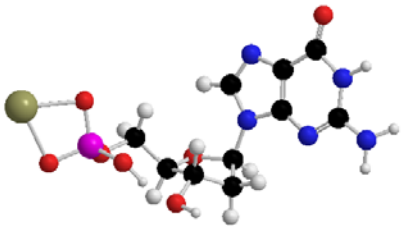

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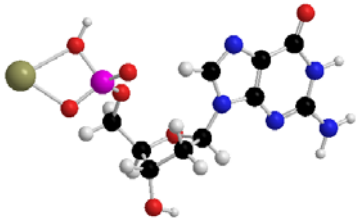
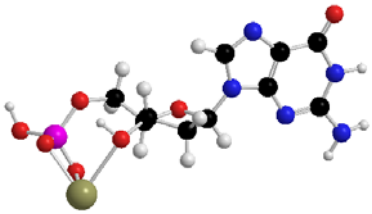
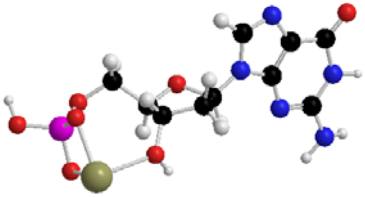


dGMPA10



dGMPA11



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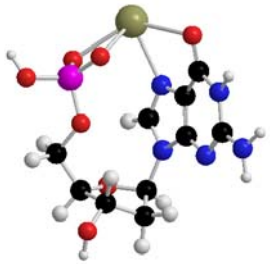
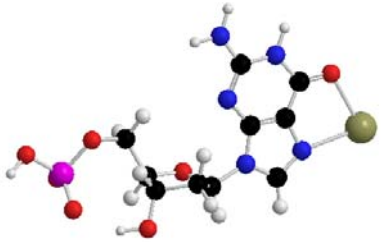


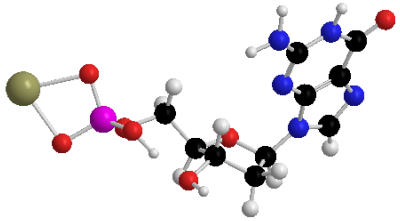
dGMPA13

2.2 *Syn* forms



dGMPS1

dGMPS2



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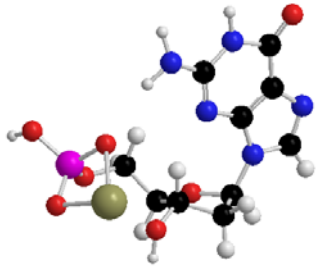

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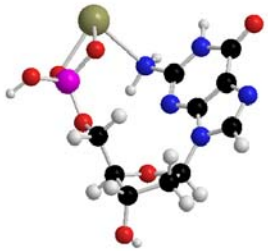
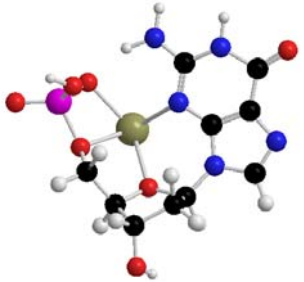


dGMPS5



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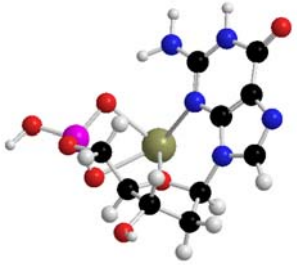
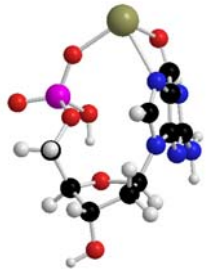


dGMPS7



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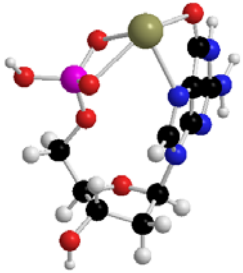
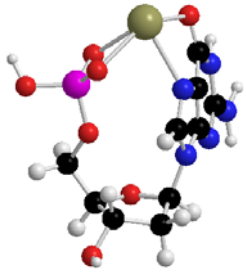


