

Electronic Supplementary Information for

Internal Electric Fields in Small Water Clusters [(H₂O)_n; n=2-6]

Saumik Sen,^{‡*a} Manjusha Boda,^{‡*a} S. Venkat Lata^a and G. Naresh Patwari^{*a}

^a Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400 076 India; E-mail: saumiksen@chem.iitb.ac.in; naresh@chem.iitb.ac.in

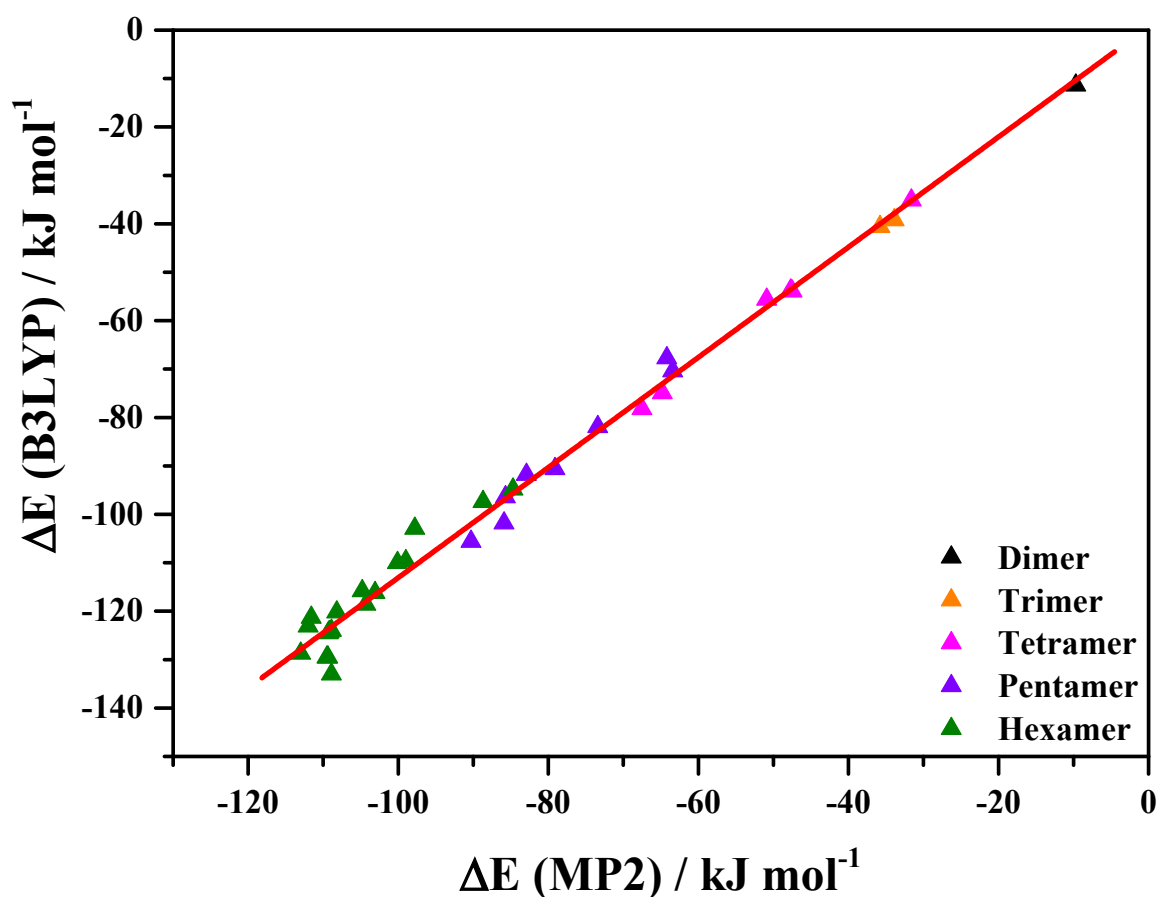


Fig. S1. Plot of ZPE and BSSE corrected stabilization energies calculated at B3LYP/6-311++G(*d,p*) against stabilization energies calculated MP2/aug-cc-pVDZ level of theory for various water clusters. The straight-line is a linear fit to the data points ($R^2 = 0.989$). From the slope it can be inferred that the B3LYP/6-311++G(*d,p*) stabilization energies are on the average ~14% higher than the stabilization energies calculated MP2/aug-cc-pVDZ level.

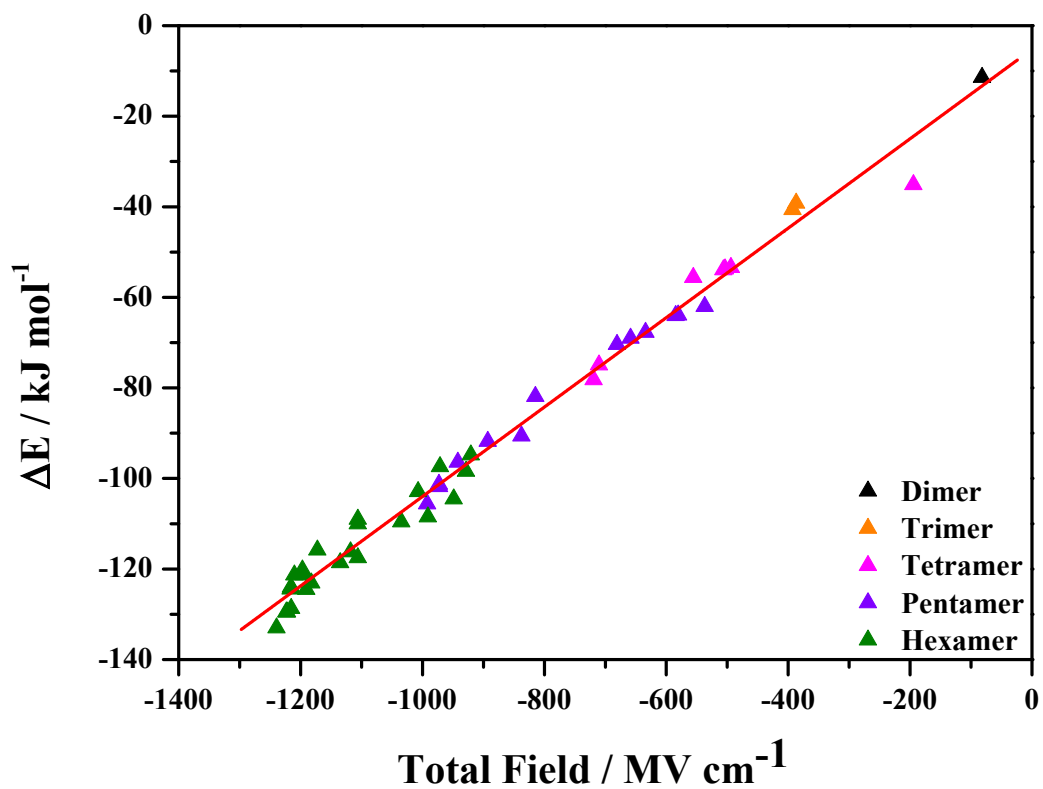


Fig. S2. Plot of total stabilization energy against total electric field calculated at B3LYP/6-311++G(*d,p*) level for several water clusters. The straight line is a linear fit ($R^2 = 0.988$) to the data points.

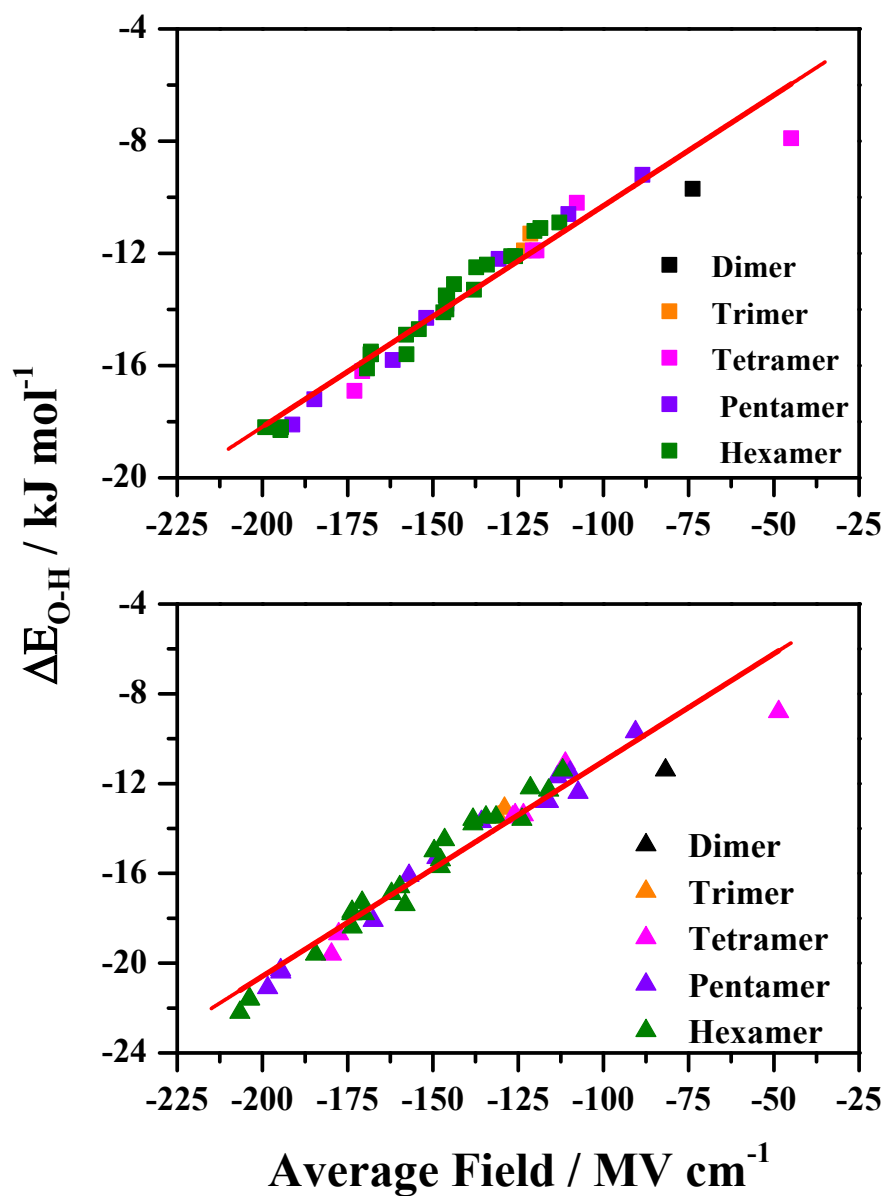


Fig. S3. Plot of average hydrogen bond stabilization energy against average electric field calculated at MP2/aug-cc-pVDZ (squares) and at B3LYP/6-311++G(*d,p*) (triangles) levels for several water clusters. The straight lines are linear fits to the data points with R^2 values of 0.951 and 0.949, respectively.

