Supplementary Information

Conformational and zwitterionic preferences of N-amidinoglycine: The effect of microsolvation and metal ion addition

Devendra K. Dhaked, Prasad V. Bharatam*

Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER),Sector-67, S. A. S. Nagar - 160 062, Punjab, India.

pvbharatam@niper.ac.in

Table of contents

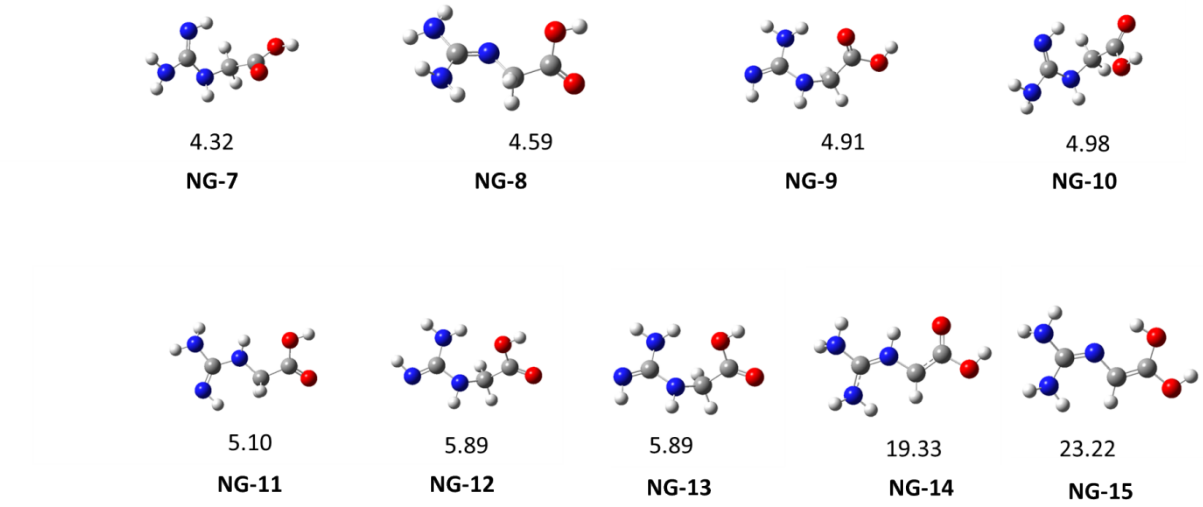


Figure S 1. B3LYP/6-311++G(d,p) optimized others structures of NG (Energy in kcal/mol).

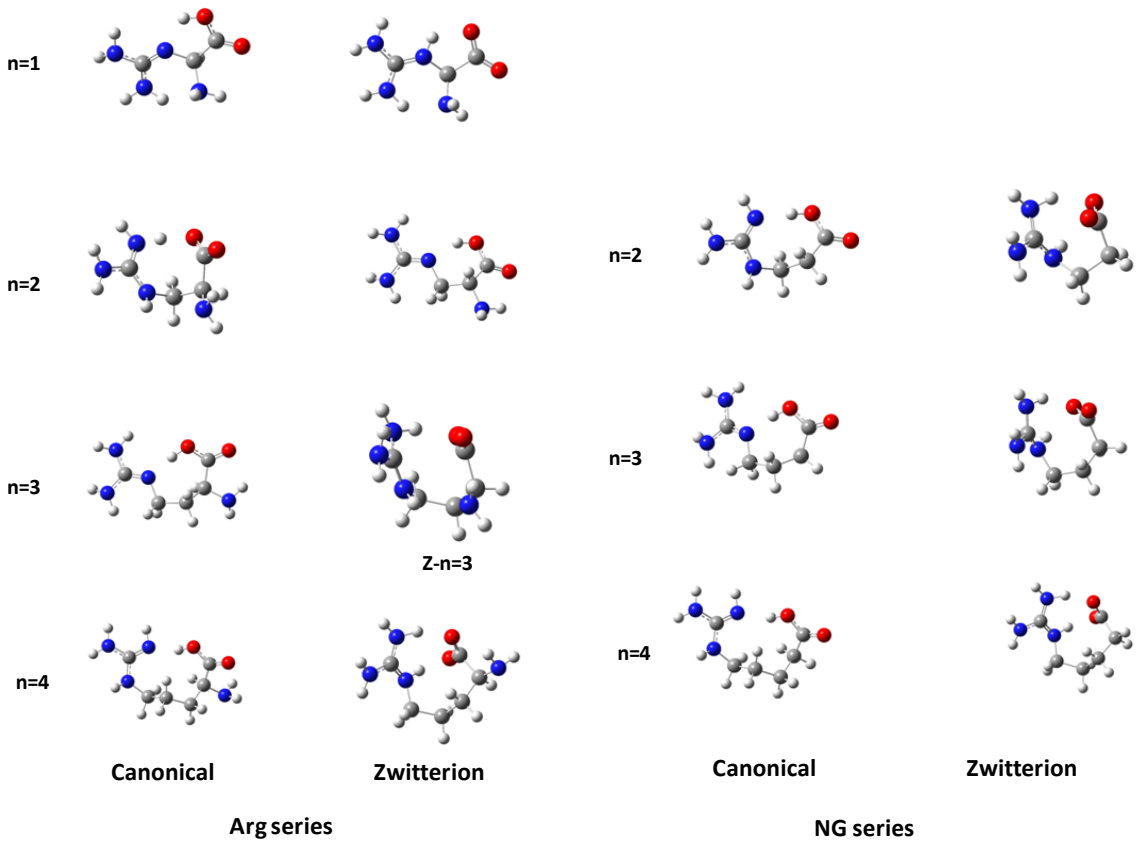


Figure S 2. Optimized canonical and zwitterionic species of Arg and NG series.

(For n=4 in Arg series the zwitterionic and canonical structures from ref 21)

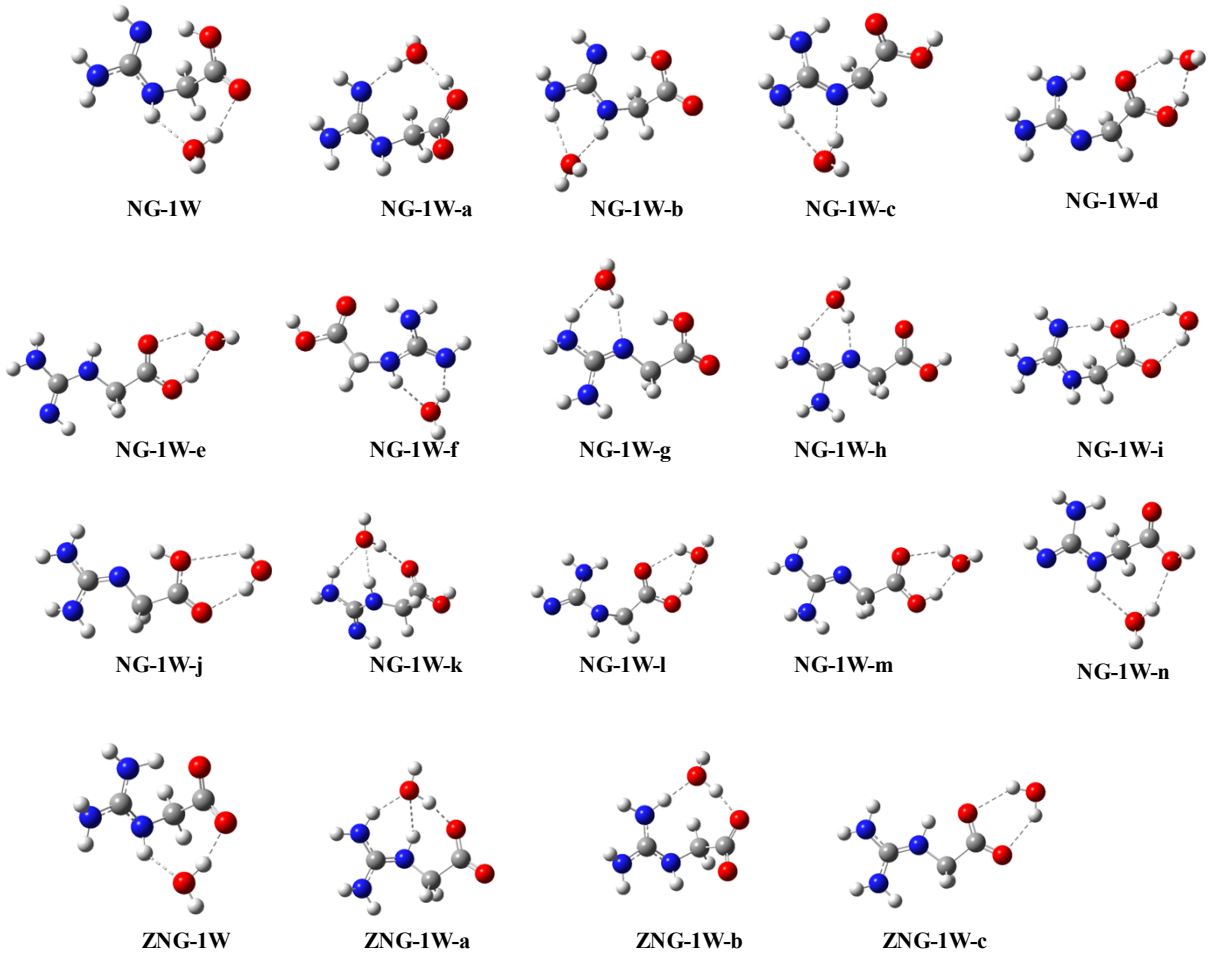


Figure S 3. ωB97XD/6-311++G(d,p) optimized geometries of canonical and zwitterionic configurations of NG with one water molecule.

Table S1. Relative energies (kcal/mol) of canonical and zwitterionic configurations of NG with one water molecule.

	B3LYP			**wB97XD**
	6-31+G(d,p)	6-311++G(d,p)	Aug-CC-pVDZ	6-311++G(d,p)
		Canonical configurations		
NG-1W	0.00	0.00	0.00	0.00
NG-1W-a	2.47	2.26	2.38	1.92
NG-1W-b	1.90	1.39	1.83	2.02
NG-1W-c	1.46	1.33	1.57	2.09
NG-1W-d	1.59	1.54	1.96	2.71
NG-1W-e	2.54	2.14	2.36	3.12
NG-1W-f	2.95	2.73	2.88	3.23
NG-1W-g	3.48	2.99	3.15	3.29
NG-1W-h	3.01	2.58	--	3.36
NG-1W-i	2.78	2.55	2.56	3.70
NG-1W-j	3.24	2.71	2.85	4.21
NG-1W-k	5.22	4.65	5.04	4.52
NG-1W-l	3.91	3.68	4.03	4.55
NG-1W-m	4.18	3.88	4.00	5.36
NG-1W-n	10.34	--	10.11	10.30
		Zwitterionic configurations		
ZNG-1W	3.06	3.47	3.32	3.64
ZNG-1W-a	5.98	5.88	6.62	6.46
ZNG-1W-b	8.07	8.22	8.61	8.40
ZNG-1W-c	12.14	12.21	12.22	13.76

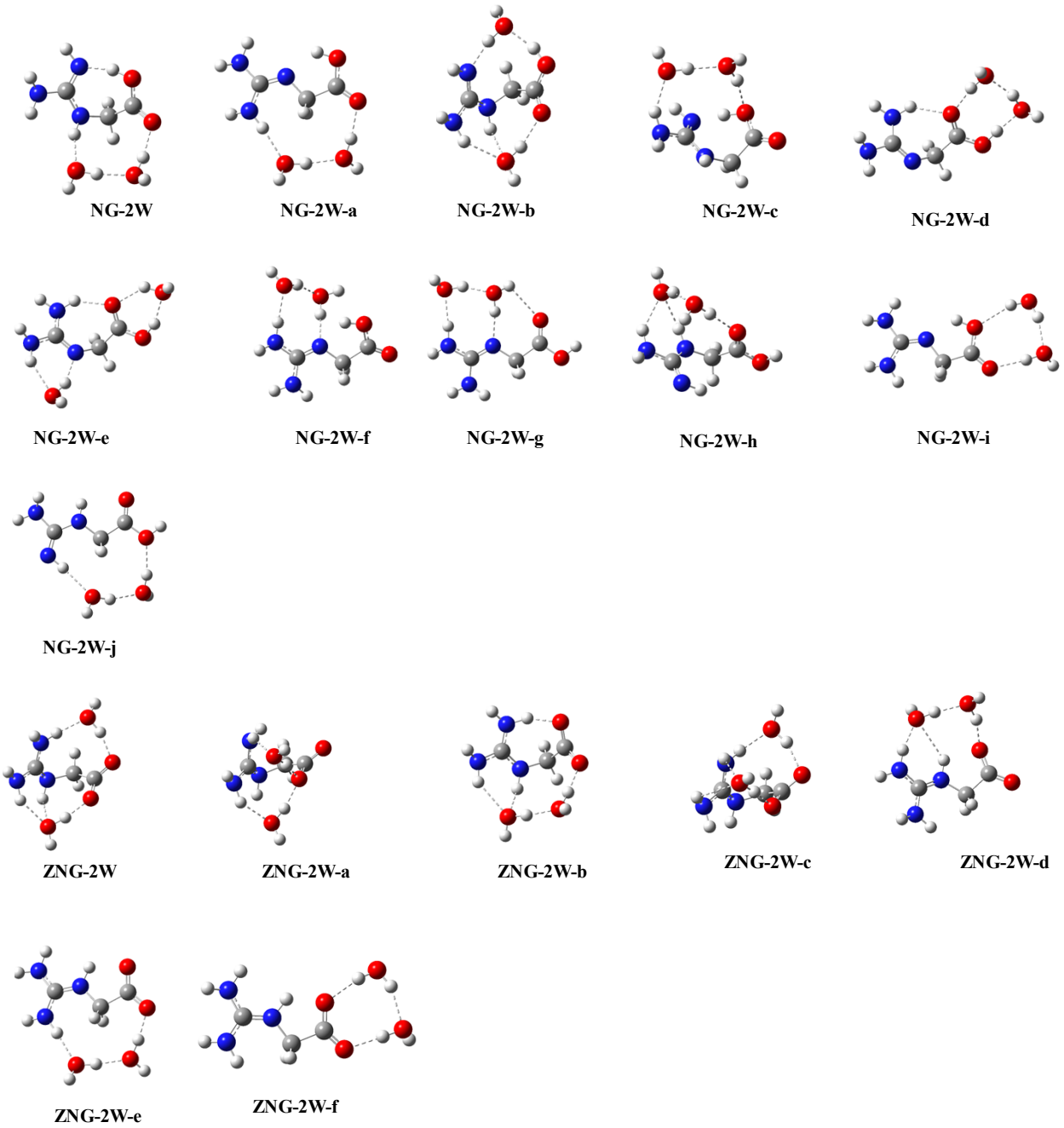


Figure S4. ωB97XD/6-311++G(d,p) optimized geometries of canonical and zwitterionic configurations of NG with two water molecules.

Table S2. Relative energies (kcal/mol) of canonical and zwitterionic configurations of NG with two water molecules.

