Al^{3+}-Dimer Speciation and Stability From Density Functional Theory Calculations.

Electronic Supplementay Information

Stuart Bogatko, Paul Geerlings

Eenheid Algemene Chemie, Vrije Universiteit Brussel (VUB), Faculteit Wetenschappen,
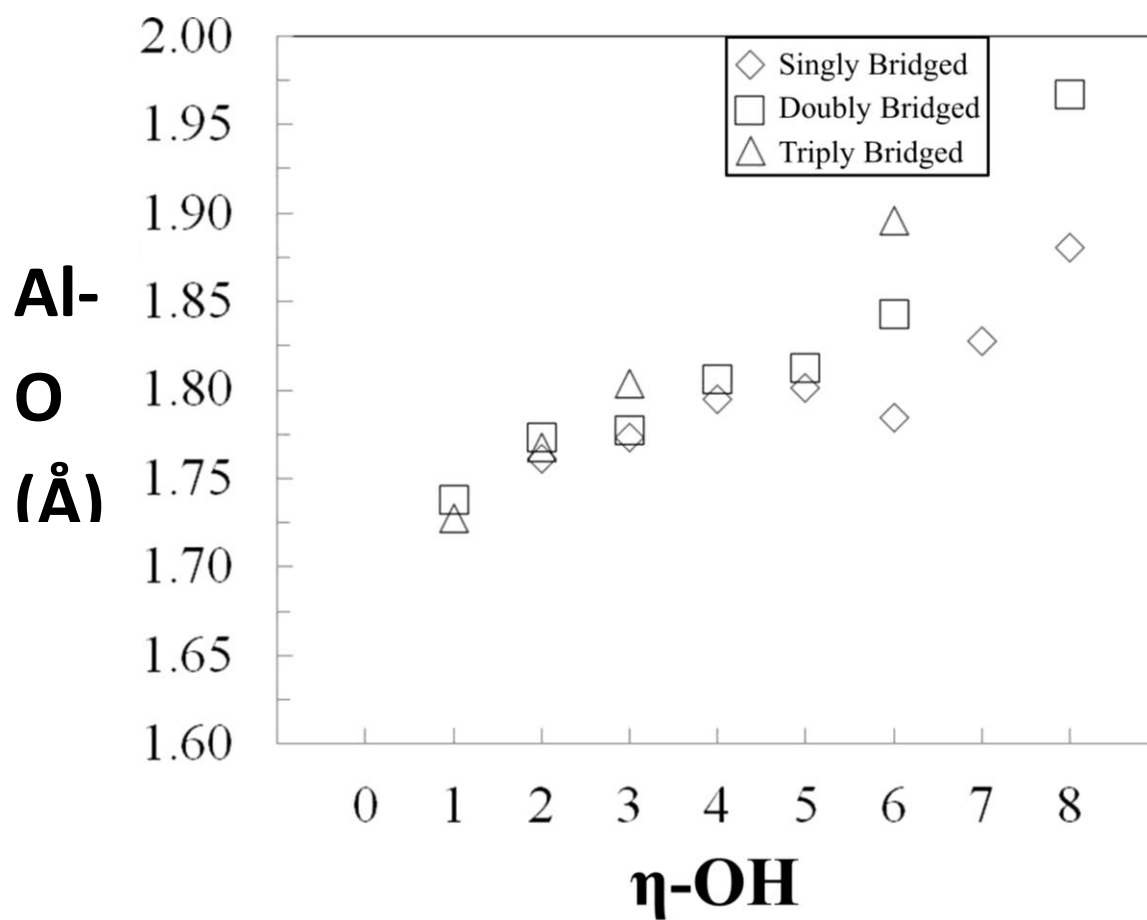
Pleinlaan 2,

1050 Brussels, Belgium.

Figure S-1. Al-O distances for the η-OH ligands as a function of number of η-OH ligandsfor the singly (diamonds), doubly (squares), and triply (triangles) bridged Al^{3+}-Dimer complexes.
