Electronic Supporting Information (ESI)

for

Effect of microhydration on the aromatic charge resonance interaction: The case of the pyrrole dimer cation

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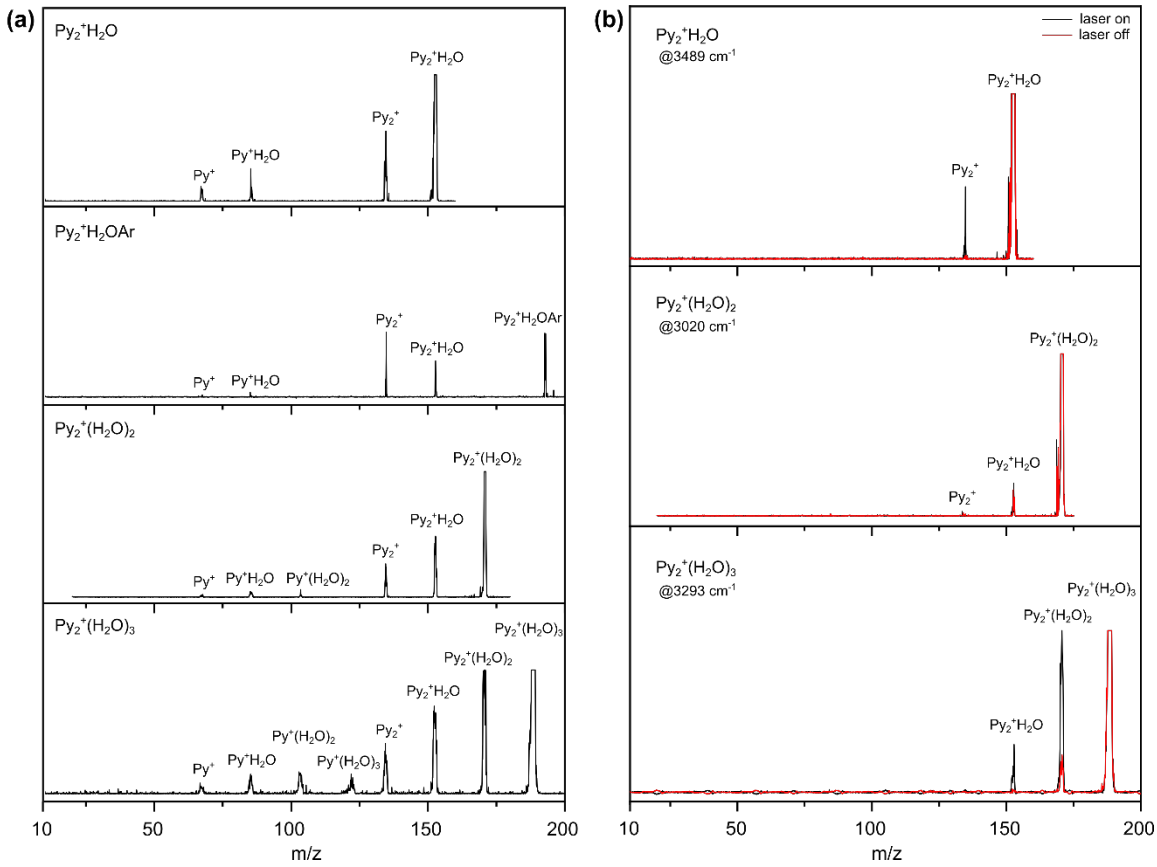
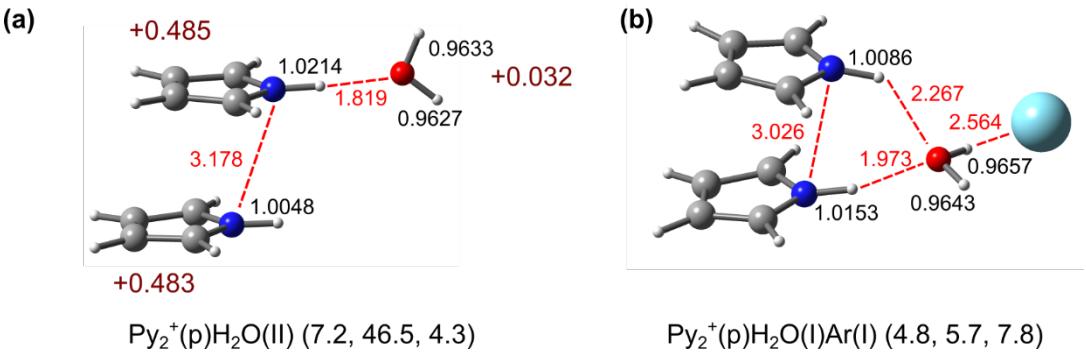


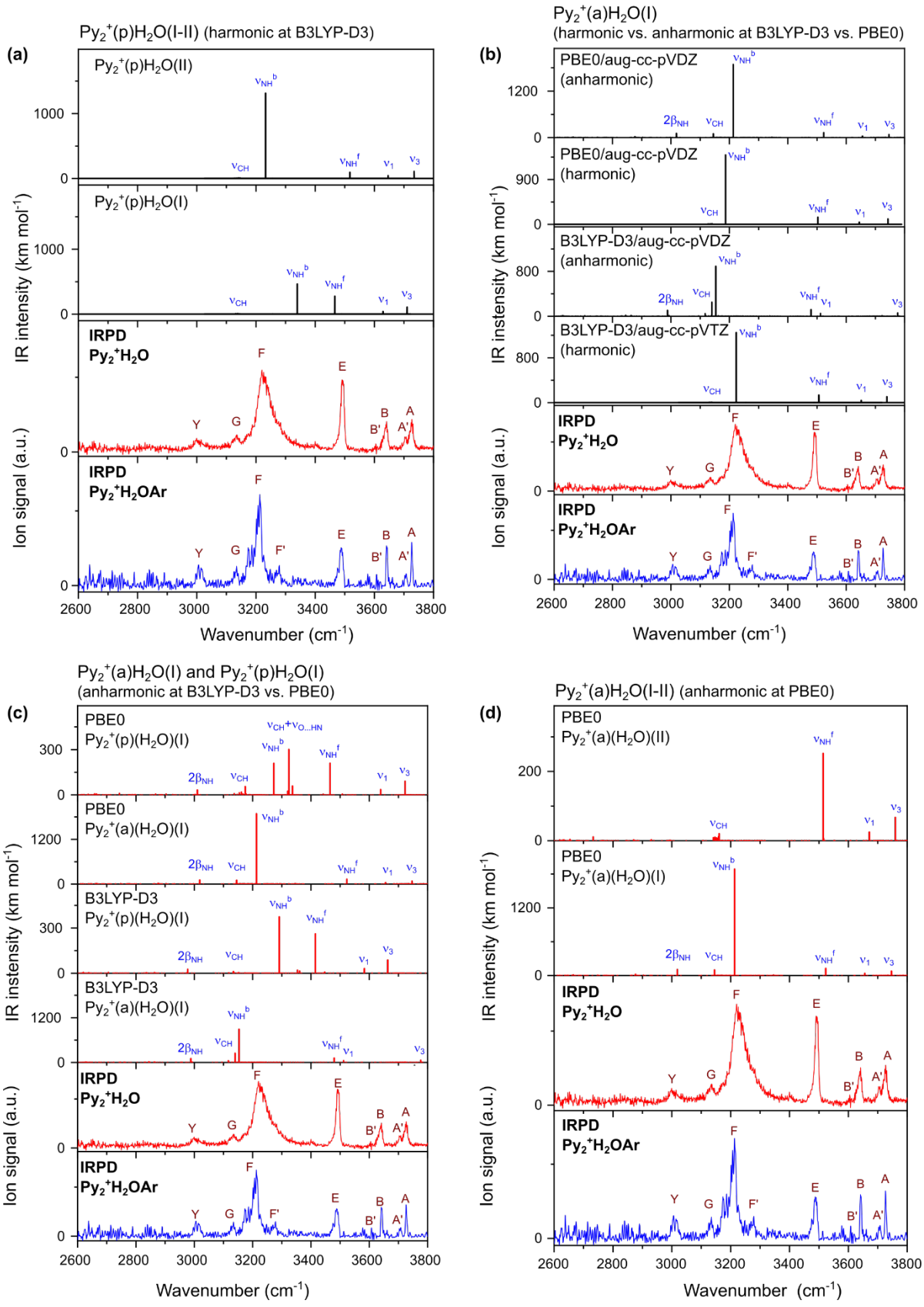
Figure S1. (a) Collision-induced dissociation (CID) and (b) laser-induced dissociation (LID) mass spectra of size-selected $Py_2^+(H_2O)_nAr_m$ clusters (n≤3 m≤1) to confirm the composition and main fragmentation channels. The progressive dissociation of H_2O molecules in the LID spectra is due to sequential resonant absorption of the fragment ions.



$Py_2^+(p)H_2O(II)$ (7.2, 46.5, 4.3)

$Py_2^+(p)H_2O(I)Ar(I)$ (4.8, 5.7, 7.8)

Figure S2. Structures of $Py_2^+(p)H_2O(II)$ and $Py_2^+(p)H_2O(I)Ar$ optimised at the B3LYP-D3/aug-cc-pVTZ level. Selected intra- and intermolecular bond lengths (in Å) are given in black and red, respectively. Values in dark red indicate NBO charges (in units of *e*). The energies in parenthesis are the relative energy, dissociation energy of the most weakly bonded ligand, and relative Gibbs free energy at 298 K (E_0, D_0, and G_0 in kJ/mol).


(a)
Py2+(p)H2O(I-II) (harmonic at B3LYP-D3)
Py2+(p)H2O(II)
Py2+(p)H2O(I)
IRPD
Py2+H2O
IRPD
Py2+H2O•Ar
IR intensity (km mol-1)
Ion signal (a.u.)
Wavenumber (cm-1)
(b)
Py2+(a)H2O(I)
(harmonic vs. anharmonic at B3LYP-D3 vs. PBE0)
PBE0/aug-cc-pVDZ
(anharmonic)
PBE0/aug-cc-pVDZ
(harmonic)
B3LYP-D3/aug-cc-pVDZ
(anharmonic)
B3LYP-D3/aug-cc-pVTZ
(harmonic)
IRPD
Py2+H2O
IRPD
Py2+H2O•Ar
IR intensity (km mol-1)
Ion signal (a.u.)
Wavenumber (cm-1)
(c)
Py2+(a)H2O(I) and Py2+(p)H2O(I)
(anharmonic at B3LYP-D3 vs. PBE0)
PBE0
Py2+(p)(H2O)(I)
PBE0
Py2+(a)(H2O)(I)
B3LYP-D3
Py2+(p)(H2O)(I)
B3LYP-D3
Py2+(a)(H2O)(I)
IRPD
Py2+H2O
IRPD
Py2+H2O•Ar
IR intensity (km mol-1)
Ion signal (a.u.)
Wavenumber (cm-1)
(d)
Py2+(a)H2O(I-II) (anharmonic at PBE0)
PBE0
Py2+(a)(H2O)(II)
PBE0
Py2+(a)(H2O)(I)
IRPD
Py2+H2O
IRPD
Py2+H2O•Ar
IR intensity (km mol-1)
Ion signal (a.u.)
Wavenumber (cm-1)

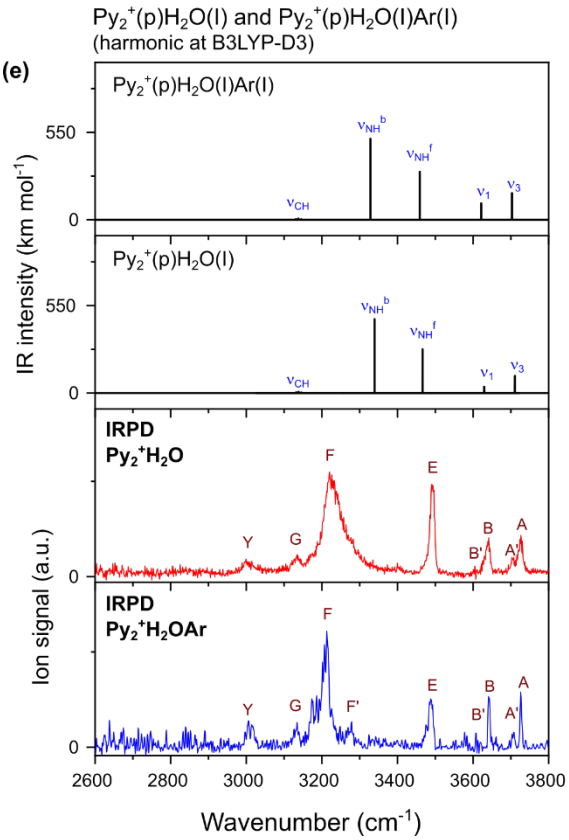
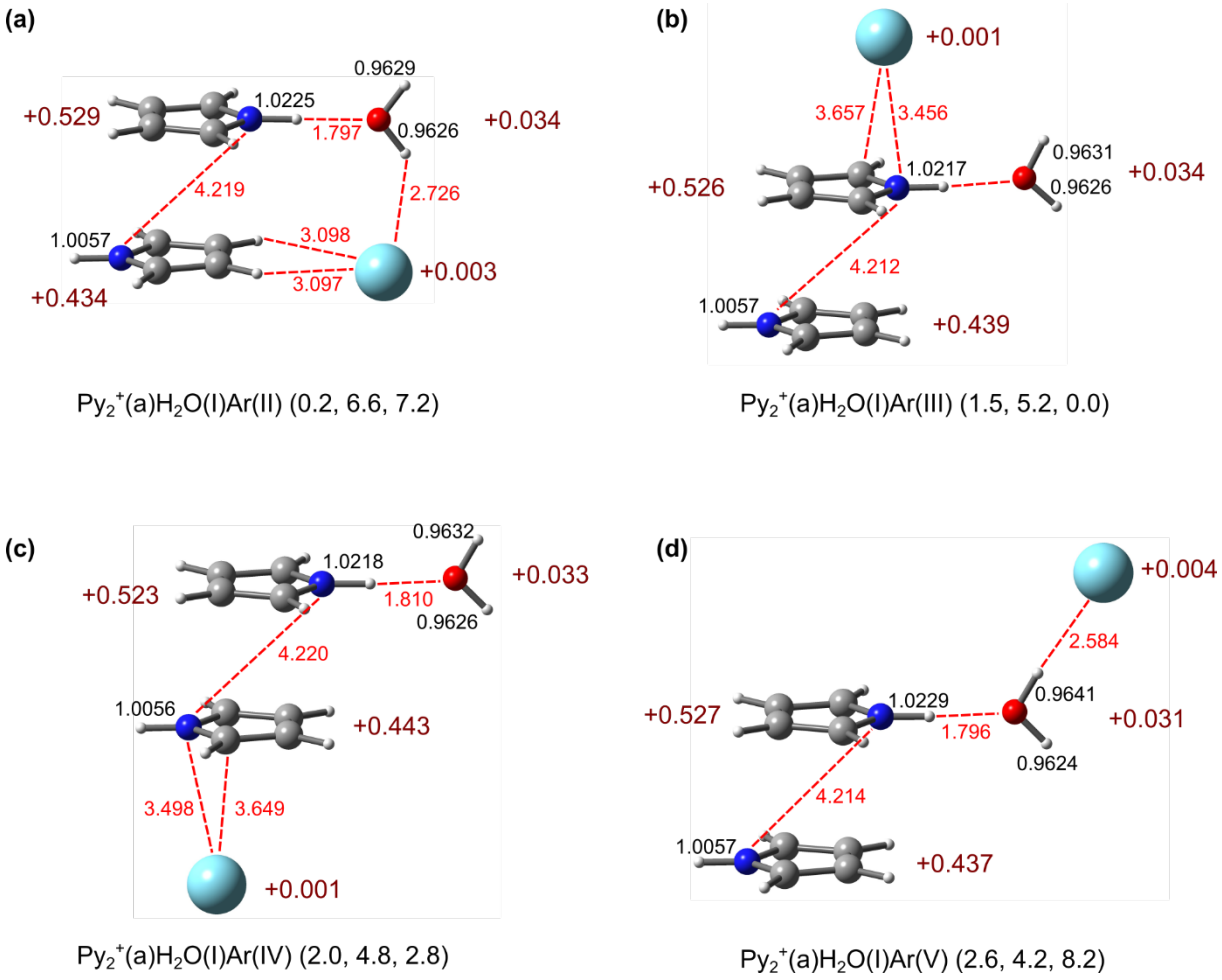


Figure S3. Comparison between IRPD spectra of $Py_2^+H_2OAr_m$ (m=0-1) and (a) harmonic IR spectra of $Py_2^+(p)H_2O$(I-II) computed at the B3LYP-D3/aug-cc-pVTZ level, (b) harmonic and anharmonic IR spectra computed for $Py_2^+(a)H_2O$(I) with reduced basis sets and different DFT functionals, (c) anharmonic IR spectra of $Py_2^+(a/p)H_2O$(I) computed at the B3LYP-D3/aug-cc-pVDZ and PBE0/aug-cc-pVDZ levels, (d) anharmonic IR spectra of $Py_2^+(a)H_2O$(I-II) computed at the PBE0/aug-cc-pVDZ level, and (e) harmonic IR spectra of $Py_2^+(p)H_2O$(I) and $Py_2^+(p)H_2O$(I)Ar(I) computed at the B3LYP-D3/aug-cc-pVTZ level. The harmonic spectra are scaled, while the anharmonic spectra are unscaled.



$Py_2^+(a)H_2O(I)Ar(II)$ (0.2, 6.6, 7.2)

$Py_2^+(a)H_2O(I)Ar(III)$ (1.5, 5.2, 0.0)

$Py_2^+(a)H_2O(I)Ar(IV)$ (2.0, 4.8, 2.8)

$Py_2^+(a)H_2O(I)Ar(V)$ (2.6, 4.2, 8.2)

Figure S4. Structures of $Py_2^+(a)H_2O(I)Ar$(II-V) optimised at the B3LYP-D3/aug-cc-pVTZ level. Selected intra- and intermolecular bond lengths (in Å) are given in black and red, respectively. The energies in parenthesis are the relative energy, dissociation energy of the most weakly bonded ligand, and relative Gibbs free energy at 298 K (E_0, D_0, and G_0 in kJ/mol).

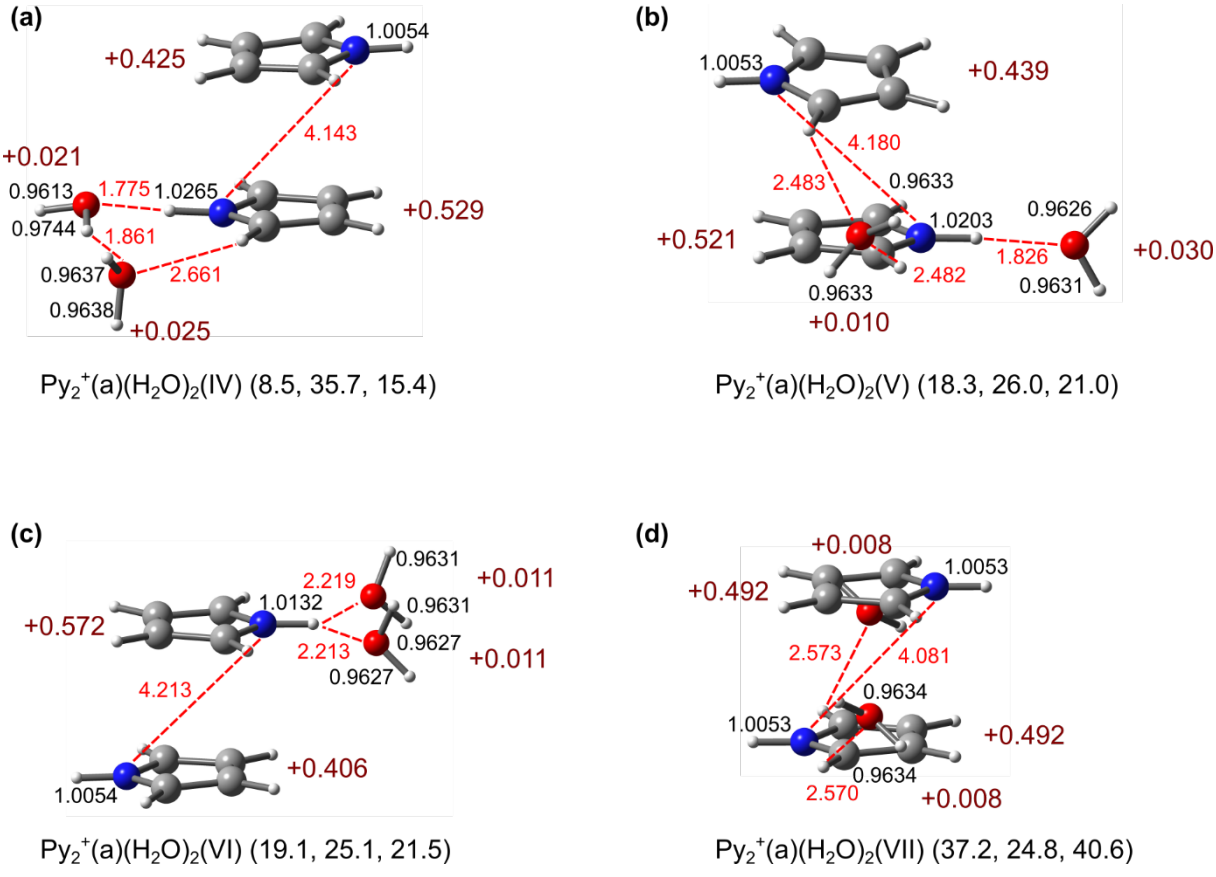
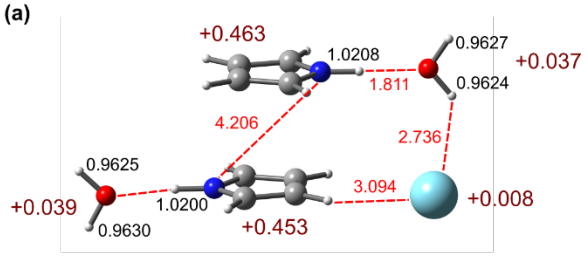
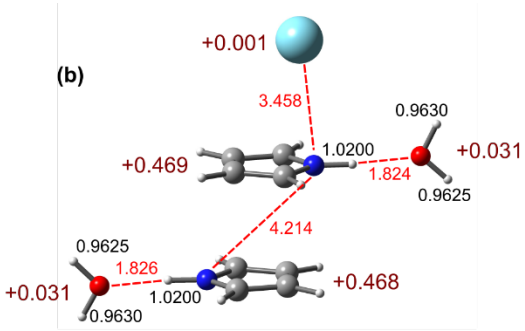


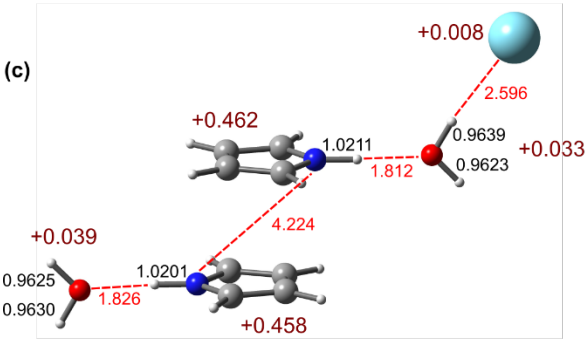
Figure S5. (a-d) Structures of $Py_2^+(a)(H_2O)_2$(IV-VII) optimised at the B3LYP-D3/aug-cc-pVTZ level. Selected intra- and intermolecular bond lengths (in Å) are given in black and red, respectively. Values in dark red indicate NBO charges (in units of *e*). The energies in parenthesis are the relative energy, dissociation energy of the most weakly bonded ligand, and relative Gibbs free energy at 298 K (E_0, D_0, and G_0 in kJ/mol).