Entry	B3LYP			wB97XD
	6-31+G(d,p)	6-311++G(d,p)	Aug-CC-pVDZ	6-311++G(d,p)
Canonical configurations				
NG-2W	0.00	0.00	0.00	0.00
NG-2W-a	1.24	0.85	0.80	0.86
NG-2W-b	3.57	3.31	3.44	1.41
NG-2W-c	3.87	3.76	4.39	3.39
NG-2W-d	3.65	3.45	4.01	4.56
NG-2W-e	4.82	4.54	4.68	5.14
NG-2W-f	7.58	5.90	5.94	5.60
NG-2W-g	5.74	5.24	5.52	5.61
NG-2W-h	8.47	7.60	8.16	6.99
NG-2W-i	8.96	8.16	8.33	9.95
NG-2W-j	14.81	13.82	14.01	14.48
Zwitterionic configurations				
ZNG-2W	2.02	2.08	2.65	0.18
ZNG-2W-a	4.12	3.93	5.31	0.84
ZNG-2W-b	1.34	1.54	1.03	1.08
ZNG-2W-c	7.34	7.14	7.99	4.76
ZNG-2W-d	5.08	4.85	5.65	5.46
ZNG-2W-e	6.22	6.37	6.11	6.06
ZNG-2W-f	15.42	15.07	15.30	16.94

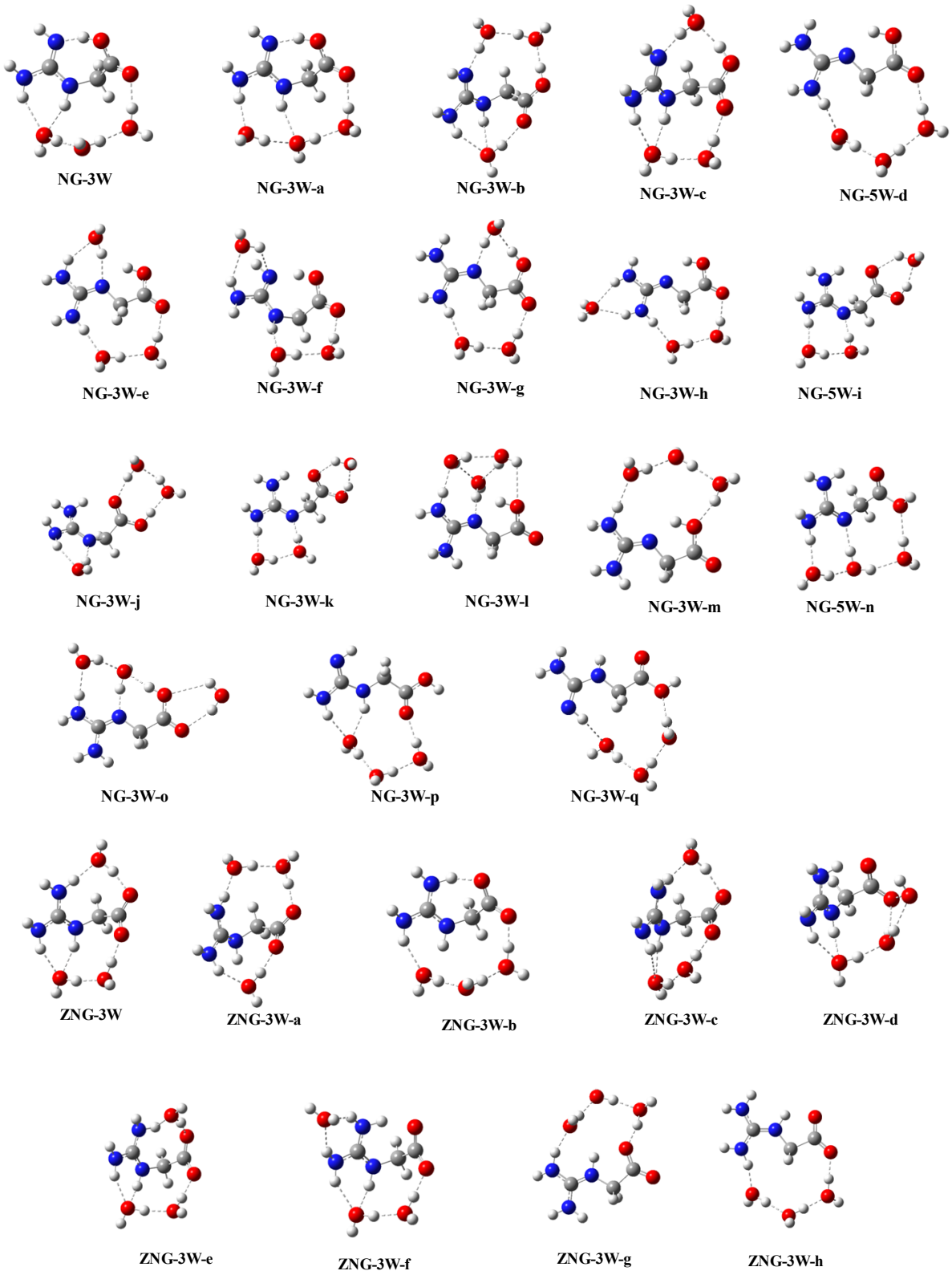


Figure S5. ωB97XD/6-311++G(d,p) optimized geometries of canonical and zwitterionic configurations of NG with three water molecules.

Table S3. Relative energies (kcal/mol) of canonical and zwitterionic configurations of NG with three water molecules.

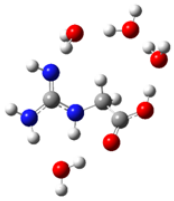
Entry	B3LYP			wB97XD
	6-31+G(d,p)	6-311++G(d,p)	Aug-CC-pVDZ	6-311++G(d,p)
Canonical configurations				
NG-3W	0.00	0.00	0.00	0.00
NG-3W-a	0.85	1.11	0.51	0.29
NG-3W-b	2.49	2.35	2.22	0.77
NG-3W-c	2.80	2.85	2.53	1.39
NG-3W-d	2.52	2.01	2.16	2.86
NG-3W-e	6.27	5.92	5.08	4.53
NG-3W-f	4.91	4.77	4.36	4.97
NG-3W-g	6.16	6.01	5.23	5.26
NG-3W-h	6.17	5.78	5.23	5.61
NG-3W-i	5.38	5.25	5.16	5.77
NG-3W-j	5.28	5.13	4.91	5.80
NG-3W-k	11.84	--	5.77	6.40
NG-3W-l	9.40	9.28	9.16	7.81
NG-3W-m	6.82	6.25	6.82	7.84
NG-3W-n	9.75	9.56	9.34	9.58
NG-3W-o	12.58	12.37	11.11	12.52
NG-3W-p	12.91	12.17	--	13.23
NG-3W-q	17.80	16.94	--	18.05
Zwitterionic configurations				
ZNG-3W	0.09	0.21	0.24	-1.25
ZNG-3W-a	0.53	0.61	0.98	-0.67
ZNG-3W-b	-0.29	0.01	0.00	-0.03
ZNG-3W-c	3.16	3.17	0.46	0.52
ZNG-3W-d	2.22	2.24	2.52	0.68
ZNG-3W-e	2.54	2.55	2.74	0.86
ZNG-3W-f	4.21	4.18	3.90	3.26
ZNG-3W-g	5.10	4.86	5.61	5.92
ZNG-3W-h	5.14	--	5.08	6.13

NG-4W

NG-4W-a

NG-4W-b

NG-4W-c



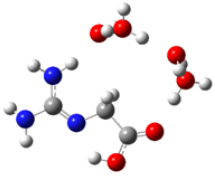
NG-4W-d

NG-4W-e

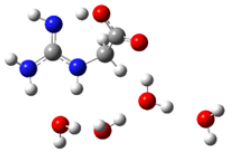
NG-4W-f

NG-4W-g

NG-4W-h

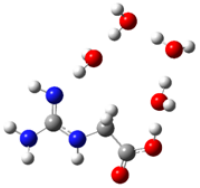


NG-4W-i

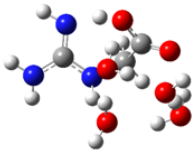


NG-4W-j

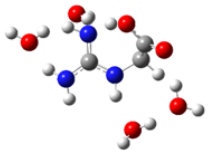
NG-4W-k



NG-4W-l

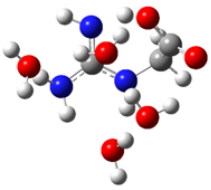


NG-4W-m

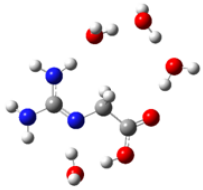


NG-4W-n

NG-4W-o



NG-4W-p

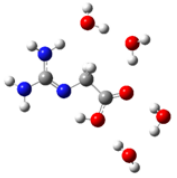


NG-4W-q

NG-4W-r

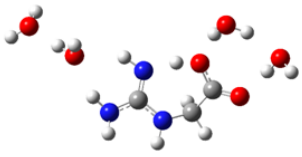
NG-4W-s

NG-4W-t



NG-4W-v

NG-4W-u



NG-4W-w

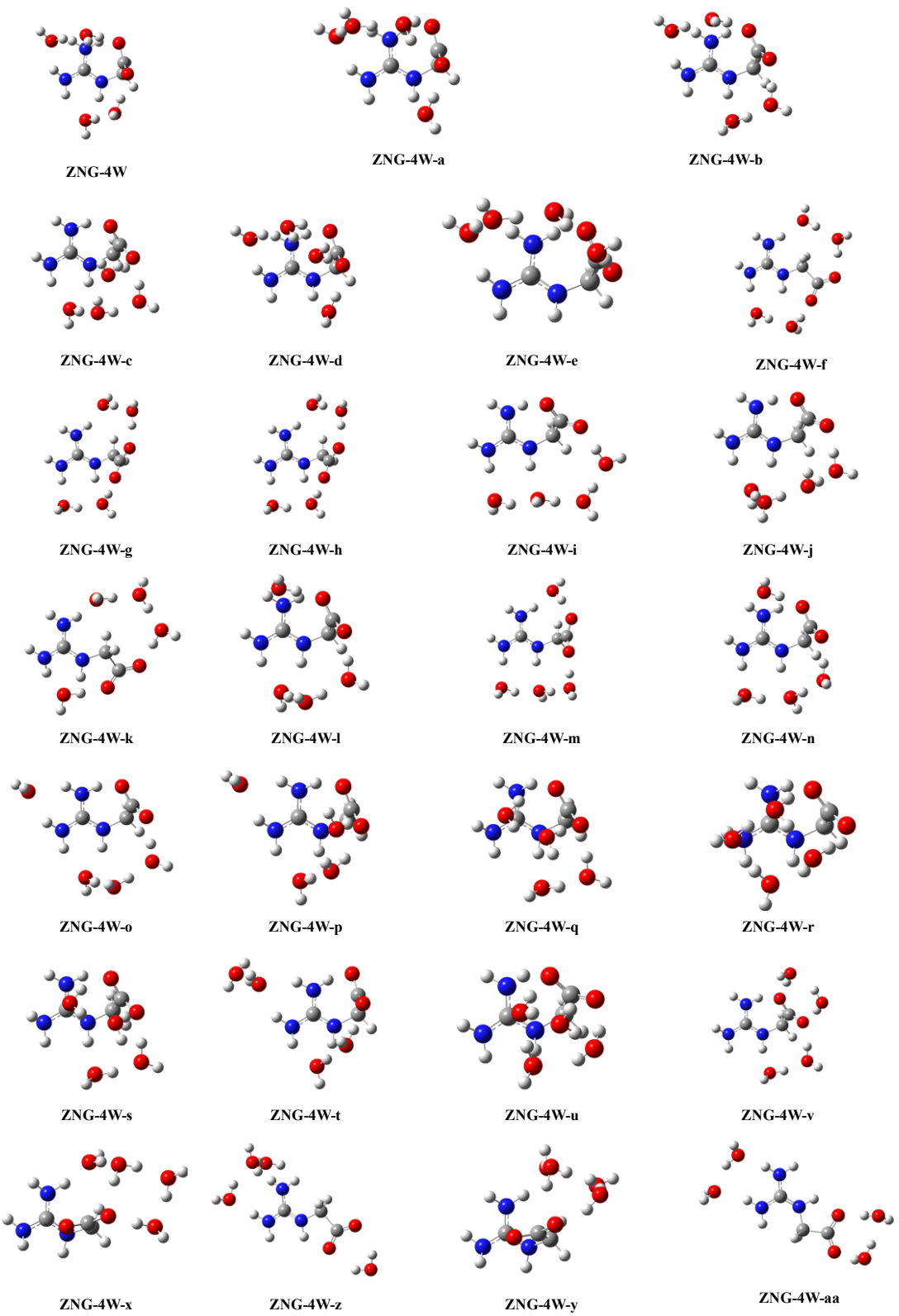
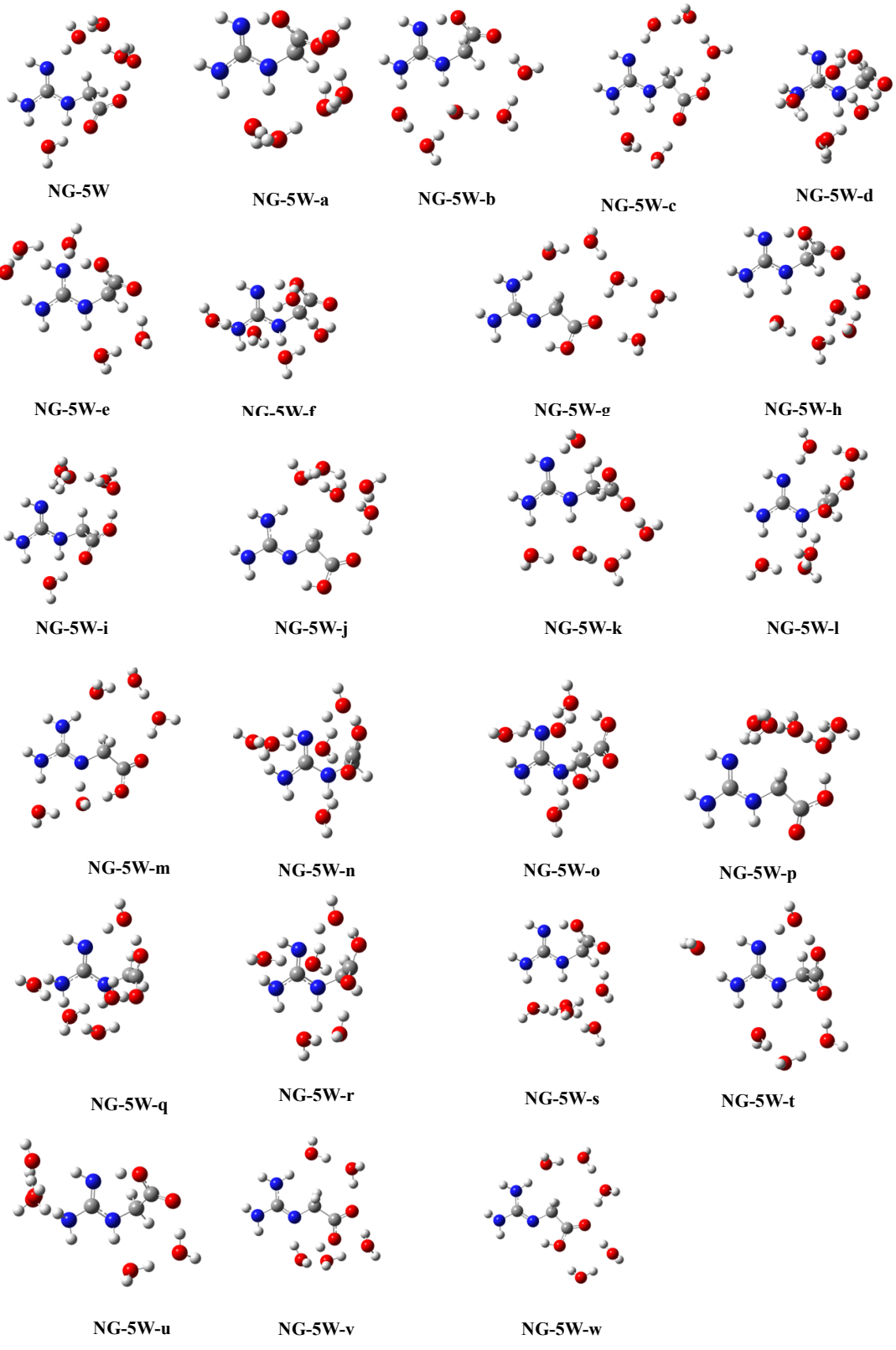


Figure S6. B3LYP/6-311++G(d,p) optimized geometries of canonical and zwitterionic configurations of NG with four water molecules.

Table S4. Relative energies (kcal/mol) of canonical and zwitterionic configurations of NG with four water molecule.

	B3LYP			wB97XD
	6-31+G(d,p)	6-311++G(d,p)	Aug-CC-pVDZ	6-311++G(d,p)
Canonical configurations				
NG-4W	1.04	0.96	1.27	0.00
NG-4W-a	0.00	0.00	0.00	0.19
NG-4W-b	0.00	-0.03	0.31	0.62
NG-4W-c	2.93	2.96	3.38	1.81
NG-4W-d	3.02	1.88	2.18	1.88
NG-4W-e	3.25	3.18	3.18	--
NG-4W-f	3.26	3.29	2.98	--
NG-4W-g	3.30	3.05	2.89	--
NG-4W-h	3.69	2.95	3.76	--
NG-4W-i	3.97	3.25	3.84	--
NG-4W-j	4.05	--	--	--
NG-4W-k	4.14	--	--	--
NG-4W-l	4.85	--	--	--
NG-4W-m	4.89	--	--	--
NG-4W-n	5.57	--	--	--
NG-4W-o	6.17	--	--	--
NG-4W-p	6.66	--	--	--
NG-4W-q	6.78	--	--	--
NG-4W-r	6.79	--	--	--
NG-4W-s	8.85	--	--	--
NG-4W-t	9.97	--	--	--
NG-4W-u	10.22	--	--	--
NG-4W-v	10.89	--	--	--
NG-4W-w	14.08	--	--	--
Zwitterionic configurations				
ZNG-4W	-3.94	-3.97	-2.87	-6.45
ZNG-4W-a	-3.05	-2.95	-2.12	-4.96
ZNG-4W-b	-2.74	-2.86	-2.10	-6.44
ZNG-4W-c	-2.38	-2.35	-1.85	-3.98
ZNG-4W-d	-2.29	-2.37	-1.30	-5.45
ZNG-4W-e	-1.95	-1.98	-0.76	--
ZNG-4W-f	-1.60	-1.82	-1.76	--
ZNG-4W-g	-1.27	-1.10	-0.76	--
ZNG-4W-h	-1.25	-1.43	-0.47	--
ZNG-4W-i	-0.81	-0.55	-0.45	--
ZNG-4W-j	-0.59	--	--	--
ZNG-4W-k	-0.31	--	--	--
ZNG-4W-l	0.14	--	--	--
ZNG-4W-m	0.27	--	--	--

ZNG-4W-n	0.38	--	--	--
ZNG-4W-o	1.23	--	--	--
ZNG-4W-p	3.12	--	--	--
ZNG-4W-q	4.03	--	--	--
ZNG-4W-r	4.11	--	--	--
ZNG-4W-s	4.18	--	--	--
ZNG-4W-t	5.63	--	--	--
ZNG-4W-u	5.65	--	--	--
ZNG-4W-v	5.80	--	--	--
ZNG-4W-w	5.80	--	--	--
ZNG-4W-x	8.93	--	--	--
ZNG-4W-y	14.08	--	--	--
ZNG-4W-z	18.24	--	--	--
ZNG-4W-aa	18.57	--	--	--