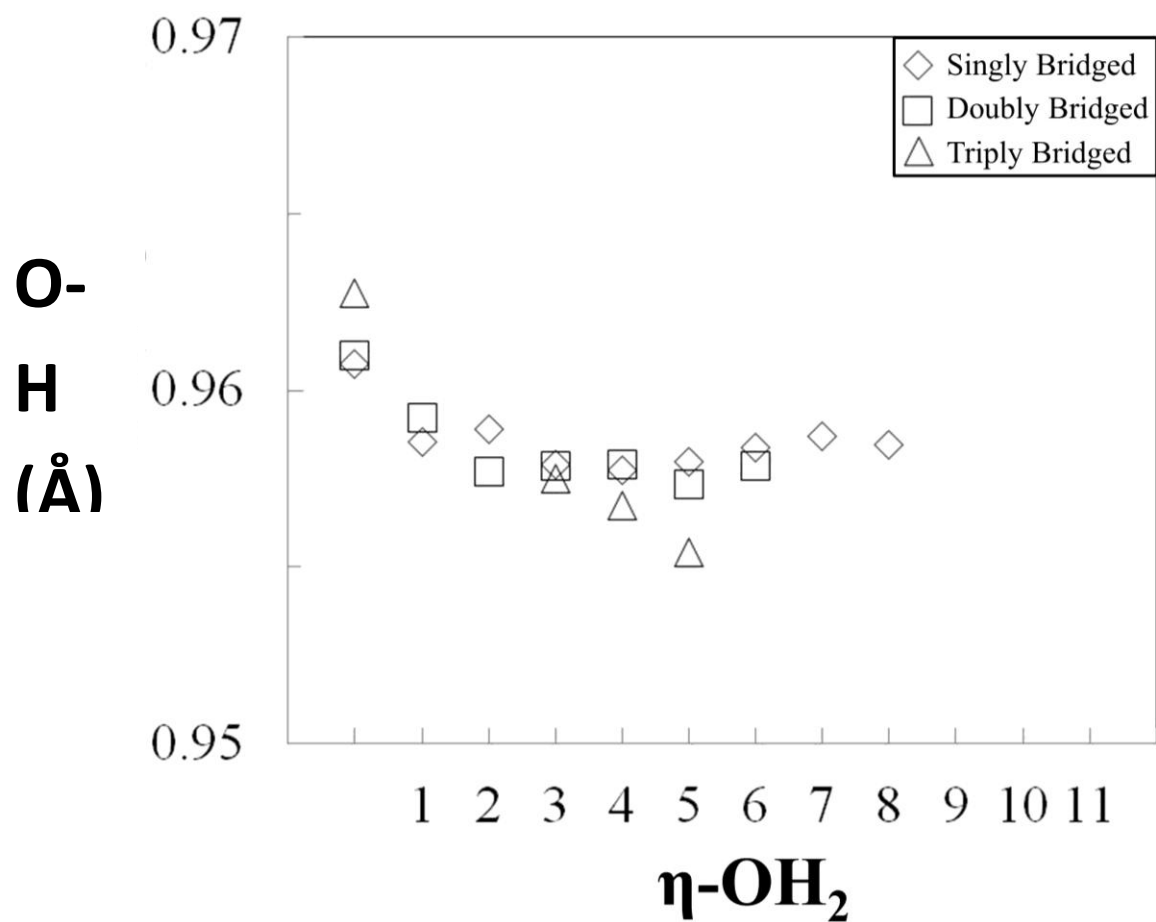
Figure S-2. Hydroxide O-H distances for the η-OH ligands as a function of number of η-OH ligands for the singly (diamonds), doubly (squares), and triply (triangles) bridged Al^{3+}-Dimer complexes.

