Electronic Supplementary Information for

A theoretical study on hydrated sodium ion-phenylalanine clusters $Na^+(Phe)(H_2O)_n$ (n = 0-6; Phe = phenylalanine)

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Table S1. The singlet-triplet splitting energy $\Delta E_{S\text{-}T}$ for $Na^+(Phe)(H_2O)_n$ (n=0-6) given in eV.

$Na^+(Phe)(H_2O)_n$	Singlet(eV)	Triplet(eV)	$\Delta E_{S\text{-}T}$(eV)
n=0	-19516.82	-19513.16	3.66
n=1	-21598.37	-21594.67	3.70
n=2	-23679.77	-23676.08	3.69
n=3	-25761.27	-25757.59	3.68
n=4	-27842.67	-27839.03	3.64
n=5	-29924.10	-29920.48	3.62
n=6	-32005.50	-32001.80	3.70

To determine the spin state of the $Na^+(Phe)(H_2O)_n$ (n=0-6), the singlet and triplet states were calculated. As shown in Table S1, the single and triplet bond energies of these are all positive. The singlet state is more stable than the triplet state by more than 3.62 eV at the BP86-D3(BJ)/TZVPP level of theory. Therefore, the electron singlet ground state of the $Na^+(Phe)(H_2O)_n$ (n=0-6) system is confirmed.

Table S2. Test calculations on binding energy of one water molecule from Na^+(Phe) and Na^+(Phe)$(H_2O)_1$ to Na^+(Phe)$(H_2O)_1$ and Na^+(Phe)$(H_2O)_2$, respectively, by using different functionals with def2-TZVPP basis set. The AE and RMSD are average error and root mean square deviation, respectively.

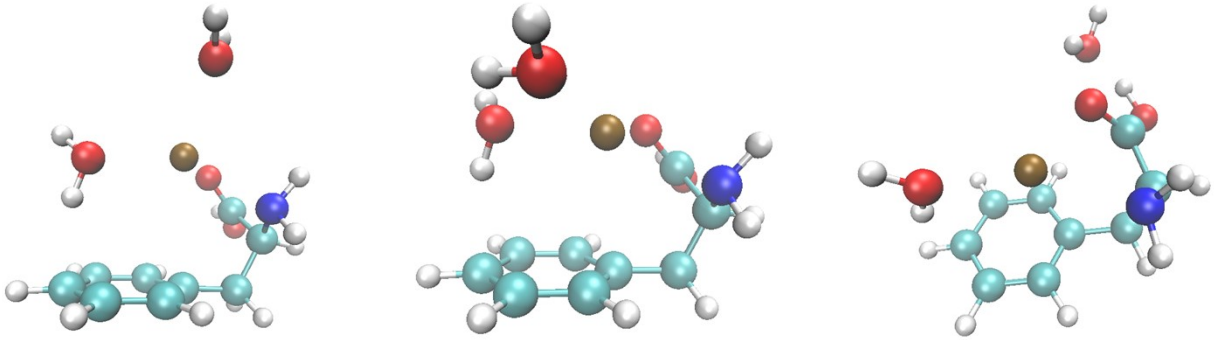
Functional	Na^+(Phe)$(H_2O)_1$		Na^+(Phe)$(H_2O)_2$		AE/RMSD
	$\Delta \boldsymbol{H}$ (kcal mol^{-1})	$\Delta \boldsymbol{G}$ (kcal mol^{-1})	$\Delta \boldsymbol{H}$ (kcal mol^{-1})	$\Delta \boldsymbol{G}$ (kcal mol^{-1})	
BP86-D3(BJ)	16.45(2.85)	8.78(0.88)	12.98(0.68)	5.91(0.61)	1.26/1.56
B3LYP-D3(BJ)	18.04(4.44)	10.42(2.52)	14.42(2.12)	7.14(1.84)	2.73/2.91
M06-2X-D3(zero)	16.31(2.71)	8.92(1.02)	13.18(0.88)	4.82(0.48)	1.28/1.53
PBE-D3(BJ)	17.27(3.57)	9.75(1.85)	14.22(1.92)	6.74(1.44)	2.20/2.34
PBE0-D3(BJ)	16.99(3.39)	10.26(2.36)	14.04(1.74)	5.88(0.58)	2.02/2.26
ωB97XD	15.71(2.11)	9.13(1.23)	11.84(0.46)	3.15(2.15)	1.49/1.64
Experimental values	13.6	7.9	12.3	5.3	/

Table S3. The Mayer bond order of $Na{-}N_{Phe}$, $Na{-}O_{Phe}$, and $Na{-}O_{H2O}$ bond in $Na^{+}(Phe)(H_2O)_n$.

$Na^{+}(Phe)(H_2O)_n$	Bond	Mayer bond order
n=0	Na−N(Phe, d_1)	0.161
	Na−O(Phe, d_2)	0.149
n=1	Na−N(Phe, d_1)	0.147
	Na−O(Phe, d_2)	0.142
	Na−O(H_2O, d_3)	0.107
n=2	Na−N(Phe, d_1)	0.123
	Na−O(Phe, d_2)	0.122
	Na−O(H_2O, d_3)	0.097
	Na−O(H_2O, d_4)	0.102
n=3	Na−N(Phe, d_1)	0.149
	Na−O(Phe, d_2)	0.101
	Na−O(H_2O, d_3)	0.119
n=4	Na−N(Phe, d_1)	0.119
	Na−O(Phe, d_2)	0.093
	Na−O(H_2O, d_3)	0.114
	Na−O(H_2O, d_4)	0.116
n=5	Na−O(Phe, d_1)	0.069
	Na−O(H_2O, d_2)	0.126
	Na−O(H_2O, d_3)	0.122
	Na−O(H_2O, d_4)	0.165
n=6	Na−O(H_2O, d_1)	0.122
	Na−O(Phe, d_2)	0.088
	Na−O(H_2O, d_3)	0.120