NG-5W
NG-5W-a
NG-5W-b
NG-5W-c
NG-5W-d
NG-5W-e
NG-5W-f
NG-5W-g
NG-5W-h
NG-5W-i
NG-5W-j
NG-5W-k
NG-5W-l
NG-5W-m
NG-5W-n
NG-5W-o
NG-5W-p
NG-5W-q
NG-5W-r
NG-5W-s
NG-5W-t
NG-5W-u
NG-5W-v
NG-5W-w

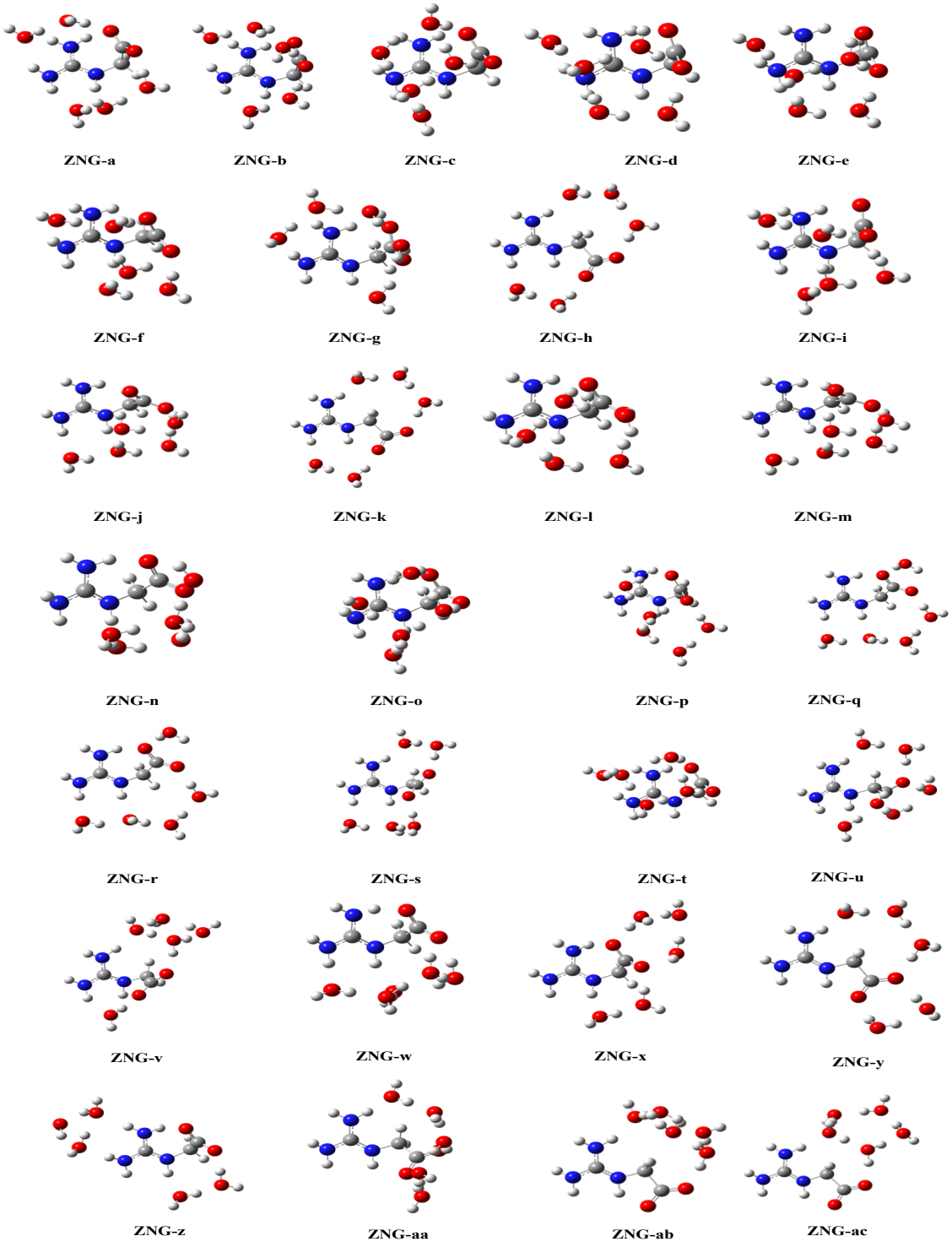
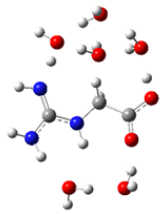


Figure S7 B3LYP/6-311++G(d,p) optimized geometries of canonical and zwitterionic configurations of NG with five water molecules.

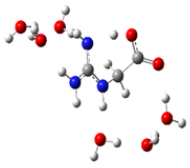
Table S5. Relative energies (kcal/mol) of canonical and zwitterionic configurations of NG with five-water molecule.

	B3LYP			wB97XD
	6-31+G(d,p)	6-311++G(d,p)	Aug-CC-pVDZ	6-311++G(d,p)
Canonical configurations				
NG-5W	3.16	2.87	2.18	0.00
NG-5W-a	0.00	0.00	0.00	0.57
NG-5W-b	1.90	1.87	1.56	2.30
NG-5W-c	2.18	1.71	1.44	1.52
NG-5W-d	2.32	2.54	2.55	0.49
NG-5W-e	3.42	3.27	2.87	--
NG-5W-f	3.88	4.02	4.01	--
NG-5W-g	3.94	3.11	3.32	--
NG-5W-h	4.23	4.06	3.66	--
NG-5W-i	4.75	4.41	3.74	--
NG-5W-j	5.08	--	--	--
NG-5W-k	5.24	--	--	--
NG-5W-l	5.55	--	--	--
NG-5W-m	5.84	--	--	--
NG-5W-n	5.96	--	--	--
NG-5W-o	6.14	--	--	--
NG-5W-p	6.19	--	--	--
NG-5W-q	6.22	--	--	--
NG-5W-r	6.25	--	--	--
NG-5W-s	6.61	--	--	--
NG-5W-t	7.10	--	--	--
NG-5W-u	7.68	--	--	--
NG-5W-v	9.41	--	--	--
NG-5W-w	9.98	--	--	--
Zwitterionic configurations				
ZNG-5W	-6.04	-5.83	-5.05	-10.05
ZNG-5W-a	-5.03	-5.09	-4.44	-7.03
ZNG-5W-b	-4.45	-4.68	-3.92	-8.59
ZNG-5W-c	-4.39	-4.25	-3.32	-8.00
ZNG-5W-d	-4.05	-3.96	-3.44	-8.49
ZNG-5W-e	-4.03	-3.96	-3.43	--
ZNG-5W-f	-3.70	-3.74	-3.33	--
ZNG-5W-g	-3.23	-3.50	-3.06	--
ZNG-5W-h	-3.14	-3.47	-3.19	--
ZNG-5W-i	-3.05	-3.09	-2.57	--
ZNG-5W-j	-2.65	--	--	--
ZNG-5W-k	-2.63	--	--	--

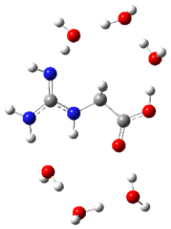
ZNG-5W-l	-1.69	--	--	--
ZNG-5W-m	-1.69	--	--	--
ZNG-5W-n	-1.30	--	--	--
ZNG-5W-o	-0.52	--	--	--
ZNG-5W-p	0.43	--	--	--
ZNG-5W-q	0.71	--	--	--
ZNG-5W-r	0.71	--	--	--
ZNG-5W-s	1.31	--	--	--
ZNG-5W-t	1.52	--	--	--
ZNG-5W-u	3.53	--	--	--
ZNG-5W-v	5.62	--	--	--
ZNG-5W-w	5.64	--	--	--
ZNG-5W-x	6.59	--	--	--
ZNG-5W-y	6.82	--	--	--
ZNG-5W-z	7.69	--	--	--
ZNG-5W-aa	7.89	--	--	--
ZNG-5W-bb	11.22	--	--	--
ZNG-5W-cc	13.56	--	--	--



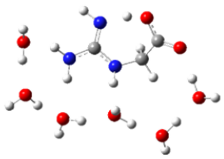
NG-6W



NG-6W-a

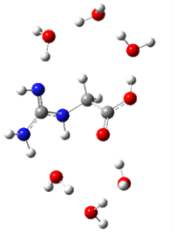


NG-6W-b

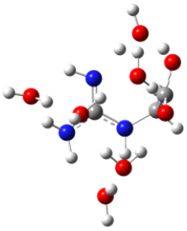


NG-6W-c

NG-6W-d



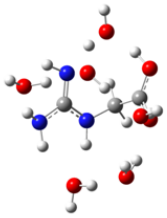
NG-6W-e



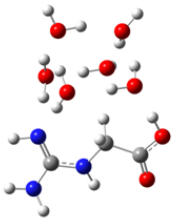
NG-6W-f

NG-6W-g

NG-6W-h

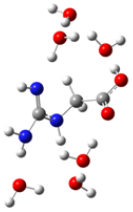


NG-6W-i

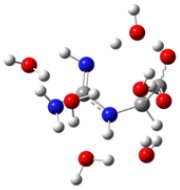


NG-6W-J

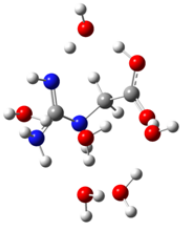
NG-6W-k



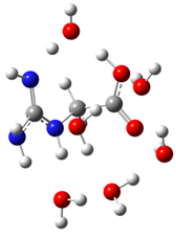
NG-6W-L



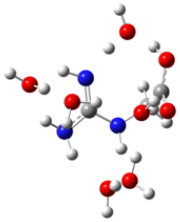
NG-6W-m



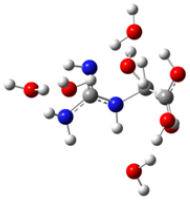
NG-6W-n



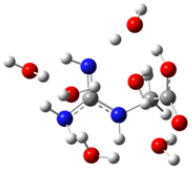
NG-6W-o



NG-6W-p

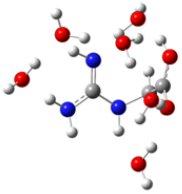


NG-6W-q

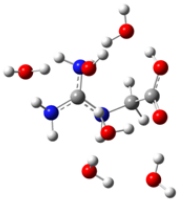


NG-6W-r

NG-6W-s

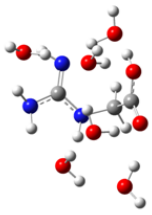


NG-6W-u



NG-6W-t

NG-6W-v



NG-6W-w

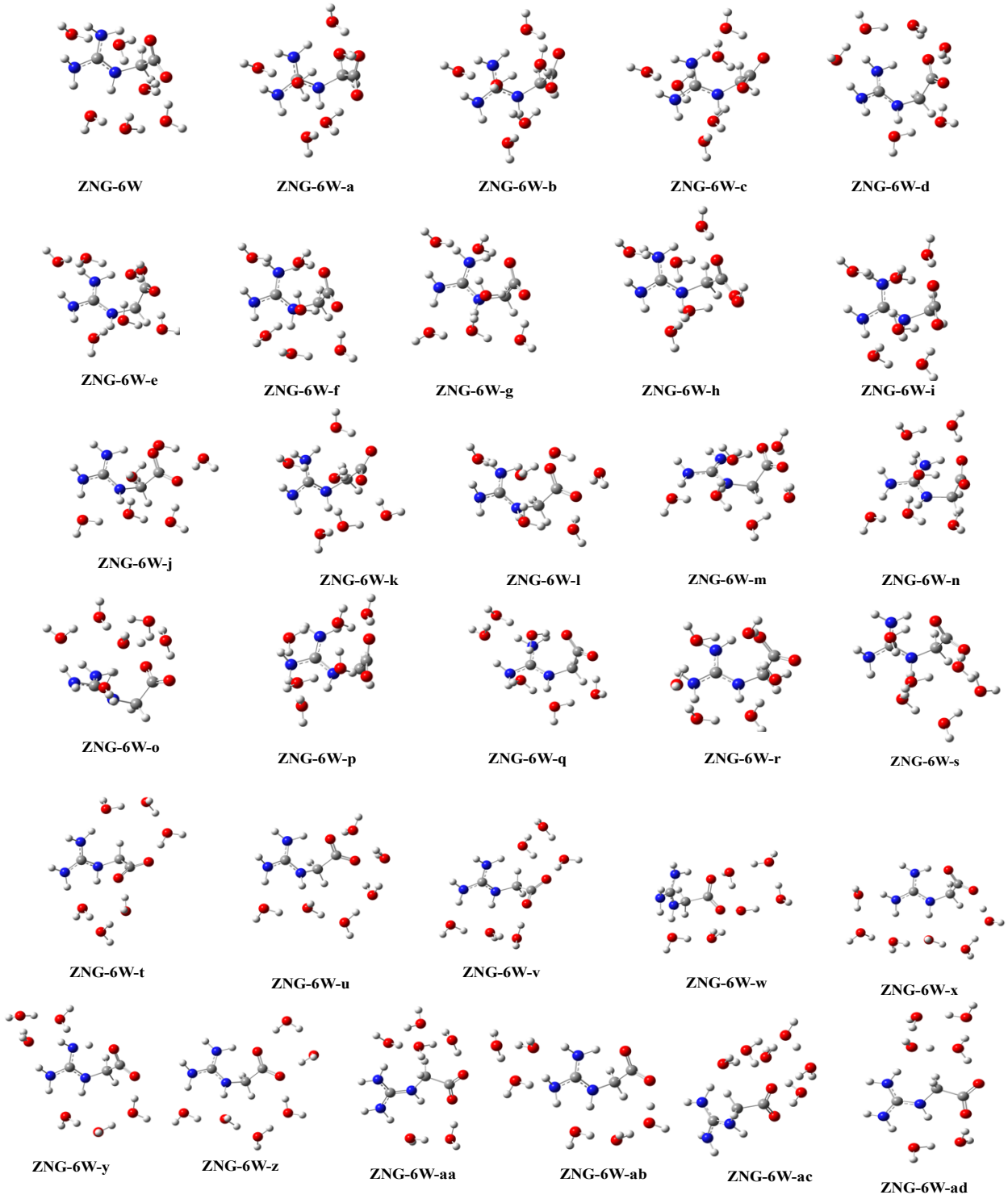


Figure S8. B3LYP/6-311++G(d,p) optimized geometries of canonical and zwitterionic configurations of NG with six water molecules.

Table S6. Relative energies (kcal/mol) of canonical and zwitterionic configurations of NG with six water molecule.

	B3LYP			wB97XD
	6-31+G(d,p)	6-311++G(d,p)	Aug-CC-pVDZ	6-311++G(d,p)
Canonical configurations				
NG-6W	0.20	-0.09	-0.65	0.00
NG-6W-a	0.00	0.00	0.00	0.86
NG-6W-b	0.77	0.17	0.27	2.40
NG-6W-c	1.12	1.16	0.99	3.50
NG-6W-d	1.58	1.43	1.58	1.40
NG-6W-e	1.77	1.25	1.53	--
NG-6W-f	1.81	1.78	1.70	--
NG-6W-g	2.18	1.66	1.18	--
NG-6W-h	2.52	2.39	2.47	--
NG-6W-i	2.57	2.50	2.47	--
NG-6W-j	3.05	--	--	--
NG-6W-k	3.46	--	--	--
NG-6W-l	3.48	--	--	--
NG-6W-m	3.55	--	--	--
NG-6W-n	3.61	--	--	--
NG-6W-o	4.13	--	--	--
NG-6W-p	4.31	--	--	--
NG-6W-q	4.32	--	--	--
NG-6W-r	4.52	--	--	--
NG-6W-s	5.52	--	--	--
NG-6W-t	6.31	--	--	--
NG-6W-u	6.90	--	--	--
NG-6W-v	7.09	--	--	--
NG-6W-w	7.28	--	--	--
Zwitterionic configurations				
ZNG-6W-	-10.98	-10.96	-9.83	-13.63
ZNG-6W-a	-10.43	-10.48	-9.51	-13.16
ZNG-6W-b	-9.74	-9.83	-8.90	-12.22
ZNG-6W-c	-9.33	-9.36	-8.33	-13.47
ZNG-6W-d	-8.81	-9.10	-8.21	-10.36
ZNG-6W-e	-8.56	-8.57	-7.46	--
ZNG-6W-f	-8.47	-8.36	-7.74	--
ZNG-6W-g	-8.35	-8.43	-7.73	--
ZNG-6W-h	-7.89	-7.83	-6.85	--
ZNG-6W-i	-7.38	-7.48	-6.95	--
ZNG-6W-j	-7.35	--	--	--

ZNG-6W-k	-7.28	--	--	--
ZNG-6W-l	-6.96	--	--	--
ZNG-6W-m	-6.88	--	--	--
ZNG-6W-n	-6.03	--	--	--
ZNG-6W-o	-5.68	--	--	--
ZNG-6W-p	-5.47	--	--	--
ZNG-6W-q	-4.97	--	--	--
ZNG-6W-r	-4.35	--	--	--
ZNG-6W-s	-3.34	--	--	--
ZNG-6W-t	-2.51	--	--	--
ZNG-6W-u	-2.46	--	--	--
ZNG-6W-v	-2.27	--	--	--
ZNG-6W-w	-0.95	--	--	--
ZNG-6W-x	-0.74	--	--	--
ZNG-6W-y	-0.72	--	--	--
ZNG-6W-z	-0.26	--	--	--
ZNG-6W-aa	0.13	--	--	--
ZNG-6W-ab	0.81	--	--	--
ZNG-6W-ac	1.13	--	--	--
ZNG-6W-ad	1.41	--	--	--

Table S7. Relative energies (kcal/mol) of charge-solvated and salt-bridge structures of NG with alkali metal cations at B3LYP/6-31+G(d,p), B3LYP /6-311++G(d,p), BHandHLYP/6-311++G(d,p) and M06/6-311++G(d,p) levels of theory.