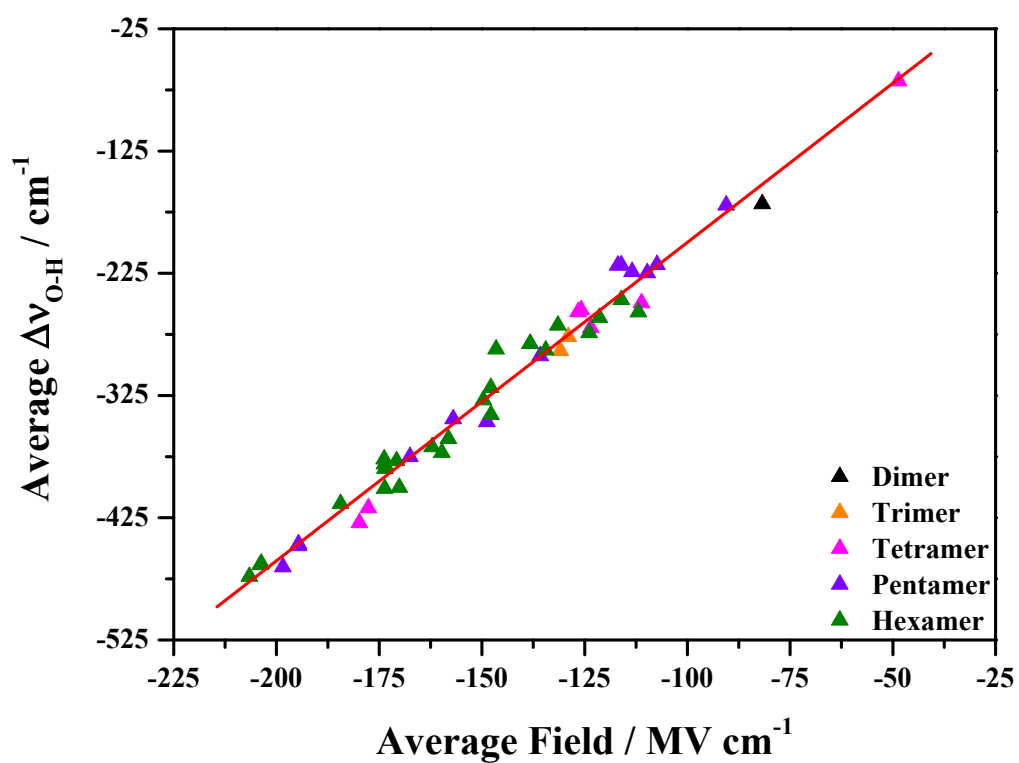


Fig. S4. Plot of average red-shift in the O–H stretching frequencies against average electric field calculated at B3LYP/6-311++G(*d,p*) level for several water clusters. The straight line is a linear fit ($R^2 = 0.979$) to the data points, which corresponds to the Stark tuning rate of $2.60 \text{ cm}^{-1}/(\text{MV cm}^{-1})$.

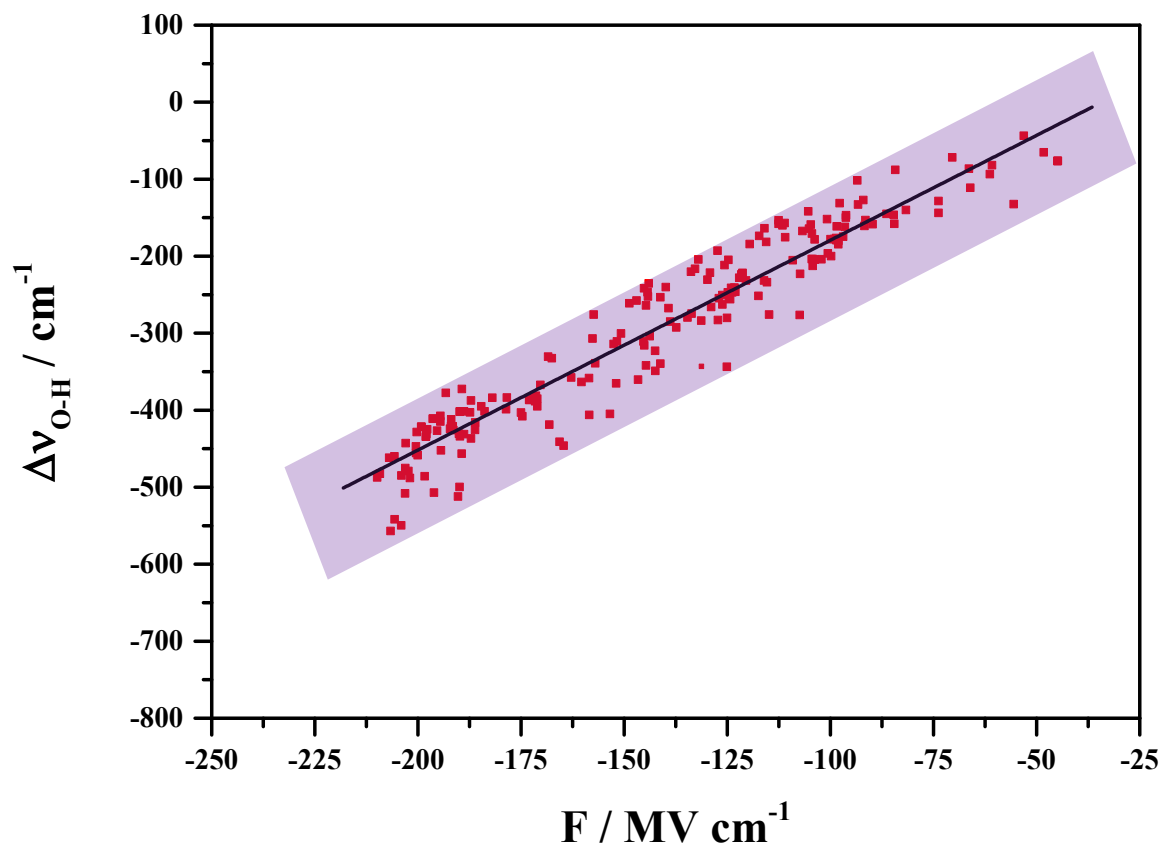


Figure S5. Plot of red-shift in the O–H stretching frequencies against the corresponding electric field calculated at MP2/aug-cc-pVDZ level for several water clusters. The shaded region indicates linear trend. The straight line is a linear fit to data points (206) with R^2 value of 0.921 and residuals within ± 100 cm⁻¹. The corresponding Stark tuning rate is 2.72 cm⁻¹/(MV cm⁻¹).

Table S1. Unscaled vibrational frequencies (cm^{-1}) for free and hydrogen bonded O–H groups and the electric fields (MV cm^{-1}) produced at hydrogen bonded O–H group for the water clusters W_n ($n = 2-6$) calculated at various levels of theory. Vibrational frequencies listed in Columns (a) and (b) are the selectively labelled hydrogen bonded O–H group in the deuterated water cluster and O–D group in the water cluster

Structure	MP2/aug-cc-pVDZ				Elec. Field	B3LYP/6-311++G(d,p)		
	$\nu_{\text{O-H}} \text{free}$	$\nu_{\text{O-H}} \text{H-bond}$	$\nu_{\text{O-H}} \text{H-bond}$ (a)	$\nu_{\text{O-D}} \text{H-bond}$ (b)		$\nu_{\text{O-H}} \text{free}$	$\nu_{\text{O-H}} \text{H-bond}$	Elec. Field
W	3875							
	2811 (O–D)							
W2	3926	3704	3731	2707	-73.79	3915	3706	-81.79
	3904					3893		
	3797					3815		
W3_1	3896	3641	3633	2636	-124.07	3895	3630	-131.83
	3894	3632	3628	2632	-123.76	3893	3619	-131.23
	3890	3574	3647	2646	-122.08	3888	3561	-129.66
W3_2	3900	3649	3651	2649	-121.57	3901	3641	-129.06
	3899	3648	3652	2650	-121.33	3899	3640	-128.98
	3899	3596	3653	2651	-121.27	3899	3587	-128.96
W4_1	3886	3524	3488	2530	-173.01	3886	3508	-179.82
	3885	3486	3488	2530	-173.00	3885	3471	-179.80
	3885	3486	3488	2530	-173.00	3885	3470	-179.78
	3884	3396	3488	2530	-172.99	3885	3377	-179.73
W4_2	3888	3532	3490	2531	-171.06	3889	3520	-178.09
	3887	3505	3490	2531	-171.06	3889	3493	-178.07
	3887	3488	3507	2545	-170.31	3888	3476	-177.17
	3886	3409	3507	2545	-170.30	3887	3396	-177.15
W4_3	3902	3779	3434	2491	-165.66	3896	3757	-167.24
	3894	3708	3707	2691	-106.79	3892	3704	-107.69
	3885	3686	3748	2720	-91.99	3883	3683	-98.89
		3675	3716	2696	-89.75		3681	-92.71
		3410	3728	2705	-84.64		3381	-89.11

W4_4	3927	3765	3533	2564	-144.67	3919	3743	-151.73
	3895	3663	3623	2629	-117.42	3892	3670	-124.55
	3886	3610	3718	2699	-111.07	3886	3595	-117.81
	3798	3504	3710	2693	-105.17	3817	3486	-109.41
W4_5	3927	3763	3514	2550	-146.63	3920	3739	-152.09
	3899	36634	3711	2694	-115.97	3894	3669	-122.57
	3888	3623	3641	2642	-115.36	3890	3610	-121.77
	3798	3488	3716	2697	-104.76	3817	3478	-109.86
W4_6	3924	3863	3798	2757	-44.94	3908	3842	-48.69
	3924	3838	3798	2757	-44.91	3907	3815	-48.69
	3796	3745	3798	2757	-44.83	3809	3753	-48.55
	3793	3737	3798	2757	-44.83	3803	3745	-48.47
W4_7						3895	3691	-169.77
						3890	3669	-132.61
						3886	3623	-108.65
						3873	3483	-82.81
W5_1	3889	3494	3450	2503	-192.20	3890	3478	-199.14
	3887	3487	3454	2505	-191.98	3889	3467	-199.03
	3887	3442	3454	2505	-191.54	3886	3422	-198.70
	3885	3433	3449	2502	-191.38	3884	3412	-198.34
	3883	3354	3473	2520	-188.83	3883	3327	-197.00
W5_2	3893	3515	3444	2498	-190.06	3898	3498	-198.04
	3892	3496	3472	2519	-187.35	3895	3484	-196.20
	3890	3464	3459	2509	-186.09	3892	3450	-194.58
	3880	3439	3491	2533	-181.97	3883	3424	-192.76
	3879	3371	3491	2533	-178.45	3882	3353	-191.26
W5_3	3899	3771	3423	2483	-194.40	3895	3757	-198.62
	3886	3698	3441	2496	-189.79	3887	3694	-195.03
	3884	3647	3418	2480	-189.39	3886	3628	-192.33
	3883	3462	3732	2710	-129.03	3884	3448	-140.81
		3419	3733	2710	-105.36		3403	-115.62
	3351	3670	2663	-103.75		3334	-99.56	