Table S4. Electron density (ρ_r), Laplacian electron density [$\nabla^2\rho(r)$], total energy density (H_r), ratio of the potential energy density (V_r) to kinetic energy density (G_r), and ratio of G_r to ρ_r at the BCPs of the Na−O_{H2O}, Na−O_{Phe}, and Na−N_{Phe} bonds by atoms in molecules (AIM) analysis

BCP		ρ_r	$\nabla^2\rho(r)$	H_r	$\lvert V_r\rvert/G_r$	G_r/ρ_r
n=0	Na−N(Phe, d_1)	0.018	0.091	0.0041	0.78	1.05
	Na−O(Phe, d_2)	0.021	0.13	0.0064	0.76	1.29
n=1	Na−N(Phe, d_1)	0.018	0.094	0.0041	0.79	1.05
	Na−O(Phe, d_2)	0.021	0.13	0.0063	0.76	1.29
	Na−O(H_2O, d_3)	0.024	0.16	0.0074	0.77	1.39
n=2	Na−N(Phe, d_1)	0.018	0.092	0.0041	0.78	1.06
	Na−O(Phe, d_2)	0.019	0.12	0.0061	0.75	1.28
	Na−O(H_2O, d_3)	0.019	0.13	0.0066	0.74	1.33
	Na−O(H_2O, d_4)	0.023	0.15	0.0073	0.77	1.37
n=3	Na−N(Phe, d_1)	0.016	0.078	0.0036	0.77	1.01
	Na−O(Phe, d_2)	0.017	0.11	0.0056	0.74	1.25
	Na−O(H_2O, d_3)	0.023	0.15	0.0072	0.77	1.37
n=4	Na−N(Phe, d_1)	0.016	0.083	0.0038	0.78	1.03
	Na−O(Phe, d_2)	0.016	0.098	0.0052	0.73	1.23
	Na−O(H_2O, d_3)	0.021	0.14	0.0069	0.75	1.35
	Na−O(H_2O, d_4)	0.021	0.14	0.0070	0.76	1.35
n=5	Na−O(Phe, d_1)	0.012	0.077	0.0046	0.69	1.23
	Na−O(H_2O, d_2)	0.019	0.12	0.0061	0.75	1.28
	Na−O(H_2O, d_3)	0.020	0.13	0.0067	0.75	1.33
	Na-O(H_2O, d_4)	0.025	0.16	0.0068	0.79	1.33
n=6	Na−O(H_2O, d_1)	0.024	0.16	0.0075	0.78	1.39
	Na−O(Phe, d_2)	0.022	0.16	0.0078	0.75	1.43
	Na−O(H_2O, d_3)	0.023	0.15	0.0073	0.77	1.38



	① N/O/O/O/Ring Pentadentate	② N/O/O/O/Ring Pentadentate	③ N/O/O/Ring Quadridentate
Δ(E+ZPE)	0.00 kcal mol^{-1}	0.17 kcal mol^{-1}	0.18 kcal mol^{-1}
ΔH	0.00 kcal mol^{-1}	-0.12 kcal mol^{-1}	-0.17 kcal mol^{-1}
ΔG	0.00 kcal mol^{-1}	1.16 kcal mol^{-1}	1.27 kcal mol^{-1}

Fig. S1 The three lowest structures of energy of optimized geometries of the $Na^+(Phe)(H_2O)_2$, which have very small differences in energy. We take the energy of structure one as the zero point.

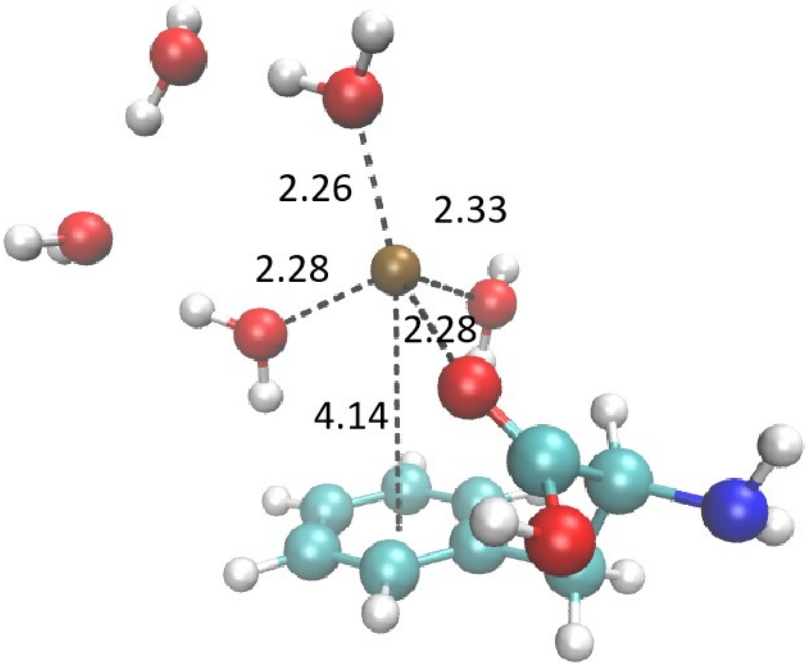


Fig. S2 Another geometric optimization of $Na^+(Phe)(H_2O)_5$ at BP86-D3(BJ)/def2-TZVPP level.

This structure was depicted in Figure 5 of the J. Phys. Chem. B 2008, 112, 12783–12789.[2] This structure is about 17.8 kcal mol^{-1} higher in energy than the lowest-energy structures of $Na^+(Phe)(H_2O)_5$ in our manuscript. We think this structure maybe one meta-stable structure.

