Collision-induced dissociation of protonated uracil water clusters probed by molecular dynamics simulations

Electronic Supplementary Material

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1 Validation of D_{NH} Parameter

To determine an appropriate D_{NH} parameter for the SCC-DFTB simulations of $(H_2O)_{1-7,11,12}UH^+$ clusters, three D_{NH} values were tested, 0.00, 0.12 and 0.14, by calculating the binding energy of two $(H_2O)U$ isomers, which structures are displayed in Figure S1, using MP2/Def2TZVP and SCC-DFTB methods. The results are shown in Table S1. The relative binding energy E_{Re} (E_{Re}=$E_{bind_{DFTB}}$-$E_{bind_{MP2}}$) for isomer a is less than 2.0 kcal.mol^{-1} when different D_{NH} parameters are used. For isomer b, the E_{Re} is 0.0 kcal.mol^{-1} when D_{NH} is 0.12 and 0.14 and it is only 0.3 kcal.mol^{-1} when D_{NH} is 0.0. This indicates that the value of D_{NH} has only a minor effect on the binding energy calculation of $(H_2O)U$. We thus decided to use D_{NH} equal to 0.12 for all the simulations.

Table S1 Binding energy of two (H_2O)U isomers using MP2/Def2TZVP and SCC-DFTB methods. All values are given in kcal.mol^{-1}.

isomer	$E_{bind_{MP2}}$	$E_{bind_{DFTB}}$ $D_{NH_{0.0}}$	E_{Re}	$E_{bind_{DFTB}}$ $D_{NH_{0.12}}$	E_{Re}	$E_{bind_{DFTB}}$ $D_{NH_{0.14}}$	E_{Re}
a	-8.3	-8.6	-0.3	-9.8	-1.5	-10.0	-1.7
b	-6.9	-6.6	0.3	-6.9	0.0	-6.9	0.0

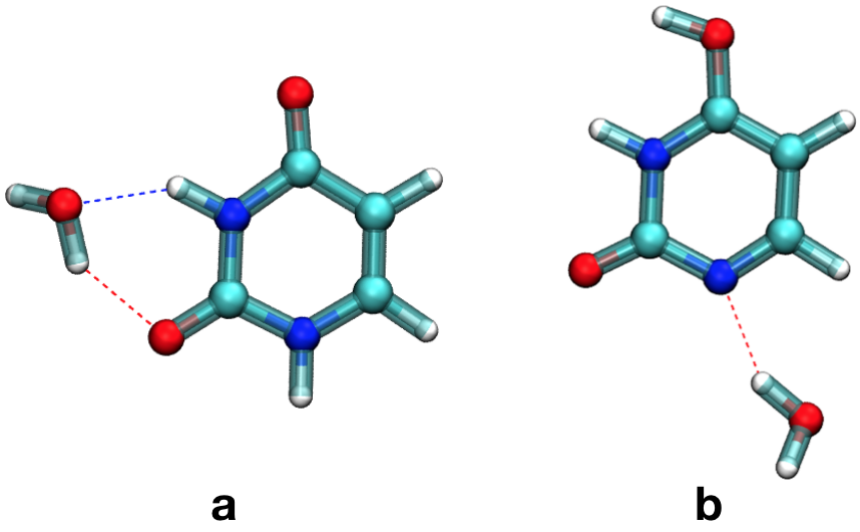

Figure S1 Structure of isomer a and b of (H_2O)U.

2 Statistical Convergence

In order to ensure that statistical convergence is reached in the collision trajectories, initial conditions have to reproduce all possible collision orientation with good statistics. The procedure described in the main text to generate initial conditions fulfil this requirement. As a visual proof, Figure S2 a, b and c represents initial conditions generated for isomer 3b generated using 200, 400 and 600 random orientations and an impact parameter of 0.0. In these pictures, $(H_2O)_3UH^+$ is fixed and all initial positions for argon are superimposed. It worth pointing out that in practice, in the collision trajectories, argon is fixed and uracil is rotated. Figure S2 d presents the same data for 200 random orientations and for impact parameter 0.0 and 6.0. These Figures demonstrate that the more simulations are performed, the more colliding opportunities of Ar at all possible orientations are obtained. The same data for isomers 4b, 5d, 6f, 7a and 12f are provided in Figure S3 to S7, respectively. In addition, to confirm that statistical convergence is reached for the properties discussed in the main text, Table S2 and S3 present the P_{NUL} and σ_{frag} values for the lowest-energy isomer and the isomer which P_{NUL} fits best to the experiment (bold) obtained for 200, 400, and 600 initial random orientations per impact parameter value. Whatever the considered isomer, the three P_{NUL} and σ_{frag} values are very close. Indeed, the largest difference is observed for isomer 7a which has P_{NUL} values of 29.5 and 31.3 % for 200 and 600 random orientations, respectively. This demonstrates that even for 200 initial random orientations, simulation are close to statistical convergence. In the present study, all results discussed in the main text were obtained with 600 initial random orientations per b value which insures statistical convergence of the results independently of cluster size.

Table S2 P_{NUL} and σ_{frag} values for the lowest-energy isomer (roman) and the isomer which P_{NUL} fits best to the experiment (bold) of $(H_2O)_{1-6}UH^+$ obtained from simulations consisting in 200, 400, and 600 initial random orientations per impact parameter.

Cluster	**Random Orientations**	P_{NUL} **(%)**	σ_{frag} **(Å^2)**
1a	200	0.1	28.4
1a	400	0.1	28.3
1a	600	0.2	28.9
1b	200	0.2	26.3
1b	400	0.1	25.7
1b	600	0.	25.9
2a	200	0.0	35.9
2a	400	0.0	36.5
2a	600	0.0	36.3
2b	200	0.0	34.7
2b	400	0.1	34.8
2b	600	0.1	34.9
3a	200	5.4	37.4
3a	400	5.2	36.2
3a	600	5.7	36.3
3b	200	0.0	41.2
3b	400	0.0	41.5
3b	600	0.0	41.9
4a	200	26.9	40.1
4a	400	28.2	40.3
4a	600	29.4	40.1
4b	200	2.7	45.3
4b	400	2.6	45.6
4b	600	2.6	45.2
5a	200	45.7	37.2
5a	400	46.1	37.8
5a	600	46.6	38.2
5d	200	0.1	47.3
5d	400	0.1	47.3
5d	600	0.1	47.5
6a	200	38.0	46.6
6a	400	38.0	45.6
6a	600	39.3	45.8
6f	200	18.9	54.2
6f	400	19.0	55.2
6f	600	18.5	55.0

Table S3 P_{NUL} and σ_{frag} values for the lowest-energy isomer (roman) and the isomer which P_{NUL} fits best to the experiment (bold) of $(H_2O)_{7,11,12}UH^+$ obtained from simulations consisting in 200, 400, and 600 initial random orientations per impact parameter.

Cluster	**Random Orientations**	P_{NUL} **(%)**	σ_{frag} **(Å^2)**
7a	200	29.5	54.8
7a	400	31.3	53.4
7a	600	31.3	53.4
7d	200	22.6	55.3
7d	400	22.9	54.3
7d	600	23.0	54.0
11a	200	26.7	53.8
11a	400	28.2	53.5
11a	600	28.3	52.9
11d	200	14.5	55.2
11d	400	15.4	56.1
11d	600	15.6	56.5
12a	200	8.0	59.2
12a	400	7.5	60.5
12a	600	7.6	60.2
12c	200	10.4	55.3
12c	400	10.8	55.8
12c	600	10.8	55.4

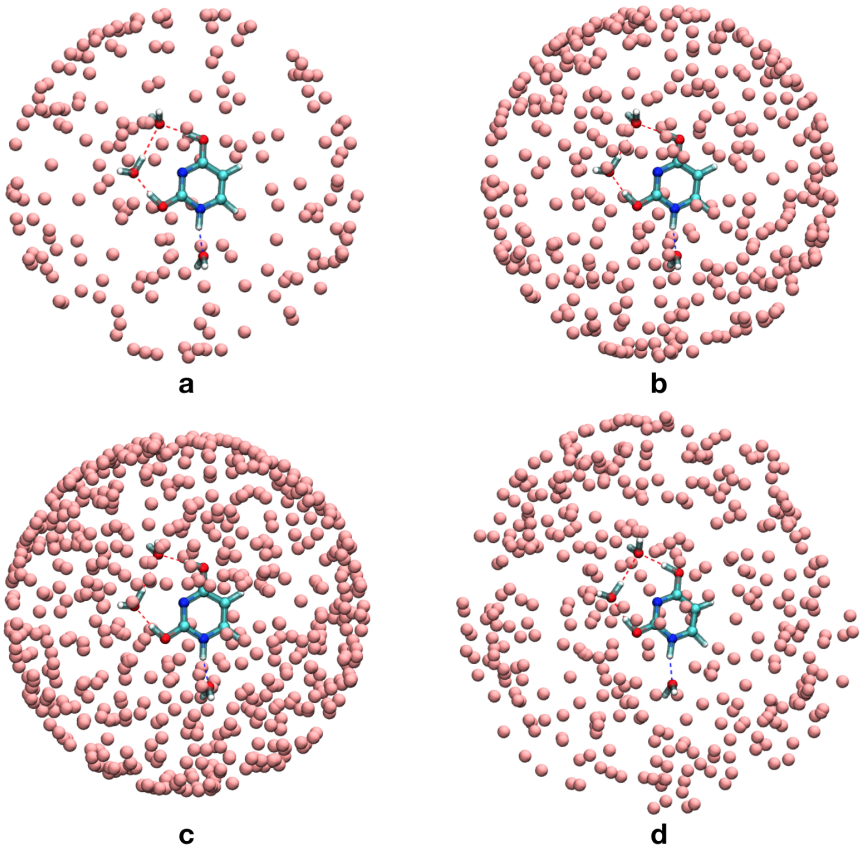

Figure S2 Schematic representation of the initial conditions for the collision simulations of isomer 3b. 200 (a), 400 (b) and 600 (c) random orientations are generated with a unique impact parameter equal to 0.0. (d) 200 orientations are generated with impact parameters 0.0 and 6.0.

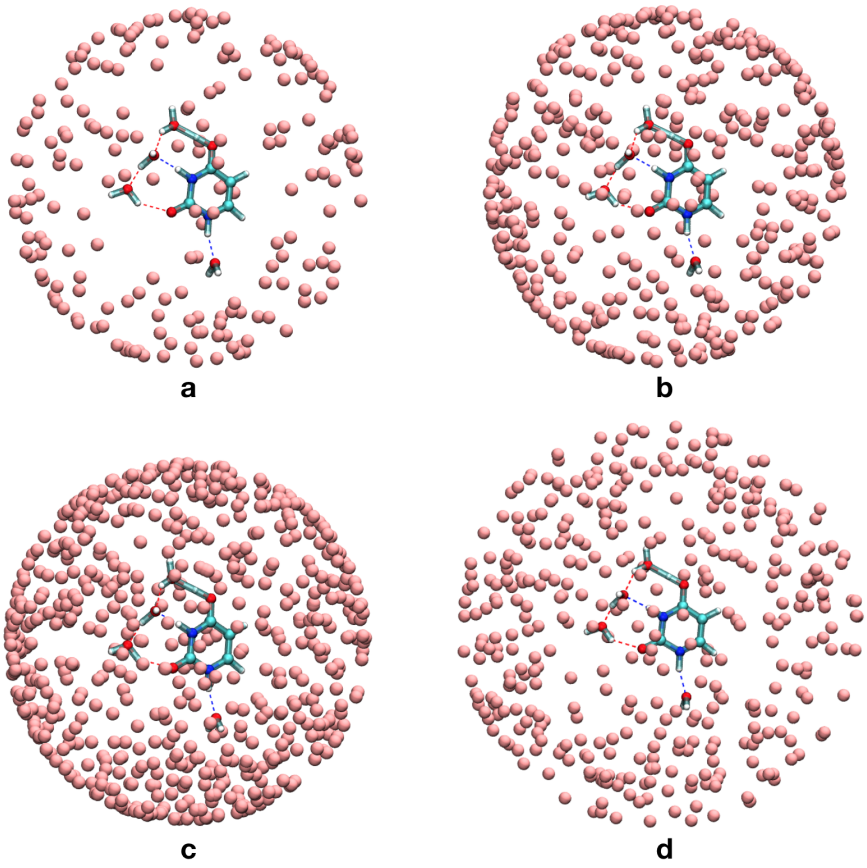

Figure S3 Schematic representation of the initial conditions for the collision simulations of isomer 4b. 200 (a), 400 (b) and 600 (c) random orientations are generated with a unique impact parameter equal to 0.0. (d) 200 orientations are generated with impact parameters 0.0 and 6.5.

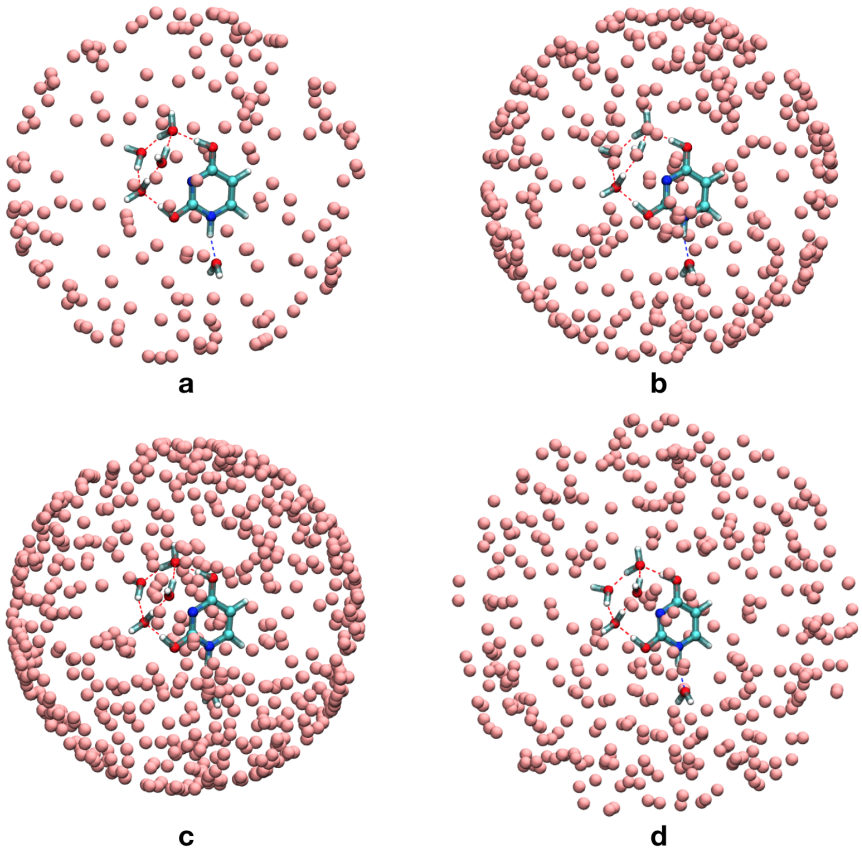

Figure S4 Schematic representation of the initial conditions for the collision simulations of isomer 5d. 200 (a), 400 (b) and 600 (c) random orientations are generated with a unique impact parameter equal to 0.0. (d) 200 orientations are generated with impact parameters 0.0 and 6.5.

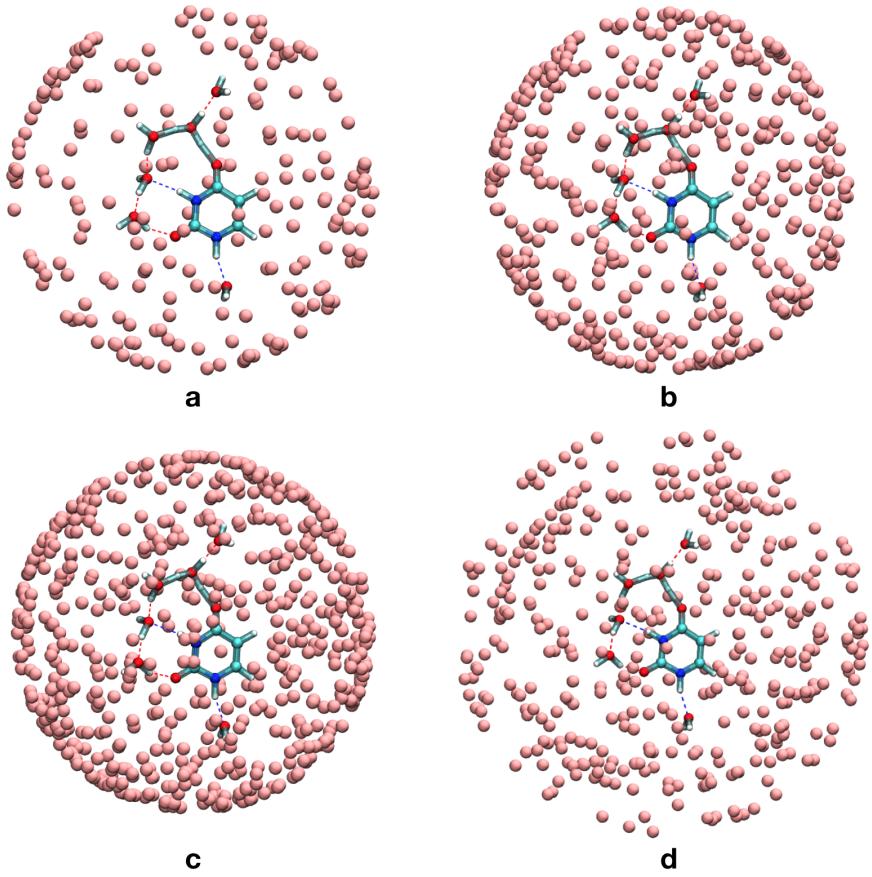

Figure S5 Schematic representation of the initial conditions for the collision simulations of isomer 6f. 200 (a), 400 (b) and 600 (c) random orientations are generated with a unique impact parameter equal to 0.0. (d) 200 orientations are generated with impact parameters 0.0 and 7.5.

