Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Reactivity of the $O_2^+.(H_2O)_n$ and $NO^+.(H_2O)_n$ Cluster Ions in the D-region of the Ionosphere

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Coordinates of the lowest energy structures of $O_2^+.(H_2O)_n$. Note *n*=1 is a doublet state and *n*=2-5 correspond to quartet states.

n=1:

O	1.0225656361	-0.5763585740	-0.0068485324
O	1.0210815466	0.5768486201	0.0068697997
H	-2.1142503269	-0.7537688472	0.0178607089
O	-1.5148078673	-0.0002989362	-0.0001016434
H	-2.1151831692	0.7524651102	-0.0162270623

n=2:

O	-1.6997644705	-0.1611392162	0.2020932842
O	-2.8353945674	-0.3768206215	-0.1627880670
H	1.7000568705	0.2830334532	-0.0603079978
O	2.8751620413	-0.5979692772	0.1166921745
H	3.2169620164	-1.2458247454	-0.5279920189
O	0.9322359287	0.9793810210	-0.1289914648
H	0.0362210517	0.5935017256	-0.0732718589
H	1.0260359887	1.7051416977	0.5106596259

n=3:

O	-2.1628880404	-0.0847685257	-0.1737866279
O	-3.3596119623	-0.0532924546	0.0345315824
O	1.9166579104	-2.1999737575	-0.2905700283
H	2.2746872091	-2.9639470955	0.1946031429
H	1.1774699198	-0.8649815062	0.2899094962
O	1.9190913057	1.9997062088	-0.1889146099
H	1.9231567954	2.3817886900	-1.0735993995
H	2.1758103933	2.6974558763	0.4247303615
O	0.7310311091	-0.0162159547	0.5749116292
H	1.2001691576	0.8479519886	0.2163928763
H	-0.2178958973	-0.0383861669	0.3741117699

n=4:

O	-2.0361325554	-0.0909270389	0.7380027673
O	-3.2313523719	0.0938078954	0.8788877817
O	0.1016376777	-2.1605395659	-0.7370120894
H	0.5313760925	-2.7204204868	-1.3921204897
H	-0.4702458275	-2.7412557193	-0.2235159042
O	0.9778501025	-0.0116211908	0.2683982367
H	0.5337271627	0.7766245841	-0.1256399325
H	0.6652408415	-0.8818839691	-0.1512773453
O	0.0295143495	2.2862753287	-0.7584198956
H	1.9870955265	0.0926408379	0.2872015543
H	-0.8418970998	2.7097567909	-0.8361126984
O	3.4972389909	0.1909679286	0.3926856514
H	4.0815281255	0.6178779708	-0.2426393379
H	3.9524064139	0.2284187246	1.2408424231

n=5:

O	2.0756424813	-1.5968512273	-0.4624089681
O	3.1307074763	-1.0077185637	-0.6414546632
O	-1.0328644045	-1.3979886848	-0.2097988115
H	0.7360963488	0.9561141323	0.4370575877
H	-0.7711381116	-2.1137755559	-0.7965274742
O	-1.4878119847	2.7805071311	-0.8009496765
H	-1.4159177872	3.3045712460	-1.6052678363
H	-1.9514001522	3.3360781165	-0.1665298543
O	1.7525155913	1.2323610709	1.6083044583
H	1.7089592540	0.8501141321	2.4905290329
O	0.1145951877	0.8220268863	-0.3370520031
H	-0.3803151294	-0.0740116964	-0.2912076105
H	-0.5021581706	1.6002968251	-0.4692744057
H	2.6793357979	1.4489013164	1.4629417544
O	-3.7348622439	-1.5304003127	0.6397594874
H	-4.5185607075	-2.0975552080	0.5597554138
H	-1.9693835465	-1.5371477421	0.0067281938

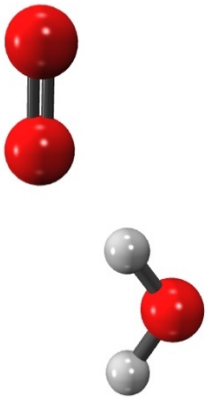

Figure S1: Minimum energy structure of the quartet state of $O_2^+.(H_2O)$.

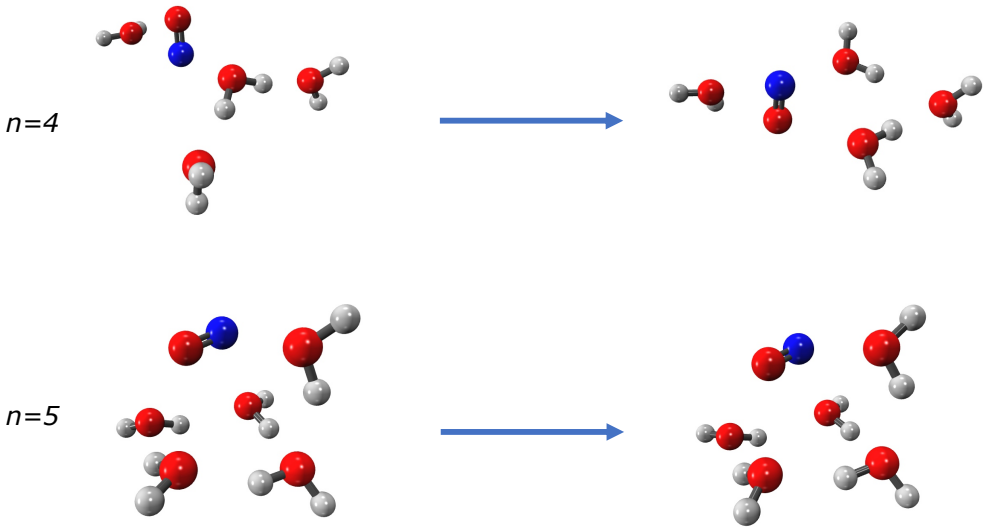

Figure S2: Initial and final structures of the AIMD MP2/6-311++G** simulations of $NO^+.(H_2O)_4$ and $NO^+.(H_2O)_5$ with thermal initial velocities.