https://www.overleaf.com/project/5e96c098d2b3c9000134390e

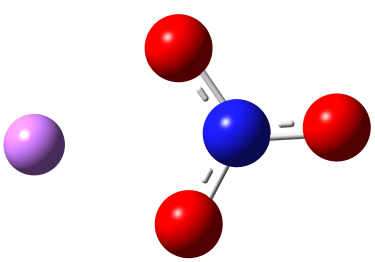
Supporting Information

S.1 Calculated Gibbs free energies for the nitrate monohydrate clusters

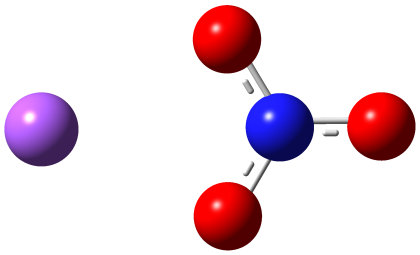
Table S.1 Gibbs free energies in Hartree calculated at ωB97XD/aug-cc-pVTZ level of theory

Dielectric constant	water	nitrate	1b	1m
78.3553	-76.442607	-280.492279	-356.930708	-356.93028
75	-76.442607	-280.492279	-356.930648	-356.930222
72	-76.442607	-280.492279	-356.930589	-356.930165
70	-76.442607	-280.492279	-356.930547	-356.930119
67	-76.442607	-280.492279	-356.93048	-356.930051
65	-76.442607	-280.492279	-356.930415	-356.930002
62	-76.442607	-280.492279	-356.930338	-356.929935
60	-76.442607	-280.492279	-356.930203	-356.92988
55	-76.442607	-280.492279	-356.930054	-356.929725
50	-76.442607	-280.492279	-356.929875	-356.929538

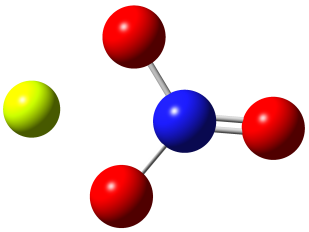
S.2 CIP structures



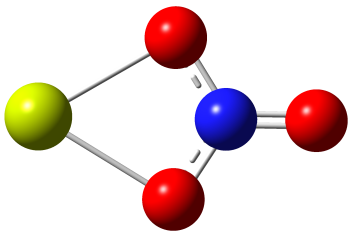
(a) $LiNO_3$



(b) $NaNO_3$

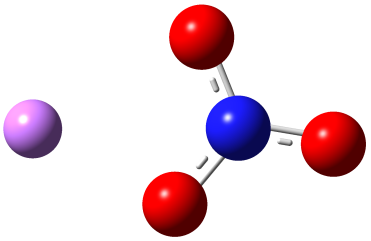


(c) $BeNO_3^+$

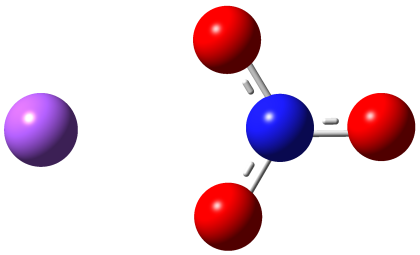


(d) $MgNO_3^+$

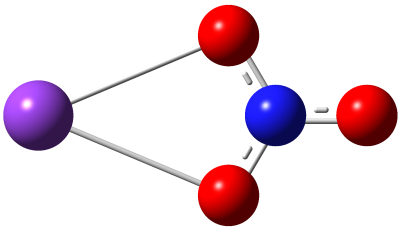
Figure S.1: Ion pair structures Optimized at the byωB97X-D/aug-cc-pVTZ level



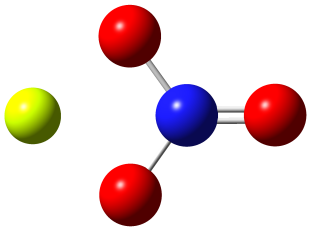
(a) $LiNO_3$



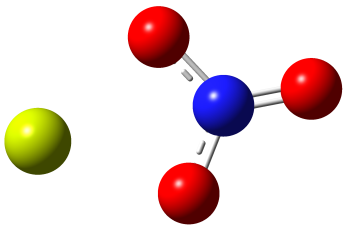
(b) $NaNO_3$



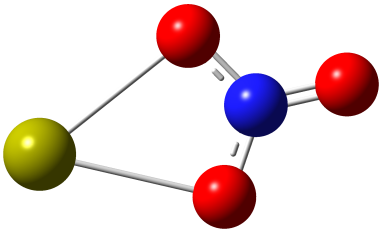
(c) KNO_3



(d) $BeNO_3^+$



(e) $MgNO_3^+$



(f) $CaNO_3^+$

Figure S.2: Ion pair structures Optimized at the ωB97X-D/6-311++G(d,p) level