dGMPS9



dGMPS10

2.3 Summary

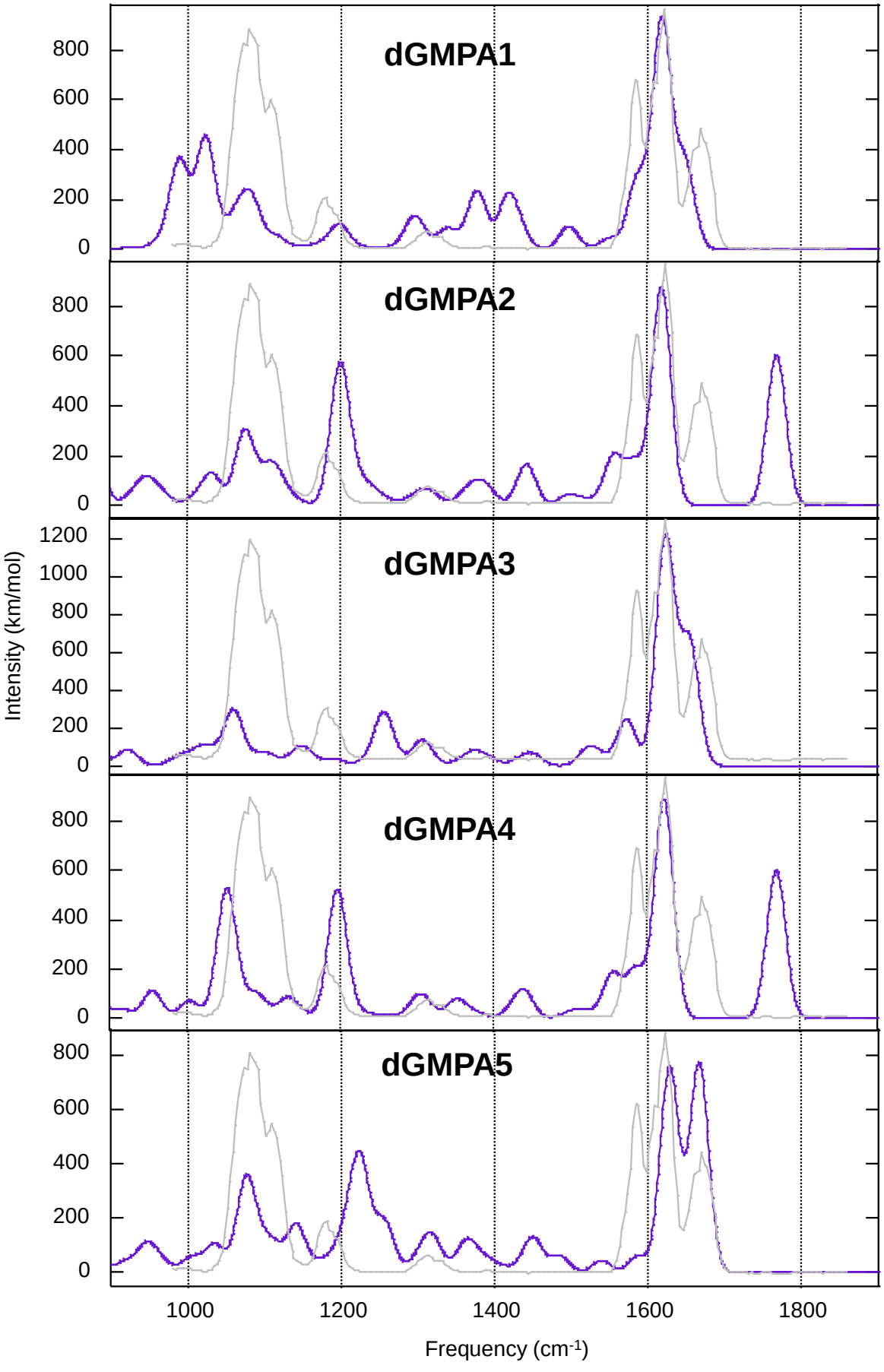
Structures	Interaction sites									Sugar conformation[(a)]	Intramolecular H bonds
	Phopshate	O4'	OH 3'	OH 5'	C=O (6)	NH_2	N1	N3	N7		
Anti forms											
dGMPA1					O				O	C2'-endo/C1'-exo ($^2T_1$)	
dGMPA2	O (O/O)									C3'-endo/C2'-exo ($^3T_2$)	
dGMPA3	O (O/O)				O					C3'-endo/C2'-exo ($^3T_2$)	NH(7)→ Phos
dGMPA4	O (O/O)									C3'-endo (^3E)	OH(3')→ Phos
dGMPA5	O (O/O)									C3'-endo/C2'-exo ($^3T_2$)	
dGMPA6	O (O/O)									C3'-endo (^3E)	OH(3')→ Phos
dGMPA7	O (O/O)									C3'-endo/C2'-exo ($^3T_2$)	OH(3')→ Phos
dGMPA8	O (O/O)									C3'-endo/C2'-exo ($^3T_2$)	Phos → OH(3')
dGMPA9	O (O/O)									C3'-endo/C2'-exo ($^3T_2$)	Phos → OH(3')
dGMPA10	O (O/OH)									C2'-endo/C3'-exo ($^2T_3$)	
