Electronic Supporting Information (ESI)

Microhydration of Substituted Diamondoid Radical Cations of Biological Relevance: Infrared Spectra of Amantadine$^+$-$(H_2O)_{n=1-3}$ Clusters

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Figure S1. Typical mass spectrum of the ion source for an expansion of Ama^+ and W seeded in Ar carrier gas at 5 bar, illustrating the efficient production of $Ama^+W_{n=1-3}$ (red). The protonated $AmaH^+W_{n=1-3}$ cluster series is indicated by asterisks. Bare protonated water clusters (W_mH^+) and W_pH^+-N_2 clusters are indicated as well. The N_2-tagged clusters are produced from N_2 impurity in the gas inlet system.

Figure S2. Collision-induced dissociation (CID) mass spectrum of mass-selected Ama^+W_3 clusters to illustrate the efficient production of Ama^+W_n clusters in the electron ionization source and to ensure their composition (only loss of W ligands is observed). For the CID spectra, the octupole is filled with N_2 collision gas to induce dissociation (10^{-5} mbar) at a collision energy of around 10 eV in the laboratory frame.

Figure S3. Calculated equilibrium structures (in Å and degrees) of Ad, Ad^+, Ama, and Ama^+ in their ground electronic state (B3LYP-D3/cc-pVTZ).

Figure S4. Calculated equilibrium structures (in Å and degrees) of W, Ama, $Ama^{(+)}$, Ama^+W(**I**), NH_3, NH_3^+, CH_3NH_2, $CH_3NH_2^+$, $CH_3NH_2^+W$, $CH_3NH_2^+W_2$, and $CH_3NH_2^+W_3$ in their ground electronic state (B3LYP-D3/cc-pVTZ).

Figure S5. LUMO**,** HOMO and HOMO-1 orbitals of Ama and Ama^+ evaluated at the B3LYP-D3/cc-pVTZ level.

Figure S6. NBO charge distribution (in m*e*) of W, Ama, Ama^+, and Ama^+W(**I-III**) in their ground electronic states calculated at the B3LYP-D3/cc-pVTZ level.

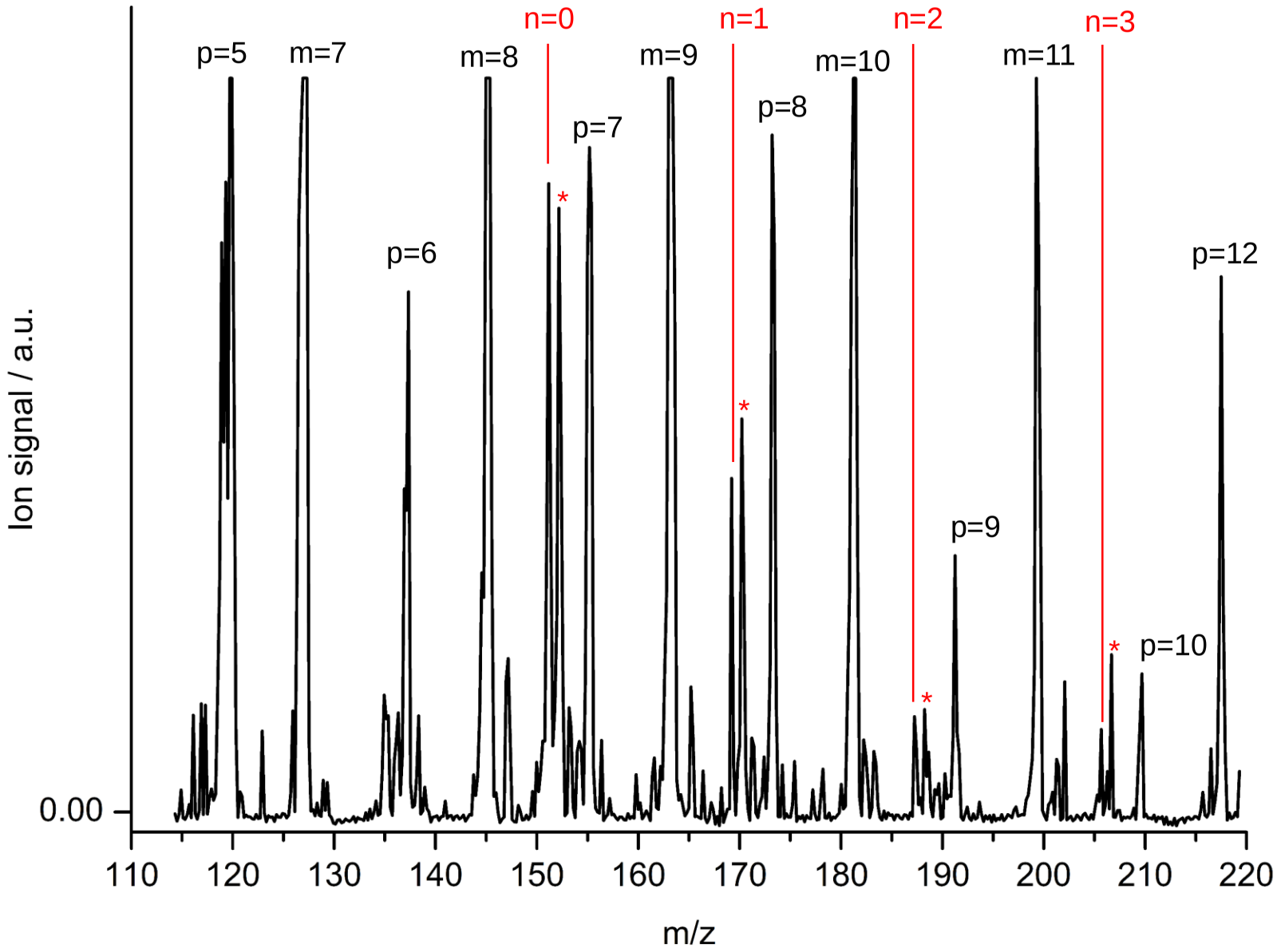
Figure S7. NBO charge distribution (in m*e*) of Ama^+W_2(**I-V**) in their ground electronic states calculated at the B3LYP-D3/cc-pVTZ level.

Figure S8. Calculated equilibrium structures (in Å and degrees) of Ama^+W_3(**VII-IX**) in their ground electronic state (B3LYP-D3/cc-pVTZ).

Figure S9. NBO charge distribution (in m*e*) of Ama^+W_3(**I-IX**) in their ground electronic states calculated at the B3LYP-D3/cc-pVTZ level.

Figure S10. Plot of the water binding energies (D_0) of the most stable isomers of Ama^+W_{1-3} (crosses) as a function of the cluster size *n* (surface solvation). A linear fit is drawn to illustrate the decrease of the binding energies by increasing the number of solvent molecules. For comparison, the binding energies of Ama^+W(**II**,**III**) representing interior ion solvation are included (filled squares). The experimental value for the sublimation enthalpy of bulk ice suggests that D_0 of larger Ama^+W_n converges to values much higher than D_0 of **II/III**, predicting that in such clusters indeed the hydrophobic adamantyl cage will reside at the surface of the water droplet.

Figure S1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n=1
n=2
n=3
p=5
m=7
m=8
m=9
m=10
m=11
p=6
p=7
p=8
p=9
p=10
p=12
*
*
*
*
Ion signal / a.u.
0.00
110
120
130
140
150
160
170
180
190
200
210
220
m/z

Figure S2

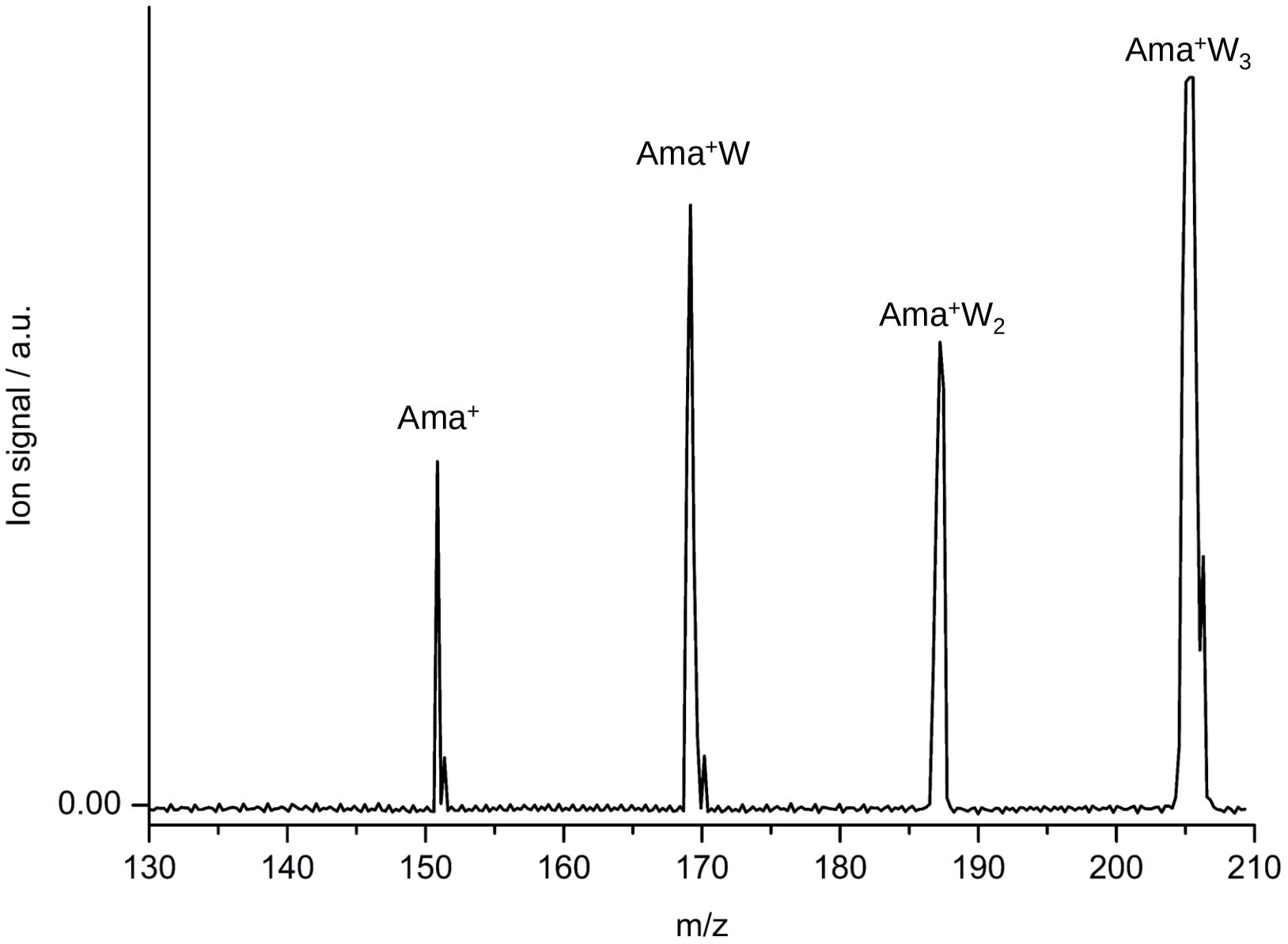
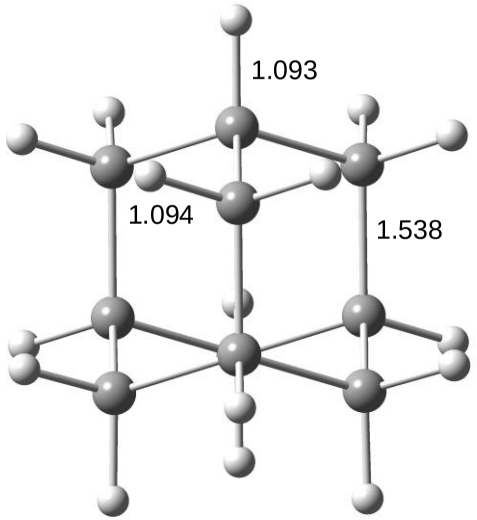
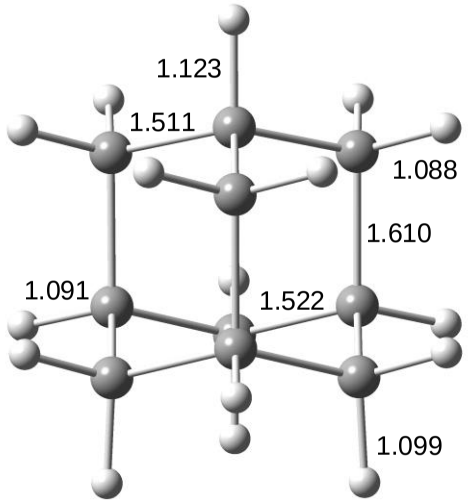

Ama+W3
Ama+W
Ama+W2
Ama+
Ion signal / a.u.
0.00
130
140
150
160
170
180
190
200
210
m/z

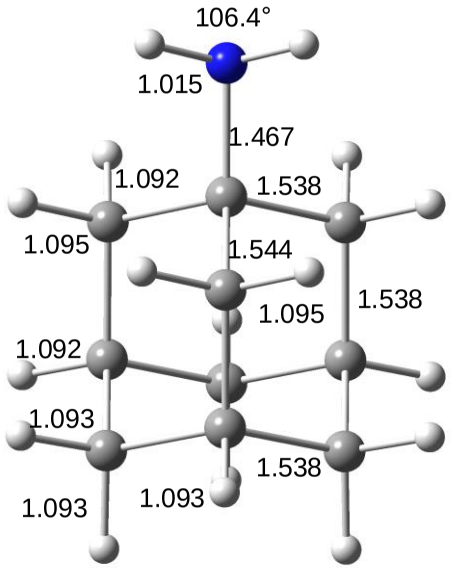
Figure S3



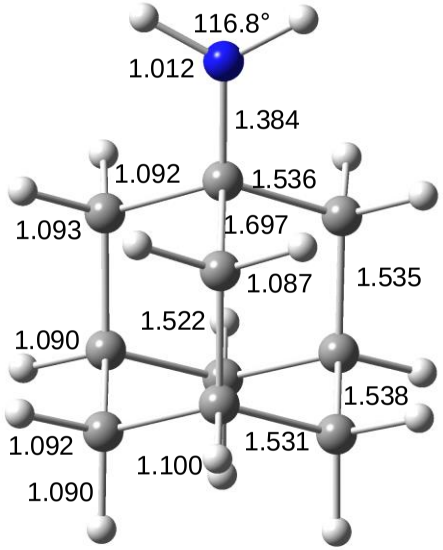
Ad (T_D)



Ad^+ (C_{3v})

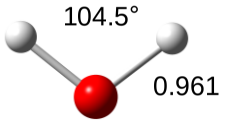


Ama (C_s)

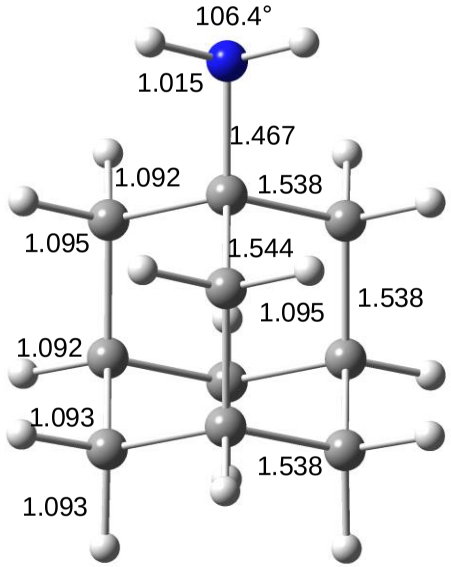


Ama^+ (C_s)