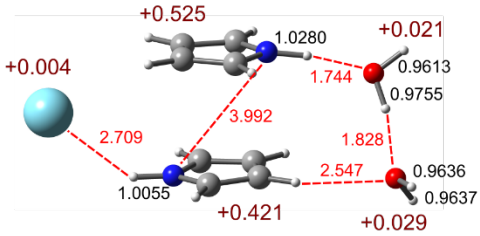
$Py_2^+(a)(H_2O)_2(I)Ar(I)$ (0.0, 6.7, 0.0)



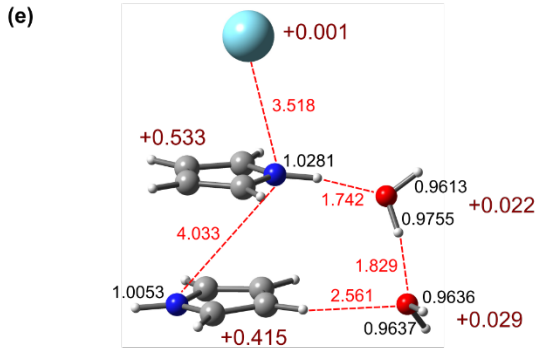
$Py_2^+(a)(H_2O)_2(I)Ar(II)$ (2.4, 4.3, 0.2)



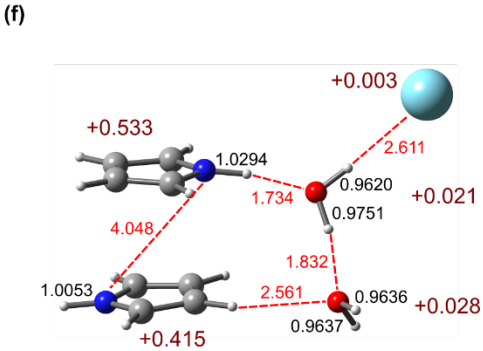
$Py_2^+(a)(H_2O)_2(I)Ar(III)$ (3.5, 3.2, 7.0)



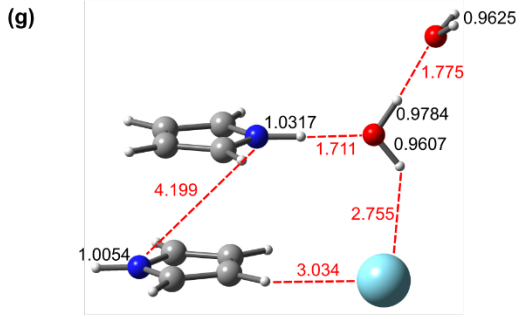
$Py_2^+(a)(H_2O)_2(II)Ar(I)$ (4.9, 6.8, 12.2)



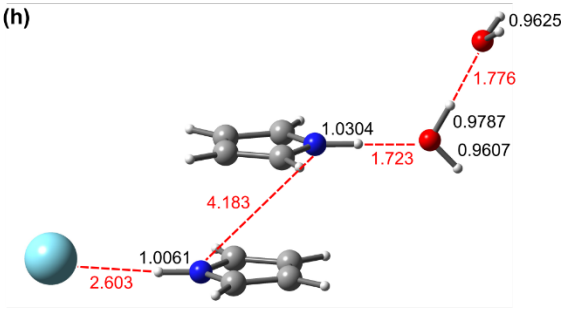
$Py_2^+(a)(H_2O)_2(II)Ar(II)$ (7.4, 4.3, 13.8)



$Py_2^+(a)(H_2O)_2(II)Ar(III)$ (8.2, 3.5, 15.4)

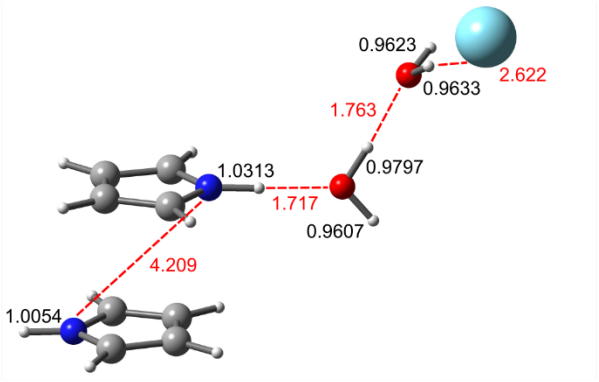


$Py_2^+(a)(H_2O)_2(III)Ar(I)$ (5.7, 6.5, 10.3)



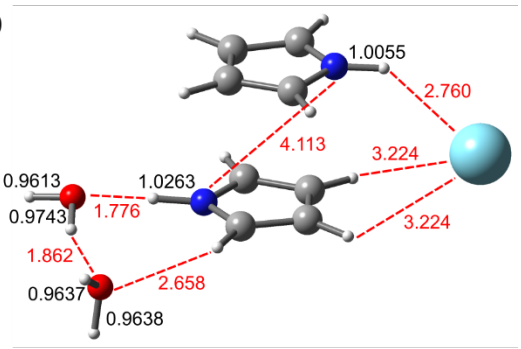
$Py_2^+(a)(H_2O)_2(III)Ar(II)$ (5.7, 6.5, 2.4)

(i)



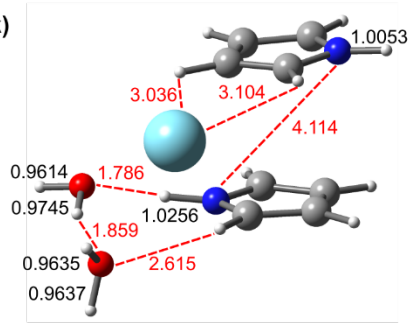
$Py_2^+(a)(H_2O)_2(III)Ar(III)$ (8.6, 3.5, 10.7)

(j)



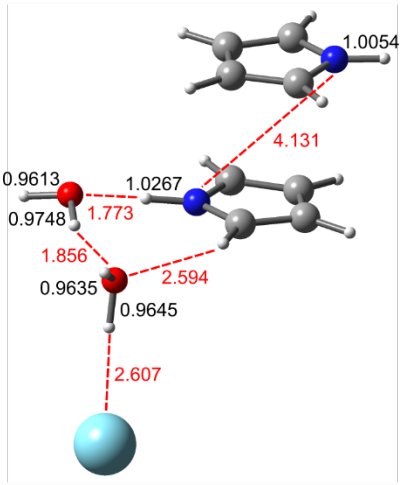
$Py_2^+(a)(H_2O)_2(IV)Ar(I)$ (8.0, 7.2, 14.2)

(k)



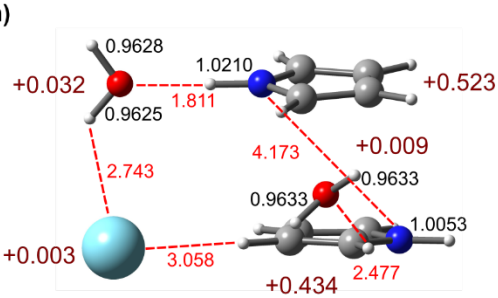
$Py_2^+(a)(H_2O)_2(IV)Ar(II)$ (8.5, 6.7, 16.8)

(l)



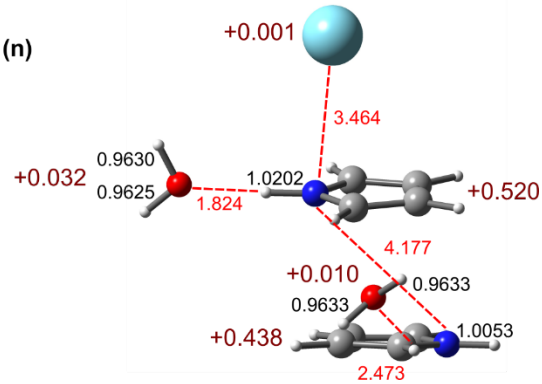
$Py_2^+(a)(H_2O)_2(IV)Ar(III)$ (10.6, 4.6, 13.0)

(m)



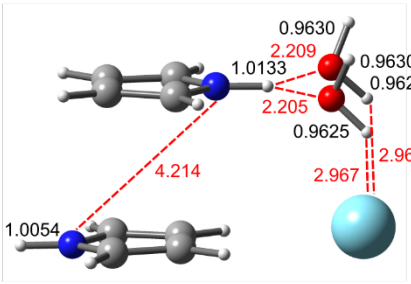
$Py_2^+(a)(H_2O)_2(V)Ar(I)$ (18.7, 6.7, 23.0)

(n)



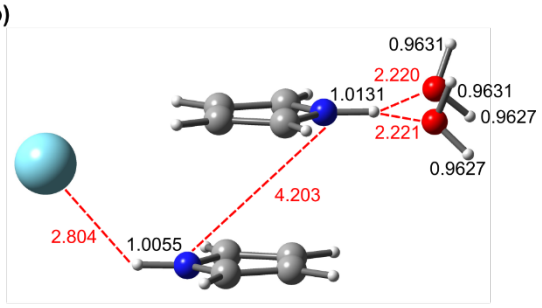
$Py_2^+(a)(H_2O)_2(V)Ar(II)$ (20.1, 4.9, 21.7)

(o)



$Py_2^+(a)(H_2O)_2(VI)Ar(I)$ (18.2, 7.7, 25.3)

(p)



$Py_2^+(a)(H_2O)_2(VI)Ar(II)$ (18.2, 7.6, 24.5)

Figure S6. (a-p) Structures of $Py_2^+(a)(H_2O)_2(I\text{-}VI)Ar$ optimised at the B3LYP-D3/aug-cc-pVTZ level. Selected intra- and intermolecular bond lengths (in Å) are given in black and red, respectively. Values in dark red indicate NBO charges (in units of *e*). The energies in parenthesis are the relative energy, dissociation energy of the most weakly bonded ligand, and relative Gibbs free energy at 298 K (E_0, D_0, and G_0 in kJ/mol).

$Py_2^+(p)(H_2O)_2(I)$ (-1.0, 48.9, 6.0)

$Py_2^+(p)(H_2O)_2(II)$ (3.4, 44.5, 9.8)

Figure S7. (a-b) Structures of $Py_2^+(p)(H_2O)_2$(I-II) optimised at the B3LYP-D3/aug-cc-pVTZ level. Selected intra- and intermolecular bond lengths (in Å) are given in black and red, respectively. Values in dark red indicate NBO charges (in units of *e*). The energies in parenthesis are the relative energy, dissociation energy of the most weakly bonded ligand, and relative Gibbs free energy at 298 K (E_0, D_0, and G_0 in kJ/mol). The relative energy and Gibbs free energy are referenced to $Py_2^+(a)(H_2O)_2$(I) in Figure 5.

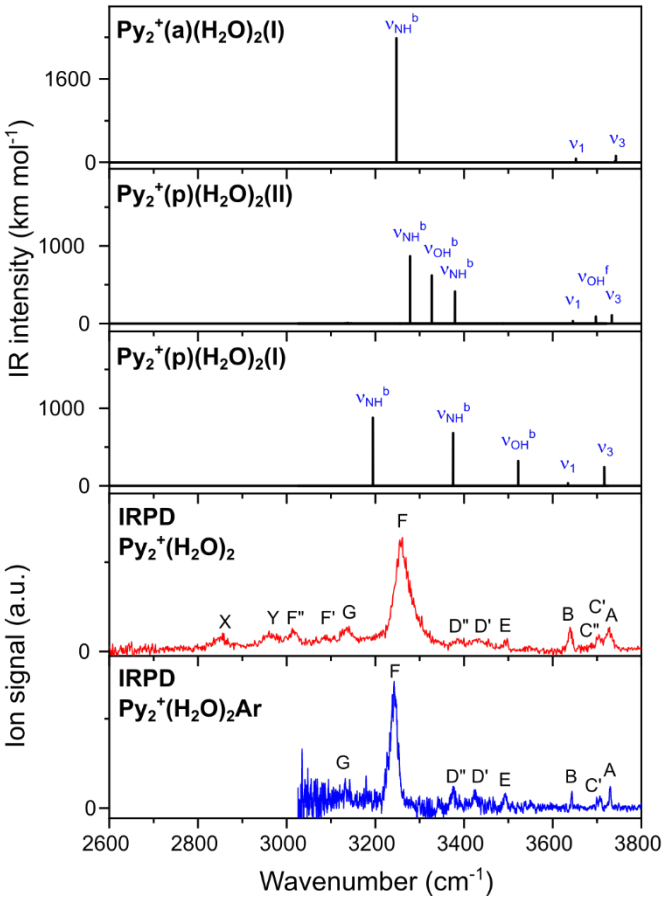
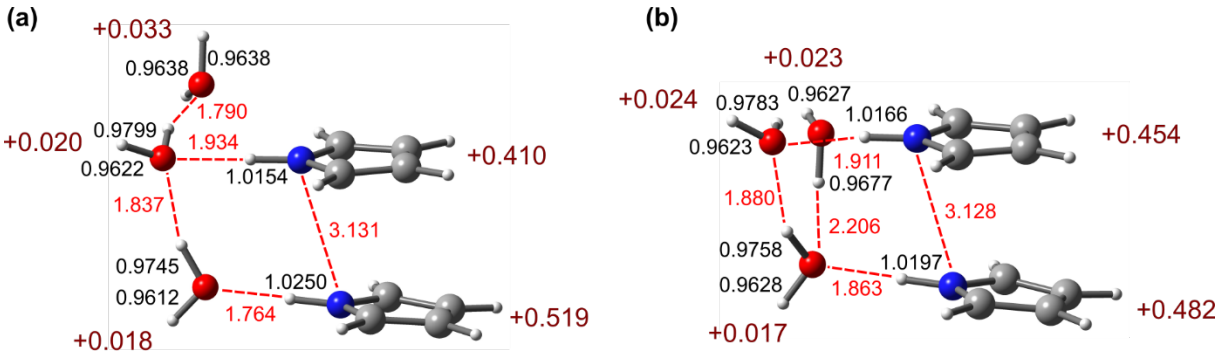


Figure S8. Comparison between the IRPD spectra ($Py_2^+(H_2O)_2$ and $Py_2^+(H_2O)_2Ar$) and the IR spectra of $Py_2^+(p)(H_2O)_2$(I-II) and $Py_2^+(a)(H_2O)_2$(I) computed at the B3LYP-D3/aug-cc-pVTZ level.



$Py_2^+(p)(H_2O)_3$(I) (-7.7, 43.3, 4.9)

$Py_2^+(p)(H_2O)_3$(II) (-5.0, 40.6, 14.1)

Figure S9. (a-b) Structures of $Py_2^+(p)(H_2O)_3$(I-II) optimised at the B3LYP-D3/aug-cc-pVTZ level. Selected intra- and intermolecular bond lengths (in Å) are given in black and red, respectively. Values in dark red indicate NBO charges (in units of *e*). The energies in parenthesis are the relative energy, dissociation energy of the most weakly bonded ligand, and relative Gibbs free energy at 298 K (E_0, D_0, and G_0 in kJ/mol). The relative energy is referenced to $Py_2^+(a)(H_2O)_3$(I) and Gibbs free energy is referenced to $Py_2^+(a)(H_2O)_3$(II) in Figure 5.

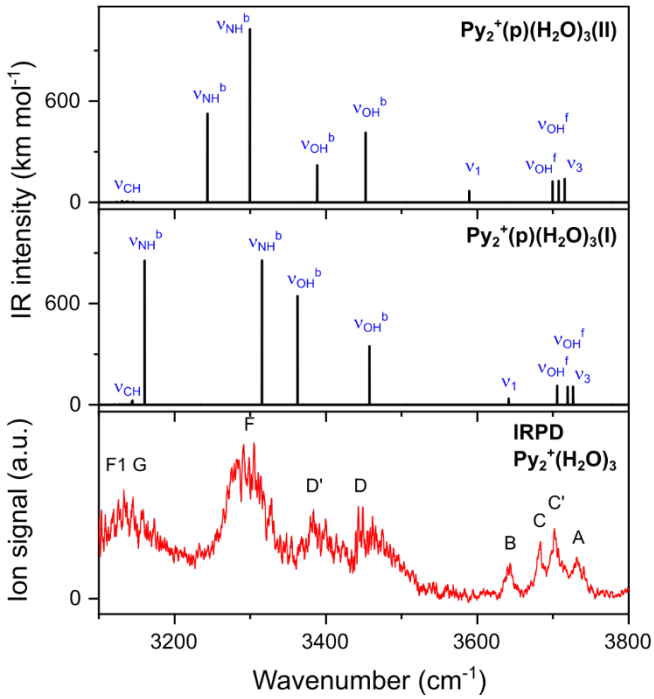


Figure S10. IRPD spectra of $Py_2^+(H_2O)_3$ in the CH, NH, and OH stretch range compared to the linear IR absorption spectra of $Py_2^+(p)(H_2O)_3$(I-II). The calculated transitions are compiled in Table S8.

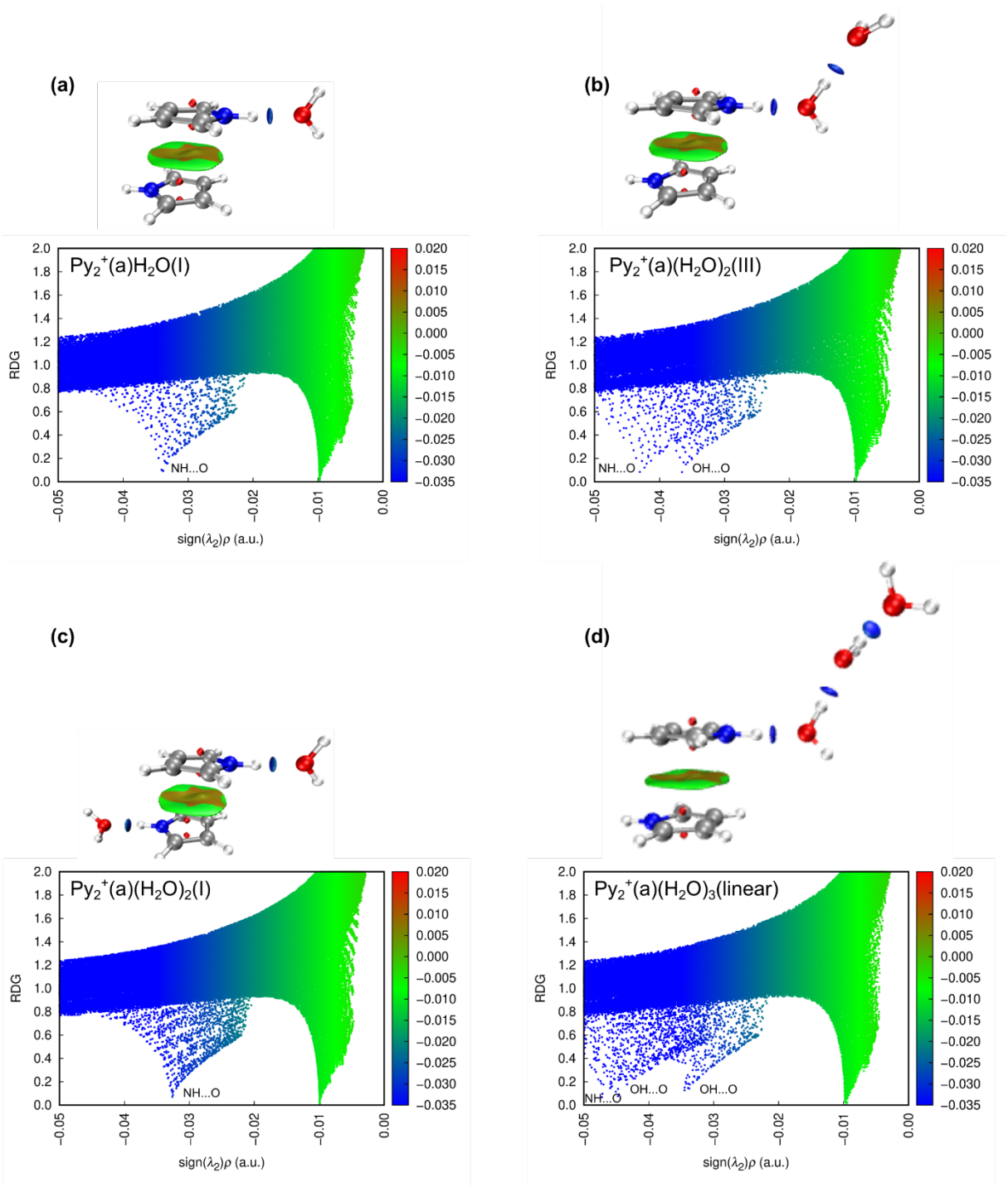


Figure S11. (a-d) Noncovalent (NCI) interactions in $Py_2^+(a)(H_2O)_n$ (n=1-3) visualised via the reduced electron density gradient (RDG), $s(\rho) \sim |\nabla(\rho)|/\rho^{4/3}$ as a function of the oriented electron density ρ^*=sign(λ_2)ρ. Blue: attractive interactions (negative λ_2), red: repulsive interactions (positive λ_2), and green: weak van der Waals contact (λ_2 close to zero).

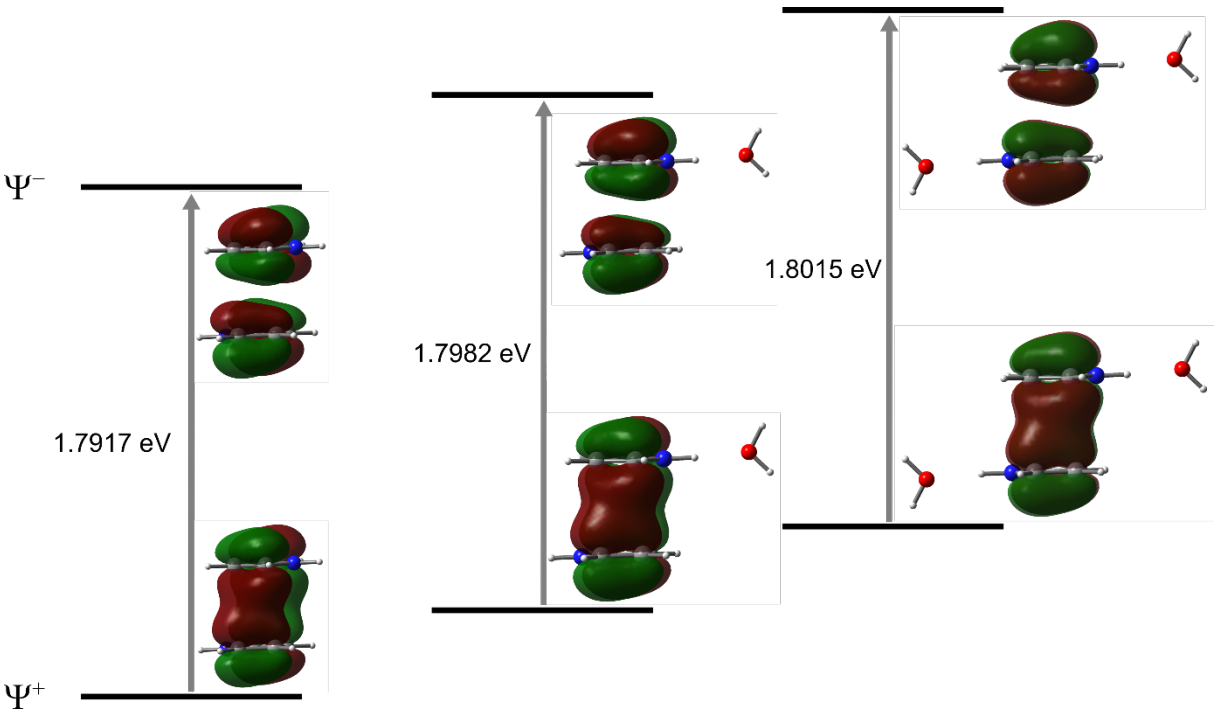


Figure S12. Frontier MOs and the vertical TD-DFT transition energies of the CR band computed for Py_2^+(a), Py_2^+(a)H_2O(I), Py_2^+(a)$(H_2O)_2$(I) at the B3LYP-D3/aug-cc-pVTZ level.

