

Electronic Supplementary Information

Supplementary information for the communication *Chemically accurate energy barriers of small gas molecules in clathrate hydrates*
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Table 1 CCSD(T)/aug-cc-pVTZ interaction energy of CH₄-6H₂O as a function of water ring diameter (d) and gas molecule centre of mass-ring separation (R). Distances in Å, energy in kJ/mol.

$d \backslash R$	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5
5.4	51.26	43.22	-56.66	-144.32	-183.82	-193.97	-194.03	-192.27	-190.86	-190.00
5.6	-19.50	-24.87	-93.07	-154.69	-182.79	-189.59	-189.03	-187.28	-185.95	-185.15
5.8	-64.89	-68.19	-114.22	-156.86	-176.35	-180.59	-179.57	-177.84	-176.59	-175.85
6.2	-106.10	-107.08	-127.22	-146.52	-154.99	-155.94	-154.42	-152.83	-151.73	-151.09
6.4	-111.67	-112.03	-125.03	-137.57	-142.76	-142.77	-141.16	-139.64	-138.63	-138.03
6.6	-111.62	-111.60								
6.8	-108.01	-107.75								

Table 2 CCSD(T)/aug-cc-pVTZ interaction energy of CO₂-6H₂O as a function of water ring diameter (d) and gas molecule centre of mass-ring separation (R). Distances in Å, energy in kJ/mol.

$d \backslash R$	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5
5.2	-118.03	-114.65	-116.57	-136.22	-164.32	-183.86	-190.86	-191.03	-189.45	-188.09
5.4	-149.40	-146.71	-147.21	-159.55	-177.64	-190.09	-194.08	-193.50	-191.89	-190.60
5.6	-164.37	-162.32	-162.09	-169.47	-180.55	-187.89	-189.67	-188.54	-186.92	-185.71
5.8	-168.26	-166.79	-166.25	-170.34	-176.62	-180.40	-180.62	-179.11	-177.50	-176.36
6.2	-156.81	-156.06	-155.47	-156.26	-157.42	-157.32	-155.87	-154.03	-152.51	-151.50
6.4	-146.50	-145.96	-145.44	-145.48	-145.43	-144.44	-142.65	-140.79	-139.34	-138.40

Table 3 CCSD(T)/aug-cc-pVTZ interaction energy of H₂-6H₂O as a function of water ring diameter (d) and gas molecule centre of mass-ring separation (R). Distances in Å, energy in kJ/mol.

$d \backslash R$	0.0000	0.37305	0.87305	1.37305	1.87305	2.37305	2.87305	3.37305	3.87305	4.37305
4.8	-96.36	-102.11	-121.55	-140.27	-150.40	-153.48	-153.44	-152.65	-151.93	-151.44
5.0	-134.92	-139.15	-153.30	-166.88	-174.14	-176.19	-175.93	-175.14	-174.47	-174.01
5.2	-160.02	-163.07	-173.24	-182.94	-188.02	-189.27	-188.84	-188.07	-187.44	-187.01
5.4	-171.78	-173.90	-180.98	-187.70	-191.12	-191.77	-191.24	-190.50	-189.92	-189.53
5.6	-173.75	-175.10	-179.80	-184.32	-186.54	-186.81	-186.24	-185.55	-185.02	-184.66
5.8	-169.37	-170.23	-173.25	-176.11	-177.41	-177.38	-176.80	-176.17	-175.69	-175.36
6.2	-150.31	-150.61	-151.64	-152.53	-152.73	-152.38	-151.83	-151.32	-150.94	-150.68
6.4	-138.66	-138.85	-139.37	-139.71	-139.61	-139.17	-138.65	-138.20	-137.86	-137.63