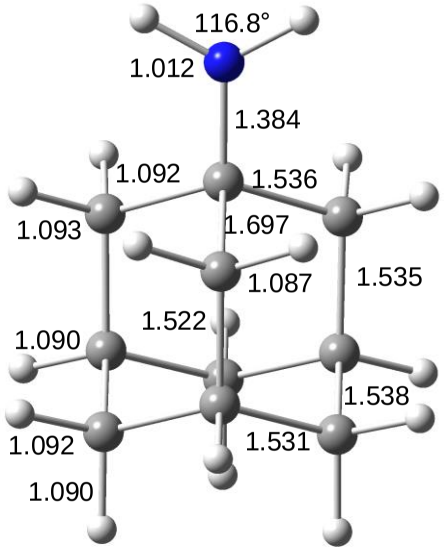
Figure S4



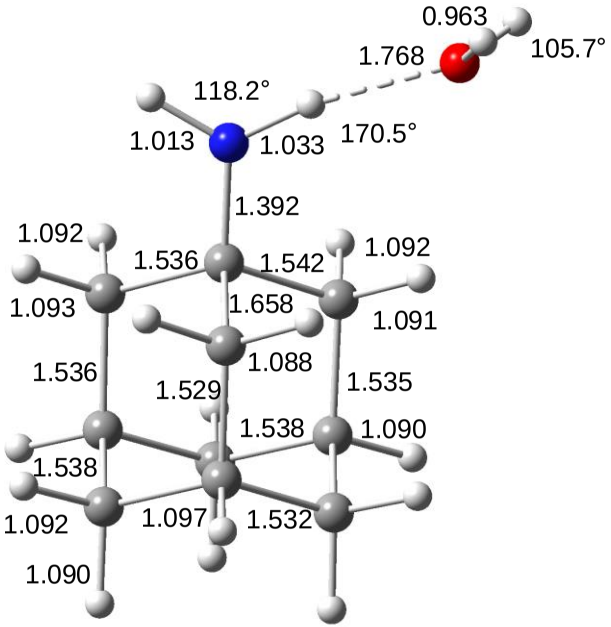
W (C_{2v})



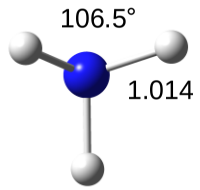
Ama (C_s)



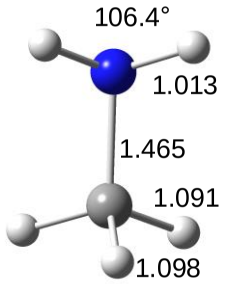
Ama$^+$ (C_s)



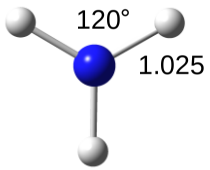
Ama$^+$W(**I**)



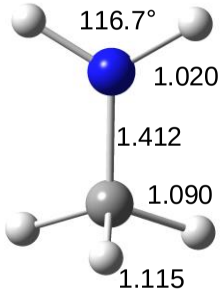
NH_3 (C_{3v})



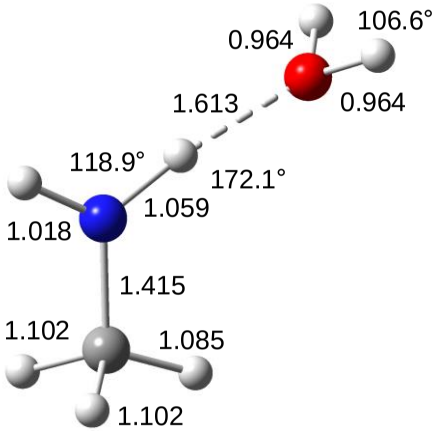
CH_3NH_2 (C_s)



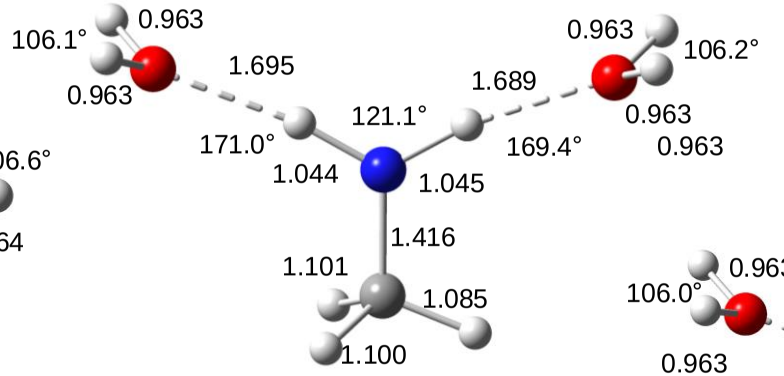
NH_3^+ (C_{3v})



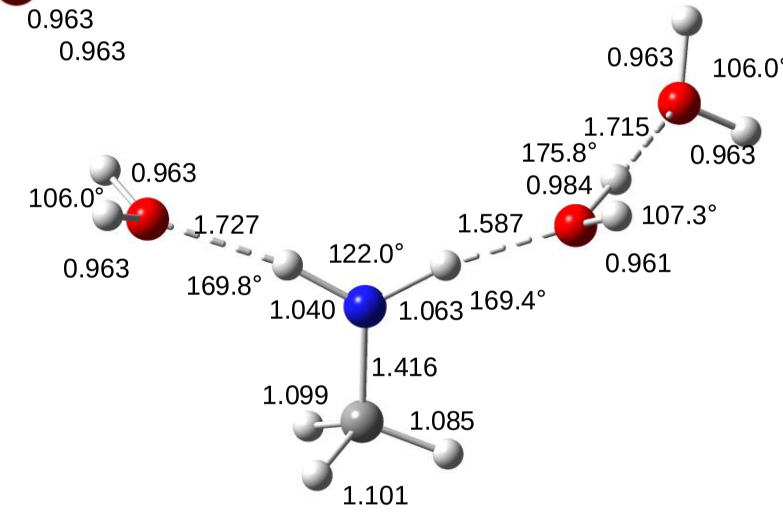
$CH_3NH_2^+$ (C_s)



$CH_3NH_2^+W$

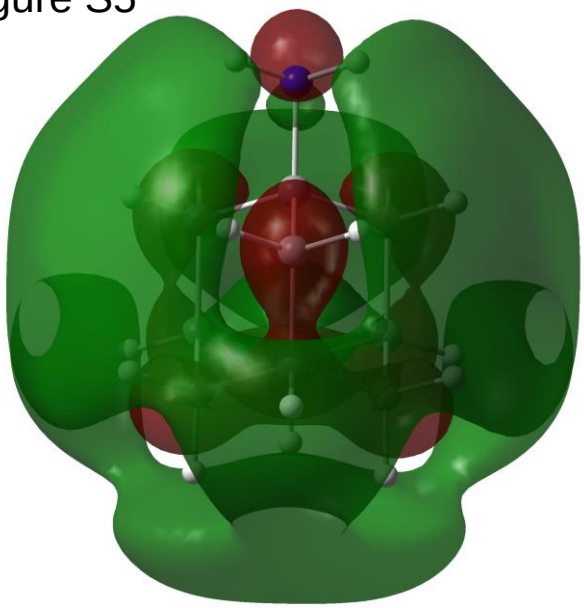


$CH_3NH_2^+W_2$

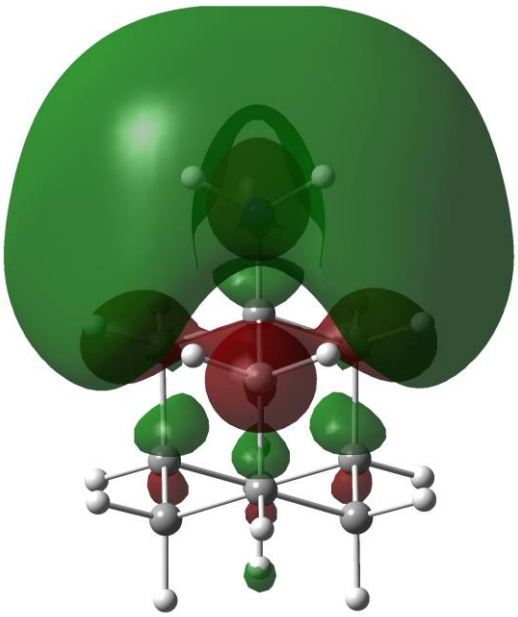


$CH_3NH_2^+W_3$

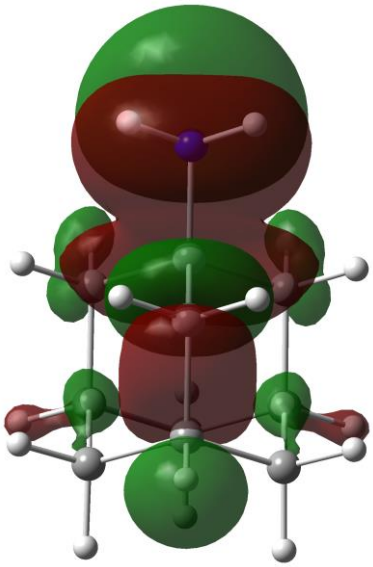
Figure S5



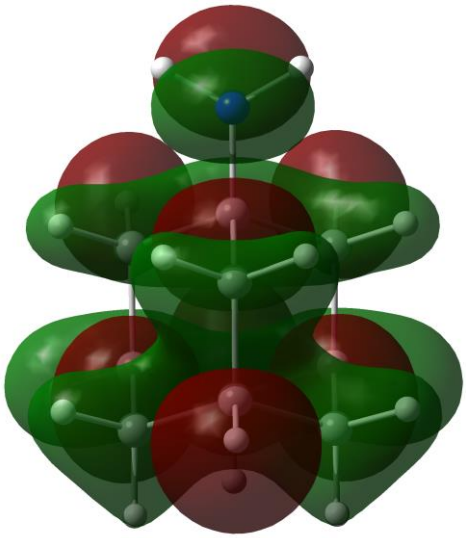
Ama LUMO



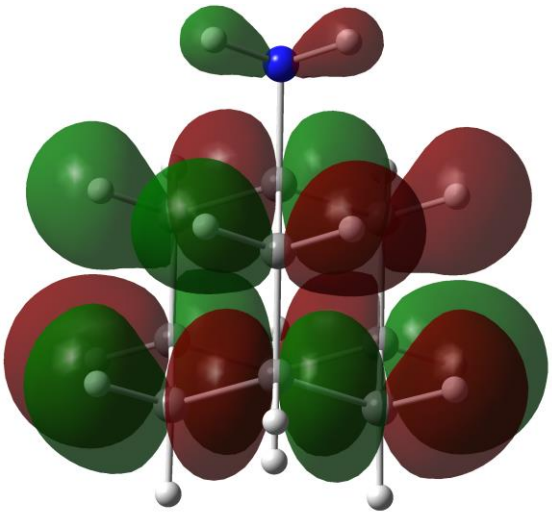
Ama^{+} LUMO



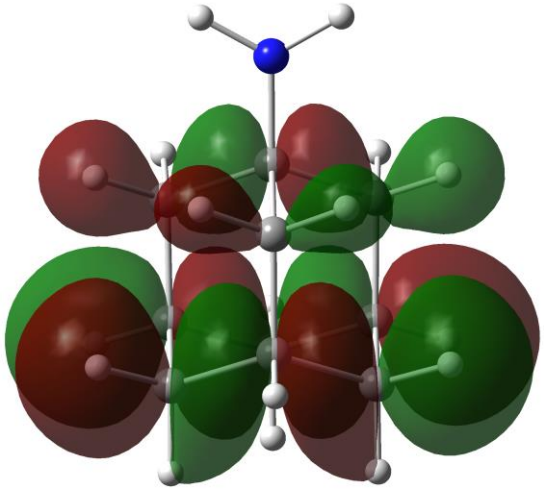
Ama HOMO



Ama^{+} HOMO

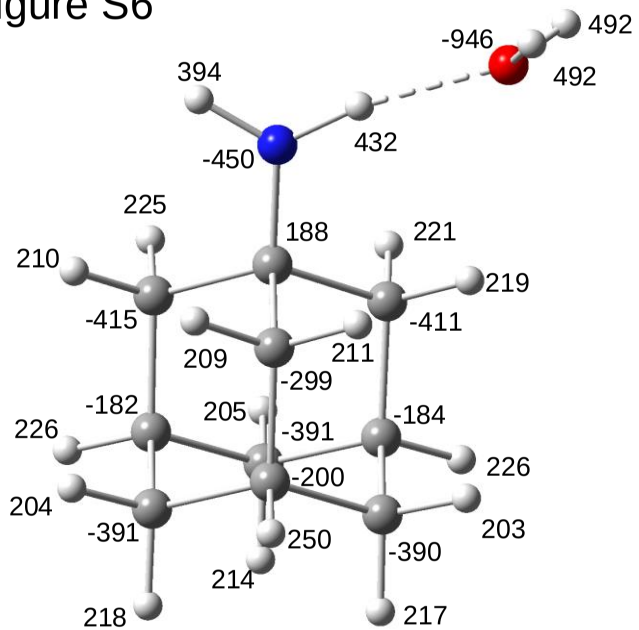


Ama HOMO

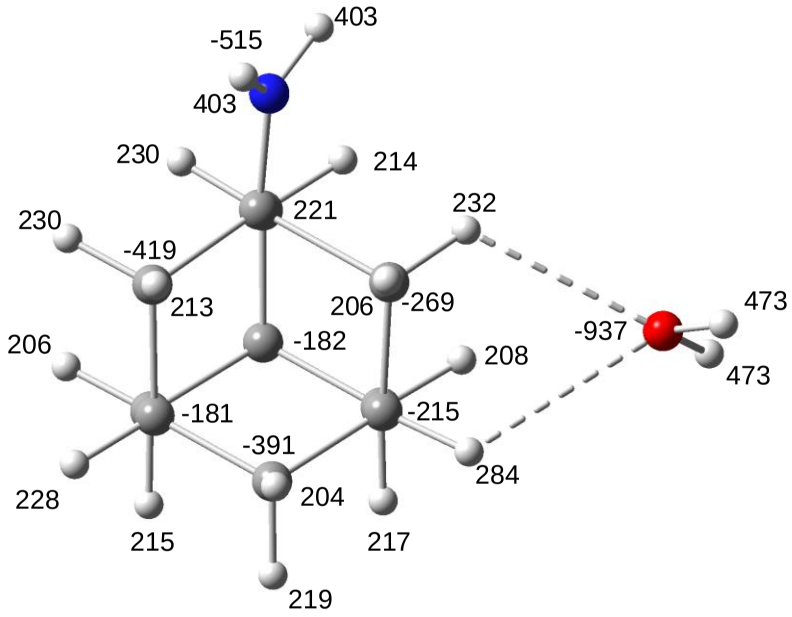


Ama^{+} HOMO-1

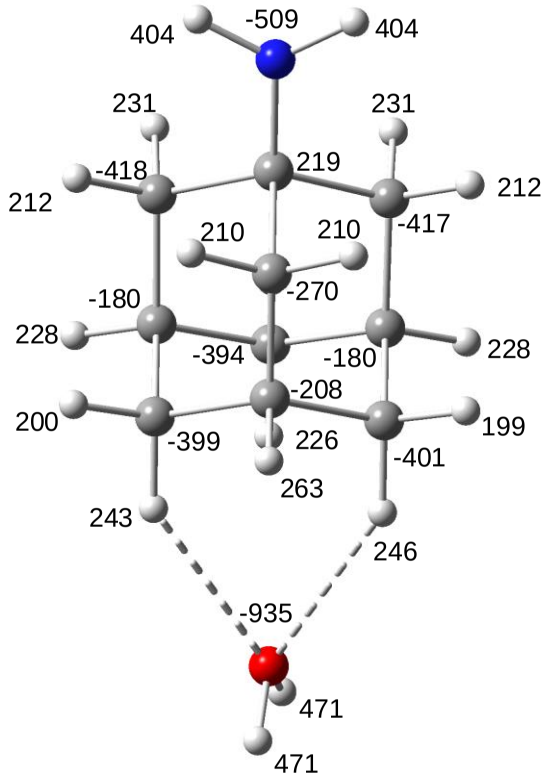
Figure S6



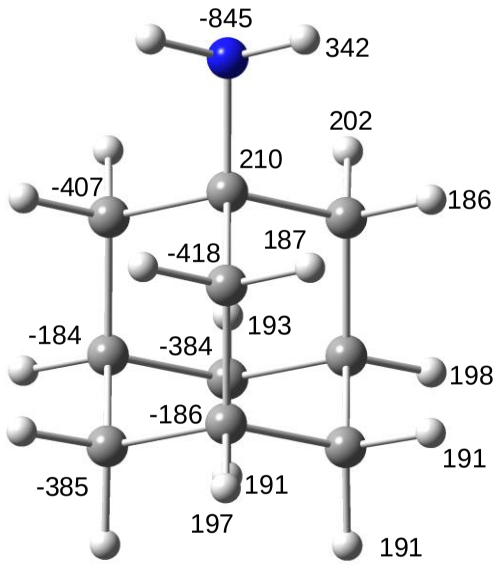
Ama^{+}W(**I**)