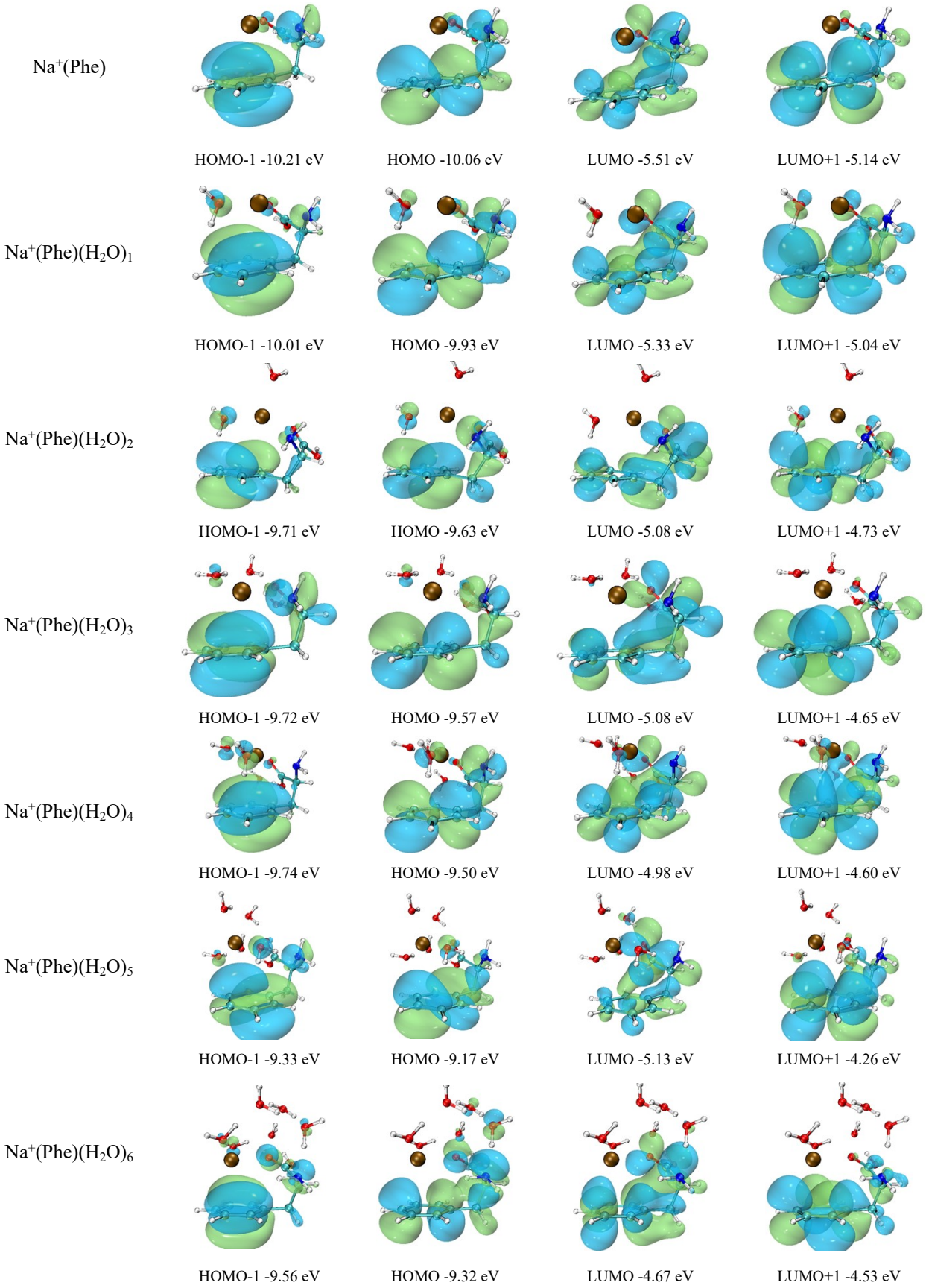
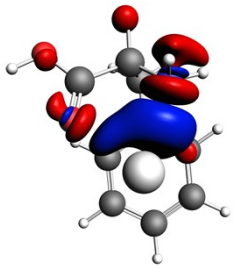


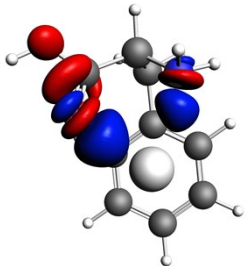
Fig. S2 Selected molecular orbitals (isovalue = 0.02) of $Na^+(Phe)(H_2O)_n$ (n=0-6) with energy eigenvalues given in eV.

$Na^+(Phe)$



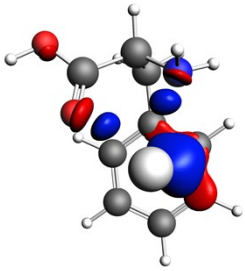
$\Delta\rho_1$： ΔE_1 = -4.6 kcal·mol^{-1}

$|v_1|$ = 0.16



$\Delta\rho_2$： ΔE_2 = -3.2 kcal·mol^{-1}

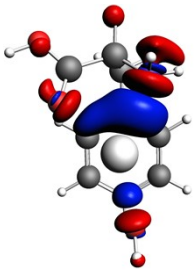
$|v_2|$ = 0.11



$\Delta\rho_3$： ΔE_3 = -2.6 kcal·mol^{-1}

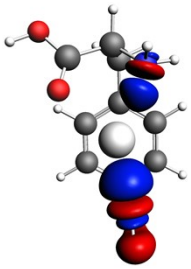
$|v_3|$ = 0.10

$Na^+(Phe)(H_2O)_1$



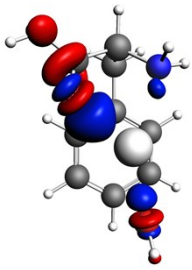
$\Delta\rho_1$： ΔE_1 = -4.7 kcal·mol^{-1}