W5_4	3899	3714	3325	2410	-204.05	3898	3695	-204.32
	3890	3666	3389	2458	-198.37	3890	3669	-203.24
	3886	3634	3658	2656	-132.78	3889	3640	-135.01
	3882	3627	3682	2673	-127.37	3883	3628	-130.91
		3392	3670	2662	-109.11		3368	-112.26
		3281	3671	2663	-104.50		3261	-107.00
W5_5	3927	3730	3368	2442	-196.09	3920	3721	-201.76
	3887	3565	3467	2514	-174.66	3887	3563	-182.01
	3885	3506	3511	2547	-160.34	3886	3492	-166.94
	3882	3451	3568	2590	-157.66	3884	3431	-160.65
	3797	3328	3718	2699	-120.17	3817	3310	-126.31
W5_6	3894	3682	3628	2634	-144.32	3893	3652	-147.56
	3893	3636	3628	2634	-144.32	3893	3628	-147.56
	3893	3621	3620	2626	-124.60	3892	3615	-130.00
	3892	3621	3620	2626	-124.60	3890	3608	-130.00
		3576	3634	2636	-123.24		3562	-129.79
		3540	3634	2636	-123.24		3534	-129.78
W5_7	3916	3830	3470	2517	-153.44	3902	3816	-154.62
	3886	3808	3695	2683	-98.10	3884	3787	-99.53
	3787	3743	3695	2683	-98.09	3796	3729	-99.53
		3713	3746	2720	-73.78		3721	-75.50
		3693	3746	2720	-73.78		3695	-75.50
		3653	3781	2745	-61.34		3663	-64.63
		3445	3781	2745	-61.33		3428	-64.63
W5_8	3928	3785	3526	2560	-142.45	3919	3756	-144.52
	3903	3722	3708	2693	-129.14	3894	3705	-137.46
	3897	3685	3678	2669	-100.59	3885	3685	-108.00
	3799	3665	3675	2666	-99.83	3817	3650	-103.15
		3644	3728	2706	-96.19		3623	-97.27
		3497	3742	2716	-93.27		3514	-90.30
W5_9						3899	3502	-197.83
						3895	3483	-196.27

						3893	3450	-196.05
						3883	3428	-191.62
						3879	3354	-191.36
W5_10						3917	3791	-160.34
						3889	3741	-121.39
						3885	3688	-115.03
						3816	3670	-97.20
							3629	-94.08
							3392	-70.68
W5_11						3920	3751	-140.48
						3918	3745	-129.92
						3892	3668	-106.32
						3818	3593	-104.57
						3816	3515	-103.38
W5_12						3918	3756	-143.70
						3916	3739	-127.46
						3887	3667	-104.50
						3817	3613	-102.74
						3815	3487	-102.11
W5_13						3895	3764	-144.27
						3895	3737	-127.12
						3894	3667	-113.99
						3886	3600	-95.12
						3803	3515	-56.50
W6_1	3889	3735	3362	2439	-214.12	3888	3724	-218.11
	3886	3586	3390	2458	-203.99	3887	3582	-208.45
	3885	3570	3367	2441	-203.10	3887	3564	-206.27
	3882	3516	3577	2598	-167.42	3885	3506	-173.10
	3877	3415	3574	2593	-150.76	3876	3399	-156.19
		3362	3559	2582	-145.13		3344	-153.18
		3286	3723	2702	-100.82		3266	-100.22
W6_2	3895	3762	3255	2359	-222.10	3896	3748	-218.23

	3883	3724	3472	2519	-174.98	3885	3716	-177.71
	3880	3671	3536	2564	-156.99	3884	3676	-161.43
	3878	3591	3710	2693	-153.97	3879	3592	-158.78
		3534	3509	2546	-151.92		3523	-154.84
		3484	3598	2612	-107.42		3477	-110.10
		3443	3704	2689	-104.48		3433	-107.09
		3225	3725	2704	-96.22		3199	-94.22
W6_3	3885	3805	3224	2337	-230.86	3884	3777	-226.98
	3884	3772	3456	2508	-168.12	3883	3757	-170.78
	3880	3755	3542	2571	-167.52	3881	3738	-162.87
		3678	3582	2598	-137.36		3697	-142.28
		3667	3690	2679	-119.57		3684	-116.16
		3564	3752	2724	-113.04		3555	-115.14
		3534	3700	2686	-96.89		3542	-97.94
		3437	3789	2751	-92.10		3422	-95.98
		3196	3735	2711	-81.67		3180	-81.93
W6_4	3893	3500	3440	2496	-198.05	3896	3485	-206.21
	3893	3489	3441	2496	-198.02	3896	3475	-206.21
	3888	3476	3463	2513	-196.36	3887	3457	-204.67
	3888	3436	3464	2513	-196.35	3887	3417	-204.66
	3883	3413	3473	2520	-189.85	3884	3394	-200.23
	3883	3356	3473	2520	-189.80	3884	3332	-200.23
W6_5	3893	3501	3446	2500	-200.26	3895	3484	-206.94
	3891	3487	3450	2503	-197.74	3894	3472	-205.07
	3886	3475	3448	2501	-195.36	3888	3456	-205.04
	3886	3432	3467	2516	-194.55	3886	3414	-204.39
	3885	3417	3460	2510	-194.54	3885	3396	-203.02
	3885	3356	3480	2525	-184.65	3885	3331	-199.01
W6_6	3887	3712	3266	2367	-221.86	3899	3663	-228.55
	3886	3633	3463	2512	-191.94	3887	3639	-219.15
	3883	3609	3375	2447	-189.90	3885	3614	-214.64
	3875	3578	3611	2622	-144.67	3878	3584	-143.78

	3827	3470	3619	2625	-124.30	3876	3397	-143.33
		3346	3643	2642	-116.07		3279	-122.39
		3232	3693	2682	-115.54		3216	-118.77
W6_7	3896	3755	3356	2434	-215.79	3893	3729	-219.35
	3889	3686	3413	2475	-206.96	3890	3690	-212.65
	3885	3628	3428	2486	-200.47	3885	3624	-207.20
	3882	3456	3416	2478	-200.07	3883	3436	-205.02
	3880	3418	3721	2703	-127.15	3880	3395	-137.03
		3374	3714	2697	-120.34		3354	-119.68
		3304	3652	2649	-107.31		3281	-114.06
W6_8	3896	3753	3392	2461	-209.20	3895	3728	-214.34
	3890	3683	3415	2477	-205.67	3894	3690	-211.78
	3886	3638	3396	2463	-202.32	3887	3629	-208.06
	3885	3463	3444	2498	-197.94	3886	3448	-205.19
	3880	3419	3721	2703	-134.47	3879	3398	-141.82
		3380	3708	2693	-122.97		3358	-122.82
		3322	3662	2657	-104.27		3297	-111.88
W6_9	3888	3494	3453	2505	-199.18	3888	3472	-206.71
	3888	3476	3453	2505	-199.18	3887	3453	-206.68
	3888	3476	3453	2505	-199.18	3887	3453	-206.62
	3887	3421	3453	2505	-199.17	3886	3394	-206.61
	3887	3421	3453	2505	-199.17	3886	3393	-206.48
	3887	3349	3453	2505	-199.16	3886	3316	-206.46
W6_10	3893	3811	3318	2406	-206.64	3890	3818	-207.38
	3888	3789	3444	2498	-188.81	3889	3755	-194.26
	3888	3680	3487	2531	-187.14	3888	3690	-193.26
	3887	3645	3476	2522	-178.61	3888	3633	-187.51
		3504	3692	2680	-128.56		3490	-126.36
		3466	3773	2740	-105.21		3449	-114.79
		3402	3671	2663	-104.23		3379	-108.99
		3287	3803	2760	-70.46		3265	-64.63
W6_11	3904	3786	3376	2449	-212.00	3901	3766	-213.37

	3903	3777	3387	2456	-201.91	3897	3748	-205.56
	3885	3685	3633	2638	-145.17	3888	3689	-146.80
	3878	3671	3768	2737	-140.59	3880	3659	-136.20
		3644	3653	2652	-129.16		3647	-131.64
		3611	3774	2741	-123.04		3634	-124.38
		3405	3697	2682	-99.97		3388	-109.10
		3320	3695	2681	-98.53		3302	-105.32
W6_12	3892	3660	3497	2539	-193.24	3892	3637	-193.78
	3892	3627	3490	2532	-172.02	3890	3615	-177.66
	3887	3578	3486	2529	-171.59	3890	3562	-177.56
	3884	3520	3480	2524	-171.07	3886	3509	-175.39
	3883	3487	3639	2642	-144.02	3884	3477	-146.39
		3479	3620	2627	-127.01		3468	-133.14
		3394	3624	2629	-126.19		3383	-130.99
W6_13	3898	3710	3146	2278	-224.45	3896	3697	-234.79
	3892	3606	3638	2639	-151.34	3894	3612	-154.03
	3886	3598	3564	2586	-145.29	3886	3588	-150.60
	3883	3582	3571	2591	-143.81	3885	3571	-149.81
	3846	3543	3667	2659	-141.45	3852	3542	-148.37
		3525	3590	2603	-138.80		3516	-141.69
		3114	3600	2610	-133.63		3048	-138.87
W6_14	3905	3821	3502	2542	-189.31	3899	3823	-186.53
	3902	3729	3517	2552	-162.83	3896	3712	-166.20
	3885	3689	3468	2517	-158.48	3888	3689	-158.22
	3884	3673	3561	2583	-152.54	3887	3665	-155.21
		3562	3716	2698	-126.55		3555	-129.67
		3519	3817	2772	-113.13		3527	-112.78
		3492	3697	2683	-99.05		3492	-101.72
		3411	3713	2693	-96.48		3415	-95.66
W6_15	3928	3702	3362	2438	-190.26	3921	3700	-188.90
	3890	3698	3473	2522	-183.82	3890	3678	-184.21
	3884	3628	3693	2682	-147.49	3887	3636	-147.51

	3881	3594	3644	2646	-129.81	3883	3594	-130.31
	3799	3554	3592	2606	-127.25	3819	3551	-129.18
		3463	3595	2608	-125.03		3453	-128.07
		3328	3670	2665	-124.70		3318	-126.52
W6_16	3893	3822	3449	2503	-186.16	3889	3813	-189.42
	3883	3807	3516	2550	-158.49	3886	3798	-159.96
	3882	3696	3532	2566	-131.26	3882	3729	-126.68
		3678	3531	2566	-125.08		3686	-122.34
		3664	3698	2684	-98.57		3670	-99.54
		3551	3690	2678	-98.06		3549	-98.87
		3536	3721	2700	-91.49		3542	-83.01
		3479	3788	2749	-66.41		3477	-65.41
		3409	3793	2752	-60.82		3395	-61.99
W6_17	3905	3780	3429	2487	-164.67	3897	3758	-164.49
	3893	3744	3635	2639	-139.91	3893	3720	-142.69
	3890	3700	3628	2632	-124.85	3889	3691	-131.44
	3881	3679	3628	2632	-123.01	3881	3685	-128.51
		3630	3717	2698	-112.57		3620	-112.03
		3624	3713	2695	-98.47		3616	-103.26
		3564	3743	2717	-97.73		3554	-99.18
		3405	3730	2705	-86.39		3386	-89.73
W6_18	3926	3757	3617	2626	-147.00	3918	3738	-150.00
	3896	3692	3535	2565	-141.20	3896	3666	-146.66
	3894	3657	3654	2653	-133.78	3894	3661	-137.94
	3887	3628	3591	2605	-131.29	3890	3618	-135.56
	3797	3600	3643	2643	-120.42	3816	3594	-126.33
		3546	3715	2697	-111.60		3534	-118.35
		3502	3696	2683	-103.81		3495	-105.69
W6_19	3886	3848	3307	2397	-227.27			
	3885	3701	3248	2353	-223.41			
	3883	3653	3564	2585	-151.74			
	3881	3600	3614	2624	-148.71			