dGMPA11	O (O/O)		O							C3'-endo/C4'-exo ($^3T_4$)	
dGMPA12	O (O/O)		O							O4'-endo/C1'-exo ($^OT_1$)	
dGMPA13	O (O/O)				O				O	C3'-endo/C2'-exo ($^3T_2$)	
Syn forms											
dGMPS1					O				O	C2'-endo/C1'-exo ($^2T_1$)	OH(3')→ Phos
dGMPS2	O (O/O)		O							C3'-endo/C2'-exo ($^3T_2$)	
dGMPS3	O (O/O)									C3'-endo/C2'-exo ($^3T_2$)	Phos → OH(3')
dGMPS4	O (O/O)		O							C3'-endo/C2'-exo ($^3T_2$)	
dGMPS5	O (O/O)					O				C2'-endo/C3'-exo ($^2T_3$)	
dGMPS6	O (O)	O		O				O		C2'-endo/C3'-exo ($^2T_3$)	
dGMPS7	O (O/O)	O						O		C3'-endo/C2'-exo ($^3T_2$)	
dGMPS8	O (O)				O				O	C2'-endo/C3'-exo ($^2T_3$)	Phos → O (4')
dGMPS9	O (O/O)				O				O	C3'-endo/C2'-exo ($^3T_2$)	
dGMPS10	O (O/O)				O				O	C3'-endo/C2'-exo ($^3T_2$)	