$|v_1|$ = 0.15



$\Delta\rho_2$： ΔE_2 = -3.4 kcal·mol^{-1}

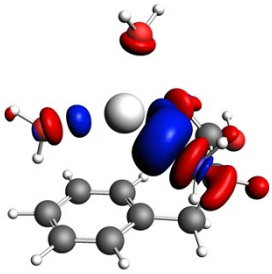
$|v_2|$ = 0.11



$\Delta\rho_3$： ΔE_3 = -3.1 kcal·mol^{-1}

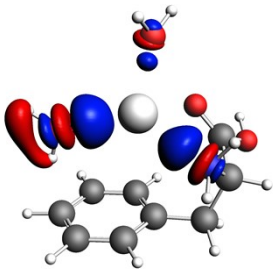
$|v_3|$ = 0.11

$Na^+(Phe)(H_2O)_2$



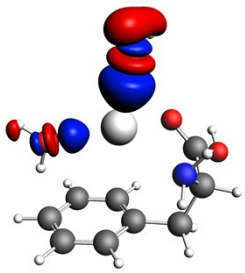
$\Delta\rho_1$： ΔE_1 = -4.5 kcal·mol^{-1}

$|v_1|$ = 0.15



$\Delta\rho_2$： ΔE_2 = -3.4 kcal·mol^{-1}

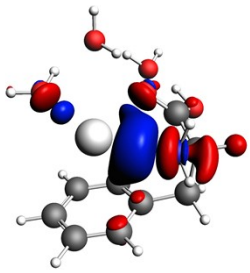
$|v_2|$ = 0.11



$\Delta\rho_3$： ΔE_3 = -3.2 kcal·mol^{-1}

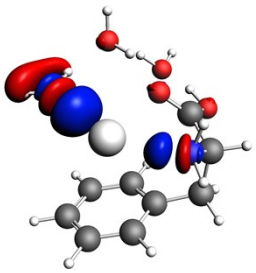
$|v_3|$ = 0.11

$Na^+(Phe)(H_2O)_3$



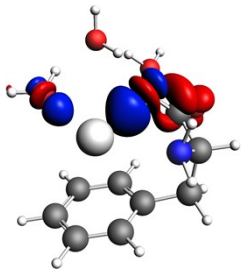
$\Delta\rho_1$： ΔE_1 = -4.6 kcal·mol^{-1}

