Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

The Ehrenfest Force Topology: A physically intuitive approach for analyzing chemical interactions

Supplementary material

Table S1(a) QTAIM BCP data for the twelve molecular graphs, see Figure 2. All units are atomic units. The bond-path length is denoted by BPL and $\rho(\mathbf{r}_b)$ is the electronic density at the QTAIM BCP. The trace (i.e. the Laplacian) of the QTAIM Hessian and its eigenvalues (λ_1, λ_2 and λ_3, respectively) are listed next, ϵ is the QTAIM ellipticity and the QTAIM stiffness is shown as $\mathbb{S}$. For data at QTAIM BCPs that are symmetrically equivalent only one entry is shown. For the organization of the data for the water-dimer, W4 and W6 see Figure 3(a), 3(c) and 3(d) respectively. The BCPs involving a hydrogen nuclei between two nearest-neighbour oxygen nuclei, e.g. O1−H2--O4 are shown in pairs (sigma BCP O1−H2 and hydrogen BCP H2--O4). The remaining sigma BCPs that are not close to being collinear with any hydrogen-bond BCPs are referred to as 'dangling' BCPs, and are shown distanced from the pairs. The same scheme is used for the clusters W4 and W6.

Molecular graph	BCP	BPL	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r}_b)$	λ_1	λ_2	λ_3	ϵ	$\mathbb{S}$
H_2									
	H1−H2	1.3800	0.2730	-1.3504	-1.0111	-1.0111	0.6717	0.0000	1.5053
H_2O									
	O2−H1	1.7968	0.3780	-2.7083	-1.9623	-1.9211	1.1751	0.0215	1.6699
$(H_2O)_2$									
	O4−H5	1.7979	0.3766	-2.7315	-1.9744	-1.9346	1.1775	0.0206	1.6767
	O1−H3	1.7950	0.3792	-2.6916	-1.9522	-1.9135	1.1741	0.0202	1.6627
	O1−H2	1.8111	0.3673	-2.6968	-1.9525	-1.9145	1.1702	0.0199	1.6685
	H2--O4	3.7171	0.0246	0.0822	-0.0360	-0.0352	0.1534	0.0226	0.2347
CH_2O									
	O1=C2	2.2648	0.4352	-0.0404	-1.2632	-1.1639	2.3868	0.0854	0.5293
	C2−H3	2.0781	0.2870	-1.1297	-0.8207	-0.8091	0.5001	0.0143	1.6411
CH_3NO									
	C1=O2	2.2850	0.4322	-0.3523	-1.2412	-1.1222	2.0111	0.1060	0.6172
	C1−N3	2.5632	0.3314	-1.0945	-0.8060	-0.7121	0.4235	0.1319	1.9030
	N3−H4	1.8853	0.3536	-2.0099	-1.4516	-1.3873	0.8290	0.0463	1.7509
	N3−H5	1.8802	0.2888	-2.0039	-1.4537	-1.3855	0.8353	0.0492	1.7403
	C1−H6	2.0744	0.2888	-1.1434	-0.8348	-0.8122	0.5036	0.0278	1.6577
C_3H_3NO									
	O1=C2	2.5586	0.2991	-0.3929	-0.6761	-0.5930	0.8763	0.1401	0.7716
	O1−C3	2.5849	0.2847	-0.2834	-0.5937	-0.5329	0.8432	0.1141	0.7041
	C2=N4	2.4342	0.3991	-1.3409	-1.0525	-0.7934	0.5049	0.3265	2.0843
	C2−H5	2.0203	0.3044	-1.2799	-0.9206	-0.8720	0.5127	0.0557	1.7955
	C3−C6	2.5498	0.3508	-1.1094	-0.8231	-0.6049	0.3186	0.3607	2.5833