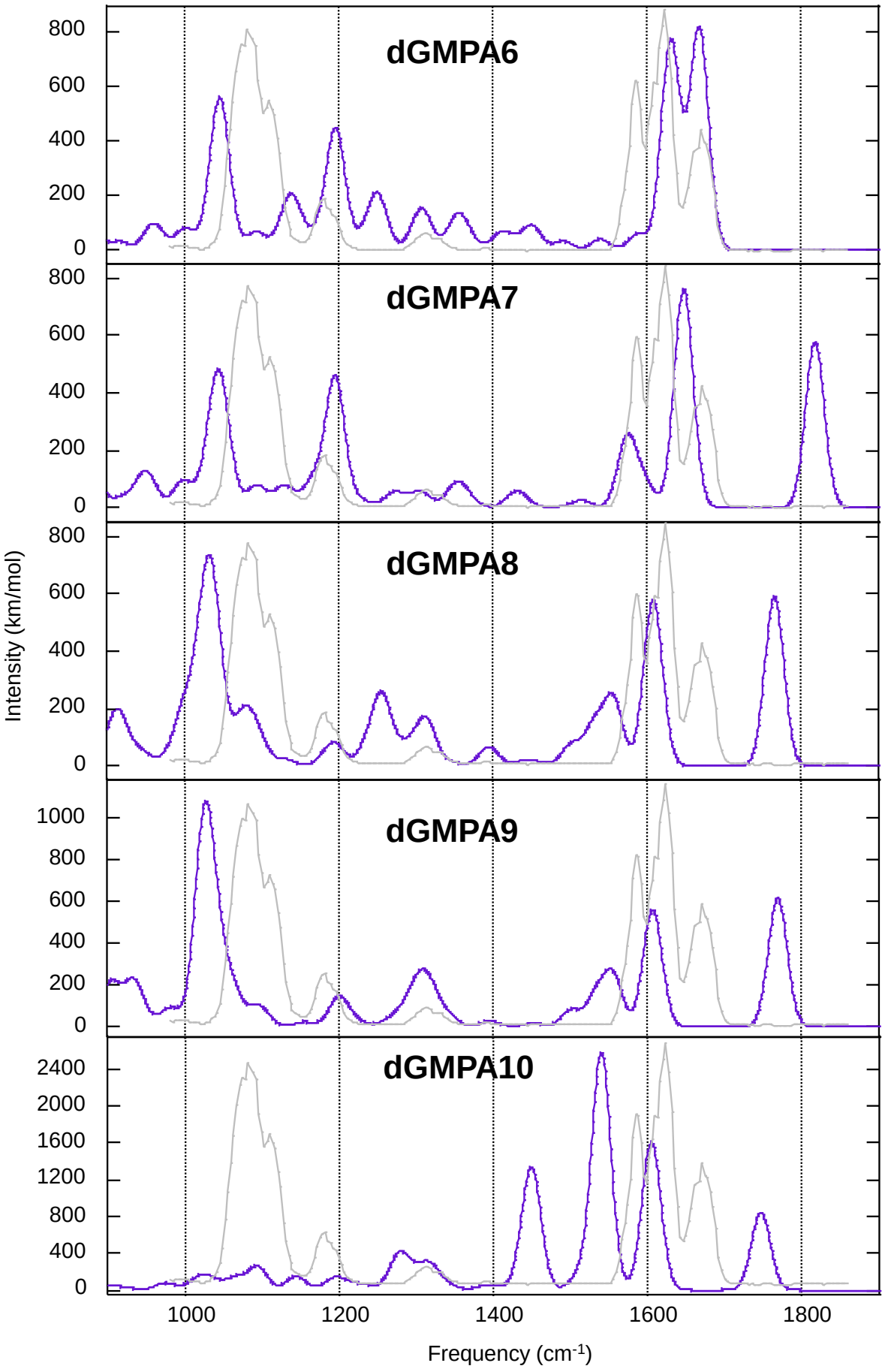
(a) Four ring atoms are considered as planar (E forms) when their associated torsional angle is greater than 179°

