Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary information

Atmospheric Implication of the Hydrogen Bonding Interaction in Hydrated Clusters of HONO and Dimethylamine in the Nighttime

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Table S1 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of $H_2O{-}HONO$ (A).

O	-2.856564	-0.198268	0.000018
H	-3.345315	0.629432	-0.000117
H	-1.927138	0.057505	0.000002
N	0.899892	-0.433405	-0.000019
O	2.242941	-0.131191	0.000004
H	2.315894	0.846265	0.000036
O	0.195788	0.517039	0.000004

Total energy: -282.2607891 a.u.
Zero point correction 0.042948 a.u.

Table S2 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of $H_2O{-}HONO$ (B).

O	2.897117	0.006514	-0.000013
H	3.030251	-0.945510	0.000023
H	1.940788	0.127085	0.000006
N	-0.901028	-0.438469	0.000013
O	-2.244214	-0.136610	-0.000015
H	-2.316918	0.840950	-0.000026
O	-0.196268	0.510941	0.000016

Total energy: -282.2609686 a.u.
Zero point correction 0.043054 a.u.

Table S3 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of $H_2O{-}HONO$ (C).

O	2.627487	0.103976	0.000003
H	2.893412	-0.819808	-0.000022
H	1.663111	0.088715	0.000002
N	-0.553458	0.169979	0.000001
O	-1.125128	-1.095907	0.000001
H	-2.095853	-0.967029	-0.000001
O	-1.325668	1.055464	-0.000002

Total energy: -282.2610338 a.u.
Zero point correction 0.043159 a.u.

Table S4 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of H_2O−HONO (D).

O	-2.627732	-0.143203	-0.000014
H	-2.976132	0.752724	0.000083
H	-1.668545	-0.041596	0.000013
N	0.544920	0.143185	0.000013
O	1.222812	-1.061141	0.000002
H	2.178824	-0.847414	-0.000023
O	1.236346	1.096094	-0.000009

Total energy: -282.2609246 a.u.
Zero point correction 0.043193a.u.

Table S5 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of H_2O−HONO (E).

O	-2.822761	-0.252871	-0.000031
H	-3.406084	0.511167	-0.000021
H	-1.930195	0.111191	0.000026
N	0.854622	-0.353441	0.000082
O	2.225145	-0.011129	-0.000069
H	2.665185	-0.874610	-0.000009
O	0.183708	0.604793	0.000028

Total energy: -282.2622332 a.u.
Zero point correction 0.043237 a.u.

Table S6 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of H_2O−HONO (F).

O	-2.545750	-0.221830	-0.148697
H	-1.641703	-0.096237	0.164594
H	-2.958042	-0.810820	0.489176
N	1.433927	0.208710	-0.312586
O	0.237867	0.802160	0.256296
H	0.188390	1.664372	-0.182990
O	1.604616	-0.857615	0.107066

Total energy: -282.2636615 a.u.
Zero point correction 0.043160 a.u.

Table S7 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−H_2O (G).

O	-1.973336	-0.047026	-0.084661
H	-1.624560	-0.941863	0.012528
H	-2.680599	0.043522	0.561571
N	1.371945	0.006692	0.018811
O	0.550455	1.097234	-0.001947
H	-0.393185	0.780107	-0.022910
O	0.809721	-1.041284	0.001250

Total energy: -282.2701629 a.u.
Zero point correction 0.044611 a.u.

Table S8 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−H_2O (H).

O	-2.348261	-0.167071	-0.067888
H	-2.248059	-1.123779	-0.119016
H	-2.957271	-0.003501	0.659213
N	0.894338	-0.388781	0.001261
O	0.242708	0.845683	-0.021027
H	-0.705795	0.587237	-0.037890
O	2.061897	-0.270924	0.025023

Total energy: -282.2707417 a.u.
Zero point correction 0.044310 a.u.

Table S9 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of DMA−HONO (A).