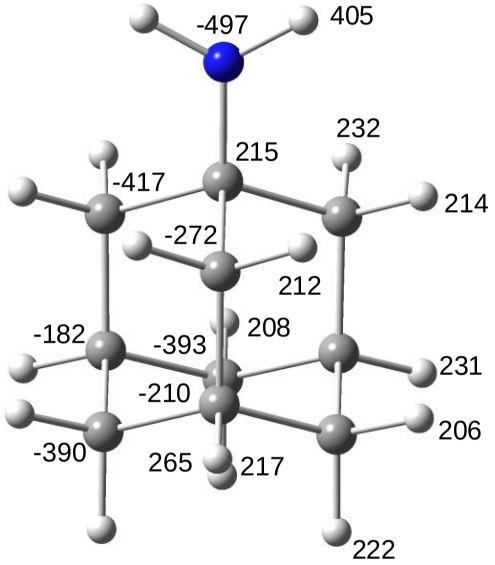
Ama^{+}W(**II**)



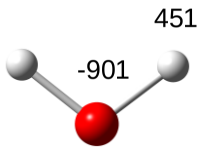
Ama^{+}W(**III**)



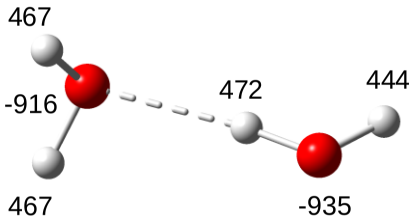
Ama (C_s)



Ama^{+} (C_s)

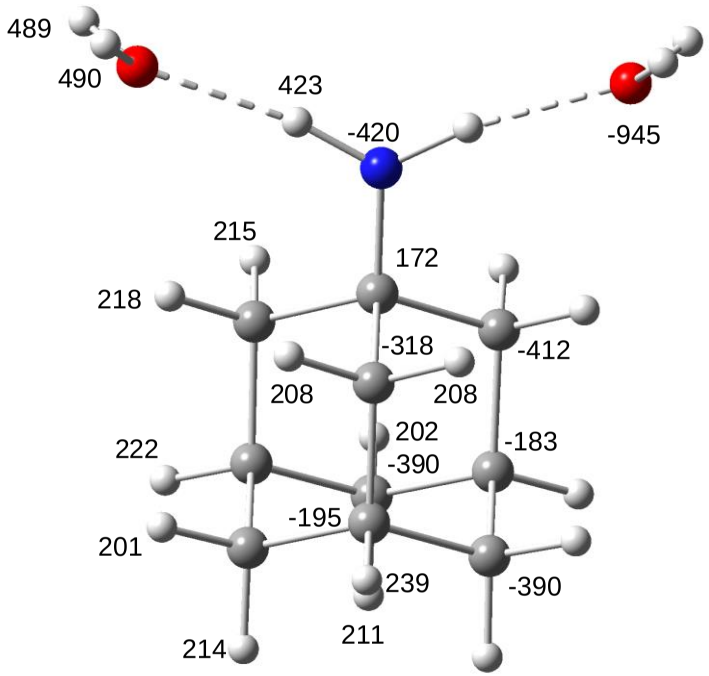


W (C_{2v})

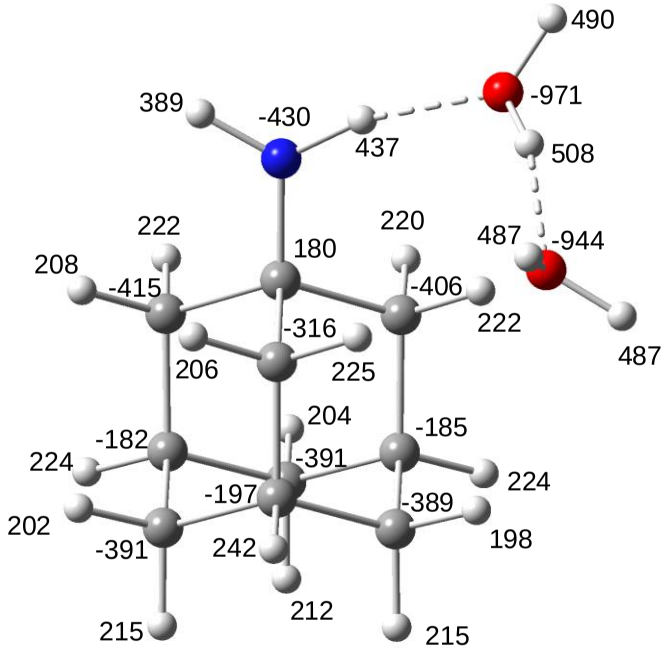


W_2 (C_s)

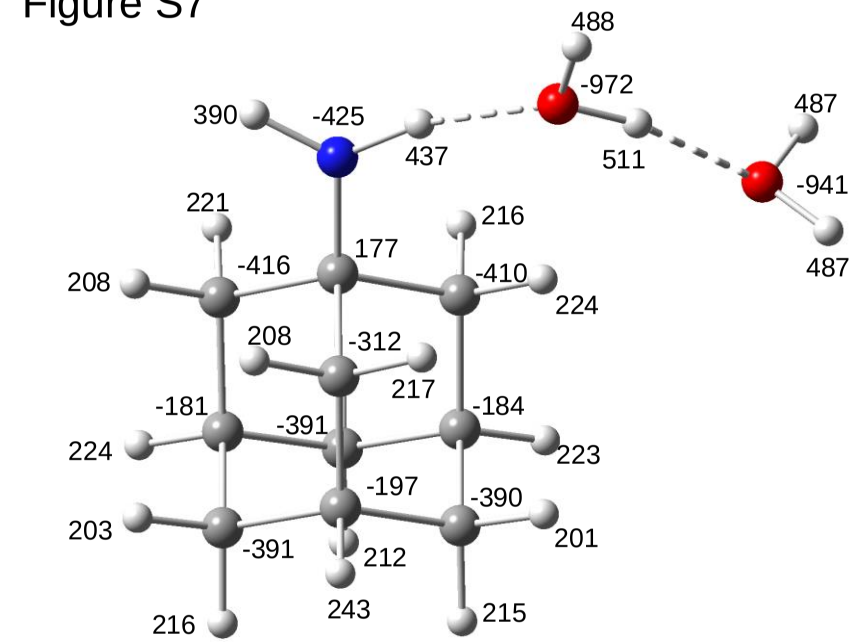
Figure S7



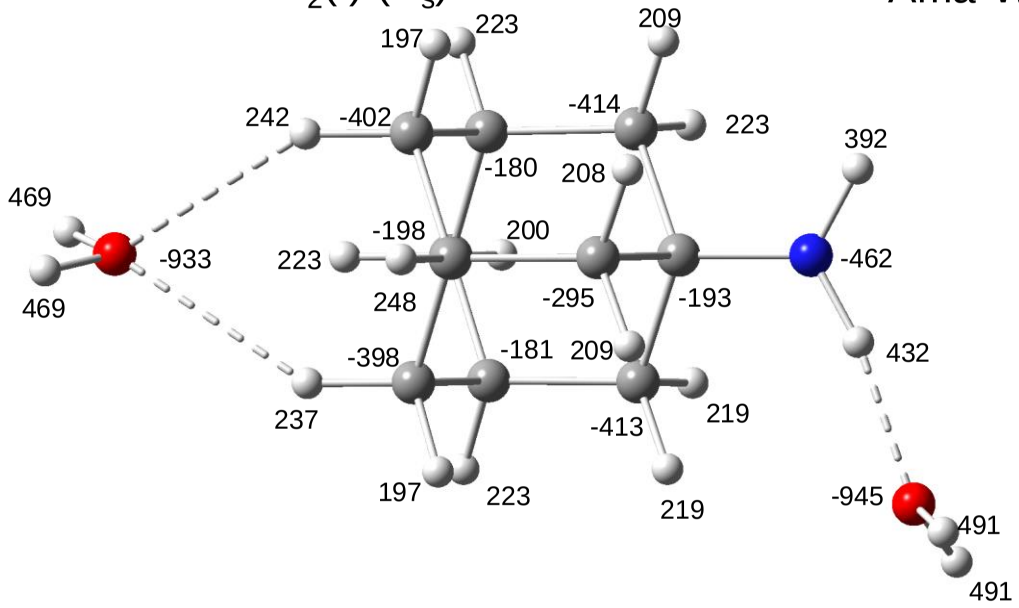
$Ama^{+}W_2$(**I**) (C_s)



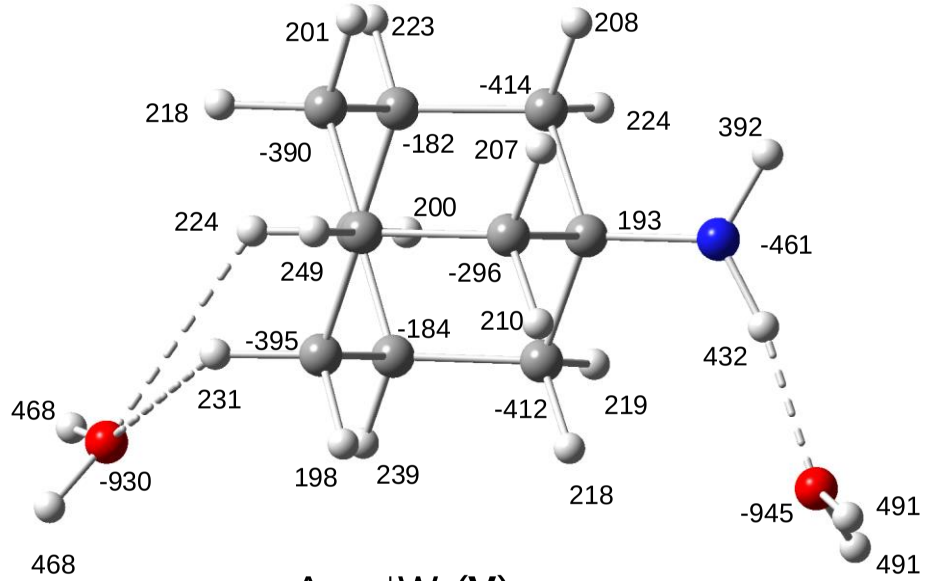
$Ama^{+}W_2$(**II**)



$Ama^{+}W_2$(**III**)

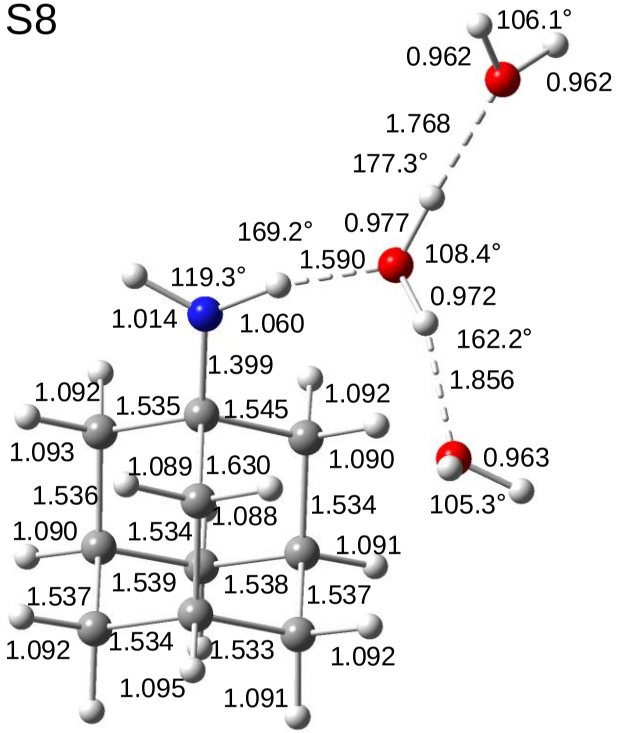


$Ama^{+}W_2$(**IV**)

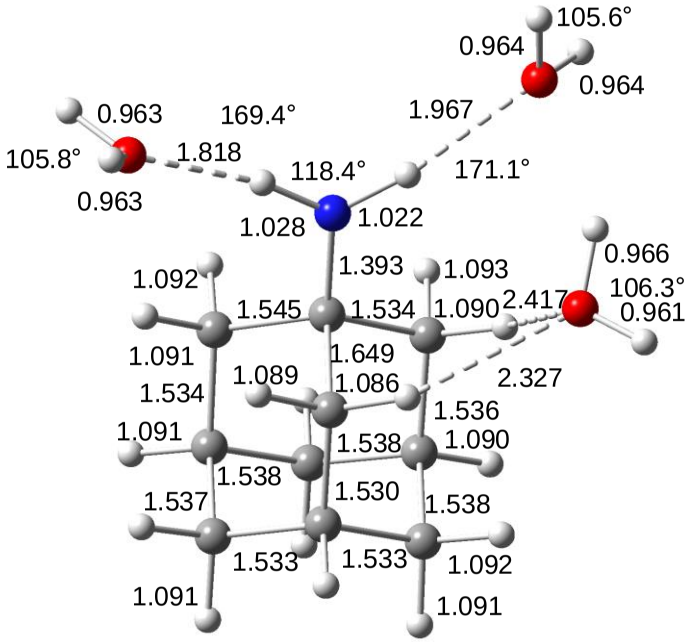


$Ama^{+}W_2$(**V**)

Figure S8



$Ama^{+}W_3$(**VII**)