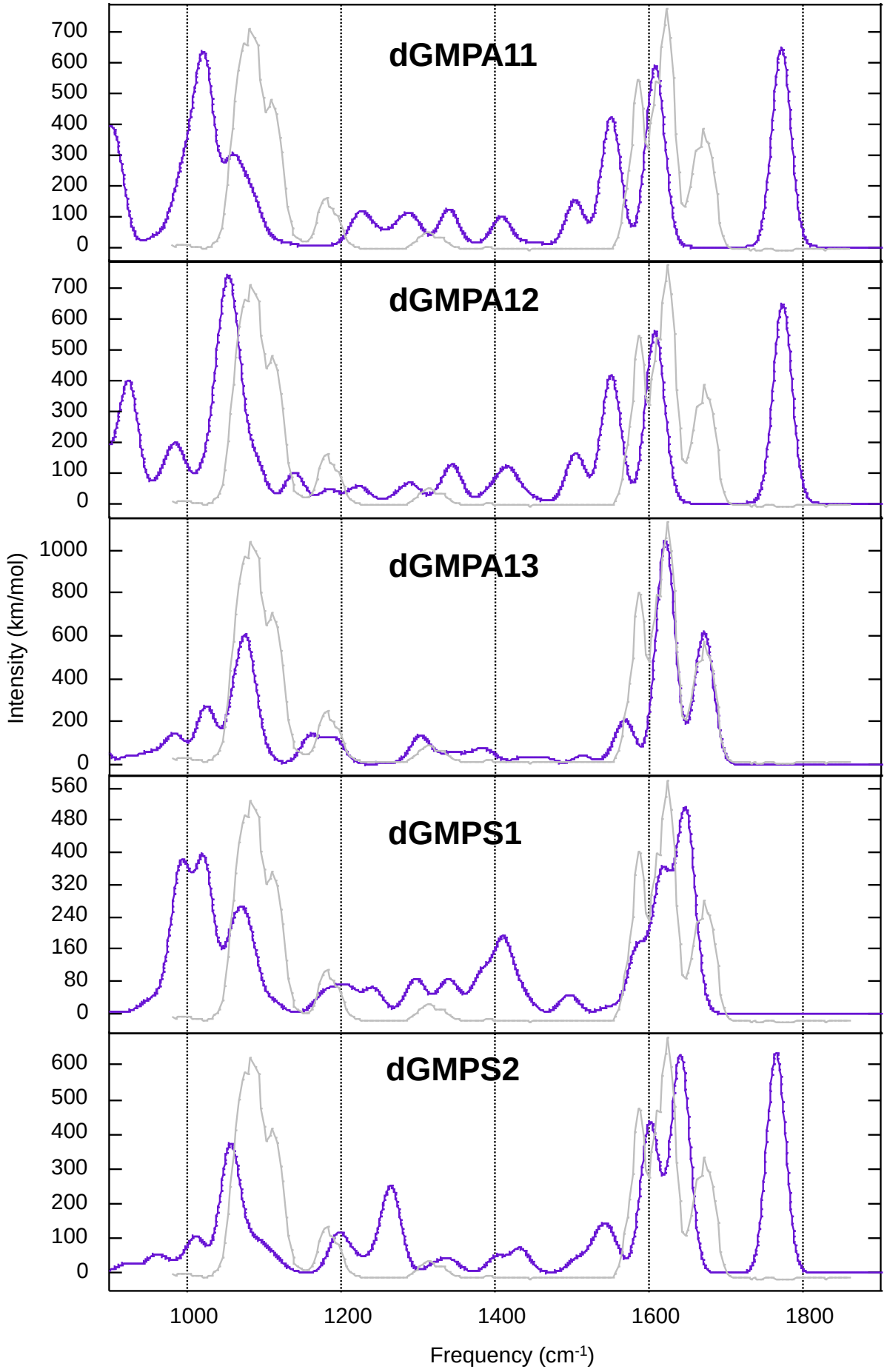
3S. Total energy, thermal correction to Gibbs free energy (TCG) and ZPE (Hartree) of the various structures considered during this study.