Cations	CS-1	CS-2	CS-3	CS-4	SB-1	SB-2
			B3LYP/6-31+G(d,p)			
Li^+	3.88	5.11	15.39	NA	0.78	0.00
Na^+	9.03	8.94	16.03	11.88	0.93	0.00
K^+	11.07	10.24	14.67	8.62	1.24	0.00
Rb^+	11.33	10.31	13.86	6.71	1.71	0.00
Cs^+	11.27	10.19	13.07	5.44	1.94	0.00
			B3LYP/6-311++G(d,p)			
Li^+	3.69	4.84	15.07	NA	0.73	0.00
Na^+	8.57	8.59	15.57	11.96	0.93	0.00
K^+	10.54	9.74	14.24	8.84	1.09	0.00
Rb^+	10.56	9.69	12.99	6.41	1.59	0.00
Cs^+	10.50	9.58	12.21	5.06	1.80	0.00
			BHandHLYP/6-311++G(d,p)			
Li^+	2.38	3.39	14.17	17.08	0.36	0.00
Na^+	7.28	7.24	14.43	12.21	0.48	0.00
K^+	9.29	8.48	12.94	8.66	0.55	0.00
Rb^+	9.16	8.28	11.51	6.00	0.87	0.00
Cs^+	9.03	8.10	10.69	4.54	1.09	0.00
			M06/6-311++G(d,p)			
Li^+	3.24	3.75	13.13	14.54	0.47	0.00
Na^+	7.73	7.46	13.12	10.69	0.78	0.00
K^+	8.93	7.80	11.15	7.67	0.43	0.00
Rb^+	8.65	7.34	9.70	5.30	0.85	0.00
Cs^+	8.22	6.95	8.82	3.76	0.74	0.00

Table S8. Relative energies (kcal/mol) of charge-solvated and salt-bridge structures of NG with alkaline earth cations at B3LYP/6-31+G(d,p), B3LYP/6-311++G(d,p), BHandHLYP/6-311++G(d,p) and M06/6-311++G(d,p) levels of theory.

Cations	CS-1	CS-2	CS-3	CS-4	CS-5	SB-1
			B3LYP/6-31+G(d,p)			
Be^{2+}	-24.22	-12.51	9.75	-23.44	0.00	0.70
Mg^{2+}	3.51	10.18	22.93	1.12	0.00	1.99
Ca^{2+}	14.98	14.02	24.82	13.52	0.00	2.45
Sr^{2+}	16.49	15.03	24.70	15.83	0.00	2.22
Ba^{2+}	18.47	16.59	24.37	18.55	0.00	2.14
			B3LYP/6-311++G(d,p)			
Be^{2+}	-26.30	-13.95	8.72	-24.78	0.00	0.76
Mg^{2+}	2.35	9.10	21.84	0.17	0.00	2.00
Ca^{2+}	14.01	12.99	24.46	13.06	0.00	2.50
Sr^{2+}	14.92	13.68	23.01	14.34	0.00	2.20
Ba^{2+}	17.01	15.35	22.89	17.15	0.00	2.16
			BHandHLYP/6-311++G(d,p)			
Be^{2+}	-28.14	-15.01	9.38	-25.63	0.00	0.93
Mg^{2+}	1.14	8.45	21.52	-0.75	0.00	2.42
Ca^{2+}	13.47	12.97	24.31	12.56	0.00	2.92
Sr^{2+}	14.53	13.58	22.82	13.95	0.00	2.65
Ba^{2+}	16.77	15.28	22.81	16.92	0.00	2.57
			M06/6-311++G(d,p)			
Be^{2+}	-25.62	-13.68	7.88	-23.01	0.00	1.13
Mg^{2+}	2.24	8.49	19.94	0.62	0.00	1.95
Ca^{2+}	13.27	12.34	22.02	12.07	0.00	2.42
Sr^{2+}	13.62	12.28	19.88	12.68	0.00	1.99
Ba^{2+}	15.78	13.75	19.69	15.42	0.00	2.41

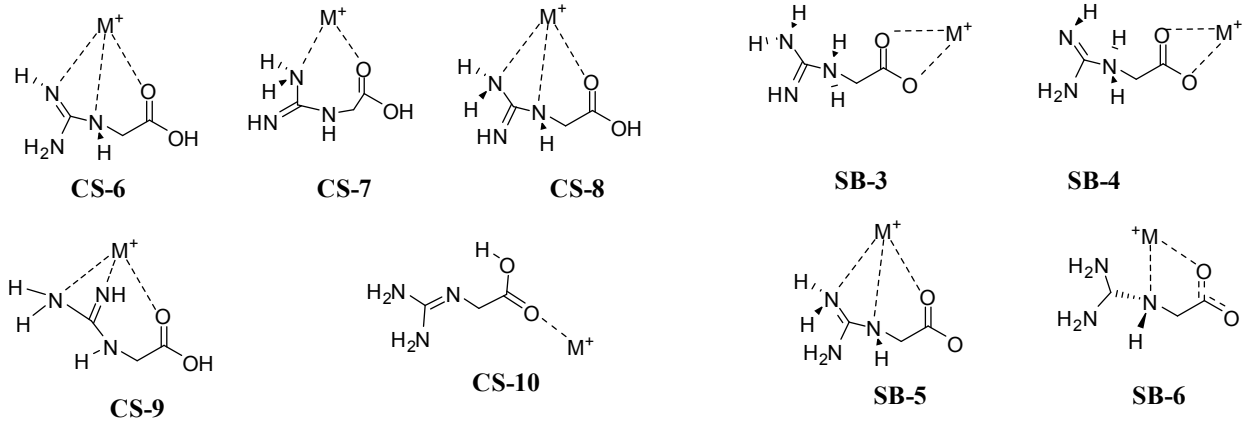


Figure S9.Some other initial guess for metal complexation.

CS-6 converged to **CS-1** after optimization. **CS-7** converged to **CS-8**. **CS-8** of Li^+ bound complex is found to be about 30 kcal/mol less stable than **CS-1**. **CS-9** and **CS-10** converged to **CS-3** and **CS-2**, respectively. **SB-3** and **SB-4** are found to be highly unstable compared to most preferred SB complex by about 29 and 36 kcal/mol in Li^+ bound complex. Both **SB-5** and **SB-6** converged to **SB-2**. So these are not considered for other metal ions.

Table S9. Cartesian coordinates of canonical and zwitterionic configurations of NG in the presence of one water molecule at ωB97XD/6-311++G (d,p) level.

NG-1W

N	-0.566052	0.668798	0.554203
N	-2.604309	1.059566	-0.433819
C	-1.705597	0.125032	0.029892
H	-3.494388	0.717190	-0.753356
N	-1.849891	-1.157852	-0.015812
H	-0.317294	-1.874579	-0.351576
H	-2.635389	1.944195	0.046718
C	0.461806	-0.188631	1.113369
H	-0.009245	-0.914296	1.779924
H	1.145079	0.434355	1.687063
C	1.274650	-0.922256	0.038238
O	2.411815	-0.600992	-0.228579
O	0.655039	-1.902868	-0.584749
H	-2.776702	-1.444734	-0.305780
H	-0.205905	1.520371	0.136679
O	1.779203	2.181021	-0.289802
H	2.279158	1.350104	-0.323772
H	2.202845	2.771654	-0.911858

NG-1W-a

N	0.976020	-0.747404	0.754553
N	2.920571	-0.220470	-0.375916
C	1.657452	0.180509	0.005264
H	3.319877	0.246318	-1.172309
N	1.162375	1.346928	-0.233582
H	3.158293	-1.195849	-0.302624
C	-0.422306	-0.535678	1.057839
H	-0.574362	0.499323	1.350824
H	-0.690156	-1.167765	1.908352
C	-1.326077	-0.973275	-0.105014
O	-1.153331	-2.045895	-0.623357
O	-2.311709	-0.164609	-0.458246
H	1.828596	1.938598	-0.717484
H	1.191920	-1.711460	0.547420
H	-0.451141	2.086138	-0.086312
O	-1.410913	2.315651	-0.012820
H	-2.147009	0.759902	-0.163911
H	-1.495565	3.020909	0.627510

NG-1W-b

N	0.447608	-0.207628	0.442106
N	2.206093	1.188564	-0.101418
C	0.854164	1.052386	0.129792
H	2.473343	1.954709	-0.696215
N	-0.015918	2.008894	0.104978
H	-1.482186	1.314534	-0.439306
H	2.735312	0.338278	-0.239836
C	-0.870676	-0.488034	0.973294
H	-1.112607	0.255788	1.739973
H	-0.855914	-1.474506	1.432799
C	-1.996950	-0.489790	-0.071652
O	-2.688965	-1.457507	-0.254733
O	-2.166020	0.646216	-0.729374
H	0.401225	2.917434	-0.053271
H	1.092767	-0.970052	0.302262
O	2.871175	-1.820758	-0.324097
H	2.810410	-2.310702	-1.146541
H	3.424418	-2.345278	0.257504

NG-1W-c

N	-0.518380	0.338608	0.311980
N	-2.382424	-0.910757	-0.196854
C	-1.046055	-0.822862	0.101932
H	-2.658981	-1.623930	-0.851577
N	-0.385475	-2.019568	0.241778
H	0.572798	-2.031626	-0.084421
H	-2.849164	-0.015843	-0.311368
C	0.790339	0.417177	0.918478
H	0.925471	-0.336635	1.709966
H	0.910920	1.402786	1.367476
C	1.924097	0.191796	-0.064941
O	2.797655	1.204168	-0.103493
O	2.060969	-0.798810	-0.744095
H	-0.914410	-2.862807	0.095098
H	3.489062	0.966607	-0.734266
O	-2.637419	2.042349	-0.215145
H	-1.753618	1.671035	-0.000295
H	-2.498048	2.674126	-0.919894

NG-1W-d

N	-1.403036	0.912010	-0.387148
N	-3.329922	-0.311452	-0.666229
C	-2.090210	-0.121703	-0.072596
H	-3.527975	-1.250681	-0.977424
N	-1.763674	-1.050674	0.893814
H	-0.790991	-1.327996	0.904630
H	-3.518484	0.387600	-1.369157
C	-0.263852	1.264229	0.424112
H	-0.456639	1.118239	1.500803
H	-0.030646	2.317614	0.269395
C	0.988845	0.460515	0.136787
O	2.080152	1.199886	0.040857
O	1.001245	-0.756358	0.041201
H	-2.431044	-1.782673	1.071626
H	2.854403	0.609366	-0.097708
O	3.733970	-0.934647	-0.300659
H	2.867488	-1.368868	-0.274818
H	4.178692	-1.241084	-1.091419

NG-1W-e

N	-1.169598	-0.272125	0.193429
N	-3.253970	-1.225828	-0.029603
C	-2.516914	-0.047218	-0.022024
H	-4.245663	-1.040691	-0.043984
N	-3.103267	1.072700	-0.208912
H	-2.448837	1.843818	-0.283811
H	-2.990424	-1.900523	0.673231
C	-0.215731	0.793669	0.074826
H	-0.286837	1.499137	0.908453
H	-0.340111	1.377312	-0.850595
C	1.184940	0.231760	0.039175
O	1.426468	-0.949712	-0.089336
O	2.102728	1.176212	0.135538
H	2.993255	0.759107	0.077001
H	-0.810981	-1.177253	-0.077819
O	4.190058	-0.523610	-0.022585
H	3.498486	-1.190777	-0.131456
H	4.851156	-0.685740	-0.696219

NG-1W-f

N	0.466595	-0.344113	-0.028220
N	0.274688	1.938749	0.327584
C	1.111022	0.865420	0.092272
H	0.726097	2.838834	0.326580
N	2.396329	0.900298	0.006239
H	-0.602628	1.913611	-0.180462
C	-0.763287	-0.663116	0.647389
H	-0.836240	-0.175190	1.629154
H	-0.802979	-1.738217	0.822975
C	-2.015407	-0.258727	-0.110228
O	-2.110961	0.676298	-0.862339
O	-3.053011	-1.045145	0.203461
H	2.754375	1.847324	-0.030663
H	1.108513	-1.117649	-0.172697
H	-3.829972	-0.703589	-0.256126
O	3.016682	-1.761889	-0.353898
H	3.097742	-0.788943	-0.240399
H	3.606157	-2.156277	0.288020

NG-1W-g

N	0.332093	-0.083251	0.078418
N	2.623760	0.127805	-0.108278
C	1.490843	-0.638809	-0.043116
H	3.386774	-0.223871	-0.662763
N	1.716296	-1.993819	-0.109767

H	0.964555	-2.607767	0.152153
H	2.470646	1.129871	-0.153309
C	-0.834522	-0.915416	0.252499
H	-0.925657	-1.326654	1.265027
H	-0.874378	-1.760846	-0.451677
C	-2.119219	-0.136518	-0.022937
O	-1.951309	1.019321	-0.666328
O	-3.199969	-0.552312	0.285165
H	-0.995970	1.150765	-0.784257
H	2.629199	-2.318946	0.162399
O	1.132193	2.619017	0.248713
H	0.947489	3.245444	0.948116
H	0.622364	1.813112	0.442621

NG-1W-h

N	-0.410989	-0.059580	0.026446
N	-2.700833	0.162170	0.099840
C	-1.567865	-0.611517	-0.002181
H	-3.495666	-0.147522	-0.436950
N	-1.814423	-1.966919	-0.131604
H	-1.039262	-2.588489	0.027494
H	-2.680736	-2.297892	0.262224
H	-2.515957	1.159995	0.035035
C	0.760309	-0.878232	0.027912
H	0.831426	-1.548647	-0.844262
H	0.848935	-1.519786	0.919324
C	2.008916	-0.021935	-0.013369
O	2.057845	1.169377	-0.125631
O	3.111318	-0.794132	0.079292
H	3.875055	-0.207408	0.034165
O	-1.095520	2.639251	0.081934
H	-0.607983	3.312152	-0.391366
H	-0.529411	1.842035	0.072627

NG-1W-i

N	-1.426833	0.894719	-0.282683
N	-3.215610	-0.453865	-0.802238
C	-2.072705	-0.291028	-0.053214
H	-3.740212	-1.299624	-0.654595
N	-1.574754	-1.137876	0.780217
H	0.099628	-1.033272	0.661917
H	-3.773507	0.365346	-0.982105
C	-0.289857	1.317939	0.514176
H	-0.538948	1.179814	1.570028
H	-0.117469	2.377182	0.333360
C	1.028938	0.586651	0.230936
O	2.022072	1.185842	-0.100198
O	1.016533	-0.724191	0.397841
H	-2.187505	-1.918120	0.981503
H	-1.512336	1.288055	-1.205683
O	4.009102	-0.974026	-0.548692
H	3.597961	-0.104919	-0.471967
H	3.312857	-1.557681	-0.242529

NG-1W-j

N	-1.098158	0.327516	0.077616
N	-3.193326	1.271902	-0.112035
C	-2.367056	0.172423	-0.003729
H	-4.071656	1.216972	0.380579
N	-3.032734	-1.030256	0.003190
H	-2.484940	-1.869258	-0.085251
H	-2.709574	2.146019	0.022629
C	-0.235322	-0.826856	0.050768
H	-0.372461	-1.459989	-0.837667
H	-0.343857	-1.471164	0.933825
C	1.221473	-0.375371	0.029821
O	1.384555	0.940660	0.049782
O	2.142148	-1.149312	-0.001282
H	0.477454	1.314424	0.074123
H	-3.928072	-1.064272	-0.456355
O	4.596991	0.498984	-0.071177
H	3.954853	-0.221187	-0.052549
H	4.043653	1.280491	-0.040475

NG-1W-k

N	-0.548579	-0.373965	1.004273
N	-2.468035	-0.324874	-0.279094
C	-1.269684	-0.962526	-0.036642
H	-2.944725	-0.709081	-1.079843
N	-0.945071	-2.011233	-0.694553
H	-0.103503	-2.448298	-0.334903
H	-2.435486	0.687715	-0.254223
C	0.872762	-0.527088	1.057510
H	1.165456	-1.578669	1.080769
H	1.248475	-0.092856	1.988930
C	1.616577	0.164318	-0.077830
O	1.207939	1.107022	-0.710808
O	2.824002	-0.366515	-0.278907
H	3.255693	0.132047	-0.983987
H	-0.897221	0.527860	1.296990
O	-1.188092	2.382505	0.089999
H	-1.264009	3.324361	-0.059531
H	-0.361599	2.095107	-0.329077

NG-1W-l

N	-1.418769	0.756444	-0.489218
N	-1.679151	-1.249669	0.642348
C	-2.299022	-0.228507	-0.058628
H	-2.271024	-2.034071	0.861685
N	-3.543249	-0.093465	-0.320105
H	-0.759797	-1.501359	0.296859
C	-0.296891	1.195862	0.304681
H	-0.487012	1.101424	1.382656
H	-0.107962	2.251776	0.109579
C	0.992109	0.438512	0.041829

O	1.045180	-0.705979	-0.361865
O	2.057387	1.155921	0.356871
H	-4.067956	-0.926447	-0.071381
H	-1.921375	1.491292	-0.960779
H	2.863110	0.605344	0.226474
O	3.829439	-0.785290	-0.269313
H	3.019610	-1.276532	-0.467788
H	4.387362	-1.357018	0.258697