$|v_1|$ = 0.16



$\Delta\rho_2$： ΔE_2 = -3.2 kcal·mol^{-1}

$|v_2|$ = 0.11



$\Delta\rho_3$： ΔE_3 = -3.1 kcal·mol^{-1}

$|v_3|$ = 0.11

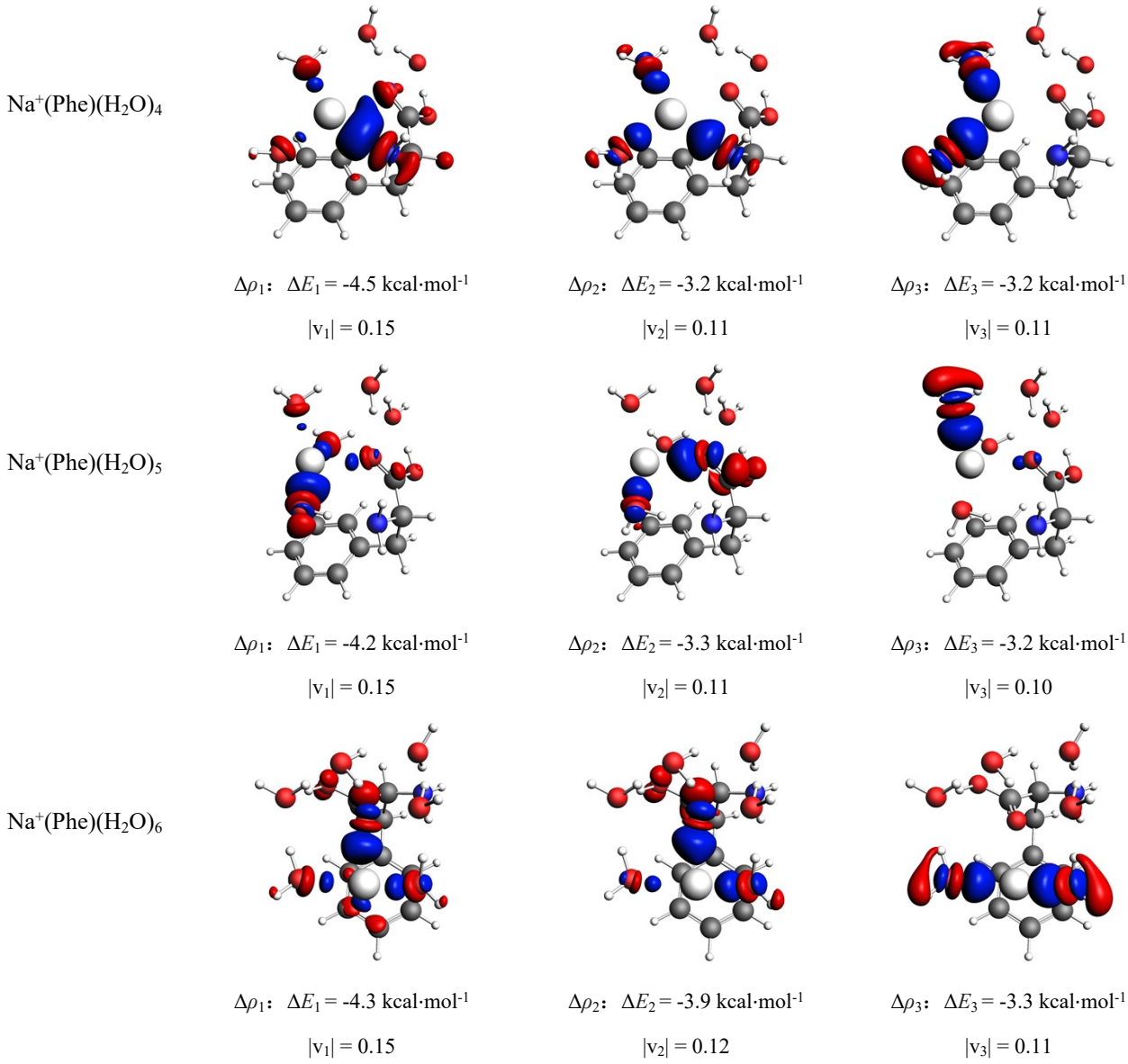
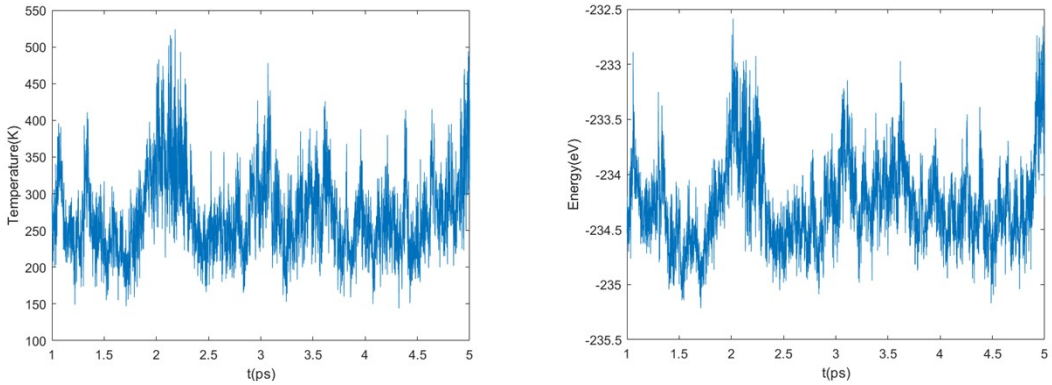
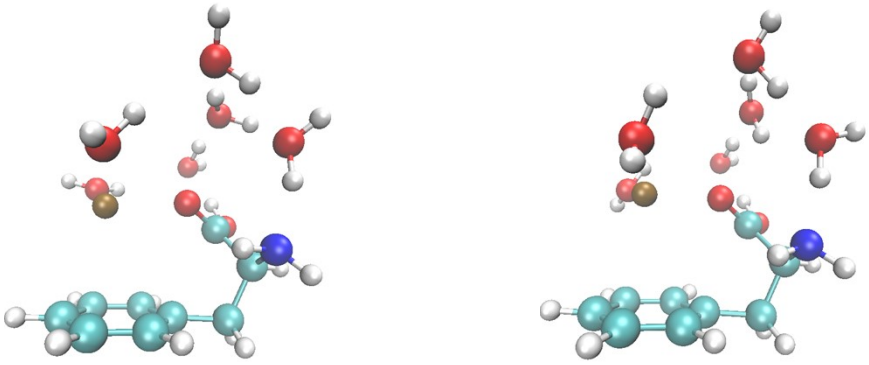


Fig. S3 Deformation densities $\Delta\rho_{1-3}$ (isovalue = 0.0008) of the orbital interaction in $Na^+(Phe)(H_2O)_n$ between Na^+ (singlet) and $(Phe)(H_2O)_n$ (singlet) as interacting fragments with the association interaction energies ΔE (in kcal·mol^{-1}) and their energy eigenvalues ν (in e) which indicates the amount of donated and accepted charge. The direction of the charge flow is red → blue.



(a) **(b)**



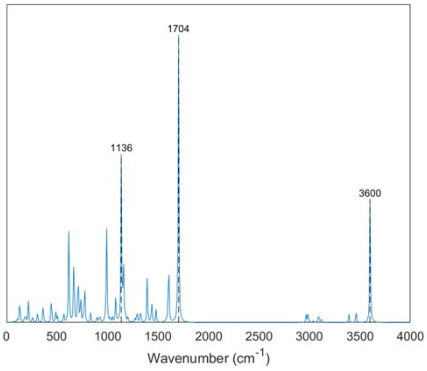
1.54 ps 4.42 ps

$D_{cation-\pi}$ = 2.93 $D_{cation-\pi(max)}$ = 3.11

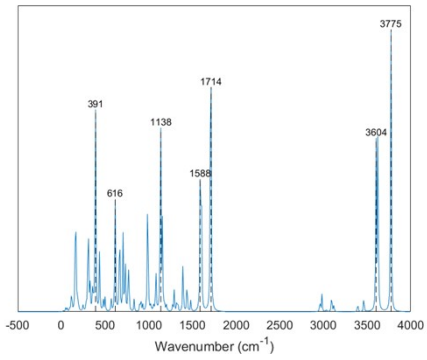
$\theta_{cation-\pi(max)}$ = 12.52 $\theta_{cation-\pi}$ = 9.79

(c)

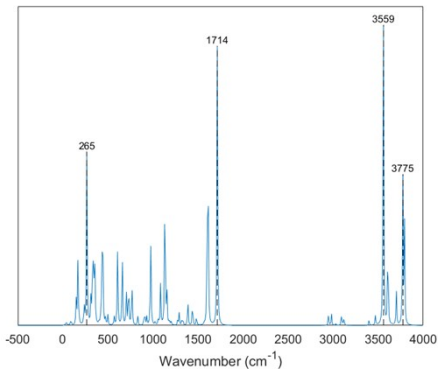
Fig. S4 The AIMD simulation at 300K of $Na^+(Phe)(H_2O)_6$; (a) Temperature-time curve ; (b) Energy-time curve; (c) Selected two other molecular dynamics trajectories.