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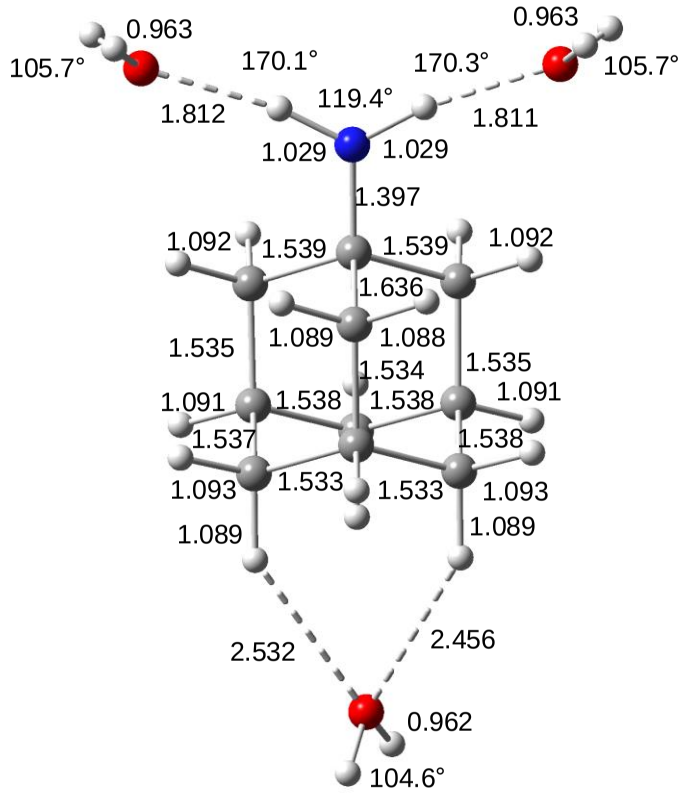
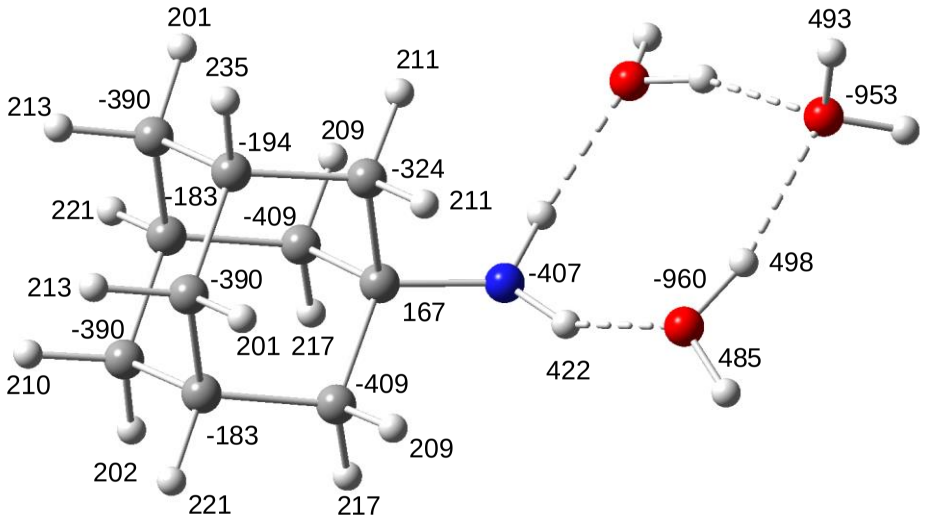
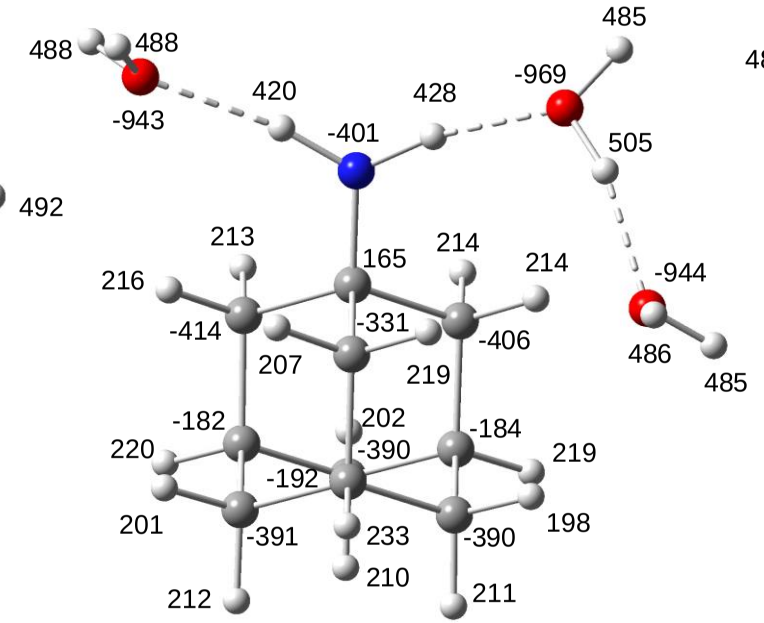


$Ama^{+}W_3$(**IX**)

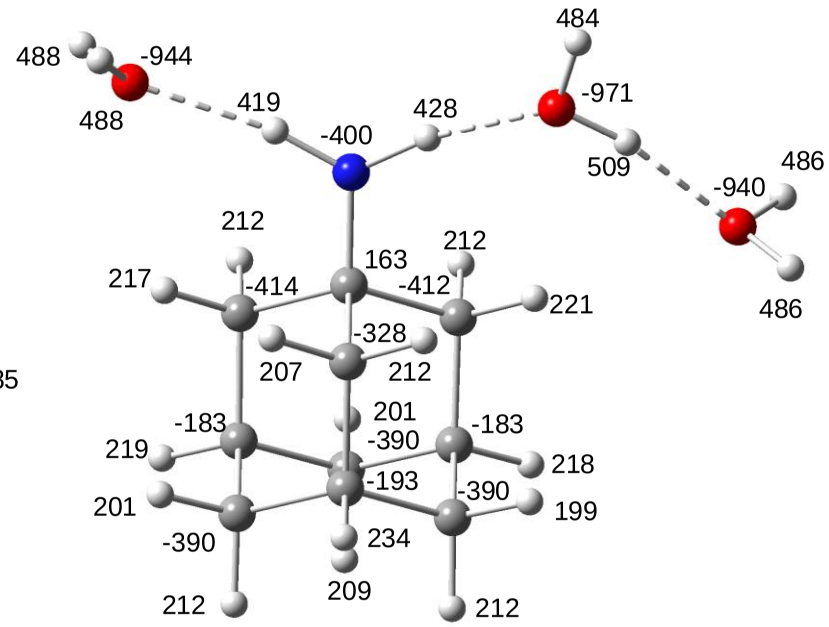
Figure S9



$Ama^{+}W_3$(**I**) (C_S)



$Ama^{+}W_3$(**II**)



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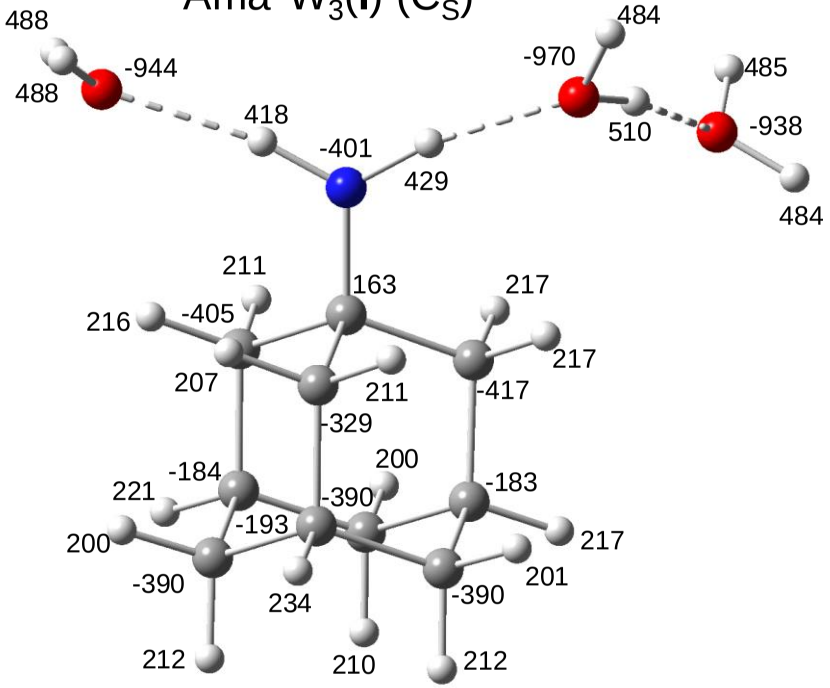
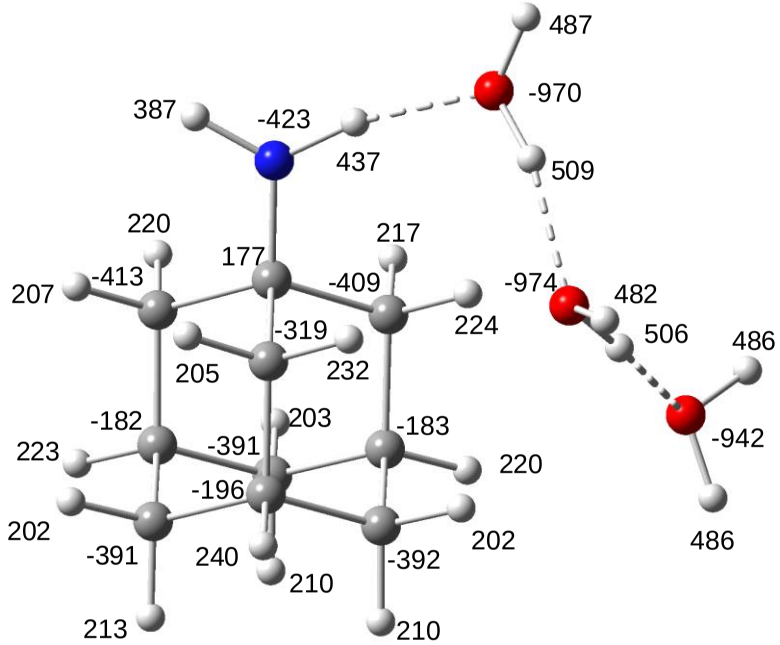


$Ama^{+}W_3$(**IV**)



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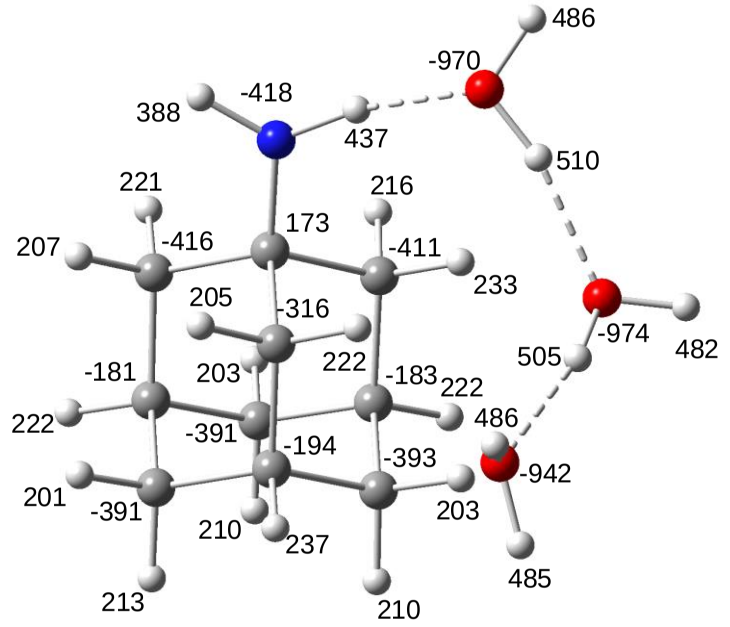
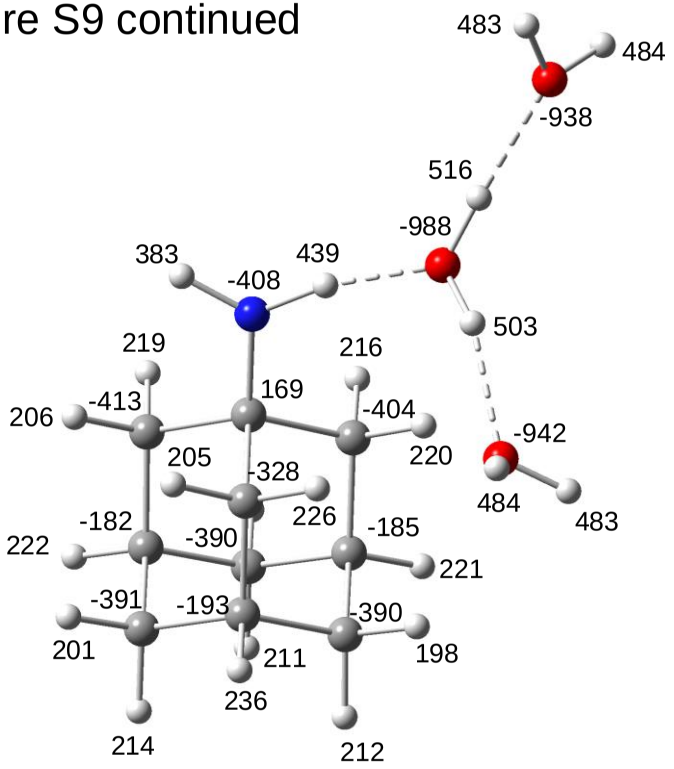
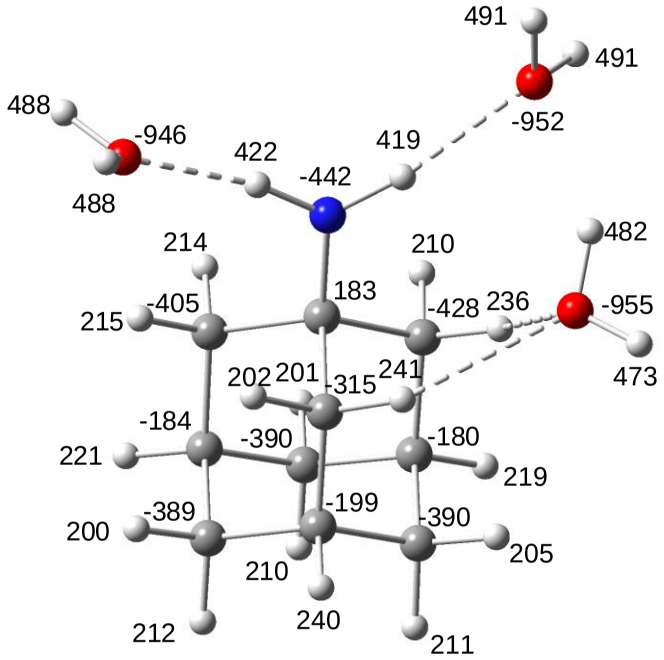


$Ama^{+}W_3$(**VI**)

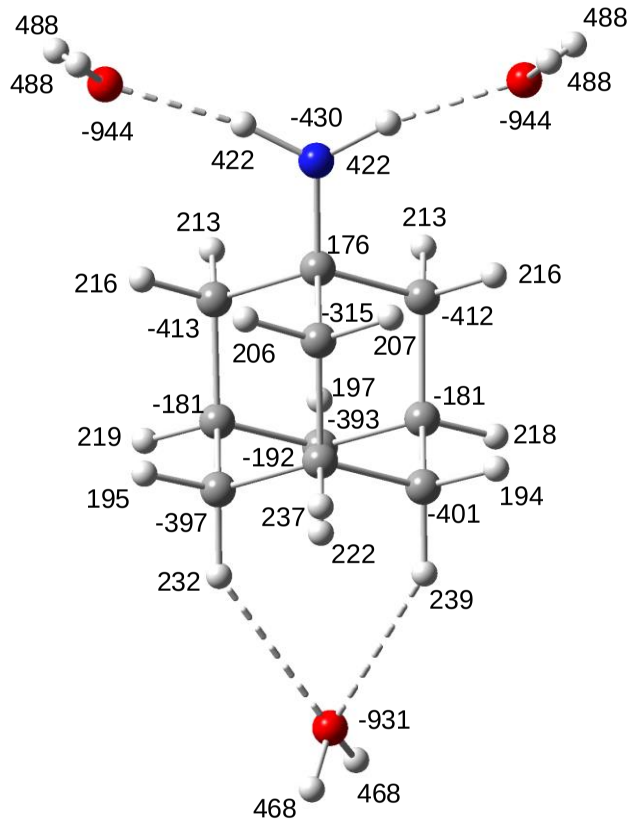
Figure S9 continued



Ama^{+}W$_3$(**VII**)



Ama^{+}W$_3$(**VIII**)



Ama^{+}W$_3$(**IX**)