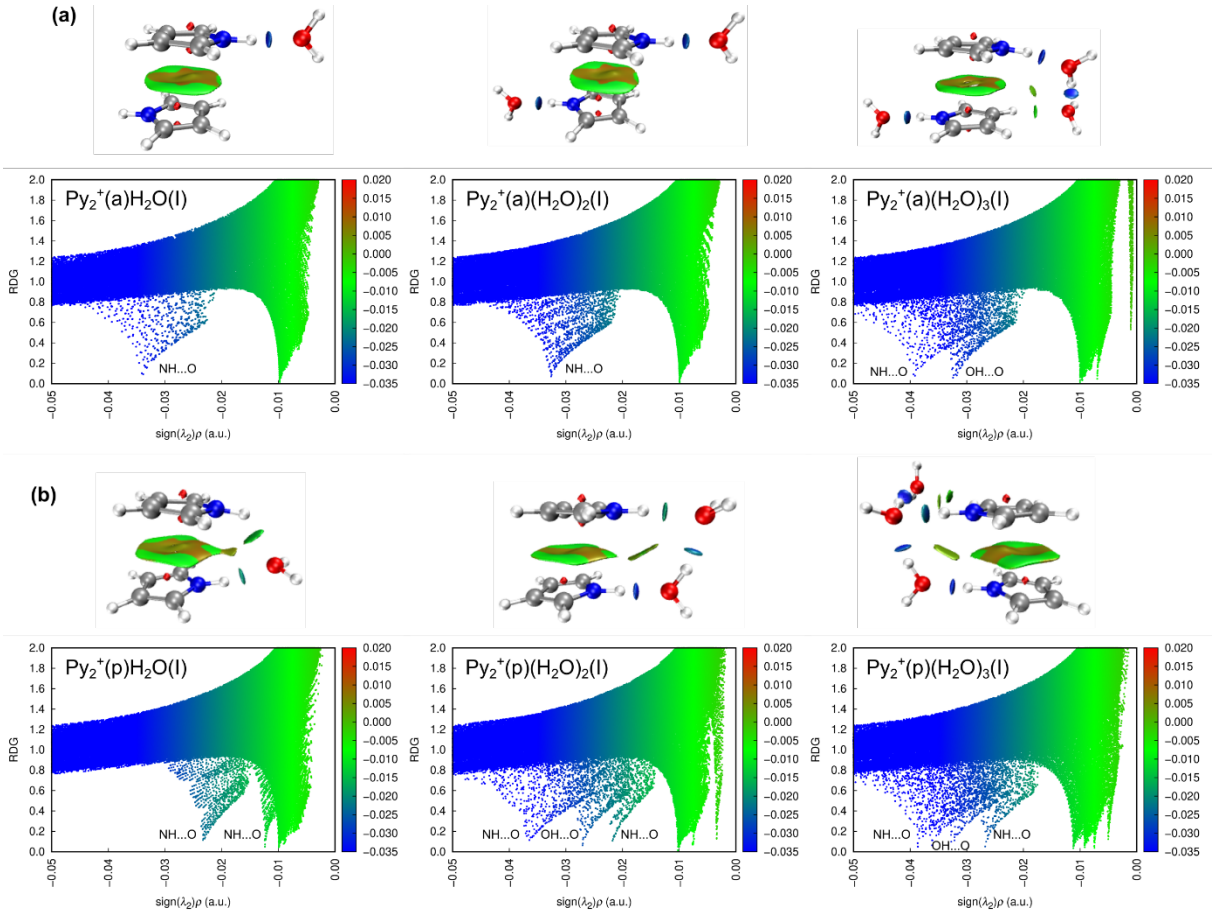


Figure S13. Noncovalent (NCI) interactions calculated for (a) $Py_2^+(a)(H_2O)_n$ and (b) $Py_2^+(p)(H_2O)_n$ (n=1-3) visualised via the reduced electron density gradient (RDG), $s(\rho) \sim |\nabla(\rho)|/\rho^{4/3}$ as a function of the oriented electron density $\rho^*=\text{sign}(\lambda_2)\rho$. Blue: attractive interactions (negative λ_2), red: repulsive interactions (positive λ_2), and green: weak van der Waals contact (λ_2 close to zero).

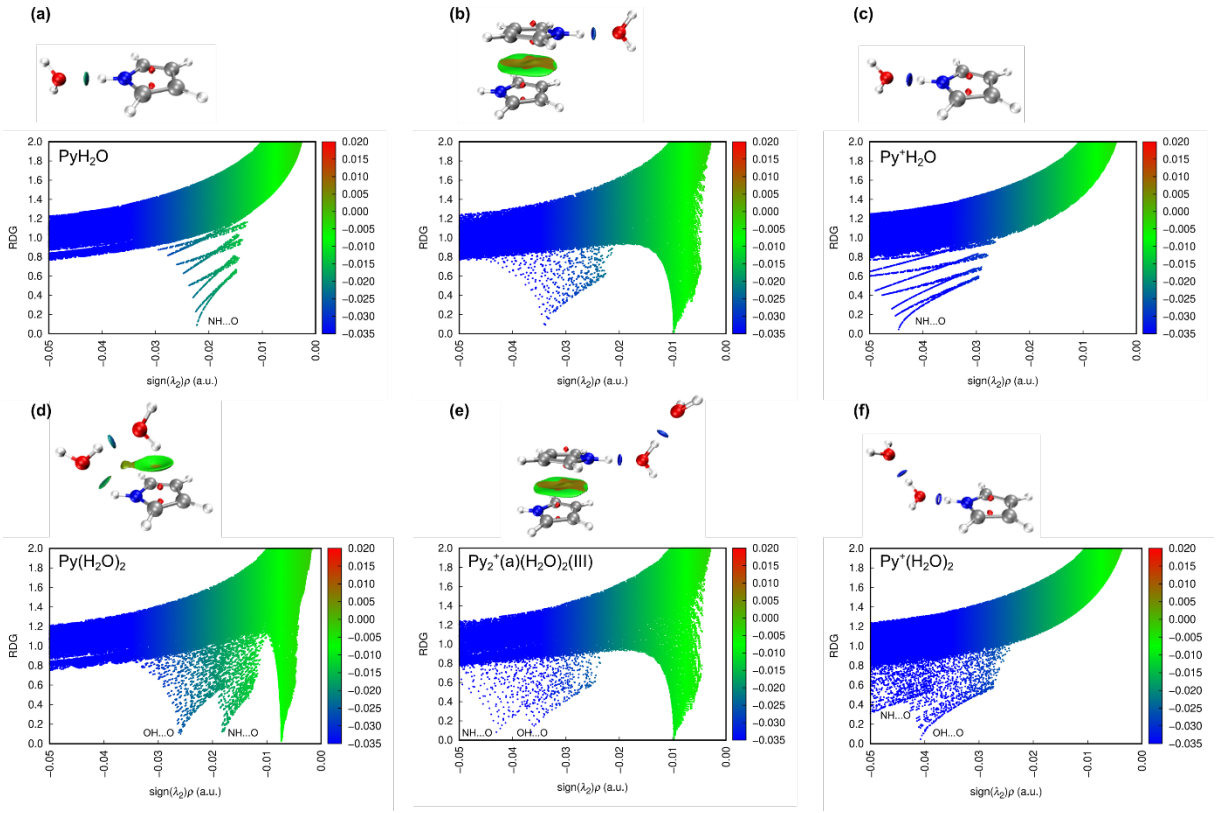


Figure S14. Noncovalent (NCI) interactions in (a-c) $Py^{q}H_2O$ and (d-f) $Py^{q}(H_2O)_2$ (q=0, +0.5, +1.0) visualised via the reduced electron density gradient (RDG), $s(\rho) \sim |\nabla(\rho)|/\rho^{4/3}$ as a function of the oriented electron density $\rho^{*}=\text{sign}(\lambda_2)\rho$. Blue: attractive interactions (negative λ_2), red: repulsive interactions (positive λ_2), and green: weak van der Waals contact (λ_2 close to zero).

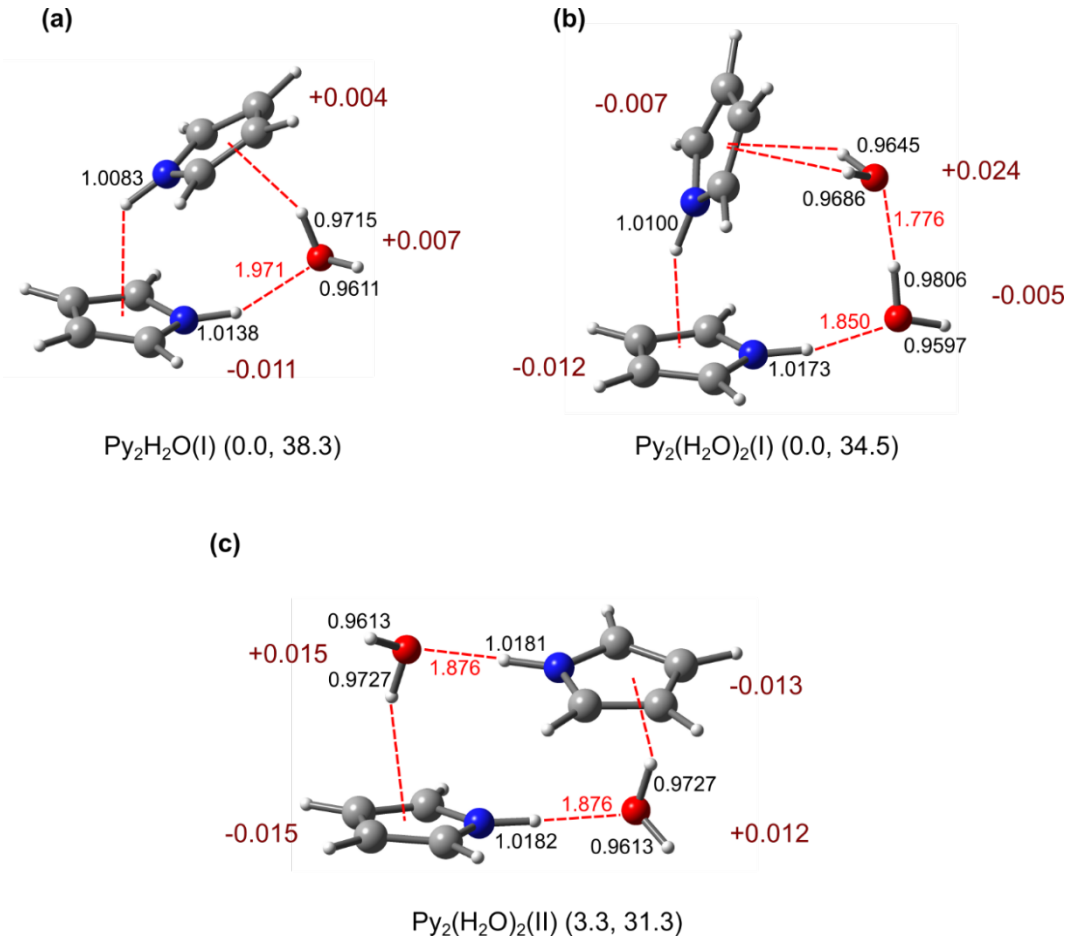


Figure S15. (a-c) Structures of neutral $Py_2(H_2O)_n$ (n=1-2) optimised at the B3LYP-D3/aug-cc-pVTZ level. Selected intra- and intermolecular bond lengths (in Å) are given in black and red, respectively. Values in dark red indicate NBO charges (in units of e). The energies in parenthesis are the relative energy and dissociation energy of the most weakly bonded ligand (E_0 and D_0 in kJ/mol).

Table S1. Positions (in cm^{-1}) and Suggested Vibrational Assignments of the Transitions Observed in the IRPD Spectra of $Py_2^+(H_2O)_nAr_m$ (n=0-3, m=0 and 1) Compared to Frequencies of the Most Stable Isomers Calculated at the B3LYP-D3/aug-cc-pVTZ Level.

	exp [a]	structure	calc [b]	mode
H_2O	3657		3657 (5)	ν_1
	3756		3756 (63)	ν_3
$(H_2O)_2$	3601		3540 (342)	ν_{OH} [b]
	3654		3652 (10)	ν_1
	3735		3728 (86)	ν_{OH} [f]
	3746		3747 (84)	ν_3
Py^+Ar	G 3131 (23), 3145 (16)	Py^+Ar(H) $Py^+Ar(\pi)$	3117 (13), 3121 (9), 3128 (26), 3140 (19) 3118 (13), 3123 (10), 3129 (28), 3141(16)	ν_{CH}
	F 3423 (32)	Py^+Ar(H)	3412 (522)	ν_{NH} [b]
	E 3450 (11)	$Py^+Ar(\pi)$	3462 (203)	ν_{NH} [f]
Py_2^+	G 3126 (29)	Py_2^+(a)	3121 (1), 3122 (0), 3131 (0), 3131 (16), 3138 (0), 3138 (19), 3144 (1), 3145 (0)	ν_{CH}
	E 3479 (19)	Py_2^+(a)	3500 (288), 3501 (0)	ν_{NH} [f]
	F* 3028 (116)	$Py_2(OC)^+$	2792 (3561)	ν_{NH} [b]
	X 2888 (68)	$Py_2(OC)^+$	--	FR
$Py_2^+H_2O$	Y 3006 (49)	$Py_2^+(a)H_2O(I)$	--	$2\beta_{NH}$
	G 3134 (29)	$Py_2^+(a)H_2O(I)$	3121 (1), 3122 (0), 3130 (4), 3131 (8), 3136 (5), 3139 (7), 3143 (3), 3145 (0)	ν_{CH}
	Y′ 3175 (nr)	$Py_2^+(a)H_2O(I)$	--	$2\beta_{OH}$
	F 3228 (58)	$Py_2^+(a)H_2O(I)$	3223 (1248)	ν_{NH} [b]
	F′ 3282 (nr)	$Py_2^+(p)H_2O(I)$	3339 (465)	ν_{NH} [b]
	E 3492 (13)	$Py_2^+(a)H_2O(I)$	3506 (135)	ν_{NH} [f]
	B′ 3605 (xx)	$Py_2^+(p)H_2O(I)$	3651 (40)	ν_1
	B 3639 (15)	$Py_2^+(a)H_2O(I)$	3651 (39)	ν_1
	A′ 3705 (13)	$Py_2^+(p)H_2O(I)$	3713 (108)	ν_3
	A 3725 (15)	$Py_2^+(a)H_2O(I)$	3739 (105)	ν_3
$Py_2^+H_2OAr$	Y 3010 (27)	$Py_2^+(a)H_2O(I)Ar(I)$	--	$2\beta_{NH}$
	G 3133 (17)	$Py_2^+(a)H_2O(I)Ar(I)$	3121 (1), 3122 (0), 3130 (3),	ν_{CH}

			3131 (7), 3135 (4), 3138 (7), 3143 (3), 3145 (0)	
	Y′ 3175 (28)	$Py_2^+(a)H_2O(I)Ar(I)$	--	$2\beta_{OH}$
	F 3210 (23)	$Py_2^+(a)H_2O(I)Ar(I)$	3226 (1276)	ν_{NH}^b
	F′ 3274 (20)	$Py_2^+(p)H_2O(I)Ar(I)$	3328 (510)	ν_{NH}^b
	E 3488 (14)	$Py_2^+(a)H_2O(I)Ar(I)$	3494 (315)	ν_{NH}^f
	B′ 3607 (nr)	$Py_2^+(p)H_2O(I)Ar(I)$	3649 (42)	ν_1
	B 3642 (6)	$Py_2^+(a)H_2O(I)Ar(I)$	3650 (39)	ν_1
	A′ 3706 (10)	$Py_2^+(p)H_2O(I)Ar(I)$	3737 (108)	ν_3
	A 3727 (4)	$Py_2^+(a)H_2O(I)Ar(I)$	3740 (105)	ν_3
$Py_2^+H_2OAr$ (colder)	G 3141 (nr)	$Py_2^+(a)H_2O(I)Ar(I)$	3121 (1), 3122 (0), 3130 (3), 3131 (7), 3135 (4), 3138 (7), 3143 (3), 3145 (0)	ν_{CH}
	Y′ 3178 (16)	$Py_2^+(a)H_2O(I)Ar(I)$	--	$2\beta_{OH}$
	F 3213 (15)	$Py_2^+(a)H_2O(I)Ar(I)$	3226 (1276)	ν_{NH}^b
	E 3489 (10)	$Py_2^+(a)H_2O(I)Ar(I)$	3494 (315)	ν_{NH}^f
	B 3642 (4)	$Py_2^+(a)H_2O(I)Ar(I)$	3650 (39)	ν_1
	A 3727 (5)	$Py_2^+(a)H_2O(I)Ar(I)$	3740 (105)	ν_3
$Py_2^+(H_2O)_2$	X 2852 (37)	$Py_2^+(a)(H_2O)_2(II\text{-}III)$	--	FR
	Y 2967 (64)	$Py_2^+(a)(H_2O)_2(I\text{-}III)$	--	$2\beta_{NH}$
	F″ 3014 (19)	$Py_2^+(a)(H_2O)_2(III)$	3068 (2001)	ν_{NH}^b
	F′ 3093 (57)	$Py_2^+(a)(H_2O)_2(II)$	3107 (1281)	ν_{NH}^b
	G 3136 (15)	$Py_2^+(a)(H_2O)_2(I\text{-}III)$	3120 (1), 3121 (0), 3129 (0), 3130 (8), 3136 (0), 3136 (7), 3143 (3), 3144 (0)	ν_{CH}
	F 3260 (41)	$Py_2^+(a)(H_2O)_2(I)$	3247 (2381), 3253 (2)	ν_{NH}^b
	D″ 3388 (21)	$Py_2^+(a)(H_2O)_2(III)$	3384 (795)	ν_{OH}^b
	D′ 3430 (55)	$Py_2^+(a)(H_2O)_2(II)$	3433 (420)	ν_{OH}^b
	E 3493 (13)	$Py_2^+(a)(H_2O)_2(II\text{-}III)$	3510 (128)	ν_{NH}^f
	B 3639 (10)	$Py_2^+(a)(H_2O)_2(I)$	3652 (72), 3652 (1)	ν_1
		$Py_2^+(a)(H_2O)_2(II)$	3631 (31)	ν_1
	C″ 3684 (nr)	$Py_2^+(a)(H_2O)_2(III)$	3655 (26)	ν_1
	C′ 3703 (12)	$Py_2^+(a)(H_2O)_2(II)$	3718 (108)	ν_{OH}^f
		$Py_2^+(a)(H_2O)_2(II)$	3728(102)	ν_3
		$Py_2^+(a)(H_2O)_2(III)$	3722 (78)	ν_{OH}^f

	A 3726 (19)	$Py_2^+(a)(H_2O)_2(I)$	3742 (178), 3741 (27)	ν_3
		$Py_2^+(a)(H_2O)_2(III)$	3746 (111)	ν_3
$Py_2^+(H_2O)_2Ar$	G 3135 (nr)	$Py_2^+(a)(H_2O)_2(I\text{-}III)Ar(I)$	3121 (1), 3124 (1), 3130 (3), 3131 (4), 3136 (2), 3137 (5), 3144 (3), 3145 (1)	ν_{CH}
	F 3242 (19)	$Py_2^+(a)(H_2O)_2(I)Ar(I)$	3239 (1663), 3254 (720)	ν_{NH}^b
	D″ 3376 (9)	$Py_2^+(a)(H_2O)_2(III)Ar(II)$	3386 (790)	ν_{OH}^b
	D′ 3424 (11)	$Py_2^+(a)(H_2O)_2(II)Ar(I)$	3434 (418)	ν_{OH}^b
	E 3493 (8)	$Py_2^+(a)(H_2O)_2(II\text{-}III)Ar(II)$	3500 (280)	ν_{NH}^f
	B 3643 (3)	$Py_2^+(a)(H_2O)_2(I)Ar(I)$	3651 (39), 3653 (24)	ν_1
	C″ 3700 (3)	$Py_2^+(a)(H_2O)_2(II)Ar(I)$	3718 (107)	ν_{OH}^f
	C′ 3706 (9)	$Py_2^+(a)(H_2O)_2(III)Ar(II)$	3722 (79)	ν_{OH}^f
	A 3730 (4)	$Py_2^+(a)(H_2O)_2(I)Ar(I)$	3741 (100), 3743 (130)	ν_3
$Py_2^+(H_2O)_3$	F1/G 3139 (85) (nr)	$Py_2^+(a)(H_2O)_3(I\text{-}II)$	3118 (1), 3119 (0), 3127 (4), 3129 (5), 3135 (3), 3137 (4), 3142 (314), 3142 (267), 3147 (747)	ν_{CH} ν_{NH}^b/ν_{CH}
	F 3293 (63)	$Py_2^+(a)(H_2O)_3(I)$	3268 (1052)	ν_{NH}^b
	D′ 3388 (37)	$Py_2^+(a)(H_2O)_3(I)$	3400 (744)	ν_{OH}^b
	D 3459 (84)	$Py_2^+(a)(H_2O)_3(I)$	3442 (405)	ν_{OH}^b
	B 3642 (10)	$Py_2^+(a)(H_2O)_3(I)$	3643 (30), 3652 (34)	ν_1
		$Py_2^+(a)(H_2O)_3(II)$	3653 (35), 3656 (25)	ν_1
	C 3683 (12)	$Py_2^+(a)(H_2O)_3(I)$	3719 (105)	ν_{OH}^f
	C′ 3702 (9)	$Py_2^+(a)(H_2O)_3(II)$	3724 (79)	ν_{OH}^f
	A 3732 (20)	$Py_2^+(a)(H_2O)_3(I)$	3731 (100), 3742 (99)	ν_3
		$Py_2^+(a)(H_2O)_3(II)$	3743 (101), 3748 (109)	ν_3

[a] Peak positions and widths (in parenthesis) are obtained from deconvolution. [b] IR intensities in parenthesis are given in km mol^{-1}. nr = not resolved, FR = Fermi resonance.

Table S2. Calculated NH and CH stretching frequencies of isomeric Py_2^+ obtained at the B3LYP-D3/aug-cc-pVTZ level. The calculated frequencies are scaled by factors of 0.9619 for both NH and CH modes, respectively.

structure	symmetry	calc (km mol^{-1})	mode	remark
Py_2^+(a)	C_{2h}	3121 (1), 3122 (0), 3131 (0), 3131 (16), 3138 (0), 3138 (19), 3144 (1), 3145 (0)	ν_{CH}	
		3500 (288)	ν_{NH}^f	Antisym.
		3501 (0)	ν_{NH}^f	Sym.
Py_2^+(p)	C_s	3124 (0), 3125 (2), 3130 (7), 3133 (7), 3137 (5), 3140 (12), 3146 (0), 3146 (4)	ν_{CH}	
		3499 (131)	ν_{NH}^f	Antisym.
		3510 (120)	ν_{NH}^f	Sym.