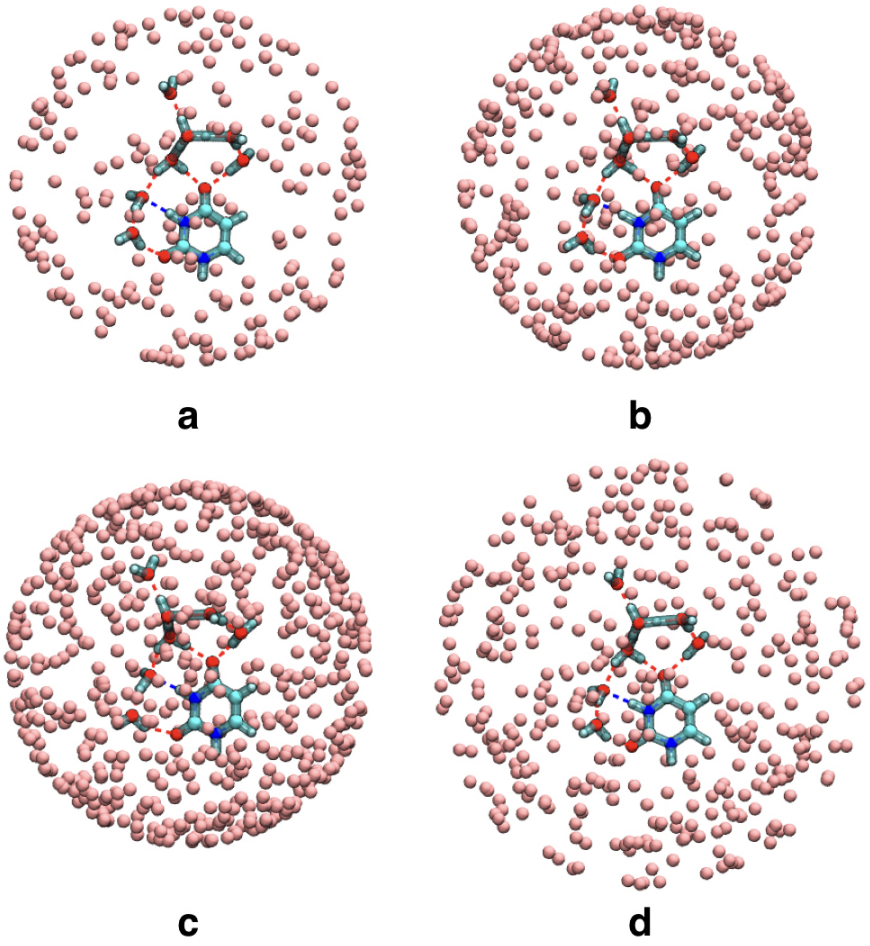

Figure S6 Schematic representation of the initial conditions for the collision simulations of isomer 7a. 200 (a), 400 (b) and 600 (c) random orientations are generated with a unique impact parameter equal to 0.0. (d) 200 orientations are generated with impact parameters 0.0 and 7.5.

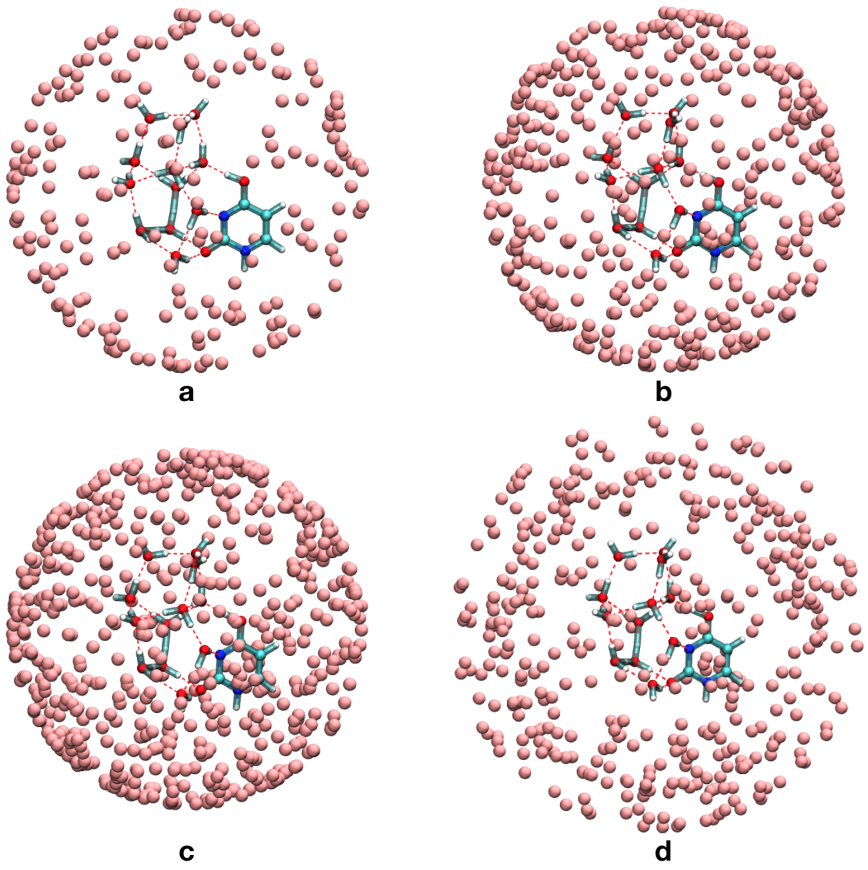

Figure S7 Schematic representation of the initial conditions for the collision simulations of isomer 12f. 200 (a), 400 (b) and 600 (c) random orientations are generated with a unique impact parameter equal to 0.0. (d) 200 orientations are generated with impact parameters 0.0 and 7.5.

Table S4 R_{max} value (Å), number of b values and dissociation probability at R_{max} for all considered isomers. R_{max} is calculated as $\lfloor 2R \rfloor/2 + 1.5$ Å, where R is the radius of the considered isomer. Dissociation probability at R_{max}, evaluated over 600 collision trajectories, indicates how converged are the results with respect to the number of b values. The lower the dissociation probability at R_{max}, the better is the convergence. The maximum dissociation probability at R_{max} is 2.7%, which indicates that the present definition of R_{max} is good enough to insure convergency.

Isomers	R_{max}(Å)	Number of b Values	Dissociation Probability at R_{max} (%)
1a	5.5	12	0.0
1b	5.5	12	0.0
2a	5.5	12	0.2
2b	5.5	12	0.0
3a	5.5	12	0.0
3b	6.5	14	0.0
4a	6.5	14	1.0
4b	6.5	14	0.0
5a	5.5	12	0.0
5b	6.5	14	0.0
5c	7.0	15	0.3
5d	6.5	14	1.5
6a	7.0	15	0.7
6b	6.5	14	2.7
6c	7.0	15	0.8
6d	6.0	13	0.0
6e	7.0	15	0.2
6f	8.0	17	0.0
7a	7.5	16	0.7
7b	7.0	15	1.5
7c	7.0	15	2.3
7d	7.5	16	0.2
11a	7.5	16	0.0
11b	7.5	16	0.0
11c	7.5	16	0.0
11d	7.5	16	0.3
11e	7.5	16	0.0
11f	7.0	15	0.0
12a	8.0	17	0.8
12b	7.0	15	0.0
12c	7.0	15	0.0
12d	7.0	15	0.0
12e	7.0	15	0.0
12f	7.5	16	0.0

3 Time-dependent proportion of fragments

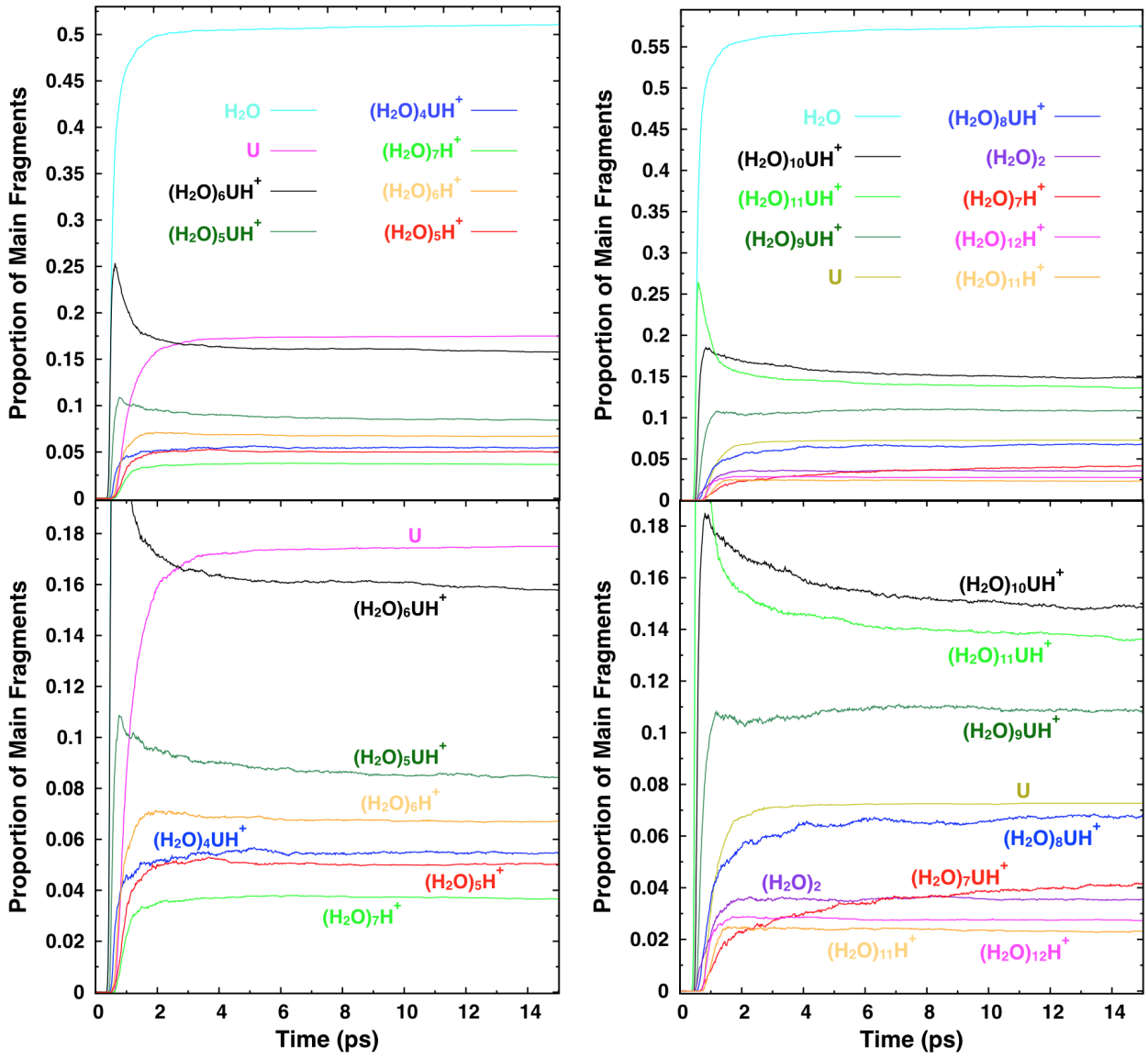

Figure S8 Time-dependent proportions of the main fragments obtained from the dissociation of isomers 7d (left) and 12c (right). Bottom panels correspond to a zoom over the lower proportions.

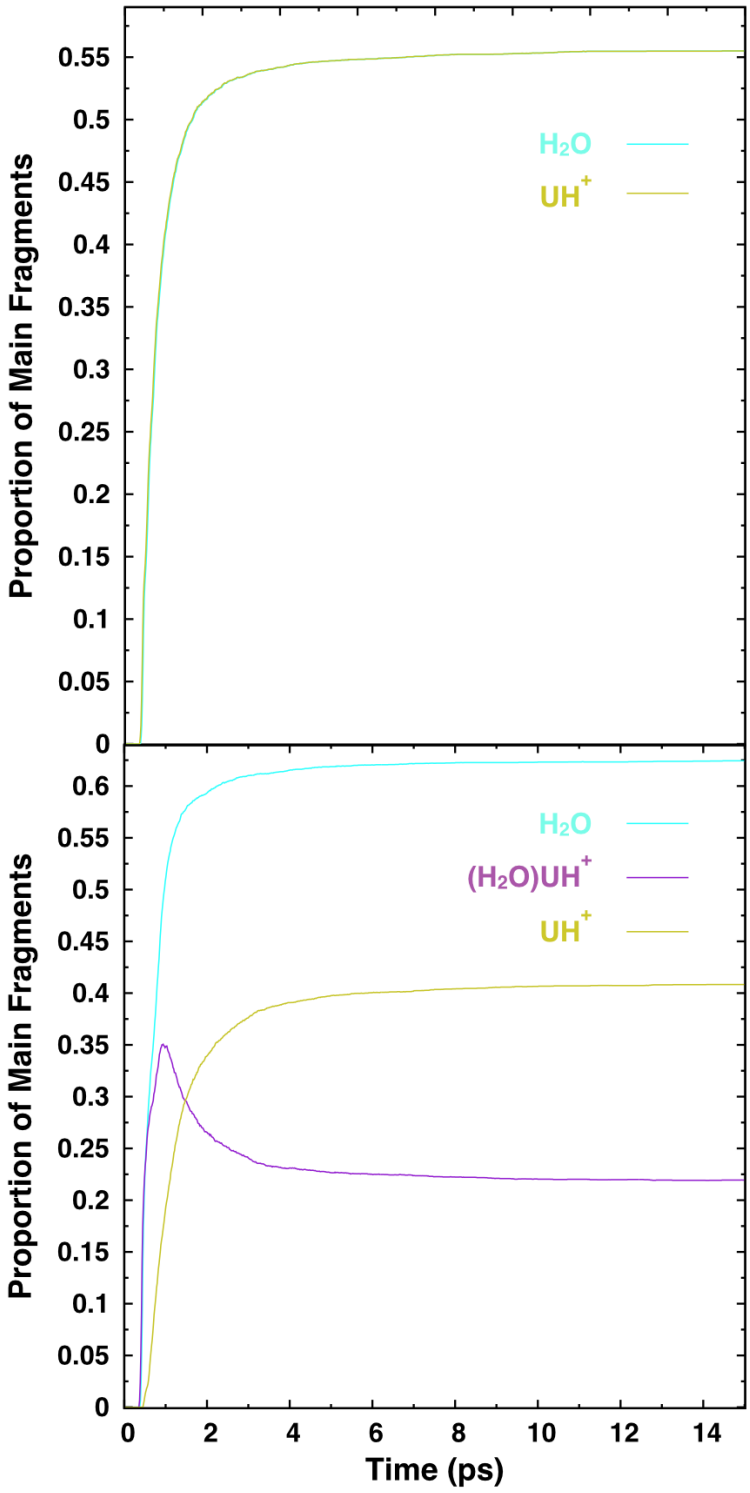

Figure S9 Time-dependent proportions of the main fragments obtained from the dissociation of isomers 1a (top) and 2a (bottom).