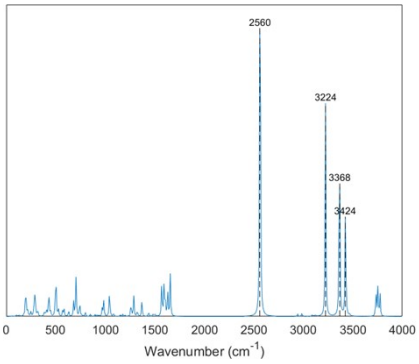
$Na^+(Phe)$



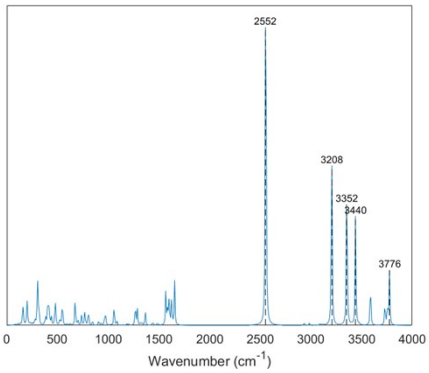
$Na^+(Phe)(H_2O)_1$



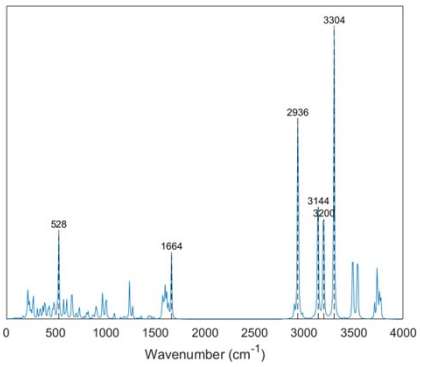
$Na^+(Phe)(H_2O)_2$



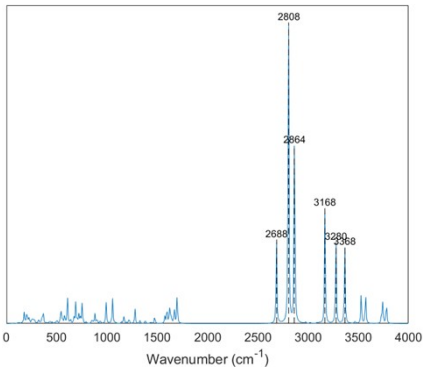
$Na^+(Phe)(H_2O)_3$



$Na^+(Phe)(H_2O)_4$



$Na^+(Phe)(H_2O)_5$



$Na^+(Phe)(H_2O)_6$

Fig. S5 Simulated infrared spectra for $Na^+(Phe)(H_2O)_n$ (n=0-6).

Cartesian coordinates

(1) Na^+(Phe)
BP86-D3(BJ)/def-TZVPP, Singlet
Energy = -717.230 a.u.
Gibbs free energy = -717.082 a.u.

C	3.04931500	-0.65386600	0.22019500
C	2.83856300	0.71250700	-0.00923200
C	1.65942800	1.14502600	-0.62898800
C	0.66925000	0.22426600	-1.02056400
C	0.91174900	-1.14663900	-0.81882300
C	2.08924400	-1.58314800	-0.20018200
H	3.97073300	-0.99422300	0.69320700
H	3.59983000	1.43913300	0.27698800
H	1.51143100	2.21006200	-0.82017400
H	0.17416700	-1.88019800	-1.14985200
H	2.26314800	-2.65024900	-0.05873000
C	-0.66059100	0.70471900	-1.54959500
H	-0.54794300	1.68569700	-2.03446400
H	-1.06099000	0.01609900	-2.30568200
C	-1.73656600	0.86749700	-0.42949200
H	-2.64944100	1.25527400	-0.90972000
N	-1.23503500	1.73857900	0.65419500
H	-0.85658800	2.59502600	0.24156900
H	-2.02058800	2.03817600	1.23902700
C	-2.07645500	-0.49513700	0.16813700
O	-1.60146500	-0.93415300	1.21022700
O	-2.93365400	-1.17942000	-0.59734800
H	-3.09214300	-2.05395100	-0.18293100
Na	0.28826900	0.22057500	1.92178300

(2) Na^+(Phe)(H_2O)
BP86-D3(BJ)/def-TZVPP, Singlet
Energy = -793.725 a.u.
Gibbs free energy = -793.560 a.u.

Na	-0.23928200	1.80960100	0.25221500
O	-2.41156600	2.32504400	-0.04954500
H	-2.99944900	3.08702600	-0.16927100
H	-2.95287000	1.53274800	-0.22627100
C	-2.88820000	-0.81703800	-0.61927000
C	-2.61137600	-0.95620900	0.74630400
C	-1.29996100	-1.19179000	1.17392800
C	-0.24714500	-1.30131000	0.24956500
C	-0.53970500	-1.15611000	-1.11901100
C	-1.84624200	-0.91158400	-1.55118800
H	-3.91609600	-0.68065700	-0.96067800
H	-3.41849400	-0.90707900	1.47797100
H	-1.09949700	-1.33088900	2.23833900
H	0.25665600	-1.26648900	-1.85728900
H	-2.05614800	-0.82236900	-2.61729600
C	1.16507200	-1.57270500	0.71645100
H	1.14434000	-2.05635300	1.70441800
H	1.67074400	-2.26866600	0.03326000
C	2.05927600	-0.30476900	0.85098400
H	3.03970100	-0.64281300	1.22500900
N	1.41679600	0.69412200	1.72760300
H	1.09520900	0.22883700	2.58007800
H	2.11437200	1.37864800	2.03298700
C	2.29231300	0.32145800	-0.52107500
O	1.68176400	1.28897300	-0.95908700
O	3.23122200	-0.33497300	-1.21573700
H	3.32050700	0.09157900	-2.09401800

(3) Na^+(Phe)(H_2O)$_2$
BP86-D3(BJ)/def-TZVPP, Singlet
Energy = -870.215 a.u.
Gibbs free energy = -870.034 a.u.