O	1.776056	1.025473	-0.355430
H	1.617142	1.768511	0.245005
O	1.725829	-1.106161	-0.108085
N	1.576972	-0.116252	0.488049
N	-1.583559	-0.055747	0.573267
H	-0.811338	-0.073420	1.225605
C	-1.644870	1.216533	-0.127606
H	-1.627085	2.035591	0.592341
H	-0.827546	1.365413	-0.850056
H	-2.586163	1.281661	-0.677059
C	-1.539160	-1.209395	-0.309906
H	-0.706877	-1.186285	-1.030685
H	-1.454184	-2.121929	0.278961
H	-2.468749	-1.262867	-0.880128

Total energy: -341.0224247 a.u.
Zero point correction 0.113480 a.u.

Table S10 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of DMA−HONO (B).

O	-2.170654	0.790050	-0.475148
H	-2.551660	0.659556	-1.355994
O	-1.303046	-0.543187	0.963207
N	-1.790676	-0.536139	-0.095247
N	1.773868	-0.150805	0.457972
H	1.108436	-0.377761	1.184328
C	1.588782	-1.026425	-0.685130
H	1.601188	-2.067126	-0.362303
H	0.649233	-0.849354	-1.235879
H	2.410463	-0.883337	-1.390169
C	1.686301	1.262926	0.121105
H	0.750312	1.539298	-0.387389
H	1.773521	1.863658	1.026033
H	2.515273	1.529772	-0.538034

Total energy: -341.0220537 a.u.
Zero point correction 0.113180 a.u.

Table S11 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of DMA−HONO (C).

O	1.840273	-1.113475	0.355738
H	1.815494	-1.852726	-0.269097
O	1.894342	1.018778	0.089215
N	1.903555	0.028862	-0.520565
N	-1.189473	-0.104308	-0.047771
H	-0.576305	-0.398900	0.701003
C	-2.363582	-0.962800	-0.099133
H	-2.056571	-2.007634	-0.152153
H	-3.038706	-0.844456	0.763024
H	-2.938334	-0.738355	-1.000104
C	-1.516427	1.306722	0.099924
H	-2.140989	1.526875	0.979717
H	-0.600076	1.891178	0.175778
H	-2.059954	1.646196	-0.784184

Total energy: -341.0226746 a.u.
Zero point correction 0.113216 a.u.

Table S12 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of DMA−HONO (D).

O	-1.863379	0.702239	-0.604220
H	-2.302867	1.483666	-0.237898
O	-1.338613	-1.211245	0.209605
N	-1.862194	-0.214434	0.501102
N	1.460700	0.278439	-0.558811
H	0.579629	0.126809	-1.031078
C	1.287801	1.237385	0.517696
H	0.834757	2.150230	0.131033
H	0.665417	0.868016	1.350856
H	2.263073	1.499326	0.933472
C	2.018468	-0.990419	-0.113921
H	1.451429	-1.462618	0.703200
H	2.056852	-1.688597	-0.949634
H	3.040491	-0.834614	0.238284

Total energy: -341.0226824 a.u.
Zero point correction 0.113264 a.u.

Table S13 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of DMA−HONO (E).

O	-1.956184	0.808859	-0.375237
H	-2.104631	1.036435	0.564817
O	-1.408365	-0.998832	0.674244
N	-1.485995	-0.506667	-0.393124
N	1.502860	0.296312	-0.563226
H	0.731661	0.233037	-1.213488
C	1.218059	1.241490	0.498798
H	0.872035	2.183586	0.075864
H	0.463252	0.882532	1.220472
H	2.131215	1.440708	1.063471
C	1.892895	-1.020137	-0.085855
H	1.163390	-1.472337	0.603473
H	2.029341	-1.693740	-0.931216
H	2.846351	-0.946066	0.441342

Total energy: -341.0219859 a.u.
Zero point correction 0.113392 a.u.

Table S14 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of DMA−HONO (F).