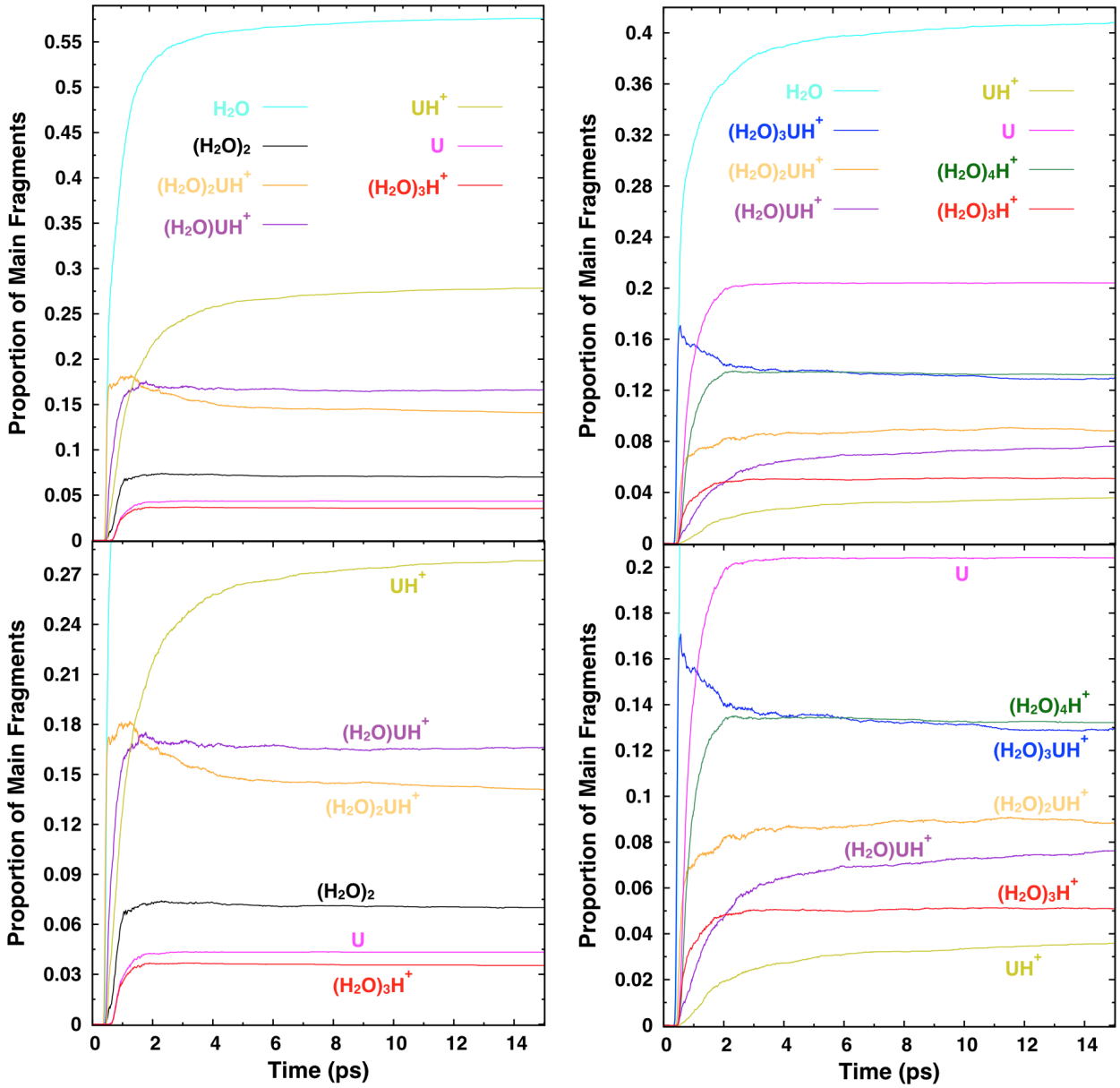

Figure S10 Time-dependent proportions of the main fragments obtained from the dissociation of isomers 3a (left) and 4a (right). Bottom panels correspond to a zoom over the lower proportions.

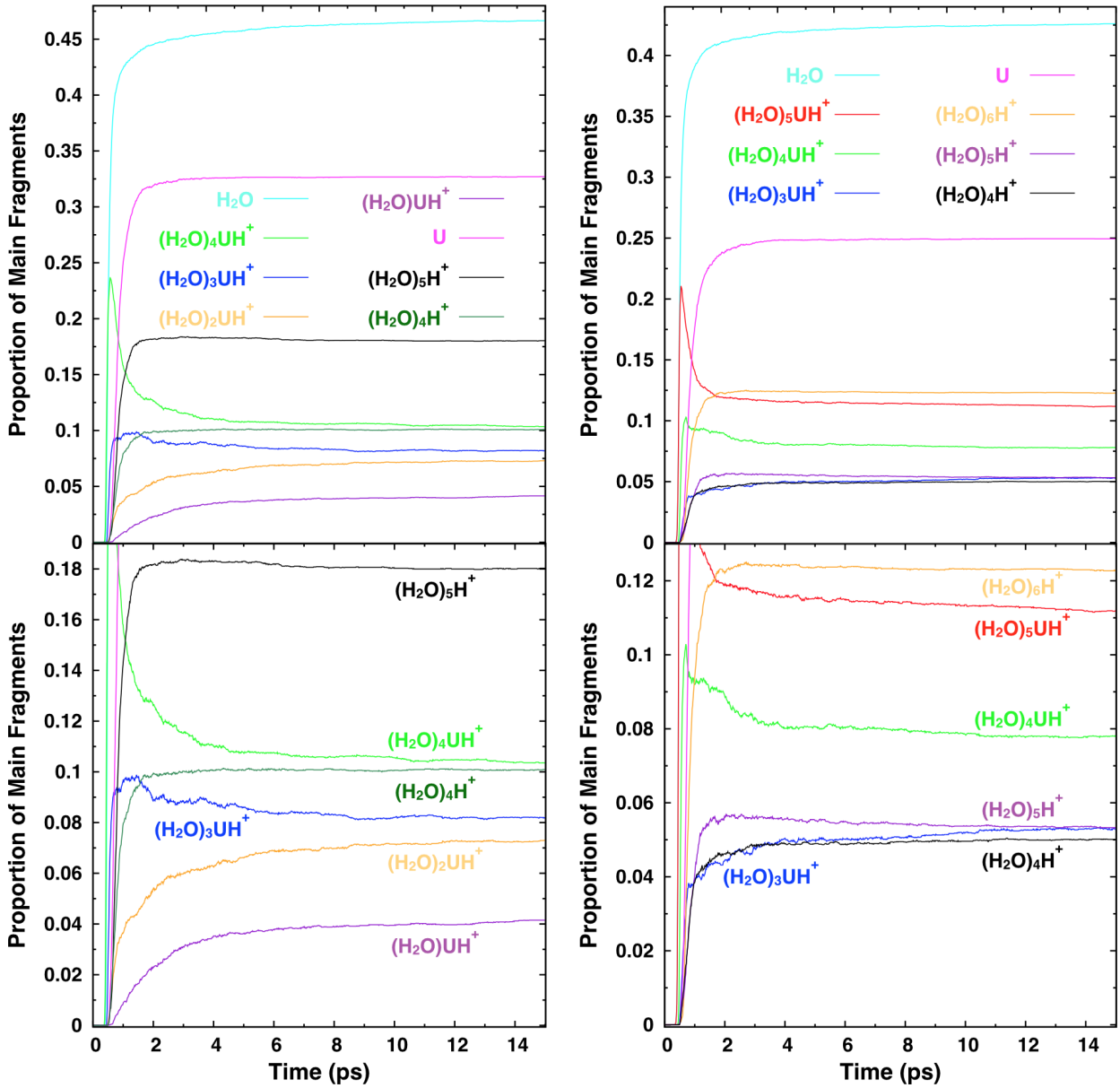

Figure S11 Time-dependent proportions of the main fragments obtained from the dissociation of isomers 5a (left) and 6a (right). Bottom panels correspond to a zoom over the lower proportions.

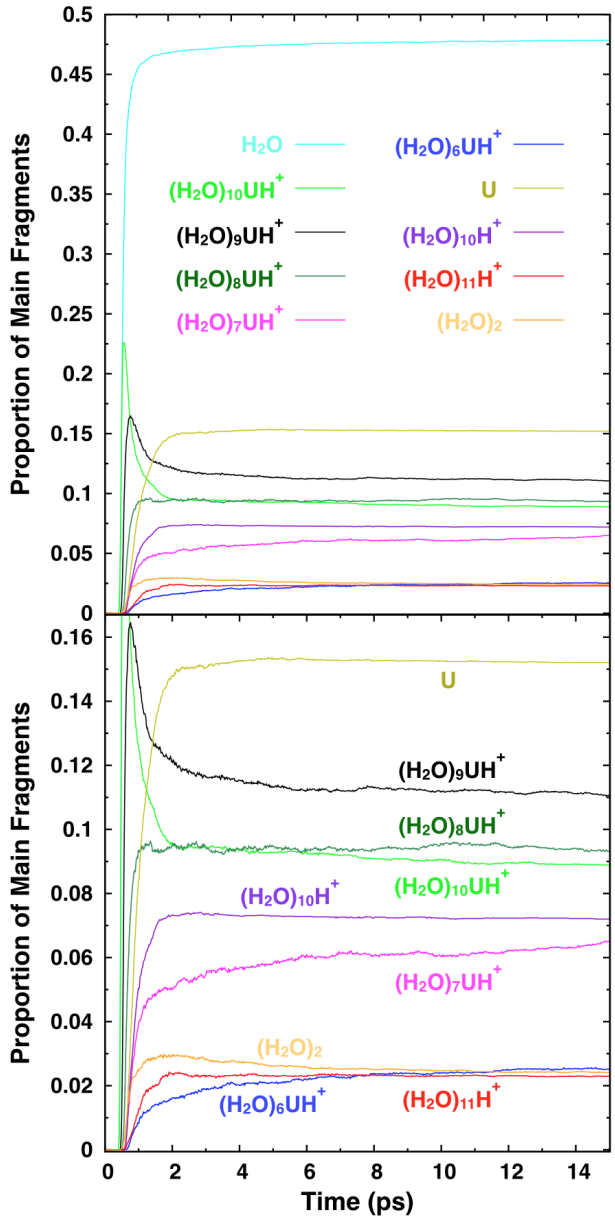

Figure S12 Time-dependent proportions of the main fragments obtained from the dissociation of isomer 11a. Bottom panels correspond to a zoom over the lower proportions.

4 Comparison of P_{NUL} and σ_{frag} including Experimental Data with Ne

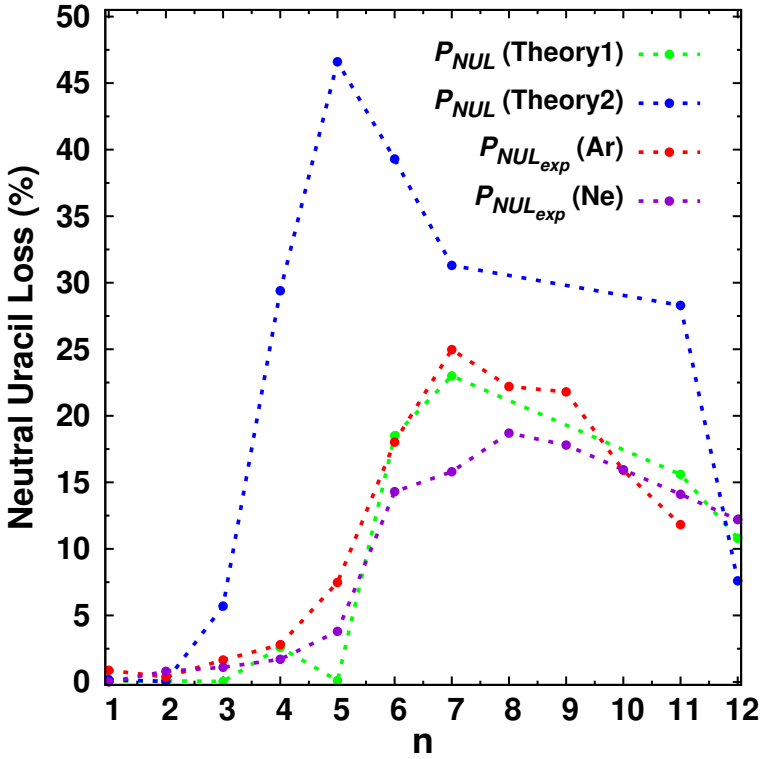

Figure S13 Theoretical (green and blue lines) and experimental (red line for Ar and purple for Ne) P_{NUL} values for the $(H_2O)_nUH^+$ clusters (n=1-7,11,12 for theory, n=1-11 for experiments with Ar and n=1-12 for experiments with Ne). Theory 1 (green line) is obtained from the isomers which P_{NUL} matches best to the experimental data while Theory 2 (blue line) is obtained from lowest-energy isomers.

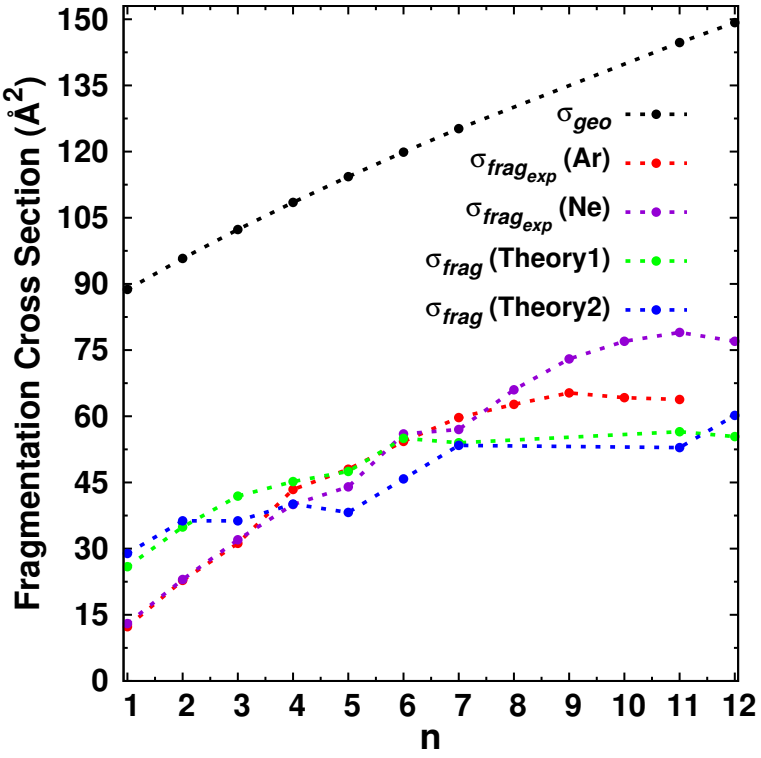

Figure S14 Theoretical (green and blue lines) and experimental (red line for Ar and purple for Ne) σ_{frag} values for the $(H_2O)_nUH^+$ clusters (n=1-7,11,12 for theory, n=1-11 for experiments with Ar and n=1-12 for experiments with Ne). Theory 1 (green line) is obtained from the isomers which P_{NUL} matches best to the experimental data while Theory 2 (blue line) is obtained from lowest-energy isomers.

5 Mass Spectrum of Fragments with Excess Proton

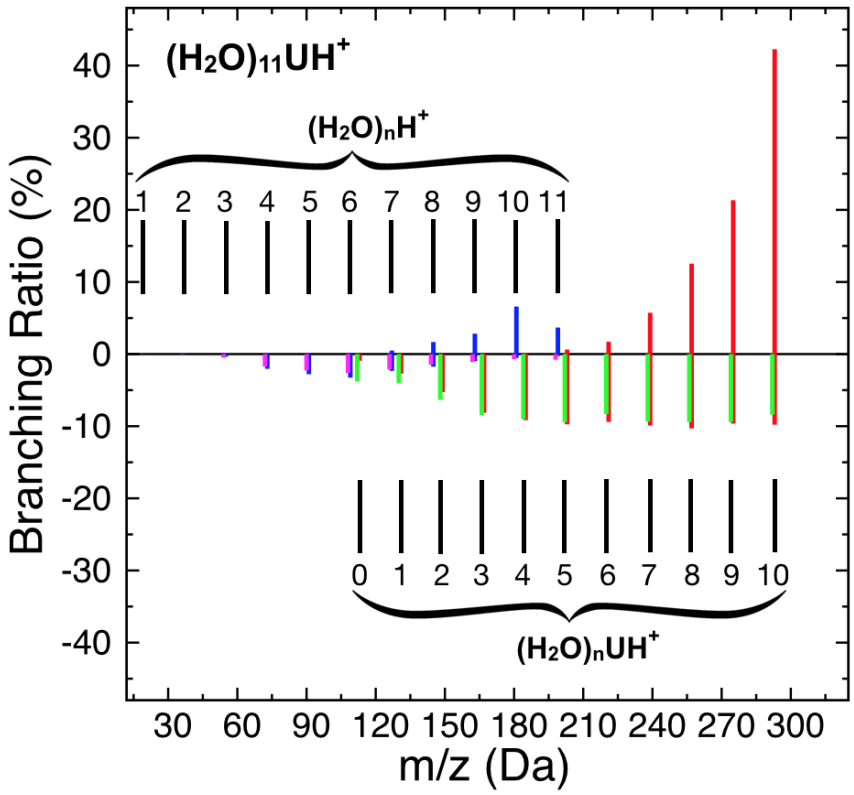

Figure S15 Simulated mass spectra of the charged fragments after 15 ps simulation time for isomer 11d (positive area) together with the experimental ones (negative area). For collisions with Argon, fragments $(H_2O)_nH^+$ are plotted in blue whereas $(H_2O)_nUH^+$ fragments are plotted in red. For collisions with Neon Fragments $(H_2O)_nH^+$ are plotted in pink whereas fragments $(H_2O)_nUH^+$ are plotted in green.