Figure S10

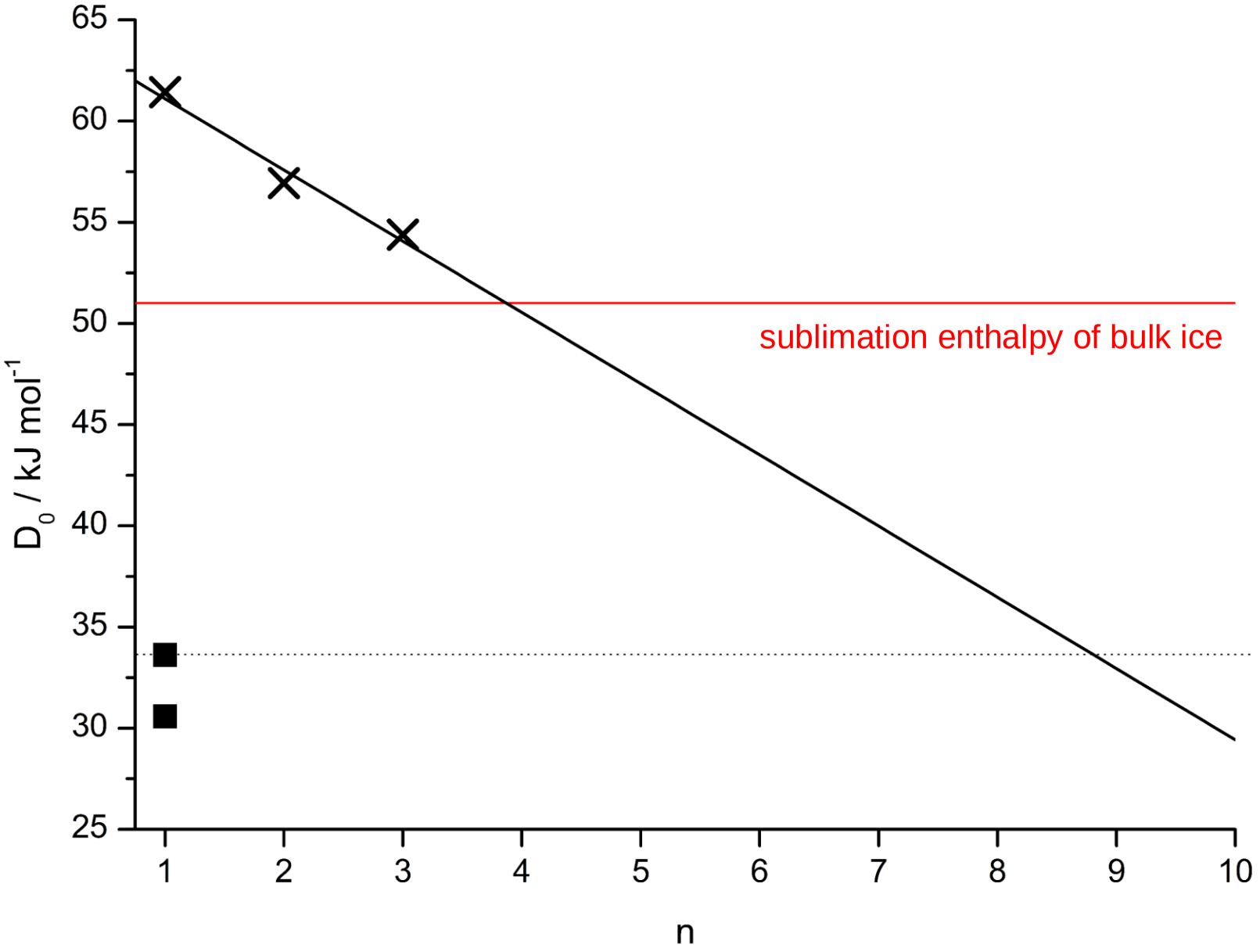

65
60
55
50
45
40
35
30
25
D_0 / kJ mol^{-1}
1
2
3
4
5
6
7
8
9
10
n
sublimation enthalpy of bulk ice

Table S1a. Various energies of the Ama^+W(**I-III**) isomers calculated at the B3LYP-D3/cc-pVTZ level. Energies are given in kJ mol^{-1}.

	E_0	E_e	G	D_0
Ama^+W(**I**)	0	0	0	61.43
Ama^+W(**II**)	27.82	30.99	25.24	33.61
Ama^+W(**III**)	30.86	34.42	26.73	30.57

Table S1b. Various energies of the Ama^+W_2(**I-V**) isomers calculated at the B3LYP-D3/cc-pVTZ level. Energies are given in kJ mol^{-1}.

	E_0	E_e	G	D_0 Ama^+W(**I**)+W	D_0 Ama^+W(**III**)+W	D_0^{total}
Ama^+W_2(**I**)	0	0	0	56.94		118.37
Ama^+W_2(**II**)	5.36	2.22	9.59	51.58		113.01
Ama^+W_2(**III**)	5.66	2.73	9.04	51.28		112.72
Ama^+W_2(**IV**)	28.57	31.01	25.85	28.37	59.23	89.80
Ama^+W_2(**V**)	31.03	33.82	27.52	25.91	56.76	87.34

Table S1c. Various energies of the Ama^+W_3(**I-IX**) isomers calculated at the B3LYP-D3/cc-pVTZ level. Energies are given in kJ mol^{-1}.

	E_0	E_e	G	D_0 Ama^+W_2(**I**)+W	D_0 Ama^+W_2(**II**)+W	D_0 Ama^+W_2(**III**)+W	D_0 Ama^+W_2(**IV**)+W	D_0^{total}
Ama^+W_3(**I**)	0	0	5.13	49.25				167.63
Ama^+W_3(**II**)	0.22	3.80	0	49.03	54.39			167.40
Ama^+W_3(**III**)	0.64	4.45	0.10	48.62		54.27		166.99
Ama^+W_3(**IV**)	1.52	5.30	0.52	47.73		53.39		166.10
Ama^+W_3(**V**)	4.30	5.19	12.0		50.31	-		163.32
Ama^+W_3(**VI**)	5.48	6.84	11.62		49.13	-		162.15
Ama^+W_3(**VII**)	9.37	13.00	9.98		45.24	45.54		158.26
Ama^+W_3(**VIII**)	14.41	19.16	13.47	34.84				153.21
Ama^+W_3(**IX**)	23.69	31.98	18.30	25.57	30.92		54.14	143.94

Table S2. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of Ama, Ama^+, W, and Ama^+W(**I-III**) compared to experimental values of Ama^+W.[a]

Mode	Ama	Ama^+	W	Ama^+W(**I**)	Ama^+W(**II**)	Ama^+W(**III**)	Ama^+W Exp.
ν_{CH}	2845 (13)	2803 (76)		2831 (59)	2811 (121)	2793 (77)	***J*** 2858 (20)
ν_{CH2}	2848 (30)	2870 (4)		2869 (11)	2869 (4)	2867 (4)	
ν_{CH2}	2853 (39)	2874 (16)		2879 (12)	2873 (17)	2872 (15)	
ν_{CH2}	2854 (29)	2882 (16)		2881 (14)	2882 (16)	2882 (21)	
ν_{CH2}	2855 (18)	2884 (20)		2882 (22)	2883 (18)	2882 (29)	
ν_{CH2}	2856 (25)	2887 (10)		2884 (14)	2891 (14)	2883 (17)	
ν_{CH2}/ν_{CH}	2875 (119)	2910 (5)		2906 (23)	2908 (4)	2907 (2)	
ν_{CH2}/ν_{CH}	2876 (105)	2911 (28)		2909 (14)	2909 (34)	2908 (37)	
ν_{CH2}/ν_{CH}	2880 (66)	2912 (1)		2911 (14)	2911 (2)	2910 (3)	
ν_{CH2}/ν_{CH}	2884 (26)	2913 (10)		2915 (7)	2911 (15)	2910 (12)	
ν_{CH2}	2888 (12)	2922 (6)		2919 (5)	2922 (10)	2921 (11)	
ν_{CH2}	2889 (33)	2922 (11)		2922 (7)	2926 (8)	2941 (8)	
ν_{CH2}	2894 (102)	2927 (4)		2923 (12)	2928 (8)	2947 (1)	
ν_{CH2}	2898 (5)	2932 (27)		2927 (36)	2931 (28)	2951 (1)	***I*** 2937 (35)
ν_{CH2}	2903 (80)	2984 (7)		2973 (7)	3001 (4)	2984 (8)	
ν_{NH}[b]				3022 (1267)			***H*** 2992 (66)
$2\beta_{CH2}$				2969[b] 2940 (12)[c]			***I*** 2937 (35)
$\beta_{NH}+\beta_{OH}$				3196[b] 3167 (136)[c]			***K*** 3187 (20)
ν_{NH}[f]				3378 (95)			***E*** 3368 (27)
ν_{NH}[s]	3285 (3)	3322 (223)			3329 (208)	3326 (227)	
ν_{NH}[a]	3358 (0.2)	3438 (67)			3445 (62)	3442 (64)	
ν_{OH}[s]			3658 (3)	3650 (51)	3653 (30)	3652 (23)	***C*** 3627 (31)
ν_{OH}[a]			3754 (40)	3736 (110)	3740 (71)	3741 (69)	***A*** 3717 (28)

[a] IR intensities in km mol^{-1} are given in parentheses. [b] Harmonic value. [c] Result of anharmonic calculation. The experimental values with width (fwhm in parenthesis) are assigned to the most dominant vibrations.

Table S3. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of Ama^+ and Ama^+W_2(**I-IV**).[a]

Mode	Ama^+	Ama^+W_2(**I**)	Ama^+W_2(**II**)	Ama^+W_2(**III**)	Ama^+W_2(**IV**)	Ama^+W_2(**V**)
ν_{CH}	2803 (76)	2849 (36)	2839 (201)	2837 (896)	2821 (57)	2824 (59)
ν_{CH2}	2870 (4)	2876 (0.4)	2868 (199)	2868 (15)	2867 (10)	2868 (12)
ν_{CH2}	2874 (16)	2876 (17)	2877 (75)	2878 (14)	2876 (8)	2876 (9)
ν_{CH2}	2882 (16)	2877 (27)	2879 (13)	2879 (33)	2878 (33)	2878 (28)
ν_{CH2}	2884 (20)	2880 (25)	2881 (16)	2882 (16)	2878 (26)	2879 (36)
ν_{CH2}	2887 (10)	2881 (9)	2887 (7)	2885 (8)	2880 (20)	2881 (11)
ν_{CH2}/ν_{CH}	2910 (5)	2904 (39)	2904 (28)	2903 (27)	2904 (31)	2906 (26)
ν_{CH2}/ν_{CH}	2911 (28)	2907 (23)	2909 (10)	2909 (12)	2907 (12)	2909 (9)
ν_{CH2}/ν_{CH}	2912 (1)	2909 (1)	2911 (16)	2911 (23)	2908 (17)	2914 (10)
ν_{CH2}/ν_{CH}	2913 (10)	2915 (3)	2912 (10)	2912 (7)	2913 (10)	2920 (14)
ν_{CH2}	2922 (6)	2917 (0.03)	2918 (7)	2917 (10)	2919 (14)	2925 (13)
ν_{CH2}	2922 (11)	2919 (12)	2919 (7)	2919 (5)	2937 (9)	2927 (10)
ν_{CH2}	2927 (4)	2921 (24)	2924 (40)	2924 (39)	2944 (1)	2937 (8)
ν_{CH2}	2932 (27)	2923 (46)	2933 (15)	2935 (8)	2948 (1)	2946 (9)
ν_{CH2}	2984 (7)	2962 (12)	2970 (4)	2967 (10)	2971 (9)	2972 (8)
ν_{NH}^{b}			2870 (1094)	2853 (711)		
$\nu_{NH}^{b}{}_{s}$		3034 (1065)				
$\nu_{NH}^{b}{}_{a}$		3139 (901)				
$\beta_{NH}+\beta_{OH}$		3131				
ν_{NH}^{f}			3374 (75)	3369 (51)		
ν_{NH}^{s}	3322 (223)				3044 (1259)	3042 (1255)
ν_{NH}^{a}	3438 (67)				3383 (93)	3383 (94)
ν_{OH}^{b}			3415 (494)	3383 (612)		
ν_{OH}^{s}		3652 (48)	3647 (33)	3651 (33)	3651 (50)	3652 (48)
ν_{OH}^{s}		3653 (41)			3654 (20)	3652 (49)
ν_{OH}^{f}			3727 (124)	3722 (111)		
ν_{OH}^{a}		3741 (5)	3735 (100)	3740 (100)	3739 (107)	3739 (107)
ν_{OH}^{a}		3741 (201)			3744 (67)	

[a] IR intensities in km mol^{-1} are given in parentheses.

Table S4. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of $Ama^{+}W_3$(**I**,**V-VII**,**IX**).[a]

Mode	$Ama^{+}W_3$(**I**)	$Ama^{+}W_3$(**V**)	$Ama^{+}W_3$(**VI**)	$Ama^{+}W_3$(**VII**)	$Ama^{+}W_3$(**IX**)
ν_{CH}	2853 (34)	2845 (10)	2849 (7)	2851 (12)	2841 (31)
ν_{CH2}	2873 (4)	2868 (13)	2868 (13)	2866 (15)	2874 (2)
ν_{CH2}	2875 (16)	2877 (19)	2877 (19)	2876 (28)	2875 (35)
ν_{CH2}	2876 (29)	2879 (21)	2878 (21)	2877 (19)	2876 (11)
ν_{CH2}	2877 (22)	2887 (15)	2885 (14)	2880 (20)	2877 (15)
ν_{CH2}	2880 (15)	2890 (12)	2888 (17)	2887 (7)	2878 (40)
ν_{CH2}/ν_{CH}	2905 (47)	2906 (41)	2903 (26)	2903 (37)	2901 (44)
ν_{CH2}/ν_{CH}	2907 (17)	2908 (4)	2908 (13)	2907 (10)	2904 (25)
ν_{CH2}/ν_{CH}	2909 (2)	2910 (16)	2911 (19)	2909 (17)	2907 (5)
ν_{CH2}/ν_{CH}	2913 (2)	2913 (12)	2915 (9)	2910 (17)	2916 (11)
ν_{CH2}	2913 (2)	2915 (21)	2917 (13)	2916 (7)	2918 (20)
ν_{CH2}	2916 (7)	2920 (20)	2918 (21)	2916 (9)	2936 (8)
ν_{CH2}	2918 (33)	2926 (29)	2924 (34)	2921 (48)	2941 (2)
ν_{CH2}	2921 (52)	2954 (11)	2947 (2)	2935 (14)	2945 (3)
ν_{CH2}	2961 (10)	2975 (2)	2985 (5)	2970 (3)	2961 (13)
$\nu_{NH}{}^{b}{}_{s}$	3020 (1420)				3051 (1071)
$\nu_{NH}{}^{b}{}_{a}$	3103 (456)				3158 (850)
$\nu_{NH}{}^{b}$		2789 (1555)	2776 (1574)	2589 (2353)	
$\nu_{NH}{}^{f}$		3369 (81)	3366 (72)	3406 (491)	
$\nu_{OH}{}^{b}$	3519 (225)	3313 (658)	3316 (688)	3365 (446)	
$\nu_{OH}{}^{b}$	3539 (527)	3415 (385)	3427 (375)	3506 (626)	
$\nu_{OH}{}^{s}$					3654 (47)
$\nu_{OH}{}^{s}$				3649 (26)	3654 (24)
$\nu_{OH}{}^{s}$	3637 (17)	3651 (32)	3649 (33)	3665 (18)	3655 (35)
$\nu_{OH}{}^{f}$	3724 (209)	3715 (96)	3717 (91)		
$\nu_{OH}{}^{f}$	3727 (35)	3727 (118)	3724 (122)		
$\nu_{OH}{}^{a}$	3720 (110)				3742 (67)
$\nu_{OH}{}^{a}$				3737 (90)	3743 (132)
$\nu_{OH}{}^{a}$		3739 (93)	3737 (93)	3757 (97)	3745 (68)

[a] IR intensities in km mol^{-1} are given in parentheses.