	N4−C6	2.6250	0.3155	-0.9964	-0.6910	-0.6273	0.3219	0.1016	2.1468
	C3−H7	2.0155	0.3023	-1.2566	-0.9015	-0.8560	0.5009	0.0531	1.7997
	C6−H8	2.0192	0.2999	-1.2338	-0.8770	-0.8456	0.4889	0.0371	1.7939
CH_4									
	C1−H2	2.0442	0.2839	-1.0854	-0.7655	-0.7655	0.4455	0.0000	1.7183
C_2H_2									
	C1≡C2	2.2593	0.4339	-1.4740	-0.7629	-0.7629	0.0518	0.0000	14.7305
	C1−H3	1.9925	0.3009	-1.2725	-0.8842	-0.8842	0.4959	0.0000	1.7830
C_2H_4									
	C2=C4	2.5026	0.3614	-1.1816	-0.8382	-0.6353	0.2919	0.3193	2.8713
	H1−C2	2.0329	0.2924	-1.1625	-0.8184	-0.8105	0.4664	0.0097	1.7546
N_4H_4									
	N1−N2	2.7796	0.2952	-0.5206	-0.6901	-0.6438	0.8133	0.0718	-0.8485
	N1−H4	1.9107	0.3584	-1.9327	-1.4365	-1.3764	0.8802	0.0437	-1.6321
W4									
	O4−H6	1.8372	0.3489	-2.5751	-1.8754	-1.8422	1.1424	0.0181	-1.6416
	H6--O1	3.3790	0.0384	0.1059	-0.0653	-0.0638	0.2350	0.0233	-0.2778
	O1−H2	1.7950	0.3781	-2.7170	-1.9649	-1.9300	1.1779	0.0181	-1.6681
W6									
	O4−H6	1.8529	0.3334	-2.3792	-1.7868	-1.7558	1.1633	0.0177	1.5359
	H6--O1	3.2069	0.0501	0.1131	-0.0913	-0.0896	0.2939	0.0182	0.3105
	O7−H8	1.8274	0.3495	-2.5466	-1.8866	-1.8520	1.1920	0.0187	1.5827
	H8--O10	3.4012	0.0387	0.1026	-0.0641	-0.0629	0.2296	0.0198	0.2793
	O1−H2	1.8202	0.3559	-2.5767	-1.9087	-1.8769	1.2089	0.0170	1.5788
	H2--O16	3.6027	0.0317	0.0884	-0.0473	-0.0454	0.1811	0.0429	0.2613
	O13−H15	1.8160	0.3570	-2.6276	-1.9333	-1.8972	1.2030	0.0190	1.6071
	H15--O4	3.5362	0.0315	0.0948	-0.0497	-0.0470	0.1914	0.0572	0.2594
	O10−H12	1.7966	0.3719	-2.6753	-1.9814	-1.9459	1.2520	0.0182	1.5826
	H12--O13	4.1788	0.0156	0.0583	-0.0185	-0.0174	0.0942	0.0649	0.1964
	O1−H3	1.7992	0.3702	-2.6595	-1.9698	-1.9371	1.2473	0.0169	1.5792
	H3--O7	4.0827	0.0172	0.0622	-0.0215	-0.0200	0.1037	0.0767	0.2075
	O16−H18	1.8002	0.3695	-2.6486	-1.9661	-1.9308	1.2483	0.0183	1.5750
	H18--O7	3.9632	0.0193	0.0650	-0.0256	-0.0238	0.1143	0.0731	0.2236
	O10−H11	1.8030	0.3674	-2.6659	-1.9690	-1.9336	1.2367	0.0183	1.5922
	H11--O4	3.8522	0.0221	0.0729	-0.0301	-0.0287	0.1317	0.0507	0.2287
	O16−H17	1.8026	0.3674	-2.6526	-1.9643	-1.9289	1.2406	0.0183	1.5833
	H17--O13	3.7915	0.0233	0.0736	-0.0329	-0.0321	0.1385	0.0241	0.2373
	O4−H5	1.7836	0.3790	-2.6815	-1.9987	-1.9651	1.2823	0.0171	1.5587
	O7−H9	1.7840	0.3796	-2.6670	-1.9950	-1.9585	1.2865	0.0186	1.5508
	O13−H14	1.7842	0.3793	-2.6840	-2.0012	-1.9636	1.2808	0.0192	1.5625

Table S1(b) Stress tensor BCP data calculated at the Ehrenfest Hessian BCPs for the twelve molecular graphs, see Figure 2. All units are atomic units. The trace of the stress tensor and its eigenvalues (λ_1^σ, λ_2^σ and λ_3^σ, respectively) are listed next, ϵ_σ is the stress tensor ellipticity and the stress tensor stiffness is shown as $\mathbb{S}_\sigma$. For more explanation, see the caption of Table 1 in the main text.