O	-2.518308	0.594646	-0.015022
H	-2.427158	0.567788	0.959287
O	-1.164291	-1.052569	0.315109
N	-1.724578	-0.432218	-0.516700
N	1.683048	0.198328	0.588769
H	0.956671	-0.230075	1.146484
C	2.300767	-0.800613	-0.271642
H	2.631696	-1.649154	0.326520
H	1.632670	-1.173271	-1.063087
H	3.179782	-0.368463	-0.754221
C	1.151716	1.333962	-0.145201
H	0.447662	1.056923	-0.946885
H	0.641975	2.014081	0.537798
H	1.973310	1.882691	-0.610018

Total energy: -341.0207222 a.u.
Zero point correction 0.113153 a.u.

Table S15 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA (G).

O	1.132830	-0.852321	0.107257
H	0.188869	-0.554525	-0.109732
O	3.034936	0.106609	0.074866
N	1.885727	0.276957	-0.131722
N	-1.393545	0.016516	-0.406477
H	-1.512633	0.073692	-1.411024
C	-2.384791	-0.907564	0.151452
H	-2.305859	-1.873093	-0.345993
H	-2.176401	-1.055310	1.211330
H	-3.413213	-0.540449	0.052604
C	-1.471477	1.363207	0.169422
H	-1.242503	1.307159	1.233798
H	-0.725853	2.001993	-0.300162
H	-2.462199	1.818066	0.054338

Total energy: -341.0391591 a.u.
Zero point correction 0.114663 a.u.

Table S16 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA (H).

O	-1.196106	0.000135	0.940327
H	-0.188719	0.000092	0.829492
O	-2.831708	-0.000031	-0.425269
N	-1.653469	-0.000054	-0.358848
N	1.476738	0.000016	0.451112
H	2.040995	0.000046	1.292356
C	1.738831	-1.222576	-0.315775
H	1.569143	-2.093140	0.316001
H	1.041444	-1.269823	-1.151869
H	2.759738	-1.264586	-0.712898
C	1.738905	1.222507	-0.315910
H	1.041522	1.269704	-1.152011
H	1.569270	2.093152	0.315768
H	2.759815	1.264411	-0.713039

Total energy: -341.0394833 a.u.
Zero point correction 0.114818 a.u.

Table S17 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA (I).

O	1.228318	-1.043009	0.451952
H	0.342120	-0.620996	0.130798
O	1.954389	0.744033	-0.492632
N	2.264922	-0.249103	0.093250
N	-1.127311	0.047114	-0.322296
H	-0.981620	0.274699	-1.299200
C	-2.276290	-0.850740	-0.186397
H	-2.128476	-1.731003	-0.810396
H	-2.350957	-1.179335	0.850462
H	-3.224603	-0.375306	-0.463288
C	-1.261614	1.288656	0.445546
H	-1.320029	1.044883	1.506752
H	-0.378299	1.903766	0.283967
H	-2.155645	1.861516	0.174769

Total energy: -341.037847 a.u.
Zero point correction 0.114278 a.u.

Table S18 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA (J).

O	-1.396033	-0.000020	-1.075418
H	-0.388366	-0.000013	-0.843401
O	-1.500665	0.000019	1.068995
N	-2.135061	-0.000002	0.056699
N	1.254214	-0.000007	-0.520564
H	1.794498	-0.000017	-1.377404
C	1.533322	1.222367	0.240584
H	1.359792	2.092613	-0.390869
H	0.846833	1.269986	1.085222
H	2.560103	1.258330	0.621597
C	1.533329	-1.222358	0.240618
H	0.846838	-1.269958	1.085256
H	1.359804	-2.092623	-0.390811
H	2.560109	-1.258305	0.621634

Total energy: -341.0387203 a.u.
Zero point correction 0.114558 a.u.

Table S19 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA−H_2O (A).

