Journal of the Korean Chemical Society
2015, *Vol. 59, No. 2*
Printed in the Republic of Korea
http://dx.doi.org/10.5012/jkcs.2015.59.2.1

SUPPORTING INFORMATION

H_2O_n-H_2O_m (n=1-4, m=1-4) 이중합체의 수소결합에 따른 구조적 특성 및 결합에너지에 관한 이론 연구

송희성 · 서현일 · 신창호[†] · 김승준*
한남대학교 생명나노과학대학 화학과
[†]KT&G 중앙연구원
(접수 2015. 1. 19; 게재확정 2015. 2. 23)

Theoretical Study on the Hydrogen-Bonding Effect of H_2O_n-H_2O_m (n=1-4, m=1-4) Dimers

Hui-Seong Song, Hyun-Il Seo, Chang-Ho Shin[†], and Seung-Joon Kim*
Department of Chemistry, HanNam University, Daejeon 300-791, Korea
[†]KT&G Central Research Institute, Daejeon 305-805, Korea
(Received January 19, 2015; Accepted February 23, 2015)

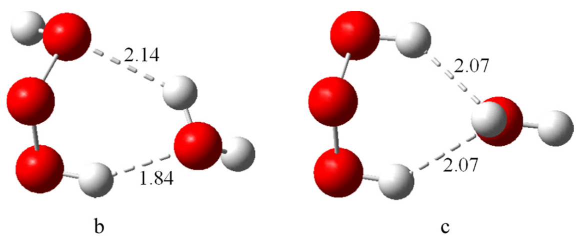

***Figure* S1.** Optimized structures of H_2O_3-H_2O at the MP2/cc-pVTZ level of theory. Bond lengths are in Å.

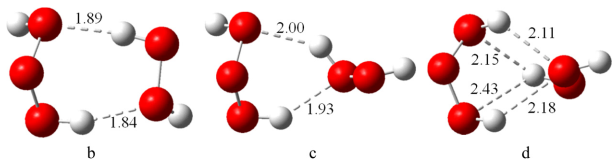

***Figure* S2.** Optimized structures of H_2O_3-H_2O_2 at the MP2/cc-pVTZ level of theory. Bond lengths are in Å.

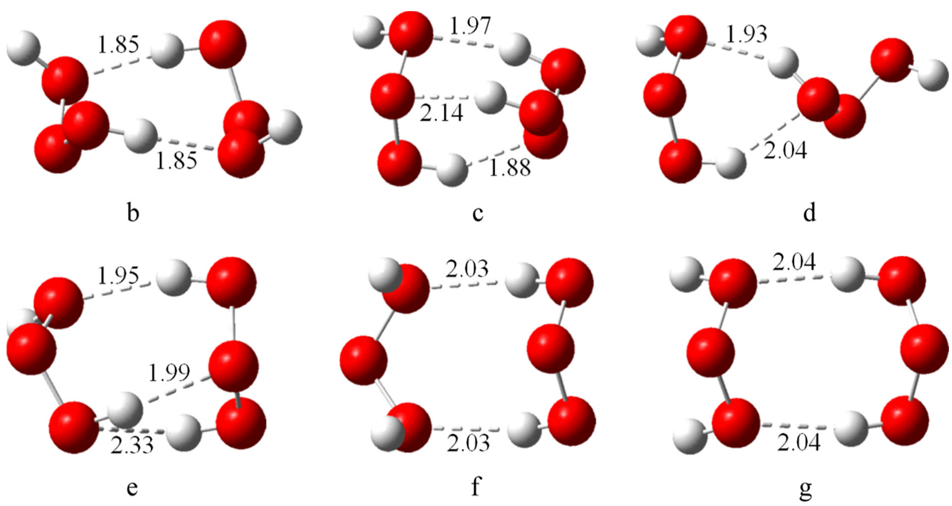

***Figure* S3.** Optimized structures of H_2O_3-H_2O_3 at the MP2/cc-pVTZ level of theory. Bond lengths are in Å.

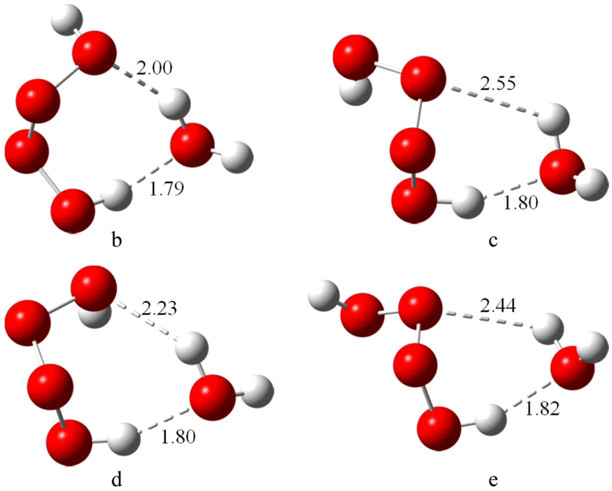

***Figure* S4.** Optimized structures of H_2O_4-H_2O at the MP2/cc-pVTZ level of theory. Bond lengths are in Å.

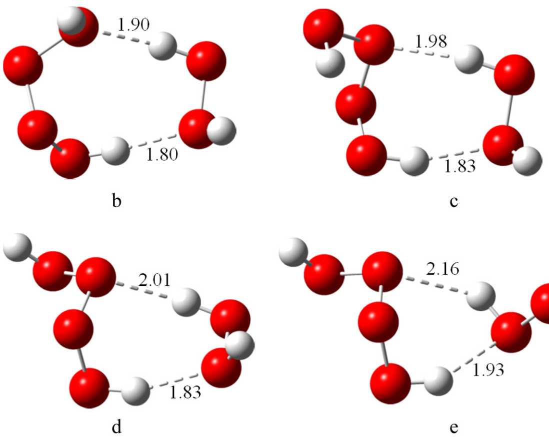