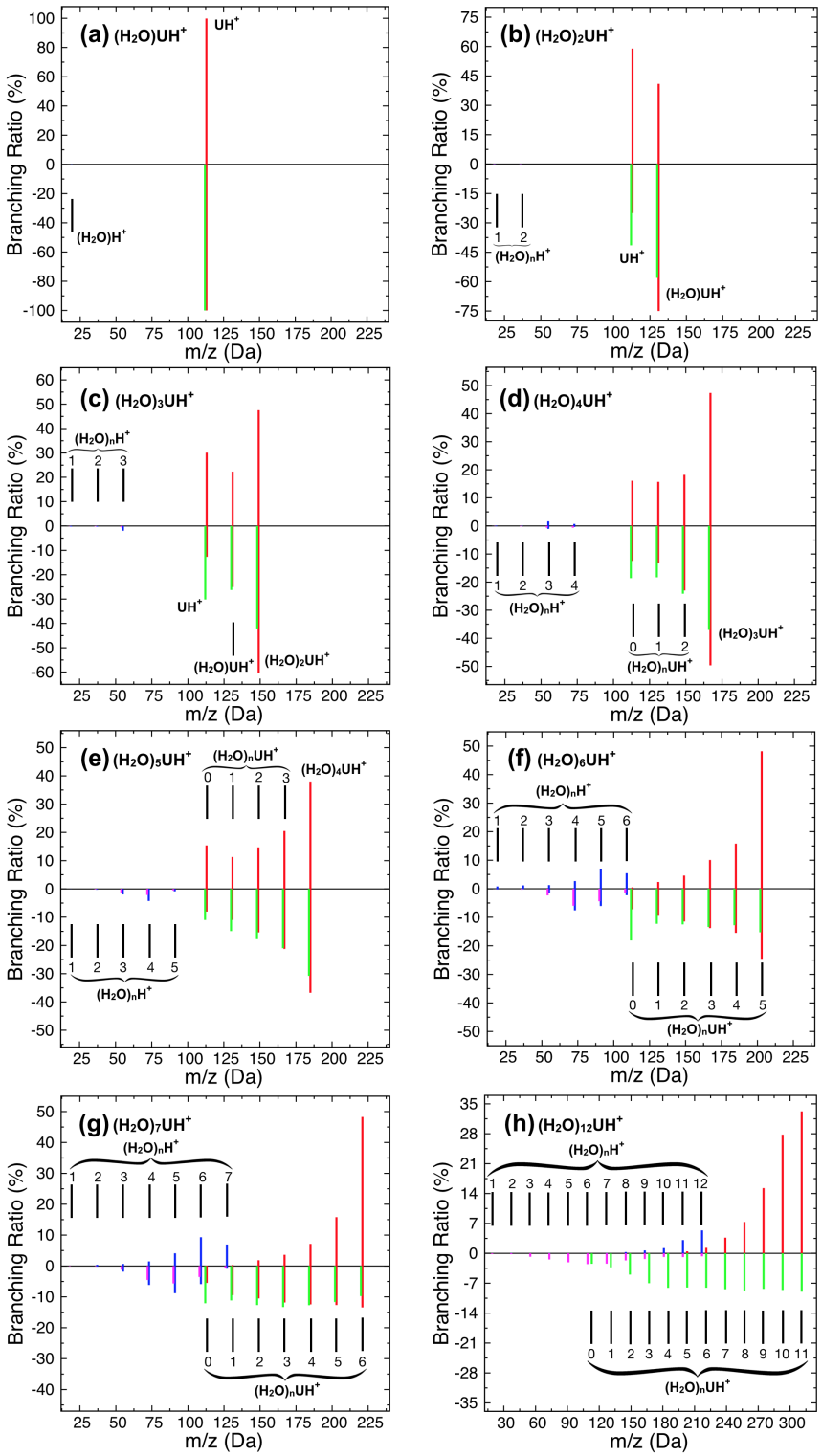

Figure S16 Simulated mass spectra of the charged fragments after 15 ps simulation time for isomers (a) 1a, (b) 2b, (c) 3b, (d) 4b, (e) 5d, (f) 6f, (g) 7d, (h) 12c (positive area) together with the experimental ones (negative area). For collisions with Argon, fragments $(H_2O)_nH^+$ are plotted in blue whereas $(H_2O)_nUH^+$ fragments are plotted in red. For collisions with Neon Fragments $(H_2O)_nH^+$ are plotted in pink whereas fragments $(H_2O)_nUH^+$ are plotted in green.

6 Energy Conservation

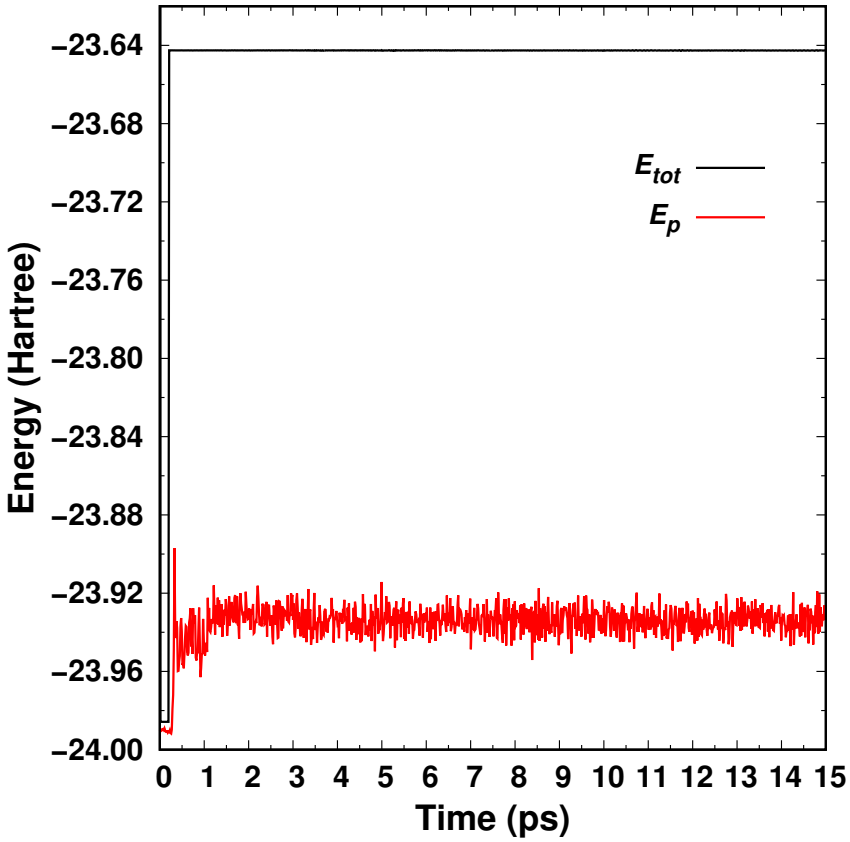

Figure S17 Total energy E_{tot} (black line) and potential energy E_p (red line) of a randomly selected trajectory of isomer 1a.

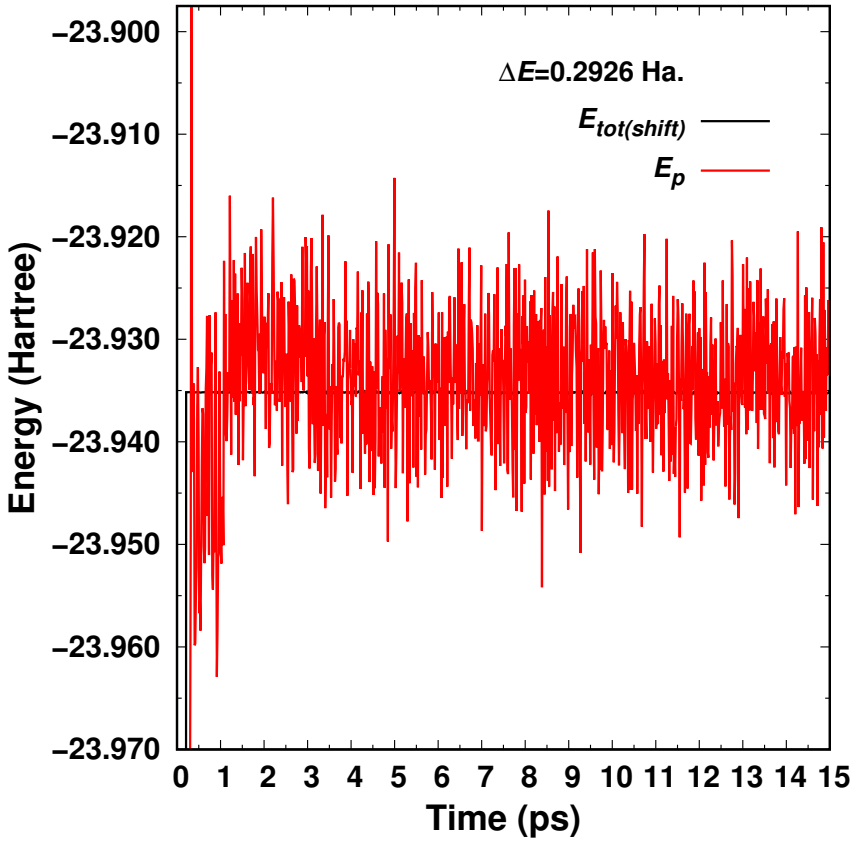

Figure S18 Shifted total energy $E_{tot(shift)}$ (black line), pan down 0.2926 Hartree of the total energy, and potential energy E_p (red line) of a the same randomly selected trajectory of isomer 1a than presented in Figure S17.

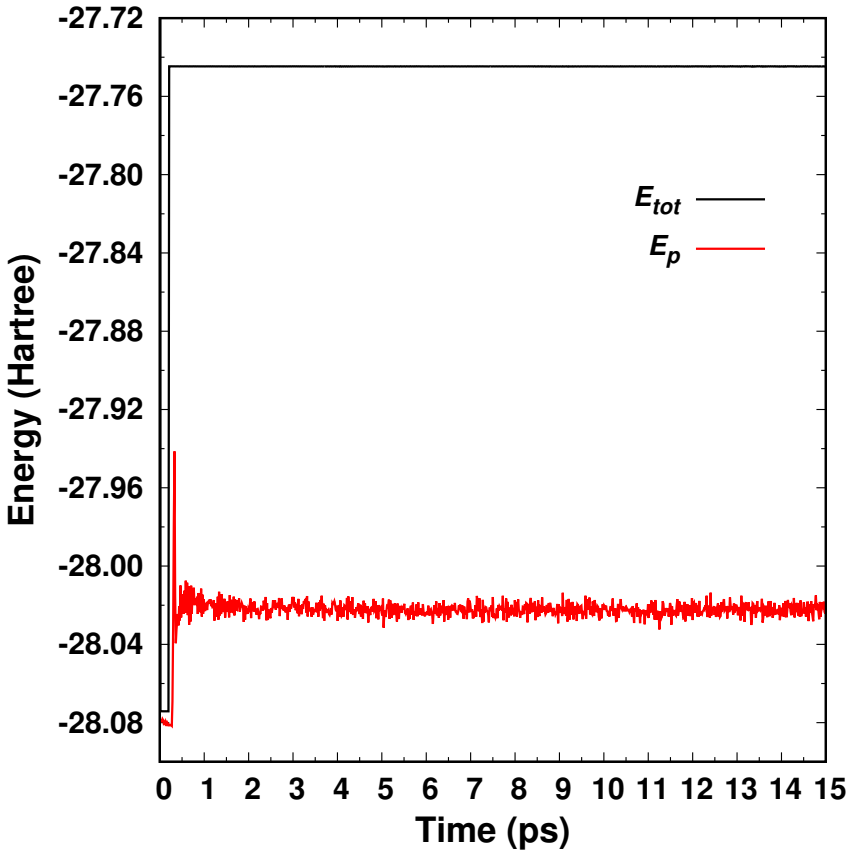

Figure S19 Total energy E_{tot} (black line) and potential energy E_p (red line) of a randomly selected trajectory of isomer 2b.

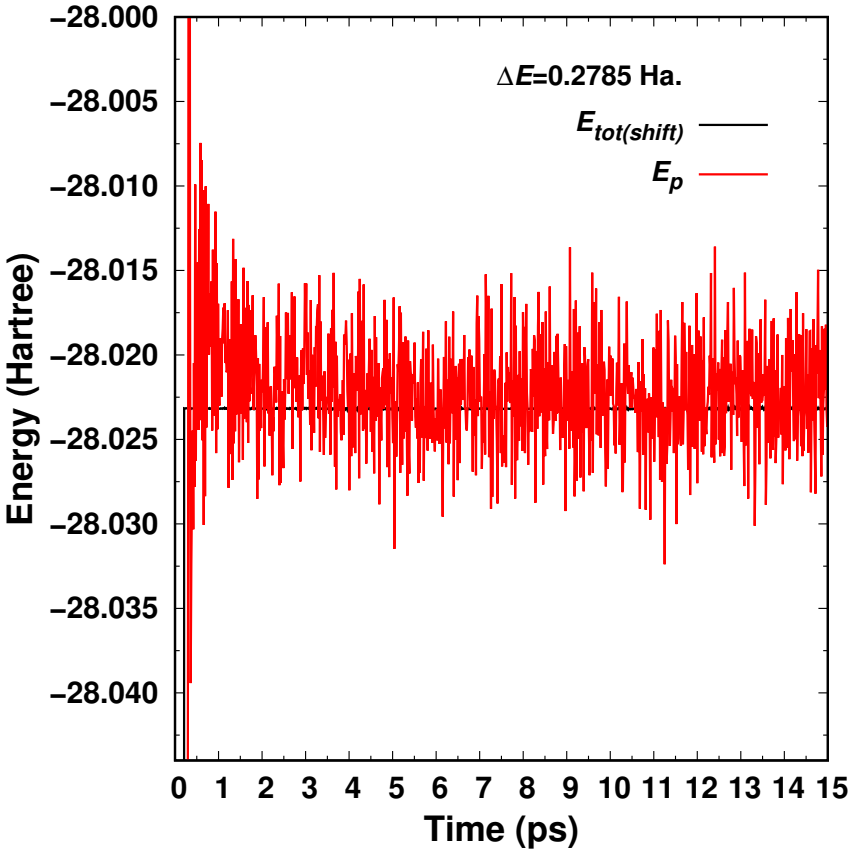

Figure S20 Shifted total energy $E_{tot(shift)}$ (black line), pan down 0.2785 Hartree of the total energy, and potential energy E_p (red line) of a the same randomly selected trajectory of isomer 2b than presented in Figure S19.

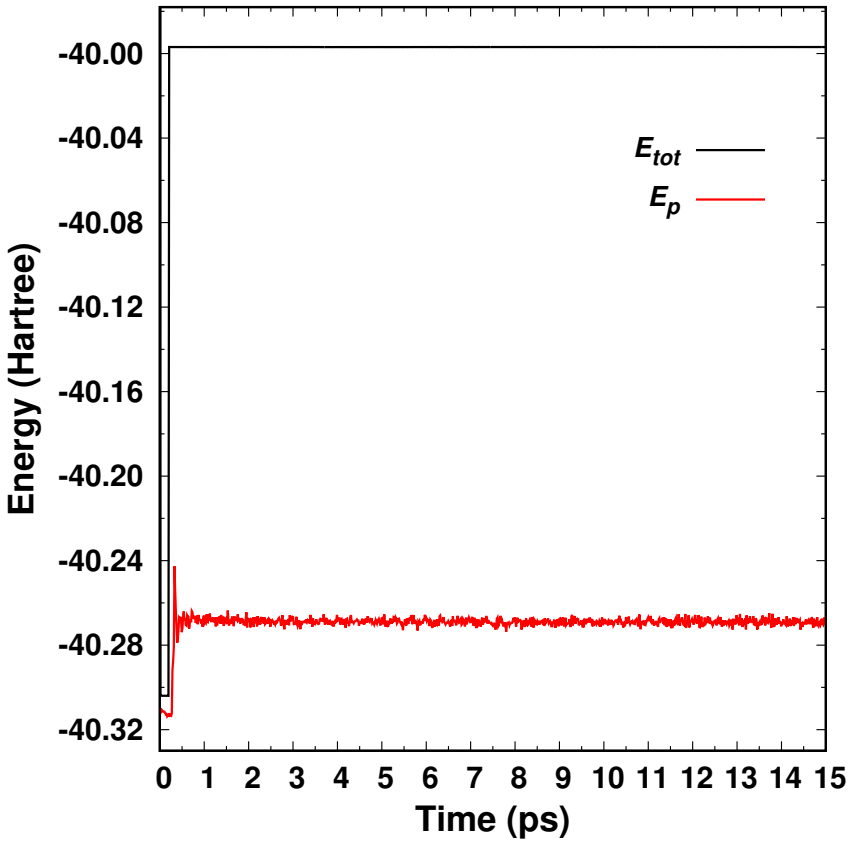

Figure S21 Total energy E_{tot} (black line) and potential energy E_p (red line) of a randomly selected trajectory of isomer 5d.

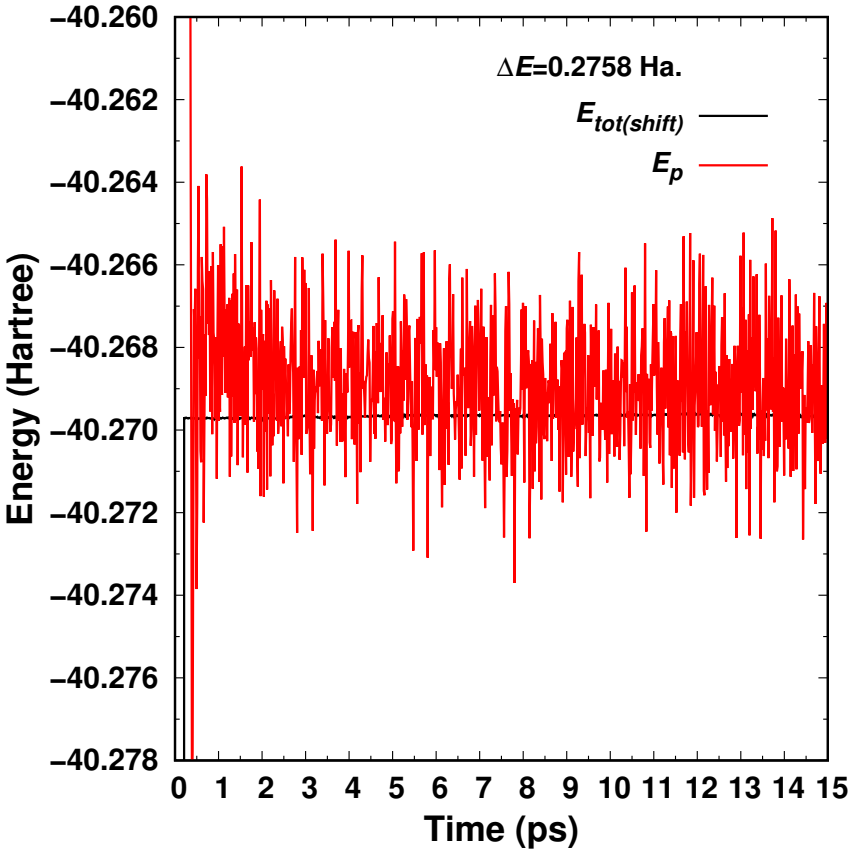

Figure S22 Shifted total energy $E_{tot(shift)}$ (black line), pan down 0.2758 Hartree of the total energy, and potential energy E_p (red line) of a the same randomly selected trajectory of isomer 5d than presented in Figure S21.

