Supporting Information

A Face-sharing Bi-icosahedral Model for Al_{23}^-

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1. Full citation of Gaussian 09

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2. Results

Table S1. Atomic Coordinates of Structure 1

Atom	X	Y	Z
Al1	-0.010088	3.273765	1.511195
Al2	1.627642	1.150858	1.879481
Al3	-0.01214	4.388427	-0.91696
Al4	1.523458	2.231297	-0.63272
Al5	2.882801	0.111583	-0.20627
Al6	2.729265	-1.27559	2.296806
Al7	3.953448	-2.32658	0.191268
Al8	-0.00819	2.669647	-3.0088
Al9	1.489166	0.403399	-2.63378
Al10	2.672295	-1.92215	-2.07367

Al11	-1.63535	1.142476	1.879596
Al12	0.003088	-1.22277	2.447962
Al13	-1.53393	2.221452	-0.63384
Al14	0.001228	-0.08958	-0.20927
Al15	1.270537	-2.58188	0.308351
Al16	-1.49415	0.3953	-2.63539
Al17	0.006214	-2.13019	-2.12357
Al18	-2.72417	-1.29072	2.29784
Al19	-2.8799	0.093519	-0.20647
Al20	-1.25529	-2.58579	0.309345
Al21	-2.66115	-1.93849	-2.07493
Al22	-3.93933	-2.34833	0.190508
Al23	-0.00546	1.630331	4.043311

Table S2. Atomic Coordinates of Structure 2

Atom	X	Y	Z
Al1	-2.60907	-1.47313	1.590959
Al2	-2.73088	0.640102	3.431458
Al3	1.419064	2.800252	-1.93428
Al4	1.072813	0.710984	0.44528
Al5	1.87693	-4.00031	0.053517
Al6	-1.06024	2.167639	1.924511
Al7	1.019679	0.065435	-2.24635
Al8	1.093936	3.410469	0.777903
Al9	-0.30669	-0.54325	2.624117
Al10	1.895648	-1.80358	1.789092
Al11	-1.00307	-0.46536	-0.37912
Al12	-3.1797	1.02773	0.588131
Al13	-0.93669	2.289451	-0.74157
Al14	0.260513	-2.66817	-1.739
Al15	2.621781	-1.54733	-0.82682
Al16	-0.43108	-2.88445	0.960308
Al17	3.285491	1.062208	-1.06037
Al18	1.450832	1.537155	3.003877
Al19	-2.60689	-2.44937	-1.01508
Al20	-2.76664	0.890938	-1.99837
Al21	-0.64793	1.874755	-3.57364
Al22	-1.20778	-1.00025	-3.16987
Al23	3.489942	0.358073	1.495302

Table S3. Atomic Coordinates of Structure 3

Atom	X	Y	Z
Al1	-2.61793	-2.51396	0.614131
Al2	0.000031	-1.92871	0.47083
Al3	-1.53798	-0.74126	2.535499
Al4	-4.26733	-0.51213	1.758219
Al5	-2.61785	1.788826	1.869601
Al6	-4.3E-05	1.372573	1.434294
Al7	-1.53798	2.566076	-0.62597
Al8	-1.7E-05	0.554632	-1.90466
Al9	-1.54008	-1.82641	-1.90983
Al10	-2.61732	0.725336	-2.48401
Al11	-4.2675	-1.26546	-1.32223
Al12	-4.26717	1.780259	-0.43598
Al13	-2.02243	-0.00067	0.000186
Al14	1.540221	-1.82642	-1.90979
Al15	1.538038	2.566118	-0.62593
Al16	2.617315	0.725269	-2.48402
Al17	1.537867	-0.74118	2.535478
Al18	2.618025	-2.51382	0.614172
Al19	2.617769	1.788857	1.869664
Al20	4.26724	-0.51211	1.758405
Al21	4.267593	-1.26539	-1.32222
Al22	4.267111	1.780214	-0.43604
Al23	2.022412	-0.00063	0.000185