Table S3. Calculated NH, OH and CH stretching frequencies of $Py_2^+(a)H_2O$(II) and $Py_2^+(a)H_2O$(I)Ar(II-V) obtained at the B3LYP-D3/aug-cc-pVTZ level. The calculated frequencies are scaled by factors of 0.9619 and 0.9631 for NH/CH and OH modes, respectively.

structure	calc (km mol^{-1})	mode	remark
$Py_2^+(a)H_2O$(II)	3122 (6), 3122 (0), 3131 (12), 3131 (6), 3137 (0), 3138 (41), 3144 (0), 3145 (5)	ν_{CH}	
	3505 (262)	ν_{NH}^{f}	Antisym.
	3505 (1)	ν_{NH}^{f}	Sym.
	3642 (30)	ν_1	
	3728 (83)	ν_3	
$Py_2^+(a)H_2O$(I)Ar(II)	3121 (1), 3125 (1), 3130 (4), 3132 (7), 3135 (5), 3139 (6), 3143 (5), 3146 (0)	ν_{CH}	
	3212 (1223)	ν_{NH}^{b}	
	3506 (138)	ν_{NH}^{f}	
	3651 (29)	ν_1	
	3741 (134)	ν_3	
$Py_2^+(a)H_2O$(I)Ar(III)	3121 (1), 3122 (0), 3130 (4), 3131 (8), 3136 (5), 3139 (7), 3143 (3), 3145 (0)	ν_{CH}	
	3225 (1219)	ν_{NH}^{b}	
	3506 (135)	ν_{NH}^{f}	
	3651 (37)	ν_1	
	3740 (104)	ν_3	
$Py_2^+(a)H_2O$(I)Ar(IV)	3121 (1), 3123 (0), 3130 (4), 3132 (7), 3136 (5), 3140 (7), 3143 (3), 3146 (0)	ν_{CH}	
	3225 (1255)	ν_{NH}^{b}	
	3506 (130)	ν_{NH}^{f}	
	3651 (39)	ν_1	
	3739 (104)	ν_3	
$Py_2^+(a)H_2O$(I)Ar(V)	3120 (1), 3122 (0), 3130 (4), 3131 (8), 3136 (5), 3139 (7), 3143 (5), 3145 (0)	ν_{CH}	
	3206 (1373)	ν_{NH}^{b}	
	3506 (135)	ν_{NH}^{f}	
	3644 (109)	ν_1	OH…Ar
	3733 (165)	ν_3	OH…Ar

Table S4. Calculated NH, OH, and CH stretching frequencies of $Py_2^+(p)H_2O$(I-II) and $Py_2^+(p)H_2O$(I)Ar obtained at the B3LYP-D3/aug-cc-pVTZ level. The calculated frequencies are scaled by factors of 0.9619 and 0.9631 for NH/CH and OH modes, respectively.

structure	calc (km mol^{-1})	mode	remark
$Py_2^+(p)H_2O$(I)	3123 (0), 3123 (1), 3130 (3), 3132 (5), 3137 (2), 3138 (8), 3144 (0), 3145 (4)	ν_{CH}	
	3339 (465)	ν_{NH}^{b}	Bottom Py
	3466 (276)	ν_{NH}^{f}	Top Py
	3632 (40)	ν_1	
	3713 (108)	ν_3	
$Py_2^+(p)H_2O$(II)	3123 (1), 3123 (1), 3128 (4), 3133 (4), 3136 (3), 3141 (8), 3146 (5), 3147 (4)	ν_{CH}	
	3232 (1312)	ν_{NH}^{b}	Top Py
	3517 (94)	ν_{NH}^{f}	Bottom Py
	3649 (42)	ν_1	
	3737 (108)	ν_3	
$Py_2^+(p)H_2O$(I)Ar(I)	3122 (0), 3123 (1), 3130 (3), 3132 (5), 3136 (3), 3137 (2), 3137 (8), 3144 (0), 3145 (4)	ν_{CH}	
	3328 (510)	ν_{NH}^{b}	Bottom Py
	3459 (302)	ν_{NH}^{f}	Top Py
	3622 (105)	ν_1	
	3703 (168)	ν_3	

Table S5. Calculated NH, OH and CH stretching frequencies of $Py_2^+(a)(H_2O)_2$(II–VI) and $Py_2^+(a)(H_2O)_2$(I-VI)Ar obtained at the B3LYP-D3/aug-cc-pVTZ level. The calculated frequencies are scaled by factors of 0.9619 and 0.9631 for NH/CH and OH modes, respectively.

structure	calc (km mol^{-1})	mode	remark
$Py_2^+(a)(H_2O)_2$(II)	3118 (42), 3119 (4), 3128 (12), 3129 (6), 3136 (4), 3138 (9), 3143 (1), 3144 (9)	ν_{CH}	
	3107 (1281)	ν_{NH}^{b}	
	3510 (128)	ν_{NH}^{f}	
	3433 (420)	ν_{OH}^{b}	
	3631 (31)	ν_1	
	3718 (108)	ν_{OH}^{f}	
	3728 (102)	ν_3	
$Py_2^+(a)(H_2O)_2$(III)	3120 (1), 3122 (0), 3129 (4), 3131 (6), 3134 (4), 3139 (6), 3143 (1), 3146 (1)	ν_{CH}	
	3068 (2001)	ν_{NH}^{b}	
	3509 (129)	ν_{NH}^{f}	
	3384 (795)	ν_{OH}^{b}	
	3655 (26)	ν_1	
	3722 (78)	ν_{OH}^{f}	
	3746 (111)	ν_3	
$Py_2^+(a)(H_2O)_2$(IV)	3118 (3), 3123 (1), 3126 (2), 3132 (6)	ν_{CH}	
	3132 (30), 3139 (623), 3139 (65), 3144 (479), 3146 (72)	$\nu_{NH}^{b} + \nu_{CH}$	
	3509 (130)	ν_{NH}^{f}	
	3459 (427)	ν_{OH}^{b}	
	3641 (30)	ν_1	
	3719 (116)	ν_{OH}^{f}	
	3727 (99)	ν_3	
$Py_2^+(a)(H_2O)_2$(V)	3121 (4), 3122 (1), 3131 (5), 3132 (8), 3137 (11), 3139 (19), 3144 (4), 3146 (6)	ν_{CH}	
	3248 (1140)	ν_{NH}^{b}	
	3510 (123)	ν_{NH}^{f}	
	3644 (27)	ν_1	CH…O
	3651 (36)	ν_1	NH…O
	3731 (80)	ν_3	CH…O
	3741 (103)	ν_3	NH-…O
$Py_2^+(a)(H_2O)_2$(VI)	3122 (1), 3123 (1), 3132 (5), 3134 (9), 3140	ν_{CH}	

	(4), 3146 (10), 3146 (0), 3152 (3)		
	3397 (480)	$\nu_{NH}{}^{b}$	
	3509 (130)	$\nu_{NH}{}^{f}$	
	3649 (16)	ν_1	Out-of-phase
	3650 (44)	ν_1	In-phase
	3737 (0)	ν_3	Out-of-phase
	3737 (165)	ν_3	In-phase
$Py_2^+(a)(H_2O)_2$(VII)	3123 (7), 3124 (0), 3134 (10), 3134 (0), 3143 (0), 3143 (51), 3148 (0), 3149 (0)	ν_{CH}	
	3509 (240)	$\nu_{NH}{}^{f}$	Out-of-phase
	3509 (0)	$\nu_{NH}{}^{f}$	In-phase
	3643 (52)	ν_1	Out-of-phase
	3643 (0)	ν_1	In-phase
	3729 (20)	ν_3	Out-of-phase
	3729 (137)	ν_3	In-phase
$Py_2^+(a)(H_2O)_2$(I)Ar(II)	3120 (1), 3121 (0), 3130 (0), 3130 (8), 3136 (0), 3137 (7), 3143 (3), 3144 (0)	ν_{CH}	
	3249 (2360)	$\nu_{NH}{}^{b}$	Out-of-phase
	3256 (0)	$\nu_{NH}{}^{b}$	In-phase
	3652 (71)	ν_1	Out-of-phase
	3652 (1)	ν_1	In-phase
	3742 (22)	ν_3	In-phase
	3742 (181)	ν_3	Out-of-phase
$Py_2^+(a)(H_2O)_2$(I)Ar(III)	3121 (1), 3121 (0), 3130 (0), 3130 (8), 3136 (0), 3137 (7), 3143 (4), 3144 (0)	ν_{CH}	
	3235 (1742)	$\nu_{NH}{}^{b}$	NH…OH…Ar
	3253 (770)	$\nu_{NH}{}^{b}$	NH…OH
	3647 (102)	ν_1	OH…Ar
	3652 (35)	ν_1	
	3735 (158)	ν_3	OH…Ar
	3742 (103)	ν_3	
$Py_2^+(a)(H_2O)_2$(II)Ar(I)	3121 (1), 3128 (15), 3130 (4), 3137 (3), 3138 (11), 3143 (0), 3144 (13)	ν_{CH}	
	3113 (1233), 3118 (104)	$\nu_{NH}{}^{b} \pm \nu_{CH}$	
	3508 (172)	$\nu_{NH}{}^{f}$	
	3434 (418)	$\nu_{OH}{}^{b}$	
	3642 (31)	ν_1	

	3718 (107)	ν_{OH}^{f}	
	3729 (102)	ν_3	
$Py_2^+(a)(H_2O)_2(II)Ar(II)$	3119 (66), 3120 (1), 3128 (14), 3130 (3), 3137 (4), 3138 (9), 3143 (0)	ν_{CH}	
	3110 (1232)	ν_{NH}^{b}	
	3510 (128)	ν_{NH}^{f}	
	3434 (423)	ν_{OH}^{b}	
	3641 (31)	ν_1	
	3718 (106)	ν_{OH}^{f}	
	3729 (102)	ν_3	
$Py_2^+(a)(H_2O)_2(II)Ar(III)$	3118 (16), 3119 (1), 3127 (10), 3129 (5), 3136 (4), 3138 (8), 3143 (0), 3143 (5)	ν_{CH}	
	3089 (1435)	ν_{NH}^{b}	
	3510 (129)	ν_{NH}^{f}	
	3441 (414)	ν_{OH}^{b}	
	3642 (30)	ν_1	
	3708 (235)	ν_{OH}^{f}	
	3729 (100)	ν_3	
$Py_2^+(a)(H_2O)_2(III)Ar(I)$	3120 (1), 3125 (1), 3129 (4), 3133 (5), 3135 (4), 3140 (5), 3143 (1), 3147 (1)	ν_{CH}	
	3052 (1967)	ν_{NH}^{b}	
	3390 (834)	ν_{OH}^{b}	
	3508 (131)	ν_{NH}^{f}	
	3655 (27)	ν_1	Terminal H_2O
	3723 (105)	ν_{OH}^{f}	
	3747 (110)	ν_3	Terminal H_2O
$Py_2^+(a)(H_2O)_2(III)Ar(II)$	3120 (1), 3121 (0), 3129 (4), 3131 (5), 3135 (4), 3139 (6), 3143 (2), 3145 (1)	ν_{CH}	
	3074 (2016)	ν_{NH}^{b}	
	3386 (790)	ν_{OH}^{b}	
	3500 (280)	ν_{NH}^{f}	NH…Ar
	3655 (26)	ν_1	Terminal H_2O
	3722 (79)	ν_{OH}^{f}	
	3746 (110)	ν_3	Terminal H_2O
$Py_2^+(a)(H_2O)_2(III)Ar(III)$	3120 (1), 3122 (0), 3129 (4), 3131 (6), 3135 (4), 3139 (6), 3143 (1), 3145 (1)	ν_{CH}	
	3060 (2074)	ν_{NH}^{b}	

	3368 (860)	ν_{OH}^{b}	
	3509 (129)	ν_{NH}^{f}	
	3651 (65)	ν_1	OH…Ar
	3722 (76)	ν_{OH}^{f}	
	3741 (170)	ν_3	OH…Ar
$Py_2^+(a)(H_2O)_2(IV)Ar(I)$	3119 (3), 3123 (1), 3126 (1), 3131 (7), 3133 (11)	ν_{CH}	
	3138 (5), 3140 (401), 3145 (149), 3147 (729)	$\nu_{NH}^{b}+\nu_{CH}$	
	3460 (423)	ν_{OH}^{b}	
	3508 (162)	ν_{NH}^{f}	NH…Ar
	3641 (30)	ν_1	
	3719 (116)	ν_{OH}^{f}	
	3727 (98)	ν_3	
$Py_2^+(a)(H_2O)_2(IV)Ar(II)$	3117 (3), 3122 (1), 3125 (4), 3131 (4), 3131 (4)	ν_{CH}	
	3137 (46), 3138 (775), 3142 (15), 3157 (397)	$\nu_{NH}^{b}+\nu_{CH}$	
	3451 (440)	ν_{OH}^{b}	
	3509 (130)	ν_{NH}^{f}	
	3635 (64)	ν_1	OH…Ar
	3719 (111)	ν_{OH}^{f}	
	3721 (164)	ν_3	OH…Ar
$Py_2^+(a)(H_2O)_2(IV)Ar(III)$	3118 (2), 3124 (1), 3127 (4), 3132 (7), 3134 (5)	ν_{CH}	
	3139 (4), 3141 (39), 3148 (3), 3157 (1090)	$\nu_{NH}^{b}+\nu_{CH}$	
	3457 (412)	ν_{OH}^{b}	
	3510 (128)	ν_{NH}^{f}	
	3641 (26)	ν_1	
	3718 (115)	ν_{OH}^{f}	
	3729 (101)	ν_3	
$Py_2^+(a)(H_2O)_2(V)Ar(I)$	3121 (3), 3125 (4), 3131 (4), 3133 (9), 3137 (11), 3140 (16), 3144 (5), 3147 (4)	ν_{CH}	
	3237 (1129)	ν_{NH}^{b}	
	3509 (125)	ν_{NH}^{f}	
	3644 (27)	ν_1	CH…O
	3652 (27)	ν_1	NH…O
	3731 (79)	ν_3	CH…O
	3742 (129)	ν_3	NH…O

$Py_2^+(a)(H_2O)_2(V)Ar(II)$	3121 (4), 3122 (2), 3131 (6), 3131 (8), 3137 (9), 3139 (22), 3144 (3), 3145 (7)		
	3249 (1116)		
	3510 (123)		
	3643 (27)		
	3652 (35)		
	3731 (79)		
	3741 (102)		
$Py_2^+(a)(H_2O)_2(VI)Ar(I)$	3122 (0), 3126 (2), 3133 (2), 3134 (10), 3140 (3), 3145 (9), 3148 (0), 3151 (3)	ν_{CH}	
	3396 (477)	ν_{NH}^{b}	
	3509 (133)	ν_{NH}^{f}	
	3650 (11)	ν_1	Out-of-phase
	3651 (39)	ν_1	In-phase
	3738 (6)	ν_3	Out-of-phase
	3739 (165)	ν_3	In-phase
$Py_2^+(a)(H_2O)_2(VI)Ar(II)$	3122 (1), 3125 (0), 3132 (5), 3136 (9), 3139 (4), 3145 (9), 3146 (0), 3151 (3)	ν_{CH}	
	3400 (487)	ν_{NH}^{b}	
	3508 (152)	ν_{NH}^{f}	
	3648 (15)	ν_1	Out-of-phase
	3649 (44)	ν_1	In-phase
	3736 (0)	ν_3	Out-of-phase
	3737 (165)	ν_3	In-phase

Table S6. Calculated NH, OH and CH stretching frequencies of $Py_2^+(p)(H_2O)_2$(I-II) obtained at the B3LYP-D3/aug-cc-pVTZ level. The calculated frequencies are scaled by factors of 0.9619 and 0.9631 for NH/CH and OH modes, respectively.

structure	calc, (km mol^{-1})	mode	remark
$Py_2^+(p)(H_2O)_2$(I)	3122 (0), 3123 (1), 3129 (2), 3132 (3), 3136 (1), 3138 (6), 3144 (3), 3145 (7)	ν_{CH}	
	3194 (877)	ν_{NH}^{b}	bottom
	3375 (678)	ν_{NH}^{b}	Top
	3522 (320)	ν_{OH}^{b}	
	3634 (34)	ν_1	
	3716 (122)	ν_{OH}^{f}	
	3716 (118)	ν_3	
$Py_2^+(p)(H_2O)_2$(II)	3122 (0), 3123 (0), 3130 (1), 3132 (4), 3136 (1), 3138 (7), 3145 (0), 3145 (4)	ν_{CH}	
	3278 (867)	ν_{NH}^{b}	Bottom
	3379 (411)	ν_{NH}^{b}	Top
	3328 (620)	ν_{OH}^{b}	
	3645 (32)	ν_1	
	3697 (91)	ν_{OH}^{f}	
	3733 (107)	ν_3	

Table S7. Calculated NH, OH and CH stretching frequencies of $Py_2^+(a)(H_2O)_3$(II-III) obtained at the B3LYP-D3/aug-cc-pVTZ level. The calculated frequencies are scaled by factors of 0.9619 and 0.9631 for NH/CH and OH modes, respectively.

structure	Calc (km mol^{-1})	mode	remark
$Py_2^+(a)(H_2O)_3$(II)	3120 (1), 3121 (0), 3130 (3), 3130 (5), 3136 (1), 3137 (4), 3143 (2), 3144 (9)	ν_{CH}	
	3108 (1973)	ν_{NH}^{b}	
	3265 (1093)	ν_{NH}^{b}	
	3400 (744)	ν_{OH}^{b}	
	3653 (35)	ν_1	NH…O
	3656 (25)	ν_1	OH…O
	3724 (79)	ν_{OH}^{f}	
	3743 (101)	ν_3	NH…O
	3748 (109)	ν_3	OH…O
$Py_2^+(a)(H_2O)_3$(III)	3118 (3), 3122 (0), 3126 (4), 3130 (4), 3133 (3), 3137 (3), 3142 (10), 3144(1)	ν_{CH}	
	3172 (1277)	ν_{NH}^{b}	
	3267 (1060)	ν_{NH}^{b}	
	3464 (418)	ν_{OH}^{b}	
	3642 (29)	ν_1	Cyclic
	3653 (35)	ν_1	
	3720 (112)	ν_{OH}^{f}	
	3729 (97)	ν_3	Cyclic
	3743 (100)	ν_3	

Table S8. Calculated NH, OH, and CH stretching frequencies of $Py_2^+(p)(H_2O)_3$(I-II) at the B3LYP-D3/aug-cc-pVTZ level. The calculated frequencies are scaled by factors of 0.9619 and 0.9631 for NH/CH and OH modes, respectively.

structure	calc (km mol^{-1})	mode
$Py_2^+(p)(H_2O)_3$(I)	3145 (25), 3144 (83), 3139 (4), 3135 (2), 3132 (3), 3128 (4), 3122 (1), 3120 (3)	ν_{CH}
	3161 (854)	ν_{NH}^{b}
	3316 (855)	ν_{NH}^{b}
	3363 (644)	ν_{OH}^{b}
	3458 (347)	ν_{OH}^{b}
	3641 (37)	ν_1
	3706 (112)	ν_{OH}^{f}
	3720 (107)	ν_{OH}^{f}
	3727 (108)	ν_3
$Py_2^+(p)(H_2O)_3$(II)	3139 (5), 3137 (5), 3133 (3), 3131 (7), 3124 (4)	ν_{CH}
	3244 (525)	ν_{NH}^{b}
	3300 (1026)	ν_{NH}^{b}
	3389 (219)	ν_{OH}^{b}
	3453 (413)	ν_{OH}^{b}
	3589 (67)	ν_1
	3700 (123)	ν_{OH}^{f}
	3708 (126)	ν_{OH}^{f}
	3716 (138)	ν_3

Table S9. Calculated NH, OH and CH stretching frequencies of the linear $Py_2^+(H_2O)_3$ obtained at the B3LYP-D3/aug-cc-pVTZ level. The calculated frequencies are scaled by factors of 0.9619 and 0.9631 for NH/CH and OH modes, respectively.

structure	calc (km mol^{-1})	mode	remark
Linear	3118 (4), 3119 (7), 3128 (0), 3129 (13), 3135 (3), 3138 (7), 3143 (0), 3144 (2)	ν_{CH}	
	2937 (1969)	ν_{NH}^{b}	
	3512 (145)	ν_{NH}^{f}	
	3451 (520)	ν_1	double donor H_2O
	3518 (631)	ν_3	double donor H_2O
	3644 (25)	ν_1	
	3657 (16)	ν_1	
	3732 (93)	ν_3	
	3749 (104)	ν_3	

Table S10. Total binding energies *(D_0^t)* of selected clusters and their estimated H-bond cooperativity obtained at the B3LYP-D3/aug-cc-pVTZ level.

	Clusters	Total binding energy (D_0^t), kJ mol^{-1}	Cooperativity,[a] %
1	Py_2^+(a)	107.4	--
2	Py_{2+}(a)$(H_2O)_2$(I)	197.9	-1
3	Py_2^+(a)$(H2O)_2$(III)	192.4	13
4	$Py_2^+(H_2O)_3$(I)	234.4	9
5	$Py_2^+(H_2O)_3$(linear)	225.9	20
6	Py_2^+(p)	99.9	--
7	Py_2^+(p)$(H_2O)_2$(I)	198.8	-1
8	Py_2^+(p)$(H_2O)_3$(I)	242.1	13

[a]The cooperativity is quantified by comparing the total binding energy of the clusters with the sum of the individual intermolecular interaction energies in the clusters. D_0 values of the individual interactions: Py_2^+(a) 107.4, Py_2^+(p) 99.9, Py^+H_2O 65.5, $(H_2O)_2$ 13.0, Py_2^+(p)H_2O 42.6, Py_2^+(a)H_2O(CH…O H-bonded) 0.4 kJ mol^{-1}.

Table S11. Comparison of TD-DFT transition energies of CR and local excitation (LE) bands of various dimers at various DFT levels with the aug-cc-pVTZ basis set and their measured CR transitions.

Cluster	Experiment	Functionals	Transition energy
Benzene dimer cation (Bz_2^+)[1,2]	CR 1160 nm CR 920 nm LE 580 nm LE 430 nm	B3LYP-D3	CR 1108.8 nm, 789.2 nm LE 405.9 nm
		CAM-B3LYP-D3	CR 923.4 nm, 866.2 nm LE 382 nm
		B3PW91-D3	CR 1036.4 nm, 734.6 nm LE 409.7 nm
		M06-2X	CR 1024.3 nm, 916.4 nm LE 380.7 nm
Benzene-Naphthalene cation ($BzNp^+$)[3]	CR 920 nm LE 580 nm LE 430 nm	B3LYP-D3	CR 957.2 nm LE 563.8 nm, 405.2 nm
		CAM-B3LYP-D3	CR 872.1 nm LE 568.7 nm, 381.8 nm
		B3PW91-D3	CR 896.9 nm LE 560.5 nm, 405.9 nm
		M06-2X	CR 895.7 nm LE 591.9 nm, 371.0 nm
Benzene-Toluene cation ($BzTol^+$)[4,5]	CR 1175 nm CR 920 nm CR 670 nm LE 420 nm	B3LYP-D3	CR 1014.4 nm, 827.0 nm LE 404.2 nm
		CAM-B3LYP-D3	CR 912.0 nm, 849.2 nm LE 377.6 nm
		B3PW91-D3	CR 943.3 nm, 775.8 nm LE 404.0 nm
		M06-2X	CR 943.5 nm, 823.4 nm LE 378.1 nm

Table S12. The TD-DFT transition energies of the CR band for $Py_2^+(a)$, $Py_2^+(a)H_2O$, $Py_2^+(a)(H_2O)_2$ at various DFT levels with the aug-cc-pVTZ basis set.

Cluster	Functionals	Transition energy of CR
$Py_2^+(a)$	CAM-B3LYP-D3	750.2 nm (1.6526 eV)
	M06-2X	828.2 nm (1.4971 eV)
$Py_2^+(a)H_2O(I)$	CAM-B3LYP-D3	689.5 nm (1.6682 eV)
	M06-2X-D3	815.5 nm (1.5204 eV)
$Py_2^+(a)(H_2O)_2(I)$	CAM-B3LYP-D3	745.2 nm (1.6637 eV)
	M06-2X	821.8 nm (1.5087 eV)

Notes and References

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4 K. Ohashi, Y. Nakane, Y. Inokuchi, Y. Nakai and N. Nishi, *Chem. Phys.*, 1998, **239**, 429.

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Cartesian coordinates (Å) and energies (hartree) of the relevant structures (B3LYP-D3/aug-cc-pVTZ)

Py

	Atomic Number		Coordinates (Angstroms)	
		X	Y	Z
1	7	0	0	1.118892
2	1	0	0	2.121967
3	6	0	1.12204	0.330562
4	6	0	-1.12204	0.330562
5	6	0	0.710862	-0.9801
6	6	0	-0.71086	-0.9801
7	1	0	2.107478	0.761394
8	1	0	-2.10748	0.761394
9	1	0	1.356665	-1.84126
10	1	0	-1.35667	-1.84126

Sum of electronic and zero-point Energies= 10.173471

Sum of electronic and thermal Energies= -210.169533

Sum of electronic and thermal Enthalpies= -210.168588

Sum of electronic and thermal Free Energies=-210.199188

Py^+

1	7	0	0	1.139358
2	1	0	0	2.149563
3	6	0	1.105943	0.351665
4	6	0	-1.10594	0.351665
5	6	0	0.683921	-1.01345
6	6	0	-0.68392	-1.01345
7	1	0	2.100752	0.768682
8	1	0	-2.10075	0.768682
9	1	0	1.348426	-1.86053
10	1	0	-1.34843	-1.86053

Sum of electronic and zero-point Energies= -209.876150

Sum of electronic and thermal Energies= -209.872164

Sum of electronic and thermal Enthalpies= -209.871220

Sum of electronic and thermal Free Energies= -209.902561

Ar

1	18	0	0	0

Sum of electronic and zero-point Energies= -527.560002

Sum of electronic and thermal Energies= -527.558586

Sum of electronic and thermal Enthalpies= -527.557642

Sum of electronic and thermal Free Energies= -527.575214

H_2O

1	8	0	0	0.116996
2	1	0	0.76341	-0.46799
3	1	0	-0.76341	-0.46799

Sum of electronic and zero-point Energies= -76.444964

Sum of electronic and thermal Energies= -76.442129

Sum of electronic and thermal Enthalpies= -76.441184

Sum of electronic and thermal Free Energies= -76.462606

$(H_2O)_2$

1	8	1.389074	0.001186	0.112327
2	1	1.725605	-0.77043	-0.35443
3	1	1.729078	0.761783	-0.36974
4	8	-1.51063	-0.00131	-0.1213
5	1	-1.92582	0.008305	0.745089
6	1	-0.5564	0.001355	0.050824

Sum of electronic and zero-point Energies= -152.894893

Sum of electronic and thermal Energies= -152.889113

Sum of electronic and thermal Enthalpies= -152.888169

Sum of electronic and thermal Free Energies= -152.921056

Py_2^+(a)

1	6	1.562634	0.60234	1.112731
2	6	1.562634	-0.73394	0.696537
3	6	1.562634	-0.73394	-0.69654
4	6	1.562634	0.60234	-1.11273
5	7	1.580394	1.38897	0
6	1	1.594577	2.395019	0
7	1	1.59127	1.024466	2.102133
8	1	1.591628	-1.58615	1.352511
9	1	1.591628	-1.58615	-1.35251

10	1	1.59127	1.024466	-2.10213
11	6	-1.56263	-0.60234	-1.11273
12	6	-1.56263	0.733936	-0.69654
13	6	-1.56263	0.733936	0.696537
14	6	-1.56263	-0.60234	1.112731
15	7	-1.58039	-1.38897	0
16	1	-1.59458	-2.39502	0
17	1	-1.59127	-1.02447	-2.10213
18	1	-1.59163	1.586152	-1.35251
19	1	-1.59163	1.586152	1.352511
20	1	-1.59127	-1.02447	2.102133

Sum of electronic and zero-point Energies= -420.090494

Sum of electronic and thermal Energies= -420.081137

Sum of electronic and thermal Enthalpies= -420.080193

Sum of electronic and thermal Free Energies= -420.126263

Py_2^+(p)