Molecular graph	BCP	$Tr[\sigma(\mathbf{r}_b^\mathbf{F})]$	λ_1^σ	λ_2^σ	λ_3^σ	ϵ_σ	$\mathbb{S}_\sigma$
H_2							
	H1−H2	-0.3376	-0.2528	-0.2528	0.1679	0.0000	1.5053
H_2O							
	O2−H1	-0.7576	-0.5279	-0.4979	0.2682	0.0602	1.9685
$(H_2O)_2$							
	O4−H4	-0.7552	-0.5259	-0.4969	0.2676	0.0584	1.9652
	O1−H3	-0.7609	-0.5283	-0.5012	0.2685	0.0540	1.9672
	O1−H2	-0.7374	-0.5118	-0.4834	0.2578	0.0587	1.9855
	H2--O4	-0.0204	-0.0119	-0.0113	0.0029	0.0525	4.1597
CH_2O							
	O1=C2	-1.1698	-0.6719	-0.6676	0.1697	0.0063	3.9583
	C2−H3	-0.3492	-0.2346	-0.2250	0.1104	0.0430	2.1260
CH_3NO							
	C1=O2	-1.1180	-0.6489	-0.6407	0.1715	0.0128	3.7828
	C1−N3	-0.5670	-0.3566	-0.3235	0.1131	0.1022	3.1526
	N3−H4	-0.5745	-0.3931	-0.3673	0.1859	0.0703	2.1151
	N3−H5	-0.5810	-0.3981	-0.3703	0.1874	0.0751	2.1246
	C1−H6	-0.3528	-0.2354	-0.2285	0.1111	0.0300	2.1190
C_3H_3NO							
	O1=C2	-0.5858	-0.3813	-0.3572	0.1527	0.0673	2.4964
	O1−C3	-0.5428	-0.3581	-0.3365	0.1518	0.0644	2.3597
	C2=N4	-0.7720	-0.4637	-0.4306	0.1223	0.0769	3.7917
	C2−H5	-0.3895	-0.2558	-0.2517	0.1180	0.0161	2.1683
	C3−C6	-0.5512	-0.3294	-0.2879	0.0661	0.1444	4.9869
	N4−C6	-0.4965	-0.3101	-0.3005	0.1140	0.0318	2.7190
	C3−H7	-0.3907	-0.2579	-0.2508	0.1180	0.0282	2.1857
	C6−H8	-0.3865	-0.2533	-0.2504	0.1172	0.0115	2.1619
CH_4							
	C1−H2	-0.3645	-0.2383	-0.2383	0.1121	0.0000	2.1253
C_2H_2							
	C1≡C2	-1.0023	-0.4916	-0.4916	-0.0191	0.0000	25.7755
	C1−H3	-0.3978	-0.2568	-0.2568	0.1158	0.0000	2.2179
C_2H_4							
	C1=C2	-0.5934	-0.3476	-0.3079	0.0621	0.1287	5.5969
	C1−H3	-0.3755	-0.2461	-0.2442	0.1148	0.0081	2.1442
N_4H_4							
	N1−N2	-0.3879	-0.2679	-0.2586	0.1385	0.0358	1.9337
	N1−H4	-0.5611	-0.3868	-0.3652	0.1908	0.0592	2.0269
W4							
	O4−H6	-0.6937	-0.4806	-0.4552	0.2421	0.0557	1.9849
	H6--O1	-0.0376	-0.0222	-0.0210	0.0056	0.0542	3.9799