O	1.499246	0.096984	-0.493658
H	1.058333	0.904718	-0.116616
O	3.344673	-0.923060	-0.181319
N	2.727011	0.016214	0.161265
N	-1.679340	-0.262228	-0.147739
H	-0.939677	-0.679521	-0.702602
C	-1.786112	-0.984251	1.122154
H	-0.814259	-0.997981	1.612746
H	-2.488840	-0.464084	1.773991
H	-2.133830	-2.017225	0.998089
C	-2.926589	-0.250895	-0.910881
H	-3.685209	0.301016	-0.354257
H	-2.770231	0.254070	-1.863516
H	-3.317713	-1.256898	-1.108876
O	-0.180705	1.954374	0.449673
H	-0.383569	2.771351	-0.013412
H	-0.888205	1.291140	0.214567

Total energy: -417.5163687 a.u.
Zero point correction 0.139265 a.u.

Table S20 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA−H_2O (B).

O	1.175040	0.076452	-0.587401
H	0.175970	-0.123353	-0.403776
O	3.033770	-0.710862	0.097870
N	1.865163	-0.852537	0.166216
N	-1.405936	-0.168550	-0.051719
H	-1.619680	0.818875	-0.149849
C	-2.211206	-0.961267	-0.981721
H	-2.065924	-0.592439	-1.996067
H	-1.882682	-2.000428	-0.947085
H	-3.281387	-0.932964	-0.745598
C	-1.576301	-0.562523	1.349680
H	-1.200650	-1.576494	1.487416
H	-0.996133	0.106525	1.982545
H	-2.623858	-0.533825	1.670594
O	-0.170514	2.580103	0.033854
H	0.612875	2.058753	-0.190968
H	0.085553	3.500160	-0.071028

Total energy:	-417.516985 a.u.
Zero point correction	0.138070 a.u.

Table S21 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA−H_2O (C).

O	1.068762	0.906173	-0.516036
H	0.264848	0.204894	-0.395014
O	2.141691	-0.695157	0.421119
N	2.221579	0.418841	-0.000593
N	-1.023294	-0.607672	-0.175513
H	-1.763321	0.004529	-0.500352
C	-0.993093	-1.857195	-0.937604
H	-0.944969	-1.633935	-2.002453
H	-0.096757	-2.413636	-0.663409
H	-1.867361	-2.488415	-0.746107
C	-1.153166	-0.805764	1.272023
H	-0.255777	-1.302228	1.640547
H	-1.240019	0.166155	1.753406
H	-2.025213	-1.414202	1.532992
O	-1.398323	2.359910	-0.041749
H	-0.443073	2.320801	-0.187544
H	-1.635829	3.288215	-0.112508

Total energy:	-417.515765 a.u.
Zero point correction	0.137360 a.u.

Table S22 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA−H_2O (D).

O	2.287427	0.687987	-0.005081
H	1.467583	1.261825	-0.000569
O	2.646946	-1.408914	0.000702
N	1.795025	-0.591206	0.002562
N	-1.482679	-0.238657	0.010080
H	-0.635563	-0.797819	0.005667
C	-2.280625	-0.563158	1.191750
H	-1.670715	-0.449542	2.087339
H	-3.122279	0.127464	1.262409
H	-2.681717	-1.584121	1.170283
C	-2.205855	-0.432750	-1.247178
H	-3.044718	0.262873	-1.293178
H	-1.543032	-0.218833	-2.084338
H	-2.599851	-1.450317	-1.360521
O	-0.004501	2.051783	-0.026981
H	-0.210515	2.685204	0.665379
H	-0.665718	1.300911	0.042481

Total energy:	-417.5192978 a.u.
Zero point correction	0.139652 a.u.

Table S23 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA−H_2O (E).