Table S4. Atomic Coordinates of Al_{33}^-

Atom	X	Y	Z
Al1	-4.426128	2.690808	0.000387
Al2	-1.854191	2.159537	0.000562
Al3	-3.403253	1.282483	-2.289428
Al4	-6.119529	0.964363	-1.587916
Al5	-4.469298	-1.339701	-2.251689
Al6	-1.893013	-1.056394	-1.705199
Al7	-3.423856	-2.694342	-0.000641
Al8	-1.892951	-1.057119	1.704948
Al9	-3.403475	1.281576	2.289972
Al10	-4.469124	-1.340899	2.251150
Al11	-6.119535	0.963600	1.588278
Al12	-6.145053	-1.778403	-0.000247

Al13	-3.984300	0.031053	0.000050
Al14	-0.608358	1.289472	2.350666
Al15	-0.660849	-3.010864	-0.000876
Al16	0.614410	-1.284824	2.375478
Al17	-0.608457	1.290407	-2.350258
Al18	0.665849	3.024853	0.000721
Al19	0.614352	-1.284059	-2.375653
Al20	1.888467	1.034672	-1.636114
Al21	1.888534	1.034033	1.636342
Al22	1.850588	-2.120149	-0.000450
Al23	-0.033407	-0.021616	0.000019
Al24	3.441014	2.709730	0.000547
Al25	6.144501	1.803811	0.000239
Al26	4.460544	1.337970	-2.250649
Al27	3.405630	-1.284203	-2.295777
Al28	6.117291	-0.979565	-1.618832
Al29	4.424588	-2.686919	-0.000346
Al30	6.117316	-0.980205	1.618451
Al31	4.460711	1.337004	2.250975
Al32	3.405634	-1.285035	2.295361
Al33	4.015348	-0.031076	-0.000071