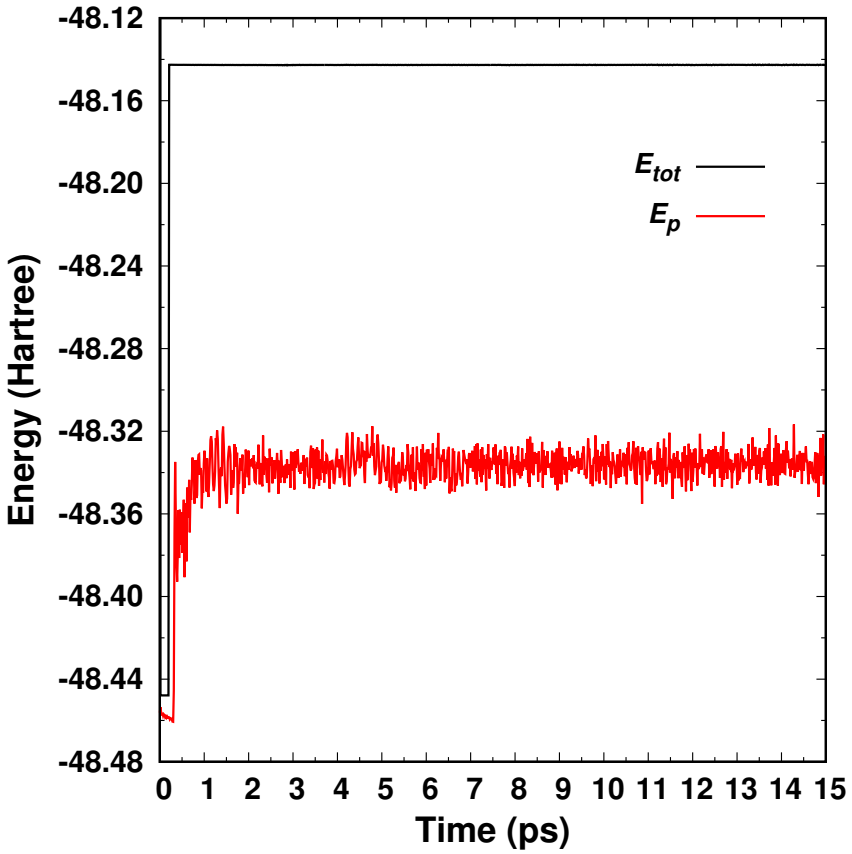

Figure S23 Total energy E_{tot} (black line) and potential energy E_p (red line) of a random selected trajectory of isomer 7d.

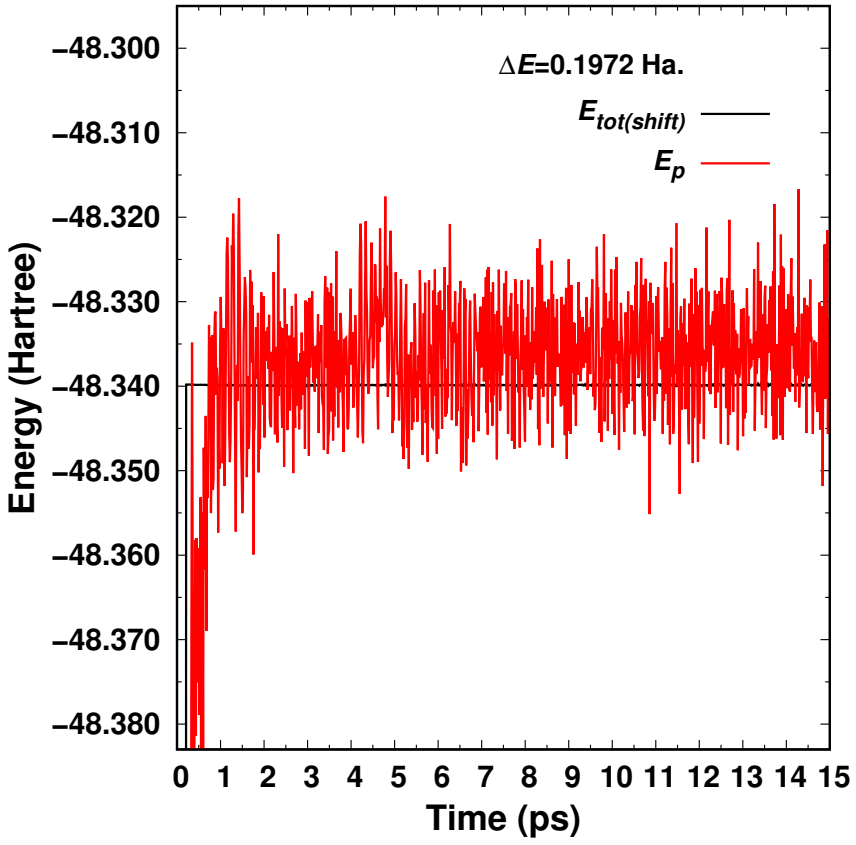

Figure S24 Shifted total energy $E_{tot(shift)}$ (black line), pan down 0.1972 Hartree of the total energy, and potential energy E_p (red line) of a the same randomly selected trajectory of isomer 7d than presented in Figure S23.

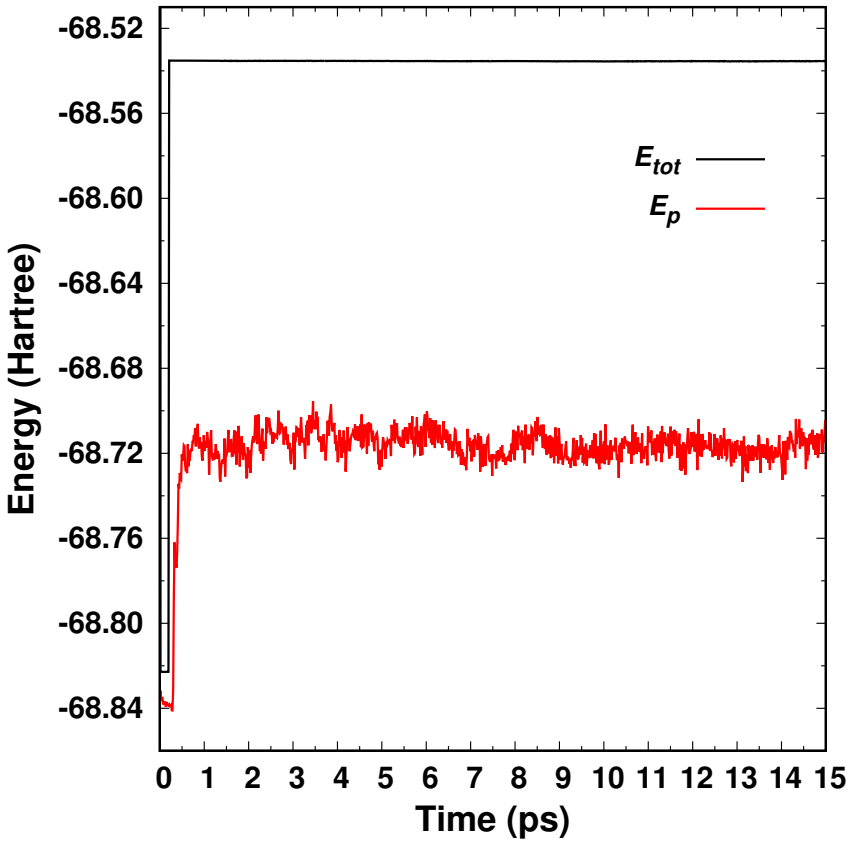

Figure S25 Total energy E_{tot} (black line) and potential energy E_p (red line) of a random selected trajectory of isomer 12c.

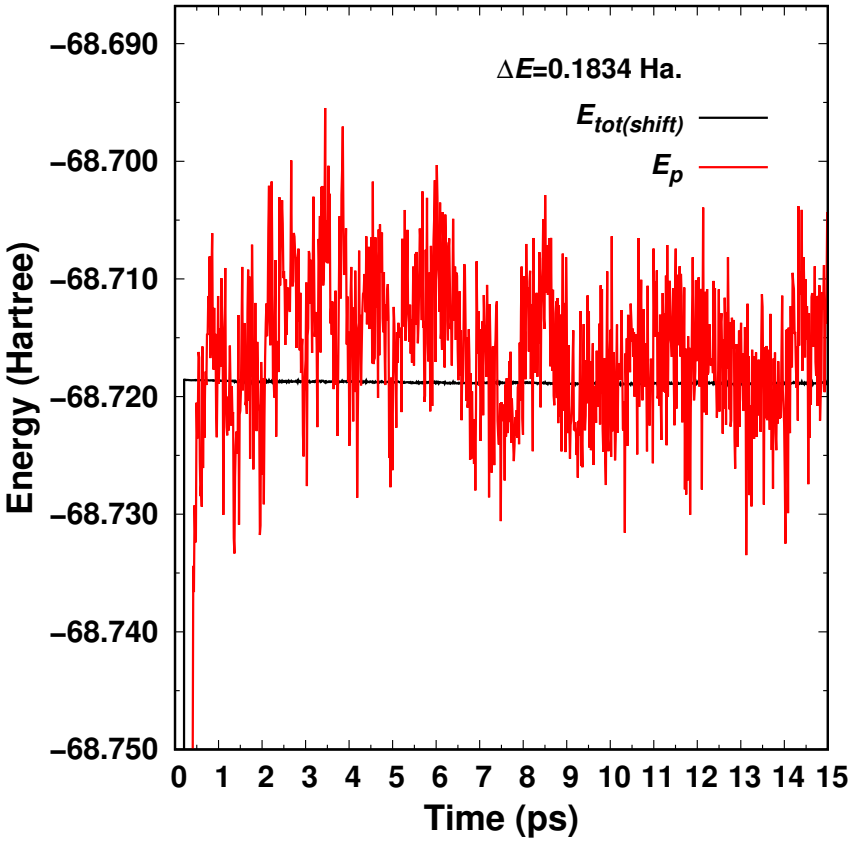

Figure S26 Shifted total energy $E_{tot(shift)}$ (black line), pan down 0.1834 Hartree of the total energy, and potential energy E_p (red line) of a the same randomly selected trajectory of isomer 12c than presented in Figure S25.

7 Influence of Equilibration Time prior to Collision

Table S5 P_{PU} (in %), P_{NUL} (in %), σ_{frag} (in Å^2) of the first low-energy isomers of $(H_2O)_{1-7,11,12}UH^+$ clusters obtained from simulations consisting in 200 initial random orientations per impact parameter. $t_{0.2ps}$ designates simulations with an equilibration time prior to collision of 0.2 ps. t_{2ps} designates simulations with an equilibration time prior to collision of 2.0 ps. $P_{NUL_{exp}}$ and $\sigma_{frag_{exp}}$ are the experimental values for P_{NUL} and σ_{frag}, respectively. For $(H_2O)_{12}UH^+$, experimental values were obtained for collision with Ne, whereas all other theoretical and experimental data are for collision with Ar.

Isomers	Simu	$t_{0.2ps}$ P_{PU}	t_{2ps} P_{PU}	$t_{0.2ps}$ P_{NUL}	t_{2ps} P_{NUL}	$P_{NUL_{exp}}$	$t_{0.2ps}$ σ_{frag}	t_{2ps} σ_{frag}	$\sigma_{frag_{exp}}$
1a	200	100	100	0.1	0.5	0.9	28.4	29.0	12.3
2a	200	100	100	0.0	0.4	0.4	35.9	37.4	22.8
3a	200	100	100	5.4	6.7	1.7	37.4	38.53	31.2
4a	200	98.2	99.2	26.9	28.7	2.8	40.1	43.5	43.4
5a	200	79.3	78.5	45.7	43.0	7.5	37.2	39.9	48.0
6a	200	43.3	43.6	38.0	38.4	18.0	46.6	48.4	54.3
7a	200	27.1	30.1	29.5	31.9	18.0	54.8	57.6	54.3
11a	200	4.2	4.9	26.7	29.9	11.8	53.8	56.6	63.8
12a	200	6.45	6.34	8.0	9.0	12.2	59.2	65.1	77.0

8 Coordinates of Isomers

Table S6 Optimized Cartesian coordinates of 1a at MP2/Def2TZVP level. Electronic energy is equal to -490.77283 Hartree.

Symbol	x	y	z
H	26.294494	28.036899	25.037455
H	24.003324	24.527660	24.958922
C	24.956798	25.032176	24.976864
C	25.052011	26.392772	24.998859
H	24.175839	27.029868	24.999342
C	26.163160	24.304111	24.978498
O	26.274285	23.018341	24.959860
N	27.324587	24.976727	25.001251
H	25.375313	22.542648	24.942934
C	27.473791	26.372392	25.024363
O	28.539373	26.922788	25.044210
N	26.242384	27.023141	25.021269
H	28.193913	24.445535	25.002328
O	23.994477	21.850593	24.917577
H	23.716709	21.322401	25.678546
H	23.733027	21.346170	24.135006

Table S7 Optimized Cartesian coordinates of 1b at MP2/Def2TZVP level. Electronic energy is equal to -490.771635 Hartree.

Symbol	x	y	z
H	28.236659	24.392567	24.962164
H	24.044319	24.465897	25.072636
C	24.991893	24.980172	25.035482
C	25.086867	26.338845	25.001751
H	24.212764	26.978391	25.010451
C	26.193199	24.249964	25.020112
O	26.170478	22.955644	25.050439
N	27.359822	24.915408	24.973627
H	27.092155	22.559874	25.034880
C	27.507072	26.315257	24.937549
O	28.577818	26.856582	24.896475
N	26.281390	26.967126	24.955378
H	26.334709	27.980579	24.930681
O	28.700103	22.261830	24.998700
H	29.082209	21.818365	24.227516
H	29.123465	21.853775	25.767887

Table S8 Optimized Cartesian coordinates of 2a at MP2/Def2TZVP level. Electronic energy is equal to -567.1110192 Hartree.

Symbol	x	y	z
H	23.673322	21.309237	25.752543
H	23.941239	24.468078	24.988674
C	24.878672	25.002026	24.989286
C	24.932166	26.363355	24.987704
H	24.039552	26.976791	24.985793
C	26.111194	24.312555	24.991572
O	26.244471	23.023508	24.993169
N	27.252205	25.005072	24.992682
H	28.177017	24.512233	24.989934
C	27.350760	26.397493	24.990090
O	28.402117	26.986107	24.989218
N	26.108002	27.023644	24.988437
H	26.136777	28.037799	24.986487
O	29.812927	24.203270	24.939298
H	30.379835	24.984769	24.957918
H	25.355755	22.545386	24.990294
O	23.947394	21.827128	24.983768
H	30.388918	23.435867	25.029532
H	23.680167	21.312433	24.210435

Table S9 Optimized Cartesian coordinates of 2b at MP2/Def2TZVP level. Electronic energy is equal to -567.1107287 Hartree.

Symbol	x	y	z
H	31.204769	25.237452	25.198863
H	24.086648	24.436308	25.034415
C	25.012376	24.992349	25.020860
C	25.035931	26.351639	25.002975
H	24.148047	26.969434	25.001032
C	26.268597	24.336662	25.019603
O	26.301813	23.032339	25.033970
N	27.420983	24.998925	25.004394
H	29.914706	24.364238	25.043870
C	27.393606	26.318633	24.986171
O	28.477991	27.023833	24.969020
N	26.230252	27.006147	24.985285
H	26.274384	28.020376	24.969037
O	30.300421	25.235670	24.863550
H	29.274416	26.380928	24.956184
H	29.168496	21.632783	25.698177
O	28.923885	22.257605	25.000758
H	27.252632	22.730555	25.025325
H	29.193287	21.826412	24.177190

Table S10 Optimized Cartesian coordinates of 3a at MP2/Def2TZVP level. Electronic energy is equal to -643.4491802 Hartree.