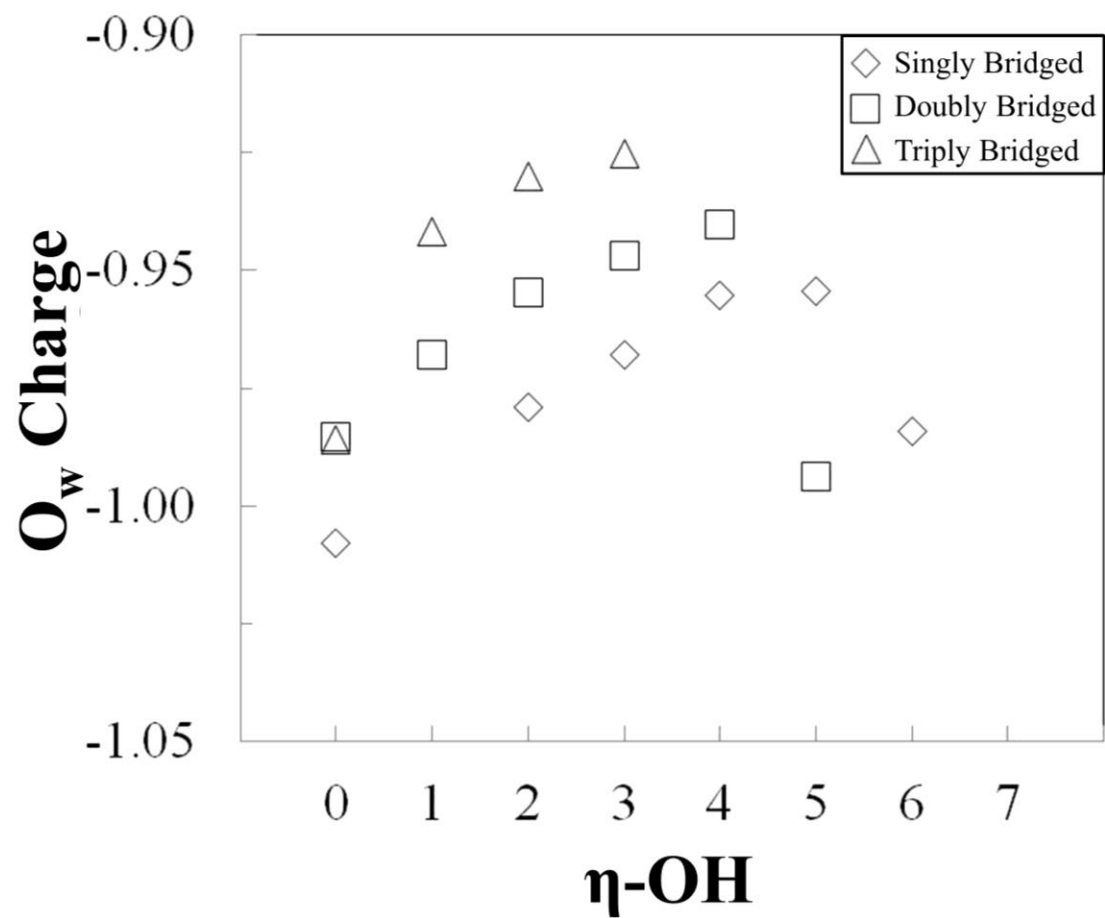Figure S-3. Average water O Natural Charges as a function of the number of η-OH ligands for the singly (diamonds), doubly (squares), and triply (triangles) bridged Al^{3+}-Dimer complexes.