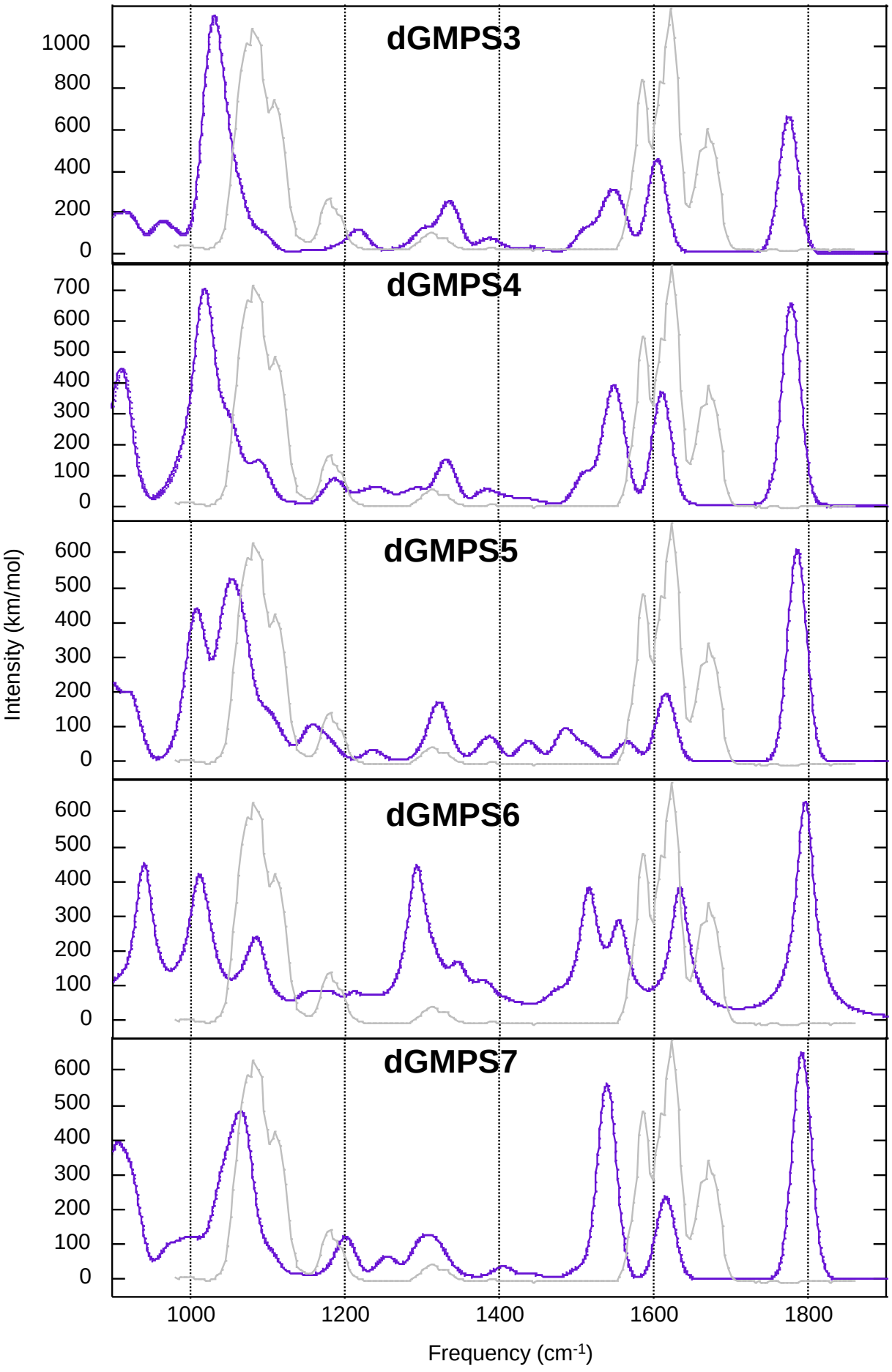
Structure	B3LYP/6-31G(d,p)			B3LYP//6-311+G(2df,2p)
	E	ZPE	TCG	E
dGMPA1	-1533.845199	0.266534	0.209900	-1534.329415
dGMPA2	-1533.956524	0.268431	0.212373	-1534.443255
dGMPA3	-1533.955654	0.267647	0.216837	-1534.434760
dGMPA4	-1533.951044	0.269049	0.212966	-1534.437542
dGMPA5	-1533.930100	0.268004	0.211968	-1534.41654
dGMPA6	-1533.93549	0.268700	0.212493	-1534.421218
dGMPA7	-1533.917473	0.267758	0.211300	-1534.404346
dGMPA8	-1533.928523	0.268243	0.213293	-1534.414012
dGMPA9	-1533.928081	0.267856	0.211509	-1534.414562
dGMPA10	-1533.881039	0.265704	0.206523	
dGMPA11	-1533.929477	0.266978	0.211334	-1534.414943
dGMPA12	-1533.93568	0.266842	0.211183	-1534.422404
dGMPA13	-1533.993128	0.268303	0.216814	-1534.475306
dGMPS1	-1533.841038	0.266733	0.210618	
dGMPS2	-1533.951487	0.269717	0.218234	-1534.431864
dGMPS3	-1533.929210	0.267705	0.212417	-1534.416566
dGMPS4	-1533.942752	0.267361	0.214402	-1534.425433
dGMPS5	-1533.928814	0.267843	0.214730	-1534.412366
dGMPS6	-1533.945020	0.267200	0.214716	-1534.424076
dGMPS7	-1533.961591	0.267712	0.215996	-1534.442794
dGMPS8	-1533.965819	0.268626	0.217449	-1534.448121
dGMPS9	-1533.987905	0.268021	0.215972	-1534.471506
dGMPS10	-1533.989783	0.267613	0.215146	-1534.474311