***Figure* S5.** Optimized structures of H_2O_4-H_2O_2 at the MP2/cc-pVTZ level of theory. Bond lengths are in Å.

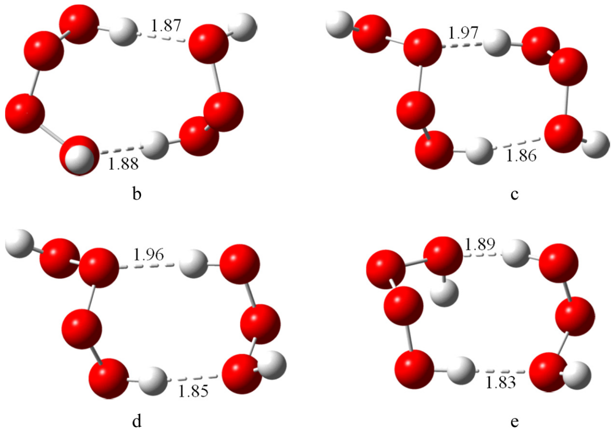

***Figure* S6.** Optimized structures of H_2O_4-H_2O_3 at the MP2/cc-pVTZ level of theory. Bond lengths are in Å.

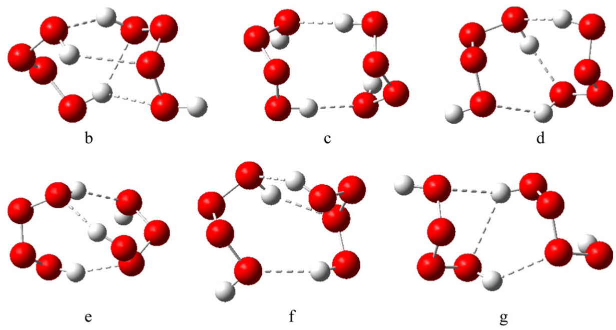

***Figure* S7.** Optimized structures of H_2O_4-H_2O_4 at the MP2/cc-pVTZ level of theory. Bond lengths are in Å.

***Table* S1.** The Binding energies in kcal/mol of H_2O_3-H_2O_n at the various levels of theory

		B3LYP				CAM-B3LYP				MP2						CCSD(T)					
		cc-pvDZ		cc-pvTZ		cc-pvDZ		cc-pvTZ		cc-pvDZ			cc-pvTZ			cc-pvDZ			cc-pvTZ		
		ΔE	$ΔE_0$	ΔE	$ΔE_0$	ΔE	$ΔE_0$	ΔE	$ΔE_0$	ΔE	$ΔE_0$	$ΔE^*$	ΔE	$ΔE_0$	$ΔE^*$	ΔE	$ΔE_0$	$ΔE^*$	ΔE	$ΔE_0$	$ΔE^*$
H_2O_3-H_2O	a	−14.07	−11.24	−9.56	−7.14	−15.70	−12.75	−10.97	−8.43	−13.06	−10.32	−6.89	−10.31	−7.83	−6.44	−12.58	−9.84	−6.46	−10.07	−7.58	−6.22
	b	−13.17	−10.47	−8.90	−6.64	−14.72	−11.91	−10.26	−7.86	−12.13	−9.55	−6.44	−9.63	−7.29	−6.02	−11.68	−9.10	−6.02	−9.39	−7.04	−5.80
	c	−10.35	−7.91	−6.65	−4.53	−12.01	−9.36	−8.03	−5.74	−9.64	−7.22	−4.39	−7.55	−5.31	−4.09	−9.31	−6.88	−4.10	−7.44	−5.19	−4.00
H_2O_3-H_2O_2	a	−14.13	−11.75	−9.97	−7.91	−15.97	−13.50	−11.58	−9.43	−13.44	−10.97	−7.91	−11.12	−8.97	−7.65	−12.97	−10.50	−7.41	−10.90	−8.75	−7.41