Na	0.66480200	1.63917800	0.04877300
O	-1.33805300	2.66305000	-0.22933200
H	-1.66624300	3.50354300	-0.58328800
H	-2.09545200	2.04370900	-0.26309400
O	2.36956500	3.22957700	0.06854500
H	2.43936800	4.10704900	0.47732000
H	3.13569200	3.16855900	-0.52471000
C	-3.26842600	0.15962400	-0.58278400
C	-3.03850900	0.05486000	0.79476900
C	-1.93251600	-0.65985100	1.26661700
C	-1.04785600	-1.28927800	0.37770600
C	-1.28525600	-1.16880800	-1.00289200
C	-2.38157200	-0.44897800	-1.48125000
H	-4.15298800	0.67954100	-0.95405700
H	-3.73308300	0.50837300	1.50270800
H	-1.78074600	-0.76450000	2.34288500
H	-0.62800300	-1.67565300	-1.71185100
H	-2.56219900	-0.38496900	-2.55451200
C	0.10786300	-2.11433400	0.89559300
H	-0.08986600	-2.41780200	1.93447100
H	0.21018500	-3.03882900	0.31100300
C	1.48570700	-1.39495500	0.88921800
H	2.21566900	-2.10648300	1.31153000
N	1.41477700	-0.12646000	1.63408600
H	0.91913600	-0.28257000	2.51463300
H	2.35742900	0.17732800	1.89241700
C	1.92817400	-1.11209600	-0.54345700
O	1.89016500	-0.01817000	-1.09063000
O	2.35424700	-2.22772000	-1.15793500
H	2.60179100	-1.99403600	-2.07687700

(4) Na^+(Phe)(H_2O)$_3$
BP86-D3(BJ)/def-TZVPP, Singlet
Energy = -946.709 a.u.
Gibbs free energy = -946.498 a.u.

C	-2.57616000	1.83739100	-1.00614600
C	-3.29100900	0.91735500	-0.22927200
C	-2.82869800	-0.39809600	-0.09839200
C	-1.64551800	-0.81348700	-0.73575900
C	-0.95228900	0.11463700	-1.53442300
C	-1.41161000	1.42949700	-1.66583600
H	-2.93969800	2.85918900	-1.11678900
H	-4.21793300	1.21799400	0.26067300
H	-3.40009800	-1.11453600	0.49550400
H	-0.05034700	-0.19674500	-2.06460500
H	-0.86395600	2.13265300	-2.29361100
C	-1.08555100	-2.19630400	-0.50130800
H	-1.89042500	-2.89358300	-0.22517800
H	-0.61227800	-2.58917900	-1.41043800
C	-0.02489300	-2.22945300	0.63901400
H	0.33710000	-3.26979200	0.71674800
N	-0.60152200	-1.71452900	1.89623500
H	-1.46164000	-2.22876300	2.10122500

H	0.03600700	-1.91388500	2.67182200
C	1.17901800	-1.37062000	0.26034900
O	1.44328200	-0.32462700	0.88129400
O	1.85320100	-1.82160900	-0.76420600
H	2.53957200	-1.12043200	-1.10845300
Na	-0.55015900	0.81524200	1.55235200
O	0.61777900	2.74410400	1.29338400
H	1.52379500	2.62853000	0.91666100
H	0.42831900	3.69344700	1.25836600
O	3.34303600	0.01496000	-1.75596100
H	3.44966400	0.78338400	-1.14097200
H	4.20933500	-0.16629700	-2.15393100
O	3.06238400	1.72486600	0.38377300
H	3.81439800	1.88216600	0.97886400
H	2.62339300	0.88281000	0.68895800

(5) $Na^+(Phe)(H_2O)_4$
BP86-D3(BJ)/def-TZVPP, Singlet
Energy = -1023.199 a.u.
Gibbs free energy = -1022.971 a.u.

Na	-0.37915200	1.19944700	1.24359500
O	4.12074200	-0.36153900	-1.37868900
H	3.96123800	0.59702200	-1.18514000
H	4.29131400	-0.45029300	-2.32962800
O	0.70675800	2.95832100	0.23337100
H	0.46511100	3.85389500	-0.04524200
H	1.64578200	2.82740100	-0.03897700
O	-2.59920100	1.70219600	1.51814700
H	-3.16668000	2.39175500	1.89515400
H	-3.12529400	1.27985700	0.81088800
O	3.28093800	1.93306800	-0.16279200
H	3.96673900	2.31332600	0.41149800
H	2.83983700	1.20573400	0.36023100
C	-2.94144500	0.79928800	-1.73012800
C	-3.54151400	-0.16781600	-0.91494300
C	-2.76891800	-1.19869400	-0.36550000
C	-1.39574600	-1.29563100	-0.63586400
C	-0.81034600	-0.32922100	-1.47497100
C	-1.57187400	0.71537600	-2.00633000
H	-3.54064600	1.59820500	-2.16758700
H	-4.61649300	-0.13804900	-0.72820500
H	-3.24720700	-1.95466500	0.26054800
H	0.24675000	-0.40613100	-1.73683000
H	-1.10041300	1.45204700	-2.65699400
C	-0.57644700	-2.41843400	-0.04127000
H	-1.24983000	-3.18106700	0.37624700
H	0.02633800	-2.91383600	-0.81448900
C	0.38406600	-1.97249500	1.09330900
H	0.83663900	-2.89344200	1.50311700
N	-0.33624000	-1.17843000	2.10226700
H	-1.22640300	-1.63153800	2.31992500
H	0.19535400	-1.16065100	2.97605600
C	1.54885800	-1.15108200	0.54026500
O	1.71544800	0.03845900	0.86324100
O	2.31407100	-1.82002000	-0.28332600
H	3.05237100	-1.22609700	-0.71300800

(6)$Na^+(Phe)(H_2O)_5$
BP86-D3(BJ)/def-TZVPP, Singlet
Energy = -1099.690 a.u.
Gibbs free energy = -1099.437 a.u.