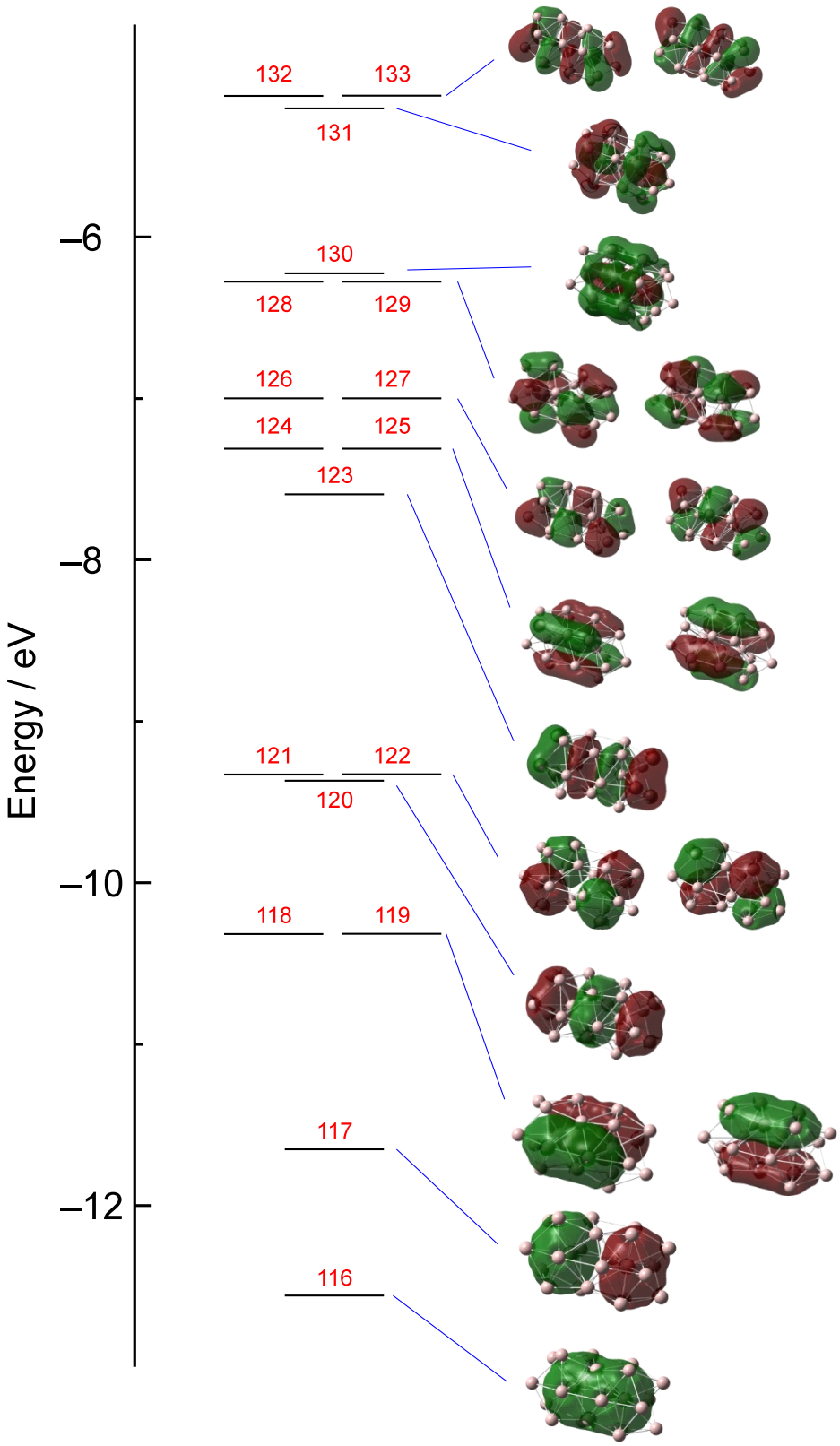

Figure S1. Energy diagram and shapes of the low-lying occupied SAOs (#116–#133) of structure **3**. The isovalue is 0.020.