	b	−13.36	−11.10	−9.22	−7.26	−15.05	−12.73	−10.73	−8.69	−12.61	−10.31	−7.27	−10.29	−8.25	−6.97	−12.16	−9.87	−6.79	−10.08	−8.03	−6.73
	c	−11.88	−9.72	−7.93	−6.19	−13.48	−11.21	−9.28	−7.44	−11.27	−9.16	−6.28	−9.00	−7.19	−6.01	−10.88	−8.77	−5.86	−8.81	−6.99	−5.79
	d	−9.92	−8.12	−5.98	−4.30	−11.89	−9.94	−7.13	−5.64	−9.73	−8.09	−4.63	−7.13	−5.56	−4.17	−9.58	−7.95	−4.45	−7.15	−5.59	−4.16
H_2O_3-H_2O_3	a	−14.07	−12.10	−9.81	−8.15	−15.91	−13.85	−11.46	−9.69	−13.47	−11.43	−8.32	−11.19	−9.39	−8.00	−13.03	−10.98	−7.83	−10.99	−9.19	−7.77
	b	−14.15	−12.06	−9.57	−7.84	−15.90	−13.73	−11.12	−9.30	−13.69	−11.51	−8.04	−10.98	−9.13	−7.66	−13.33	−11.15	−7.62	−10.84	−9.00	−7.50
	c	−11.37	−9.17	−7.19	−5.36	−13.48	−11.14	−9.01	−7.03	−11.05	−8.83	−5.54	−9.09	−7.08	−5.67	−11.04	−8.82	−5.44	−9.20	−7.19	−5.71
	d	−10.59	−8.81	−6.88	−5.47	−12.14	−10.28	−8.21	−6.71	−10.39	−8.64	−5.79	−8.23	−6.73	−5.53	−10.07	−8.33	−5.44	−8.09	−6.59	−5.36
	e	−9.61	−7.64	−5.66	−4.07	−11.44	−9.33	−7.19	−5.50	−9.22	−7.34	−3.93	−7.20	−5.54	−4.14	−9.19	−7.31	−3.86	−7.32	−5.67	−4.22
	f	−6.38	−4.76	−3.12	−1.85	−7.99	−6.21	−4.35	−2.98	−6.12	−4.52	−1.35	−4.32	−2.95	−1.69	−6.13	−4.53	−1.36	−4.48	−3.11	−1.84
	g	−5.14	−3.73	−2.33	−1.24	−6.39	−4.87	−3.36	−2.18	−4.83	−3.43	−1.01	−3.37	−2.22	−1.12	−4.81	−3.42	−0.97	−3.50	−2.35	−1.24