1	6	1.449062	1.110809	-0.53758
2	6	2.04218	0.69853	0.66615
3	6	2.045638	-0.68926	0.672157
4	6	1.454548	-1.11478	-0.52775
5	7	1.122216	-0.00583	-1.24542
6	1	0.716937	-0.0109	-2.16543
7	1	1.301201	2.097758	-0.93954
8	1	2.420248	1.357439	1.428171
9	1	2.426752	-1.33962	1.439977
10	1	1.310809	-2.10587	-0.92094
11	6	-1.74304	1.113735	-0.08667
12	6	-1.20324	0.701513	1.132771
13	6	-1.20289	-0.69428	1.137806
14	6	-1.74241	-1.11547	-0.07851
15	7	-2.06201	-0.00352	-0.80696
16	1	-2.54561	-0.00684	-1.68938
17	1	-1.95076	2.101685	-0.4602
18	1	-0.8757	1.357354	1.919511
19	1	-0.8749	-1.34422	1.929236
20	1	-1.94945	-2.10617	-0.44505

Sum of electronic and zero-point Energies= -420.087601

Sum of electronic and thermal Energies= -420.078127

Sum of electronic and thermal Enthalpies= -420.077182

Sum of electronic and thermal Free Energies= -420.124899

$Py_2^+(a)H_2O(I)$

1	7	-2.62766	-0.15662	0.000312
2	1	-3.41329	0.471234	0.000649
3	6	-2.00645	-0.63907	-1.11361
4	6	-2.00659	-0.64047	1.113674
5	6	-0.97393	-1.48229	-0.69847
6	6	-0.97401	-1.48316	0.69764
7	1	-2.35107	-0.39189	-2.10238
8	1	-2.35119	-0.3944	2.102729
9	1	-0.3284	-2.03995	-1.35379
10	1	-0.32854	-2.04158	1.352351
11	7	1.538685	0.49356	-0.00042
12	1	2.333013	-0.14935	-0.00071
13	6	0.921195	0.984685	-1.10676
14	6	0.922299	0.98462	1.106643
15	6	-0.11087	1.844662	-0.69379
16	6	-0.11021	1.844525	0.694795
17	1	1.260229	0.733495	-2.09686
18	1	1.262258	0.733163	2.096353
19	1	-0.74821	2.409486	-1.35118
20	1	-0.74697	2.409218	1.35286
21	8	3.8077	-1.19725	0.000033
22	1	4.704377	-0.84557	-0.00044
23	1	3.900404	-2.15543	0.000096

Sum of electronic and zero-point Energies= -496.553096

Sum of electronic and thermal Energies= -496.539955

Sum of electronic and thermal Enthalpies= -496.539011

Sum of electronic and thermal Free Energies= -496.595350

$Py_2^+(a)H_2O(II)$

1	7	0.429374	1.854818	-0.94965
2	1	0.360168	2.093219	-1.92425
3	6	-0.6234	1.544617	-0.13949
4	6	1.59229	1.753616	-0.24699

5	6	-0.11269	1.277725	1.13673
6	6	1.273288	1.399799	1.06759
7	1	-1.64214	1.542501	-0.48651
8	1	2.545378	1.962544	-0.70084
9	1	-0.70799	1.039793	2.000335
10	1	1.984041	1.280151	1.86634
11	7	0.41976	-1.85722	0.949643
12	1	0.35062	-2.09574	1.924218
13	6	-0.63242	-1.5409	0.141111
14	6	1.582234	-1.76218	0.24536
15	6	-0.12202	-1.27629	-1.13577
16	6	1.263329	-1.40617	-1.06865
17	1	-1.65067	-1.53317	0.489497
18	1	2.534802	-1.97654	0.697764
19	1	-0.71733	-1.03472	-1.99835
20	1	1.973637	-1.29017	-1.86833
21	8	-3.51179	0.008239	-0.00006
22	1	-4.10419	-0.30722	-0.69135
23	1	-4.09966	0.328953	0.692678

Sum of electronic and zero-point Energies= -496.546335

Sum of electronic and thermal Energies= -496.533145

Sum of electronic and thermal Enthalpies= -496.532201

Sum of electronic and thermal Free Energies= -496.588184

Py_2^+(a)H_2O(l)Ar(l)

1	7	1.460401	0.891346	0.000138
2	1	2.372836	0.466433	0.000681
3	6	0.743084	1.212954	-1.11315
4	6	0.742705	1.215063	1.112686
5	6	-0.46067	1.788293	-0.69866
6	6	-0.46087	1.789568	0.69685
7	1	1.136647	1.053945	-2.10177
8	1	1.135986	1.057742	2.101693
9	1	-1.2202	2.175969	-1.35435
10	1	-1.22034	2.178974	1.351602
11	7	-2.422	-0.74724	0.000459
12	1	-3.35353	-0.32751	0.001168
13	6	-1.70342	-1.07029	-1.10694

14	6	-1.70266	-1.0726	1.106797
15	6	-0.49087	-1.64848	-0.69553
16	6	-0.49038	-1.64975	0.693521
17	1	-2.09552	-0.9112	-2.09651
18	1	-2.09369	-0.91433	2.096917
19	1	0.266549	-2.0364	-1.35368
20	1	0.267513	-2.03893	1.350389
21	8	-5.05528	0.290486	0.001265
22	1	-5.82548	-0.28781	-0.00068
23	1	-5.40028	1.189158	0.004264
24	18	4.785633	-0.46262	0.000694

Sum of electronic and zero-point Energies= -1024.115679

Sum of electronic and thermal Energies= -1024.099796

Sum of electronic and thermal Enthalpies= -1024.098852

Sum of electronic and thermal Free Energies= -1024.166527

Py_2^+(a)H_2O(I)Ar(II)

1	7	2.398467	-1.74461	0.003893
2	1	3.391916	-1.90102	0.004898
3	6	1.621782	-1.60988	1.116943
4	6	1.62364	-1.61295	-1.11059
5	6	0.303976	-1.41498	0.69998
6	6	0.305093	-1.41668	-0.69611
7	1	2.035722	-1.69658	2.10622
8	1	2.039025	-1.70234	-2.09902
9	1	-0.54491	-1.31313	1.352227
10	1	-0.5427	-1.31629	-1.35001
11	7	0.052557	1.761751	-0.00043
12	1	-0.96149	1.893251	0.002139
13	6	0.8351	1.644818	1.104123
14	6	0.828528	1.639578	-1.10877
15	6	2.166597	1.470524	0.688344
16	6	2.162611	1.467127	-0.69976
17	1	0.422498	1.724295	2.094969
18	1	0.410295	1.714389	-2.09761
19	1	3.015606	1.388747	1.343979
20	1	3.007821	1.382413	-1.35992
21	8	-2.74186	2.135157	0.006795

22	1	-3.20116	2.98142	0.006741
23	1	-3.42512	1.457061	0.007738
24	18	-3.33077	-1.26771	-0.00311

Sum of electronic and zero-point Energies= -1024.115621

Sum of electronic and thermal Energies= -1024.100052

Sum of electronic and thermal Enthalpies= -1024.099108

Sum of electronic and thermal Free Energies= -1024.163996

Py_2^+(a)H_2O(I)Ar(III)

1	7	3.22108	-0.91119	0.015812
2	1	3.60111	-1.8422	0.028609
3	6	2.9202	-0.19952	-1.10754
4	6	2.910039	-0.17273	1.119686
5	6	2.428412	1.044997	-0.70878
6	6	2.42247	1.061578	0.68726
7	1	3.105278	-0.59442	-2.09107
8	1	3.086326	-0.54445	2.113797
9	1	2.140296	1.839391	-1.3744
10	1	2.128064	1.871392	1.331179
11	7	-0.73129	0.544575	-0.00467
12	1	-1.13249	1.484225	-0.00561
13	6	-0.43221	-0.18581	-1.10979
14	6	-0.43827	-0.18519	1.103087
15	6	0.049395	-1.43976	-0.69559
16	6	0.045428	-1.43914	0.69284
17	1	-0.60728	0.19723	-2.10013
18	1	-0.6193	0.198815	2.091981
19	1	0.332243	-2.24359	-1.35224
20	1	0.32503	-2.24233	1.351665
21	8	-1.9886	3.075841	0.0008
22	1	-2.94874	3.151498	0.001669
23	1	-1.65227	3.977777	-0.00168
24	18	-3.81727	-1.01113	0.001934

Sum of electronic and zero-point Energies= -1024.115091

Sum of electronic and thermal Energies= -1024.099150

Sum of electronic and thermal Enthalpies= -1024.098206

Sum of electronic and thermal Free Energies= -1024.166742

$Py_2^+(a)H_2O(I)Ar(IV)$

1	7	1.478982	-1.18343	0.002789
2	1	1.921369	-2.08649	0.000729
3	6	1.134544	-0.4738	-1.10901
4	6	1.129438	-0.48137	1.117831
5	6	0.569776	0.732602	-0.69062
6	6	0.566609	0.727859	0.705106
7	1	1.34279	-0.84107	-2.0985
8	1	1.333099	-0.8554	2.105743
9	1	0.234089	1.518482	-1.34387
10	1	0.22772	1.509225	1.362102
11	7	-2.55762	0.048304	-0.00169
12	1	-2.99408	0.972194	0.00017
13	6	-2.21257	-0.65846	-1.11005
14	6	-2.21809	-0.66588	1.103573
15	6	-1.65697	-1.8823	-0.7003
16	6	-1.66041	-1.88696	0.68836
17	1	-2.40675	-0.28121	-2.09913
18	1	-2.41701	-0.29524	2.094209
19	1	-1.32616	-2.66521	-1.35981
20	1	-1.33296	-2.67432	1.344253
21	8	-3.86629	2.558667	0.000853
22	1	-4.82639	2.63522	-0.00108
23	1	-3.52985	3.460581	0.003801
24	18	4.352275	0.811641	-0.00291

Sum of electronic and zero-point Energies= -1024.114919

Sum of electronic and thermal Energies= -1024.099029

Sum of electronic and thermal Enthalpies= -1024.098085

Sum of electronic and thermal Free Energies= -1024.165671

$Py_2^+(a)H_2O(I)Ar(V)$

1	7	-3.90571	-0.17448	0.000907
2	1	-4.69637	0.446972	0.001687
3	6	-3.28138	-0.65208	-1.1134
4	6	-3.2795	-0.65252	1.113991
5	6	-2.2415	-1.48616	-0.6989
6	6	-2.24033	-1.48646	0.6974
7	1	-3.6288	-0.40801	-2.10196

8	1	-3.62528	-0.40887	2.103223
9	1	-1.59154	-2.03838	-1.35445
10	1	-1.58934	-2.03902	1.351627
11	7	0.251895	0.509894	-5.7E-05
12	1	1.047892	-0.13249	-8.7E-05
13	6	-0.36795	0.99725	-1.10646
14	6	-0.36847	0.99652	1.106391
15	6	-1.40593	1.850913	-0.69418
16	6	-1.40622	1.850496	0.69417
17	1	-0.02683	0.748044	-2.09635
18	1	-0.02795	0.746485	2.096275
19	1	-2.04643	2.411749	-1.35191
20	1	-2.047	2.410949	1.351967
21	8	2.5044	-1.18296	-7.9E-05
22	1	3.404218	-0.83679	0.000106
23	1	2.590838	-2.14145	-0.00079
24	18	5.851427	-0.0084	0.000071

Sum of electronic and zero-point Energies= -1024.114695

Sum of electronic and thermal Energies= -1024.099180

Sum of electronic and thermal Enthalpies= -1024.098235

Sum of electronic and thermal Free Energies= -1024.163620

$Py_2^+(p)H_2O(l)$

1	7	-1.56578	-0.9798	-7.9E-05
2	1	-2.37999	-0.38517	0.000042
3	6	-0.87722	-1.36642	-1.11219
4	6	-0.87716	-1.36681	1.111873
5	6	0.268004	-2.05173	-0.69721
6	6	0.26804	-2.052	0.696569
7	1	-1.25347	-1.17471	-2.10199
8	1	-1.25346	-1.17558	2.101754
9	1	0.9941	-2.50226	-1.35047
10	1	0.994151	-2.50279	1.349636
11	7	0.294147	1.40673	-4.6E-05
12	1	-0.66885	1.726438	-0.00025
13	6	1.022756	1.108308	1.109115
14	6	1.023643	1.10918	-1.10896
15	6	2.282284	0.64377	0.693795

16	6	2.282807	0.644328	-0.69306
17	1	0.642265	1.288634	2.099151
18	1	0.643925	1.290541	-2.09911
19	1	3.083648	0.350706	1.349179
20	1	3.084666	0.351776	-1.34807
21	8	-2.64978	1.89139	0.000088
22	1	-3.07364	2.300431	-0.76377
23	1	-3.07261	2.300552	0.764454

Sum of electronic and zero-point Energies= -496.551703

Sum of electronic and thermal Energies= -496.538932

Sum of electronic and thermal Enthalpies= -496.537988

Sum of electronic and thermal Free Energies= -496.592982

$Py_2^+(p)H_2O(II)$

1	7	1.623332	0.368593	0.00041
2	1	2.459594	-0.2179	0.000589
3	6	1.01098	0.872444	-1.10837
4	6	1.010667	0.872942	1.108818
5	6	-0.0228	1.723864	-0.69581
6	6	-0.02297	1.724184	0.695623
7	1	1.359817	0.631898	-2.09811
8	1	1.359264	0.63289	2.098765
9	1	-0.67009	2.279399	-1.35056
10	1	-0.67056	2.279838	1.349968
11	7	-0.99412	-1.43361	0.000079
12	1	-0.18995	-2.03598	0.000225
13	6	-1.61947	-0.95918	1.113432
14	6	-1.61872	-0.95875	-1.11354
15	6	-2.70682	-0.18125	0.695011
16	6	-2.70635	-0.18099	-0.69554
17	1	-1.3018	-1.23992	2.102014
18	1	-1.30046	-1.23928	-2.10199
19	1	-3.40345	0.314108	1.348451
20	1	-3.40254	0.314631	-1.34925
21	8	4.034778	-1.1269	-0.00024
22	1	4.879572	-0.66392	-0.00164
23	1	4.250741	-2.06504	0.002249

Sum of electronic and zero-point Energies= -496.550337

Sum of electronic and thermal Energies= -496.537014

Sum of electronic and thermal Enthalpies= -496.536069

Sum of electronic and thermal Free Energies= -496.593699

$Py_2^+(p)H_2O(l)Ar(l)$

1	7	0.447993	1.771292	-0.22525
2	1	-0.47476	1.797682	-0.63149
3	6	0.717087	1.562413	1.095566
4	6	1.613723	1.734389	-0.93204
5	6	2.100379	1.425418	1.240717
6	6	2.662415	1.532475	-0.03028
7	1	-0.06354	1.567492	1.836246
8	1	1.631316	1.891954	-1.99641
9	1	2.616669	1.28056	2.173128
10	1	3.705502	1.48848	-0.28906
11	7	0.528784	-1.24537	-0.4505
12	1	-0.35317	-0.90081	-0.81687
13	6	1.679257	-1.37573	-1.16446
14	6	0.774096	-1.54474	0.853153
15	6	2.688221	-1.81843	-0.29233
16	6	2.122624	-1.92315	0.969535
17	1	1.705473	-1.20758	-2.22675
18	1	-0.0076	-1.52806	1.592117
19	1	3.704124	-2.03231	-0.57476
20	1	2.603939	-2.23641	1.879363
21	8	-1.88969	0.196866	-1.38971
22	1	-2.71122	0.092563	-0.89296
23	1	-2.15578	0.167597	-2.31612
24	18	-4.89265	-0.17741	0.426245

Sum of electronic and zero-point Energies= -1024.113865

Sum of electronic and thermal Energies= -1024.098607

Sum of electronic and thermal Enthalpies= -1024.097663

Sum of electronic and thermal Free Energies= -1024.163785

$Py_2^+(a)(H_2O)_2(l)$

1	7	-2.00396	-0.6659	0.000169
2	1	-2.89824	-0.17495	-4.3E-05
3	6	-1.30985	-1.04074	-1.10743

4	6	-1.31049	-1.04113	1.108132
5	6	-0.14497	-1.70283	-0.6952
6	6	-0.14542	-1.70304	0.696466
7	1	-1.68843	-0.8523	-2.09694
8	1	-1.68965	-0.85286	2.097451
9	1	0.585317	-2.14164	-1.35189
10	1	0.58423	-2.14245	1.353471
11	7	2.004106	0.66616	0.000261
12	1	2.897987	0.174419	0.000534
13	6	1.309839	1.039851	-1.10773
14	6	1.310629	1.042597	1.107824
15	6	0.145509	1.703257	-0.69618
16	6	0.145921	1.704781	0.695536
17	1	1.688852	0.851335	-2.09706
18	1	1.689867	0.855477	2.097341
19	1	-0.58438	2.142056	-1.35332
20	1	-0.58352	2.145152	1.352133
21	8	-4.55295	0.596069	-0.00073
22	1	-5.37171	0.089135	-0.00129
23	1	-4.81585	1.521935	0.000174
24	8	4.551911	-0.59839	-0.00069
25	1	5.370346	-0.09093	-0.00287
26	1	4.81543	-1.52407	0.002074

Sum of electronic and zero-point Energies= -573.014907

Sum of electronic and thermal Energies= -572.997684

Sum of electronic and thermal Enthalpies= -572.996739

Sum of electronic and thermal Free Energies= -573.064336

$Py_2^+(a)(H_2O)_2(II)$

1	7	0.124344	1.662857	-0.00844
2	1	1.133702	1.66753	-0.20476
3	6	-0.85778	1.677684	-0.94182
4	6	-0.42964	1.451178	1.214006
5	6	-2.09589	1.512389	-0.28915
6	6	-1.82533	1.370815	1.063892
7	1	-0.63999	1.833267	-1.9841
8	1	0.175532	1.406218	2.102697
9	1	-3.05851	1.525891	-0.7698

10	1	-2.53172	1.247493	1.86612
11	7	-1.97503	-1.79169	0.110531
12	1	-2.93289	-1.95794	0.366644
13	6	-1.53421	-1.52111	-1.14943
14	6	-0.91982	-1.76856	0.978004
15	6	-0.1492	-1.35056	-1.09099
16	6	0.235984	-1.5086	0.243224
17	1	-2.20532	-1.50373	-1.99006
18	1	-1.05136	-1.97323	2.025939
19	1	0.488038	-1.14912	-1.93409
20	1	1.235738	-1.45271	0.638692
21	8	2.815319	1.368666	-0.5469
22	1	3.507875	2.007987	-0.73594
23	1	3.251316	0.55493	-0.23151
24	8	3.757029	-1.07696	0.417629
25	1	4.144098	-1.70794	-0.19943
26	1	4.314861	-1.10988	1.202679

Sum of electronic and zero-point Energies= -573.013008

Sum of electronic and thermal Energies= -572.996956

Sum of electronic and thermal Enthalpies= -572.996012

Sum of electronic and thermal Free Energies= -573.060114

$Py_2^+(a)(H_2O)_2(III)$

1	7	-0.84251	0.540419	-4.2E-05
2	1	-1.64704	-0.10405	-8.9E-05
3	6	-0.21681	1.020162	1.104349
4	6	-0.21684	1.020411	-1.10434
5	6	0.832978	1.863657	0.693441
6	6	0.832956	1.863822	-0.69327
7	1	-0.55927	0.772499	2.094184
8	1	-0.55936	0.773028	-2.09423
9	1	1.480744	2.415241	1.351893
10	1	1.480673	2.415596	-1.35161
11	7	3.298321	-0.21026	-0.00012
12	1	4.098771	0.398155	-0.00021
13	6	2.664463	-0.67678	1.113984
14	6	2.664168	-0.67674	-1.11407
15	6	1.611131	-1.49132	0.698814

16	6	1.610953	-1.49131	-0.69866
17	1	3.015322	-0.43837	2.102618
18	1	3.014814	-0.43838	-2.10279
19	1	0.948633	-2.03023	1.352831
20	1	0.948355	-2.03027	-1.35253
21	8	-3.02714	-1.13113	-0.00023
22	1	-3.94422	-0.7891	-7.4E-05
23	1	-3.09183	-2.08973	-0.00027
24	8	-5.57069	-0.0823	0.000152
25	1	-6.14597	-0.02518	-0.7694
26	1	-6.14567	-0.02436	0.769867

Sum of electronic and zero-point Energies= -573.012827

Sum of electronic and thermal Energies= -572.996395

Sum of electronic and thermal Enthalpies= -572.995451

Sum of electronic and thermal Free Energies= -573.061222

$Py_2^+(a)(H_2O)_2$(IV)

1	7	-0.81706	1.010356	0.539239
2	1	-1.5555	0.542054	1.076881
3	6	0.250111	1.688459	1.029677
4	6	-0.70269	0.914465	-0.81064
5	6	1.063625	2.077832	-0.05133
6	6	0.465176	1.593127	-1.20547
7	1	0.359067	1.88383	2.082359
8	1	-1.45652	0.411941	-1.39329
9	1	1.961175	2.665866	0.02758
10	1	0.797468	1.720687	-2.22082
11	7	2.760758	-0.71939	-0.63122
12	1	3.518548	-0.38573	-1.2015
13	6	2.671354	-0.57491	0.721643
14	6	1.650194	-1.36389	-1.09452
15	6	1.481049	-1.17195	1.139399
16	6	0.841522	-1.66698	0.000572
17	1	3.453638	-0.10367	1.29036
18	1	1.528409	-1.59325	-2.13846
19	1	1.147415	-1.24781	2.159204
20	1	-0.09317	-2.19755	-0.04041
21	8	-2.86834	-0.5859	1.469196

22	1	-3.40792	-0.68936	0.664481
23	1	-3.46318	-0.64527	2.222069
24	8	-3.88379	-0.64809	-1.1341
25	1	-4.1342	-1.48339	-1.54441
26	1	-4.56612	-0.02018	-1.39701

Sum of electronic and zero-point Energies= -573.011671

Sum of electronic and thermal Energies= -572.995726

Sum of electronic and thermal Enthalpies= -572.994782

Sum of electronic and thermal Free Energies= -573.058489

$Py_2^+(a)(H_2O)_2(V)$

1	7	-1.60568	-0.25261	-0.51519
2	1	-2.3874	-0.14408	0.131531
3	6	-0.78159	0.747243	-0.92991
4	6	-1.20183	-1.4242	-1.072
5	6	0.159058	0.197091	-1.81836
6	6	-0.09825	-1.16516	-1.89993
7	1	-0.89945	1.766114	-0.60404
8	1	-1.72084	-2.34674	-0.87708
9	1	0.919673	0.755435	-2.33455
10	1	0.415964	-1.89803	-2.49654
11	7	2.496269	-0.63288	0.193653
12	1	3.281535	-0.61306	-0.43375
13	6	1.852553	0.466413	0.682525
14	6	1.883687	-1.76274	0.649167
15	6	0.820765	0.018841	1.511903
16	6	0.835651	-1.37688	1.484654
17	1	2.153352	1.470193	0.438499
18	1	2.239686	-2.74257	0.383033
19	1	0.155864	0.656229	2.067061
20	1	0.188483	-2.05037	2.01833
21	8	-3.84283	0.103481	1.205554
22	1	-4.70594	0.359391	0.863411
23	1	-3.98516	-0.13322	2.127653
24	8	0.792396	3.491438	-0.03744
25	1	0.689712	4.061541	0.73223
26	1	1.003561	4.094604	-0.75829

Sum of electronic and zero-point Energies= -573.007955

Sum of electronic and thermal Energies= -572.990843

Sum of electronic and thermal Enthalpies= -572.989899

Sum of electronic and thermal Free Energies= -573.056333

$Py_2^+(a)(H_2O)_2$(VI)

1	7	1.181603	-0.00122	0.62249
2	1	1.989933	-0.00319	0.011649
3	6	0.547013	1.107707	1.078748
4	6	0.54415	-1.10766	1.080698
5	6	-0.52597	0.695768	1.892166
6	6	-0.52782	-0.69149	1.893361
7	1	0.905637	2.089583	0.826236
8	1	0.900185	-2.09096	0.830059
9	1	-1.1899	1.354804	2.423474
10	1	-1.19357	-1.34787	2.425678
11	7	-2.94026	0.001591	-0.24818
12	1	-3.7635	0.00337	0.328958
13	6	-2.28857	1.114445	-0.69313
14	6	-2.2904	-1.11395	-0.68889
15	6	-1.20608	0.696916	-1.46602
16	6	-1.20722	-0.70106	-1.46341
17	1	-2.64671	2.103783	-0.46906
18	1	-2.65009	-2.10187	-0.46107
19	1	-0.52109	1.34963	-1.97737
20	1	-0.52335	-1.35682	-1.97236
21	8	3.042807	1.824744	-0.67574
22	1	3.831703	2.10957	-0.20235
23	1	3.196271	2.083749	-1.59013
24	8	3.042046	-1.82525	-0.6749
25	1	3.195852	-2.08437	-1.58919
26	1	3.829811	-2.11197	-0.20076