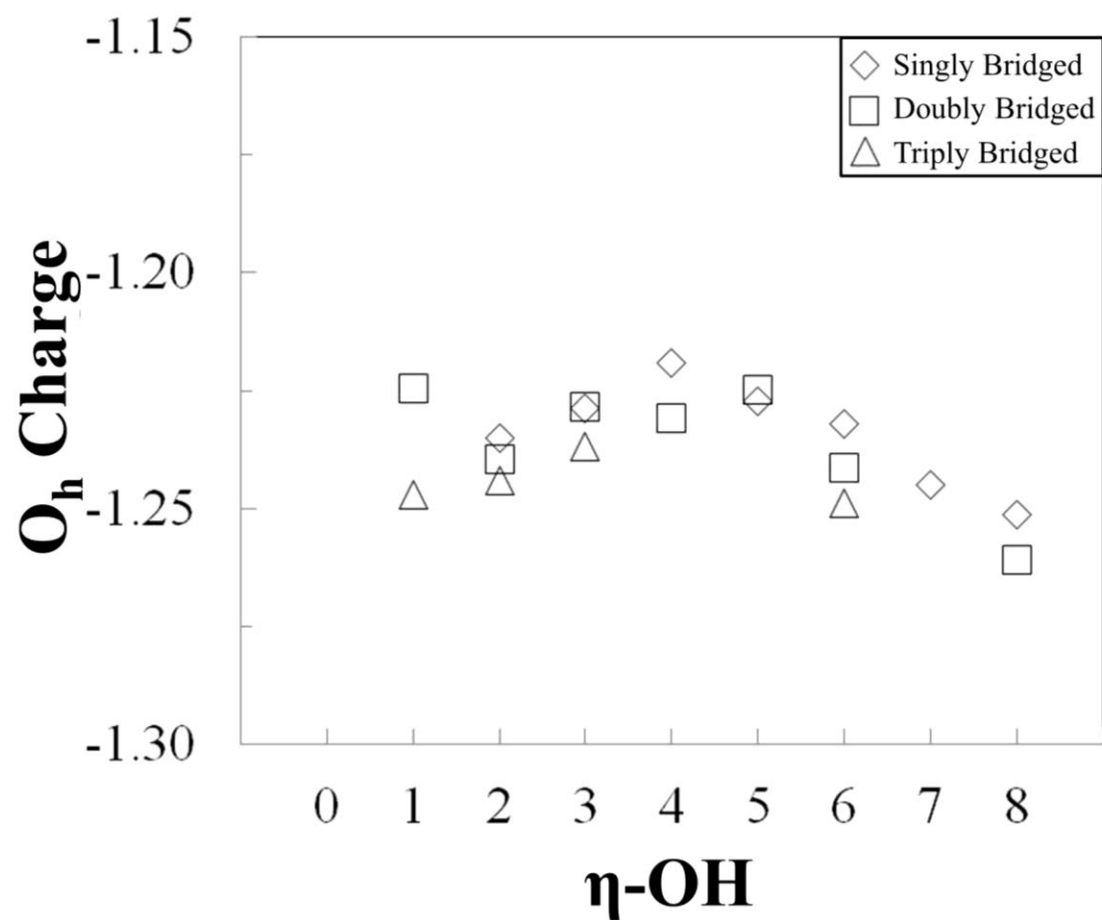
Figure S-4. Average hydroxide O Natural Charges as a function of number of η-OH ligands for the singly (diamonds), doubly (squares), and triply (triangles) bridged Al^{3+}-Dimer complexes.

Figure S-5. Average water O Natural Charges as a function of number of η-OH_2 ligands for the singly (diamonds), doubly (squares), and triply (triangles) bridged Al^{3+}-Dimer complexes.