		3580	3621	2629	-141.20
		3538	3609	2619	-128.89
		3316	3714	2695	-91.75
		3194	3831	2781	-53.12
W6_20	3900	3769	3387	2458	-209.85
	3889	3681	3399	2466	-203.06
	3884	3644	3432	2490	-202.98
	3881	3456	3419	2480	-200.43
	3880	3422	3750	2724	-130.11
		3378	3693	2681	-128.69
		3320	3671	2663	-102.18
W6_21	3899	3842	3333	2417	-205.66
	3883	3808	3544	2573	-168.44
	3878	3729	3671	2665	-132.01
		3729	3802	2761	-118.19
		3680	3701	2687	-117.24
		3644	3599	2611	-114.83
		3586	3699	2684	-110.94
		3526	3764	2732	-66.05
		3305	3810	2766	-48.28
W6_22	3890	3800	3493	2535	-171.36
	3887	3757	3599	2613	-157.38
	3879	3648	3622	2631	-144.23
	3878	3624	3552	2577	-142.47
		3592	3612	2621	-126.16
		3584	3663	2658	-125.66
		3514	3787	2748	-84.28
		3468	3742	2717	-55.55
W6_23	3924	3780	3232	2341	-214.14
	3904	3738	3438	2494	-187.14
	3883	3692	3607	2618	-139.22
	3877	3604	3595	2608	-134.65

	3796	3566	3721	2702	-112.53			
		3429	3773	2737	-93.46			
		3197	3717	2696	-84.49			
W6_24						3898	3738	-213.18
						3896	3687	-213.03
						3886	3639	-208.26
						3884	3438	-207.66
						3880	3406	-138.20
							3372	-127.01
							3303	-109.09
W6_25						3893	3753	-207.36
						3891	3659	-205.45
						3888	3606	-203.25
						3882	3457	-201.87
						3881	3415	-147.16
							3362	-118.41
							3310	-111.81
W6_26						3916	3723	-218.43
						3888	3537	-207.31
						3887	3458	-200.45
						3883	3416	-187.56
						3883	3372	-171.26
						3815	3285	-121.20
W6_27						3896	3799	-219.90
						3894	3693	-155.81
						3884	3689	-146.48
						3879	3664	-131.84
							3628	-130.15
							3594	-117.79
							3548	-109.99
							3232	-94.09
W6_28						3895	3819	-210.37

	3885	3746	-187.61
	3882	3715	-139.48
	3872	3663	-120.97
		3634	-117.60
		3601	-115.82
		3451	-53.57
		3251	-45.72
W6_29	3920	3714	-220.87
	3892	3666	-210.73
	3888	3593	-154.23
	3881	3541	-144.07
	3864	3346	-132.08
	3818	3240	-86.89
W6_30	3888	3758	-164.91
	3883	3753	-132.69
	3882	3684	-131.77
	3881	3671	-117.68
		3621	-112.14
		3594	-100.90
		3517	-85.64
		3497	-82.73

Table S2. Average values of the free and hydrogen bonded O–H stretching frequencies (cm^{-1}), their shifts and the average electric field (MV cm^{-1}) produced at hydrogen bonded O–H groups for the water clusters calculated at various levels of theory. Vibrational frequency shifts listed in Columns (a) and (b) are the average of selectively labelled hydrogen bonded O–H group in the deuterated water cluster and O–D group in the water cluster

Structure	MP2/aug-cc-pVDZ						B3LYP/6-311++G(d,p)				
	$\nu_{\text{O-H}} \text{free}$	$\nu_{\text{O-H}} \text{H-bond}$	$ \Delta\nu_{\text{O-H}} $	$ \Delta\nu_{\text{O-H}} \text{H-bond}$	$ \Delta\nu_{\text{O-D}} \text{H-bond}$	Elec. Field	$\nu_{\text{O-H}} \text{free}$	$\nu_{\text{O-H}} \text{H-bond}$	$ \Delta\nu_{\text{O-H}} $	Elec. Field	
			(a)	(b)							
W2	3876	3704	172	144	103	-73.79	3874	3706	168	-81.79	
W3_1	3893	3616	277	239	172	-123.31	3892	3604	288	-130.91	
W3_2	3899	3631	268	223	161	-121.39	3899	3623	276	-129.00	
W4_1	3885	3473	412	387	280	-173.00	3885	3456	429	-179.78	
W4_2	3887	3483	404	376	273	-170.68	3888	3471	417	-177.62	
W4_3	3893	3652	241	208	150	-107.77	3891	3641	250	-111.13	
W4_4	3876	3635	241	229	164	-119.58	3878	3624	254	-125.87	
W4_5	3878	3634	244	229	165	-120.68	3880	3624	256	-126.57	
W4_6	3859	3796	63	76	53	-44.88	3857	3789	68	-48.60	
W4_7	--	--	--	--	--	--	3886	3616	270	-123.46	
W5_1	3886	3442	444	419	304	-191.19	3886	3421	465	-198.44	
W5_2	3887	3457	430	403	292	-184.78	3890	3442	448	-194.57	
W5_3	3888	3558	330	305	220	-151.95	3888	3544	344	-156.99	
W5_4	3889	3552	337	309	224	-146.03	3890	3544	346	-148.79	
W5_5	3876	3516	360	348	252	-161.78	3879	3503	376	-167.53	
W5_6	3893	3613	280	247	178	-130.72	3892	3600	292	-135.78	
W5_7	3863	3698	165	173	123	-88.55	3861	3691	170	-90.56	
W5_8	3882	3666	216	199	142	-110.25	3879	3655	224	-113.45	
W5_9	--	--	--	--	--	--	3890	3443	446	-194.63	
W5_10	--	--	--	--	--	--	3877	3652	225	-109.79	
W5_11	--	--	--	--	--	--	3873	3654	219	-116.93	
W5_12	--	--	--	--	--	--	3871	3652	219	-116.10	
W5_13	--	--	--	--	--	--	3875	3657	218	-107.40	
W6_1	3884	3496	388	367	266	-169.33	3885	3484	401	-173.65	

W6_2	3884	3554	330	311	225	-146.01	3886	3545	341	-147.80
W6_3	3883	3601	282	267	192	-134.13	3883	3595	288	-134.45
W6_4	3888	3445	443	416	301	-194.74	3889	3427	462	-203.70
W6_5	3888	3445	443	416	301	-194.51	3889	3425	464	-203.91
W6_6	3872	3512	360	351	254	-157.76	3885	3485	400	-170.09
W6_7	3886	3517	369	346	250	-168.30	3886	3501	385	-173.57
W6_8	3887	3523	364	341	246	-168.12	3888	3507	381	-173.70
W6_9	3888	3439	449	422	306	-199.17	3887	3414	473	-206.59
W6_10	3889	3573	316	292	211	-146.21	3889	3560	329	-149.65
W6_11	3893	3612	281	252	181	-143.80	3891	3604	287	-146.55
W6_12	3887	3535	352	327	236	-157.88	3889	3521	368	-162.13
W6_13	3881	3525	356	335	244	-154.11	3883	3511	372	-159.74
W6_14	3894	3612	282	251	181	-137.30	3892	3610	282	-138.25
W6_15	3876	3567	309	299	215	-146.91	3880	3561	319	-147.82
W6_16	3886	3627	259	239	172	-112.93	3885	3629	256	-111.91
W6_17	3892	3641	251	222	160	-118.45	3890	3629	261	-121.42
W6_18	3880	3626	254	239	172	-127.01	3883	3615	268	-131.50
W6_19	3884	3554	330	311	225	-145.76	--	--	--	--
W6_20	3887	3524	363	339	245	-168.19	--	--	--	--
W6_21	3887	3650	237	217	156	-120.18	--	--	--	--
W6_22	3883	3623	260	241	173	-125.89	--	--	--	--
W6_23	3877	3572	305	291	211	-137.95	--	--	--	--
W6_24	--	--	--	--	--	--	3889	3512	377	-173.78
W6_25	--	--	--	--	--	--	3887	3509	378	-170.76
W6_26	--	--	--	--	--	--	3879	3465	414	-184.37
W6_27	--	--	--	--	--	--	3889	3606	283	-138.26
W6_28	--	--	--	--	--	--	3884	3610	274	-123.89
W6_29	--	--	--	--	--	--	3877	3517	360	-158.14

W6_30	--	--	--	--	--	--	3883	3637	246	-116.06
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Cartesian coordinates of various hydrogen bonded water clusters considered in the present investigation at MP2/aug-cc-pVDZ level of theory. Coordinates at B3LYP/6-311++G(d,p) level are given for which MP2 level structures are not found.

W2 (MP2)

O	1.51646400	-0.00360900	-0.12278400
H	1.91858900	0.02249200	0.75387900
H	0.55948300	0.00381700	0.05212700
O	-1.38925800	0.00326900	0.11222200
H	-1.75205700	0.75060000	-0.38183500
H	-1.74366100	-0.77418700	-0.33967300

W3_1 (MP2)

O	1.28725000	-0.97617200	-0.09356500
H	1.95714400	-1.24334100	0.54730400
H	1.22682000	-0.00292300	-0.01153400
O	0.20524800	1.60086300	0.11059600
H	0.13294400	2.24412100	-0.60533400
H	-0.61025300	1.06362900	0.05106700
O	-1.49421100	-0.61724300	-0.08366700
H	-2.05963900	-1.04472100	0.57085600
H	-0.63331200	-1.07634600	-0.01927400

W3_2 (MP2)

O	-0.76899200	-1.42238300	-0.06857800
H	-0.93398900	-2.15183300	0.54054500
H	0.18752500	-1.23526200	0.00582000
O	1.61587300	0.04507200	-0.06722200
H	0.97679300	0.78075500	0.00848300
H	2.33765800	0.27151100	0.53113500
O	-0.84643300	1.37642500	-0.06667000
H	-1.40921600	1.88760900	0.52678100
H	-1.16235800	0.45430400	0.00699800

W4_1 (MP2)

O	-0.12975700	1.93850600	-0.00526600
H	-0.30301000	2.50928800	-0.76388200
H	-0.87500000	1.29429400	0.00394100
O	0.12974200	-1.93852400	-0.00530400
H	0.30296600	-2.50907200	-0.76410700
H	0.87499400	-1.29432300	0.00416600
O	-1.93858600	-0.12976800	0.00551400
H	-2.50891500	-0.30281900	0.76452100
H	-1.29439400	-0.87502600	-0.00390500
O	1.93856800	0.12974900	0.00502700
H	2.50925400	0.30294400	0.76372900