Sum of electronic and zero-point Energies= -573.007625

Sum of electronic and thermal Energies= -572.990380

Sum of electronic and thermal Enthalpies= -572.989436

Sum of electronic and thermal Free Energies= -573.056151

$Py_2^+(a)(H_2O)_2$(VII)

1	7	0.001446	1.783075	0.992031

2	1	0.002715	1.95829	1.981964
3	6	1.115245	1.604353	0.22587
4	6	-1.11422	1.604535	0.228597
5	6	0.695328	1.35683	-1.08522
6	6	-0.69761	1.356862	-1.08348
7	1	2.110953	1.660546	0.629149
8	1	-2.10899	1.660899	0.634152
9	1	1.351893	1.207805	-1.924
10	1	-1.35634	1.207755	-1.92055
11	7	-0.00177	-1.78287	-0.99274
12	1	-0.00324	-1.95826	-1.98264
13	6	-1.11539	-1.60456	-0.22626
14	6	1.114054	-1.60377	-0.22965
15	6	-0.69522	-1.35669	1.084664
16	6	0.69772	-1.35616	1.082538
17	1	-2.11129	-1.66133	-0.62899
18	1	2.108752	-1.66023	-0.63535
19	1	-1.35162	-1.20793	1.923628
20	1	1.356707	-1.20668	1.919334
21	8	3.968727	-0.00084	0.001566
22	1	4.560423	-0.33831	0.682831
23	1	4.55822	0.334948	-0.68244
24	8	-3.9684	0.000063	0.000879
25	1	-4.56174	0.336571	-0.67944
26	1	-4.55621	-0.33772	0.68535

Sum of electronic and zero-point Energies= -573.000728

Sum of electronic and thermal Energies= -572.983460

Sum of electronic and thermal Enthalpies= -572.982516

Sum of electronic and thermal Free Energies= -573.048876

Py_2+(a)($H_2O)_2$(l)Ar(l)

1	7	-0.93024	1.764434	0.000006
2	1	-1.94268	1.634225	0.000333
3	6	-0.1467	1.854686	1.10719
4	6	-0.14738	1.854268	-1.10768
5	6	1.181013	2.038376	0.695018
6	6	1.180591	2.03811	-0.69638
7	1	-0.56824	1.820117	2.096647

8	1	-0.56952	1.819323	-2.09687
9	1	2.021918	2.1753	1.351708
10	1	2.02109	2.174803	-1.35364
11	7	2.261385	-0.97516	0.000063
12	1	3.274675	-0.85802	0.000061
13	6	1.477413	-1.06096	1.107896
14	6	1.477449	-1.06146	-1.10774
15	6	0.149254	-1.2366	0.696036
16	6	0.14927	-1.2369	-0.69584
17	1	1.899431	-1.02873	2.097216
18	1	1.899483	-1.02966	-2.09707
19	1	-0.6935	-1.36722	1.351168
20	1	-0.69346	-1.36782	-1.35093
21	8	-3.74525	1.459714	0.000908
22	1	-4.3871	2.177276	0.001109
23	1	-4.25405	0.642757	0.001009
24	8	5.099572	-0.78041	0.000487
25	1	5.65951	-1.5639	0.001772
26	1	5.699651	-0.02787	-0.00111
27	18	-3.41363	-1.96095	-0.00023

Sum of electronic and zero-point Energies= -1100.577460

Sum of electronic and thermal Energies= -1100.557692

Sum of electronic and thermal Enthalpies= -1100.556748

Sum of electronic and thermal Free Energies= -1100.633921

Py_2^+(a)$(H_2O)_2$(I)Ar(II)

1	7	-1.34203	0.542548	0.003558
2	1	-1.98768	1.332149	0.002421
3	6	-0.85525	-0.07842	-1.10306
4	6	-0.85344	-0.07411	1.1118
5	6	-0.04517	-1.14548	-0.68997
6	6	-0.04402	-1.14274	0.701593
7	1	-1.13376	0.239517	-2.09255
8	1	-1.13019	0.247785	2.100512
9	1	0.452283	-1.83787	-1.34586
10	1	0.45431	-1.83269	1.35939
11	7	2.858157	0.198766	-0.00171
12	1	3.488222	-0.60342	-0.00104

13	6	2.365958	0.813956	-1.10993
14	6	2.370504	0.8195	1.105447
15	6	1.558098	1.883399	-0.69909
16	6	1.560903	1.886809	0.692642
17	1	2.637907	0.488957	-2.09903
18	1	2.646619	0.499488	2.095023
19	1	1.058673	2.572981	-1.35646
20	1	1.064066	2.579584	1.348618
21	8	-3.26541	2.633521	-0.00192
22	1	-4.2087	2.439827	-0.00319
23	1	-3.19268	3.59325	-0.00021
24	8	4.716942	-1.95471	-0.0016
25	1	5.66769	-1.80164	-0.00563
26	1	4.603761	-2.9105	0.004394
27	18	-3.83284	-1.85581	-0.00266

Sum of electronic and zero-point Energies= -1100.576538

Sum of electronic and thermal Energies= -1100.556749

Sum of electronic and thermal Enthalpies= -1100.555805

Sum of electronic and thermal Free Energies= -1100.633846

$Py_2^+(a)(H_2O)_2(I)Ar(III)$

1	7	0.786101	-0.44396	0.000227
2	1	1.632633	0.126936	0.00013
3	6	0.126784	-0.87646	1.107714
4	6	0.126443	-0.87619	-1.10716
5	6	-0.97729	-1.63655	0.696073
6	6	-0.97751	-1.63639	-0.69534
7	1	0.48778	-0.65552	2.097054
8	1	0.487152	-0.65505	-2.09655
9	1	-1.66668	-2.13681	1.353
10	1	-1.66713	-2.13646	-1.35217
11	7	-3.32037	0.543856	-9.3E-05
12	1	-4.17034	-0.0201	-0.00026
13	6	-2.66002	0.974782	1.107803
14	6	-2.65944	0.97449	-1.10775
15	6	-1.55422	1.731333	0.696161
16	6	-1.55386	1.731163	-0.69571
17	1	-3.02205	0.755398	2.097095

18	1	-3.02099	0.75495	-2.09718
19	1	-0.86315	2.2294	1.352977
20	1	-0.86251	2.229163	-1.35228
21	8	3.188855	1.055231	-0.00013
22	1	4.056641	0.635718	-0.0002
23	1	3.354821	2.003069	0.000036
24	8	-5.75458	-0.92868	-0.00077
25	1	-6.61356	-0.49335	-0.00116
26	1	-5.93778	-1.87357	-0.00023
27	18	6.491418	-0.26626	-0.00027

Sum of electronic and zero-point Energies= -1100.576124

Sum of electronic and thermal Energies= -1100.556721

Sum of electronic and thermal Enthalpies= -1100.555777

Sum of electronic and thermal Free Energies= -1100.631263

$Py_2^+(a)(H_2O)_2(II)Ar(I)$

1	7	-1.06534	1.67398	0.020538
2	1	-2.0841	1.615313	0.144938
3	6	-0.15418	1.749694	1.020079
4	6	-0.41461	1.501611	-1.16043
5	6	1.13439	1.665536	0.455763
6	6	0.968536	1.510736	-0.91307
7	1	-0.45383	1.888585	2.044202
8	1	-0.95243	1.420539	-2.08893
9	1	2.058934	1.735008	1.001518
10	1	1.73639	1.430735	-1.66241
11	7	1.195979	-1.61626	0.038599
12	1	2.176579	-1.67464	-0.17601
13	6	0.679185	-1.38477	1.275892
14	6	0.183535	-1.66834	-0.8767
15	6	-0.71211	-1.32384	1.154615
16	6	-1.02224	-1.5047	-0.19537
17	1	1.308567	-1.31616	2.145608
18	1	0.379035	-1.85464	-1.91804
19	1	-1.40084	-1.17812	1.968205
20	1	-2.004	-1.52343	-0.63662
21	8	-3.76997	1.227114	0.364703
22	1	-4.50554	1.832249	0.49441

23	1	-4.14347	0.382422	0.050593
24	8	-4.53981	-1.28982	-0.57251
25	1	-4.93353	-1.92109	0.039967
26	1	-5.04635	-1.37242	-1.38806
27	18	4.414071	-0.14679	-0.18531

Sum of electronic and zero-point Energies= -1100.575598

Sum of electronic and thermal Energies= -1100.557012

Sum of electronic and thermal Enthalpies= -1100.556068

Sum of electronic and thermal Free Energies= -1100.629281

$Py_2^+(a)(H_2O)_2(II)Ar(II)$

1	7	-0.73781	0.43741	-0.14215
2	1	-0.48886	1.412748	-0.35128
3	6	-0.9511	-0.53665	-1.05929
4	6	-0.73468	-0.11453	1.098401
5	6	-1.13252	-1.75735	-0.3789
6	6	-0.99683	-1.49061	0.975354
7	1	-0.99782	-0.31729	-2.1117
8	1	-0.58878	0.487118	1.978443
9	1	-1.36109	-2.7002	-0.84428
10	1	-1.09517	-2.18143	1.794381
11	7	2.083737	-2.42442	0.189395
12	1	1.995069	-3.39054	0.452804
13	6	2.001672	-1.94595	-1.08375
14	6	2.270884	-1.38532	1.055956
15	6	2.173578	-0.56142	-1.03275
16	6	2.344383	-0.21009	0.309277
17	1	1.868322	-2.60297	-1.92511
18	1	2.376408	-1.54976	2.113875
19	1	2.182292	0.095425	-1.88476
20	1	2.511383	0.777889	0.703033
21	8	0.218029	2.973687	-0.66403
22	1	-0.22829	3.794599	-0.88983
23	1	1.083381	3.210658	-0.28109
24	8	2.732744	3.321122	0.501516
25	1	3.482155	3.545709	-0.06123
26	1	2.83369	3.862667	1.29214
27	18	-4.24737	0.39542	0.093233

Sum of electronic and zero-point Energies= -1100.574658

Sum of electronic and thermal Energies= -1100.556023

Sum of electronic and thermal Enthalpies= -1100.555079

Sum of electronic and thermal Free Energies= -1100.628679

$Py_2^+(a)(H_2O)_2(II)Ar(III)$

1	7	0.113788	-1.23491	0.251151
2	1	-0.76909	-0.71965	0.130333
3	6	0.821663	-1.82188	-0.74452
4	6	0.84874	-1.26344	1.392755
5	6	2.041327	-2.285	-0.212
6	6	2.056953	-1.93385	1.129701
7	1	0.42362	-1.90869	-1.74053
8	1	0.47205	-0.84965	2.311943
9	1	2.791092	-2.83041	-0.75809
10	1	2.82278	-2.14452	1.855574
11	7	3.683577	0.610564	-0.23867
12	1	4.618079	0.265995	-0.1021
13	6	2.982221	0.540343	-1.40502
14	6	2.9085	1.189814	0.725251
15	6	1.73152	1.121464	-1.18807
16	6	1.686018	1.530464	0.147558
17	1	3.415799	0.128335	-2.29923
18	1	3.281174	1.353163	1.721155
19	1	0.961557	1.235067	-1.93082
20	1	0.869906	2.027307	0.643569
21	8	-2.07126	0.392084	-0.14103
22	1	-3.01188	0.19477	-0.18365
23	1	-1.98353	1.328339	0.116905
24	8	-1.48956	3.02182	0.611893
25	1	-1.55252	3.71724	-0.05224
26	1	-1.86685	3.398349	1.414634
27	18	-5.5016	-0.58911	-0.22531

Sum of electronic and zero-point Energies= -1100.574334

Sum of electronic and thermal Energies= -1100.555896

Sum of electronic and thermal Enthalpies= -1100.554952

Sum of electronic and thermal Free Energies= -1100.628064

$Py_2^+(a)(H_2O)_2(III)Ar(I)$

1	7	0.41398	-1.32558	-0.07955
2	1	1.332234	-0.85567	-0.06155
3	6	-0.28158	-1.73019	1.013558
4	6	-0.30985	-1.60747	-1.19125
5	6	-1.4854	-2.32094	0.585048
6	6	-1.50406	-2.24338	-0.79916
7	1	0.117437	-1.61188	2.006104
8	1	0.062223	-1.37952	-2.17514
9	1	-2.22303	-2.76591	1.229479
10	1	-2.25878	-2.61522	-1.46966
11	7	-3.47353	0.250573	0.10959
12	1	-4.38043	-0.18315	0.125538
13	6	-2.71287	0.525938	1.208709
14	6	-2.804	0.633548	-1.01508
15	6	-1.53456	1.131466	0.773908
16	6	-1.59093	1.197961	-0.62081
17	1	-3.06486	0.316092	2.203373
18	1	-3.23543	0.518353	-1.99384
19	1	-0.74866	1.492948	1.412844
20	1	-0.85841	1.622962	-1.28344
21	8	2.868614	-0.10565	0.014207
22	1	3.723146	-0.5813	0.041331
23	1	3.070568	0.833213	-0.01099
24	8	5.220137	-1.53281	0.103005
25	1	5.790017	-1.7186	-0.65002
26	1	5.764221	-1.65349	0.887699
27	18	1.497558	3.094017	-0.06329

Sum of electronic and zero-point Energies= -1100.575299

Sum of electronic and thermal Energies= -1100.556362

Sum of electronic and thermal Enthalpies= -1100.555418

Sum of electronic and thermal Free Energies= -1100.629981

$Py_2^+(a)(H_2O)_2(III)Ar(II)$

1	7	-1.73055	-0.49535	0.02144
2	1	-2.64415	-0.01876	0.022
3	6	-1.03075	-0.85547	-1.08427
4	6	-1.02043	-0.84163	1.124826

5	6	0.161211	-1.48189	-0.67499
6	6	0.167814	-1.47314	0.712139
7	1	-1.41904	-0.68398	-2.07328
8	1	-1.39932	-0.65806	2.115318
9	1	0.89964	-1.90371	-1.3339
10	1	0.912387	-1.88678	1.369325
11	7	2.166525	1.023723	-0.01131
12	1	3.057384	0.556296	-0.01532
13	6	1.451557	1.363525	-1.12136
14	6	1.467612	1.374799	1.10527
15	6	0.272435	1.980405	-0.70109
16	6	0.282429	1.987416	0.695699
17	1	1.831964	1.185596	-2.1118
18	1	1.862213	1.207077	2.091932
19	1	-0.48055	2.388512	-1.35192
20	1	-0.46091	2.402499	1.353158
21	8	-4.20584	0.708684	0.0121
22	1	-5.03182	0.183998	-0.00276
23	1	-4.46695	1.633043	0.031178
24	8	-6.46818	-0.85928	-0.03443
25	1	-7.02318	-1.05088	0.728257
26	1	-7.0177	-1.0096	-0.81024
27	18	5.17828	-0.95351	-0.01342

Sum of electronic and zero-point Energies= -1100.575287

Sum of electronic and thermal Energies= -1100.556172

Sum of electronic and thermal Enthalpies= -1100.555228

Sum of electronic and thermal Free Energies= -1100.633027

Py_2^+(a)$(H_2O)_2$(III)Ar(III)

1	7	0.498259	0.423617	0.401763
2	1	-0.27525	-0.2579	0.373785
3	6	1.302979	0.656742	1.469114
4	6	0.902234	1.202858	-0.633
5	6	2.241909	1.644565	1.114813
6	6	1.990298	1.987446	-0.20486
7	1	1.151124	0.149569	2.406179
8	1	0.391508	1.185309	-1.58023
9	1	2.985653	2.059102	1.772397

10	1	2.495221	2.727291	-0.80074
11	7	4.587762	-0.03173	-0.48176
12	1	5.363888	0.606973	-0.45855
13	6	4.167883	-0.79881	0.565386
14	6	3.77839	-0.2479	-1.55827
15	6	3.07481	-1.55046	0.135188
16	6	2.830061	-1.20435	-1.19651
17	1	4.681601	-0.79075	1.510546
18	1	3.946233	0.249132	-2.49749
19	1	2.547509	-2.27523	0.729909
20	1	2.074245	-1.60586	-1.84812
21	8	-1.58806	-1.36394	0.366208
22	1	-2.48702	-1.12412	0.672957
23	1	-1.63687	-2.2715	0.054897
24	8	-4.06851	-0.60472	1.254128
25	1	-4.80572	-0.35832	0.685207
26	1	-4.45565	-0.86873	2.09465
27	18	-6.89208	0.302251	-0.75941

Sum of electronic and zero-point Energies= -1100.574174

Sum of electronic and thermal Energies= -1100.555339

Sum of electronic and thermal Enthalpies= -1100.554394

Sum of electronic and thermal Free Energies= -1100.629843

$Py_2^+(a)(H_2O)_2(IV)Ar(I)$

1	7	-1.44866	-0.54309	-1.02472
2	1	-2.4012	-0.17425	-1.12453
3	6	-0.42237	-0.4141	-1.90233
4	6	-0.99536	-1.141	0.107258
5	6	0.727777	-0.98532	-1.32685
6	6	0.368015	-1.4416	-0.06654
7	1	-0.56195	0.032152	-2.87161
8	1	-1.66166	-1.34068	0.929672
9	1	1.688879	-1.06301	-1.80366
10	1	0.990287	-1.95034	0.648364
11	7	1.741738	1.447404	0.642412
12	1	2.675834	1.119338	0.818113
13	6	1.320307	2.034928	-0.51271
14	6	0.683656	1.300661	1.490834

15	6	-0.04344	2.30583	-0.38448
16	6	-0.44222	1.845979	0.872162
17	1	2.002972	2.251531	-1.31546
18	1	0.803058	0.86616	2.467611
19	1	-0.65212	2.799106	-1.12158
20	1	-1.42584	1.904404	1.303426
21	8	-4.02445	0.390977	-0.67753
22	1	-4.32694	-0.16785	0.061042
23	1	-4.79774	0.612159	-1.20405
24	8	-4.25603	-1.34125	1.50551
25	1	-4.59922	-1.02426	2.3484
26	1	-4.64129	-2.21659	1.386142
27	18	4.106724	-1.18934	0.325908

Sum of electronic and zero-point Energies= -1100.574421

Sum of electronic and thermal Energies= -1100.555849

Sum of electronic and thermal Enthalpies= -1100.554905

Sum of electronic and thermal Free Energies= -1100.628516

$Py_2^+(a)(H_2O)_2(IV)Ar(II)$

1	7	0.083892	0.373573	0.948805
2	1	-0.39792	-0.43338	1.361986
3	6	0.999024	1.176265	1.54635
4	6	-0.01237	0.706545	-0.36441
5	6	1.482318	2.088071	0.588659
6	6	0.847065	1.793688	-0.60927
7	1	1.23066	1.085872	2.593407
8	1	-0.69284	0.184601	-1.01617
9	1	2.191086	2.874133	0.781996
10	1	0.955152	2.301287	-1.55177
11	7	3.721275	0.215248	-1.00265
12	1	4.249774	0.912904	-1.49732
13	6	3.840082	-0.06643	0.325982
14	6	2.755422	-0.57808	-1.55163
15	6	2.943745	-1.09223	0.629212
16	6	2.264659	-1.41354	-0.54846
17	1	4.559	0.439045	0.94654
18	1	2.513991	-0.52617	-2.59864
19	1	2.828604	-1.55316	1.594285

20	1	1.510028	-2.16908	-0.67726
21	8	-1.26821	-1.97554	1.458824
22	1	-1.88316	-1.98918	0.702611
23	1	-1.70014	-2.43033	2.1873
24	8	-2.63849	-1.52847	-0.92856
25	1	-2.78351	-2.22786	-1.57517
26	1	-3.46871	-1.03928	-0.88721
27	18	-5.28968	0.71084	-0.24047

Sum of electronic and zero-point Energies= -1100.573439

Sum of electronic and thermal Energies= -1100.554992

Sum of electronic and thermal Enthalpies= -1100.554048

Sum of electronic and thermal Free Energies= -1100.628967

$Py_2^+(a)(H_2O)_2(IV)Ar(III)$

1	7	0.238864	-1.79807	0.073986
2	1	-0.41346	-2.03812	-0.68019
3	6	1.558826	-2.0972	0.144561
4	6	-0.08681	-0.96677	1.098744
5	6	2.096349	-1.46587	1.282931
6	6	1.063112	-0.75868	1.881323
7	1	2.030047	-2.74605	-0.57309
8	1	-1.09755	-0.61668	1.223339
9	1	3.114442	-1.55468	1.619462
10	1	1.103742	-0.17619	2.785057
11	7	2.486078	1.646744	0.138492
12	1	3.060242	2.057297	0.854373
13	6	2.927228	0.801786	-0.83458
14	6	1.137753	1.826727	0.008949
15	6	1.833043	0.454476	-1.62981
16	6	0.712504	1.099964	-1.10182
17	1	3.96593	0.535074	-0.92098
18	1	0.590463	2.472564	0.672184
19	1	1.872333	-0.17637	-2.50024
20	1	-0.29602	1.056975	-1.47215
21	8	-1.84842	-1.88936	-1.73219
22	1	-2.59775	-1.67664	-1.14666
23	1	-2.1884	-2.44413	-2.4399
24	8	-3.51864	-1.09616	0.360391

25	1	-4.08793	-0.32425	0.26861
26	1	-4.03954	-1.74467	0.847023
27	18	-2.47815	2.16404	0.32491

Sum of electronic and zero-point Energies= -1100.574233

Sum of electronic and thermal Energies= -1100.555710

Sum of electronic and thermal Enthalpies= -1100.554766

Sum of electronic and thermal Free Energies= -1100.627527

$Py_2^+(a)(H_2O)_2(V)Ar(I)$

1	7	-0.07795	1.614957	-0.71092
2	1	-1.05247	1.820976	-0.48678
3	6	0.948712	1.604259	0.180847
4	6	0.391155	1.262633	-1.93616
5	6	2.126209	1.271683	-0.51237
6	6	1.775507	1.049666	-1.83745
7	1	0.812461	1.837373	1.222552
8	1	-0.25928	1.209277	-2.79204
9	1	3.106445	1.219089	-0.07297
10	1	2.423669	0.790037	-2.65595
11	7	2.110025	-1.9125	-0.28465
12	1	3.093304	-2.09531	-0.38651
13	6	1.520376	-1.37987	0.824848
14	6	1.169406	-2.11538	-1.25067
15	6	0.150371	-1.28071	0.569715
16	6	-0.06811	-1.73381	-0.73274
17	1	2.078086	-1.11927	1.70729
18	1	1.426342	-2.53449	-2.2077
19	1	-0.58388	-0.92323	1.268981
20	1	-1.00737	-1.80681	-1.25154
21	8	-2.76445	2.233726	-0.06233
22	1	-3.1557	3.112699	-0.0986
23	1	-3.48852	1.624196	0.112778
24	8	1.957188	0.846614	3.209744
25	1	1.464862	0.660886	4.016651
26	1	2.735278	1.330075	3.507822
27	18	-3.52452	-1.09757	0.448307

Sum of electronic and zero-point Energies= -1100.570508

Sum of electronic and thermal Energies= -1100.550921

Sum of electronic and thermal Enthalpies= -1100.549977

Sum of electronic and thermal Free Energies= -1100.625164

$Py_2^+(a)(H_2O)_2(V)Ar(II)$

1	7	-0.84245	-0.57755	0.398379
2	1	-1.21988	-0.82349	1.313719
3	6	-0.42781	0.663189	0.025489
4	6	-0.67659	-1.43551	-0.64059
5	6	-0.01521	0.599834	-1.31676
6	6	-0.16146	-0.71718	-1.73158
7	1	-0.45735	1.507721	0.691664
8	1	-0.95113	-2.4731	-0.56119
9	1	0.333463	1.436976	-1.89492
10	1	0.044847	-1.1286	-2.704
11	7	3.072957	-0.08772	-0.97193
12	1	3.427448	0.304361	-1.82704
13	6	2.658437	0.632782	0.1109
14	6	2.892169	-1.41761	-0.73384
15	6	2.239905	-0.27452	1.087429
16	6	2.377293	-1.55771	0.555073
17	1	2.692734	1.707941	0.137593
18	1	3.160119	-2.16197	-1.46303
19	1	1.886992	-0.00651	2.067352
20	1	2.159363	-2.4945	1.03693
21	8	-2.02709	-1.19386	2.906622
22	1	-2.97198	-1.07116	3.046458
23	1	-1.70434	-1.66255	3.682929
24	8	1.100795	3.418194	0.946496
25	1	1.334898	3.752605	1.819048
26	1	0.872261	4.204799	0.439537
27	18	-3.89617	0.378335	-0.92955

