Table 1: Intermolecular parameters of the CC-pol-8s stationary point structures of water dimer. Distances in Å, angles in degrees. See Ref. [1] for definitions and atom labeling.

No.	index	$r_{H_2O_2}$	$\theta_{O_1H_2O_2}$	$\theta_{H_3O_2O_1}$	$\theta_{H_4O_2O_1}$	$\tau_{O_2H_2O_1H_1}$	$\tau_{H_3O_2O_1H_2}$	$\tau_{H_4O_2O_1H_2}$
1	0	1.9468	171.03	108.82	108.82	180.00	123.23	−123.23
2	1	1.9648	167.68	106.78	135.97	142.59	160.00	26.13
3	2	1.9687	166.52	110.27	145.04	180.00	180.00	0.00
4	1	2.2666	114.70	131.47	47.02	−133.75	111.16	180.00
5	1	2.2685	112.71	143.42	48.56	−151.15	−116.32	−167.86
6	3	2.2721	110.11	155.29	50.60	180.00	180.00	180.00
7	2	3.4247	56.92	53.05	53.05	180.00	−97.86	97.86
8	3	3.1220	92.07	70.83	70.83	−63.23	180.00	66.11
9	1	2.5515	110.11	127.66	127.66	0.00	−90.00	90.00
10	2	2.7073	111.15	127.66	127.66	0.00	0.00	180.00

References

[1] G. S. Tschumper, M. N. Leininger, B. C. Hoffman, E. F. Valeev, H. F. Schaefer III, and M. Quack, J. Chem. Phys. **116**, 690 (2002).