***Table* S2.** The Binding energies in kcal/mol of H_2O_4-H_2O_n at the various levels of theory

		B3LYP				CAM-B3LYP				MP2						CCSD(T)					
		cc-pvDZ		cc-pvTZ		cc-pvDZ		cc-pvTZ		cc-pvDZ			cc-pvTZ			cc-pvDZ			cc-pvTZ		
		ΔE	$ΔE_0$	ΔE	$ΔE_0$	ΔE	$ΔE_0$	ΔE	$ΔE_0$	ΔE	$ΔE_0$	$ΔE^*$	ΔE	$ΔE_0$	$ΔE^*$	ΔE	$ΔE_0$	$ΔE^*$	ΔE	$ΔE_0$	$ΔE^*$
H_2O_4-H_2O	a	−14.75	−11.98	−10.15	−7.68	−16.34	−13.48	−11.58	−8.99	−13.75	−11.02	−7.48	−10.92	−8.42	−6.97	−13.33	−10.60	−7.09	−10.77	−8.28	−6.84
	b	−15.18	−12.36	−10.40	−7.90	−16.53	−13.65	−11.63	−9.06	−13.35	−10.58	−6.95	−10.47	−7.97	−6.48	−13.04	−10.27	−6.64	−10.40	−7.90	−6.43
	c	−13.16	−10.66	−9.10	−7.16	−14.77	−12.15	−10.35	−8.23	−12.54	−10.08	−7.02	−9.84	−7.75	−6.53	−12.00	−9.54	−6.53	−9.52	−7.43	−6.25
	d	−13.77	−11.11	−9.25	−6.93	−15.31	−12.55	−10.62	−8.23	−12.75	−10.15	−6.64	−9.98	−7.65	−6.22	−12.37	−9.77	−6.29	−9.85	−7.52	−6.11
	e	−12.33	−9.90	−8.20	−6.27	−13.62	−11.11	−9.29	−7.20	−11.10	−8.74	−5.61	−8.45	−6.39	−5.13	−10.66	−8.30	−5.21	−8.23	−6.18	−4.95
H_2O_4-H_2O_2	a	−13.85	−11.63	−9.64	−7.66	−15.62	−13.29	−11.18	−9.10	−13.34	−11.04	−7.77	−10.82	−8.77	−7.36	−12.95	−10.64	−7.35	−10.71	−8.65	−7.22
	b	−13.21	−11.10	−9.42	−7.55	−14.77	−12.60	−10.83	−8.89	−11.98	−9.81	−6.80	−9.98	−8.06	−6.75	−11.68	−9.50	−6.46	−9.92	−8.00	−6.67
	c	−11.31	−9.31	−7.44	−5.74	−13.03	−11.01	−8.91	−7.09	−11.06	−9.08	−6.23	−8.79	−6.97	−5.80	−10.60	−8.62	−5.73	−8.55	−6.72	−5.53
	d	−11.73	−9.64	−7.93	−6.14	−13.25	−11.13	−9.30	−7.46	−10.93	−8.81	−6.06	−8.84	−7.00	−5.80	−10.61	−8.49	−5.68	−8.58	−6.74	−5.48
	e	−10.08	−8.23	−6.42	−4.95	−11.35	−9.44	−7.49	−5.95	−9.36	−7.57	−4.97	−7.11	−5.60	−4.54	−9.03	−7.24	−4.61	−6.96	−5.45	−4.37
H_2O_4-H_2O_3	a	−14.47	−12.54	−10.00	−8.33	−16.34	−14.32	−11.62	−9.86	−14.20	−12.19	−8.67	−11.54	−9.80	−8.26	−13.90	−11.88	−8.30	−11.50	−9.75	−8.18
	b	−13.68	−11.73	−9.11	−7.48	−15.78	−13.69	−10.91	−9.14	−13.56	−11.61	−8.04	−11.10	−9.35	−7.82	−13.42	−11.47	−7.81	−11.13	−9.38	−7.79
	c	−14.07	−12.19	−9.69	−8.12	−15.74	−13.79	−11.16	−9.50	−13.39	−11.45	−7.90	−10.80	−9.13	−7.63	−13.11	−11.16	−7.55	−10.77	−9.10	−7.57
	d	−12.16	−10.33	−7.92	−6.40	−13.67	−11.81	−9.28	−7.72	−11.80	−9.94	−6.69	−9.30	−7.73	−6.34	−11.56	−9.71	−6.37	−9.23	−7.66	−6.22
	e	−11.29	−9.56	−7.47	−6.06	−12.75	−10.98	−8.81	−7.34	−10.63	−8.88	−6.10	−8.58	−7.07	−5.80	−10.33	−8.58	−5.74	−8.47	−6.96	−5.65
H_2O_4-H_2O_4	a	−13.38	−11.65	−8.97	−7.44	−15.30	−13.43	−10.59	−8.94	−13.37	−11.52	−7.95	−10.64	−9.03	−7.51	−13.06	−11.21	−7.58	−10.64	−9.02	−7.46
	b	−13.14	−11.35	−6.72	−5.70	−15.30	−13.41	−9.83	−8.30	−13.32	−11.57	−9.81	−10.34	−8.80	−7.12	−13.17	−11.42	−7.28	−10.38	−8.84	−7.07
	c	−12.17	−10.53	−7.94	−6.52	−13.86	−12.08	−9.34	−7.79	−12.12	−10.41	−6.95	−9.63	−8.18	−6.63	−11.98	−10.26	−6.73	−9.75	−8.29	−6.70
	d	−14.22	−12.30	−8.64	−7.15	−16.11	−14.05	−10.22	−8.62	−13.14	−11.29	−6.78	−9.97	−8.37	−6.59	−13.00	−11.15	−6.56	−10.10	−8.50	−6.66
	e	−14.61	−12.43	−8.73	−7.01	−16.54	−14.21	−10.38	−8.53	−13.51	−11.43	−6.11	−10.41	−8.57	−6.58	−13.57	−11.48	−6.07	−10.68	−8.85	−6.78
	f	−12.56	−10.66	−7.40	−5.99	−14.76	−12.78	−9.24	−7.71	−12.60	−10.82	−6.97	−9.61	−8.10	−6.51	−12.35	−10.56	−6.66	−9.59	−8.09	−6.43
	g	−9.24	−8.08	−5.39	−4.66	−11.22	−9.93	−6.91	−6.04	−9.64	−8.48	−2.82	−7.26	−6.43	−5.26	−9.26	−8.10	−5.21	−7.10	−6.27	−5.06