Sum of electronic and zero-point Energies= -1100.569809

Sum of electronic and thermal Energies= -1100.550030

Sum of electronic and thermal Enthalpies= -1100.549086

Sum of electronic and thermal Free Energies= -1100.625641

$Py_2^+(a)(H_2O)_2(VI)Ar(I)$

1	7	0.293881	-1.43221	-0.0008

2	1	1.289098	-1.24165	-0.00106
3	6	-0.47705	-1.57019	1.106638
4	6	-0.47657	-1.57161	-1.10842
5	6	-1.79543	-1.84189	0.692516
6	6	-1.79511	-1.84271	-0.69465
7	1	-0.04638	-1.49554	2.089154
8	1	-0.04553	-1.49782	-2.09086
9	1	-2.62471	-2.03402	1.35035
10	1	-2.62416	-2.03538	-1.35263
11	7	-3.06119	1.118197	-0.00014
12	1	-4.05207	0.948108	-0.00038
13	6	-2.28381	1.240554	1.114258
14	6	-2.28355	1.242409	-1.11421
15	6	-0.97446	1.478954	0.699306
16	6	-0.97434	1.480036	-0.69866
17	1	-2.70498	1.188928	2.102793
18	1	-2.7045	1.192071	-2.10292
19	1	-0.13687	1.646059	1.352389
20	1	-0.1365	1.647976	-1.35119
21	8	2.527519	-1.06423	1.819986
22	1	3.019145	-1.81022	2.179463
23	1	3.088531	-0.29753	1.974426
24	8	2.532929	-1.06902	-1.81314
25	1	3.094476	-0.3036	-1.97196
26	1	3.024473	-1.81759	-2.16729
27	18	2.600522	1.860057	-0.00218

Sum of electronic and zero-point Energies= -1100.570539

Sum of electronic and thermal Energies= -1100.550858

Sum of electronic and thermal Enthalpies= -1100.549914

Sum of electronic and thermal Free Energies= -1100.624292

$Py_2^+(a)(H_2O)_2(VI)Ar(II)$

1	7	-1.64502	-0.80161	0.002942
2	1	-2.63139	-0.57046	0.002587
3	6	-0.87977	-0.97117	-1.10481
4	6	-0.87881	-0.96421	1.110938
5	6	0.427963	-1.28607	-0.6903
6	6	0.428614	-1.28167	0.697178

7	1	-1.30875	-0.88626	-2.08725
8	1	-1.30693	-0.87333	2.093211
9	1	1.251257	-1.50712	-1.34603
10	1	1.252477	-1.49879	1.353501
11	7	1.807057	1.595713	-0.01008
12	1	2.779597	1.340224	-0.0112
13	6	1.035043	1.754397	-1.12282
14	6	1.039619	1.762222	1.104606
15	6	-0.25884	2.067338	-0.70626
16	6	-0.25601	2.072012	0.691116
17	1	1.450283	1.673197	-2.11184
18	1	1.45892	1.688434	2.092496
19	1	-1.08578	2.281773	-1.35969
20	1	-1.08021	2.291221	1.34641
21	8	-3.8753	-0.41293	-1.82905
22	1	-4.38512	-1.17813	-2.11553
23	1	-4.40473	0.34815	-2.08833
24	8	-3.86873	-0.38191	1.837579
25	1	-4.37977	0.387806	2.107997
26	1	-4.39548	-1.13874	2.115592
27	18	4.092043	-1.13751	0.006216

Sum of electronic and zero-point Energies= -1100.570525

Sum of electronic and thermal Energies= -1100.551448

Sum of electronic and thermal Enthalpies= -1100.550504

Sum of electronic and thermal Free Energies= -1100.624590

$Py_2^+(p)(H_2O)_2(l)$

1	7	0.712865	-1.32751	0.012217
2	1	-0.26296	-1.63469	0.000584
3	6	1.476051	-1.09648	-1.08688
4	6	1.442651	-1.06257	1.124612
5	6	2.759637	-0.70328	-0.66048
6	6	2.739351	-0.68176	0.723465
7	1	1.09728	-1.26924	-2.07898
8	1	1.036565	-1.20714	2.110372
9	1	3.586004	-0.4687	-1.30834
10	1	3.546483	-0.42742	1.387959
11	7	-1.14547	1.180934	0.002186

12	1	-2.08964	0.81614	0.02437
13	6	-0.39529	1.504545	1.095776
14	6	-0.42881	1.452429	-1.1265
15	6	0.826991	2.010354	0.652187
16	6	0.806342	1.977392	-0.74385
17	1	-0.78056	1.391768	2.094234
18	1	-0.84246	1.290003	-2.1066
19	1	1.619538	2.367957	1.28499
20	1	1.579159	2.305096	-1.41607
21	8	-1.96554	-2.16655	-0.05224
22	1	-2.25816	-3.08272	-0.06165
23	1	-2.76092	-1.6121	-0.01302
24	8	-3.8937	-0.07569	0.050183
25	1	-4.47965	0.063154	-0.70332
26	1	-4.45013	0.028081	0.831145

Sum of electronic and zero-point Energies= -573.015282

Sum of electronic and thermal Energies= -572.999509

Sum of electronic and thermal Enthalpies= -572.998565

Sum of electronic and thermal Free Energies= -573.062034

$Py_2^+(p)(H_2O)_2(II)$

1	7	-0.14507	1.603152	0.314506
2	1	-1.06577	1.426193	0.699443
3	6	1.00619	1.66827	1.040572
4	6	0.165767	1.536987	-1.00989
5	6	2.084889	1.693953	0.149081
6	6	1.55843	1.612555	-1.13664
7	1	0.990335	1.734412	2.114469
8	1	-0.59978	1.484744	-1.76414
9	1	3.120982	1.77303	0.427451
10	1	2.100046	1.615586	-2.06609
11	7	0.009179	-1.36758	0.405523
12	1	-0.90586	-1.09539	0.757689
13	6	0.320613	-1.53257	-0.90854
14	6	1.147068	-1.44315	1.146996
15	6	1.700834	-1.77191	-1.00574
16	6	2.218136	-1.7153	0.281046
17	1	-0.43819	-1.52371	-1.67113

18	1	1.127219	-1.35424	2.219057
19	1	2.236232	-1.96383	-1.91898
20	1	3.241612	-1.85446	0.582069
21	8	-2.43659	0.00674	1.194069
22	1	-3.17532	-0.06895	0.551492
23	1	-2.8424	-0.02352	2.066523
24	8	-4.34618	-0.20538	-0.75519
25	1	-4.84056	-1.01716	-0.91248
26	1	-4.94664	0.514336	-0.97795

Sum of electronic and zero-point Energies= -573.013626

Sum of electronic and thermal Energies= -572.997897

Sum of electronic and thermal Enthalpies= -572.996953

Sum of electronic and thermal Free Energies= -573.060603

$Py_2^+(a)(H_2O)_3(I)$

1	7	1.141479	1.645269	-0.05803
2	1	2.116772	1.365739	0.095108
3	6	0.47707	1.531112	-1.23798
4	6	0.261357	1.992805	0.91412
5	6	-0.86928	1.86235	-1.02365
6	6	-1.00616	2.152321	0.329067
7	1	0.989739	1.263413	-2.14521
8	1	0.577873	2.136232	1.932397
9	1	-1.63025	1.897847	-1.78332
10	1	-1.89584	2.463605	0.847806
11	7	-1.90763	-1.02775	0.157048
12	1	-2.90458	-0.91156	-0.01935
13	6	-0.97182	-1.35186	-0.77751
14	6	-1.29545	-0.85314	1.357687
15	6	0.276975	-1.41944	-0.14774
16	6	0.073698	-1.10444	1.194156
17	1	-1.24693	-1.54501	-1.79966
18	1	-1.85539	-0.60085	2.241198
19	1	1.209751	-1.67701	-0.6193
20	1	0.812343	-1.06459	1.975337
21	8	3.66368	0.574107	0.376442
22	1	4.530323	0.974222	0.489244
23	1	3.806656	-0.34112	0.071946

24	8	-4.71583	-0.80863	-0.30011
25	1	-5.30965	-1.56042	-0.20309
26	1	-5.27343	-0.06243	-0.54214
27	8	3.749479	-2.07114	-0.53182
28	1	4.229151	-2.29983	-1.33553
29	1	3.949537	-2.77384	0.096388

Sum of electronic and zero-point Energies= -649.473804

Sum of electronic and thermal Energies= -649.453826

Sum of electronic and thermal Enthalpies= -649.452882

Sum of electronic and thermal Free Energies= -649.527016

$Py_2^+(a)(H_2O)_3$(II)

1	7	1.370281	-0.49293	0.000203
2	1	2.229266	0.072426	0.00012
3	6	0.703506	-0.91395	1.105654
4	6	0.703141	-0.91354	-1.10521
5	6	-0.41575	-1.65626	0.695169
6	6	-0.41597	-1.656	-0.69464
7	1	1.067713	-0.69815	2.094984
8	1	1.067029	-0.69733	-2.09457
9	1	-1.11414	-2.14302	1.352739
10	1	-1.11456	-2.14255	-1.35216
11	7	-2.7052	0.582501	0.00002
12	1	-3.56557	0.036051	-0.00016
13	6	-2.03487	0.998004	1.108353
14	6	-2.03455	0.998162	-1.10804
15	6	-0.91341	1.728695	0.696894
16	6	-0.9132	1.728802	-0.69613
17	1	-2.40169	0.786104	2.097434
18	1	-2.40094	0.786209	-2.09727
19	1	-0.20918	2.209208	1.352764
20	1	-0.20875	2.209399	-1.35171
21	8	3.722268	0.961868	-0.0003
22	1	4.595281	0.52123	-0.00036
23	1	3.891053	1.90756	-0.00017
24	8	-5.17306	-0.84746	-0.00084
25	1	-6.02408	-0.39692	-0.00158
26	1	-5.37306	-1.78886	-0.00025

27	8	6.131037	-0.38368	-0.00047
28	1	6.695362	-0.50875	-0.76999
29	1	6.695201	-0.50899	0.769132

Sum of electronic and zero-point Energies= -649.473639

Sum of electronic and thermal Energies= -649.453320

Sum of electronic and thermal Enthalpies= -649.452376

Sum of electronic and thermal Free Energies= -649.528337

$Py_2^+(a)(H_2O)_3$(III)

1	7	1.423155	0.865447	-0.70075
2	1	2.256956	0.341362	-0.98311
3	6	0.461528	1.37405	-1.51263
4	6	1.051319	1.03694	0.594749
5	6	-0.54745	1.928412	-0.70879
6	6	-0.17654	1.717227	0.614724
7	1	0.556201	1.34626	-2.58411
8	1	1.685386	0.70363	1.398804
9	1	-1.42304	2.436385	-1.07299
10	1	-0.70321	2.025461	1.500711
11	7	-2.30696	-0.73843	0.127757
12	1	-3.17587	-0.32367	0.461885
13	6	-1.95414	-0.88404	-1.17722
14	6	-1.30652	-1.21906	0.915618
15	6	-0.69943	-1.50523	-1.22829
16	6	-0.29284	-1.71609	0.086808
17	1	-2.61086	-0.57785	-1.97272
18	1	-1.38698	-1.2117	1.98854
19	1	-0.17409	-1.77801	-2.12645
20	1	0.617998	-2.18064	0.420688
21	8	3.665454	-0.75999	-0.87553
22	1	4.043625	-0.64428	0.014644
23	1	4.39661	-0.9326	-1.47517
24	8	-4.79238	0.308371	1.058301
25	1	-5.55928	-0.25672	1.198918
26	1	-5.08739	1.204706	1.247568
27	8	4.175833	-0.18447	1.816379
28	1	4.379975	-0.88875	2.441513
29	1	4.763711	0.542744	2.049205

Sum of electronic and zero-point Energies= -649.472571

Sum of electronic and thermal Energies= -649.452642

Sum of electronic and thermal Enthalpies= -649.451698

Sum of electronic and thermal Free Energies= -649.526183

$Py_2^+(a)(H_2O)_3$(linear)

1	7	0.137653	0.476063	-0.19369
2	1	0.920191	-0.20154	-0.21731
3	6	-0.58088	0.879898	-1.27066
4	6	-0.35563	1.079882	0.91535
5	6	-1.55697	1.800615	-0.84012
6	6	-1.41628	1.925535	0.532818
7	1	-0.34822	0.529323	-2.26129
8	1	0.078076	0.909721	1.885625
9	1	-2.25097	2.315854	-1.4807
10	1	-1.97651	2.55937	1.197541
11	7	-3.98935	-0.12547	0.253027
12	1	-4.76822	0.510012	0.26296
13	6	-3.47033	-0.71725	-0.86147
14	6	-3.27428	-0.51114	1.348821
15	6	-2.40996	-1.52894	-0.46135
16	6	-2.2869	-1.39942	0.925349
17	1	-3.89982	-0.55815	-1.83484
18	1	-3.52938	-0.16897	2.336277
19	1	-1.82142	-2.14893	-1.11432
20	1	-1.5844	-1.89961	1.568303
21	8	2.227881	-1.25637	-0.3503
22	1	3.13373	-0.91414	-0.54078
23	1	2.322707	-2.18286	-0.11651
24	8	4.637041	-0.21249	-0.90559
25	1	5.356788	-0.09103	-0.25681
26	1	5.056237	-0.31632	-1.76405
27	8	6.640035	0.158669	0.981513
28	1	7.055988	1.013135	1.133745
29	1	7.284755	-0.5037	1.249416

Sum of electronic and zero-point Energies= -649.470542

Sum of electronic and thermal Energies= -649.451811

Sum of electronic and thermal Enthalpies= -649.450867

Sum of electronic and thermal Free Energies= -649.522873

$Py_2^+(p)(H_2O)_3(I)$

1	7	-0.74986	-0.91734	-0.78752
2	1	-1.57032	-0.4053	-1.09686
3	6	0.306714	-1.30566	-1.55733
4	6	-0.54622	-1.33184	0.494407
5	6	1.203154	-2.00564	-0.74543
6	6	0.66946	-2.01887	0.543954
7	1	0.337075	-1.10269	-2.61363
8	1	-1.27869	-1.13786	1.259463
9	1	2.123849	-2.45225	-1.07583
10	1	1.090912	-2.48008	1.419304
11	7	1.26884	1.287464	0.144384
12	1	0.369129	1.737574	-0.05212
13	6	1.688715	0.883062	1.373616
14	6	2.216578	0.979895	-0.77212
15	6	2.972834	0.327854	1.24403
16	6	3.306336	0.386254	-0.09921
17	1	1.088049	1.048703	2.250685
18	1	2.104791	1.246073	-1.80836
19	1	3.566872	-0.06526	2.050265
20	1	4.217069	0.052272	-0.56486
21	8	-3.19604	0.632829	-0.95943
22	1	-3.62884	0.253875	-0.16614
23	1	-3.87483	0.736426	-1.63351
24	8	-3.95468	-0.54574	1.401456
25	1	-4.30287	-0.01993	2.13024
26	1	-4.44462	-1.37545	1.42277
27	8	-1.21235	2.473462	-0.3142
28	1	-2.0164	1.986458	-0.57095
29	1	-1.41497	3.411787	-0.36265

Sum of electronic and zero-point Energies= -649.476730

Sum of electronic and thermal Energies= -649.458249

Sum of electronic and thermal Enthalpies= -649.457305

Sum of electronic and thermal Free Energies= -649.526490

$Py_2^+(p)(H_2O)_3(II)$

1	7	0.593034	1.424216	-0.3855
2	1	1.499683	1.208638	-0.79168
3	6	-0.52105	1.82975	-1.06154
4	6	0.30976	1.358897	0.943995
5	6	-1.54128	2.049253	-0.12992
6	6	-1.0225	1.75043	1.1277
7	1	-0.50893	1.979435	-2.12716
8	1	1.062008	1.054641	1.651691
9	1	-2.53362	2.391313	-0.36361
10	1	-1.52725	1.817495	2.075002
11	7	-0.8718	-1.33701	-0.25822
12	1	0.108459	-1.54619	-0.44553
13	6	-1.46199	-1.40027	0.970385
14	6	-1.79236	-0.95692	-1.17603
15	6	-2.81786	-1.08345	0.82454
16	6	-3.02919	-0.8036	-0.51882
17	1	-0.90666	-1.69885	1.842036
18	1	-1.55011	-0.88232	-2.22139
19	1	-3.5426	-1.06087	1.619278
20	1	-3.95374	-0.52323	-0.9926
21	8	3.225414	0.436205	-1.07189
22	1	3.531307	0.343781	-0.14729
23	1	3.956519	0.783623	-1.59224
24	8	1.91716	-1.95825	-0.61459
25	1	2.447069	-1.27474	-1.06641
26	1	2.162702	-2.80458	-1.00244
27	8	3.151814	-0.36809	1.521279
28	1	2.845332	-1.24671	1.255547
29	1	3.764821	-0.49537	2.252635

Sum of electronic and zero-point Energies= -649.475705

Sum of electronic and thermal Energies= -649.457976

Sum of electronic and thermal Enthalpies= -649.457032

Sum of electronic and thermal Free Energies= -649.522956

$Py_2H_2O(I)$

1	7	-1.52325	0.994935	-0.17903
2	6	-1.91543	0.146235	-1.17644

3	6	-1.96923	0.524769	1.024841
4	6	-2.64101	-0.87686	-0.60744
5	1	-1.64414	0.330608	-2.20072
6	1	-0.83177	1.728258	-0.28831
7	6	-2.67465	-0.63614	0.795271
8	1	-1.75229	1.047305	1.939568
9	1	-3.1094	-1.69001	-1.13524
10	1	-3.17571	-1.22923	1.541169
11	6	2.736054	-0.18819	0.691554
12	6	1.499666	-0.50486	1.21373
13	6	2.74116	-0.61911	-0.66569
14	1	3.548335	0.270441	1.229216
15	7	0.77164	-1.10968	0.228785
16	1	1.086272	-0.34882	2.19388
17	6	1.509839	-1.17641	-0.91983
18	1	3.554727	-0.53824	-1.36597
19	1	-0.20485	-1.34949	0.303579
20	1	1.100267	-1.6036	-1.81742
21	8	0.998628	2.458856	-0.2403
22	1	1.472097	2.818739	-0.99527
23	1	1.510248	1.679745	0.033661

Sum of electronic and zero-point Energies= -496.815394

Sum of electronic and thermal Energies= -496.802578

Sum of electronic and thermal Enthalpies= -496.801633

Sum of electronic and thermal Free Energies= -496.856790

$Py_2(H_2O)_2$(l)

1	7	-2.03823	0.61306	0.006292
2	6	-2.2421	-0.17297	-1.09232
3	6	-2.15997	-0.14128	1.138899
4	6	-2.50674	-1.45505	-0.65825
5	1	-2.18715	0.236816	-2.08532
6	1	-1.74477	1.586795	-0.01993
7	6	-2.4552	-1.43415	0.763848
8	1	-2.02933	0.295252	2.113312
9	1	-2.72791	-2.30193	-1.28519

10	1	-2.62614	-2.26301	1.429285
11	6	2.896258	-0.92115	0.669841
12	6	1.587774	-1.19488	1.002494
13	6	2.934838	-0.70136	-0.73589
14	1	3.729472	-0.89295	1.351015
15	7	0.843919	-1.15183	-0.1431
16	1	1.131362	-1.42473	1.948785
17	6	1.646954	-0.85201	-1.20601
18	1	3.803625	-0.48093	-1.33255
19	1	-0.1528	-1.30688	-0.1946
20	1	1.245628	-0.77927	-2.20121
21	8	-0.73733	3.13131	-0.16229
22	1	-0.80654	4.062256	0.060403
23	1	0.189461	2.86383	0.014313
24	8	1.790131	2.152953	0.308702
25	1	2.063318	1.549366	-0.39789
26	1	1.838506	1.589699	1.090184

Sum of electronic and zero-point Energies= -573.273501

Sum of electronic and thermal Energies= -573.257530

Sum of electronic and thermal Enthalpies= -573.256586

Sum of electronic and thermal Free Energies= -573.320767

$Py_2(H_2O)_2$(II)

1	7	1.361582	1.067427	-0.04057
2	6	1.766302	0.661533	1.199614
3	6	2.291434	0.699088	-0.96971
4	6	2.979031	0.02346	1.069352
5	1	1.161651	0.851458	2.068462
6	1	0.483817	1.540162	-0.2471
7	6	3.31466	0.043159	-0.31384
8	1	2.1612	0.93513	-2.01103
9	1	3.560434	-0.40092	1.869922
10	1	4.209052	-0.34615	-0.77025
11	6	-3.31651	-0.03924	-0.30592
12	6	-2.29924	-0.69567	-0.97042
13	6	-2.97207	-0.02501	1.07519
14	1	-4.21271	0.353879	-0.75536
15	7	-1.3645	-1.06951	-0.04845

16	1	-2.17626	-0.92842	-2.01336
17	6	-1.76025	-0.66669	1.195638
18	1	-3.54722	0.398319	1.880811
19	1	-0.48928	-1.5442	-0.26127
20	1	-1.15048	-0.86102	2.059921
21	8	-1.15318	2.328358	-0.71339
22	1	-1.49665	3.019921	-0.14078
23	1	-1.8209	1.621535	-0.68787
24	8	1.153516	-2.32807	-0.71456
25	1	1.496617	-3.01287	-0.1336
26	1	1.818285	-1.61835	-0.69114

Sum of electronic and zero-point Energies= -573.272264

Sum of electronic and thermal Energies= -573.256362

Sum of electronic and thermal Enthalpies= -573.255417

Sum of electronic and thermal Free Energies= -573.317805

Py_2^+(a) **CAM-B3LYP-D3**

1	6	1.522427	0.602469	1.107519
2	6	1.522427	-0.72879	0.693781
3	6	1.522427	-0.72879	-0.69378
4	6	1.522427	0.602469	-1.10752
5	7	1.54545	1.385942	0
6	1	1.559975	2.39141	0
7	1	1.553907	1.023235	2.097255
8	1	1.554968	-1.58033	1.350025
9	1	1.554968	-1.58033	-1.35003
10	1	1.553907	1.023235	-2.09726
11	6	-1.52243	-0.60247	-1.10752
12	6	-1.52243	0.728792	-0.69378
13	6	-1.52243	0.728792	0.693781
14	6	-1.52243	-0.60247	1.107519
15	7	-1.54545	-1.38594	0
16	1	-1.55998	-2.39141	0
17	1	-1.55391	-1.02324	-2.09726
18	1	-1.55497	1.580328	-1.35003
19	1	-1.55497	1.580328	1.350025
20	1	-1.55391	-1.02324	2.097255

Sum of electronic and zero-point Energies= -419.844048

Sum of electronic and thermal Energies= -419.834871

Sum of electronic and thermal Enthalpies= -419.833926

Sum of electronic and thermal Free Energies= -419.879501

Py_2^+(a) **M06-2X**

1	6	1.507384	0.634914	1.109053
2	6	1.507384	-0.69997	0.695254
3	6	1.507384	-0.69997	-0.69525
4	6	1.507384	0.634914	-1.10905
5	7	1.528336	1.41907	0
6	1	1.545157	2.426023	0
7	1	1.539345	1.059134	2.098339
8	1	1.540829	-1.55084	1.353752
9	1	1.540829	-1.55084	-1.35375
10	1	1.539345	1.059134	-2.09834
11	6	-1.50738	-0.63491	-1.10905
12	6	-1.50738	0.699968	-0.69525
13	6	-1.50738	0.699968	0.695254
14	6	-1.50738	-0.63491	1.109053
15	7	-1.52834	-1.41907	0
16	1	-1.54516	-2.42602	0
17	1	-1.53935	-1.05913	-2.09834
18	1	-1.54083	1.550838	-1.35375
19	1	-1.54083	1.550838	1.353752
20	1	-1.53935	-1.05913	2.098339

Sum of electronic and zero-point Energies= -419.883901

Sum of electronic and thermal Energies= -419.874773

Sum of electronic and thermal Enthalpies= -419.873829

Sum of electronic and thermal Free Energies= -419.919093

Py_2^+(a)H_2O(l) **CAM-B3LYP-D3**

1	7	2.595189	-0.18101	-0.00004
2	1	3.39654	0.425417	-0.00052
3	6	1.965304	-0.64714	1.109569
4	6	1.965276	-0.64881	-1.10885
5	6	0.922437	-1.46608	0.697703
6	6	0.922368	-1.46714	-0.69566
7	1	2.318319	-0.4124	2.098191