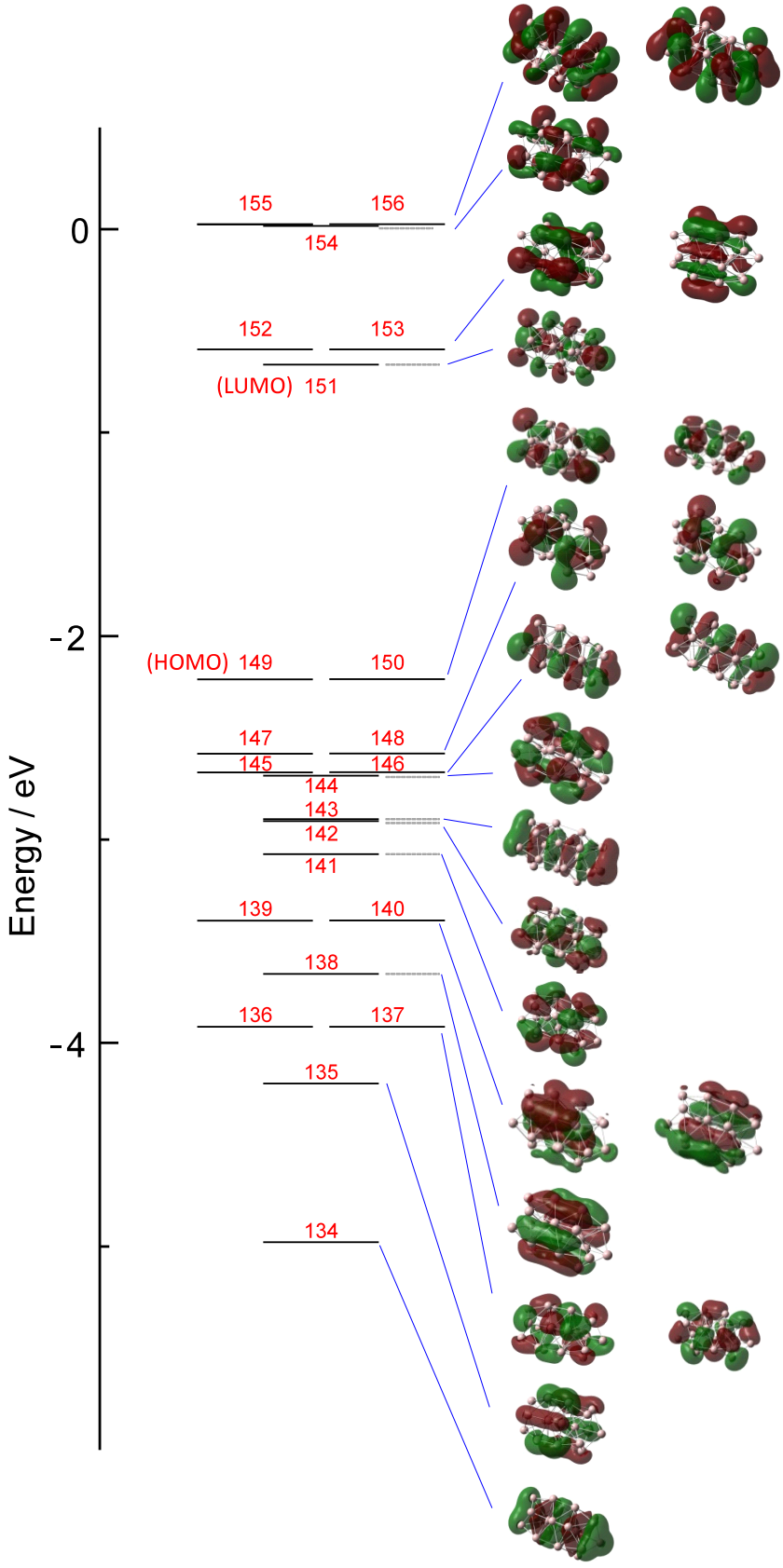

Figure S2. Energy diagram and shapes of the high-lying occupied (#134–#150) and unoccupied SAOs (#151–#156) of structure **3**. The isovalue is 0.020, except for #155 and #156 orbitals, for which the isovalue of 0.014 is used.