H 1.29437600 0.87501000 -0.00422800

W4_2 (MP2)

O 0.89958400 1.72218500 0.09384000
H 1.08469000 2.34397200 -0.62044500
H -0.07312000 1.57573300 0.05939200
O -0.89959700 -1.72222200 -0.09380800
H -1.08472800 -2.34368100 0.62076000
H 0.07312700 -1.57589600 -0.05949500
O -1.73155100 0.89162600 0.09688600
H -2.39748100 1.07955900 -0.57551800
H -1.56045900 -0.07555300 0.02241800
O 1.73157000 -0.89161300 -0.09693100
H 2.39744100 -1.07950700 0.57554400
H 1.56048400 0.07557500 -0.02255800

W4_3 (MP2)

O -1.96420800 -0.12442800 -0.78250700
H -1.42619400 0.66037900 -0.57617200
H -1.89752300 -0.22078800 -1.74100000
O 1.85648500 -0.24166000 -0.84117000
H 2.78808100 -0.08400900 -1.03630400
H 1.52334600 0.60088800 -0.48366200
O -0.06663800 -1.21492500 1.11279100
H -0.81606600 -1.23882300 0.48926000
H 0.70474200 -1.33037300 0.53076400
O 0.06115500 1.44462400 0.57490800
H 0.01995400 2.12543900 1.25726500
H 0.00930300 0.57839900 1.04766900

W4_4 (MP2)

O 1.70890300 1.41447100 -0.29574800
H 0.85791500 1.16450900 0.12855200
H 2.14093700 1.99785700 0.34031600
O -3.07108500 -0.13054400 -0.34138500
H -3.76180700 -0.06508300 0.33140100
H -3.28435600 0.56881100 -0.97330900
O 1.90102400 -1.38820200 -0.09917100
H 2.10477000 -0.45233200 -0.30022100
H 2.14705300 -1.87458400 -0.89518200
O -0.41593200 0.03974600 0.79259500
H -1.28875800 -0.07658200 0.37872600
H 0.10096800 -0.74636300 0.53938600

W4_5 (MP2)

O 0.38635500 0.02668500 0.95844200
H -0.13563600 -0.75509000 0.70307400
H 1.25153900 -0.09337000 0.52866300
O 2.95122800 -0.15193300 -0.36299900
H 2.92617100 0.25937900 -1.23733000

H	3.69647000	0.27307200	0.08159800
O	-1.60198000	1.42910900	-0.32674500
H	-0.80860400	1.15552400	0.18713700
H	-2.03865000	2.09210600	0.22166300
O	-1.77095300	-1.38402900	-0.27932000
H	-2.57646300	-1.84237900	-0.01215700
H	-2.03203300	-0.44789200	-0.38767600

W4_6 (MP2)

O	-0.00060600	1.98295000	0.00122600
H	0.76132600	1.38379700	-0.00749600
H	-0.76302300	1.38435500	-0.00206100
O	0.00071400	-1.98294500	0.00135800
H	-0.76177200	-1.38444700	-0.00166300
H	0.76257600	-1.38362800	-0.00158000
O	-2.26874600	-0.00023700	-0.00124700
H	-2.85519600	-0.00140900	0.76686300
H	-2.86367800	-0.00148900	-0.76278500
O	2.26875600	0.00034100	-0.00188400
H	2.84851700	0.00800800	0.77126500
H	2.87030700	-0.00606400	-0.75815900

W4_7 (B3LYP)

O	-1.61530000	-1.39593900	-0.24894600
H	-1.93962000	-0.50467500	-0.47625600
H	-1.57316800	-1.89380500	-1.07079000
O	2.96209500	-0.00651700	-0.45723200
H	2.97599300	0.77714800	-1.01351700
H	2.09866600	0.01184800	-0.01307500
O	0.43791100	-0.06038900	0.97021000
H	-0.15479100	-0.76322000	0.62483000
H	0.62945600	-0.28819300	1.88558900
O	-1.65492000	1.37691100	-0.30086400
H	-2.19383600	2.07650100	0.07902900
H	-0.88098900	1.27186700	0.27885000

W5_1 (MP2)

O	-1.83305500	-1.43438000	0.08445900
H	-2.28345400	-1.70997100	0.89191700
H	-1.92917300	-0.45358700	0.06040100
O	0.78470000	-2.16304400	-0.17353800
H	-0.17086700	-1.93387100	-0.08561600
H	0.84865200	-2.63713300	-1.01154900
O	-1.91422700	1.29789100	-0.09281800
H	-2.42049700	1.87501500	0.49119700
H	-0.99823700	1.66475000	-0.07926800
O	0.65582800	2.21908700	-0.05288800
H	1.28623500	1.46756000	0.05316000
H	0.96312800	2.68310800	-0.84138400

O	2.31622300	0.06609700	0.17166500
H	2.82941700	-0.07569200	0.97624800
H	1.79904500	-0.76538000	0.04985700

W5_2 (MP2)

O	0.73772100	2.13040800	-0.21254000
H	-0.17195600	1.89327700	0.08134900
H	0.62114600	2.46651600	-1.10997000
O	-1.72330400	1.25686600	0.63817400
H	-1.89247500	0.40617900	0.17166700
H	-2.54741200	1.75392300	0.57696300
O	-1.76255500	-1.12836000	-0.68318200
H	-0.95818800	-1.57647100	-0.32719200
H	-2.42212000	-1.82557300	-0.77570800
O	2.29616200	-0.11831500	-0.14175200
H	1.78045300	0.72233100	-0.15301000
H	3.09494400	0.08139900	0.36057500
O	0.54529300	-2.16338100	0.35583800
H	1.23460200	-1.47403100	0.20768400
H	0.51446000	-2.26529300	1.31534000

W5_3 (MP2)

O	1.76275200	1.45086600	0.28792900
H	1.94528600	1.78728600	1.17383600
H	1.95793200	0.48417700	0.33920500
O	1.95051600	-1.26460500	0.35782800
H	1.07819400	-1.48485900	-0.05187600
H	2.59753400	-1.79651800	-0.12100300
O	-2.50009300	-0.19865900	0.82021500
H	-2.64403400	0.04473700	1.74251400
H	-2.00968500	0.55014100	0.43072100
O	-0.75018300	1.38730600	-0.74531200
H	0.15091000	1.53522000	-0.36742400
H	-0.90074800	2.12026800	-1.35414500
O	-0.51011300	-1.51541900	-0.78681700
H	-0.58130500	-0.61321300	-1.14563000
H	-1.21710800	-1.50315700	-0.11693800

W5_4 (MP2)

H	0.51356100	-0.83802700	1.21331300
O	-0.02787000	-0.16705000	1.70053100
H	0.10523300	-0.34666900	2.63906800
H	1.30980800	-2.55902900	-0.31241900
O	1.36247800	-1.62706300	-0.06934000
H	0.93665100	-1.13196400	-0.81834000
H	0.59446500	1.42685000	0.78952100
O	0.79899700	2.04984600	0.06637100
H	1.70497000	2.33573700	0.23760400
H	-2.96337100	-0.70319100	0.05985500
O	-2.22384200	-0.10608200	-0.10424400

H	-1.65348600	-0.17841600	0.68456600
H	-0.83853100	-0.06354500	-1.46959600
O	0.07867600	0.00248300	-1.79651300
H	0.38318900	0.84118100	-1.39801300

W5_5 (MP2)

H	0.07448200	-1.27456400	-0.48506200
O	0.75178500	-1.93941900	-0.19902700
H	0.91095300	-2.48279300	-0.98056600
H	-3.40078200	-0.54207500	1.30672200
O	-3.40078400	0.11529500	0.59820100
H	-4.17797800	-0.10415900	0.06751600
H	2.05625800	-0.86869100	0.33703400
O	2.65659900	-0.12656500	0.58475300
H	2.88515000	-0.28982800	1.50794100
H	1.43829700	2.52536400	-0.75796900
O	0.98885000	1.96326700	-0.11521000
H	1.66927500	1.31173300	0.16883700
H	-0.36012000	0.84926700	-0.65657500
O	-0.91632600	0.07471500	-0.88563400
H	-1.73653000	0.17739900	-0.37253500

W5_6 (MP2)

H	-2.83541900	-0.98595200	-1.77415400
O	-2.36586300	-1.08533700	-0.93705400
H	-2.73727800	-0.39518900	-0.35154000
H	-2.69683100	1.03778200	1.82643000
O	-2.48720000	1.03373000	0.88463300
H	-1.52033000	0.88856300	0.83614100
H	2.69687000	-1.03749500	1.82653800
O	2.48723300	-1.03361900	0.88474200
H	1.52035900	-0.88848400	0.83623300
H	2.73727400	0.39515600	-0.35161700
O	2.36582600	1.08523200	-0.93719400
H	2.83537900	0.98578900	-1.77428900
H	-0.61031500	-0.49005800	-0.49270900
O	0.00000000	-0.00001500	0.09384000
H	0.61031300	0.48996200	-0.49276800

W5_7 (MP2)

H	3.04439300	-0.00001600	0.76599100
O	2.59546500	0.00000800	-0.09069400
H	3.31310900	0.00000900	-0.73831500
H	1.05760400	-1.35906000	-0.15825100
O	0.21927600	-1.83282200	-0.03721100
H	-0.35843900	-1.45933900	-0.72479500
H	-2.60483500	0.00009000	-1.66790900
O	-1.75181800	0.00002500	-1.21714100
H	-1.95443400	-0.00000400	-0.25192400
H	-0.87232900	-0.75904400	1.34165900

O	-1.46365200	-0.00006200	1.50402600
H	-0.87237800	0.75898000	1.34176900
H	1.05759700	1.35912000	-0.15819200
O	0.21925000	1.83284500	-0.03714600
H	-0.35846600	1.45931600	-0.72470400

W5_8 (MP2)

O	1.49709000	0.01870300	1.49487600
H	1.80635800	0.78257900	0.97566200
H	1.83972000	-0.74534400	0.99859500
O	1.45490200	-1.94081500	-0.65029100
H	1.30023000	-2.86663200	-0.87143600
H	0.59315600	-1.49900500	-0.77047400
O	-0.60355100	-0.03036400	-0.28622800
H	-1.55053700	-0.01406000	-0.06260400
H	-0.11113500	-0.01182300	0.56434500
O	-3.45121400	0.05056200	0.17059300
H	-3.98132700	0.02031300	-0.63677300
H	-3.88297100	-0.57633600	0.76574500
O	1.38894200	1.96814100	-0.66188200
H	0.55077100	1.48071600	-0.77430300
H	1.14638000	2.89976900	-0.72531100

W5_9 (B3LYP)