8	1	2.318257	-0.41568	-2.09787
9	1	0.26948	-2.01466	1.352916
10	1	0.269217	-2.01665	-1.3499
11	7	-1.51293	0.501449	0.000086
12	1	-2.32007	-0.12622	0.000695
13	6	-0.88635	0.976249	1.100554
14	6	-0.8856	0.97318	-1.10127
15	6	0.160207	1.81369	0.689237
16	6	0.160585	1.811882	-0.6916
17	1	-1.23068	0.735287	2.091251
18	1	-1.22928	0.729538	-2.09153
19	1	0.806277	2.366948	1.347336
20	1	0.80711	2.36327	-1.35081
21	8	-3.79359	-1.13596	0.000121
22	1	-4.68449	-0.77298	-0.0014
23	1	-3.89315	-2.09228	0.002228

Sum of electronic and zero-point Energies= -496.279568

Sum of electronic and thermal Energies= -496.266603

Sum of electronic and thermal Enthalpies= -496.265658

Sum of electronic and thermal Free Energies= -496.321650

$Py_2^+(a)H_2O(l)$ M06-2X

1	7	2.611391	-0.19059	0.002139
2	1	3.426894	0.399164	0.004352
3	6	1.972592	-0.6503	1.111397
4	6	1.976185	-0.64689	-1.11046
5	6	0.912935	-1.45056	0.695869
6	6	0.915114	-1.44834	-0.70077
7	1	2.330855	-0.42151	2.100506
8	1	2.337504	-0.41509	-2.09776
9	1	0.250835	-1.99047	1.350678
10	1	0.254827	-1.986	-1.35925
11	7	-1.51657	0.502576	0.000178
12	1	-2.33516	-0.1109	0.000245
13	6	-0.88021	0.964956	1.102377
14	6	-0.88111	0.966202	-1.1018
15	6	0.185149	1.785844	0.691716
16	6	0.184714	1.78658	-0.69094

17	1	-1.22876	0.724608	2.092721
18	1	-1.23036	0.727245	-2.09224
19	1	0.840927	2.32515	1.353149
20	1	0.840102	2.326485	-1.35227
21	8	-3.84584	-1.1033	-0.00002
22	1	-4.72953	-0.7246	0.000381
23	1	-3.96736	-2.05654	-0.00089

Sum of electronic and zero-point Energies= -496.310202

Sum of electronic and thermal Energies= -496.297275

Sum of electronic and thermal Enthalpies= -496.296331

Sum of electronic and thermal Free Energies= -496.352079

$Py_2^+(a)(H_2O)_2(I)$ CAM-B3LYP-D3

1	7	-1.97232	-0.66523	-0.00053
2	1	-2.87215	-0.18477	-4.4E-05
3	6	-1.27427	-1.02494	-1.10349
4	6	-1.27374	-1.02602	1.101727
5	6	-0.1061	-1.67146	-0.69469
6	6	-0.10572	-1.67218	0.69167
7	1	-1.65657	-0.84482	-2.09291
8	1	-1.6556	-0.84697	2.091513
9	1	0.626686	-2.10404	-1.35217
10	1	0.627366	-2.10557	1.348287
11	7	1.972287	0.665079	0.000585
12	1	2.87275	0.185796	0.001104
13	6	1.274996	1.026085	-1.10239
14	6	1.272496	1.023703	1.102828
15	6	0.105984	1.671152	-0.69356
16	6	0.104524	1.669822	0.692804
17	1	1.65822	0.847747	-2.09178
18	1	1.653421	0.842935	2.092655
19	1	-0.62649	2.104358	-1.35099
20	1	-0.62936	2.101715	1.349519
21	8	-4.51852	0.56336	0.001849
22	1	-5.32928	0.045891	0.002503
23	1	-4.78908	1.485799	0.001438
24	8	4.519813	-0.56061	0.001643
25	1	5.330504	-0.04304	0.003147

26	1	4.79047	-1.48302	0.000054

Sum of electronic and zero-point Energies= -572.713541

Sum of electronic and thermal Energies= -572.696694

Sum of electronic and thermal Enthalpies= -572.695750

Sum of electronic and thermal Free Energies= -572.761810

$Py_2^+(a)(H_2O)_2(I)$ M06-2X

1	7	-1.98806	-0.65111	-3.1E-05
2	1	-2.89288	-0.17944	-0.00069
3	6	-1.28592	-1.00749	-1.10366
4	6	-1.2874	-1.00715	1.104543
5	6	-0.10946	-1.64535	-0.69314
6	6	-0.11035	-1.6451	0.695766
7	1	-1.67086	-0.82843	-2.09329
8	1	-1.67358	-0.82789	2.093653
9	1	0.626038	-2.07333	-1.3521
10	1	0.624607	-2.07245	1.355717
11	7	1.988382	0.6519	-0.00017
12	1	2.89213	0.178187	-0.00094
13	6	1.286397	1.008699	-1.1038
14	6	1.287988	1.008429	1.104437
15	6	0.110536	1.647469	-0.69329
16	6	0.111502	1.647287	0.695714
17	1	1.670907	0.828598	-2.09341
18	1	1.673965	0.828568	2.093521
19	1	-0.62467	2.076452	-1.3519
20	1	-0.62295	2.075766	1.355497
21	8	-4.575	0.550997	-0.00216
22	1	-5.37466	0.017623	-0.00261
23	1	-4.86881	1.465697	-0.00243
24	8	4.572613	-0.55598	-0.00202
25	1	5.37348	-0.02442	-0.00134
26	1	4.86435	-1.47134	-0.00425

Sum of electronic and zero-point Energies= -572.735108

Sum of electronic and thermal Energies= -572.718083

Sum of electronic and thermal Enthalpies= -572.717139

Sum of electronic and thermal Free Energies= -572.784098

Bz_2^+ **B3PW91-D3**

1	6	2.356575	-0.0155	-0.81966
2	6	1.957786	-1.20143	-0.2245
3	6	1.198224	-1.18601	0.971367
4	6	0.854337	0.015533	1.565119
5	6	1.212355	1.201687	0.947679
6	6	1.972837	1.185626	-0.24784
7	1	2.951245	-0.02811	-1.72302
8	1	2.238659	-2.15186	-0.66047
9	1	0.929852	-2.12424	1.439548
10	1	0.296287	0.028093	2.490823
11	1	0.954907	2.15177	1.397836
12	1	2.264535	2.124267	-0.70182
13	6	-0.8547	0.026223	-1.56516
14	6	-1.19344	-1.18046	-0.9794
15	6	-1.95246	-1.20666	0.21654
16	6	-2.35632	-0.02606	0.819636
17	6	-1.97784	1.180115	0.255802
18	6	-1.21731	1.206949	-0.93956
19	1	-0.29691	0.047389	-2.49087
20	1	-0.92174	-2.11455	-1.45389
21	1	-2.22926	-2.16101	0.646541
22	1	-2.95097	-0.04734	1.722843
23	1	-2.27331	2.114621	0.715809
24	1	-0.96357	2.160965	-1.38349

Sum of electronic and zero-point Energies= -463.994105

Sum of electronic and thermal Energies= -463.983114

Sum of electronic and thermal Enthalpies= -463.982169

Sum of electronic and thermal Free Energies= -464.034793

Bz_2^+ **CAM-B3LYP-D3**

1	6	-2.33101	0.217346	0.820488
2	6	-2.05087	-1.0637	0.410158
3	6	-1.31127	-1.2859	-0.77546
4	6	-0.88558	-0.21853	-1.5496
5	6	-1.13113	1.064939	-1.12009
6	6	-1.85434	1.285921	0.071468
7	1	-2.90637	0.395179	1.71672

8	1	-2.4032	-1.91164	0.97999
9	1	-1.13214	-2.29994	-1.10339
10	1	-0.35415	-0.39573	-2.47208
11	1	-0.81384	1.911941	-1.71076
12	1	-2.06099	2.299904	0.38395
13	6	0.885498	-0.21755	1.549741
14	6	1.310785	-1.28554	0.776285
15	6	2.050448	-1.06436	-0.40946
16	6	2.331094	0.216365	-0.82062
17	6	1.85487	1.285545	-0.07229
18	6	1.131528	1.065568	1.119399
19	1	0.354002	-0.39399	2.472331
20	1	1.131052	-2.2993	1.104704
21	1	2.402503	-1.91279	-0.97875
22	1	2.906531	0.393388	-1.71696
23	1	2.061898	2.299265	-0.38537
24	1	0.81459	1.913068	1.709543

Sum of electronic and zero-point Energies= -463.882794

Sum of electronic and thermal Energies= -463.871898

Sum of electronic and thermal Enthalpies= -463.870954

Sum of electronic and thermal Free Energies= -463.923412

Bz_2^+ **M06-2X**

1	6	-2.24235	-0.69399	0.652703
2	6	-1.55884	-1.37993	-0.37278
3	6	-0.92188	-0.67906	-1.40732
4	6	-0.92807	0.696742	-1.39908
5	6	-1.57246	1.380005	-0.35688
6	6	-2.24918	0.676479	0.660446
7	1	-2.75645	-1.25487	1.42039
8	1	-1.5629	-2.462	-0.38332
9	1	-0.44489	-1.22474	-2.20919
10	1	-0.4564	1.256282	-2.19464
11	1	-1.58657	2.462042	-0.35551
12	1	-2.76877	1.223531	1.434354
13	6	0.928756	-0.70158	1.396042
14	6	1.573278	-1.38001	0.350317
15	6	2.249292	-0.67159	-0.66376

16	6	2.241361	0.698873	-0.64971
17	6	1.558146	1.37989	0.379382
18	6	0.921971	0.674203	1.410666
19	1	0.457757	-1.26501	2.189181
20	1	1.587569	-2.46203	0.344095
21	1	2.76887	-1.21465	-1.44047
22	1	2.75482	1.26352	-1.41507
23	1	1.562119	2.461899	0.394855
24	1	0.444687	1.215804	2.215113

Sum of electronic and zero-point Energies= -463.938367

Sum of electronic and thermal Energies= -463.927575

Sum of electronic and thermal Enthalpies= -463.926630

Sum of electronic and thermal Free Energies= -463.977612

Bz_2^+ **B3LYP-D3**

1	6	-1.69552	-1.37611	0.210162
2	6	-2.28343	-0.56377	-0.77582
3	6	-2.21305	0.804012	-0.6539
4	6	-1.55872	1.376086	0.461407
5	6	-1.00575	0.565609	1.4613
6	6	-1.06828	-0.80567	1.33542
7	1	-1.75226	-2.45235	0.120419
8	1	-2.78336	-1.01854	-1.61885
9	1	-2.65714	1.448267	-1.39934
10	1	-1.52053	2.452253	0.560252
11	1	-0.54045	1.01904	2.324086
12	1	-0.65891	-1.44876	2.100874
13	6	1.692243	-1.37678	-0.21552
14	6	1.066691	-0.80074	-1.33869
15	6	1.007138	0.571114	-1.45913
16	6	1.561857	1.376663	-0.45597
17	6	2.214944	0.79901	0.656987
18	6	2.281882	-0.56937	0.773726
19	1	1.746926	-2.45347	-0.12989
20	1	0.655835	-1.43991	-2.10661
21	1	0.543055	1.028963	-2.32025
22	1	1.525758	2.453273	-0.55072
23	1	2.660414	1.439326	1.404982

24	1	2.780525	-1.02849	1.615174

Sum of electronic and zero-point Energies= -464.184884

Sum of electronic and thermal Energies= -464.175649

Sum of electronic and thermal Enthalpies= -464.174705

Sum of electronic and thermal Free Energies= -464.220754

BzNp+ B3PW91-D3

1	6	1.423789	-0.69039	-1.5096
2	6	2.098859	-1.38472	-0.50313
3	6	2.782735	-0.69047	0.497306
4	6	2.78204	0.692493	0.49738
5	6	2.097492	1.386114	-0.50301
6	6	1.423137	0.691165	-1.50955
7	1	0.905286	-1.23758	-2.2861
8	1	2.117597	-2.46702	-0.516
9	1	3.324145	-1.23664	1.259278
10	1	3.32287	1.239112	1.259442
11	1	2.115188	2.468427	-0.51589
12	1	0.904327	1.237941	-2.28614
13	6	-0.81604	-2.43304	0.809404
14	6	-0.33475	-1.22828	1.322861
15	6	-0.81254	-0.00017	0.834595
16	6	-1.78962	-0.00069	-0.19975
17	6	-2.26048	-1.23133	-0.69438
18	6	-1.77657	-2.43282	-0.19318
19	1	0.395303	1.234264	2.120123
20	1	-0.44219	-3.36922	1.202851
21	1	0.396495	-1.23329	2.120232
22	6	-0.3359	1.228465	1.322724
23	6	-2.26163	1.229414	-0.69453
24	1	-3.01186	-1.23466	-1.47506
25	1	-2.15317	-3.36935	-0.58292
26	6	-1.77879	2.431435	-0.19351
27	6	-0.8183	2.4327	0.809091
28	1	-3.01305	1.231925	-1.47518
29	1	-2.15624	3.367563	-0.58342
30	1	-0.44535	3.369289	1.202427

Sum of electronic and zero-point Energies= -617.612824

Sum of electronic and thermal Energies= -617.599610

Sum of electronic and thermal Enthalpies= -617.598666

Sum of electronic and thermal Free Energies= -617.655255

$BzNp^+$ **CAM-B3LYP-D3**

1	6	1.561558	-0.69064	-1.50035
2	6	2.19007	-1.38286	-0.4721
3	6	2.823762	-0.6896	0.552124
4	6	2.822604	0.693029	0.551805
5	6	2.187661	1.384697	-0.47269
6	6	1.560293	0.690877	-1.5006
7	1	1.088533	-1.23453	-2.30574
8	1	2.213714	-2.46346	-0.48593
9	1	3.335027	-1.23168	1.335264
10	1	3.332987	1.236298	1.334696
11	1	2.209405	2.465325	-0.48715
12	1	1.08626	1.23362	-2.30617
13	6	-0.88166	-2.42864	0.795714
14	6	-0.39846	-1.22363	1.306051
15	6	-0.86859	-0.00023	0.812129
16	6	-1.83765	-0.00093	-0.22489
17	6	-2.30532	-1.22708	-0.71984
18	6	-1.8291	-2.42909	-0.20898
19	1	0.332193	1.229956	2.099653
20	1	-0.51287	-3.36245	1.194098
21	1	0.333444	-1.22864	2.100164
22	6	-0.39979	1.223861	1.305618
23	6	-2.30696	1.224584	-0.71993
24	1	-3.048	-1.23199	-1.50616
25	1	-2.20478	-3.36351	-0.59926
26	6	-1.83226	2.427284	-0.20932
27	6	-0.88452	2.428183	0.795106
28	1	-3.04973	1.228374	-1.50618
29	1	-2.2093	3.361166	-0.59956
30	1	-0.51671	3.362518	1.19318

Sum of electronic and zero-point Energies= -617.472353

Sum of electronic and thermal Energies= -617.459176

Sum of electronic and thermal Enthalpies= -617.458232

Sum of electronic and thermal Free Energies= -617.515605

$BzNp^+$ **M06-2X**

1	6	1.441878	-0.69338	-1.5068
2	6	2.105499	-1.38799	-0.49716
3	6	2.773081	-0.69387	0.509949
4	6	2.773726	0.691834	0.509585
5	6	2.106827	1.38605	-0.49791
6	6	1.442589	0.691549	-1.50721
7	1	0.940924	-1.23774	-2.29624
8	1	2.128349	-2.46965	-0.51248
9	1	3.30937	-1.23732	1.276184
10	1	3.310514	1.235178	1.275542
11	1	2.130721	2.467684	-0.51382
12	1	0.942149	1.235966	-2.29693
13	6	-0.8443	-2.43357	0.822768
14	6	-0.37479	-1.226	1.351144
15	6	-0.83342	0.000254	0.844678
16	6	-1.77384	0.000943	-0.22125
17	6	-2.22958	-1.22655	-0.73277
18	6	-1.76625	-2.43222	-0.2107
19	1	0.336623	1.228816	2.167788
20	1	-0.48644	-3.36879	1.229999
21	1	0.335011	-1.23001	2.167641
22	6	-0.3732	1.225826	1.351303
23	6	-2.22808	1.229115	-0.73254
24	1	-2.95126	-1.22719	-1.53976
25	1	-2.13149	-3.36656	-0.61255
26	6	-1.7632	2.434104	-0.21029
27	6	-0.84117	2.434092	0.823116
28	1	-2.9498	1.230781	-1.53949
29	1	-2.12728	3.368973	-0.61194
30	1	-0.48208	3.368781	1.230471

Sum of electronic and zero-point Energies= -617.552921

Sum of electronic and thermal Energies= -617.539741

Sum of electronic and thermal Enthalpies= -617.538797

Sum of electronic and thermal Free Energies= -617.595158

$BzNp^+$ **B3LYP-D3**

1	6	2.181532	-1.38819	-0.48118
2	6	2.838412	-0.69275	0.538691
3	6	2.838549	0.692565	0.538409
4	6	2.181822	1.387726	-0.48175
5	6	1.532451	0.691618	-1.50607
6	6	1.532301	-0.69236	-1.50578
7	1	2.200801	-2.46912	-0.49373
8	1	3.358754	-1.23782	1.314098
9	1	3.359001	1.237849	1.313596
10	1	2.201301	2.46865	-0.49475
11	1	1.038322	1.237258	-2.29769
12	1	1.038	-1.23823	-2.29715
13	6	-0.86813	-2.43667	0.796421
14	6	-0.38389	-1.23095	1.30897
15	6	-0.85976	0.000061	0.819501
16	6	-1.84178	0.000232	-0.21511
17	6	-2.31545	-1.23224	-0.70851
18	6	-1.83148	-2.43595	-0.20595
19	1	0.349829	1.237106	2.102352
20	1	-0.49562	-3.37201	1.189248
21	1	0.349472	-1.23742	2.102273
22	6	-0.38356	1.230899	1.309067
23	6	-2.31507	1.232863	-0.70846
24	1	-3.06718	-1.2358	-1.48683
25	1	-2.20938	-3.37098	-0.59411
26	6	-1.83075	2.436409	-0.20583
27	6	-0.86744	2.436786	0.796577
28	1	-3.06678	1.2367	-1.48679
29	1	-2.20835	3.371564	-0.59395
30	1	-0.49467	3.371994	1.18947

Sum of electronic and zero-point Energies= -617.863929

Sum of electronic and thermal Energies= -617.850681

Sum of electronic and thermal Enthalpies= -617.849737

Sum of electronic and thermal Free Energies= -617.906833

$BzTol^+$ **B3PW91-D3**

1	6	1.220093	0.23297	1.520107

2	6	2.051725	0.950098	0.666463
3	6	2.599272	0.3392	-0.48077
4	6	2.292877	-0.97184	-0.77815
5	6	1.422499	-1.67488	0.054539
6	6	0.890529	-1.07133	1.209343
7	1	0.829762	0.699119	2.414424
8	1	2.31829	1.972469	0.903021
9	1	3.267534	0.904408	-1.11769
10	1	2.716215	-1.45187	-1.65037
11	1	1.172786	-2.70401	-0.17175
12	1	0.250677	-1.64686	1.86535
13	6	-1.4923	1.775767	0.537954
14	6	-0.63597	1.973804	-0.56853
15	6	-0.41579	0.943582	-1.48598
16	6	-1.0008	-0.28261	-1.28213
17	6	-1.84663	-0.5072	-0.16573
18	6	-2.08871	0.559252	0.731521
19	1	-1.66989	2.590881	1.22728
20	1	-0.1783	2.942498	-0.72338
21	1	0.218273	1.112587	-2.34518
22	1	-0.84385	-1.08845	-1.98761
23	1	-2.74668	0.397998	1.576144
24	6	-2.52252	-1.81415	0.016949
25	1	-2.69723	-2.03969	1.069113
26	1	-3.50919	-1.77397	-0.46256
27	1	-1.97407	-2.63101	-0.45036

Sum of electronic and zero-point Energies= -503.295727

Sum of electronic and thermal Energies= -503.283128

Sum of electronic and thermal Enthalpies= -503.282184

Sum of electronic and thermal Free Energies= -503.337767

$BzTol^+$ **CAM-B3LYP-D3**

1	6	1.243942	0.217773	1.51961
2	6	2.042854	0.962596	0.666301
3	6	2.582989	0.378697	-0.49135
4	6	2.302768	-0.93353	-0.7977
5	6	1.464797	-1.6651	0.03611
6	6	0.938423	-1.08799	1.199263

7	1	0.861102	0.661413	2.426656
8	1	2.29666	1.983312	0.915292
9	1	3.232168	0.961758	-1.12891
10	1	2.727637	-1.39348	-1.67782
11	1	1.243333	-2.69782	-0.19453
12	1	0.327747	-1.68469	1.861613
13	6	-1.52219	1.754063	0.560062
14	6	-0.67239	1.969907	-0.54839
15	6	-0.44502	0.952612	-1.47692
16	6	-1.01202	-0.27643	-1.28314
17	6	-1.84762	-0.51938	-0.16502
18	6	-2.09948	0.535438	0.744206
19	1	-1.70586	2.561302	1.253959
20	1	-0.22858	2.943922	-0.69701
21	1	0.180697	1.139514	-2.33601
22	1	-0.85144	-1.07346	-1.99458
23	1	-2.75179	0.356337	1.587205
24	6	-2.51025	-1.83242	0.010755
25	1	-2.63755	-2.08274	1.062311
26	1	-3.51502	-1.77996	-0.42217
27	1	-1.98002	-2.63286	-0.49875

Sum of electronic and zero-point Energies= -503.172396

Sum of electronic and thermal Energies= -503.159879

Sum of electronic and thermal Enthalpies= -503.158935

Sum of electronic and thermal Free Energies= -503.214782

BzTol^{+} **M06-2X**

1	6	1.191862	0.234554	1.519237
2	6	2.000131	0.989498	0.679386
3	6	2.570518	0.409186	-0.46726
4	6	2.315676	-0.91324	-0.77556
5	6	1.474228	-1.65729	0.046735
6	6	0.912952	-1.08189	1.197452
7	1	0.784404	0.674503	2.41883
8	1	2.234674	2.015517	0.930544
9	1	3.224558	0.999274	-1.0948
10	1	2.76711	-1.36939	-1.64525
11	1	1.274969	-2.69591	-0.18316

12	1	0.298528	-1.68613	1.852056
13	6	-1.5749	1.743372	0.550423
14	6	-0.70548	1.981453	-0.54256
15	6	-0.42319	0.966785	-1.4699
16	6	-0.96003	-0.27906	-1.2892
17	6	-1.81074	-0.54669	-0.18268
18	6	-2.11753	0.504858	0.724131
19	1	-1.79746	2.546858	1.238211
20	1	-0.28293	2.967457	-0.68106
21	1	0.216287	1.175468	-2.3152
22	1	-0.7606	-1.07492	-1.99427
23	1	-2.7823	0.301558	1.553148
24	6	-2.4283	-1.88369	-0.01296
25	1	-2.58237	-2.12418	1.037776
26	1	-3.41907	-1.87209	-0.48304
27	1	-1.84704	-2.66511	-0.49722

Sum of electronic and zero-point Energies= -503.231317

Sum of electronic and thermal Energies= -503.218829

Sum of electronic and thermal Enthalpies= -503.217885

Sum of electronic and thermal Free Energies= -503.272452

BzTol^{+} **B3LYP-D3**

1	6	1.292781	0.22008	1.522536
2	6	2.088971	0.963656	0.653969
3	6	2.611785	0.376096	-0.51921
4	6	2.319645	-0.93874	-0.82355
5	6	1.490432	-1.67072	0.02902
6	6	0.980396	-1.08913	1.207205
7	1	0.920807	0.667931	2.432353
8	1	2.345237	1.985816	0.896004
9	1	3.250084	0.959738	-1.16773
10	1	2.724629	-1.39967	-1.71297
11	1	1.257084	-2.70152	-0.20018
12	1	0.372615	-1.68337	1.874706
13	6	-1.52534	1.754314	0.583687
14	6	-0.70126	1.982045	-0.54352
15	6	-0.49168	0.966473	-1.48383
16	6	-1.06147	-0.26983	-1.28845

17	6	-1.879	-0.52246	-0.15491
18	6	-2.1042	0.526426	0.770951
19	1	-1.69321	2.554131	1.290918
20	1	-0.26026	2.957395	-0.69447
21	1	0.118918	1.156598	-2.35393
22	1	-0.91283	-1.06046	-2.01052
23	1	-2.73677	0.343748	1.628777
24	6	-2.54551	-1.8403	0.020693
25	1	-2.67329	-2.09371	1.072586
26	1	-3.55161	-1.79233	-0.41359
27	1	-2.01474	-2.64179	-0.48949

Sum of electronic and zero-point Energies= -503.500218

Sum of electronic and thermal Energies= -503.487581

Sum of electronic and thermal Enthalpies= -503.486637

Sum of electronic and thermal Free Energies= -503.542507