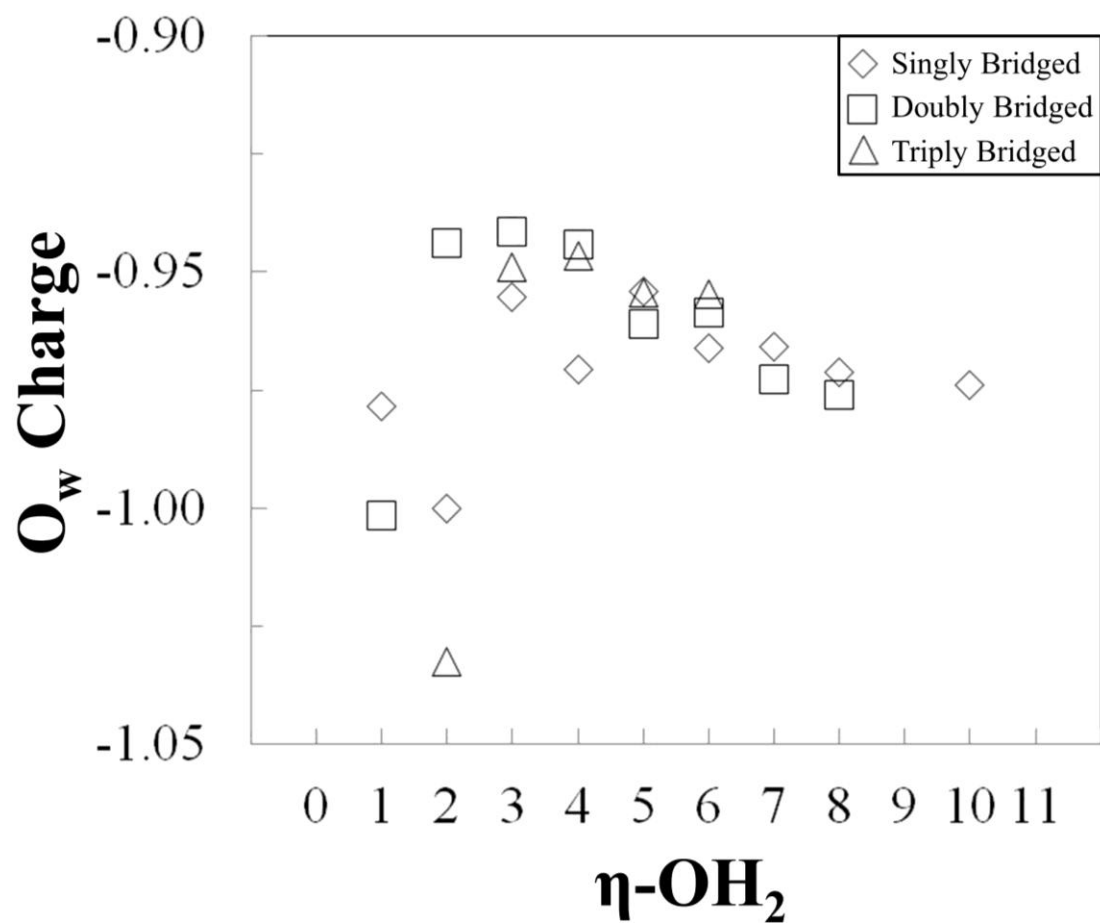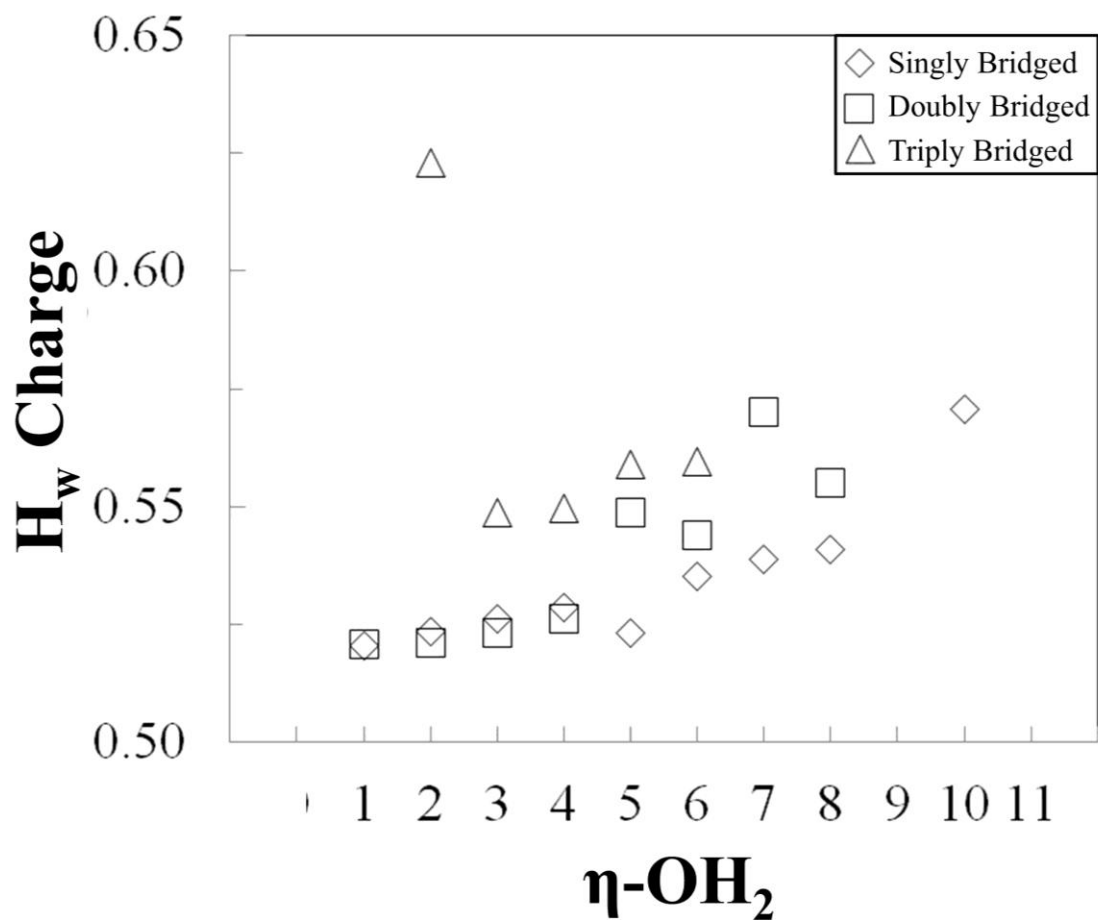
Figure S-6. Average water H Natural Charges as a function of number of η-OH$_2$ ligands for the singly (diamonds), doubly (squares), and triply (triangles) bridged Al^{3+}-Dimer complexes.