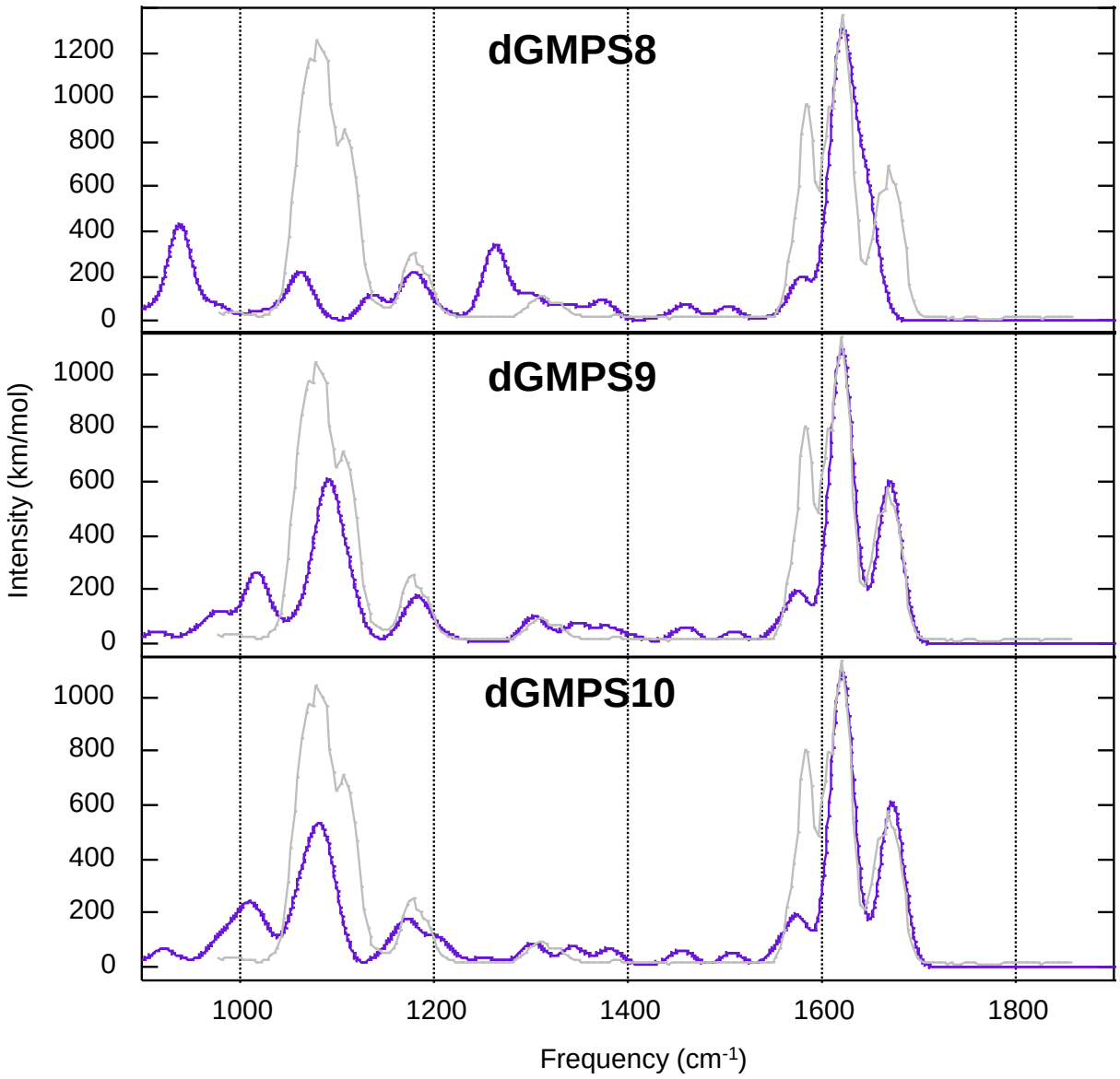
4S. DFT-computed IR absorption spectra for the [Pb(dGMP)-H]$^+$ structures. The experimental IRMPD spectrum is overlayed in grey.




dGMPA6
dGMPA7
dGMPA8
dGMPA9
dGMPA10
Intensity (km/mol)
Frequency (cm-1)
0
200
400
600
800
1000
1200
1400
1600
1800
2000
2400


dGMPA11
dGMPA12
dGMPA13
dGMPS1
dGMPS2
Intensity (km/mol)
Frequency (cm-1)
1000
1200
1400
1600
1800


dGMPS3
dGMPS4
dGMPS5
dGMPS6
dGMPS7
Intensity (km/mol)
Frequency (cm-1)
1000
1200
1400
1600
1800


dGMPS8
dGMPS9
dGMPS10
Intensity (km/mol)
Frequency (cm-1)
0
200
400
600
800
1000
1200
1400
1600
1800

5S. Evolution of [Pb(dGMP)-H]$^+$ drift time as a function of 1/E, E the electric field applied across the mobility tube. Inset shows a drift time distribution at E = 700V/m (blue) overlaid with the expected distribution (red) for a single conformation in the same experimental conditions. The expected distribution for CCS 10% higher (dashed green) is well separated, showing that only one family of conformations is observed experimentally. From the slope can be deduced the collisional cross section of the main conformation of [Pb(dGMP)-H]$^+$in the gas phase : 99.6 Å^2