NG-1W-m

N	1.160698	-0.434006	-0.121739
N	3.328276	-1.187818	0.103217
C	2.398394	-0.159807	0.000922
H	4.166796	-1.055366	-0.443731
N	2.978063	1.098750	0.049256
H	2.355394	1.881003	0.164875
H	3.824088	1.172029	0.592052
H	2.896920	-2.086356	-0.057385
C	0.219316	0.642094	-0.091127
H	0.281325	1.291850	-0.977941
H	0.332382	1.308695	0.781170
C	-1.214795	0.154468	-0.039307
O	-1.570085	-0.998056	-0.002123
O	-2.057648	1.189999	-0.036132
H	-2.975793	0.845810	-0.003309
O	-4.268130	-0.418244	0.007588
H	-3.539594	-1.059231	0.028178
H	-4.861363	-0.647032	0.723354

NG-1W-n

N	-0.520408	0.638030	0.165971
N	-2.633212	1.285875	-0.430198
C	-1.845573	0.341432	-0.076704
H	-3.552959	0.930203	-0.670376
N	-2.173746	-0.992916	0.136528
H	-1.472397	-1.682020	-0.105320
C	0.365199	-0.166409	0.971021
H	-0.189823	-0.765418	1.695918
H	1.057343	0.488568	1.499143
C	1.128967	-1.114518	0.063740
O	2.303934	-0.603111	-0.360895
O	0.728505	-2.186042	-0.309055
H	-3.101113	-1.246761	-0.161941
H	-0.259049	1.603409	0.034805
O	1.925035	2.336007	0.009274
H	2.354338	1.563985	-0.371772
H	2.216737	3.087766	-0.506589
H	2.687144	-1.234513	-0.982914

ZNG-1W

N	-0.502477	0.604547	0.655512
N	-2.551777	1.003405	-0.337238
C	-1.580899	0.133860	0.042167
H	-3.107773	0.776786	-1.144333
N	-1.737596	-1.169995	-0.137230
H	-0.848682	-1.744803	-0.218138
H	-2.407221	1.983307	-0.158800
C	0.542618	-0.280812	1.179675
H	0.079082	-1.025140	1.829866
H	1.218148	0.344029	1.760104
C	1.281970	-0.958928	-0.013142
O	2.261863	-0.352103	-0.473725
O	0.739291	-2.011526	-0.428555
H	-2.614835	-1.517819	-0.485182
H	-0.157971	1.530593	0.397691
O	1.477195	2.231959	-0.320961
H	1.941755	1.367961	-0.439035
H	2.151526	2.908022	-0.275747

ZNG-1W-a

N	0.390785	-0.427218	0.618462
N	2.341047	0.623723	0.035126
C	1.601723	-0.487124	0.105524
H	3.310505	0.576890	-0.223064
N	2.111799	-1.665370	-0.307425
H	1.560178	-2.499700	-0.200061
H	2.856964	-1.684099	-0.981170
H	1.833200	1.516607	-0.017027
C	-0.763501	-1.228285	0.220683
H	-1.039190	-1.941730	0.999058
H	-0.563457	-1.766534	-0.708467
C	-1.971146	-0.248617	-0.032047
O	-1.711634	0.966815	0.194724
O	-2.999825	-0.790063	-0.403178
H	0.064232	0.496226	0.911169
O	0.361601	2.553333	-0.256582
H	-0.496881	2.062523	-0.202857
H	0.165447	3.465347	-0.045394

ZNG-1W-b

N	0.914515	-0.785836	0.696735
N	2.864046	-0.224882	-0.402728
C	1.635573	0.126907	0.057095
H	3.231004	0.258840	-1.204938
N	1.239875	1.384358	-0.082407
H	3.155565	-1.182325	-0.298396
C	-0.477261	-0.561153	1.088771
H	-0.604866	0.457391	1.449266
H	-0.698706	-1.242338	1.911879
C	-1.398721	-0.926372	-0.123449
O	-1.032061	-1.935533	-0.734465
O	-2.370046	-0.162388	-0.324126
H	1.891851	2.053114	-0.455604
H	1.040284	-1.736707	0.365835
H	0.251242	1.695284	-0.003021

O	-1.367259	2.225609	-0.132221
H	-1.900309	1.380104	-0.223229
H	-1.897738	2.843363	0.369006

ZNG-1W-c

N	-1.009767	0.148479	-0.068999
N	-2.927494	1.420551	0.098033
C	-2.302475	0.221479	0.007745
H	-3.870369	1.502374	-0.243504
N	-3.070640	-0.888586	0.008008
H	-2.615758	-1.786465	0.024761
H	-4.005583	-0.844815	0.375651
H	-2.360238	2.249765	0.028328
C	-0.162527	-1.029494	-0.005097
H	-0.316102	-1.690509	-0.862080
H	-0.306260	-1.581751	0.927303
C	1.304552	-0.464260	-0.051303
O	1.343299	0.791686	-0.143571
O	2.200520	-1.296916	0.008641
H	-0.337014	0.954784	-0.142146
O	4.257694	0.866984	0.111127
H	4.040654	-0.071974	0.109217
H	3.376569	1.245106	0.005539

Table S10. Cartesian coordinates of canonical and zwitterionic configurations of NG in the presence of two water molecules at ωB97XD/6-311++G (d,p) level.

NG--2W

N	-0.661091	0.598757	0.437738
N	-2.578901	1.608326	-0.357940
C	-1.937252	0.445819	0.009293
H	-3.300352	1.517158	-1.053287
N	-2.477747	-0.732465	0.009400
H	-2.018085	2.440915	-0.445667
C	0.071895	-0.485530	1.051851
H	-0.553408	-0.964641	1.811946
H	0.953214	-0.064801	1.533702
C	0.539935	-1.557180	0.058577
O	1.719393	-1.752444	-0.161670
O	-0.402204	-2.252799	-0.525381
H	-3.463298	-0.718703	-0.219712
H	-0.119435	1.429154	0.203037
O	3.236338	0.529435	-0.211432
H	3.896763	0.437497	-0.898417
H	2.800801	-0.343979	-0.143070
H	2.088448	1.870278	-0.218446
O	1.359653	2.516071	-0.113057
H	1.692649	3.186594	0.483409
H	-1.306033	-1.852555	-0.303882

NG--2W-a

N	1.188678	-0.777573	0.055915
N	3.425296	-0.265476	-0.176453
C	2.105137	0.122171	-0.021666
H	4.100953	0.278777	0.338056
N	1.907286	1.469605	0.022022
H	0.967607	1.863145	0.038046
H	3.552250	-1.259937	-0.069870
C	-0.182186	-0.340350	0.056203
H	-0.444827	0.271541	-0.817378
H	-0.450515	0.250845	0.941887
C	-1.107079	-1.544417	0.039337
O	-0.493210	-2.708821	0.038318
O	-2.314495	-1.437783	0.027859
H	0.465160	-2.483651	0.047574
H	2.619541	2.058548	-0.374716
H	-3.699035	1.375574	-0.758603
O	-3.003829	1.241845	-0.114584
H	-2.886446	0.273871	-0.036343
H	-0.903599	3.487812	0.719942
O	-0.726735	2.801747	0.076516
H	-1.558998	2.297253	-0.007090

NG--2W-b

N	0.670211	0.430872	1.032873
N	1.859505	1.852839	-0.325734
C	0.618323	1.401132	0.062543
H	1.864084	2.477195	-1.115443
N	-0.519051	1.841422	-0.365445
H	2.579226	1.138292	-0.363592
C	-0.439641	-0.476192	1.178514
H	-1.351437	0.071930	1.405608
H	-0.233219	-1.137223	2.023880
C	-0.616862	-1.387415	-0.046291
O	0.332523	-1.959656	-0.536226
O	-1.837100	-1.571361	-0.501539
H	-0.396385	2.536271	-1.093027
H	1.583451	0.020079	1.168201
H	-2.181036	1.289269	-0.211326
O	-3.029113	0.773440	-0.160899
H	-2.434152	-0.829255	-0.241410
H	-3.635228	1.251190	0.403534
H	2.095425	-1.458036	-0.389649
O	2.912065	-0.976110	-0.161180
H	3.636702	-1.591304	-0.268476

NG--2W-c

N	-0.559141	-1.524207	-0.541153
N	1.760064	-1.742006	-0.461643
C	0.612852	-1.298072	0.136409
H	2.551625	-1.112289	-0.347736

N	0.567132	-0.712342	1.288843
H	1.679105	-2.165996	-1.371377
C	-1.844339	-1.134013	0.014769
H	-1.916103	-1.529903	1.031084
H	-2.632604	-1.575167	-0.592265
C	-2.067729	0.385935	0.039757
O	-2.921194	0.926897	-0.610420
O	-1.229564	1.059327	0.826333
H	1.475548	-0.676054	1.734210
H	-0.502785	-1.557089	-1.545728
O	3.189769	0.714800	-0.142985
H	2.436690	1.327641	-0.231682
H	3.871479	1.196787	0.323671
H	0.132242	2.113062	0.032287
O	0.974252	2.385651	-0.365046
H	0.754999	3.003166	-1.062687
H	-0.537387	0.409221	1.219222

NG--2W-d

N	1.932602	-0.855133	-0.523594
N	3.709174	0.600501	-0.645086
C	2.519081	0.185654	-0.064151
H	3.796358	1.592577	-0.807215
N	2.134332	0.912891	1.044011
H	1.139825	1.078135	1.119456
H	3.945534	0.043542	-1.452692
C	0.868287	-1.450214	0.244392
H	1.082409	-1.449919	1.327350
H	0.743357	-2.488510	-0.062965
C	-0.478203	-0.763983	0.114097
O	-1.481503	-1.600736	0.008711
O	-0.604881	0.452564	0.150117
H	2.728245	1.675493	1.324077
H	-2.359458	-1.133588	-0.007226
O	-3.862959	-0.408411	-0.040242
H	-3.727796	0.554374	-0.146493
H	-4.534619	-0.673617	-0.668355
O	-2.806789	2.066422	-0.184507
H	-2.702886	2.672083	-0.917960
H	-1.949654	1.614167	-0.073963

NG--2W-e

N	-1.140543	0.348423	0.322517
N	-2.875308	-0.934927	-0.479726
C	-1.615034	-0.822692	0.052875
H	-3.022473	-1.665062	-1.157105
N	-0.982117	-2.008178	0.341832
H	0.018234	-2.014749	0.187453
H	-3.322992	-0.049313	-0.696368
C	0.033196	0.458590	1.156641
H	0.025345	-0.274529	1.979019
H	0.059892	1.454564	1.598115
C	1.340390	0.232463	0.420344
O	2.221296	1.201177	0.589697
O	1.568794	-0.764787	-0.245950
H	-1.471866	-2.861117	0.130067
H	3.049258	0.966594	0.111934
O	4.159999	-0.008664	-0.875946
H	3.440512	-0.645014	-1.000556
H	4.503625	0.203366	-1.744318
O	-3.153486	2.013751	-0.592198
H	-2.902330	2.649688	-1.261276
H	-2.315573	1.656351	-0.223325

NG--2W-f

N	-0.023374	0.469780	0.075256
N	-2.246782	1.024424	-0.127945
C	-0.943215	1.379563	0.009666
H	-2.892523	1.708837	-0.482269
N	-0.699598	2.731989	0.069738
H	0.180700	3.028436	0.454845
H	-2.456486	0.050785	-0.355116
C	1.356867	0.861405	0.240127
H	1.620337	1.104864	1.276791
H	1.648379	1.717514	-0.387039
C	2.282125	-0.275174	-0.195908
O	1.679544	-1.229972	-0.909501
O	3.451927	-0.298611	0.060418
H	0.738840	-0.978595	-0.967747
H	-1.472148	3.333182	0.303396
H	-3.569137	-2.271865	-0.400485
O	-2.756627	-1.800926	-0.584176
H	-2.097077	-2.131699	0.055561
H	-0.444774	-1.162256	0.926465
O	-0.713341	-2.066122	1.190997
H	0.065485	-2.612266	1.071033

NG--2W-g

N	0.044453	0.437407	0.078082
N	2.244561	1.151714	0.098021
C	0.902435	1.397263	0.029064
H	2.843697	1.828348	-0.346625
N	0.577051	2.738344	-0.096450
H	-0.361003	3.006614	0.148470
H	1.270629	3.394440	0.224594
H	2.561124	0.188517	-0.029426
C	-1.346189	0.785536	0.063225
H	-1.623475	1.442593	-0.777728
H	-1.678501	1.300083	0.978871
C	-2.240530	-0.426071	-0.087397
O	-1.907309	-1.554594	-0.318214
O	-3.532064	-0.067032	0.050348
H	-4.065122	-0.860125	-0.078676
H	2.485320	-1.996498	-0.123084
O	3.325583	-1.531994	-0.322340
H	3.964731	-1.883483	0.297262

O	0.858498	-2.242460	0.433353
H	0.166419	-2.762490	0.021823
H	0.521758	-1.321984	0.352414

NG--2W-h

C	1.924915	-0.377050	0.082970
C	1.219313	0.570332	1.043145
C	-0.780740	1.344193	-0.156112
H	0.823075	1.964150	-1.006292
H	-2.614180	0.576956	0.386705
H	-2.603058	1.685012	-0.932764
H	-0.767572	-0.024383	1.371379
H	1.455923	0.217551	2.051279
H	1.693422	1.552827	0.955654
N	-0.186372	1.991428	-1.091594
N	-2.155281	1.331625	-0.104505
N	-0.193542	0.661792	0.897533
O	1.405928	-1.197450	-0.630956
O	3.250947	-0.219882	0.143275
O	-2.310988	-1.354663	1.171571
H	-2.032577	-1.670984	0.287359
H	-2.799857	-2.060653	1.592266
O	-1.269344	-1.722752	-1.310342
H	-0.328809	-1.572157	-1.120357
H	-1.527464	-0.969862	-1.846711
H	3.654185	-0.859253	-0.456958

NG--2W-i

N	1.606415	0.245690	-0.171287
N	3.609626	1.375790	-0.025711
C	2.872903	0.212453	0.023006
H	4.529536	1.305159	-0.432588
N	3.614465	-0.912661	0.291129
H	3.119462	-1.762710	0.500913
H	3.081499	2.170335	-0.351172
C	0.818702	-0.945338	0.017279
H	0.922062	-1.394075	1.015839
H	1.032788	-1.730795	-0.720383
C	-0.656934	-0.598867	-0.144450
O	-0.885092	0.672518	-0.429494
O	-1.534638	-1.416449	-0.025265
H	4.472577	-0.789292	0.803355
H	0.004164	1.093242	-0.463197
O	-3.561690	1.960259	0.431520
H	-4.030726	1.133871	0.248969
H	-2.669031	1.765758	0.137861
H	-4.734064	-1.283640	0.562037
O	-4.313596	-0.768365	-0.126317
H	-3.389700	-1.062783	-0.139115

NG--2W-j

N	-1.345913	-0.641811	-0.111880
N	-3.565874	-0.114448	0.207976
C	-2.268869	0.382288	0.071111
H	-4.240187	0.636511	0.194708
N	-2.046826	1.633243	0.131016
H	-1.059675	1.877880	0.096097
H	-3.802755	-0.852889	-0.439082
C	0.058482	-0.351904	-0.055689
H	0.351695	0.193068	0.856300
H	0.368082	0.286566	-0.888424
C	0.849132	-1.628019	-0.083793
O	0.409767	-2.739321	-0.004870
O	2.181918	-1.389124	-0.182530
H	3.604733	1.241965	1.273976
O	3.287469	1.245965	0.370412
H	3.051924	0.332800	0.164064
H	1.040899	3.485275	-0.736206
O	0.957571	2.597001	-0.391216
H	1.845150	2.312585	-0.124233
H	-1.604820	-1.538530	0.274307
H	2.628974	-2.244478	-0.185447

ZNG--2W

N	0.677721	0.353769	1.087128
N	1.957261	1.635334	-0.322404
C	0.738579	1.280072	0.129900
H	2.012473	2.320616	-1.056524
N	-0.358553	1.878140	-0.325107
H	2.635529	0.872486	-0.354917
C	-0.481979	-0.524084	1.212755
H	-1.363439	0.047271	1.502118
H	-0.268521	-1.226424	2.019506
C	-0.739574	-1.338141	-0.095155
O	0.279547	-1.696833	-0.722650
O	-1.933177	-1.544417	-0.374007
H	-0.293446	2.406619	-1.178315
H	1.571418	-0.085768	1.273181
H	-1.309474	1.571687	-0.078692
O	-2.960002	0.895037	-0.221747
H	-2.780908	-0.075573	-0.308158
H	-3.820558	0.994782	0.182437
H	1.877959	-1.405841	-0.425864
O	2.774597	-1.059916	-0.157193
H	3.414091	-1.748605	-0.332308

ZNG--2W-a

N	-0.156539	-1.114824	-1.134328
N	-2.154258	-0.169030	-0.457712
C	-0.947198	-0.042454	-1.017371
H	-2.680666	0.680508	-0.325212
N	-0.569154	1.148770	-1.506417
H	-2.209701	-0.854493	0.296007
C	1.287389	-0.941609	-0.958142
H	1.750265	-0.529342	-1.856586

H	1.720373	-1.931677	-0.811924
C	1.647263	-0.044336	0.273484
O	0.728022	0.061357	1.152919
O	2.751478	0.471880	0.254174
H	-0.798669	1.936746	-0.899117
H	-0.539319	-1.938092	-0.686482
H	0.354158	1.199896	-1.907998
O	-0.821519	2.278844	1.038599
H	-0.186565	1.559663	1.257312
H	-0.569126	3.030957	1.573348
H	-0.342031	-1.190430	1.518407
O	-1.052838	-1.881496	1.479596
H	-1.104928	-2.292441	2.341314