	O1−H2	-0.7600	-0.5260	-0.5021	0.2681	0.0478	1.9620
W6							
	O4−H6	-0.7333	-0.4767	-0.4504	0.1937	0.0583	2.4604
	H6--O1	-0.0627	-0.0378	-0.0361	0.0112	0.0484	3.3677
	O7−H8	-0.7710	-0.5021	-0.4740	0.2051	0.0592	2.4479
	H8--O10	-0.0485	-0.0284	-0.0270	0.0069	0.0519	4.1105
	O1−H2	-0.7847	-0.5101	-0.4841	0.2095	0.0535	2.4347
	H2--O16	-0.0348	-0.0195	-0.0184	0.0031	0.0550	6.2115
	O13−H15	-0.7878	-0.5137	-0.4852	0.2111	0.0588	2.4338
	H15--O4	-0.0368	-0.0211	-0.0197	0.0040	0.0704	5.3092
	O1−H3	-0.8174	-0.5335	-0.5064	0.2225	0.0535	2.3975
	H3--O7	-0.0116	-0.0064	-0.0060	0.0007	0.0758	8.6430
	O16−H17	-0.8139	-0.5300	-0.5050	0.2210	0.0493	2.3975
	H17--O13	-0.0133	-0.0073	-0.0069	0.0009	0.0481	7.9412
	O16−H18	-0.8119	-0.5290	-0.5029	0.2200	0.0520	2.4046
	H18--O7	-0.0155	-0.0086	-0.0081	0.0011	0.0656	7.4814
	O10−H11	-0.8092	-0.5277	-0.5000	0.2185	0.0553	2.4147
	H11--O4	-0.0192	-0.0105	-0.0100	0.0013	0.0422	8.1394
	O10−H12	-0.8088	-0.5268	-0.5000	0.2180	0.0535	2.4162
	H12--O13	-0.0205	-0.0114	-0.0108	0.0017	0.0531	6.8240
	O4−H4	-0.8298	-0.5408	-0.5172	0.2283	0.0457	2.3694
	O7−H9	-0.8305	-0.5423	-0.5167	0.2285	0.0496	2.3737
	O13−H14	-0.8308	-0.5430	-0.5164	0.2286	0.0516	2.3759

Table S2(a) Total local energy $H(\mathbf{r}_b)$ and the $\underline{\mathbf{e_2}}$ eigenvector components at the QTAIM BCPs for the twelve molecular graphs.

Molecular graph	BCP	$H(\mathbf{r}_b)$	$\underline{\mathbf{e_2}}$		
H_2					
	H1−H2	-0.3376	1.0000	0.0000	0.0000
H_2O					
	O2−H1	-0.7588	1.0000	0.0000	0.0000
$(H_2O)_2$					
	O4−H4	-0.7622	0.5659	0.8244	-0.0122
	O1−H3	-0.7568	0.0000	0.0000	1.0000
	O1−H2	-0.7524	0.0000	0.0000	1.0000
	H2--O4	0.0007	0.9984	-0.0569	0.0000
CH_2O					
	O1=C2	-0.7957	1.0000	0.0000	0.0000
	C2−H3	-0.3158	1.0000	0.0000	0.0000
CH_3NO					
	C1=O2	-0.7969	0.0000	0.0000	1.0000
	C1−N3	-0.5183	0.0000	0.0000	1.0000
	N3−H4	-0.5599	0.0000	0.0000	1.0000
	N3−H5	-0.5610	0.0000	0.0000	1.0000
	C1−H6	-0.3193	0.0000	0.0000	1.0000
C_3H_3NO					
	O1=C2	-0.4782	0.0000	0.0000	1.0000
	O1−C3	-0.4454	0.0000	0.0000	1.0000
	C2=N4	-0.6868	0.0000	0.0000	1.0000
	C2−H5	-0.3543	0.0000	0.0000	1.0000
	C3−C6	-0.4159	0.0000	0.0000	1.0000
	N4−C6	-0.4269	0.0000	0.0000	1.0000
	C3−H7	-0.3521	0.0000	0.0000	1.0000
	C6−H8	-0.3476	0.0000	0.0000	1.0000
CH_4					
	C1−H2	-0.3203	0.7071	-0.7071	0.0000
C_2H_2					
	C1≡C2	-0.6854	1.0000	0.0000	0.0000
	C1−H3	-0.3571	1.0000	0.0000	0.0000
C_2H_4					
	C2=C4	-0.4444	1.0000	0.0000	0.0000
	H1−C2	-0.3342	1.0000	0.0000	0.0000
N_4H_4					
	N1−N2	-0.2583	-0.0492	-0.0306	0.9983
	N1−H4	-0.5396	0.9286	-0.2163	-0.3016
W4					
	O4−H6	-0.7183	0.5230	0.5951	0.6102
	H6--O1	-0.0042	0.5365	0.3814	-0.7528
	O1−H2	-0.7609	0.6290	-0.4855	-0.6072
W6					

