Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Rydberg electron capture by neutral Al hydrolysis products

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Contents:

Tables providing Al species type, number and type of coordinating ligands, total charge and Dipole moment of optimized geometry. For dimer species with identical hydroxide and water ligand coordination numbers (separated by shaded rows in the table) relative DFT energies are also provided.

Table I: Al monomer species

Al-monomers	Number of waters	number of hydroxides	number of Aluminums	Charge	Dipole Moment (Debye)
1	3	3	1	0	1.08
2	2	3	1	0	1.37
3	2	3	1	0	1.37
4	1	3	1	0	2.12

Table II: Al-F monomer species

AlF-monomers	Number of waters	number of hydroxides	number of Aluminums	Charge	Dipole Moment (Debye)
1	3	2	1	0	0.43
2	2	2	1	0	0.08
3	2	2	1	0	0.07
4	1	2	1	0	3.00

Table III: Al dimer species

Dimers	Number of waters	number of hydroxides	number of Aluminums	Charge	Dipole Moment (Debye)	Relative Energy (kcal/mol)
1	2	6	2	0	0.0154	N/A
2	3	6	2	0	1.68	1.81
3	3	6	2	0	1.59	0.34
4	3	6	2	0	2.05	0.00
5	3	6	2	0	1.52	0.93
6	3	6	2	0	2.09	0.20
7	3	6	2	0	2.16	2.40
8	3	6	2	0	2.03	0.00
9	3	6	2	0	1.68	1.81
10	3	6	2	0	1.30	2.38
11	3	6	2	0	1.94	1.70
12	3	6	2	0	1.33	2.17
13	3	6	2	0	0.85	5.93
14	3	6	2	0	6.59	14.43
15	3	6	2	0	2.29	5.71
16	3	6	2	0	3.35	5.74
17	3	6	2	0	3.30	9.35

18	3	6	2	0	4.56	9.56
19	3	6	2	0	2.98	5.89
20	3	6	2	0	3.33	7.18
21	3	6	2	0	4.87	20.79
22	3	6	2	0	3.91	21.38
23	3	6	2	0	4.00	21.37
24	4	6	2	0	3.43	2.12
25	4	6	2	0	3.18	2.44
26	4	6	2	0	9.45	18.33
27	4	6	2	0	1.82	0.27
28	4	6	2	0	1.41	0.52
29	4	6	2	0	0.01	20.26
30	4	6	2	0	2.96	17.58
31	4	6	2	0	0.00	1.80
32	4	6	2	0	0.65	0.00
33	5	6	2	0	1.65	2.07
34	5	6	2	0	1.75	0.14
35	5	6	2	0	2.78	1.96
36	5	6	2	0	1.78	0.14
37	5	6	2	0	3.25	0.10
38	5	6	2	0	3.44	0.00
39	5	6	2	0	2.68	2.99