ZNG--2W-b

N	0.188774	0.572068	0.828787
N	1.216277	2.213233	-0.409112
C	0.081982	1.583141	-0.020732
H	1.177207	2.750677	-1.258719
N	-1.116883	2.003563	-0.422339
H	2.076604	1.692448	-0.259830
C	-0.947257	-0.224011	1.292117
H	-1.659819	0.428993	1.801782
H	-0.555472	-0.953883	1.998315
C	-1.615644	-0.931349	0.075287
O	-1.121656	-2.021360	-0.270014
O	-2.530845	-0.280234	-0.471426
H	-1.163176	2.756759	-1.087289
H	1.129868	0.213712	0.967027
H	-1.886107	1.292861	-0.426943
O	1.488077	-2.284523	-0.546656
H	1.593241	-2.802362	-1.344520
H	0.506430	-2.237026	-0.388172
H	2.456563	-0.969849	-0.158383
O	2.857215	-0.145209	0.215031
H	3.650666	-0.410450	0.679863

ZNG--2W-c

N	0.412100	-1.730130	-0.140810
N	2.464544	-0.731001	0.268953
C	1.136677	-0.810305	0.507000
H	2.926404	0.068237	0.678980
N	0.592487	-0.025700	1.427920
H	2.732736	-0.880129	-0.692215
C	-0.948033	-1.376435	-0.554777
H	-1.648679	-1.510893	0.269036
H	-1.242157	-2.062785	-1.349572
C	-1.013612	0.091859	-1.098376
O	0.058293	0.542764	-1.558809
O	-2.115403	0.648614	-0.978048
H	1.004958	0.899709	1.495747
H	0.940295	-2.290018	-0.790831
H	-0.415263	-0.051999	1.613700
O	-2.251130	0.350413	1.699195
H	-2.440666	0.561381	0.757452
H	-2.749923	0.967055	2.233349
H	1.624558	3.083668	-0.231554
O	1.667704	2.141544	-0.071932
H	1.057909	1.726194	-0.722872

ZNG--2W-d

C	1.596201	-1.363225	-0.123473
C	0.067427	-1.720720	-0.092338
C	-1.926171	-0.250592	0.032630
H	-2.402868	-2.213813	0.279669
H	-3.615888	-1.114804	0.786223
H	-1.719678	1.772359	-0.052137
H	-3.373320	1.180597	0.061689
H	-0.019420	0.286700	-0.470506
H	-0.143081	-2.429450	-0.898349
H	-0.153359	-2.188430	0.871275
N	-2.775873	-1.279560	0.259419
N	-2.385675	1.003552	0.103755
N	-0.671657	-0.481218	-0.261164
O	1.817607	-0.156227	-0.421504
O	2.359509	-2.279720	0.134868
O	-0.289543	2.764187	-0.337674
H	0.587015	2.650810	0.101705
H	-0.094560	3.183629	-1.176156
O	2.170435	2.242965	0.534982
H	2.248187	1.308843	0.225246
H	2.630591	2.301720	1.370984

ZNG--2W-e

N	1.068839	-0.742770	0.050628
N	3.356158	-0.471792	-0.140334
C	2.106351	0.048296	-0.016426
H	4.136661	0.072248	0.185996
N	1.960141	1.376912	0.011564
H	1.032724	1.823294	0.049766
H	3.457988	-1.470002	-0.061503
C	-0.307588	-0.300933	0.028832
H	-0.510588	0.285722	-0.869568
H	-0.534849	0.305112	0.907891
C	-1.210197	-1.566841	0.031116
O	-0.602808	-2.647775	0.055223
O	-2.431134	-1.314878	0.009638
H	2.737202	1.958085	-0.250591
H	-3.587883	1.497612	-0.640281
O	-2.829012	1.305577	-0.090545
H	-2.772250	0.308227	-0.030826
H	-0.721162	3.500612	0.663330
O	-0.534112	2.779724	0.062200
H	-1.383048	2.290685	-0.035635
H	1.094369	-1.772363	0.075151

ZNG--2W-f

N	1.548073	0.101455	-0.099530
N	3.419682	1.441377	0.036931
C	2.836464	0.220840	0.016412
H	4.378574	1.531311	-0.253529
N	3.633225	-0.861715	0.126135
H	3.207437	-1.771604	0.187430
H	2.834328	2.248484	-0.105526
C	0.734289	-1.095224	0.022130
H	0.866617	-1.578958	0.993493
H	0.934143	-1.808573	-0.781813
C	-0.744005	-0.587104	-0.103690
O	-0.830967	0.647044	-0.298135
O	-1.611708	-1.453395	0.001342
H	4.558659	-0.763651	0.506855
H	0.872216	0.885087	-0.254962
O	-3.322664	2.045549	0.222522
H	-3.890996	1.272021	0.110128
H	-2.448044	1.682190	0.031103
H	-4.635065	-1.083674	0.738717
O	-4.294978	-0.692942	-0.065859
H	-3.362676	-0.981570	-0.104716

Table S11. Cartesian coordinates of canonical and zwitterionic configurations of NG in the presence of three water molecules at ωB97XD/6-311++G (d,p) level.

NG--3W

N	-0.702358	0.360067	0.556249
N	-2.239998	1.927137	-0.131449
C	-1.942854	0.601458	0.060621
H	-2.950476	2.126094	-0.815077
N	-2.738939	-0.399165	-0.165378
H	-1.455961	2.570506	-0.120056
C	-0.307668	-0.936335	1.057692
H	-1.086293	-1.336779	1.717299
H	0.611371	-0.813896	1.627475
C	-0.044184	-1.964031	-0.051327
O	1.060788	-2.446692	-0.223883
O	-1.071117	-2.301815	-0.782103
H	-3.657522	-0.115108	-0.479883
H	-0.078734	1.148443	0.677144
O	3.029796	-0.718710	0.451515
H	3.877697	-1.123306	0.633088
H	2.409628	-1.444132	0.224066
H	1.350478	2.567464	-0.226132
O	0.572278	2.941783	0.241045
H	0.910543	3.610622	0.836363
O	2.651400	1.633058	-0.875451
H	2.688870	1.433339	-1.810901
H	2.836318	0.790576	-0.411180
H	-1.863771	-1.697630	-0.559075

NG--3W-a

N	-0.559662	-0.280561	0.501034
N	-2.741136	-0.786824	-0.045513
C	-1.467617	-1.236689	0.169858
H	-3.334765	-1.391093	-0.587935
N	-1.071239	-2.473528	0.115428
H	-2.862251	0.208532	-0.222213
C	0.754759	-0.610886	1.000544
H	0.678344	-1.395407	1.761350
H	1.177198	0.282440	1.457283
C	1.712939	-1.088606	-0.096403
O	2.701075	-0.447561	-0.405462
O	1.409834	-2.222373	-0.668227
H	-1.822352	-3.123124	-0.077726
H	-0.800173	0.699346	0.469886
O	2.386189	2.239395	-0.182613
H	2.870109	2.666464	-0.889440
H	2.610313	1.285017	-0.235455
H	0.746735	2.587911	0.176282
O	-0.180816	2.681929	0.490241
H	-0.143633	3.220510	1.281171
H	0.485335	-2.520776	-0.357136
O	-2.621526	2.114682	-0.649784
H	-1.774245	2.495681	-0.362405
H	-2.784882	2.459401	-1.527539

NG--3W-b

N	0.892137	0.441776	0.969677
N	2.330532	1.775636	-0.229951
C	1.030105	1.389298	-0.016798
H	2.480159	2.406627	-0.999362
N	-0.010768	1.874640	-0.610620
H	3.027201	1.041663	-0.141265
C	-0.235069	-0.451475	0.947742
H	-1.161914	0.113349	0.883663
H	-0.269425	-1.000606	1.893215
C	-0.153234	-1.499776	-0.169152
O	0.906586	-1.864657	-0.630750
O	-1.284714	-2.037657	-0.561402
H	0.249796	2.526094	-1.341917
H	1.761906	0.034315	1.282787
H	-2.082551	-1.560042	-0.216196
O	3.369377	-0.942768	0.174939
H	4.086934	-1.574110	0.142391
H	2.582753	-1.381227	-0.203415
H	-4.235949	-0.900328	-0.281541
O	-3.443250	-0.697741	0.215882
H	-3.281645	0.269049	0.111979
O	-2.669287	1.837791	-0.063136
H	-1.694260	1.870447	-0.275955
H	-2.826815	2.522378	0.586863

NG--3W-c

N	0.274438	0.658986	0.796956
N	0.982551	2.429073	-0.480531
C	-0.059789	1.611978	-0.122104
H	0.854991	2.980633	-1.311133
N	-1.279943	1.727397	-0.544316
H	1.921293	2.079361	-0.319432
C	-0.643842	-0.385409	1.156280
H	-1.608712	0.041831	1.425101
H	-0.250203	-0.896274	2.038416
C	-0.797121	-1.470451	0.077560
O	0.173342	-2.036715	-0.378435
O	-2.010539	-1.817097	-0.281334
H	-1.369327	2.488535	-1.207441
H	1.263129	0.518771	0.962988
H	-2.681265	-1.121733	-0.059506
O	2.878949	-1.757137	-0.499812
H	3.138928	-2.124852	-1.344326
H	1.914139	-1.899029	-0.429893
H	3.238691	-0.167161	0.041511
O	3.202582	0.727632	0.444044
H	3.949139	0.798293	1.038192
O	-3.534668	0.309588	-0.066270
H	-2.771480	0.930950	-0.234675
H	-4.111458	0.715611	0.579483

NG--3W-d

N	1.750935	0.567387	-0.097456
N	3.810331	-0.454180	-0.144417
C	2.426914	-0.525898	-0.140127
H	4.283439	-1.153566	-0.695869
N	1.915083	-1.786879	-0.184564
H	0.942150	-1.961673	0.067308
H	4.151350	0.479339	-0.312921
C	0.313227	0.517668	-0.014066
H	-0.067396	-0.050343	0.845270
H	-0.157995	0.080529	-0.905170
C	-0.210995	1.941103	0.120563
O	0.727848	2.859437	0.188923
O	-1.390254	2.217386	0.168170
H	1.570287	2.350605	0.105300
H	2.539308	-2.540698	0.050217
H	-4.293961	1.076762	0.269644
O	-3.592269	0.673036	-0.240559
H	-2.800810	1.231900	-0.103132
H	-3.400577	-2.265968	-1.217050
O	-3.112107	-1.976198	-0.351903
H	-3.330300	-1.021434	-0.294888
O	-0.695141	-2.609768	0.681502
H	-0.883572	-3.008090	1.530589
H	-1.565858	-2.410040	0.278487

NG--3W-e

N	1.020768	-0.025387	0.003892
N	2.762585	1.413200	-0.464486
C	1.430033	1.186878	-0.217726
H	3.129388	2.292905	-0.137965
N	0.635558	2.287994	-0.241396
H	-0.366500	2.239539	-0.065850
H	3.364271	0.621830	-0.266018
C	-0.398143	-0.253728	0.068884
H	-0.961249	0.310249	-0.687703
H	-0.837901	0.008080	1.038873
C	-0.730997	-1.710849	-0.195764
O	0.275803	-2.467644	-0.586490
O	-1.855938	-2.145219	-0.080698
H	1.064829	-1.891872	-0.602732
H	0.976126	3.118242	-0.693866
H	-4.424132	-0.214915	-0.279478
O	-3.644507	-0.054178	0.252176
H	-3.103427	-0.866297	0.190424
H	-2.626375	2.884593	0.958477
O	-2.258158	2.338261	0.264385
H	-2.800131	1.525544	0.249257
O	3.445612	-1.235542	0.761721
H	3.640214	-1.596590	1.626097
H	2.504654	-0.981188	0.763302

NG--3W-f

N	0.075468	0.612965	-0.748775
N	2.156539	1.593649	-0.471984
C	1.417995	0.454139	-0.665624
H	2.983167	1.465512	0.098732
N	1.930216	-0.736245	-0.795792
H	1.646843	2.444221	-0.292836
C	-0.798470	-0.459783	-1.169129
H	-0.393720	-0.927307	-2.072434
H	-1.771965	-0.029371	-1.399050
C	-0.995450	-1.547855	-0.104899
O	-2.077780	-1.748547	0.412129
O	0.065637	-2.248510	0.202252
H	2.938993	-0.714374	-0.881387
H	-0.383031	1.443355	-0.377756
H	0.885024	-1.836999	-0.246302
O	-3.590792	0.505331	0.748828
H	-4.110257	0.415676	1.547917
H	-3.161084	-0.363368	0.610609
H	-2.467906	1.855177	0.529578
O	-1.779017	2.506220	0.284671
H	-2.234000	3.194026	-0.201154
O	3.851506	0.067638	1.439145
H	3.159072	-0.599459	1.443570
H	4.272412	0.024261	2.298088

NG--3W-g

N	1.126359	0.219316	0.066358
N	2.595949	1.931648	-0.407636
C	1.318262	1.480998	-0.135215
H	2.867109	2.801054	0.023838
N	0.366445	2.448829	-0.126733
H	-0.615004	2.248082	0.065247
H	3.305157	1.215288	-0.378654
C	-0.231143	-0.255335	0.109852
H	-0.861099	0.216366	-0.655296
H	-0.720019	-0.040066	1.070095
C	-0.427332	-1.751055	-0.111983
O	0.594758	-2.564822	-0.238573
O	-1.560939	-2.185368	-0.172404
H	0.559434	3.305702	-0.616005
H	-4.245777	-0.550342	-0.706649
O	-3.583354	-0.342637	-0.047928
H	-2.929745	-1.071785	-0.075180
H	-2.900583	2.501204	1.124365
O	-2.468914	2.120676	0.359771
H	-2.923766	1.270826	0.191584
H	2.490938	-0.770589	0.444701
O	3.090467	-1.556794	0.402940
H	3.337881	-1.784657	1.299590
H	1.479332	-2.155729	-0.117926

NG--3W-h

N	-0.270621	-1.220244	-0.038632
N	-2.553739	-1.483566	0.080515
C	-1.441531	-0.674249	-0.002972
H	-3.426350	-1.097362	-0.248340
N	-1.689200	0.658894	-0.009635
H	-0.944044	1.349963	-0.010758
H	-2.377702	-2.445144	-0.157884
C	0.868495	-0.344725	-0.031278
H	0.913205	0.309597	0.851230
H	0.923195	0.316008	-0.907698
C	2.142162	-1.170679	-0.021561
O	1.945313	-2.471022	-0.009676
O	3.248159	-0.671011	-0.021691
H	0.961549	-2.563686	-0.012289
H	-2.641939	0.977919	0.073562
H	3.648250	2.424461	0.725814
O	3.029183	2.081118	0.081772
H	3.216272	1.122326	0.011607
H	0.323274	3.493077	-0.742445
O	0.362018	2.820849	-0.062399
H	1.309015	2.599126	0.027476
O	-4.736700	0.646360	0.031838
H	-5.168765	0.599809	0.886729
H	-5.339592	1.115895	-0.546627

NG--3W-i

N	0.728897	0.060964	0.510490
N	2.324259	1.435231	-0.428203
C	1.078563	1.235568	0.085426
H	2.431155	2.132491	-1.145086
N	0.288145	2.354378	0.190016
H	-0.705371	2.213839	0.052494
H	2.962279	0.641407	-0.492388
C	-0.465732	-0.063675	1.321070
H	-0.585615	0.779186	2.016756
H	-0.392195	-0.982712	1.902919
C	-1.732027	-0.125327	0.486188
O	-2.359118	-1.285083	0.546541
O	-2.132297	0.812952	-0.185935
H	0.667426	3.228343	-0.132162
H	-3.162210	-1.244417	-0.021371
O	4.170946	-0.809051	-0.754439
H	4.921840	-0.933163	-0.174178
H	3.528013	-1.505965	-0.510040
O	2.066924	-2.279522	0.082604
H	1.553537	-1.441908	0.239553
H	1.522641	-2.826854	-0.483053
O	-4.372926	-0.536254	-1.108745
H	-3.832603	0.266680	-1.143765
H	-4.571064	-0.784673	-2.012100

NG--3W-j

N	-1.638036	-0.454446	-0.226358
N	-3.262519	1.094230	0.284339
C	-2.051598	0.767561	-0.273820
H	-3.336040	1.996309	0.725195
N	-1.403921	1.786721	-0.933598
H	-0.397398	1.788478	-0.834534
H	-3.720255	0.333431	0.777482
C	-0.539435	-0.863958	-1.065738
H	-0.587654	-0.401296	-2.065367
H	-0.583094	-1.944158	-1.204816
C	0.837768	-0.515875	-0.530998
O	1.706454	-1.488219	-0.653510
O	1.103682	0.585798	-0.069532
H	-1.848358	2.689415	-0.945078
H	2.617359	-1.219557	-0.354641
O	4.158389	-0.829587	0.129040
H	4.124091	0.032827	0.589067
H	4.692194	-1.418833	0.661703
O	-3.609442	-1.677330	1.281667
H	-2.799228	-1.481806	0.760194
H	-3.311759	-2.085043	2.094284
O	3.395155	1.558449	1.112223
H	3.247529	1.866957	2.005887
H	2.519639	1.338496	0.744170