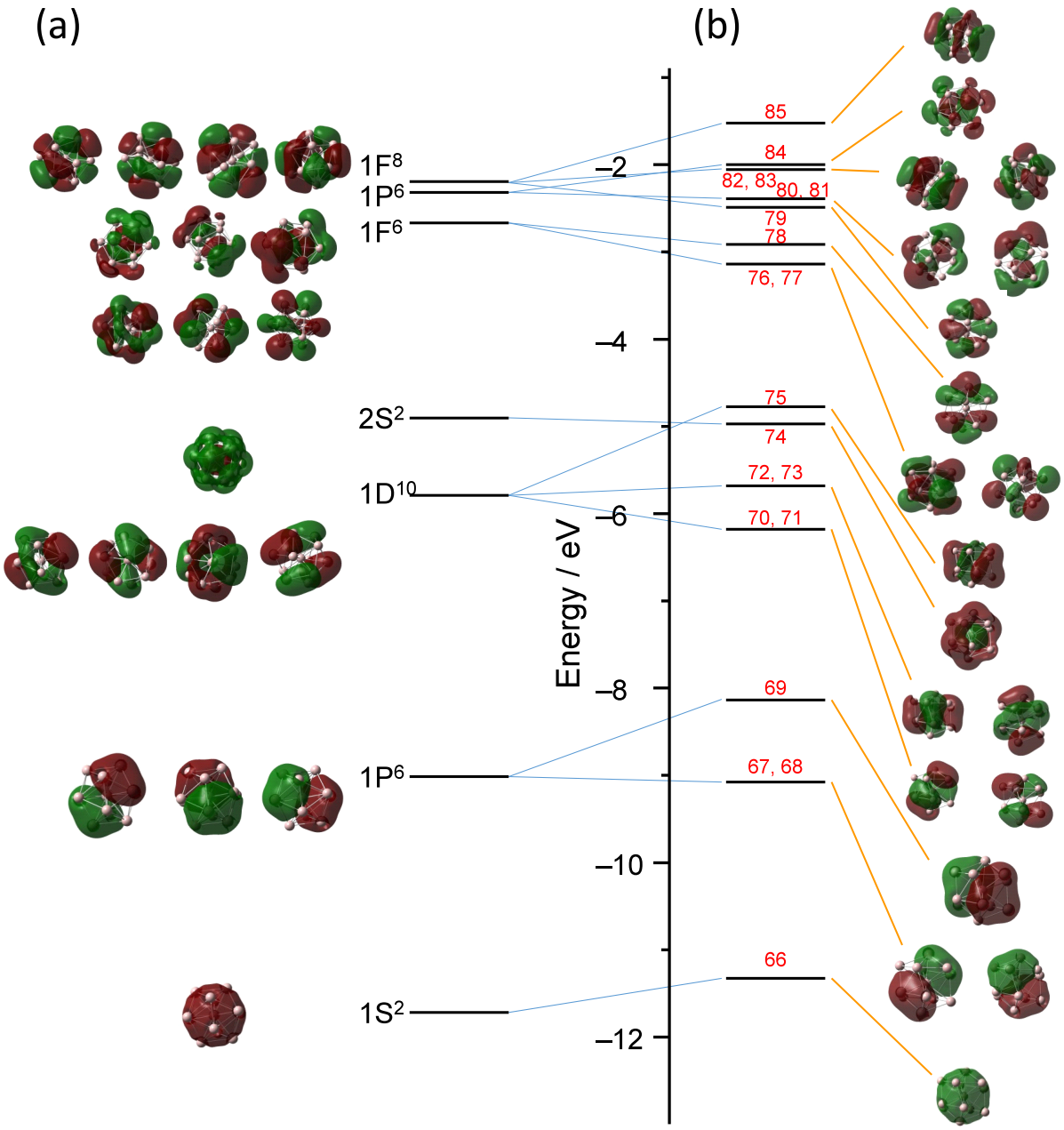

Figure S3. Energy diagram and shapes of SAOs of (a) Al_{13}^- (I_h) and (b) Al_{13}^- (D_{3d}). The isovalue is 0.020.