Symbol	x	y	z
H	29.310188	22.306065	24.923478
H	24.239998	24.526356	25.202060
C	25.175725	25.047598	25.073131
C	25.239164	26.384857	24.850351
H	24.356565	27.009526	24.795380
C	26.393007	24.326916	25.114568
O	26.377267	23.060161	25.301663
N	27.549142	25.004679	24.961316
H	28.470518	24.534531	25.086758
C	27.649426	26.374411	24.710414
O	28.709266	26.937908	24.548792
N	26.427375	27.013803	24.671460
H	26.466925	28.011875	24.496530
O	28.465819	21.851053	24.725925
H	31.815325	25.713749	23.009190
H	27.278597	22.554068	25.127878
O	31.002258	25.514327	23.486126
H	30.596359	24.401704	24.637116
H	30.541070	26.350974	23.639913
O	30.088099	23.872809	25.308592
H	28.576827	20.898372	24.825121
H	30.558667	23.980226	26.145316

Table S11 Optimized Cartesian coordinates of 3b at MP2/Def2TZVP level. Electronic energy is equal to -643.4487627 Hartree.

Symbol	x	y	z
H	29.334994	26.311976	25.041431
H	24.100090	24.540399	24.934385
C	25.043103	25.065954	24.957114
C	25.116305	26.425975	24.962076
H	24.251153	27.075541	24.943887
C	26.274604	24.372256	24.981758
O	26.269154	23.062719	24.975613
N	27.446333	24.997232	25.010942
H	27.209331	22.739933	24.989133
C	27.455945	26.319643	25.013657
O	28.572064	26.983728	25.040149
N	26.323408	27.047036	24.990019
H	26.369407	28.084355	24.990071
O	28.897553	22.220097	24.999887
H	29.105311	21.568730	25.684487
H	29.177748	21.806023	24.171425
O	30.333554	25.100955	24.961699
H	29.887496	24.252037	25.109637
H	31.217022	25.040256	25.342928
O	26.042846	29.769393	24.971371
H	26.131360	30.348279	25.738479
H	26.183501	30.335346	24.202351

Table S12 Optimized Cartesian coordinates of 4a at MP2/Def2TZVP level. Electronic energy is equal to -719.7870304 Hartree.

Symbol	x	y	z
H	29.987210	25.683685	25.020579
H	24.031466	24.491626	25.082263
C	24.981777	25.001190	25.045088
C	25.067066	26.350638	25.036919
H	24.194149	26.990088	25.064412
C	26.189893	24.227622	25.013927
O	26.221831	22.987179	25.049492
N	27.354300	24.960691	24.938645
H	28.245004	24.470037	24.858252
C	27.475745	26.339039	24.959805
O	28.554054	26.910358	24.946028
N	26.271259	26.995071	25.000809
H	26.323723	28.006011	25.012032
O	27.560898	19.127225	26.295373
H	27.776876	18.344608	25.773968
H	26.810242	18.887530	26.851699
O	29.704103	22.919690	26.892424
H	30.278778	22.711706	27.637068
H	28.840218	21.960694	26.109492
O	30.272501	24.747283	25.000758
H	30.133815	23.616720	26.351377
H	30.989026	24.694736	24.356464
O	28.188715	21.493264	25.474265
H	27.907847	20.585835	25.802159
H	27.378981	22.110175	25.284398

Table S13 Optimized Cartesian coordinates of 4b at MP2/Def2TZVP level. Electronic energy is equal to -719.7856381 Hartree.

Symbol	x	y	z
H	27.222070	22.640488	24.853616
H	24.160856	24.535037	25.183568
C	25.090987	25.079448	25.139397
C	25.145079	26.438478	25.109414
H	24.257786	27.059100	25.135728
C	26.313620	24.377925	25.089772
O	26.318135	23.093081	25.097967
N	27.460703	25.086390	25.043510
H	28.383373	24.614056	25.112222
C	27.540332	26.481141	24.991509
O	28.600910	27.068982	24.922408
N	26.317187	27.105841	25.032478
H	26.304938	28.139002	25.003253
O	30.913325	25.862524	23.756531
H	25.872066	30.407982	25.737356
H	31.726014	26.215071	23.378801
O	25.760276	29.805949	24.991508
H	25.757189	30.367734	24.206938
H	30.479889	23.912954	26.136520
O	30.030657	23.929326	25.281990
H	30.365934	26.612675	24.034114
H	30.541335	24.564876	24.713834
O	28.441253	22.021176	24.344300
H	28.570000	21.067963	24.281579
H	29.274565	22.447499	24.631855

Table S14 Optimized Cartesian coordinates of 5a at MP2/Def2TZVP level. Electronic energy is equal to -796.125622 Hartree.

Symbol	x	y	z
H	31.014571	25.368894	23.406352
H	24.100728	24.467433	24.759873
C	25.032332	25.005663	24.844897
C	25.069039	26.352630	24.923150
H	24.177068	26.965373	24.906981
C	26.266917	24.263104	24.870489
O	26.358566	23.039817	24.780676
N	27.410500	25.046505	25.013215
H	28.299488	24.558423	25.131701
C	27.474054	26.417350	25.058884
O	28.529996	27.038022	25.131768
N	26.254033	27.034732	25.020082
H	26.272254	28.045515	25.059552
O	29.585573	23.032666	21.953247
H	29.693787	22.681090	21.062363
H	29.135956	22.354057	22.496869
O	30.644033	26.761579	23.473776
H	29.929615	26.976214	24.114455
H	31.292932	27.474252	23.493960
O	29.939546	23.345607	25.459698
H	30.269029	23.185051	26.353400
H	29.526199	22.508977	25.140541
O	31.196249	24.341098	23.405722
H	30.885407	23.968899	24.282779
H	30.629901	23.858859	22.705744
O	28.482504	21.591730	24.051409
H	28.344769	20.637738	24.112285
H	27.623053	22.017027	24.299312

Table S15 Optimized Cartesian coordinates of 5b at MP2/Def2TZVP level. Electronic energy is equal to -796.1251968 Hartree.

Symbol	x	y	z
H	28.549578	22.410509	23.117682
H	24.055962	24.567324	24.805097
C	25.031829	25.019904	24.892841
C	25.193691	26.359551	24.958582
H	24.362268	27.052066	24.933920
C	26.193798	24.175072	24.915489
O	26.168524	22.943898	24.798547
N	27.399018	24.837712	25.084270
H	28.239274	24.276390	25.251965
C	27.593359	26.199645	25.099125
O	28.703900	26.716610	25.155703
N	26.436104	26.928329	25.045869
H	26.549382	27.933973	25.064469
O	29.972691	23.546077	25.956355
H	30.106412	23.845833	26.865453
H	30.538612	24.121169	25.401179
O	29.211168	23.632973	22.413401
H	29.357732	23.655948	21.460919
H	29.851092	24.247132	22.829094
O	29.650514	20.877917	25.405700
H	30.062407	21.688745	25.758001
H	30.288899	20.156895	25.427405
O	28.062031	21.698082	23.645458
H	27.294848	22.146557	24.151563
H	28.709816	21.265715	24.312920
O	30.734840	25.316421	24.012086
H	30.114762	25.992609	24.369423
H	31.546559	25.781357	23.772541

Table S16 Optimized Cartesian coordinates of 5c at MP2/Def2TZVP level. Electronic energy is equal to -796.1224153 Hartree.

Symbol	x	y	z
H	30.067484	22.349930	24.178715
H	24.013222	24.466874	25.101273
C	24.953020	24.996170	25.078364
C	25.011124	26.345679	25.078343
H	24.127598	26.970557	25.100340
C	26.176819	24.242738	25.049748
O	26.215497	23.005219	25.042998
N	27.335688	24.991958	25.033185
H	28.236485	24.497385	25.046997
C	27.423314	26.370759	25.019297
O	28.480883	26.978212	24.988486
N	26.205377	27.006497	25.047774
H	26.243856	28.017592	25.041518
O	27.627627	20.910523	24.841951
H	27.113152	21.782133	24.927993
H	27.074370	20.210138	24.386157
O	30.830953	25.982714	23.887717
H	30.154683	26.605817	24.206132
H	31.639472	26.481848	23.732637
O	30.057122	23.799252	25.088790
H	30.433279	23.751778	25.977088
H	30.501224	24.577292	24.651164
O	29.762872	21.523874	23.730831
H	30.526384	20.954010	23.586799
H	28.533092	21.075865	24.357416
O	26.281506	19.007429	23.710992
H	25.957291	18.247961	24.209408
H	25.762984	19.046260	22.899009

Table S17 Optimized Cartesian coordinates of 5d at MP2/Def2TZVP level. Electronic energy is equal to -796.1217798 Hartree.

Symbol	x	y	z
H	29.556586	22.922527	26.364223
H	24.143285	24.478148	24.903351
C	25.072061	25.027802	24.935910
C	25.110457	26.386356	24.965506
H	24.232310	27.018197	24.959447
C	26.318488	24.353980	24.945599
O	26.313241	23.052824	24.912304
N	27.483637	25.004039	24.986468
H	31.473637	25.948723	25.319898
C	27.453874	26.324568	25.016789
O	28.541948	27.038181	25.060059
N	26.305479	27.028849	25.005263
H	26.330381	28.063025	25.029932
O	29.992157	23.630737	26.873020
H	29.356543	26.433636	25.093269
H	27.254905	22.690807	24.901091
O	30.013096	23.592440	23.121341
H	30.378481	24.341271	23.624249
H	30.627335	23.409602	22.402077
O	30.631559	25.508172	25.147040
H	30.469175	23.207018	27.594807
H	30.502238	24.834888	25.871385
O	25.902135	29.751898	25.059251
H	25.955059	30.313522	25.842039
H	25.990011	30.349001	24.306437
O	28.744976	22.069112	24.871025
H	28.802983	21.117520	24.715748
H	29.247405	22.513684	24.137092

Table S18 Optimized Cartesian coordinates of 6a at MP2/Def2TZVP level. Electronic energy is equal to -872.4593536 Hartree.

Symbol	x	y	z
H	33.452909	25.090349	20.389350
H	24.097060	24.537649	24.789243
C	25.035927	25.063832	24.868963
C	25.090248	26.410429	24.951716
H	24.205306	27.033571	24.944536
C	26.262688	24.307593	24.882951
O	26.340715	23.083126	24.776004
N	27.414809	25.073079	25.031235
H	28.296236	24.568160	25.165651
C	27.497732	26.444470	25.072084
O	28.560205	27.053759	25.128376
N	26.283006	27.078035	25.040211
H	26.315133	28.088399	25.079292
O	29.205554	23.027678	21.486326
H	28.923088	22.519546	22.276948
H	28.620219	22.781907	20.762036
O	28.509310	21.806873	23.860763
H	27.656405	22.169668	24.212880
H	28.436905	20.845022	23.908111
O	30.706945	25.787758	23.999590
H	30.034423	26.381733	24.404711
H	30.671709	24.971883	24.538787
O	30.404889	25.287297	21.628514
H	30.546431	25.528614	22.669763
H	29.941999	24.393602	21.529140
O	32.572868	25.421371	20.176122
H	32.695665	26.118875	19.521564
H	31.253728	25.320232	21.105393
O	29.929566	23.553996	25.410123
H	30.254249	23.283576	26.277945
H	29.637378	22.739125	24.949875

Table S19 Optimized Cartesian coordinates of 6b at MP2/Def2TZVP level. Electronic energy is equal to -872.4589692 Hartree.

Symbol	x	y	z
H	30.259138	24.364446	20.928069
H	24.020577	24.507524	25.099527
C	24.965701	25.024872	25.039532
C	25.035088	26.370730	24.956770
H	24.157507	27.004135	24.947506
C	26.183597	24.256384	25.036240
O	26.243516	23.026600	25.079696
N	27.350157	25.009848	24.987271
H	28.237818	24.505564	25.078064
C	27.444732	26.375836	24.877086
O	28.509004	26.978864	24.793207
N	26.236046	27.021493	24.870174
H	26.279854	28.029287	24.793781
O	27.421477	21.317376	23.444848
H	28.529838	21.650494	23.370974
H	26.933821	21.877620	24.100232
O	26.971490	18.741816	23.788186
H	27.266564	20.353168	23.618706
H	26.483805	18.216099	23.144123
O	29.978664	24.241116	21.841356
H	27.222592	18.140905	24.498220
H	30.401898	24.943720	22.368975
O	30.849796	25.925977	23.922316
H	30.072589	26.460241	24.204554
H	31.614648	26.513812	23.952651
O	30.051060	23.787739	25.377058
H	30.578889	24.533319	25.013321
H	30.373554	23.628780	26.272924
O	29.696779	22.063546	23.304280
H	29.819629	22.774292	22.618570
H	29.945721	22.505337	24.146948

Table S20 Optimized Cartesian coordinates of 6c at MP2/Def2TZVP level. Electronic energy is equal to -872.4589455 Hartree.

Symbol	x	y	z
H	33.256113	28.811894	24.266165
H	24.098032	24.410678	24.678200
C	25.022738	24.956747	24.785278
C	25.047914	26.304446	24.848412
H	24.153098	26.911092	24.797533
C	26.261493	24.222573	24.857577
O	26.360347	22.998872	24.786687
N	27.395847	25.014206	25.024269
H	28.286694	24.532353	25.169003
C	27.448097	26.385053	25.058420
O	28.495713	27.015934	25.159771
N	26.225262	26.994683	24.974411
H	26.236924	28.005569	25.004588
O	31.181185	24.494116	23.468657
H	30.945549	25.603286	23.473646
H	30.649416	23.995535	22.776594
O	29.572430	23.090785	22.004100
H	29.162808	22.388480	22.545997
H	29.659402	22.752202	21.106393
O	32.554938	28.678253	23.619069
H	32.725074	29.302310	22.904645
H	29.533805	22.539625	25.189947
O	30.622991	26.833655	23.490305
H	29.906844	27.025212	24.134107
H	31.339954	27.505603	23.576396
O	29.897828	23.389944	25.528443
H	30.198457	23.231077	26.432040
H	30.894618	24.095568	24.329329
O	28.523629	21.572737	24.099214
H	27.653194	21.978061	24.335355
H	28.407451	20.616203	24.157565

Table S21 Optimized Cartesian coordinates of 6d at MP2/Def2TZVP level. Electronic energy is equal to -872.4578704 Hartree.

Symbol	x	y	z
H	29.978188	29.229288	26.092945
H	24.581259	24.746107	26.498289
C	25.543164	25.040797	26.106954
C	25.999605	26.304608	26.220971
H	25.435740	27.090769	26.705903
C	26.367446	24.045073	25.466861
O	26.087871	22.858591	25.340604
N	27.584686	24.539408	24.971397
H	28.193865	23.860209	24.515261
C	28.053912	25.815117	25.076651
O	29.154948	26.163841	24.626452
N	27.221228	26.679921	25.719598
H	27.590504	27.611855	25.882329
O	31.293066	24.523346	24.346157
H	30.167608	26.436435	28.803497
H	29.948866	21.412228	27.607315
O	31.225096	24.181715	26.858650
H	31.369506	24.335489	25.863703
H	30.636511	23.337747	26.977815
O	29.568133	28.360872	26.189120
H	27.492103	21.853246	24.893417
H	32.019186	24.667031	23.729119
O	29.738390	22.184368	27.070650
H	29.300948	21.873442	26.241352
H	29.712528	27.876267	25.356230
O	30.047192	26.226112	27.870000
H	30.784367	24.997506	27.270540
H	29.974634	27.079073	27.391279
O	28.461279	21.747971	24.761063
H	30.582474	25.167101	24.152435
H	28.587550	21.035737	24.122792

Table S22 Optimized Cartesian coordinates of 6e at MP2/Def2TZVP level. Electronic energy is equal to -872.4553511 Hartree.

Symbol	x	y	z
H	30.863119	21.346506	29.380512
H	23.979347	24.492890	24.554268
C	24.910156	25.029307	24.654120
C	24.959774	26.378558	24.631758
H	24.078675	26.995808	24.512503
C	26.130464	24.284384	24.823406
O	26.192454	23.052600	24.868811
N	27.278989	25.051361	24.928517
H	28.177387	24.556434	24.981783
C	27.355548	26.427351	24.920030
O	28.401637	27.048358	25.035473
N	26.141659	27.051844	24.765563
H	26.171811	28.062863	24.755068
O	26.655391	18.739316	25.156404
H	27.104676	20.224667	25.708607
H	26.001861	18.185880	25.599052
O	27.384461	21.089106	26.108758
H	26.949106	21.843316	25.623651
H	28.507219	21.226406	26.157177
O	29.984830	23.822726	24.986114
H	30.391564	23.775027	24.111492
H	30.416191	24.595816	25.442068
O	30.680035	26.014651	26.230308
H	31.475890	26.539126	26.366287
H	29.995344	26.611125	25.874599
O	31.094121	21.071667	28.486386
H	31.808059	20.430945	28.579362
H	26.729766	18.404265	24.255824
O	29.763142	21.433126	26.175055
H	30.225710	21.317418	27.036457
H	29.980805	22.321560	25.801523

Table S23 Optimized Cartesian coordinates of 6f at MP2/Def2TZVP level. Electronic energy is equal to -872.4551165 Hartree.