NG--3W-k

N	0.739150	0.104116	0.578230

N	2.377137	1.383580	-0.419848
C	1.116435	1.238596	0.076816
H	2.503380	2.016408	-1.191800
N	0.340153	2.374117	0.081674
H	-0.645229	2.231161	-0.103456
H	2.992023	0.569452	-0.426701
C	-0.480052	0.058649	1.357300
H	-0.612497	0.960644	1.972664
H	-0.439122	-0.803264	2.024081
C	-1.726438	-0.063003	0.499089
O	-2.415910	-1.168298	0.709423
O	-2.061442	0.788677	-0.309208
H	0.744605	3.214326	-0.295949
H	-3.199712	-1.174490	0.112931
O	-4.321377	-0.591436	-1.131309
H	-3.737073	0.172079	-1.250370
H	-4.450039	-0.983264	-1.995789
O	4.153497	-0.926963	-0.658478
H	4.847860	-1.107090	-0.025239
H	3.466022	-1.604541	-0.502749
O	1.868722	-2.292873	-0.142883
H	1.428708	-1.450189	0.144988
H	1.658397	-2.952221	0.517402

NG--3W-l

N	0.322891	0.743215	0.165577
N	-1.463310	2.049174	-0.458546
C	-0.164926	1.918425	-0.100299
H	-1.925773	2.924029	-0.279475
N	0.546952	3.090208	-0.037498
H	1.533592	3.043200	0.147222
H	-2.049641	1.207499	-0.475906
C	1.747786	0.557173	0.300719
H	2.106946	0.679762	1.328931
H	2.347532	1.227354	-0.333680
C	2.145780	-0.852388	-0.145830
O	1.191979	-1.502628	-0.814738
O	3.229484	-1.318837	0.060949
H	0.401946	-0.927600	-0.803510
H	0.253724	3.853016	-0.624646
H	-2.760113	-1.048985	-0.815685
O	-3.097968	-0.289316	-0.320590
H	-2.899618	-0.537734	0.590809
H	-0.664499	-0.358768	1.219912
O	-1.217153	-1.035894	1.676657
H	-0.921773	-1.084125	2.585682
O	-1.551719	-2.658153	-0.590361
H	-0.763780	-3.059246	-0.960883
H	-1.313101	-2.397210	0.311621

NG--3W-m

C	-0.037913	2.213772	-0.156491
C	-1.384738	1.534298	0.097854
C	-2.175156	-0.706832	0.082701
H	-3.673013	0.625870	0.482672
H	-4.197006	-0.955709	0.209616
H	-1.022927	-2.325401	-0.303928
H	-2.553087	-2.676102	0.368935
H	0.446981	0.455201	-0.467854
H	-1.695960	1.830046	1.109429
H	-2.099502	1.978840	-0.610789
N	-3.443003	-0.353551	0.497982
N	-1.994563	-2.035822	-0.172166
N	-1.200504	0.117459	-0.065869
O	0.913361	1.336718	-0.496549
O	0.155527	3.392256	-0.064975
O	3.035934	-1.889839	0.513599
H	3.266915	-0.948369	0.390917
H	3.284251	-2.104852	1.412605
O	3.532279	0.794077	0.226404
H	2.686641	1.198235	-0.026886
H	4.194771	1.176585	-0.349002
O	0.722509	-2.968146	-0.518545
H	1.515239	-2.559321	-0.120809
H	1.023146	-3.359582	-1.338400

NG--3W-n

N	-0.210326	-0.453023	0.504544
N	-1.895548	-1.807602	-0.285750
C	-0.594800	-1.612347	0.064979
H	-2.084822	-2.481243	-1.008805
N	0.214524	-2.721623	0.001782
H	1.191559	-2.577029	-0.214408
H	-2.523981	-1.001245	-0.278254
C	1.105128	-0.340753	1.100172
H	1.373969	-1.209096	1.715799
H	1.123259	0.551912	1.728283
C	2.159287	-0.214187	0.019759
O	2.485806	1.064079	-0.270807
O	2.651340	-1.136169	-0.581057
H	-0.187892	-3.579651	-0.334591
H	3.109064	1.042410	-1.008898
O	-3.717120	0.459714	-0.459870
H	-4.476740	0.555588	0.114280
H	-3.089166	1.162030	-0.183365
O	-1.688824	1.913510	0.522358
H	-1.171245	1.077669	0.559522
H	-1.096983	2.541278	0.087546
O	0.629199	3.343803	-0.423211
H	1.253549	2.616128	-0.319183
H	0.917974	4.021202	0.189275

NG--3W-o

N	0.785731	-0.497341	0.192857
N	3.086411	-0.369148	0.039466
C	1.927451	-1.088637	0.042441

H	3.903089	-0.818253	-0.340410
N	2.075196	-2.445982	-0.119957
H	1.331965	-3.044604	0.196744
H	3.024986	0.624623	-0.183931
C	-0.404175	-1.311720	0.158840
H	-0.558551	-1.875235	1.090775
H	-0.387841	-2.048212	-0.656085
C	-1.719017	-0.568532	-0.064197
O	-1.727810	0.750148	-0.201973
O	-2.745157	-1.197641	-0.126188
H	-0.866217	1.179153	-0.050903
H	2.995393	-2.836927	-0.008688
H	3.425253	3.224759	-0.545545
O	2.865186	2.456644	-0.651980
H	2.036278	2.641890	-0.178426
H	0.775533	1.117946	0.729878
O	0.562122	2.092589	0.769984
H	0.392537	2.323718	1.684177
O	-4.934925	0.783299	-0.152389
H	-4.413806	-0.028931	-0.157402
H	-4.270861	1.460384	-0.288854

NG--3W-p

C	0.055697	1.969165	-0.114329
C	-1.314210	1.387034	0.084798
C	-2.458034	-0.760596	0.078902
H	-3.616496	0.680969	0.580702
H	-1.332222	-2.461888	-0.116730
H	-2.993281	-2.676418	0.273690
H	-0.482409	-0.475299	-0.442166
H	-1.575798	1.559515	1.140929
H	-2.010813	1.997418	-0.504837
N	-3.579609	-0.330543	0.533723
N	-2.279159	-2.106229	-0.147619
N	-1.361569	0.005966	-0.276759
O	1.037905	1.354748	-0.453154
O	0.072780	3.279096	0.141992
O	3.095077	-2.151168	0.592475
H	3.396133	-1.227984	0.495477
H	3.269379	-2.403956	1.498902
O	3.651919	0.495818	0.115836
H	2.785100	0.845897	-0.138715
H	4.244532	0.702064	-0.607606
O	0.628763	-2.217586	-0.602528
H	1.482778	-2.252009	-0.129532
H	0.808897	-2.532861	-1.488536
H	0.974282	3.599308	0.019818

ZNG--3W

N	0.352945	0.562283	0.834923
N	1.285678	2.200382	-0.475922
C	0.197445	1.509013	-0.082161
H	1.219114	2.793541	-1.283763
N	-0.999649	1.819367	-0.572347
H	2.195901	1.799718	-0.252127
C	-0.687801	-0.392929	1.182752
H	-1.582829	0.134305	1.516075
H	-0.320294	-0.970584	2.032164
C	-1.019148	-1.397188	0.034962
O	-0.052779	-1.818350	-0.629241
O	-2.221924	-1.691516	-0.091032
H	-1.066023	2.544755	-1.264067
H	1.317852	0.340232	1.057726
H	-1.883952	1.356914	-0.309599
O	2.546541	-1.845889	-0.528338
H	2.820941	-2.323632	-1.310093
H	1.549198	-1.844911	-0.537601
H	3.148343	-0.440885	0.061428
O	3.255207	0.439406	0.506443
H	4.024569	0.386709	1.072291
O	-3.454111	0.606403	0.037342
H	-4.254193	0.662983	-0.483844
H	-3.167885	-0.347196	0.020129

ZNG--3W-a

N	0.956189	0.422694	1.016209
N	2.408601	1.573510	-0.342165
C	1.145388	1.301580	0.027503
H	2.567881	2.258953	-1.059949
N	0.122245	1.932669	-0.536234
H	-0.854172	1.839544	-0.221313
H	3.071179	0.798751	-0.265117
C	-0.213609	-0.450002	1.047586
H	-1.129247	0.139389	1.066448
H	-0.180025	-1.006967	1.985265
C	-0.239407	-1.472638	-0.127425
O	0.844678	-1.700920	-0.703619
O	-1.349760	-1.981432	-0.358460
H	0.272616	2.441338	-1.389717
H	-4.185225	-0.948486	-0.708210
O	-3.573858	-0.630012	-0.044322
H	-2.767962	-1.210823	-0.117099
H	-3.058208	2.310991	0.717549
O	-2.589602	1.832711	0.033876
H	-3.040400	0.956093	-0.050467
H	1.816704	-0.016066	1.322335
O	3.247893	-1.045064	0.107520
H	3.901123	-1.739707	0.040767
H	2.387454	-1.401029	-0.251102

ZNG--3W-b

N	-0.506230	0.511574	0.637671
N	-1.236339	2.530273	-0.192067
C	-1.458018	1.216380	0.039128
H	-1.766407	2.972477	-0.923215
N	-2.616797	0.641155	-0.266344

H	-0.282071	2.858048	-0.055291
C	-0.664651	-0.862179	1.113154
H	-1.554363	-0.918940	1.747458
H	0.217009	-1.087538	1.709661
C	-0.807405	-1.871197	-0.064905
O	0.182369	-2.576209	-0.335248
O	-1.916885	-1.855982	-0.643429
H	-3.329137	1.193391	-0.712149
H	0.383832	0.979974	0.772222
H	-2.583663	-0.407266	-0.411578
O	2.464353	-1.598499	0.423161
H	3.105586	-2.287712	0.593642
H	1.616925	-2.052358	0.139688
H	2.154081	1.906723	-0.189168
O	1.583583	2.508761	0.347846
H	2.165798	2.978166	0.945238
O	2.965496	0.641370	-0.926836
H	2.897452	0.449041	-1.861955
H	2.839635	-0.218567	-0.457589

ZNG--3W-c

N	0.415139	0.447214	0.918624
N	1.338774	1.993708	-0.502657
C	0.239903	1.414591	0.032351
H	1.200336	2.754217	-1.146730
N	-0.976777	1.846143	-0.297838
H	2.082410	1.342069	-0.742879
C	-0.587434	-0.582908	1.138290
H	-1.479940	-0.167279	1.606939
H	-0.158440	-1.305239	1.834465
C	-0.964171	-1.340758	-0.173056
O	-0.047656	-1.497843	-1.009549
O	-2.144340	-1.719332	-0.250670
H	-1.084214	2.359012	-1.156162
H	1.379091	0.226414	1.178692
H	-1.840229	1.427102	0.069944
O	-3.427838	0.576535	0.167629
H	-3.159990	-0.362184	0.013680
H	-4.193608	0.565442	0.739876
H	1.455101	-1.006913	-1.154417
O	2.391483	-0.653167	-1.251465
H	2.738054	-1.024769	-2.062342
O	3.099947	-0.439088	1.316932
H	3.418330	-1.174293	1.839866
H	3.100601	-0.725415	0.383636

ZNG--3W-d

N	1.107902	-0.377569	-0.820952
N	2.609470	-0.113037	0.901127
C	1.606413	-0.814422	0.327770
H	2.760414	-0.250877	1.886450
N	1.164758	-1.956019	0.858400
H	2.714630	0.845200	0.573272
C	0.026484	-1.040411	-1.550627
H	0.294918	-2.086741	-1.715731
H	-0.070408	-0.535783	-2.509566
C	-1.285889	-0.929793	-0.734000
O	-2.041448	0.022548	-1.009259
O	-1.411079	-1.762912	0.194354
H	1.564612	-2.263289	1.728845
H	1.353564	0.576596	-1.071877
H	0.161004	-2.179170	0.663573
O	-0.811488	2.324360	0.027419
H	-1.253125	2.057233	0.850661
H	-1.227972	1.723405	-0.614356
H	0.838213	2.450242	-0.152096
O	1.797245	2.335505	-0.379828
H	2.093531	3.155087	-0.774957
O	-2.584259	0.811780	1.607508
H	-2.355317	0.012050	2.084571
H	-2.722798	0.479939	0.700770

ZNG--3W-e

N	-0.546545	0.564972	-1.092772
N	-0.565356	2.384718	0.304650
C	0.130736	1.480617	-0.406805
H	-0.066142	2.984458	0.938094
N	1.463992	1.549034	-0.480120
H	-1.531212	2.154487	0.523397
C	0.067473	-0.623888	-1.688965
H	0.767242	-0.325714	-2.472928
H	-0.739496	-1.203669	-2.133740
C	0.788846	-1.440298	-0.579326
O	0.085293	-2.191982	0.116306
O	2.009421	-1.183430	-0.446292
H	1.936693	1.977992	0.304116
H	-1.548721	0.557158	-0.924574
H	1.931481	0.675197	-0.748321
O	-2.336930	-1.652390	1.013830
H	-2.342871	-2.028565	1.893963
H	-1.458123	-1.903694	0.625327
H	-2.830443	-0.087808	0.707529
O	-2.990776	0.823058	0.352867
H	-3.930098	0.897231	0.185977
O	2.692016	0.305523	1.766137
H	2.528408	-0.425394	1.138770
H	3.224128	-0.067558	2.467879

ZNG--3W-f

N	-0.256230	0.199098	-1.124718
N	1.660573	1.315296	-0.509695
C	0.999396	0.153586	-0.694672
H	2.503009	1.271455	0.047073
N	1.615594	-1.014778	-0.509669
H	1.083817	2.146579	-0.431112
C	-1.107857	-0.981057	-1.262725

H	-0.667045	-1.663745	-1.993285
H	-2.071234	-0.632432	-1.631947
C	-1.265076	-1.683976	0.118939
O	-2.127071	-1.208198	0.886674
O	-0.453774	-2.605191	0.337216
H	2.529630	-0.977550	-0.080793
H	-0.687538	1.118410	-1.110724
H	1.013760	-1.832566	-0.298548
O	-2.581505	1.362037	1.116750
H	-2.874227	1.465557	2.021784
H	-2.459128	0.378854	0.988336
H	-1.498175	2.398698	0.359373
O	-0.856681	2.845052	-0.247720
H	-1.303820	3.614496	-0.599558
O	3.890287	0.129401	1.119402
H	3.718475	-0.040774	2.048079
H	4.844070	0.139581	1.022075

ZNG--3W-g

C	-0.362216	2.035131	0.194251
C	1.127755	1.623234	-0.050162
C	2.273774	-0.567673	-0.125212
H	3.504451	0.986386	-0.590937
H	4.293116	-0.525792	-0.430555
H	1.296475	-2.282078	0.322200
H	2.917185	-2.487100	-0.311823
H	0.307058	-0.237417	0.305927
H	1.406736	1.960274	-1.052998
H	1.756287	2.127001	0.690672
N	3.434810	-0.016360	-0.547970
N	2.217534	-1.889911	0.092186
N	1.218434	0.179413	0.069739
O	-1.112023	1.054853	0.465065
O	-0.609161	3.226547	0.089502
O	-2.753582	-2.201543	-0.518195
H	-3.104709	-1.279792	-0.456108
H	-2.924853	-2.491138	-1.413741
O	-3.479598	0.352494	-0.371730
H	-2.641922	0.768011	-0.040010
H	-4.192828	0.745180	0.130076
O	-0.419113	-2.332875	0.776320
H	-1.241150	-2.319617	0.230159
H	-0.719356	-2.215866	1.678488

ZNG--3W-h

N	1.508199	-0.602732	0.046603
N	3.706229	0.060596	0.164633
C	2.382329	0.367563	0.066804
H	4.337413	0.764299	0.507613
N	2.028736	1.648748	-0.026225
H	1.061268	1.959268	-0.208855
H	3.946922	-0.887347	0.402764
C	0.068416	-0.533966	-0.112258
H	-0.212386	-0.080430	-1.065840
H	-0.400428	0.035177	0.694894
C	-0.412544	-2.025887	-0.069144
O	0.498217	-2.862043	0.051982
O	-1.639970	-2.200745	-0.163248
H	2.744537	2.349717	-0.105640
H	-4.145510	-0.597702	-0.703830
O	-3.479547	-0.367870	-0.057505
H	-2.781931	-1.082499	-0.095287
H	-2.969892	2.200013	1.508204
O	-2.650676	2.033865	0.622244
H	-3.003211	1.150163	0.351039
O	-0.397352	2.832256	-0.525943
H	-0.678011	3.155750	-1.381781
H	-1.222708	2.567221	-0.056539
H	1.747207	-1.609880	0.125533

Table S 12. Cartesian coordinates of the charge solvated and salt bridge structures of NG with alkali metal cation Li^+ M06/6-311++G (d,p) level.