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

Ama

1	6	0	-1.011128	1.127081	1.255703
2	1	0	-0.514261	1.502017	2.154656
3	1	0	-2.038105	1.501352	1.276200
4	6	0	-1.011128	-0.410783	1.256075
5	1	0	-1.521728	-0.777686	2.149414
6	6	0	-0.287239	1.641427	0.000000
7	1	0	-0.281288	2.733996	0.000000
8	6	0	1.158945	1.116612	0.000000
9	1	0	1.696050	1.483603	0.880296
10	1	0	1.696050	1.483603	-0.880296
11	6	0	0.437377	-0.927013	1.249983
12	1	0	0.460778	-2.018647	1.262920
13	1	0	0.962767	-0.582715	2.146909
14	6	0	1.182128	-0.427579	0.000000
15	6	0	0.437377	-0.927013	-1.249983
16	1	0	0.962767	-0.582715	-2.146909
17	1	0	0.460778	-2.018647	-1.262920
18	6	0	-1.736812	-0.921403	0.000000
19	1	0	-2.774040	-0.575535	0.000000
20	1	0	-1.762177	-2.014271	0.000000
21	6	0	-1.011128	1.127081	-1.255703
22	1	0	-2.038105	1.501352	-1.276200
23	1	0	-0.514261	1.502017	-2.154656
24	6	0	-1.011128	-0.410783	-1.256075
25	1	0	-1.521728	-0.777686	-2.149414
26	7	0	2.535235	-0.993222	0.000000
27	1	0	3.048130	-0.666622	-0.812633
28	1	0	3.048130	-0.666622	0.812633

Sum of electronic and zero-point Energies= -445.999992
Sum of electronic and thermal Energies= -445.991746
Sum of electronic and thermal Enthalpies= -445.990802
Sum of electronic and thermal Free Energies= -446.032017

Ama^{+}

1	6	0	-1.009933	1.119927	1.260815
2	1	0	-0.519111	1.502470	2.157785
3	1	0	-2.034331	1.491912	1.270028
4	6	0	-1.009933	-0.418569	1.258258
5	1	0	-1.512657	-0.782974	2.154281
6	6	0	-0.292961	1.610622	0.000000
7	1	0	-0.245778	2.709641	0.000000
8	6	0	1.169160	1.189049	0.000000
9	1	0	1.708022	1.497285	0.892533
10	1	0	1.708022	1.497285	-0.892533
11	6	0	0.436294	-0.931980	1.280099
12	1	0	0.450942	-2.023690	1.314481
13	1	0	0.966411	-0.567549	2.163360
14	6	0	1.172297	-0.507942	0.000000
15	6	0	0.436294	-0.931980	-1.280099
16	1	0	0.966411	-0.567549	-2.163360
17	1	0	0.450942	-2.023690	-1.314481
18	6	0	-1.725250	-0.938846	0.000000
19	1	0	-2.762343	-0.601654	0.000000
20	1	0	-1.747492	-2.030538	0.000000
21	6	0	-1.009933	1.119927	-1.260815
22	1	0	-2.034331	1.491912	-1.270028
23	1	0	-0.519111	1.502470	-2.157785
24	6	0	-1.009933	-0.418569	-1.258258
25	1	0	-1.512657	-0.782974	-2.154281
26	7	0	2.515855	-0.841720	0.000000
27	1	0	3.044730	-0.885075	-0.862169
28	1	0	3.044730	-0.885075	0.862169

Sum of electronic and zero-point Energies= -445.710234
Sum of electronic and thermal Energies= -445.701526
Sum of electronic and thermal Enthalpies= -445.700582
Sum of electronic and thermal Free Energies= -445.743151

Ama^{+}W(I)

1	6	0	-1.084402	1.829616	0.167208
2	1	0	-0.319788	2.606027	0.095819
3	1	0	-2.044656	2.333685	0.279417
4	6	0	-0.820950	0.921985	1.380298
5	1	0	-0.801583	1.524859	2.288755
6	6	0	-1.098174	0.969634	-1.100562
7	1	0	-1.248026	1.603566	-1.983264
8	6	0	0.265054	0.313728	-1.325084
9	1	0	1.076808	1.036416	-1.365971
10	1	0	0.283894	-0.314296	-2.213290
11	6	0	0.547871	0.245821	1.224827
12	1	0	0.761790	-0.383329	2.091271
13	1	0	1.347588	0.984084	1.144684
14	6	0	0.543823	-0.667013	-0.017588
15	6	0	-0.589328	-1.702432	0.025454
16	1	0	-0.582106	-2.309660	-0.883519
17	1	0	-0.402156	-2.369660	0.869507
18	6	0	-1.921201	-0.148252	1.479174
19	1	0	-2.890794	0.330974	1.620428
20	1	0	-1.752507	-0.785248	2.350078
21	6	0	-2.202529	-0.089621	-1.021476
22	1	0	-3.172436	0.398264	-0.920930
23	1	0	-2.234453	-0.681009	-1.938977
24	6	0	-1.941526	-0.994406	0.194833
25	1	0	-2.720972	-1.753703	0.259666
26	7	0	1.792892	-1.222101	-0.278827
27	1	0	1.864097	-2.078759	-0.815465
28	1	0	2.658306	-0.689408	-0.094089
29	8	0	3.965469	0.455950	0.228956
30	1	0	4.444873	0.489853	1.063842
31	1	0	4.569170	0.808964	-0.433449

Sum of electronic and zero-point Energies= -522.172208
Sum of electronic and thermal Energies= -522.160107
Sum of electronic and thermal Enthalpies= -522.159163
Sum of electronic and thermal Free Energies= -522.210491

Ama^{+}W(II)

1	6	0	-0.457668	-1.200388	0.997134
2	1	0	-1.377742	-0.915740	1.509328
3	1	0	-0.365422	-2.284424	1.068091
4	6	0	0.760796	-0.525772	1.650253
5	1	0	0.818057	-0.814129	2.700216
6	6	0	-0.519861	-0.780180	-0.472680
7	1	0	-1.424075	-1.203819	-0.932889
8	6	0	-0.756164	0.714730	-0.604509
9	1	0	-1.639142	1.049873	-0.069742
10	1	0	-0.773853	1.059410	-1.635620
11	6	0	0.597738	0.997358	1.580507
12	1	0	1.437531	1.492019	2.074240
13	1	0	-0.316259	1.315760	2.087371
14	6	0	0.589613	1.468463	0.119316
15	6	0	1.814977	0.989172	-0.669508
16	1	0	1.743015	1.304119	-1.713484
17	1	0	2.690764	1.480781	-0.239250
18	6	0	2.045744	-0.944384	0.915443
19	1	0	2.178775	-2.024124	0.991870
20	1	0	2.917739	-0.483502	1.384290
21	6	0	0.741012	-1.213973	-1.220881
22	1	0	0.849150	-2.297549	-1.169511
23	1	0	0.675449	-0.946294	-2.277446
24	6	0	1.957411	-0.534823	-0.565048
25	1	0	2.866168	-0.829151	-1.090330
26	7	0	0.330613	2.819501	-0.025113
27	1	0	0.562237	3.305557	-0.881602
28	1	0	-0.271983	3.305832	0.625927
29	8	0	-3.649475	-0.339606	-0.042481
30	1	0	-4.333888	-0.131885	-0.686910
31	1	0	-4.101464	-0.862803	0.627342

Sum of electronic and zero-point Energies= -522.161613
Sum of electronic and thermal Energies= -522.148850
Sum of electronic and thermal Enthalpies= -522.147906
Sum of electronic and thermal Free Energies= -522.200876

Ama^{+}W(III)

1	6	0	-0.522335	1.339019	0.724027
2	1	0	-0.178453	2.293404	1.128804
3	1	0	-1.610906	1.342228	0.730854
4	6	0	-0.003432	0.170683	1.581608
5	1	0	-0.348318	0.296106	2.608320
6	6	0	-0.018756	1.146983	-0.708720
7	1	0	-0.340334	1.993863	-1.334363
8	6	0	1.499304	1.216772	-0.776555
9	1	0	1.912209	2.123532	-0.341477
10	1	0	1.897156	1.058761	-1.776016
11	6	0	1.530399	0.175213	1.588789
12	1	0	1.910079	-0.629443	2.222875
13	1	0	1.917099	1.117054	1.986069
14	6	0	2.072207	-0.071868	0.173455
15	6	0	1.509956	-1.349550	-0.465449
16	1	0	1.881692	-1.460565	-1.487090
17	1	0	1.889509	-2.193688	0.115272
18	6	0	-0.516656	-1.161540	1.008904
19	1	0	-1.605458	-1.167372	1.021655
20	1	0	-0.175750	-1.996102	1.625660
21	6	0	-0.542636	-0.164342	-1.300267
22	1	0	-1.631025	-0.161401	-1.288036
23	1	0	-0.215544	-0.278437	-2.335994
24	6	0	-0.023128	-1.329001	-0.438150
25	1	0	-0.383598	-2.271673	-0.850668
26	7	0	3.449326	0.032339	0.082439
27	1	0	3.953465	-0.370695	-0.696951
28	1	0	3.966818	0.658329	0.686053
29	8	0	-3.665791	0.206845	0.075157
30	1	0	-4.251475	0.753153	-0.458977
31	1	0	-4.257762	-0.297605	0.642463

Sum of electronic and zero-point Energies= -522.160455
Sum of electronic and thermal Energies= -522.147526
Sum of electronic and thermal Enthalpies= -522.146582
Sum of electronic and thermal Free Energies= -522.200310

Ama^{+}W$_2$(I)

1	6	0	-1.121688	-1.839357	1.258909
2	1	0	-1.545081	-1.383408	2.156542
3	1	0	-1.404120	-2.892761	1.270396
4	6	0	0.409685	-1.704195	1.258200
5	1	0	0.818813	-2.174931	2.152699
6	6	0	-1.683949	-1.168486	0.000000
7	1	0	-2.777636	-1.227524	0.000000
8	6	0	-1.357982	0.328949	0.000000
9	1	0	-1.737031	0.830656	0.888436
10	1	0	-1.737031	0.830656	-0.888436
11	6	0	0.792139	-0.217285	1.275577
12	1	0	1.878353	-0.106309	1.296647
13	1	0	0.391297	0.282708	2.159073
14	6	0	0.270618	0.469928	0.000000
15	6	0	0.792139	-0.217285	-1.275577
16	1	0	0.391297	0.282708	-2.159073
17	1	0	1.878353	-0.106309	-1.296647
18	6	0	0.989971	-2.372427	0.000000
19	1	0	0.746622	-3.435857	0.000000
20	1	0	2.079645	-2.295552	0.000000
21	6	0	-1.121688	-1.839357	-1.258909
22	1	0	-1.404120	-2.892761	-1.270396
23	1	0	-1.545081	-1.383408	-2.156542
24	6	0	0.409685	-1.704195	-1.258200
25	1	0	0.818813	-2.174931	-2.152699
26	7	0	0.492303	1.849845	0.000000
27	1	0	0.494289	2.367905	-0.890186

28	1	0	0.494289	2.367905	0.890186
29	8	0	0.409685	3.015805	2.569500
30	1	0	1.178092	3.099496	3.143932
31	1	0	-0.236244	3.646347	2.904614
32	8	0	0.409685	3.015805	-2.569500
33	1	0	1.178092	3.099496	-3.143932
34	1	0	-0.236244	3.646347	-2.904614

Sum of electronic and zero-point Energies= -598.632469
Sum of electronic and thermal Energies= -598.616644
Sum of electronic and thermal Enthalpies= -598.615700
Sum of electronic and thermal Free Energies= -598.676630

$Ama^{+}W_2$(II)

1	6	0	-1.251114	1.469229	0.672748
2	1	0	-0.436895	2.178800	0.836460
3	1	0	-2.182959	1.991395	0.892668
4	6	0	-1.096739	0.250720	1.597873
5	1	0	-1.084011	0.580684	2.637333
6	6	0	-1.257590	0.989795	-0.782786
7	1	0	-1.332493	1.848327	-1.460129
8	6	0	0.076207	0.324882	-1.134218
9	1	0	0.926121	0.980880	-0.957535
10	1	0	0.096441	-0.035037	-2.161315
11	6	0	0.233361	-0.452763	1.302130
12	1	0	0.366329	-1.310034	1.964803
13	1	0	1.083081	0.212717	1.455686
14	6	0	0.231601	-0.984210	-0.147684
15	6	0	-0.958080	-1.915166	-0.416407
16	1	0	-0.947057	-2.251633	-1.456623
17	1	0	-0.849549	-2.798121	0.216891
18	6	0	-2.262815	-0.725872	1.370214
19	1	0	-3.208198	-0.237060	1.609686
20	1	0	-2.170918	-1.585378	2.037577
21	6	0	-2.425634	0.027269	-1.025043
22	1	0	-3.368995	0.535475	-0.822086
23	1	0	-2.450343	-0.289304	-2.070100
24	6	0	-2.273863	-1.189693	-0.096612
25	1	0	-3.098694	-1.882741	-0.262950
26	7	0	1.461479	-1.532869	-0.509089
27	1	0	1.505673	-2.229324	-1.244215
28	1	0	2.347217	-1.093616	-0.178355
29	8	0	3.546981	-0.068106	0.411587
30	1	0	3.533718	0.856463	0.096932
31	1	0	4.428345	-0.255769	0.745063
32	8	0	3.006212	2.450284	-0.549505
33	1	0	2.975277	3.195179	0.060712
34	1	0	3.410613	2.793369	-1.353889

Sum of electronic and zero-point Energies= -598.630431
Sum of electronic and thermal Energies= -598.615516
Sum of electronic and thermal Enthalpies= -598.614572
Sum of electronic and thermal Free Energies= -598.672609

$Ama^{+}W_2$(III)

1	6	0	-1.249516	1.584924	-0.385055
2	1	0	-0.451121	2.208408	-0.793374
3	1	0	-2.170125	2.167482	-0.433272
4	6	0	-0.942271	1.204670	1.072773
5	1	0	-0.819329	2.109989	1.668570
6	6	0	-1.404747	0.303057	-1.210828
7	1	0	-1.590673	0.553815	-2.261260
8	6	0	-0.097554	-0.494518	-1.216959
9	1	0	0.748044	0.084092	-1.582445
10	1	0	-0.183356	-1.414725	-1.791969
11	6	0	0.371630	0.413574	1.129285
12	1	0	0.614081	0.150369	2.160742
13	1	0	1.199898	1.003911	0.736562
14	6	0	0.218767	-0.906264	0.340326
15	6	0	-0.955092	-1.747777	0.854770
16	1	0	-1.052288	-2.660555	0.260936
17	1	0	-0.739848	-2.044738	1.883405

18	6	0	-2.088372	0.351281	1.640525
19	1	0	-3.017703	0.922501	1.628033
20	1	0	-1.887914	0.093010	2.682646
21	6	0	-2.554696	-0.550172	-0.662430
22	1	0	-3.487443	0.012423	-0.716790
23	1	0	-2.687127	-1.448652	-1.269132
24	6	0	-2.251998	-0.925745	0.797654
25	1	0	-3.064177	-1.534016	1.195816
26	7	0	1.419440	-1.613029	0.258936
27	1	0	1.402924	-2.620004	0.142212
28	1	0	2.315582	-1.104014	0.093497
29	8	0	3.542105	-0.052405	-0.362294
30	1	0	3.630160	0.824968	0.062268
31	1	0	4.396375	-0.275557	-0.741805
32	8	0	3.424753	2.393483	0.861182
33	1	0	3.552872	3.206560	0.361101
34	1	0	3.812764	2.556616	1.727426

Sum of electronic and zero-point Energies= -598.630317
Sum of electronic and thermal Energies= -598.615371
Sum of electronic and thermal Enthalpies= -598.614426
Sum of electronic and thermal Free Energies= -598.672817

$Ama^{+}W_2$(IV)

1	6	0	-1.282711	1.441432	0.002803
2	1	0	-0.637831	2.293912	-0.222573
3	1	0	-2.302572	1.808319	0.105946
4	6	0	-0.843582	0.766589	1.313267
5	1	0	-0.876767	1.494456	2.124710
6	6	0	-1.220741	0.406398	-1.125214
7	1	0	-1.490431	0.875991	-2.080271
8	6	0	0.212556	-0.082623	-1.336995
9	1	0	0.911724	0.729324	-1.524011
10	1	0	0.288702	-0.827894	-2.125983
11	6	0	0.599632	0.265118	1.177336
12	1	0	0.932681	-0.194535	2.110648
13	1	0	1.284352	1.083752	0.948795
14	6	0	0.679287	-0.813149	0.080723
15	6	0	-0.294852	-1.973578	0.332962
16	1	0	-0.234793	-2.700958	-0.481103
17	1	0	0.018665	-2.477227	1.250006
18	6	0	-1.779290	-0.412845	1.626280
19	1	0	-2.798454	-0.045495	1.739309
20	1	0	-1.492798	-0.884617	2.569102
21	6	0	-2.162488	-0.766128	-0.834593
22	1	0	-3.182270	-0.397429	-0.736923
23	1	0	-2.141841	-1.486428	-1.655879
24	6	0	-1.725887	-1.437013	0.479091
25	1	0	-2.386504	-2.276946	0.695791
26	7	0	1.982595	-1.226608	-0.173589
27	1	0	2.152016	-2.125693	-0.608200
28	1	0	2.771657	-0.567371	-0.093695
29	8	0	3.928059	0.773358	0.078837
30	1	0	4.410257	0.948121	0.894155
31	1	0	4.464779	1.147594	-0.627802
32	8	0	-4.707120	1.172976	0.358049
33	1	0	-5.362467	0.929651	1.019658
34	1	0	-5.174844	1.765427	-0.239183