Symbol	x	y	z
H	30.695793	20.931623	26.172193
H	24.126474	24.463034	24.982417
C	25.066838	24.991570	24.975421
C	25.131232	26.342857	25.004585
H	24.250885	26.972439	25.037212
C	26.287417	24.241084	24.930597
O	26.327227	23.000453	24.904126
N	27.443774	24.991340	24.914512
H	28.342042	24.499062	24.849367
C	27.528641	26.372576	24.956002
O	28.594791	26.972224	24.951615
N	26.318036	27.008764	24.997229
H	26.319181	28.035167	25.025493
O	27.763707	20.940754	24.973922
H	27.242196	21.820302	24.938397
H	27.220504	20.225031	25.414536
O	30.968639	25.963358	25.913431
H	30.248300	26.557695	25.631290
H	31.768742	26.491956	25.996405
O	25.738551	29.749185	25.071614
H	25.805314	30.344243	24.315470
H	25.813912	30.315600	25.848602
O	26.433675	18.997650	26.073953
H	26.093826	18.258986	25.555181
H	25.899950	19.038006	26.875966
O	29.930580	21.506276	26.061134
H	30.224250	22.335912	25.612394
H	28.676451	21.082071	25.445458
O	30.178182	23.788457	24.714058
H	30.632805	24.566688	25.140885
H	30.513764	23.754376	23.809358

Table S24 Optimized Cartesian coordinates of 7a at MP2/Def2TZVP level. Electronic energy is equal to -948.7923666 Hartree.

Symbol	x	y	z
H	30.213970	26.348420	25.840746
H	24.100219	24.323774	25.466091
C	25.022915	24.881795	25.422272
C	25.068602	26.197279	25.729948
H	24.192638	26.758905	26.028395
C	26.234951	24.215825	25.030323
O	26.310568	23.013840	24.725747
N	27.364739	25.004061	25.001303
H	28.250895	24.567237	24.704236
C	27.445642	26.340030	25.337219
O	28.486083	26.976378	25.327362
N	26.237040	26.899463	25.685744
H	26.267324	27.880983	25.929649
O	24.507767	21.104043	25.555375
H	27.431396	19.629797	26.844532
H	25.041633	21.804203	25.128747
O	28.586784	21.452764	24.835460
H	25.636510	19.535060	28.009252
H	29.290900	22.130162	24.780690
O	25.978581	19.519185	27.108960
H	29.185196	16.824119	25.195352
H	23.909501	20.760601	24.882775
O	28.426930	19.726836	26.595321
H	28.541693	20.470709	25.858659
H	30.166409	16.988837	26.377495
O	29.919841	23.795400	24.378596
H	30.305856	23.870545	23.497138
H	30.456075	24.391420	24.960823
O	29.504890	17.453030	25.851967
H	28.803110	18.855526	26.294777
H	27.760332	21.964135	24.707086
O	30.860363	25.640996	26.009025
H	25.374020	20.073398	26.552612
H	31.690155	26.062249	26.255428

Table S25 Optimized Cartesian coordinates of 7b at MP2/Def2TZVP level. Electronic energy is equal to -948.7918168 Hartree.

Symbol	x	y	z
H	31.334712	25.952683	23.968954
H	24.077994	24.634683	24.687460
C	25.040241	25.114321	24.781599
C	25.162527	26.457126	24.863434
H	24.314102	27.129052	24.840263
C	26.225771	24.297831	24.816481
O	26.260638	23.073807	24.738569
N	27.416371	25.018988	24.960959
H	28.266610	24.460188	25.058761
C	27.545978	26.379028	25.031302
O	28.637922	26.955166	25.138759
N	26.380214	27.071303	24.977389
H	26.423967	28.096478	25.031653
O	27.729370	21.324127	23.206129
H	27.168268	21.873561	23.789001
H	27.189725	20.579329	22.922068
O	30.290704	21.730176	23.492441
H	30.088038	23.128010	26.336663
H	30.810468	20.921953	23.585396
O	30.026700	23.526241	25.458901
H	30.841051	22.860584	22.141805
H	30.190509	22.797308	24.805248
O	31.803095	25.923204	22.626596
H	31.601360	25.076529	22.150450
H	30.791599	23.431358	20.691120
O	25.925454	29.823564	25.111141
H	26.039071	30.456803	24.392606
H	25.959308	30.347032	25.920597
O	31.135593	23.598479	21.574494
H	32.712805	26.170516	22.426617
H	29.344205	21.447262	23.349634
O	30.933670	25.913178	24.940428
H	30.757526	24.959779	25.185838
H	30.022650	26.379753	24.997623

Table S26 Optimized Cartesian coordinates of 7c at MP2/Def2TZVP level. Electronic energy is equal to -948.7918098 Hartree.

Symbol	x	y	z
H	31.037792	27.405512	27.045191
H	24.111597	24.408355	24.849881
C	25.027895	24.973141	24.928443
C	25.022915	26.317250	25.051556
H	24.111860	26.900913	25.078987
C	26.288227	24.271857	24.898630
O	26.432086	23.054719	24.808156
N	27.411357	25.093918	24.976278
H	28.319882	24.628069	24.876903
C	27.428967	26.453516	25.136379
O	28.459320	27.111967	25.249846
N	26.186953	27.032046	25.157443
H	26.173996	28.037446	25.265278
O	26.632369	18.902955	27.282236
H	28.513947	21.935191	26.913169
H	26.062856	18.588206	27.992903
O	29.830400	24.475970	28.255304
H	27.023199	20.555935	27.019326
H	30.206709	25.257371	27.798073
O	27.231306	21.511961	26.922559
H	29.777537	23.018507	23.711520
H	26.924121	18.118203	26.805754
O	29.523899	22.329358	26.863914
H	29.653015	23.123680	27.474810
H	30.728934	23.976303	24.533890
O	32.048134	24.863785	24.939797
H	32.787100	25.147265	24.391673
H	31.794592	25.617738	25.504901
O	29.853853	23.499224	24.545477
H	29.703105	22.657613	25.935045
H	30.176111	24.479924	29.154704
O	30.707866	26.583621	26.660834
H	26.751491	21.868736	26.150814
H	29.913380	26.836467	26.134753

Table S27 Optimized Cartesian coordinates of 7d at MP2/Def2TZVP level. Electronic energy is equal to -948.7910496 Hartree.

Symbol	x	y	z
H	29.828154	25.691022	26.850259
H	23.880589	24.229406	25.631316
C	24.756551	24.839212	25.470852
C	24.687721	26.188748	25.425310
H	23.757316	26.729229	25.543663
C	26.034295	24.197450	25.315501
O	26.240742	22.984883	25.384163
N	27.090921	25.071703	25.062723
H	27.990813	24.648261	24.815423
C	27.035969	26.438688	25.073795
O	28.044130	27.148191	24.941462
N	25.796711	26.966457	25.242004
H	25.745077	27.995247	25.250302
O	31.698714	25.096333	24.770099
H	31.139963	24.456836	24.292520
H	32.402961	25.434229	24.174510
O	33.698243	25.922597	23.145196
H	28.684861	21.331745	26.704230
H	33.769267	26.725758	22.617582
O	28.614618	22.233270	26.366389
H	29.379774	22.854761	24.825447
H	27.681735	22.351593	26.057796
O	29.143619	24.584491	27.738191
H	29.010742	23.671732	27.406211
H	29.273614	23.129529	23.302122
O	26.048956	29.728811	25.271682
H	26.967484	29.943087	25.069322
H	25.547785	30.541654	25.142148
O	29.494821	23.549556	24.143313
H	29.292215	24.527184	28.688676
H	34.603115	25.628965	23.300928
O	30.169961	26.370090	26.186623
H	30.875583	25.889292	25.543649
H	29.377922	26.706281	25.657737

Table S28 Optimized Cartesian coordinates of 11a at MP2/Def2TZVP level. Electronic energy is equal to -1254.1378075 Hartree.

Symbol	x	y	z
H	-2.192111	1.574206	3.394751
H	-0.712661	-1.607888	-4.856904
C	-0.975155	-0.828161	-4.158729
C	-1.379040	0.390583	-4.576034
H	-1.463613	0.654691	-5.622255
C	-0.889457	-1.096024	-2.744139
O	-0.519654	-2.164291	-2.254641
N	-1.274590	-0.045167	-1.926936
H	-0.670778	1.223605	3.474920
C	-1.650182	1.211825	-2.325004
O	-1.923061	2.117367	-1.545431
N	-1.703468	1.378335	-3.686867
H	-1.986738	2.295982	-4.003409
O	-0.656437	3.090289	0.709114
H	-0.254750	-3.486481	1.066632
H	2.263245	-2.813842	0.294755
O	1.783235	2.574897	0.599335
H	3.071792	3.098666	3.563461
H	2.175373	-0.555405	0.187875
O	-0.708817	-3.081678	1.837347
H	-1.363345	-3.721924	2.140237
H	2.154963	2.625528	1.535421
O	-0.985669	-0.496360	0.872856
H	0.629883	-2.237494	2.937559
H	2.069499	1.885160	3.595620
O	-1.410052	1.413703	2.853160
H	-1.256090	-0.208107	-0.910581
H	0.879301	-4.485610	-0.830641
O	1.533179	0.150761	-0.018099
H	0.776739	2.853640	0.623831
H	0.318918	-3.062641	-1.081405
O	2.636188	2.436596	3.017036
H	-1.078060	-1.400831	1.235018
H	-1.293932	0.112277	1.573992
O	0.769782	-3.625106	-0.406440
H	-1.172573	2.807429	-0.073608
H	1.788122	1.581285	0.323859
O	0.857838	0.701911	4.237683
H	1.075610	-0.198085	3.859694
H	0.881479	0.587097	5.196102
O	1.368147	-1.664155	3.206699
H	2.054163	-1.825962	2.536739
H	-1.049875	2.641344	1.480348
O	2.830476	-2.178324	0.779355
H	3.741661	-2.466261	0.648798
H	0.680866	-0.145737	0.369727

Table S29 Optimized Cartesian coordinates of 11b at MP2/Def2TZVP level. Electronic energy is equal to -1254.135561 Hartree.

Symbol	x	y	z
H	-3.166836	2.630893	-1.348966
H	-1.970295	-4.083452	2.941055
C	-1.703753	-3.038986	2.988485
C	-2.071997	-2.257704	4.025697
H	-2.650122	-2.627033	4.862910
C	-0.930346	-2.465886	1.915319
O	-0.543582	-3.093215	0.927489
N	-0.633709	-1.118415	2.055896
H	0.242356	2.084433	2.188189
C	-0.998233	-0.302589	3.102009
O	-0.708456	0.883318	3.177949
N	-1.729520	-0.935297	4.078527
H	-2.004297	-0.353760	4.858887
O	0.751584	2.462521	1.442851
H	1.650833	-0.858025	-3.767801
H	3.822805	-1.562398	-0.666085
O	2.372698	-0.219838	-3.638920
H	0.437914	-3.146713	-0.436243
H	2.830575	-0.537679	-2.842566
O	1.153760	4.291422	-2.073100
H	1.893753	4.905626	-2.112287
H	0.991199	1.668701	0.913850
O	1.220608	2.147370	-3.779928
H	1.161822	2.406111	-4.707916
H	1.715410	-0.268226	-0.319953
O	-2.311160	2.389582	-0.978945
H	-0.088686	-0.678365	1.299306
H	1.334434	3.555516	-2.694809
O	-0.455397	3.943508	-0.096051
H	0.177871	4.139926	-0.856091
H	1.796271	1.334570	-3.756628
O	2.971481	-1.359382	-1.071568
H	2.459297	-2.195337	-1.092743
H	0.049448	3.325683	0.621294
O	-0.036075	-1.809901	-3.361454
H	-0.528738	-2.327757	-4.009164
H	1.124241	-4.217990	-1.323671
O	0.996145	-3.264037	-1.244792
H	-1.918706	1.696978	-1.551199
H	-1.240874	3.425902	-0.459271
O	0.896221	0.181692	-0.028106
H	0.383452	0.364231	-0.846660
H	0.228281	-2.436522	-2.653058
O	-0.634018	0.703178	-2.297098
H	-0.114473	1.256912	-2.917937
H	-0.655985	-0.183342	-2.710828

Table S30 Optimized Cartesian coordinates of 11c at MP2/Def2TZVP level. Electronic energy is equal to -1254.135348 Hartree.

Symbol	x	y	z
H	1.004311	-0.239102	3.578099
H	1.714074	-1.187932	-4.234983
C	1.496665	-0.265525	-3.718981
C	1.728993	0.937932	-4.290291
H	2.146674	1.045508	-5.283162
C	0.931377	-0.311185	-2.399304
O	0.653911	-1.357819	-1.787333
N	0.695111	0.908934	-1.807135
H	-0.163393	1.997871	1.019266
C	0.910273	2.145257	-2.370009
O	0.661292	3.202540	-1.808014
N	1.438496	2.100406	-3.639119
H	1.608912	2.999209	-4.071743
O	-0.908135	-3.195858	1.872837
H	1.111130	0.260690	2.102624
H	-1.279294	-2.950630	1.005763
O	-0.764230	3.678892	0.502609
H	-0.268513	3.686962	-0.342526
H	-0.920562	-1.825107	-1.062847
O	2.514088	-2.874746	-0.379044
H	-2.246386	-2.607962	-1.262520
H	-2.640578	-0.858126	2.720166
O	-0.001262	1.039334	0.904673
H	-0.878071	0.621319	1.076835
H	0.592514	-2.930818	1.990744
O	1.576122	-2.661572	2.046565
H	-0.554443	4.507109	0.950442
H	1.990569	-2.785601	1.145065
O	-1.749482	-2.095006	-0.613506
H	-2.959271	0.755652	0.831347
H	0.370146	0.908504	-0.818477
O	-2.499156	-0.056211	1.148268
H	1.921759	-2.496537	-1.053389
H	-4.054530	2.869104	0.192042
O	1.550826	-0.319030	2.759827
H	1.609205	-1.626715	2.347814
H	-3.278124	-1.676068	3.887003
O	-2.434084	-1.451254	3.477710
H	-2.489353	-0.694188	0.409980
H	-1.471355	-2.751076	2.535449
O	-0.252084	-0.180652	4.740092
H	-0.162587	-0.242162	5.696436
H	-1.074550	-0.644198	4.497543
O	-3.241223	2.355203	0.222829
H	2.940559	-3.647855	-0.764051
H	-2.509074	2.991678	0.319683

Table S31 Optimized Cartesian coordinates of 11d at MP2/Def2TZVP level. Electronic energy is equal to -1254?134774 Hartree.

Symbol	x	y	z
H	-0.674207	4.057961	1.655579
H	-0.430453	-4.626479	-0.470237
C	0.016719	-3.677890	-0.725166
C	0.754074	-3.513538	-1.848504
H	0.939716	-4.314796	-2.552731
C	-0.171080	-2.557083	0.150700
O	-0.834288	-2.576764	1.199585
N	0.443650	-1.386024	-0.255939
H	0.690903	3.178946	-1.144721
C	1.180852	-1.202896	-1.399717
O	1.672590	-0.111525	-1.699158
N	1.317333	-2.314793	-2.175727
H	1.864684	-2.234946	-3.042387
O	2.694698	-2.640126	-4.583774
H	3.651794	-2.730701	-4.662810
H	2.000710	3.045961	-0.200456
O	-2.534263	1.490769	-0.700082
H	2.394253	-2.344358	-5.451319
H	-0.968749	1.835910	-1.536360
O	2.724278	1.817187	0.283267
H	-0.255874	5.575140	1.560326
H	-2.050007	2.307284	0.855747
O	0.565479	0.717599	1.631172
H	2.758768	1.164444	-0.435416
H	-3.311023	0.592820	4.121903
O	0.038475	4.674532	1.389350
H	0.849562	4.199994	0.162947
H	-1.961172	-0.031539	3.655343
O	-2.983245	-0.638268	0.803586
H	-2.068323	2.057059	2.391905
H	-0.113780	-1.605269	4.239643
O	-0.470816	-1.104151	3.496174
H	-0.588192	-1.745227	2.760186
H	0.449225	1.317409	-1.969157
O	-0.095238	2.120304	-1.876091
H	0.375958	-0.568020	0.374701
H	-2.442286	-1.438788	0.892081
O	-2.695794	0.555133	3.379757
H	-3.108991	-0.315845	1.713500
H	-3.321292	1.711529	-1.213395
O	-1.559573	2.496540	1.683307
H	0.449006	0.214452	2.458972
H	2.132258	1.401721	0.943571
O	1.350464	3.746300	-0.593744
H	-2.721774	0.616261	-0.266687
H	-0.147549	1.395555	1.648056

Table S32 Optimized Cartesian coordinates of 11e at MP2/Def2TZVP level. Electronic energy is equal to -1254.134745 Hartree.

Symbol	x	y	z
H	-2.140272	-1.956669	-2.109823
H	-2.888484	2.844708	2.455498
C	-1.916606	2.375122	2.448529
C	-0.985830	2.660409	3.383693
H	-1.154936	3.362998	4.189353
C	-1.600277	1.435714	1.403283
O	-2.355228	1.121885	0.480156
N	-0.332410	0.870848	1.481652
H	-0.497517	1.244464	-2.202583
C	0.622857	1.154531	2.415411
O	1.747401	0.643701	2.414428
N	0.249529	2.069085	3.360036
H	0.948908	2.291582	4.056628
O	1.292371	1.645952	-2.272749
H	1.854133	1.702492	-1.458726
H	1.539753	2.394914	-2.828527
O	2.920944	1.387547	-0.179991
H	3.491240	0.621972	-0.371089
H	2.677859	1.289198	0.752904
O	0.289629	-1.399862	-0.067829
H	4.879908	-1.510954	-0.842485
H	0.958812	-1.837469	0.491393
O	1.727115	-1.074866	-2.429112
H	2.617730	-1.229279	-2.060158
H	1.675934	-0.109447	-2.589100
O	-2.025529	-1.452466	-3.041585
H	0.860752	-2.064568	-3.677235
H	-1.261417	-1.868880	-3.551360
O	2.533138	-1.891571	1.572419
H	0.734803	-1.296503	-0.939936
H	2.723202	-2.548182	2.253770
O	-1.404324	0.881742	-2.197875
H	-1.767126	1.036576	-1.307670
H	-1.771681	-0.497857	-2.800942
O	-2.183774	-2.503586	-0.818656
H	-1.344051	-2.264323	-0.380533
H	-2.904507	-2.133199	-0.259193
O	-3.989112	-1.183756	0.709005
H	-4.949414	-1.258901	0.730952
H	-3.782364	-0.239887	0.630445
O	0.080377	-2.469145	-4.105825
H	0.301080	-2.661328	-5.022786
H	2.340684	-1.053318	2.039597
O	3.972639	-1.206519	-0.720422
H	3.650023	-1.614451	0.108132
H	-0.096315	0.124444	0.798906

Table S33 Optimized Cartesian coordinates of 11f at MP2/Def2TZVP level. Electronic energy is equal to -1254.134109 Hartree.