O	-2.70561500	-2.27985200	1.47091100
H	-3.39809500	-1.61377200	1.27392100
H	-2.99233000	-2.73761600	2.27569800
O	-3.13429500	0.62113700	-1.87059300
H	-3.72507400	0.88997300	-2.59335200
H	-3.68966000	0.47931500	-1.05187200
O	1.02765000	-1.02964700	2.04417300
H	1.92869500	-1.32886000	1.83634600
H	1.08592000	-0.03063200	2.00021000
O	-3.90296500	0.17564700	0.64074200
H	-2.99690100	0.53591300	0.83884800
H	-4.53734600	0.69289700	1.16394600
C	3.00650500	-2.02309500	-0.77221900
C	3.74989200	-1.12826900	0.00509300
C	3.36300000	0.21284000	0.09111000
C	2.23255200	0.68192200	-0.59316300
C	1.50978800	-0.21935800	-1.39096800
C	1.88963800	-1.56210400	-1.47718900
H	3.31289600	-3.06664000	-0.84980200
H	4.64031600	-1.47142500	0.53337200
H	3.95455500	0.90671400	0.69191200
H	0.65342600	0.13043800	-1.97006100
H	1.32215400	-2.23992300	-2.11581000
C	1.79128300	2.11925100	-0.45612100
H	2.63287900	2.73882000	-0.11294500
H	1.46998400	2.52632200	-1.42402900
C	0.62851100	2.32401900	0.55297000
H	0.41294000	3.41046000	0.56861200
N	0.97884300	1.78981300	1.87477900
H	1.83065100	2.24294800	2.21226300
H	0.24247200	1.99578600	2.55359300
C	-0.66326100	1.67688600	0.07411400
O	-1.27838400	0.83301000	0.74335300
O	-1.07003300	2.12606300	-1.09924200
H	-1.89717800	1.62261000	-1.40276300
O	-1.53571000	-1.68853400	-1.55298000
H	-1.92138400	-2.50503900	-1.90724300
H	-2.13429300	-0.96868700	-1.85345000
Na	-0.66356100	-1.57213100	0.63604200

(7) $Na^+(Phe)(H_2O)_6$
BP86/def-QZVPPD, Singlet
Energy = -1176.180 a.u.
Gibbs free energy = -1175.906 a.u.

O	-2.79518000	1.78458600	1.18887600
H	-3.35540200	2.52655000	1.46742000
H	-1.83613100	2.13243000	1.16151700
O	-3.70861600	-0.39191200	-0.50880600
H	-3.54571900	-0.89836000	0.31548100
H	-3.47163800	0.51864900	-0.22559000
O	-2.17550700	-1.10591700	-2.48560800
H	-2.81597700	-0.87423300	-1.71782600
H	-2.72368100	-1.27652300	-3.26934500
O	-0.37709900	-2.87949700	-1.33935000
H	-1.04398400	-2.34862600	-1.84345500
H	-0.42446300	-3.77969900	-1.69277000
C	3.52044100	-1.37754800	0.54066100
C	3.33215200	-0.33034400	1.45113200
C	2.77933600	0.88121500	1.02287200
C	2.38641900	1.06282900	-0.31397200
C	2.58286400	0.00530700	-1.21883000
C	3.15255000	-1.20223200	-0.80100200

H	3.98106900	-2.31116600	0.86633800
H	3.63839600	-0.44887500	2.49084000
H	2.68027600	1.70428700	1.73348900
H	2.29701100	0.13409700	-2.26447500
H	3.32015500	-2.00100800	-1.52454600
C	1.71228600	2.33333000	-0.76873400
H	2.16444400	3.21201000	-0.28457600
H	1.83696100	2.45902400	-1.85329700
C	0.18142900	2.36599800	-0.45343600
H	-0.25916700	3.22419100	-0.97781400
N	-0.16136900	2.46828500	0.97628700
H	0.27817400	1.69561000	1.48687600
H	0.20344300	3.34112100	1.36399600
C	-0.45783300	1.08722100	-0.97187500
O	-0.59742800	0.10641300	-0.24047200
O	-0.80279900	1.12151900	-2.24579100
H	-1.27257600	0.23941200	-2.47054700
O	-0.41137700	-1.70121200	2.55552500
H	-1.34354300	-1.35169200	2.56351100
H	-0.27727600	-2.14132700	3.40708700
O	-2.91399600	-0.69069700	2.25067100
H	-2.87791500	0.28524500	2.03307400
H	-3.59714000	-0.79546500	2.93224500
Na	0.42658300	-1.76587000	0.46791800

References

1. H.Wincel, "Hydration Energies of Sodiated Amino Acids from Gas-Phase Equilibria Determinations," *J. Phys. Chem. A,* 2007, **111**, 5784-5791.

2. F. Costanzo, RG. Della Valle, "Car-Parrinello MD Simulations for the Na^+-Phenylalanine Complex in Aqueous Solution," *J. Phys. Chem. B*, 2008, **112**, 12783–12789