H	2.44950800	-1.19653700	1.02628900
O	2.16295800	-0.85668900	0.17371400
H	1.38571100	-1.40411600	-0.07851100
H	-3.10068300	-0.64446000	0.38313700
O	-2.14343900	-0.59338500	0.44494600
H	-1.89571300	0.33872000	0.24110200
H	-0.92871800	-1.71881400	-0.14358200
O	-0.13418600	-2.21175300	-0.44796200
H	-0.33987700	-3.14747800	-0.38057900
H	2.03806400	2.33651400	0.43257600
O	1.44106000	1.77856300	-0.07280400
H	1.76645400	0.85408100	0.02189700
H	-0.29605700	1.93002900	-0.07420200
O	-1.27802500	1.92814000	-0.14904200
H	-1.46563800	2.29305300	-1.01894300

W5_10 (B3LYP)

O	-3.89183300	0.05842700	0.15793300
O	-1.04143900	-0.16542700	0.46990300
O	2.88631400	-0.36769200	0.94779600
O	1.03465500	-1.09948700	-1.18767900
O	1.20762900	1.50226000	-0.43959600
H	-4.27197700	-0.35314600	-0.62514300
H	-4.43885300	-0.22820900	0.89658600
H	-0.63246800	0.70582500	0.37036900
H	-1.99857900	-0.04037800	0.36787600

H	2.75948200	-0.49292400	1.89272600
H	2.45586000	0.47703700	0.73224200
H	1.72781500	-1.30412600	-0.53998700
H	0.20786200	-1.10762200	-0.67107000
H	1.44260400	2.23335900	-1.01812700
H	1.18563800	0.68554700	-0.99232700

W5_11 (B3LYP)

O	-1.18430600	-0.07057500	0.85310700
H	-2.04073900	-0.37186800	0.51228700
H	-1.14918900	0.88859000	0.69908600
O	-0.15117800	2.40914300	-0.12429500
H	0.32410800	3.10675900	0.33467700
H	0.52347800	1.75565300	-0.40309900
O	1.17411500	0.04091300	-0.63245800
H	1.98591300	-0.37515400	-0.30641500
H	0.43379300	-0.31845900	-0.10682200
O	3.69677200	-1.17342500	0.15883200
H	4.25835200	-1.41780200	-0.58390300
H	4.28009900	-0.76429400	0.80591800
O	-3.65758100	-1.11674100	-0.24685200
H	-3.60249600	-1.31936000	-1.18651800
H	-4.03589000	-1.89859100	0.16811400

W5_12 (B3LYP)

O	-0.23576400	2.33306500	-0.73455000
H	-0.39219000	3.23197300	-0.43213000
H	-0.87925400	1.77095200	-0.25206400
O	-3.09229800	-1.69889000	-0.33711500
H	-3.38004300	-1.51485800	-1.23736900
H	-3.89483500	-1.89259700	0.15828500
O	-1.44630800	0.40045700	0.81147100
H	-1.93840100	-0.34885300	0.44245700
H	-0.52718100	0.09988500	0.93932900
O	1.34850600	0.40699700	0.66587000
H	2.04050800	-0.13041100	0.25200500
H	1.16694800	1.15095500	0.06728800
O	3.46985700	-1.29222100	-0.35458700
H	4.20229400	-1.36893200	0.26557500
H	3.25020800	-2.19337400	-0.61209200

W5_13 (B3LYP)

O	-3.08703900	-0.78567000	-0.55911300
H	-3.78700500	-1.27370300	-0.11616100
H	-2.25678900	-1.00667700	-0.08804100
O	2.00033700	-1.25372000	-0.09310500
H	2.04497100	-1.63122300	-0.97947500
H	2.39975500	-1.91083400	0.48897400
O	-0.70585900	-0.57472100	0.80378600
H	0.19432400	-0.74269400	0.48896600

H	-0.86391000	0.38061000	0.71254800
O	-2.15494300	1.75762800	0.10890100
H	-2.13392500	2.45719300	-0.54959000
H	-2.72423300	1.05220700	-0.25407700
O	3.97331900	0.92632600	-0.22745000
H	3.21135800	0.34187700	-0.10720400
H	3.70893700	1.77449700	0.13990900

W6_1 (MP2)

O	-0.12527400	-1.54786500	0.89586200
H	-0.96988900	-1.51995500	0.37758500
H	-0.28596600	-2.16847100	1.61727500
O	0.03469500	1.37663800	0.95362200
H	0.05664000	0.42501800	1.15641100
H	0.88256700	1.52845600	0.48532700
O	2.46509200	1.40024600	-0.44915800
H	2.53274300	0.42307900	-0.51317100
H	3.28420100	1.67690100	-0.02025100
O	2.30782600	-1.37655800	-0.44903200
H	1.44364500	-1.55164600	-0.01999700
H	2.29032400	-1.88857500	-1.26671400
O	-2.41664400	-1.20396100	-0.48108600
H	-2.47878200	-0.21634700	-0.51424600
H	-2.51701000	-1.49008500	-1.39723700
O	-2.25926300	1.49319700	-0.46276300
H	-1.40867400	1.57742500	0.03937600
H	-2.88125200	2.07062500	-0.00392500

W6_2 (MP2)

O	-0.69345600	0.51870600	1.66723400
H	-0.19010200	1.11122900	1.07936000
H	-0.27855300	-0.34643400	1.50036700
O	-0.74465300	-0.42607300	-1.65419600
H	-0.27044200	0.41700300	-1.53681700
H	-1.61974200	-0.25260700	-1.24880000
O	0.86495700	1.70447400	-0.50112100
H	1.69327800	1.19982900	-0.32403100
H	1.14894800	2.58252800	-0.78279100
O	0.58225200	-1.73403700	0.26768300
H	0.49234500	-2.69417000	0.23282400
H	0.06082300	-1.38463200	-0.50737300
O	2.81085000	-0.11823800	0.08350500
H	2.15364400	-0.84026200	0.19661800
H	3.29271600	-0.08692400	0.91954500
O	-2.89254400	-0.01346100	0.07849300
H	-2.25151200	0.26784400	0.77003000
H	-3.65065500	0.57562200	0.16828600

W6_3 (MP2)

O	1.45528800	-0.19779300	-1.46655400
H	0.55046500	-0.60804900	-1.56934400
H	1.93799300	-0.41302800	-2.27360200
O	0.57920300	2.02967300	0.10453800
H	1.02165900	1.62513700	0.86825500
H	0.94737600	1.50918900	-0.63391500
O	-1.99036600	1.07307000	0.16292100
H	-1.12768800	1.55196900	0.16012500
H	-2.66277500	1.75471200	0.28160800
O	1.78954000	-0.39687100	1.27839600
H	1.89781200	-0.49727600	0.30897500
H	2.56350000	-0.81794900	1.67231700
O	-1.01958600	-1.17877700	-1.42312700
H	-1.00724000	-1.52523700	-0.50304100
H	-1.58555900	-0.39546900	-1.30986700
O	-0.94770500	-1.39379000	1.36326200
H	-1.43763800	-0.55416200	1.31396900
H	-0.02889400	-1.11393300	1.52903600

W6_4 (MP2)

O	-2.73499000	0.37759000	-0.27793300
H	-2.31930600	-0.51373700	-0.34442600
H	-3.04994800	0.56709000	-1.17037200
O	2.73511500	-0.37816800	-0.27839800
H	3.05077600	-0.56718300	-1.17068300
H	2.31955700	0.51319800	-0.34467200
O	1.48648200	2.03935200	-0.45295200
H	0.60809000	2.11564100	-0.01170500
H	1.92079400	2.88596200	-0.29671400
O	-0.97876400	2.21831400	0.70655000
H	-1.09011400	2.17963200	1.66392700
H	-1.62513700	1.56110300	0.35321400
O	-1.48614600	-2.03962800	-0.45349500
H	-1.92005400	-2.88654500	-0.29781000
H	-0.60798500	-2.11547200	-0.01167400
O	0.97828000	-2.21765600	0.70772400
H	1.62505200	-1.56124100	0.35377500
H	1.08845800	-2.17687100	1.66516900

W6_5 (MP2)

O	2.48857100	-0.66469100	-0.66873000
H	2.26880600	0.27273900	-0.45922000
H	2.41051500	-0.73061500	-1.62827400
O	-2.60905500	0.58425900	-0.36604700
H	-2.93710700	0.65947300	-1.27039100
H	-2.30100700	-0.34917800	-0.28963900
O	-0.80321100	2.47388200	0.40771800
H	-1.45382400	1.78917600	0.12241000
H	-1.10408600	2.74558500	1.28323900
O	-1.69381000	-1.97514600	-0.19951100

H	-2.22647900	-2.70998400	0.12609400
H	-0.79358000	-2.12097400	0.17746700
O	0.84015900	-2.33500300	0.73283200
H	1.06130700	-2.18861500	1.66050700
H	1.46021100	-1.75060700	0.23481300
O	1.83912200	1.87025600	0.10585300
H	0.88422600	2.09022100	0.21625300
H	2.23682000	2.66432800	-0.27017600

W6_6 (MP2)

O	-0.99497800	1.78567400	0.73009500
H	-1.60787700	1.01309000	0.70186400
H	-0.91676000	2.04601600	-0.19987300
O	1.49221500	0.86608900	1.01055700
H	2.01478100	1.38767400	1.63207500
H	0.56541800	1.22912200	1.06311800
O	-2.37298800	-0.56107300	0.50382800
H	-1.78680300	-0.94724400	-0.19541900
H	-3.27597700	-0.71223900	0.20040200
O	-0.50080500	-1.39990200	-1.26066700
H	-0.09056300	-0.58277200	-1.59874600
H	0.18407700	-1.75326700	-0.65680600
O	0.82473900	1.15350100	-1.70319600
H	1.46153800	1.30629800	-2.41252900
H	1.35651800	1.10774100	-0.88418600
O	1.47622400	-1.93158400	0.70430000
H	1.17495600	-2.40240500	1.49165200
H	1.52543600	-0.99365600	0.97911000

W6_7 (MP2)

O	-2.70234700	-0.33436400	1.10970700
O	-0.89893500	-1.67816900	-0.67976300
O	-1.45646500	1.14571000	-0.94170000
O	0.70410900	2.29809200	0.17381500
O	2.72058000	0.49008000	0.31175700
O	1.71484500	-2.01316600	0.01015700
H	-3.66136800	-0.30654600	1.21118100
H	-2.49600700	0.34585300	0.43922100
H	-1.53986900	-1.60546400	0.05020500
H	-0.96686600	-0.78849200	-1.07110000
H	-0.67634800	1.61051800	-0.54316900
H	-1.74319700	1.71087900	-1.66910600
H	0.60442700	2.62082000	1.07801200
H	1.45799300	1.65992200	0.21844800
H	2.39158300	-0.43783800	0.22994700
H	3.44399000	0.55227100	-0.32374300
H	1.77951000	-2.66894600	0.71453000
H	0.75184800	-1.95843700	-0.20621700

W6_8 (MP2)