Symbol	x	y	z
H	0.940888	1.033999	-2.324799
H	-1.793512	-3.668006	-0.912381
C	-0.818898	-3.395724	-0.537480
C	-0.026368	-4.285415	0.100199
H	-0.316583	-5.314089	0.271542
C	-0.346927	-2.050523	-0.722149
O	-1.003923	-1.140891	-1.252072
N	0.926747	-1.797356	-0.255832
H	-0.550196	-1.338601	3.485505
C	1.729187	-2.668091	0.434874
O	2.827482	-2.369566	0.890333
N	1.204011	-3.928969	0.574189
H	1.790789	-4.594667	1.059680
O	0.072634	0.989951	-2.765871
H	-0.353260	0.205286	-2.369133
H	-1.219802	3.531239	-1.805255
O	-3.530547	2.595193	0.401224
H	-3.058994	1.795805	0.721677
H	-4.222332	2.781348	1.047277
O	0.375624	2.295679	0.966755
H	-0.400047	1.691296	0.977543
H	0.838563	2.126548	1.808052
O	-1.761074	0.550809	0.878044
H	-1.672087	-0.004951	0.079448
H	-1.443335	-0.023780	1.610307
O	3.833711	0.122752	1.314492
H	4.786621	0.162428	1.460196
H	3.615339	-0.823477	1.160930
O	1.832376	0.957996	2.997481
H	1.296697	-0.837001	-0.388228
H	2.642987	0.691850	2.504833
O	-1.350736	3.063893	-2.717386
H	-2.316014	2.770590	-2.724777
H	-0.749121	2.221886	-2.761138
O	-0.289426	-0.885016	2.675930
H	0.480080	-0.329958	2.914905
H	2.136305	1.267714	3.859350
O	-3.762491	2.256692	-2.349510
H	-3.946720	2.373519	-1.396687
H	-4.570800	2.452716	-2.835313
O	-1.217908	4.098603	-0.415587
H	-0.513166	3.737496	0.156071
H	-2.049371	3.841168	0.022125
O	1.931349	0.799524	-0.703885
H	1.446882	1.438425	-0.130809
H	2.836246	0.787974	-0.349720

Table S34 Optimized Cartesian coordinates of 12a at MP2/Def2TZVP level. Electronic energy is equal to -1330.464509 Hartree.

Symbol	x	y	z
H	-2.392951	0.876830	2.079396
H	3.148255	-0.906869	-0.330821
C	2.241313	-1.219200	0.164156
C	1.785436	-2.487821	0.065721
H	2.298650	-3.251057	-0.504758
C	1.479187	-0.264080	0.920789
O	1.791303	0.935733	1.049028
N	0.342639	-0.746574	1.520993
H	-0.299648	-0.072103	1.995646
C	-0.136486	-2.024567	1.426390
O	-1.172533	-2.387950	1.974224
N	0.639502	-2.880029	0.690373
H	0.253826	-3.806432	0.557234
O	-2.756110	0.875330	-1.358539
H	-1.247921	1.933523	2.187233
H	-4.792980	0.611606	1.338004
O	0.098585	3.057099	1.324664
H	0.294100	-1.060682	-2.577433
H	6.249993	3.492130	-0.559416
O	1.531780	1.686979	-2.579327
H	-4.297957	-2.970427	1.857541
H	0.941613	-1.050875	-4.016653
O	-3.717255	-2.467782	1.272305
H	-2.833292	-2.463134	1.707967
H	2.357242	1.738412	-1.952307
O	1.079938	-0.762357	-3.107710
H	3.052116	1.533910	-0.097599
H	4.116825	2.407328	-0.898635
O	3.448619	1.695394	-0.978205
H	-2.546181	-4.318695	-1.406052
H	5.315410	4.520170	-1.211651
O	5.320662	3.691098	-0.720294
H	-1.395980	-2.149453	-1.367740
H	1.369103	0.715078	-2.841474
O	-1.512521	1.038507	2.455693
H	-1.649592	-0.612496	-1.537289
H	0.796893	2.370994	1.404951
O	-0.490624	2.562906	-1.338289
H	-3.270309	0.727731	-0.532559
H	-3.998032	-0.712497	1.129361
O	-0.948933	-1.289924	-1.507586
H	-1.309846	2.032896	-1.312780
H	-0.329402	2.874474	-0.424645
O	-3.946387	0.266017	1.029991
H	0.443618	3.858798	1.734732
H	0.702276	2.044534	-2.084770
O	-2.144269	-3.681475	-0.804477
H	-2.842498	-3.437789	-0.169279
H	-3.403973	1.099169	-2.037593

Table S35 Optimized Cartesian coordinates of 12b at MP2/Def2TZVP level. Electronic energy is equal to -1330.463542 Hartree.

Symbol	x	y	z
H	0.979917	0.200594	3.725824
H	-0.037536	0.698922	-5.144784
C	-0.668957	0.814189	-4.277097
C	-1.989693	1.106319	-4.374062
H	-2.508296	1.245197	-5.313492
C	-0.147179	0.670988	-2.961978
O	1.128314	0.395532	-2.851152
N	-0.882460	0.804201	-1.866842
H	1.379306	0.336516	-1.878010
C	-2.195869	1.085799	-1.983752
O	-2.957760	1.210199	-0.994070
N	-2.730095	1.238897	-3.242924
H	-3.718194	1.456968	-3.287178
O	2.051807	1.119638	3.134992
H	1.691563	1.773069	2.507969
H	2.758696	0.650705	2.653025
O	3.338769	-3.035905	1.688001
H	3.974106	-3.701706	1.976975
H	2.974722	-3.344309	0.820754
O	-1.892835	0.277473	2.857613
H	-2.262230	-0.329410	2.188797
H	-1.918512	1.150105	2.423959
O	-0.051082	-1.866377	0.203692
H	0.394528	-1.020276	-0.009444
H	-1.010107	-1.687197	0.158971
O	-1.872937	2.516979	1.116253
H	-2.270295	2.083036	0.319720
H	-2.434191	3.278582	1.309121
O	0.751006	-2.556403	2.739703
H	0.420774	-2.390473	1.828122
H	1.672263	-2.850903	2.622295
O	0.255029	-0.459562	4.016739
H	0.487610	-1.363455	3.562119
H	-0.627737	-0.148437	3.607219
O	1.654561	0.293356	-0.284923
H	2.502986	0.070281	0.152444
H	1.363996	1.146125	0.103924
O	3.767050	-0.357263	1.402743
H	4.695113	-0.129810	1.268155
H	3.744074	-1.333645	1.538630
O	0.860960	2.608113	1.025784
H	-0.122141	2.672354	1.033616
H	1.182509	3.477337	0.757394
O	-2.743991	-1.074252	0.519039
H	-3.528078	-1.635599	0.479746
H	-2.939523	-0.289349	-0.040623
O	2.038350	-3.474402	-0.595973
H	1.965637	-4.212080	-1.210038
H	1.146778	-3.086744	-0.505703

Table S36 Optimized Cartesian coordinates of 12c at MP2/Def2TZVP level. Electronic energy is equal to -1330.463377 Hartree.

Symbol	x	y	z
H	3.129800	-0.166963	1.008327
H	-1.715322	-3.913701	2.620911
C	-1.472806	-3.031456	2.048561
C	-2.421911	-2.186713	1.572387
H	-3.482835	-2.332282	1.729171
C	-0.125334	-2.711160	1.734782
O	0.800613	-3.534120	2.140318
N	0.211973	-1.619470	1.055128
H	1.702684	-3.295000	1.752866
C	-0.754861	-0.799265	0.586499
O	-0.471512	0.227369	-0.081064
N	-2.065726	-1.096595	0.847762
H	-2.784598	-0.491135	0.431434
O	1.843865	2.549524	1.381159
H	0.921866	2.770698	1.722188
H	1.878370	2.743342	0.367741
O	-0.526390	3.425405	-2.394561
H	-0.810219	4.277150	-2.748056
H	-1.129609	3.216001	-1.639295
O	3.692729	-1.055166	-0.632347
H	3.004759	-0.711793	-1.243922
H	4.540585	-0.921554	-1.071745
O	1.948838	2.845975	-1.121541
H	1.956155	1.932059	-1.480318
H	1.199710	3.273972	-1.574727
O	-0.573798	3.089705	2.110826
H	-0.819497	3.834673	2.669934
H	-1.206712	3.051246	1.364114
O	-3.866664	0.566379	-0.628569
H	-3.557121	0.242816	-1.510029
H	-4.830626	0.569855	-0.656284
O	2.417482	0.124530	1.605232
H	2.057910	1.538983	1.513363
H	1.695543	-0.522794	1.446524
O	3.151546	-3.131921	1.125637
H	3.372736	-2.524345	0.392897
H	3.744931	-3.887793	1.062868
O	-0.393420	1.023289	-3.776590
H	-0.279183	1.114981	-4.730495
H	-0.451391	1.939554	-3.426335
O	-2.640896	-0.386117	-2.804017
H	-2.979475	-0.966714	-3.493658
H	-1.873823	0.080166	-3.191569
O	1.578545	0.199703	-1.837675
H	0.859517	0.106821	-1.166786
H	1.099071	0.226398	-2.684049
O	-1.855148	2.487120	-0.241345
H	-2.777365	2.187574	-0.338315
H	-1.367138	1.623525	-0.191991

Table S37 Optimized Cartesian coordinates of 12d at MP2/Def2TZVP level. Electronic energy is equal to -1330.462419 Hartree.

Symbol	x	y	z
H	2.584647	-0.812765	-3.918001
H	-0.897937	0.386081	4.156224
C	-1.045501	-0.233913	3.285613
C	-2.076453	-1.102690	3.194715
H	-2.810865	-1.226226	3.980163
C	-0.102119	-0.155832	2.203782
O	0.909196	0.561074	2.203045
N	-0.376563	-0.968783	1.121544
H	0.301227	-0.956483	0.340657
C	-1.423232	-1.843714	1.001388
O	-1.613929	-2.545952	0.012554
N	-2.245031	-1.894408	2.096222
H	-3.031989	-2.524293	2.021608
O	-2.068620	2.656745	1.438087
H	-1.357312	-0.485643	-2.244295
H	0.615684	3.301003	0.300043
O	2.912468	0.089520	-4.075342
H	-1.131079	-2.516332	-1.656748
H	-2.648038	3.197133	1.986302
O	1.826502	2.647774	0.632085
H	2.100985	-3.246132	-3.246000
H	4.097293	-0.910129	1.956734
O	-1.530534	0.301810	-1.700778
H	1.624242	1.866276	1.186616
H	-2.608065	1.908761	1.070026
O	-3.242708	0.557715	0.316035
H	-1.065614	3.323881	0.533674
H	1.875177	0.585994	-1.455227
O	1.763828	-2.362791	-3.055081
H	-0.399804	3.427165	-0.987767
H	2.479637	-1.068146	-0.003609
O	-0.945179	-2.319972	-2.604726
H	0.784357	-2.444823	-3.036206
H	3.651967	0.011309	-4.686356
O	1.780479	-0.950342	-0.685208
H	-1.218329	1.079945	-2.191915
H	-1.594826	-2.826563	-3.107553
O	2.033910	1.455807	-1.897118
H	1.933303	-1.602136	-1.398568
H	-4.160024	0.559639	0.019416
O	3.212471	-0.974337	1.582302
H	-2.696920	0.414411	-0.497002
H	2.553304	1.190827	-2.686801
O	-0.305312	3.713078	-0.031887
H	2.233298	2.311430	-0.189923
H	0.667414	2.234338	-2.360321
O	-0.223348	2.686394	-2.438947
H	-0.208588	3.212875	-3.247688
H	2.641688	-0.382733	2.098342

Table S38 Optimized Cartesian coordinates of 12e at MP2/Def2TZVP level. Electronic energy is equal to -1330.46171 Hartree.

Symbol	x	y	z
H	2.155585	-0.508733	0.288100
H	-2.702565	-1.913433	-2.811800
C	-1.834922	-1.419893	-2.401417
C	-1.410098	-0.207735	-2.838155
H	-1.904563	0.357485	-3.617503
C	-1.068734	-2.012474	-1.365802
O	-1.478482	-3.181290	-0.921512
N	0.013530	-1.461432	-0.847891
H	-0.892533	-3.491901	-0.181737
C	0.419648	-0.263291	-1.312530
O	1.455620	0.301569	-0.866708
N	-0.304511	0.358536	-2.295186
H	0.008193	1.279019	-2.624800
O	-2.417247	2.042467	1.125086
H	-2.018161	2.574938	0.388411
H	-3.145498	2.576376	1.465097
O	0.412901	3.039478	-2.978470
H	1.295467	3.129204	-2.560026
H	0.459119	3.495532	-3.827252
O	2.512364	-3.485367	0.801674
H	1.615302	-3.827870	0.979674
H	3.139431	-4.100551	1.196943
O	1.298292	3.986353	0.852183
H	1.925584	3.630575	0.190794
H	1.694793	4.791756	1.204719
O	-1.100452	3.583438	-0.571809
H	-0.323035	3.914972	-0.085971
H	-0.811371	3.522387	-1.495183
O	-1.219122	-2.027720	2.744056
H	-1.817103	-1.530670	2.123864
H	-1.709462	-2.126716	3.569758
O	2.573285	-0.921343	1.111207
H	2.610003	-1.919326	0.982845
H	1.909829	-0.694505	1.944442
O	-0.187700	-4.070852	1.290483
H	-0.508314	-4.941020	1.560446
H	-0.564277	-3.422565	1.933580
O	0.076854	2.030985	2.566581
H	-0.820179	2.064269	2.191701
H	0.583203	2.708379	2.086459
O	1.061574	-0.387523	2.950234
H	0.718975	0.543950	2.861034
H	0.273319	-0.964737	2.960232
O	2.540031	2.715926	-1.291068
H	2.234270	1.784683	-1.154023
H	3.484430	2.664984	-1.483722
O	-2.655228	-0.673705	0.961739
H	-3.548326	-0.920739	0.697287
H	-2.636081	0.309948	0.986672

Table S39 Optimized Cartesian coordinates of 12f at MP2/Def2TZVP level. Electronic energy is equal to -1330.46062 Hartree.

Symbol	x	y	z
H	1.153606	-3.052276	1.279699
H	0.311306	4.054870	-3.190128
C	0.713861	3.061461	-3.064249
C	1.611618	2.527808	-3.928795
H	1.989739	3.047345	-4.799298
C	0.316860	2.243072	-1.971754
O	-0.551491	2.739458	-1.135236
N	0.794973	1.018218	-1.776144
H	-0.833659	2.058379	-0.440178
C	1.679805	0.498834	-2.656286
O	2.146938	-0.658834	-2.538931
N	2.077849	1.268274	-3.721359
H	2.730634	0.839575	-4.366559
O	-3.400921	1.646549	2.481800
H	-4.036079	2.372243	2.490031
H	-2.746797	1.823903	3.204857
O	3.726238	-1.495053	-0.339733
H	4.668927	-1.687087	-0.412185
H	3.422702	-1.268398	-1.238700
O	0.391767	-2.362263	-1.587552
H	1.015865	-1.684951	-1.985481
H	-0.496522	-1.905588	-1.261487
O	-1.405942	1.678948	4.226273
H	-0.674666	1.198972	3.788657
H	-1.007846	2.306214	4.837959
O	-0.079025	-2.675731	2.607692
H	-0.996572	-2.839705	2.286864
H	0.012641	-3.183230	3.423544
O	-2.586095	-2.784322	1.527120
H	-3.181952	-2.168131	2.031823
H	-3.101455	-3.586200	1.374470
O	1.614062	-3.215866	0.433151
H	2.461968	-2.737078	0.440716
H	0.871284	-2.762308	-0.760207
O	-1.473919	1.029872	0.597582
H	-2.263208	1.360928	1.078832
H	-0.876404	0.706166	1.321664
O	0.146086	0.139928	2.555716
H	0.999743	0.282654	2.077004
H	0.088180	-0.824248	2.703763
O	-1.723192	-1.374016	-0.741917
H	-2.129114	-1.921220	-0.039444
H	-1.684254	-0.467429	-0.368724
O	-4.081155	-1.027187	2.825541
H	-4.478260	-1.149864	3.693843
H	-3.942782	-0.063951	2.720405
O	2.123401	0.569122	0.826472
H	2.861647	-0.023390	0.607173
H	1.625537	0.659667	-0.005873