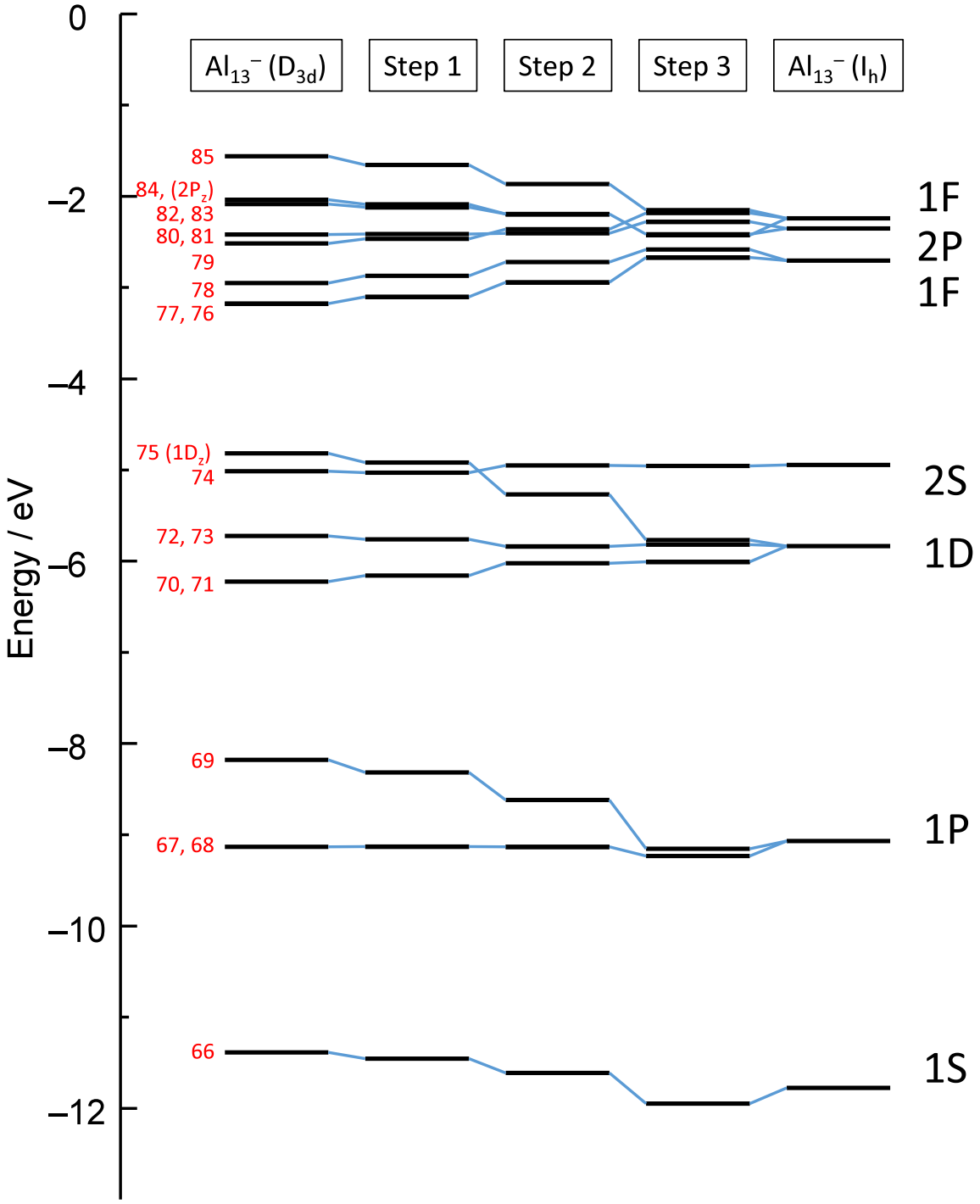

Figure S4. Evolution of the energy levels of SAOs of Al_{13}^- at three optimization steps during the optimization process (Figure S6).