O	1.09131300	2.22632200	0.22202200
H	1.17304400	2.61571200	1.10097600
H	1.75049300	1.48971300	0.20890000
O	1.36407100	-2.12392000	0.29052700
H	1.61986600	-3.00397200	-0.00953800
H	0.47282900	-1.96096100	-0.10702700
O	2.84244900	0.15445400	0.17287700
H	3.43895000	0.10376000	-0.58376100
H	2.37662500	-0.71578100	0.19060000
O	-3.03034700	-0.21186200	0.83693600
H	-2.52305300	0.52768000	0.45031500
H	-3.08115800	-0.01613100	1.78039700
O	-1.04406300	-1.50671900	-0.78983300
H	-1.76556800	-1.47616200	-0.13577800
H	-1.00080900	-0.57084400	-1.05815400
O	-1.28230400	1.37107000	-0.73810600
H	-1.55356500	1.99882200	-1.41889700
H	-0.43660500	1.73340600	-0.37342500

W6_9 (MP2)

O	2.70475700	0.08680500	0.14269200
H	3.22390200	-0.02240600	0.94845000
H	2.23269700	-0.77212800	0.03048400
O	1.27721400	2.38572800	-0.14248100
H	1.63140100	2.78079500	-0.94818300
H	1.78499100	1.54736500	-0.03047700
O	-1.42754000	2.29899600	0.14239600
H	-1.59267200	2.80337200	0.94801600
H	-0.44760200	2.31967500	0.03045200
O	-2.70476600	-0.08683500	-0.14250400
H	-3.22402300	0.02233700	-0.94819900
H	-2.23251600	0.77205600	-0.03063800
O	1.42749400	-2.29894100	-0.14281100
H	1.59269100	-2.80325600	-0.94844900
H	0.44758000	-2.31966300	-0.03079700
O	-1.27718800	-2.38574900	0.14272200
H	-1.63109700	-2.78068100	0.94860800
H	-1.78511900	-1.54749800	0.03062200

W6_10 (MP2)

O	-0.35895500	-1.89970700	-0.12401900
H	-0.68124300	-1.48273600	-0.93797600
H	0.61639800	-1.76386000	-0.13762600
O	-2.17950900	0.21742500	-1.31186800
H	-2.44580900	0.07806000	-0.38291500
H	-3.00457300	0.29540200	-1.80641300
O	-1.75104400	-0.22547000	1.40828300
H	-2.08278500	-0.55588100	2.25125800
H	-1.19113600	-0.95086400	1.02282400
O	2.34054600	-1.38193900	-0.02835900

H	2.43901500	-0.40165700	-0.05353400
H	2.94346600	-1.71089400	-0.70598300
O	2.34259300	1.35025300	-0.13291500
H	1.40022600	1.61323900	-0.00197600
H	2.84600700	1.91913700	0.46160500
O	-0.30797100	1.92913200	0.19443600
H	-0.71227300	1.33338400	0.85228600
H	-0.81257300	1.70911200	-0.60602200

W6_11 (MP2)

O	1.66344700	0.74318300	-1.12567600
H	2.43279700	0.42063800	-0.62710500
H	1.05624200	-0.01816500	-1.04551800
O	0.03874900	-1.35887500	-0.09502000
H	-0.41147300	-0.73822100	0.51192100
H	-0.71699700	-1.77594400	-0.54149900
O	-1.58714500	0.65582900	1.06098700
H	-1.76593500	0.84819800	1.98962800
H	-1.08273200	1.43829200	0.72220600
O	2.75148800	-1.26413400	0.66665000
H	1.86332600	-1.61943000	0.47839500
H	3.31208100	-2.03813000	0.79563800
O	-2.78789400	-1.34382300	-0.57370300
H	-2.64542400	-0.51965100	-0.07278000
H	-3.49826900	-1.14480700	-1.19504500
O	0.03912800	2.55805300	0.06173700
H	0.71781600	1.99529200	-0.38909100
H	-0.20361900	3.23006200	-0.58655200

W6_12 (MP2)

O	1.28905300	-1.93158700	-0.24363000
H	1.15858200	-2.43318000	-1.05776000
H	0.56116500	-1.26735200	-0.23231200
O	-0.47726000	0.15970400	-0.01721700
H	-1.14600600	0.34423300	-0.70523500
H	0.15436000	0.91429200	-0.01825200
O	1.60242300	1.94075700	0.15695800
H	1.85237100	2.62146000	-0.47948100
H	2.33256900	1.28012500	0.12461400
O	-2.94478200	0.17214900	-1.32654900
H	-3.22376100	0.01766800	-0.40097300
H	-3.53172700	0.86507400	-1.65277900
O	3.37203000	-0.15999200	0.04141800
H	2.72236700	-0.89171500	-0.07139500
H	3.88608700	-0.40310900	0.82124400
O	-2.83755500	-0.17755400	1.44575300
H	-1.88298600	-0.09218600	1.24696600
H	-2.91429800	-0.98312500	1.97148900

W6_13 (MP2)

O	2.55603500	1.46480600	0.41670100
O	2.77948300	-1.24426600	-0.29011200
O	0.03972500	-1.42110500	0.44424700
O	0.01222600	1.00447500	-0.57000300
O	-2.65790600	1.50906300	-0.02558600
O	-2.75200200	-1.29287900	0.01383600
H	3.33876500	2.00357200	0.25331800
H	2.79988000	0.55799500	0.13256800
H	1.84843300	-1.49182900	-0.11304300
H	2.92463800	-1.49399100	-1.21138800
H	0.02643600	-0.46867400	0.12899800
H	0.10387200	-1.36378600	1.40799500
H	-0.80563700	1.47603000	-0.31781800
H	0.78082100	1.50390400	-0.23535800
H	-3.15788600	1.86407200	0.71905700
H	-2.81773100	0.54112000	-0.00076300
H	-1.80327200	-1.52455100	0.09416100
H	-3.05880400	-1.76462000	-0.77039900

W6_14 (MP2)

O	-2.27270000	-0.55542100	1.27122900
H	-2.55169800	-1.41588700	1.60790400
H	-1.32460600	-0.48308900	1.51470600
O	2.32325600	-1.77040900	-0.15961600
H	2.90608300	-2.34960300	-0.66435200
H	1.85268200	-1.23870000	-0.82741100
O	0.47361800	-0.11731900	1.41551900
H	1.15106100	-0.76789400	1.65581900
H	0.50452200	-0.14972700	0.43065400
O	0.59005400	0.13329300	-1.34101600
H	0.78407500	1.07597400	-1.19127800
H	-0.37039000	0.09210800	-1.55199900
O	-2.14459500	-0.14918300	-1.46914900
H	-2.31135900	-0.29525400	-0.51080000
H	-2.74708700	0.56166500	-1.72051000
O	0.97413100	2.46148900	0.25156200
H	1.60494300	3.13635100	0.52946800
H	0.95166900	1.81445300	0.97956700

W6_15 (MP2)

O	-2.52900200	0.33864500	-0.08745300
H	-2.26720200	-0.17652800	0.69987300
H	-2.17644600	-0.21286100	-0.81375500
O	3.75554000	-0.09210600	0.02133300
H	4.18348900	0.00762300	-0.83924100
H	4.26974200	0.47060000	0.61497900
O	-1.00642900	-1.19322200	1.80466900
H	-0.20135700	-0.85842600	1.35739700
H	-0.85752900	-1.02800500	2.74356700
O	-0.85936300	-1.18293900	-1.85254600

H	-0.92859600	-2.14304700	-1.77573900
H	-0.11926700	-0.94077100	-1.25776200
O	0.89643500	-0.11328400	0.06520100
H	0.56851200	0.81446900	0.01255300
H	1.86884200	-0.06427500	0.06590000
O	-0.54965200	2.19710200	0.03550100
H	-0.63179700	2.85530000	-0.66511100
H	-1.36862100	1.64236100	-0.03628800

W6_16 (MP2)

O	0.21969200	-1.55245500	-0.40131300
O	0.52713500	0.94479000	-1.66487000
O	-1.47029200	1.50723200	0.33448300
O	0.44933800	0.06051000	1.89908500
O	2.75002200	-0.07281500	0.03701200
O	-2.50216600	-0.94921000	-0.28827700
H	0.28417700	-0.78127700	-1.00804600
H	0.25734900	-1.12385000	0.48265400
H	1.39075300	1.08628100	-1.24559900
H	-0.11038500	1.39148200	-1.07726800
H	-1.99993500	0.69448700	0.15061500
H	-2.11295300	2.22114300	0.42572000
H	1.33739500	0.35540200	1.64121900
H	-0.14886300	0.76127000	1.58028100
H	3.68756000	-0.29922800	-0.00657400
H	2.27852200	-0.89382000	-0.19156200
H	-3.02341800	-1.51941700	0.29034900
H	-1.63002600	-1.39689000	-0.37074700

W6_17 (MP2)

O	-3.34417400	-1.04764900	0.01985800
H	-2.36600900	-1.07223600	0.02886300
H	-3.60384400	-1.62910900	-0.70534600
O	-0.67651700	-0.18357900	0.04795400
H	-1.14555400	0.67222100	0.10740300
H	-0.05284400	-0.20962700	0.79476400
O	3.26496600	1.18219700	-0.25651400
H	2.89270700	0.84707200	0.57801500
H	3.31460300	2.13960800	-0.14911900
O	1.73867000	-1.05371800	-1.27498000
H	2.28063000	-0.25269100	-1.38517100
H	0.82863500	-0.70783000	-1.22704900
O	-2.74996700	1.68679000	-0.08328800
H	-3.26366200	0.85405100	-0.06581100
H	-3.18385100	2.26429900	0.55644600
O	1.80458900	-0.65034800	1.41188300
H	1.89261300	-1.05221100	0.51306600
H	2.10604000	-1.32309300	2.03463800

W6_18 (MP2)

O	-1.94314700	0.46357200	0.89044800
H	-1.04439000	0.09024000	0.83397500
H	-2.54058500	-0.26020700	0.63290700
O	2.67469000	-1.50425800	-1.05904400
H	1.83394900	-1.03013500	-0.88764500
H	2.43274600	-2.43653500	-1.11302500
O	-3.84776800	-1.55339700	0.06914600
H	-4.20124100	-1.38090500	-0.81376400
H	-4.63060300	-1.62680900	0.63100100
O	0.78338700	0.23076700	0.02941700
H	0.46070600	1.04021200	-0.41569500
H	1.57254800	0.49572800	0.54029300
O	-0.93096400	2.20829000	-0.98806200
H	-0.97690200	3.14303600	-0.75285000
H	-1.50797700	1.75018400	-0.33729000
O	3.42885300	0.25364100	0.99382900
H	3.46948600	-0.50479700	0.37783000
H	3.81185500	-0.06893600	1.81838700

W6_19 (MP2)

O	0.18936800	0.86209100	2.00699500
H	0.78415900	1.17159100	1.30023500
H	-0.65808500	1.25665000	1.75327400
O	1.48067600	1.36235100	-0.54524500
H	1.74258000	0.42853800	-0.76469900
H	2.19411700	1.92204300	-0.87399300
O	-1.27766100	1.62548500	-0.63556500
H	-0.30702600	1.63051600	-0.77873400
H	-1.62307300	2.33939800	-1.18530400
O	1.82891300	-1.25132000	-0.96104100
H	2.63190600	-1.76242100	-0.80304100
H	1.18444500	-1.55287600	-0.26177600
O	-2.30509200	-0.99330400	-0.54608800
H	-2.43551500	-1.36271100	-1.42829000
H	-2.01315800	-0.07170800	-0.70087500
O	-0.00226300	-1.77512200	0.90989600
H	0.04532900	-0.97166100	1.46639700
H	-0.85720900	-1.66880400	0.44519000