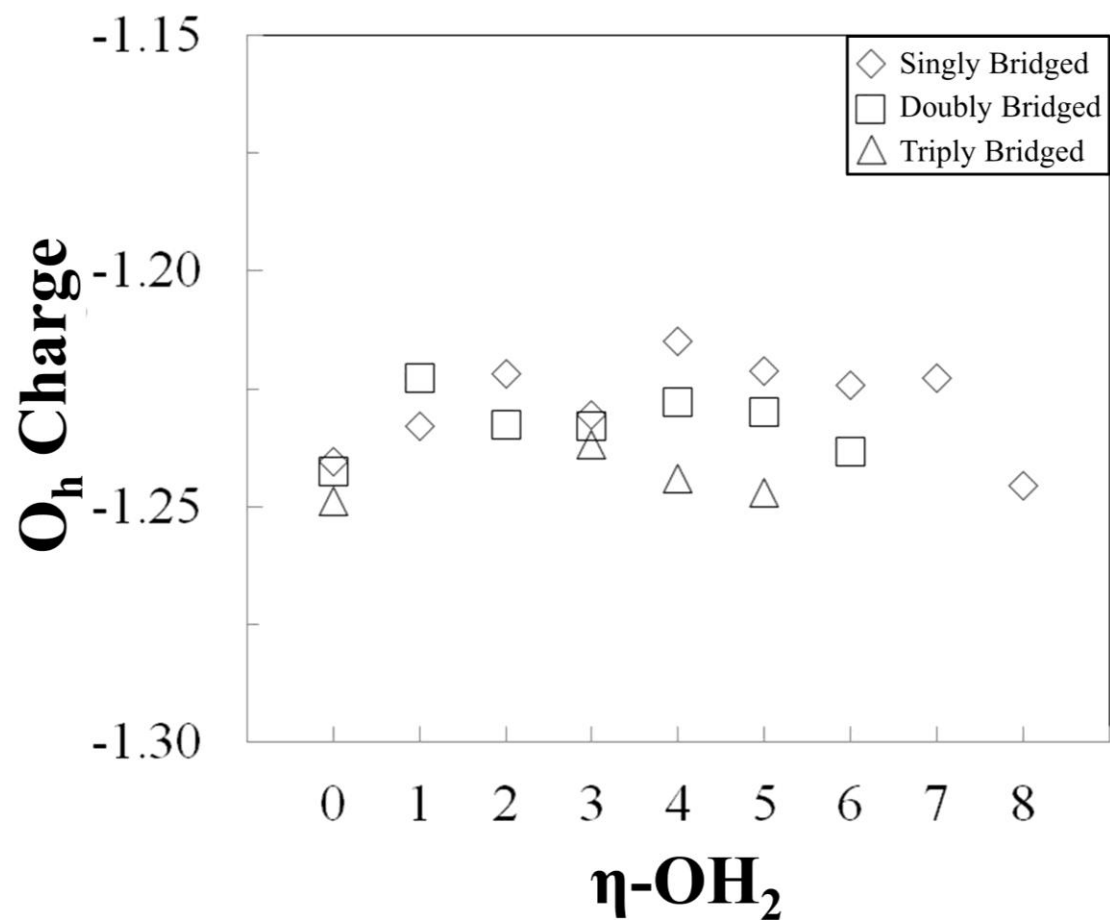
Figure S-7. Average hydroxide O Natural Charges as a function of number of η-OH$_2$ ligands for the singly (diamonds), doubly (squares), and triply (triangles) bridged Al^{3+}-Dimer complexes.