CS-1

N	0.599591	-0.887775	-0.156317
N	2.855891	-0.549406	-0.363134
C	1.658000	-0.033220	-0.003029
H	3.665677	0.048260	-0.416763
N	1.464534	1.179364	0.425317
H	3.021114	-1.544228	-0.366937
C	-0.608886	-0.825836	0.626040
H	-0.393566	-0.365834	1.599216
H	-0.978710	-1.836120	0.811462
C	-1.704340	0.000086	-0.014191
O	-2.845499	-0.636469	-0.096701
O	-1.554310	1.148246	-0.388667
H	2.349424	1.612083	0.678969
H	0.745997	-1.717556	-0.712136
H	-3.526691	-0.055975	-0.474780
Li	-0.064512	2.241230	-0.076690

CS-2

N	0.513096	0.381649	0.004530
N	2.756363	0.883084	0.087207
C	1.752587	-0.028068	0.001704
H	3.717371	0.584529	0.143175
N	2.132668	-1.321316	-0.091507
H	1.480299	-2.041739	-0.353710
H	3.106179	-1.582364	-0.088448
H	2.554308	1.778649	0.500618
C	-0.505698	-0.641351	0.012572
H	-0.453113	-1.310052	0.886631

H	-0.488785	-1.297419	-0.876318
C	-1.867376	-0.008663	0.011185
O	-2.050918	1.190517	-0.094743
O	-2.835789	-0.884140	0.118722
H	-3.695312	-0.434066	0.095611
Li	-0.406415	2.105340	-0.217921

CS-3

N	0.601634	-1.178472	-0.071016
N	2.496003	-0.036554	-0.742966
C	1.497324	-0.176247	0.171384
H	3.350589	0.390505	-0.412977
N	1.400725	0.712393	1.113784
H	0.771200	0.413284	1.855067
H	2.579710	-0.665956	-1.527126
C	-0.767320	-1.113677	0.362737
H	-0.866046	-1.121241	1.458056
H	-1.294500	-2.009787	0.028622
C	-1.519985	0.104089	-0.138495
O	-1.012622	1.143787	-0.513436
O	-2.815364	-0.086862	-0.077723
H	-3.289101	0.714714	-0.353065
H	0.836301	-1.888374	-0.749927
Li	0.595695	2.114963	-0.013915

CS-4

N	-0.560816	0.295347	0.043673
N	-2.693696	1.125048	-0.078107
C	-1.837996	0.075242	0.004233
H	-3.645499	1.021525	0.238182
N	-2.411471	-1.153499	0.027946
H	-1.848340	-1.987192	0.013587
H	-2.291903	2.044639	0.017026
C	0.363418	-0.798455	0.013113
H	0.295012	-1.446703	-0.877524
H	0.327072	-1.466331	0.890884
C	1.733462	-0.185636	-0.001960
O	1.730517	1.135901	0.017119
O	2.803168	-0.769109	-0.027513
H	0.734184	1.363291	0.038152
H	-3.383224	-1.267763	-0.215224
Li	3.883934	0.796337	-0.022945

SB-1

N	-0.582143	0.258026	0.000266
N	-2.718494	1.112240	-0.000071
C	-1.886812	0.066306	0.000029
H	-3.719195	0.993715	-0.000274
N	-2.389241	-1.170418	-0.000135
H	-1.785892	-1.978136	-0.000267
H	-2.363105	2.055961	0.000179
C	0.435020	-0.774231	0.000187
H	0.373163	-1.411142	-0.890651
H	0.373348	-1.411074	0.891087
C	1.799447	-0.094458	0.000006
O	1.827984	1.163585	-0.000067
O	2.810015	-0.817187	-0.000068
H	-3.383867	-1.334668	-0.000241
H	-0.175371	1.197013	0.000136
Li	3.773384	0.844166	-0.000215

SB-2

N	0.788478	-0.932639	-0.164489
N	2.951015	-0.168399	-0.388023
C	1.682810	0.049926	-0.022572
H	3.594566	0.597881	-0.514039
N	1.308211	1.213785	0.482307
H	0.312923	1.472107	0.371059
H	3.306326	-1.103102	-0.520684
C	-0.482739	-1.034867	0.547497
H	-0.321427	-0.798097	1.606710
H	-0.816097	-2.070931	0.489924
C	-1.590821	-0.126319	0.030028
O	-2.733585	-0.590050	-0.102891
O	-1.315496	1.092128	-0.197486
H	1.997422	1.904028	0.740054
H	1.043985	-1.703874	-0.765123
Li	-3.238160	1.187900	-0.614392

Table S13. Cartesian coordinates of the charge solvated and salt bridge structures of NG with alkali metal cation Cs^+ M06/6-311++G (d,p) level.

CS-1

N	-2.448553	-0.528032	-0.350057
N	-2.174952	-2.797392	-0.460263
C	-1.747338	-1.617269	0.095923
H	-1.714159	-3.644874	-0.166086
N	-0.768147	-1.469535	0.922996
H	-3.156623	-2.905127	-0.672996
C	-2.506785	0.710268	0.363217
H	-2.288280	0.522222	1.422892
H	-3.514481	1.134099	0.319433
C	-1.522024	1.759110	-0.091365
O	-1.928732	2.969058	0.275037
O	-0.485489	1.549875	-0.671768
H	-0.512446	-2.374023	1.316405
H	-3.017481	-0.633400	-1.175934
H	-1.272292	3.624862	-0.002085
Cs	1.948872	-0.062240	-0.015694

CS-2

N	-1.254148	-0.507595	0.283650
N	-0.812901	-2.744896	0.493439
C	-1.646488	-1.715545	0.080928
H	-1.179965	-3.685292	0.446209
N	-2.788241	-2.101655	-0.545568
H	-3.412058	-1.425406	-0.953105
H	-3.070216	-3.066796	-0.598615
H	-0.369204	-2.553625	1.381269
C	-2.160022	0.549777	-0.054577
H	-3.073322	0.553411	0.561246
H	-2.510910	0.523432	-1.104975
C	-1.511866	1.903520	0.080700
O	-0.325958	2.117345	0.132800
O	-2.429872	2.863679	0.087998
H	-1.984926	3.723070	0.126933
Cs	1.882628	-0.015718	-0.070696

CS-3

N	2.096705	1.352349	-0.408571
N	0.088035	2.505713	-0.549975
C	0.924514	1.700449	0.215784
H	-0.477586	3.111616	0.032405
N	0.502528	1.316559	1.361999
H	1.187505	0.760661	1.866558
H	0.518596	3.018568	-1.308575
C	2.901564	0.254925	0.031941
H	3.190276	0.358815	1.086227
H	3.849176	0.250813	-0.513989
C	2.247281	-1.100670	-0.143031
O	1.118971	-1.290737	-0.522838
O	3.092572	-2.063325	0.196931
H	2.668484	-2.925982	0.077545
H	2.237981	1.664414	-1.357837
Cs	-1.856687	-0.377400	-0.013226

CS-4

N	2.844391	-0.293783	0.076819
N	4.811879	-1.465011	-0.106770
C	4.131104	-0.285181	-0.012642
H	5.752725	-1.506049	0.255855
N	4.909991	0.832419	-0.032070
H	4.479383	1.740514	-0.092401
H	4.257553	-2.293516	0.047718
C	2.122523	0.944159	0.045271
H	2.306004	1.559402	-0.852016
H	2.306441	1.597552	0.914618
C	0.643222	0.635769	0.053384
O	0.367106	-0.664846	0.110392
O	-0.232181	1.464977	0.012690
H	1.265191	-1.101139	0.126988
H	5.852963	0.771959	-0.384606
Cs	-2.848083	-0.153702	-0.019686

SB-1

N	-2.803939	-0.211057	-0.001690
N	-4.715166	-1.495384	0.003428
C	-4.112372	-0.298047	-0.000079
H	-5.717994	-1.584476	-0.007498
N	-4.865043	0.808136	-0.001323
H	-4.434040	1.719659	-0.002226
H	-4.169480	-2.342399	0.001652
C	-2.014473	1.005700	0.000211
H	-2.205538	1.611590	0.893613
H	-2.205212	1.614268	-0.891448
C	-0.523396	0.593875	-0.000373
O	-0.303250	-0.641163	-0.002413
O	0.282908	1.528367	0.001208
H	-5.871220	0.764129	0.008288
H	-2.176661	-1.028303	-0.003514
Cs	2.791516	-0.170421	0.000169

SB-2

N	-3.154696	0.787077	-0.314379
N	-4.883804	-0.711049	-0.599546
C	-3.677616	-0.417984	-0.086926
H	-5.209537	-1.663497	-0.645583
N	-3.007928	-1.293834	0.639653
H	-5.507600	0.014336	-0.916523
C	-2.076121	1.405518	0.461630
H	-2.304007	1.288807	1.528448
H	-2.082957	2.470430	0.231140
C	-0.664340	0.844223	0.204007
O	0.227830	1.667156	-0.006806
O	-0.534774	-0.413772	0.281980
H	-1.966564	-1.156335	0.671676
H	-3.565994	1.336058	-1.055392
H	-3.452945	-2.144820	0.947064
Cs……	2.588702	-0.229781	-0.082083

Table S 14. Cartesian coordinates of the charge solvated and salt bridge structures of NG with alkaline earth metal cation Be^{2+} M06/6-311++G (d,p) level.

CS-1

N	0.623767	-0.961577	-0.192684
N	2.872182	-0.460026	-0.234076
C	1.632270	-0.070971	-0.021844
H	3.630317	0.207377	-0.324225
N	1.329197	1.199175	0.310922
H	3.124538	-1.438955	-0.314643
C	-0.633835	-0.992583	0.536680
H	-0.491584	-0.728330	1.596652

H	-1.029257	-2.010347	0.521173
C	-1.683253	-0.051470	-0.004335
O	-2.849359	-0.517707	-0.135724
O	-1.411323	1.155855	-0.262036
H	2.119442	1.745949	0.646044
H	0.851778	-1.812772	-0.695696
H	-3.528517	0.126149	-0.428961
Be	-0.064595	1.763222	-0.017600

CS-2

N	0.471138	0.285941	-0.042325
N	2.674551	0.921777	0.244322
C	1.790966	-0.038051	-0.004117
H	3.668571	0.763016	0.123333
N	2.203352	-1.276175	-0.216655
H	1.620805	-1.984081	-0.642581
H	3.170679	-1.538605	-0.062067
H	2.422893	1.755556	0.757591
C	-0.550019	-0.768145	0.123616
H	-0.475304	-1.290704	1.087442
H	-0.541596	-1.529444	-0.671038
C	-1.871527	-0.063633	0.030929
O	-1.851673	1.176692	-0.224095
O	-2.927463	-0.734277	0.195601
H	-3.761438	-0.226864	0.110805
Be	-0.382833	1.552493	-0.318874

CS-3

N	-0.552309	1.361688	-0.274007
N	-2.023949	-0.438692	-0.817688
C	-1.391944	0.408931	0.131705
H	-2.996710	-0.675125	-0.594534
N	-1.335530	-0.259673	1.258413
H	-0.939227	0.180062	2.087294
H	-1.907134	-0.221823	-1.809488
C	0.846583	1.237566	0.135788
H	1.017753	1.518666	1.183747
H	1.456413	1.930604	-0.451043
C	1.389324	-0.177781	-0.071803
O	0.681647	-1.209511	-0.186388
O	2.657345	-0.215995	-0.104345
H	3.044546	-1.111603	-0.190291
H	-0.758750	1.906227	-1.107818
Be	-0.827523	-1.394629	0.216710

CS-4

N	-0.547444	-0.389941	0.791240
N	-2.616104	-0.800087	-0.386899
C	-1.679385	0.033815	-0.023197
N	-1.500817	1.307812	-0.253282
H	-2.618328	-1.771738	-0.092483
C	0.592162	-1.099422	0.146543
H	0.321905	-1.545619	-0.819457
H	0.962361	-1.910446	0.781268
C	1.678179	-0.067880	-0.066086
O	2.797899	-0.500407	-0.465850
O	1.412744	1.138011	0.143539
H	-2.138234	1.857330	-0.824553
H	-0.823379	-0.801859	1.684764
H	3.479227	0.187633	-0.614310
H	-3.413978	-0.494044	-0.939760
Be	-0.087478	1.338587	0.500510

SB-1

N	-0.667487	0.285529	0.322735
N	-2.772919	1.095428	-0.131532
C	-1.962932	0.060063	0.013682
H	-3.778251	0.977207	-0.156741
N	-2.405359	-1.178497	-0.163623
H	-1.955009	-1.980310	0.256594
H	-2.423400	2.038887	-0.238138
C	0.372243	-0.707647	0.234479
H	0.196195	-1.398414	-0.603060
H	0.473889	-1.336016	1.136243
C	1.710511	-0.109899	0.008542
O	1.961488	1.150069	-0.022193
O	2.766557	-0.820527	-0.148938
H	-3.326658	-1.343404	-0.551922
H	-0.439709	1.184437	0.733934
Be	3.407502	0.587238	-0.235284

SB-2

N	0.762389	-0.728301	-0.247736
N	3.014015	-0.315014	-0.498540
C	1.843401	0.048157	-0.006534
H	3.795552	0.328745	-0.529178
N	1.724506	1.150678	0.723783
H	3.188024	-1.254191	-0.834748
C	-0.406698	-0.824103	0.585678
H	-0.223157	-0.422776	1.594302
H	-0.685873	-1.872052	0.753929
C	-1.614626	-0.128273	0.049341
O	-2.804152	-0.401708	0.444698
O	-1.598788	0.806078	-0.835169
H	0.849488	1.650219	0.794338
H	0.871485	-1.438345	-0.962769
H	2.547172	1.642528	1.052386
Be	-3.139498	0.701169	-0.589490

Table S15. Cartesian coordinates of the charge solvated and salt bridge structures of NG with alkaline earth metal cation Ba^{2+} M06/6-311++G (d,p) level.

CS-1

N	-1.985536	-0.570554	-0.577678
N	-2.113672	-2.847526	-0.199175
C	-1.472482	-1.695481	0.049993
H	-1.723569	-3.732225	0.094638
N	-0.391595	-1.572764	0.774502
H	-3.066179	-2.866595	-0.536486
C	-2.364129	0.601774	0.192494
H	-2.368365	0.374555	1.267881
H	-3.383021	0.909064	-0.057429
C	-1.448759	1.786697	0.026604
O	-2.073511	2.914663	0.178648
O	-0.244898	1.689828	-0.171266
H	-0.271148	-2.401778	1.355883
H	-2.624009	-0.772845	-1.337861
H	-1.472760	3.677327	0.132010
Ba	1.725074	-0.022240	-0.045996

CS-2

N	-0.980947	0.652922	-0.000032
N	0.297238	2.544038	0.000730
C	-1.009762	1.936779	0.000011
H	0.400099	3.157205	0.811407
N	-2.078456	2.739319	-0.000298
H	-3.021855	2.374207	-0.001714
H	-1.989101	3.745853	-0.000427
H	0.400327	3.158888	-0.808639
C	-2.179378	-0.142143	-0.000358
H	-2.817183	0.027275	-0.882058
H	-2.818033	0.027798	0.880606
C	-1.769826	-1.594465	0.000069
O	-0.599926	-1.947595	-0.000222
O	-2.786710	-2.403520	0.000602
H	-2.504913	-3.333728	0.000643
Ba	1.580941	-0.305421	-0.000071

CS-3

N	1.962307	1.471625	-0.259498
N	-0.200123	2.241902	-0.715375
C	0.702715	1.670692	0.192931
H	-0.745322	2.989152	-0.289913
N	0.181731	1.236690	1.291817
H	0.876556	0.985140	1.991623
H	0.189870	2.549680	-1.601593
C	2.776945	0.367192	0.178052
H	3.006399	0.396307	1.252546
H	3.751184	0.414745	-0.314506
C	2.147547	-0.979665	-0.121691
O	0.967840	-1.147236	-0.400532
O	3.018370	-1.937512	-0.004946
H	2.632665	-2.812690	-0.176308
H	2.314668	2.038044	-1.020031
Ba	-1.630113	-0.408629	-0.005578

CS-4

N	-1.258727	0.648499	0.881208
N	-2.277781	2.540703	-0.101343
C	-1.241820	1.694127	-0.111387
N	-0.223509	1.703231	-0.901014
H	-3.047332	2.444113	0.546234
C	-2.199638	-0.443893	0.569567
H	-3.034130	-0.124017	-0.068730
H	-2.659614	-0.810796	1.494138
C	-1.540948	-1.633644	-0.082522
O	-2.420319	-2.518768	-0.443531
O	-0.335523	-1.751186	-0.231266
H	-0.288918	2.424751	-1.617390
H	-1.516599	1.046477	1.782782
H	-2.007400	-3.305883	-0.837542
H	-2.324784	3.322420	-0.742318
Ba	1.663216	-0.049715	0.061345

SB-1

N	-2.697645	-0.268581	0.000000
N	-4.720258	-1.375607	-0.000194
C	-4.026382	-0.238685	0.000023
H	-5.729542	-1.378033	0.000066
N	-4.672788	0.925446	0.000169
H	-4.184667	1.807861	0.000655
H	-4.261257	-2.273809	-0.000900
C	-1.843458	0.899052	0.000018
H	-2.006273	1.523736	0.887630
H	-2.006393	1.523795	-0.887515
C	-0.385307	0.489046	-0.000016
O	-0.089445	-0.735454	0.000304
O	0.454569	1.415066	-0.000309
H	-5.681646	0.964712	-0.000344
H	-2.197306	-1.154665	0.000543
Ba	2.594854	-0.148496	-0.000001

SB-2

N	-2.935068	0.780635	-0.370091
N	-4.795049	-0.566338	-0.594929
C	-3.578888	-0.361558	-0.093629
H	-5.218043	-1.483619	-0.583550
N	-2.990394	-1.268920	0.672507
H	-5.356022	0.194242	-0.951498
C	-1.885453	1.375259	0.449046
H	-2.137866	1.259423	1.511169
H	-1.857299	2.444102	0.237912
C	-0.491575	0.803406	0.239221
O	0.462236	1.599034	0.123890
O	-0.339338	-0.459127	0.239661
H	-1.967787	-1.251169	0.728661
H	-3.323584	1.358620	-1.103312

H	-3.509177	-2.056710	1.032826	Ba	2.377958	-0.234008	-0.094658