W6_20 (MP2)

O	3.06150500	-0.32065200	0.83545700
H	2.61234400	0.41698600	0.38055500
H	3.28282600	0.01763100	1.71125400
O	-0.87774900	2.29618300	0.20041200
H	-0.82860400	2.62033100	1.10789000
H	-1.60748700	1.63030400	0.20879100
O	-1.62716000	-2.07944600	0.19283900
H	-0.68012700	-1.95496400	-0.06522600
H	-1.94919600	-2.76926900	-0.40035100
O	0.91789000	-1.60392500	-0.60481000

H	1.63451300	-1.60578900	0.05305200
H	0.96457600	-0.68698700	-0.93310100
O	1.37189900	1.22228900	-0.84072900
H	1.62513000	1.75568400	-1.60388600
H	0.56426800	1.66006600	-0.47191500
O	-2.79969300	0.37335600	0.11272400
H	-3.56547100	0.35464000	0.69884600
H	-2.42631000	-0.54107100	0.14694700

W6_21 (MP2)

O	-0.27947400	-1.29233800	-1.39726100
H	0.10240700	-2.12909400	-1.69207200
H	-0.11853500	-1.26507700	-0.43122700
O	-0.72634500	1.79284800	0.43510800
H	0.00820900	1.73385900	-0.23055600
H	-0.72157500	2.70119100	0.75979500
O	-2.77356900	-0.35507200	0.08772400
H	-2.38213800	-0.76802100	-0.69737400
H	-2.36175200	0.52524100	0.08926100
O	2.54823900	-0.54082000	0.64591000
H	3.26749200	-0.48679200	1.28651100
H	1.75443100	-0.76263100	1.16635900
O	-0.13190500	-0.72846800	1.41089500
H	-0.33079400	0.22198300	1.26143600
H	-1.01656000	-1.09933900	1.55637100
O	1.25104600	1.15167800	-1.27291800
H	0.79595600	0.38267100	-1.66344600
H	1.89892000	0.72337700	-0.68072400

W6_22 (MP2)

O	-2.95044700	0.21303000	-0.54602200
H	-3.82978400	0.45608500	-0.23221200
H	-2.53835200	-0.29245900	0.18845400
O	-1.08921400	-0.70437600	1.28447500
H	-0.66002600	0.06185500	0.86733500
H	-0.53395300	-1.44902100	0.97606900
O	1.80677500	1.64764000	0.97049700
H	1.68916100	1.36359800	1.88653500
H	0.90720900	1.86443600	0.65678400
O	1.91469100	-0.16121600	-1.09477800
H	2.07560900	0.42903500	-0.32277800
H	2.72954000	-0.13002600	-1.61132500
O	0.77933700	-2.46869000	0.07240000
H	0.47951900	-3.10388300	-0.58970500
H	1.24480400	-1.77448100	-0.43724700
O	-0.48035500	1.51293500	-0.60927400
H	-1.42215600	1.28211300	-0.74805200
H	0.01214200	0.97816700	-1.25225500

W6_23 (MP2)

O	0.50757900	-1.49317600	0.52981400
O	1.88734700	0.68572000	1.17674500
O	0.08893500	2.23873200	-0.33774500
O	-1.43139100	-0.09464900	-0.79202400
O	-4.12243200	-0.35882700	0.24574300
O	3.02211900	-0.94644300	-0.87872300
H	-0.24242000	-1.10409800	0.01841600
H	1.15822600	-1.75450600	-0.14263500
H	1.32633400	-0.13761200	1.10752900
H	2.04452000	0.82133900	2.11918700
H	0.78725800	1.82474200	0.21076600
H	0.55570600	2.56583300	-1.11707200
H	-1.05368200	0.80071200	-0.67583000
H	-2.33251500	-0.05833900	-0.42773000
H	-4.69726700	-0.73525700	-0.43407900
H	-4.11976500	-1.02243100	0.94866500
H	3.00265500	-0.27981600	-0.16906400
H	3.95369300	-1.17142900	-0.98863600

W6_24 (B3LYP)

O	2.94853600	-0.31096900	1.01120700
H	2.53880500	0.45329100	0.56841900
H	3.06095300	-0.06437700	1.93317800
O	-1.02583900	2.25619300	-0.10817200
H	-1.29376900	3.07162600	0.32276500
H	-1.68743300	1.56693600	0.13932000
O	-1.56714700	-2.10662000	-0.09299500
H	-0.60845700	-1.97077700	-0.29171600
H	-1.89774500	-2.71266600	-0.76191600
O	1.01404300	-1.55106900	-0.68420800
H	1.68153600	-1.58157500	0.02047100
H	1.06044600	-0.62190900	-0.96704400
O	1.42248500	1.31279200	-0.73154900
H	1.76664100	1.81923000	-1.47337800
H	0.55784100	1.72343800	-0.48841300
O	-2.75386200	0.25085100	0.52122100
H	-3.11325100	0.13123200	1.40485800
H	-2.37130000	-0.62387700	0.26943400

W6_25 (B3LYP)

O	-2.33017300	0.29779100	0.91325100
O	-0.92113500	2.31224800	-0.25462200
O	1.55269700	1.29430000	-0.70778200
O	2.43507900	-0.44518400	1.32210800
O	1.02345000	-1.59633600	-0.84422600
O	-1.63237600	-1.95294900	-0.43437800
H	-3.26079200	0.30746500	1.15180100
H	-2.15554600	-0.56836700	0.47581500
H	-1.45419400	2.63329600	-0.98771300

H	-1.47137800	1.62937300	0.19610400
H	0.67405700	1.72592600	-0.57240500
H	2.11374700	1.94067100	-1.14642300
H	2.11985900	-0.26522100	2.21248400
H	2.20919800	0.34057300	0.79016200
H	1.51424100	-1.54577800	-0.00374200
H	1.16662100	-0.71094400	-1.21296000
H	-0.66146800	-1.88851100	-0.61164600
H	-1.81467800	-2.87743900	-0.24628800

W6_26 (B3LYP)

O	-3.89574900	-0.06227900	0.69564600
O	-1.40184500	-0.38372300	-0.75149100
O	-0.16971200	2.09962600	-0.51947500
O	2.34221700	1.61771600	0.44730800
O	2.79582100	-1.05688400	0.27131900
O	0.43305200	-2.28878100	-0.20787400
H	-4.69880800	0.05422500	0.17754100
H	-3.87964900	0.67105700	1.31963500
H	-2.24333800	-0.31970900	-0.27339600
H	-0.99600800	0.50692100	-0.70578500
H	0.73088000	1.97302400	-0.14220300
H	-0.04492400	2.63257100	-1.31003800
H	2.61756900	1.89381500	1.32591900
H	2.55042900	0.65536800	0.38574200
H	1.94872400	-1.54208500	0.12050300
H	3.41032000	-1.38939300	-0.38917800
H	0.05404600	-2.90898800	0.42085900
H	-0.27951200	-1.63221000	-0.41307400

W6_27 (B3LYP)

O	-0.78785200	-1.52454800	1.51613000
H	-1.43134600	-2.23894200	1.49282400
H	-0.37415700	-1.50546200	0.63227300
O	1.01850300	1.60151800	0.15066400
H	0.13023200	1.58750900	0.59889300
H	1.12547300	2.47829700	-0.23009300
O	3.10168600	-0.34230800	-0.20679800
H	3.70105600	-0.62950100	0.48766400
H	2.58801400	0.39218900	0.16814900
O	-2.27250400	-0.02956300	-1.40983100
H	-2.65400000	0.19355500	-2.26333300
H	-1.42679400	-0.47511200	-1.58990300
O	0.37498000	-0.87103800	-1.02364100
H	0.60293300	0.04689500	-0.77247600
H	1.24609000	-1.27541700	-1.14238200
O	-1.45964300	1.18322300	1.07995200
H	-1.36392200	0.30994900	1.50496400
H	-1.94494100	0.97776800	0.26160400

W6_28 (B3LYP)

O	0.51489100	-1.71664900	0.73503200
H	0.35591000	-2.65991800	0.83791700
H	0.21177900	-1.47714800	-0.16102900
O	0.64799700	1.78585300	-0.11994500
H	0.06873400	1.51134200	0.63957600
H	0.61727800	2.74515000	-0.17783700
O	2.94158500	-0.12828300	-0.13009500
H	2.42020900	-0.79567400	0.33566200
H	2.39730700	0.66881500	-0.06398400
O	-2.74736500	-0.22674700	-0.36263200
H	-3.53859400	0.11844100	-0.78523900
H	-2.06053200	-0.28292300	-1.05012800
O	-0.24156400	-0.30898300	-1.63705100
H	0.14250400	0.52729100	-1.28733500
H	0.24423200	-0.51288300	-2.44273100
O	-0.94519000	0.59705900	1.67410000
H	-0.47629700	-0.25276100	1.72343000
H	-1.74535900	0.39226900	1.15643900

W6_29 (B3LYP)

O	0.12950900	-1.79606300	0.09075700
O	1.83740600	0.12461700	0.85701600
O	-0.04815600	2.02691200	0.01453400
O	-1.72800300	-0.06584100	-0.78713200
O	-4.41753400	-0.07316300	0.22583800
O	4.41328800	-0.24700600	-0.40153500
H	-0.62885100	-1.26649900	-0.26441300
H	0.38241300	-2.41444900	-0.60094600
H	1.27496600	-0.65442900	0.60527300
H	1.99791500	0.04044800	1.80286900
H	0.70216300	1.49061500	0.34200800
H	0.33051900	2.70608800	-0.55067300
H	-1.29060200	0.78096700	-0.57278200
H	-2.62798000	-0.02355600	-0.42585300
H	-5.13105800	-0.31629300	-0.37281500
H	-4.61320200	-0.50836200	1.06190300
H	3.53710900	-0.07476100	-0.01700800
H	4.57453600	0.48458500	-1.00338500

W6_30 (B3LYP)

O	1.24797700	-1.36887600	-0.86215200
O	1.03986600	1.45976600	-0.80599200
O	-1.36338100	1.38702700	0.85895000
O	-1.09273900	-1.41387700	0.94998700
O	3.15306400	0.07845800	0.55962000
O	-2.89455400	-0.12583800	-0.82674300
H	1.03277300	-0.45052000	-1.11660700
H	0.52016400	-1.62165800	-0.27446800
H	1.84736300	1.35404500	-0.27509500

H	0.32817000	1.64157300	-0.17333600
H	-2.03169900	1.11637400	0.19313800
H	-1.75758100	2.08601800	1.38953100
H	-1.17655900	-1.97270300	1.72889500
H	-1.02815500	-0.49397700	1.26869400
H	4.08397700	-0.05074000	0.35798600
H	2.67123000	-0.65343300	0.12205900
H	-2.44796600	-0.89418700	-0.43238900
H	-2.76358800	-0.19406900	-1.77776300