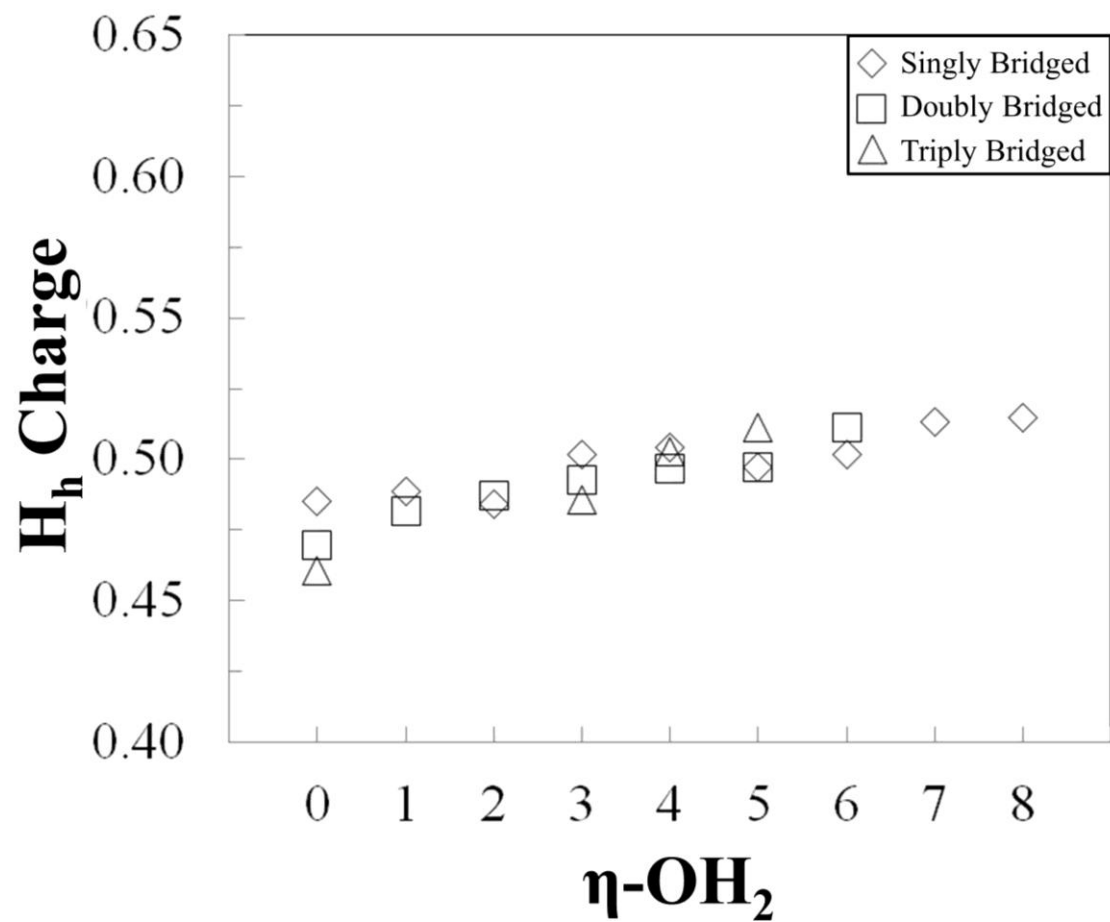
Figure S-8. Average hydroxide H Natural Charges as a function of number of η-OH$_2$ ligands for the singly (diamonds), doubly (squares), and triply (triangles) bridged Al^{3+}-Dimer complexes.