O	-0.976763	-1.228223	0.041425
H	-0.040060	-0.760156	0.009115
O	-3.000181	-0.573567	0.032828
N	-1.869677	-0.216885	0.004305
N	1.378292	-0.046186	-0.034521
H	1.141706	0.927997	-0.203267
C	2.039116	-0.165793	1.268389
H	1.411930	0.289404	2.032875
H	2.170580	-1.220124	1.513945
H	3.022437	0.317149	1.285767
C	2.184495	-0.564673	-1.142592
H	2.332580	-1.637319	-1.013475
H	1.656482	-0.404268	-2.081292
H	3.168843	-0.087383	-1.205272
O	-0.381697	2.307146	-0.130350
H	-1.072239	1.622281	-0.097037
H	-0.825097	3.133867	-0.335844

Total energy:	-417.5202591 a.u.
Zero point correction	0.138764 a.u.

Table S24 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA−H_2O (F).

O	0.651068	-0.577063	-3.596214
H	1.247408	-0.366907	-2.804845
O	-0.807678	-0.580330	-2.021190
N	-0.630181	-0.715297	-3.194925
N	0.720516	0.048304	0.603232
H	-0.130147	0.336747	0.134559
C	0.990107	0.920090	1.745232
H	1.017327	1.958847	1.417408
H	0.242868	0.825037	2.543131
H	1.964964	0.671539	2.166925
C	0.601867	-1.365184	0.968612
H	-0.153389	-1.542287	1.743974
H	0.338564	-1.941369	0.083857
H	1.563220	-1.722992	1.338856
O	2.334324	-0.042579	-1.592442
H	2.926302	0.708599	-1.683676
H	1.817701	0.080498	-0.740811

Total energy:	-417.5176626 a.u.
Zero point correction	0.139229 a.u.

Table S25 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of HONO−DMA−H_2O (G).

O	-0.964227	-1.465355	-0.481731
H	0.248299	-0.612951	-0.269710
O	-1.989665	0.193694	0.379717
N	-2.045494	-0.984248	-0.022385
N	1.153377	-0.018033	-0.042359
H	0.899817	0.928343	-0.365086
C	1.302693	0.006412	1.429904
H	0.372453	0.374321	1.854944
H	1.486860	-1.005599	1.783858
H	2.128092	0.655603	1.715619
C	2.318610	-0.549666	-0.774624
H	2.492767	-1.578899	-0.468464
H	2.105578	-0.527304	-1.840681
H	3.204829	0.047303	-0.564903
O	-0.370804	2.225346	-0.409601
H	-1.059727	1.561067	-0.164230
H	-0.764400	2.804129	-1.066902

Total energy: -417.5203318 a.u.
Zero point correction 0.140145 a.u.

Table S26 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of *cis*-HONO.

O	1.092010	0.065411	0.000000
N	-0.174455	-0.517982	0.000000
O	-1.058379	0.258521	0.000000
H	0.952141	1.034419	0.000000

Total energy: -205.7910382 a.u.
Zero point correction 0.019973 a.u.

Table S27 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of *trans*-HONO.

O	-0.890196	-0.605345	0.000000
N	0.000000	0.519339	0.000000
O	1.110612	0.174199	0.000000
H	-1.763329	-0.186202	0.000000

Total energy: -205.7921852 a.u.
Zero point correction 0.020085 a.u.

Table S28 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of H_2O.

O	0.000000	0.116983	0.000000
H	0.763571	-0.467933	0.000000
H	-0.763571	-0.467933	0.000000

Total energy: -76.4662067 a.u.
Zero point correction 0.021237 a.u.

Table S29 B3LYP-D3/aug-cc-pVTZ optimized cartesian coordinates (Å), zero point correction and total energy of DMA.

C	1.215244	-0.222479	0.020081
H	2.087742	0.425764	-0.060713
H	1.269904	-0.761034	0.979752
H	1.278261	-0.965314	-0.777860
C	-1.215243	-0.222479	0.020081
H	0.000000	1.340438	0.498948
H	-2.087742	0.425764	-0.060711
H	-1.278262	-0.965312	-0.777861
H	-1.269903	-0.761035	0.979751
N	0.000000	0.561497	-0.146040

Total energy: -135.2262358 a.u.
Zero point correction 0.092031 a.u.