Sum of electronic and zero-point Energies= -598.621590
Sum of electronic and thermal Energies= -598.605209
Sum of electronic and thermal Enthalpies= -598.604265
Sum of electronic and thermal Free Energies= -598.666415

$Ama^{+}W_2$(V)

1	6	0	-1.376163	1.147272	-0.717102
2	1	0	-0.744896	1.877628	-1.228622
3	1	0	-2.410481	1.463159	-0.841040
4	6	0	-1.039829	1.101268	0.782091
5	1	0	-1.192584	2.091123	1.208832
6	6	0	-1.173291	-0.247677	-1.313292
7	1	0	-1.368580	-0.228533	-2.393309

8	6	0	0.288476	-0.680434	-1.199658
9	1	0	0.973716	0.030008	-1.656533
10	1	0	0.464455	-1.676041	-1.601709
11	6	0	0.425323	0.690529	0.968584
12	1	0	0.684928	0.675232	2.029522
13	1	0	1.101293	1.389256	0.472603
14	6	0	0.645592	-0.734440	0.422693
15	6	0	-0.307683	-1.756434	1.059001
16	1	0	-0.146402	-2.746305	0.623479
17	1	0	-0.066110	-1.820932	2.122107
18	6	0	-1.958443	0.088634	1.484022
19	1	0	-2.993231	0.408145	1.368515
20	1	0	-1.744059	0.061818	2.555111
21	6	0	-2.094722	-1.264572	-0.631876
22	1	0	-3.134371	-0.968878	-0.774361
23	1	0	-1.975794	-2.253508	-1.080242
24	6	0	-1.763858	-1.307393	0.869622
25	1	0	-2.412231	-2.030659	1.364999
26	7	0	1.980113	-1.123094	0.459012
27	1	0	2.221680	-2.106771	0.457486
28	1	0	2.735822	-0.434758	0.321167
29	8	0	3.833527	0.932304	0.029272
30	1	0	4.436339	1.022860	-0.716272
31	1	0	4.213986	1.460450	0.739216
32	8	0	-3.692907	2.868657	0.848586
33	1	0	-3.923175	3.620606	0.293969
34	1	0	-4.289276	2.932954	1.601058

Sum of electronic and zero-point Energies= -598.620651
Sum of electronic and thermal Energies= -598.604189
Sum of electronic and thermal Enthalpies= -598.603245
Sum of electronic and thermal Free Energies= -598.665781

$Ama^{+}W_3$(I)

1	6	0	1.127917	2.292057	1.258594
2	1	0	1.486298	1.783344	2.156358
3	1	0	1.546548	3.299203	1.271851
4	6	0	-0.407939	2.359692	1.258412
5	1	0	-0.752520	2.880265	2.152348
6	6	0	1.599450	1.553033	0.000000
7	1	0	2.691129	1.470528	0.000000
8	6	0	1.076699	0.109918	0.000000
9	1	0	1.385707	-0.439413	0.887561
10	1	0	1.385707	-0.439413	-0.887561
11	6	0	-0.980612	0.934299	1.273492
12	1	0	-2.071592	0.962420	1.299694
13	1	0	-0.641617	0.389150	2.157411
14	6	0	-0.548784	0.188961	0.000000
15	6	0	-0.980612	0.934299	-1.273492
16	1	0	-0.641617	0.389150	-2.157411
17	1	0	-2.071592	0.962420	-1.299694
18	6	0	-0.896151	3.097460	0.000000
19	1	0	-0.515331	4.120069	0.000000
20	1	0	-1.986369	3.164712	0.000000
21	6	0	1.127917	2.292057	-1.258594
22	1	0	1.546548	3.299203	-1.271851
23	1	0	1.486298	1.783344	-2.156358
24	6	0	-0.407939	2.359692	-1.258412
25	1	0	-0.752520	2.880265	-2.152348
26	7	0	-0.934532	-1.155566	0.000000
27	1	0	-0.889697	-1.711021	-0.868808
28	1	0	-0.889697	-1.711021	0.868808
29	8	0	-0.216949	-2.957594	1.957874
30	1	0	-0.480164	-3.254414	2.833501
31	1	0	0.073558	-3.742017	1.465474
32	8	0	-0.216949	-2.957594	-1.957874
33	1	0	-0.480164	-3.254414	-2.833501
34	1	0	0.073558	-3.742017	-1.465474
35	8	0	0.577432	-4.934184	0.000000
36	1	0	0.114740	-5.780462	0.000000
37	1	0	1.516549	-5.154752	0.000000

Sum of electronic and zero-point Energies= -675.089807
Sum of electronic and thermal Energies= -675.071962
Sum of electronic and thermal Enthalpies= -675.071018
Sum of electronic and thermal Free Energies= -675.136539

Ama^{+}W$_3$(II)

1	6	0	1.261857	-1.751572	0.192476
2	1	0	0.304072	-2.272021	0.123900
3	1	0	2.044699	-2.511048	0.207697
4	6	0	1.322974	-0.907074	1.475479
5	1	0	1.185861	-1.550129	2.345775
6	6	0	1.452619	-0.835329	-1.022776
7	1	0	1.384056	-1.418681	-1.946394
8	6	0	0.313768	0.191240	-1.092413
9	1	0	-0.660211	-0.292557	-1.129481
10	1	0	0.422738	0.860071	-1.944616
11	6	0	0.193405	0.133376	1.457923
12	1	0	0.211605	0.731441	2.370969
13	1	0	-0.784073	-0.345981	1.397616
14	6	0	0.385184	1.085744	0.260670
15	6	0	1.756551	1.778210	0.302136
16	1	0	1.867955	2.435563	-0.562205
17	1	0	1.799304	2.399478	1.199292
18	6	0	2.681256	-0.190562	1.562074
19	1	0	3.486325	-0.925989	1.604218
20	1	0	2.739987	0.397836	2.480552
21	6	0	2.809422	-0.125071	-0.948570
22	1	0	3.612103	-0.863900	-0.946881
23	1	0	2.957324	0.507227	-1.826986
24	6	0	2.869050	0.717900	0.334992
25	1	0	3.830984	1.227886	0.394381
26	7	0	-0.680476	1.984865	0.119476
27	1	0	-0.536367	2.870965	-0.385120
28	1	0	-1.644762	1.656834	0.319602
29	8	0	-3.129262	0.796791	0.469903
30	1	0	-3.895031	0.947779	1.029933
31	1	0	-3.135279	-0.142974	0.209108
32	8	0	-0.044771	4.285587	-1.396249
33	1	0	0.332292	5.093970	-1.033519
34	1	0	-0.469074	4.543224	-2.221268
35	8	0	-2.695828	-1.806538	-0.386395
36	1	0	-3.106122	-2.110678	-1.203396
37	1	0	-2.750810	-2.552470	0.220619

Sum of electronic and zero-point Energies= -675.089723
Sum of electronic and thermal Energies= -675.070971
Sum of electronic and thermal Enthalpies= -675.070027
Sum of electronic and thermal Free Energies= -675.138493

Ama^{+}W$_3$(III)

1	6	0	-0.711051	-2.143569	0.835681
2	1	0	0.239385	-2.448279	1.279731
3	1	0	-1.415553	-2.961787	0.991097
4	6	0	-0.537317	-1.875635	-0.667962
5	1	0	-0.158225	-2.773284	-1.158222
6	6	0	-1.235172	-0.872922	1.515752
7	1	0	-1.337248	-1.038693	2.592706
8	6	0	-0.221397	0.268752	1.362026
9	1	0	0.754306	0.010550	1.769943
10	1	0	-0.572990	1.185939	1.831852
11	6	0	0.485131	-0.747453	-0.870044
12	1	0	0.636183	-0.555987	-1.934267
13	1	0	1.450990	-1.020921	-0.443344
14	6	0	-0.044350	0.550513	-0.224848
15	6	0	-1.416634	0.945924	-0.794065
16	1	0	-1.768939	1.860003	-0.312971
17	1	0	-1.298071	1.157370	-1.859112
18	6	0	-1.887753	-1.471297	-1.283308
19	1	0	-2.606384	-2.284078	-1.166222
20	1	0	-1.777130	-1.296142	-2.355860
21	6	0	-2.587811	-0.469152	0.914765

22	1	0	-3.312885	-1.268952	1.071763
23	1	0	-2.977662	0.419744	1.415829
24	6	0	-2.414287	-0.203922	-0.589281
25	1	0	-3.371688	0.086523	-1.022906
26	7	0	0.887509	1.596189	-0.279518
27	1	0	0.556493	2.569980	-0.240454
28	1	0	1.896086	1.389770	-0.136263
29	8	0	3.439283	0.842086	0.353666
30	1	0	3.734624	-0.067319	0.151354
31	1	0	4.225123	1.361524	0.542485
32	8	0	-0.298295	4.161747	-0.067812
33	1	0	-0.635933	4.671838	-0.811407
34	1	0	-0.180503	4.792902	0.649596
35	8	0	3.926218	-1.799882	-0.222896
36	1	0	4.337489	-2.081035	-1.046946
37	1	0	4.256170	-2.402026	0.452276

Sum of electronic and zero-point Energies= -675.089565
Sum of electronic and thermal Energies= -675.070808
Sum of electronic and thermal Enthalpies= -675.069864
Sum of electronic and thermal Free Energies= -675.138456

$Ama^{+}W_3$(IV)

1	6	0	1.843939	-1.414132	-1.118997
2	1	0	1.235181	-1.539872	-2.017265
3	1	0	2.669673	-2.123658	-1.188892
4	6	0	1.007124	-1.698247	0.139291
5	1	0	0.607351	-2.711820	0.092054
6	6	0	2.397641	0.014555	-1.043910
7	1	0	2.972104	0.241961	-1.947257
8	6	0	1.249800	1.032089	-1.011539
9	1	0	0.599355	0.939768	-1.879603
10	1	0	1.617231	2.055125	-0.946548
11	6	0	-0.168703	-0.712248	0.200480
12	1	0	-0.797920	-0.917480	1.068480
13	1	0	-0.799825	-0.803220	-0.684706
14	6	0	0.365442	0.724732	0.311690
15	6	0	1.292044	0.897668	1.534986
16	1	0	1.664920	1.922423	1.576276
17	1	0	0.697849	0.721825	2.433846
18	6	0	1.884007	-1.538697	1.392879
19	1	0	2.703080	-2.259215	1.367304
20	1	0	1.300227	-1.751881	2.291313
21	6	0	3.286015	0.173658	0.196303
22	1	0	4.123996	-0.522338	0.139955
23	1	0	3.707341	1.180641	0.237487
24	6	0	2.448122	-0.109123	1.453530
25	1	0	3.069355	0.009102	2.342278
26	7	0	-0.656953	1.682784	0.284107
27	1	0	-0.456626	2.638299	0.608502
28	1	0	-1.567121	1.460399	-0.168621
29	8	0	-2.939093	0.773957	-0.905893
30	1	0	-3.627625	1.189059	-1.431899
31	1	0	-3.349586	0.026696	-0.425802
32	8	0	0.217804	4.224380	1.189616
33	1	0	0.173308	4.521580	2.104425
34	1	0	0.308843	5.023539	0.660407
35	8	0	-3.775521	-1.381804	0.573786
36	1	0	-3.922720	-2.233082	0.148695
37	1	0	-4.428981	-1.327077	1.278675

Sum of electronic and zero-point Energies= -675.089228
Sum of electronic and thermal Energies= -675.070530
Sum of electronic and thermal Enthalpies= -675.069585
Sum of electronic and thermal Free Energies= -675.138296

$Ama^{+}W_3$(V)

1	6	0	0.892322	-1.509794	-0.426297
2	1	0	-0.097895	-1.731845	-0.826077
3	1	0	1.489042	-2.420603	-0.495622
4	6	0	0.785045	-1.061386	1.039997
5	1	0	0.302073	-1.844439	1.625192

6	6	0	1.556856	-0.394808	-1.241461
7	1	0	1.612785	-0.683806	-2.296967
8	6	0	0.690021	0.867776	-1.220170
9	1	0	-0.320199	0.677731	-1.574754
10	1	0	1.138779	1.681373	-1.787455
11	6	0	-0.083507	0.199595	1.128131
12	1	0	-0.186001	0.521030	2.166301
13	1	0	-1.082934	0.009552	0.741373
14	6	0	0.586326	1.349323	0.347664
15	6	0	2.011536	1.626896	0.847593
16	1	0	2.469260	2.425409	0.257553
17	1	0	1.948727	1.973705	1.881133
18	6	0	2.187205	-0.764987	1.598039
19	1	0	2.799801	-1.667287	1.564780
20	1	0	2.121714	-0.463342	2.645809
21	6	0	2.961659	-0.101440	-0.701713
22	1	0	3.578426	-0.998149	-0.773797
23	1	0	3.448375	0.671235	-1.301008
24	6	0	2.853218	0.344633	0.765259
25	1	0	3.847445	0.559401	1.157690
26	7	0	-0.214488	2.490695	0.296523
27	1	0	0.216389	3.395388	0.142677
28	1	0	-1.254839	2.406866	0.210119
29	8	0	-2.837278	1.943914	0.012550
30	1	0	-2.933872	1.182399	-0.599879
31	1	0	-3.632869	2.478806	-0.048723
32	8	0	-2.616948	-0.283376	-1.506196
33	1	0	-3.093052	-0.485999	-2.316725
34	1	0	-2.666403	-1.080518	-0.942494
35	8	0	-2.505231	-2.343630	0.333120
36	1	0	-2.301109	-3.256271	0.103475
37	1	0	-3.184705	-2.393839	1.013906

Sum of electronic and zero-point Energies= -675.088168
Sum of electronic and thermal Energies= -675.070403
Sum of electronic and thermal Enthalpies= -675.069458
Sum of electronic and thermal Free Energies= -675.133920

$Ama^{+}W_3$(VI)

1	6	0	-0.507293	-1.600694	-0.791039
2	1	0	0.550584	-1.755710	-1.009595
3	1	0	-1.043594	-2.501614	-1.092529
4	6	0	-1.035394	-0.386737	-1.572537
5	1	0	-0.887975	-0.548861	-2.641122
6	6	0	-0.713018	-1.353560	0.707870
7	1	0	-0.308712	-2.192038	1.285153
8	6	0	0.094533	-0.134961	1.165160
9	1	0	1.152961	-0.245100	0.948086
10	1	0	-0.040789	0.068934	2.225872
11	6	0	-0.242216	0.862117	-1.166569
12	1	0	-0.585831	1.733195	-1.727431
13	1	0	0.820380	0.727150	-1.364690
14	6	0	-0.472797	1.156681	0.334136
15	6	0	-1.961251	1.314796	0.665047
16	1	0	-2.091566	1.496776	1.735318
17	1	0	-2.342625	2.188569	0.132418
18	6	0	-2.528941	-0.178936	-1.272309
19	1	0	-3.096693	-1.055576	-1.588177
20	1	0	-2.913979	0.670765	-1.840320
21	6	0	-2.201416	-1.160035	1.019986
22	1	0	-2.757049	-2.054825	0.736387
23	1	0	-2.351806	-1.015665	2.092273
24	6	0	-2.728098	0.053584	0.235244
25	1	0	-3.785848	0.200866	0.453724
26	7	0	0.316963	2.216314	0.785480
27	1	0	0.006747	2.773126	1.574106
28	1	0	1.314688	2.300235	0.475180
29	8	0	2.911317	2.094948	0.074957
30	1	0	3.115719	1.252941	-0.386989
31	1	0	3.533694	2.757863	-0.235399
32	8	0	3.064171	-0.353098	-1.086020

33	1	0	3.097961	-1.097807	-0.455018
34	1	0	3.627594	-0.591303	-1.827840
35	8	0	2.824667	-2.306069	0.865453
36	1	0	2.694642	-3.229973	0.626318
37	1	0	3.446875	-2.315928	1.600853