O4−H6	-0.6722	0.2773	0.8461	0.4552
H6--O1	-0.0094	0.0862	-0.4678	0.8796
O7−H8	-0.7143	0.0470	0.1188	0.9918
H8--O10	-0.0042	0.2381	0.9709	0.0274
O1−H2	-0.7219	0.8090	0.5353	-0.2429
H2--O16	-0.0022	0.1729	0.9843	0.0359
O13−H15	-0.7338	0.4733	-0.8802	-0.0338
H15--O4	-0.0017	0.0217	-0.9918	0.1260
O10−H12	-0.7489	0.7741	-0.6328	-0.0183
H12--O13	0.0017	0.0488	-0.3139	0.9482
O1−H3	-0.7448	0.8214	-0.4936	0.2858
H3--O7	0.0014	0.3439	0.5517	0.7598
O16−H18	-0.7425	0.2230	-0.0281	-0.9744
H18--O7	0.0009	0.1207	-0.4891	0.8638
O10−H11	-0.7454	0.7769	-0.6259	-0.0685
H11--O4	0.0004	0.2052	0.4067	0.8902
O16−H17	-0.7432	0.1864	0.0547	0.9809
H17--O13	0.0000	0.2107	0.7739	-0.5973
O4−H4	-0.7539	0.2594	0.8489	0.4606
O7−H9	-0.7510	0.0510	0.1185	0.9916
O13−H14	-0.7544	0.4776	-0.8781	-0.0279

Table S2(b) Total local energy $H(\mathbf{r}_b^{\mathbf{F}})$ and the $\underline{\mathbf{e}}_{\mathbf{2}}^{\mathbf{F}}$ eigenvector components at the Ehrenfest BCPs for the twelve molecular graphs.

Molecular graph	BCP	$H(\mathbf{r}_b^{\mathbf{F}})$	$\underline{\mathbf{e}}_{\mathbf{2}}^{\mathbf{F}}$		
H_2					
	H1−H2	-0.3376	1.0000	0.0000	0.0000
H_2O					
	O2−H1	-0.5524	1.0000	0.0000	0.0000
$(H_2O)_2$					
	O4−H4	-0.5513	0.4145	-0.8973	-0.1515
	O1−H3	-0.5537	0.0000	0.0000	1.0000
	O1−H2	-0.5353	0.0000	0.0000	1.0000
	H2--O4	0.0012	0.0000	0.0000	1.0000
CH_2O					
	O1=C2	-0.7571	1.0000	0.0000	0.0000
	C2−H3	-0.3159	1.0000	0.0000	0.0000
CH_3NO					
	C1=O2	-0.7228	0.0000	0.0000	1.0000
	C1−N3	-0.4026	0.0000	0.0000	1.0000
	N3−H4	-0.4674	0.0000	0.0000	1.0000
	N3−H5	-0.4715	0.0000	0.0000	1.0000
	C1−H6	-0.3193	0.0000	0.0000	1.0000
C_3H_3NO					
	O1=C2	-0.3662	0.0000	0.0000	1.0000
	O1−C3	-0.3378	0.0000	0.0000	1.0000
	C2=N4	-0.5447	0.0000	0.0000	1.0000
	C2−H5	-0.3538	0.0000	0.0000	1.0000
	C3−C6	-0.4130	0.0000	0.0000	1.0000
	N4−C6	-0.3492	0.0000	0.0000	1.0000
	C3−H7	-0.3519	0.0000	0.0000	1.0000
	C6−H8	-0.3477	0.0000	0.0000	1.0000
CH_4					
	C1−H2	-0.3198	0.7071	-0.7071	0.0000
C_2H_2					
	C1≡C2	-0.6854	1.0000	0.0000	0.0000
	C1−H3	-0.3563	-1.0000	0.0000	0.0000
C_2H_4					
	C1=C2	-0.4444	1.0000	0.0000	0.0000
	C1−H3	-0.3342	1.0000	0.0000	0.0000
N_4H_4					
	N1−N2	-0.2578	0.0442	0.0766	-0.9961
	N1−H4	-0.4648	0.9886	-0.1456	-0.0381
W4					
	O4−H6	-0.4990	-0.0160	0.0056	0.9999
	H6--O1	-0.0030	0.0046	0.0018	1.0000
	O1−H2	-0.5536	0.1752	0.9770	0.1219
W6					