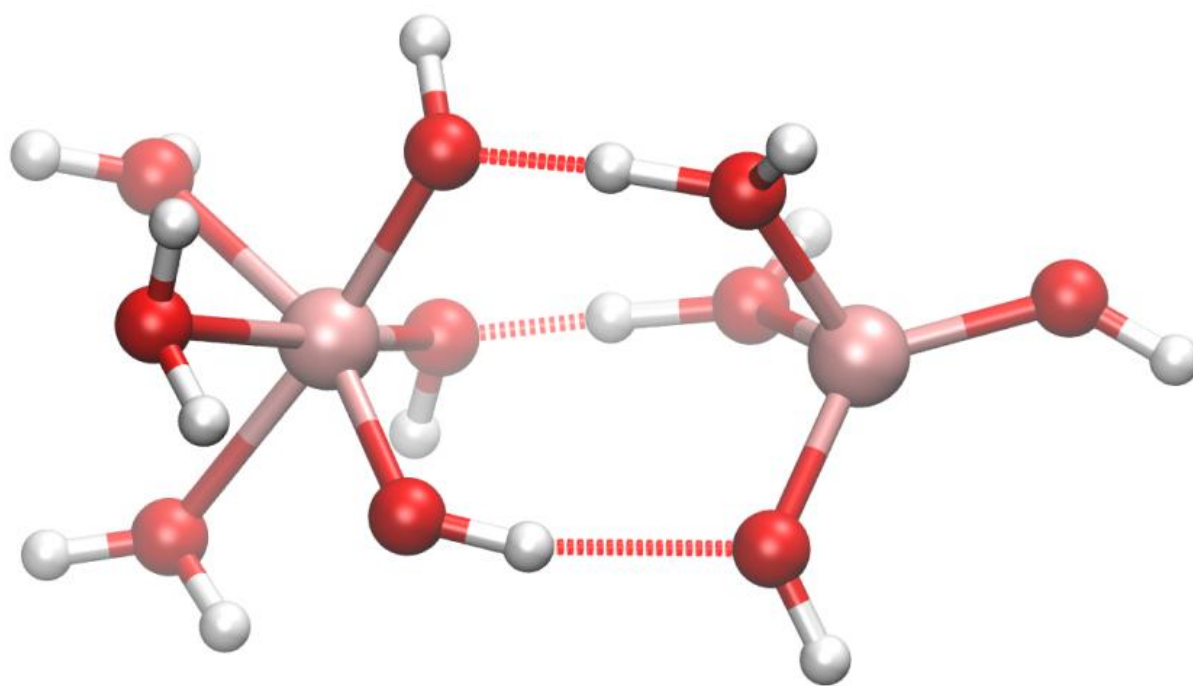
Figure S-9. HB-Bridged Al-Dimer species.