Sum of electronic and zero-point Energies= -675.087721
Sum of electronic and thermal Energies= -675.069846
Sum of electronic and thermal Enthalpies= -675.068902
Sum of electronic and thermal Free Energies= -675.134068

$Ama^{+}W_3$(VII)

1	6	0	-1.650641	1.603315	0.731929
2	1	0	-0.798247	2.269519	0.882557
3	1	0	-2.543448	2.143495	1.049649
4	6	0	-1.484066	0.322131	1.564639
5	1	0	-1.390810	0.580839	2.620146
6	6	0	-1.773192	1.223993	-0.748768
7	1	0	-1.861111	2.127147	-1.361699
8	6	0	-0.490609	0.530090	-1.225957
9	1	0	0.390282	1.147008	-1.062121
10	1	0	-0.550869	0.247008	-2.275701
11	6	0	-0.204972	-0.406975	1.133682
12	1	0	-0.061183	-1.310576	1.728831
13	1	0	0.677709	0.217600	1.270923
14	6	0	-0.324775	-0.832340	-0.346250
15	6	0	-1.562016	-1.708702	-0.587899
16	1	0	-1.633225	-1.974935	-1.646069
17	1	0	-1.444581	-2.634496	-0.020953
18	6	0	-2.699519	-0.597123	1.355717
19	1	0	-3.607756	-0.092961	1.689521
20	1	0	-2.596980	-1.501550	1.959461
21	6	0	-2.991104	0.318254	-0.968561
22	1	0	-3.899335	0.843253	-0.669871
23	1	0	-3.097017	0.072044	-2.027536
24	6	0	-2.825572	-0.962078	-0.133570
25	1	0	-3.686080	-1.613801	-0.286279
26	7	0	0.860891	-1.402316	-0.821460
27	1	0	0.820125	-2.047763	-1.602792
28	1	0	1.799573	-1.015066	-0.515704
29	8	0	3.046390	-0.201327	0.041673
30	1	0	3.980557	-0.468502	0.141896
31	1	0	3.013434	0.763777	-0.070126
32	8	0	5.687475	-0.876871	0.351501
33	1	0	6.070805	-1.147785	1.191147
34	1	0	6.293631	-1.183938	-0.329115
35	8	0	2.386550	2.498216	-0.277380
36	1	0	2.736606	3.034401	-0.997001
37	1	0	2.437171	3.057959	0.504939

Sum of electronic and zero-point Energies= -675.086239
Sum of electronic and thermal Energies= -675.067767
Sum of electronic and thermal Enthalpies= -675.066823
Sum of electronic and thermal Free Energies= -675.134692

$Ama^{+}W_3$(VIII)

1	6	0	1.777748	-1.630747	0.113992
2	1	0	1.010137	-2.371951	-0.115780
3	1	0	2.726682	-2.161671	0.202020
4	6	0	1.450470	-0.916104	1.435464
5	1	0	1.384586	-1.648939	2.240165
6	6	0	1.869757	-0.591331	-1.009550
7	1	0	2.074345	-1.089019	-1.964480
8	6	0	0.522855	0.106944	-1.206546
9	1	0	-0.289723	-0.585206	-1.405679
10	1	0	0.566171	0.871574	-1.980261
11	6	0	0.091956	-0.210828	1.308561
12	1	0	-0.164173	0.282740	2.249442
13	1	0	-0.694342	-0.926894	1.068929
14	6	0	0.162254	0.861782	0.214529
15	6	0	1.295946	1.879765	0.470565

16	1	0	1.330893	2.610545	-0.339083
17	1	0	1.056376	2.414790	1.391967
18	6	0	2.544323	0.117122	1.754597
19	1	0	3.505438	-0.384796	1.876191
20	1	0	2.325362	0.620242	2.699237
21	6	0	2.972498	0.428493	-0.704069
22	1	0	3.933198	-0.080331	-0.616056
23	1	0	3.063370	1.149944	-1.519117
24	6	0	2.635017	1.144531	0.613201
25	1	0	3.406789	1.882723	0.835767
26	7	0	-1.061674	1.478700	-0.034014
27	1	0	-1.086473	2.347150	-0.582781
28	1	0	-1.945760	1.010926	0.176225
29	8	0	-3.741938	0.385801	0.677065
30	1	0	-3.940925	0.221674	1.605695
31	1	0	-4.539977	0.779226	0.306868
32	8	0	-0.816152	3.798968	-1.642485
33	1	0	-0.692724	4.699366	-1.324601
34	1	0	-1.049350	3.879457	-2.573057
35	8	0	-2.222772	-1.644029	-0.660642
36	1	0	-2.489198	-2.519466	-0.955237
37	1	0	-3.011072	-1.233787	-0.282139

Sum of electronic and zero-point Energies= -675.084318
Sum of electronic and thermal Energies= -675.065196
Sum of electronic and thermal Enthalpies= -675.064252
Sum of electronic and thermal Free Energies= -675.133361

Ama^{+}W$_3$(IX)

1	6	0	1.013507	-1.175785	-0.414159
2	1	0	0.508669	-2.034362	-0.863662
3	1	0	2.085578	-1.365252	-0.440430
4	6	0	0.553542	-0.986627	1.040840
5	1	0	0.765788	-1.892088	1.610754
6	6	0	0.701152	0.101301	-1.202715
7	1	0	0.990196	-0.026089	-2.252107
8	6	0	-0.809902	0.362770	-1.232543
9	1	0	-1.363533	-0.476050	-1.650431
10	1	0	-1.059365	1.271805	-1.776872
11	6	0	-0.961491	-0.739981	1.072013
12	1	0	-1.308208	-0.626479	2.101573
13	1	0	-1.505828	-1.576594	0.629949
14	6	0	-1.293789	0.560029	0.317745
15	6	0	-0.528196	1.766383	0.888382
16	1	0	-0.773078	2.665621	0.320090
17	1	0	-0.865594	1.921515	1.915692
18	6	0	1.288294	0.211910	1.665398
19	1	0	2.362187	0.029168	1.655412
20	1	0	0.984969	0.341094	2.707164
21	6	0	1.442937	1.297539	-0.595308
22	1	0	2.515409	1.109716	-0.615022
23	1	0	1.249723	2.202506	-1.176478
24	6	0	0.980537	1.485243	0.858828
25	1	0	1.498657	2.338140	1.298729
26	7	0	-2.667613	0.790146	0.208564
27	1	0	-3.012006	1.740980	0.019678
28	1	0	-3.313374	-0.006573	0.127772
29	8	0	-4.199889	-1.572854	-0.072734
30	1	0	-4.556581	-2.080225	0.663804
31	1	0	-4.695052	-1.855494	-0.848467
32	8	0	-3.319047	3.482550	-0.376554
33	1	0	-3.451616	4.162159	0.292590
34	1	0	-3.722531	3.825788	-1.180437
35	8	0	4.345363	-0.520543	0.019830
36	1	0	4.953164	-0.444138	-0.722527
37	1	0	4.880252	-0.879482	0.734948

Sum of electronic and zero-point Energies= -675.080785
Sum of electronic and thermal Energies= -675.060666
Sum of electronic and thermal Enthalpies= -675.059722
Sum of electronic and thermal Free Energies= -675.131523

$CH_3NH_2^+$

1	6	0	0.012235	0.703449	0.000000
2	1	0	0.459871	1.094137	0.913952
3	1	0	-1.050687	1.038681	0.000000
4	1	0	0.459871	1.094137	-0.913952
5	7	0	0.012235	-0.708714	0.000000
6	1	0	-0.014055	-1.243325	-0.868103
7	1	0	-0.014055	-1.243325	0.868103

Sum of electronic and zero-point Energies= -95.513064
Sum of electronic and thermal Energies= -95.509141
Sum of electronic and thermal Enthalpies= -95.508197
Sum of electronic and thermal Free Energies= -95.537742

CH_3NH

1	6	0	-0.627050	0.012203	0.000027
2	1	0	-0.970053	0.581202	-0.876973
3	1	0	-0.970257	0.582386	0.876149
4	1	0	-1.125195	-0.957254	0.000539
5	7	0	0.802398	-0.152502	0.000022
6	1	0	1.211024	0.787967	-0.000028

Sum of electronic and zero-point Energies= -95.184424
Sum of electronic and thermal Energies= -95.180969
Sum of electronic and thermal Enthalpies= -95.180025
Sum of electronic and thermal Free Energies= -95.207840

$CH_3NH_2^+W$

1	6	0	1.605958	-0.433603	-0.000033
2	1	0	2.271028	-0.314791	0.870678
3	1	0	2.272207	-0.313851	-0.869663
4	1	0	1.129695	-1.407992	-0.000761
5	7	0	0.640863	0.601178	-0.000023
6	1	0	-0.397476	0.391079	0.000011
7	1	0	0.946958	1.572313	0.000084
8	8	0	-1.919614	-0.143153	0.000012
9	1	0	-2.493710	-0.194124	0.772614
10	1	0	-2.493576	-0.194043	-0.772698

Sum of electronic and zero-point Energies= -171.985432
Sum of electronic and thermal Energies= -171.978588
Sum of electronic and thermal Enthalpies= -171.977644
Sum of electronic and thermal Free Energies= -172.015873

$CH_3NH_2^+W_2$

1	6	0	0.008439	1.681966	-0.000650
2	1	0	-0.551524	2.044982	0.874628
3	1	0	-0.569835	2.045675	-0.863095
4	1	0	1.017634	2.079431	-0.009610
5	7	0	0.004482	0.266125	-0.000149
6	1	0	0.909257	-0.255999	0.000145
7	1	0	-0.909389	-0.239198	0.001134
8	8	0	2.504018	-0.815783	0.000220
9	1	0	2.986746	-1.134297	0.770571
10	1	0	2.988699	-1.132080	-0.769815
11	8	0	-2.502583	-0.818836	0.000045
12	1	0	-2.986665	-1.138478	0.769114
13	1	0	-2.978410	-1.147748	-0.770247

Sum of electronic and zero-point Energies= -248.451806
Sum of electronic and thermal Energies= -248.442380
Sum of electronic and thermal Enthalpies= -248.441436
Sum of electronic and thermal Free Energies= -248.486554

$CH_3NH_2^+W_3$

1	6	0	-0.360555	-1.584272	0.071736
2	1	0	0.112273	-1.787001	1.042825
3	1	0	0.302446	-2.064244	-0.664097
4	1	0	-1.358125	-2.008014	0.023204
5	7	0	-0.381688	-0.187448	-0.162059
6	1	0	-1.302770	0.292997	-0.385477
7	1	0	0.515624	0.335912	-0.114636
8	8	0	-2.794384	0.744983	-0.684651

9	1	0	-3.391426	1.143895	-0.011618
10	1	0	-3.134371	0.990444	-1.549524
11	8	0	-4.362394	1.781532	1.250246
12	1	0	-5.184906	1.358077	1.516530
13	1	0	-4.492178	2.724668	1.391982
14	8	0	2.130452	0.931595	0.026976
15	1	0	2.722039	1.127950	-0.707151
16	1	0	2.492653	1.393543	0.790407

Sum of electronic and zero-point Energies= -324.911228
Sum of electronic and thermal Energies= -324.898745
Sum of electronic and thermal Enthalpies= -324.897801
Sum of electronic and thermal Free Energies= -324.952075

W

1	8	0	0.000000	0.000000	0.117763
2	1	0	0.000000	0.760117	-0.471053
3	1	0	0.000000	-0.760117	-0.471053

Sum of electronic and zero-point Energies= -76.438576
Sum of electronic and thermal Energies= -76.435741
Sum of electronic and thermal Enthalpies= -76.434797
Sum of electronic and thermal Free Energies= -76.456220

W_2

1	8	0	0.004841	1.505621	0.000000
2	1	0	0.103104	0.542087	0.000000
3	1	0	0.904530	1.841770	0.000000
4	8	0	0.004841	-1.401202	0.000000
5	1	0	-0.542546	-1.609607	0.763741
6	1	0	-0.542546	-1.609607	-0.763741

Sum of electronic and zero-point Energies= -152.884652
Sum of electronic and thermal Energies= -152.878738
Sum of electronic and thermal Enthalpies= -152.877794
Sum of electronic and thermal Free Energies= -152.911316

W_3

1	8	0	-1.344244	-0.878728	0.102444
2	1	0	-1.192794	0.084933	0.041828
3	1	0	-1.842699	-1.109827	-0.685764
4	8	0	-0.095946	1.596231	-0.116948
5	1	0	-0.019943	2.146944	0.667004
6	1	0	0.666862	0.986502	-0.081273
7	8	0	1.437981	-0.709111	0.093015
8	1	0	0.534945	-1.081652	0.103237
9	1	0	1.871299	-1.094037	-0.673123

Sum of electronic and zero-point Energies= -229.340992
Sum of electronic and thermal Energies= -229.333857
Sum of electronic and thermal Enthalpies= -229.332912
Sum of electronic and thermal Free Energies= -229.369948

Ad

1	6	0	0.000000	0.000000	1.774934
2	1	0	0.621527	0.621527	2.425680
3	1	0	-0.621527	-0.621527	2.425680
4	6	0	0.889683	-0.889683	0.889683
5	1	0	1.520547	-1.520547	1.520547
6	6	0	-0.889683	0.889683	0.889683
7	1	0	-1.520547	1.520547	1.520547
8	6	0	0.000000	1.774934	0.000000
9	1	0	0.621527	2.425680	0.621527
10	1	0	-0.621527	2.425680	-0.621527
11	6	0	1.774934	0.000000	0.000000
12	1	0	2.425680	-0.621527	-0.621527
13	1	0	2.425680	0.621527	0.621527
14	6	0	0.889683	0.889683	-0.889683
15	1	0	1.520547	1.520547	-1.520547
16	6	0	0.000000	0.000000	-1.774934
17	1	0	-0.621527	0.621527	-2.425680
18	1	0	0.621527	-0.621527	-2.425680
19	6	0	0.000000	-1.774934	0.000000
20	1	0	-0.621527	-2.425680	0.621527

21	1	0	0.621527	-2.425680	-0.621527
22	6	0	-1.774934	0.000000	0.000000
23	1	0	-2.425680	-0.621527	0.621527
24	1	0	-2.425680	0.621527	-0.621527
25	6	0	-0.889683	-0.889683	-0.889683
26	1	0	-1.520547	-1.520547	-1.520547

Sum of electronic and zero-point Energies= -390.638558
Sum of electronic and thermal Energies= -390.631860
Sum of electronic and thermal Enthalpies= -390.630915
Sum of electronic and thermal Free Energies= -390.666803

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1	6	0	-1.264306	0.729947	-1.000887
2	1	0	-1.317997	0.760946	-2.097682
3	1	0	-2.157799	1.245806	-0.647152
4	6	0	0.000000	1.449632	-0.553782
5	1	0	0.000000	2.497787	-0.854160
6	6	0	-1.255418	-0.724816	-0.553782
7	1	0	-2.163147	-1.248893	-0.854160
8	6	0	0.000000	-1.459894	-1.000887
9	1	0	0.000000	-1.521892	-2.097682
10	1	0	0.000000	-2.491611	-0.647152
11	6	0	1.264306	0.729947	-1.000887
12	1	0	2.157799	1.245806	-0.647152
13	1	0	1.317997	0.760946	-2.097682
14	6	0	1.255418	-0.724816	-0.553782
15	1	0	2.163147	-1.248893	-0.854160
16	6	0	1.260725	-0.727880	1.057314
17	1	0	1.276133	-1.761607	1.396935
18	1	0	2.163663	-0.224360	1.396935
19	6	0	0.000000	1.455760	1.057314
20	1	0	-0.887530	1.985967	1.396935
21	1	0	0.887530	1.985967	1.396935
22	6	0	-1.260725	-0.727880	1.057314
23	1	0	-2.163663	-0.224360	1.396935
24	1	0	-1.276133	-1.761607	1.396935
25	6	0	0.000000	0.000000	1.463488
26	1	0	0.000000	0.000000	2.586843

Sum of electronic and zero-point Energies= -390.314906
Sum of electronic and thermal Energies= -390.307097
Sum of electronic and thermal Enthalpies= -390.306153
Sum of electronic and thermal Free Energies= -390.345713