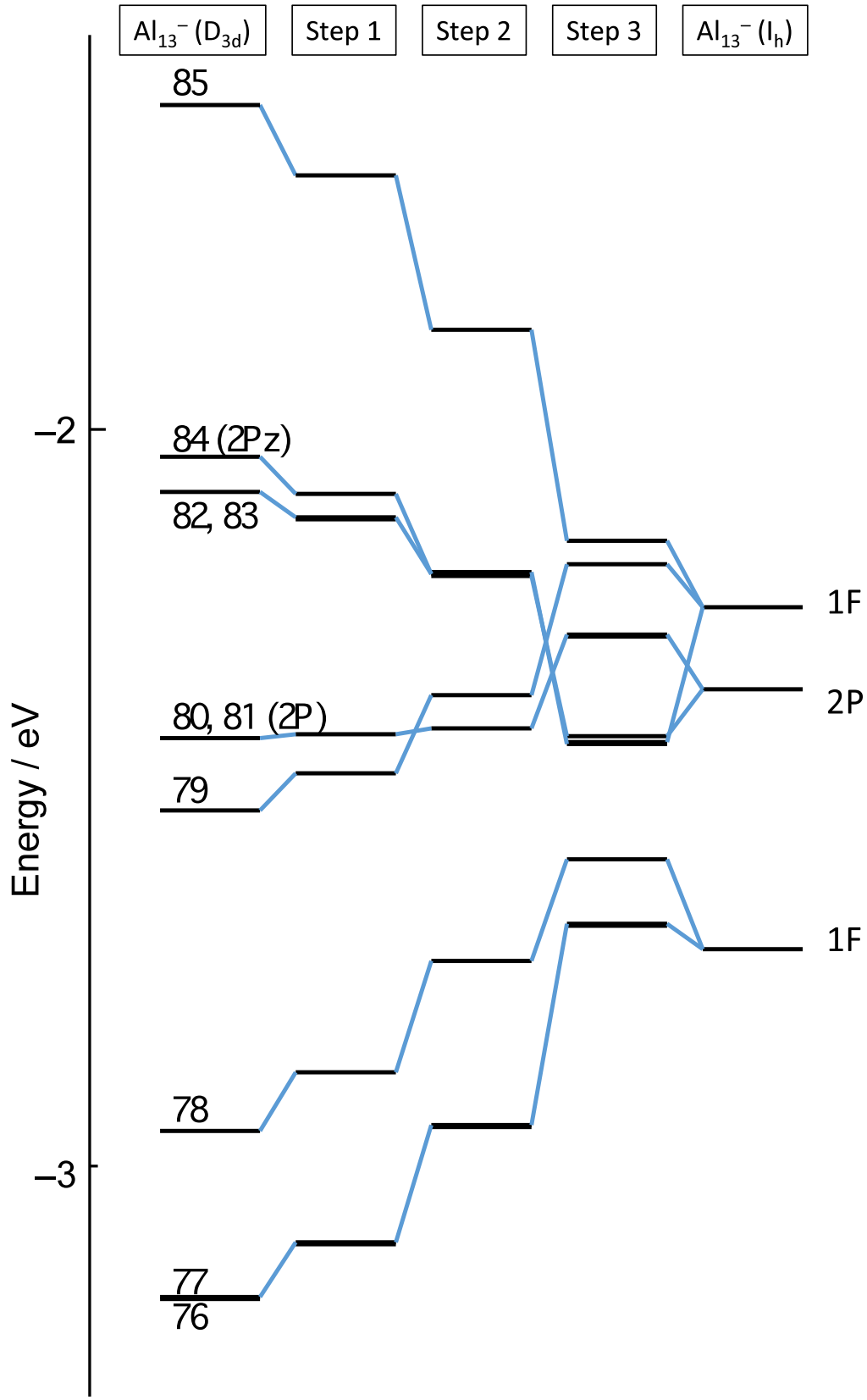

Figure S5. Evolution of the energy levels of 1F and 2P SAOs of Al_{13}^- at three steps during the optimization process (Figure S6).

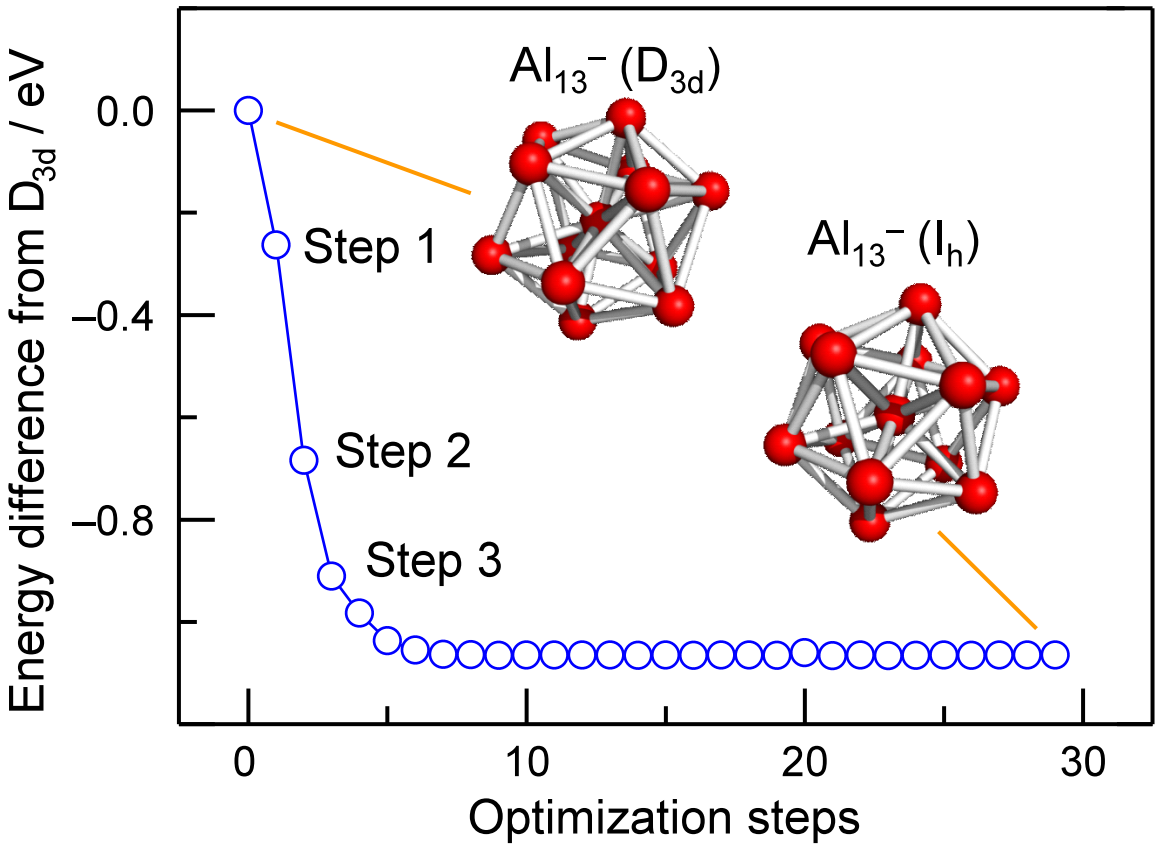

Figure S6. Evolution of the total energy of Al_{13}^- during the optimization process.