O4−H6	-0.5188	0.0787	-0.1640	-0.9833
H6--O1	-0.0101	-0.0618	0.0983	-0.9932
O7−H8	-0.5530	-0.0099	0.0088	0.9999
H8--O10	-0.0057	-0.0058	0.0716	-0.9974
O1−H2	-0.5653	0.9972	0.0753	0.0033
H2--O16	-0.0032	0.9573	0.2785	0.0780
O13−H15	-0.5690	0.6315	-0.7754	-0.0042
H15--O4	-0.0024	0.4775	-0.8774	0.0464
O1−H3	-0.5958	-0.1000	-0.0747	-0.9922
H3--O7	0.0018	0.9816	-0.1275	0.1424
O16−H17	-0.5922	-0.0006	0.6569	0.7540
H17--O13	0.0016	-0.0483	0.2766	-0.9598
O16−H18	-0.5904	-0.0959	-0.0574	0.9937
H18--O7	0.0010	0.9699	-0.1373	-0.2009
O10−H11	-0.5882	0.8988	-0.4016	0.1758
H11--O4	0.0005	0.9325	-0.0798	0.3522
O10−H12	-0.5876	0.8123	-0.5762	-0.0909
H12--O13	0.0001	0.5002	0.0563	-0.8641
O4−H4	-0.6073	0.3290	-0.9334	-0.1431
O7−H9	-0.6076	-0.1066	-0.0978	-0.9895
O13−H14	-0.6080	0.0189	-0.7429	0.6691

Table S2(c) $\underline{\mathbf{e}}_2^\sigma$ eigenvector components at the Ehrenfest BCPs for the twelve molecular graphs.

Molecular graph	BCP	$\underline{\mathbf{e}}_2^\sigma$		
H_2				
	H1−H2	1.0000	0.0000	0.0000
H_2O				
	O2−H1	0.0000	0.6050	0.7962
$(H_2O)_2$				
	O4−H4	-0.6515	-0.4616	-0.6021
	O1−H3	0.3578	-0.9338	0.0000
	O1−H2	0.9960	0.0898	0.0000
	H2--O4	0.0000	0.0000	1.0000
CH_2O				
	O1=C2	0.0000	-1.0000	0.0000
	C2−H3	1.0000	0.0000	0.0000
CH_3NO				
	C1=O2	0.1448	0.9895	0.0000
	C1−N3	0.7171	-0.6969	0.0000
	N3−H4	-0.9569	-0.2905	0.0000
	N3−H5	-0.2128	-0.9771	0.0000
	C1−H6	0.0000	0.0000	1.0000
C_3H_3NO				
	O1=C2	-0.5927	0.8055	0.0000
	O1−C3	0.9339	0.3575	0.0000
	C2=N4	0.4958	0.8685	0.0000
	C2−H5	0.9889	0.1488	0.0000
	C3−C6	-0.0613	0.9981	0.0000
	N4−C6	0.9668	-0.2557	0.0000
	C3−H7	0.7545	-0.6563	0.0000
	C6−H8	0.7383	0.6745	0.0000
CH_4				
	C1−H2	0.7071	-0.7071	0.0000
C_2H_2				
	C1≡C2	0.0000	1.0000	0.0000
	C1−H3	0.0000	-1.0000	0.0000
C_2H_4				
	C1=C2	0.0000	1.0000	0.0000
	C1−H3	1.0000	0.0000	0.0000
N_4H_4				
	N1−N2	0.5282	-0.8491	0.0000
	N1−H4	0.9739	-0.2269	0.0000
W4				
	O4−H6	-0.4301	-0.4645	0.7741
	H6--O1	-0.7146	-0.5174	-0.4708
	O1−H2	0.4786	0.8591	-0.1814
W6				

O4−H6	0.2608	0.3908	-0.8827
H6--O1	0.2808	0.8043	0.5237
O7−H8	0.4374	0.8902	-0.1272
H8--O10	-0.0061	0.0323	-0.9995
O1−H2	0.6197	0.7353	-0.2745
H2--O16	0.8696	0.4931	0.0244
O13−H15	-0.8718	-0.4623	-0.1622
H15--O4	0.9850	-0.0031	-0.1723
O1−H3	-0.4980	-0.6032	0.6230
H3--O7	-0.1251	0.2718	-0.9542
O16−H17	0.2117	-0.2487	-0.9452
H17--O13	0.9649	0.0065	0.2624
O16−H18	0.8560	-0.4624	0.2312
H18--O7	0.9726	-0.1166	-0.2012
O10−H11	-0.5390	-0.5667	-0.6232
H11--O4	0.8668	-0.3746	-0.3291
O10−H12	0.2308	0.9727	-0.0236
H12--O13	-0.2131	-0.3096	-0.9267
O4−H4	0.8078	-0.4517	0.3788
O7−H9	0.7313	-0.6806	0.0444
O13−H14	0.3825	0.2361	-0.8933