SUPPORTING INFORMATION

STRENGTHENED COOPERATIVITY OF DNA-BASED CYCLIC HYDROGEN-BONDED ROSETTES BY SUBTLE FUNCTIONALIZATION

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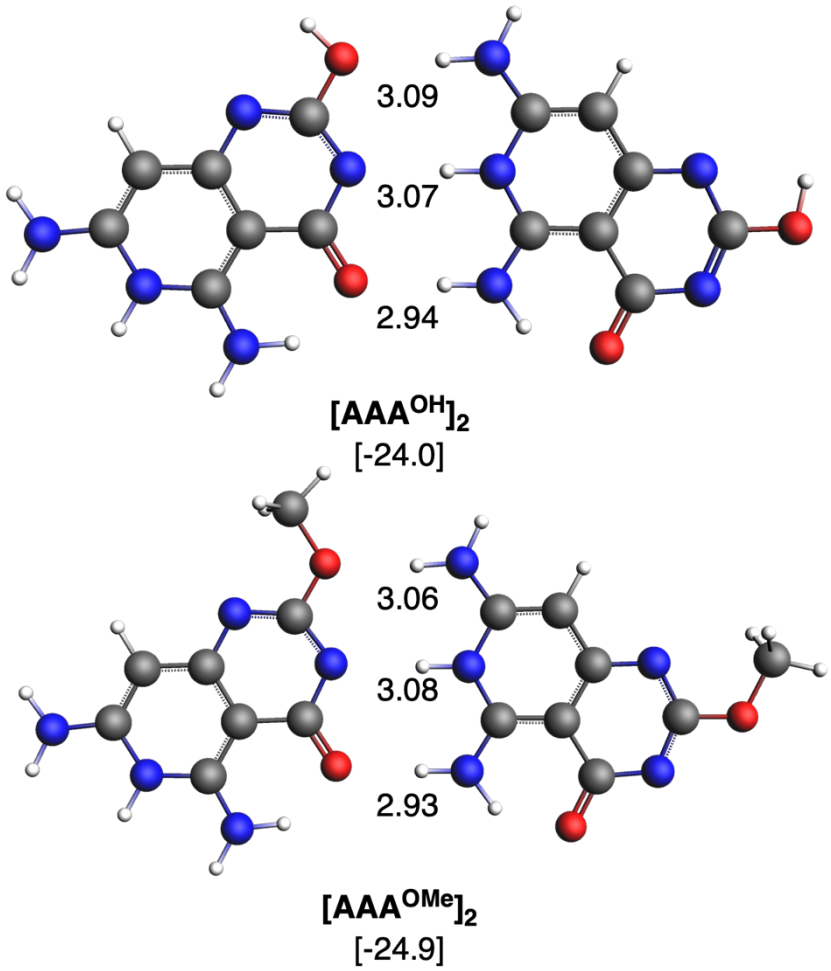

Figure S1. Optimized structures of hydrogen-bonded dimers of **AAA^{OH}** together with its tautomer with O-CH_3, both with C_s symmetry computed at ZORA-BLYP-D3(BJ)/TZ2P level. Bond lengths (in Å) and bonding energies (between brackets, in kcal mol^{-1}, computed with monomers in C_1 symmetry) are included.

Table S1. Energy decomposition analysis (in kcal mol^{-1}) for the formation of the **AAD**, **AA**, **AAA** and **AAA^{OH}** rosettes in a stepwise one-way direction, computed at ZORA-BLYP-D3(BJ)/TZ2P level.

AAD	**1+1**	**2+1**	**3+1**	**4+1**	**5+1**	**Synergy**
ΔE_{int}	-33.6	-35.7	-36.5	-37.5	-75.5	-12.7
ΔE_{oi}^{σ}	-26.6	-26.9	-27.0	-27.1	-55.6	-3.7
ΔE_{oi}^{π}	-4.4	-4.7	-4.8	-4.9	-10.5	-2.8
ΔE_{oi}	-31.0	-31.6	-31.8	-32.1	-66.1	-6.5
ΔE_{Pauli}	51.8	51.4	51.3	51.4	103.9	-1.0
ΔV_{elstat}	-47.8	-48.9	-49.3	-50.1	-100.0	-5.2
ΔE_{disp}	-6.6	-6.6	-6.7	-6.7	-13.3	0.0

AA	**1+1**	**2+1**	**3+1**	**4+1**	**5+1**	**Synergy**
ΔE_{int}	-24.2	-28.2	-29.6	-31.3	-66.6	-32.1
ΔE_{oi}^{σ}	-19.3	-20.3	-20.6	-20.9	-44.5	-9.4
ΔE_{oi}^{π}	-3.3	-3.9	-4.1	-4.5	-11.1	-7.2
ΔE_{oi}	-22.6	-24.1	-24.7	-25.3	-55.6	-16.6
ΔE_{Pauli}	39.5	39.0	38.9	38.8	79.0	-1.8
ΔV_{elstat}	-35.7	-37.7	-38.4	-39.3	-79.1	-13.7
ΔE_{disp}	-5.4	-5.4	-5.4	-5.5	-10.9	0.0

AAA	**1+1**	**2+1**	**3+1**	**4+1**	**5+1**	**Synergy**
ΔE_{int}	-26.7	-35.9	-39.9	-44.9	-92.5	-61.2
ΔE_{oi}^{σ}	-17.8	-19.6	-20.3	-20.9	-45.6	-17.1
ΔE_{oi}^{π}	-3.2	-4.2	-4.7	-5.3	-14.1	-12.0
ΔE_{oi}	-21.0	-23.8	-25.0	-26.2	-60.7	-30.1
ΔE_{Pauli}	38.9	37.9	37.7	37.5	77.1	-4.1
ΔV_{elstat}	-38.9	-44.2	-46.8	-50.4	-97.3	-27.0
ΔE_{disp}	-5.7	-5.8	-5.8	-5.8	-11.6	0.0

AAA^{OH}	**1+1**	**2+1**	**3+1**	**4+1**	**5+1**	**Synergy**
ΔE_{int}	-29.4	-39.1	-43.2	-48.4	-100.0	-66.2
ΔE_{oi}^{σ}	-21.8	-23.8	-24.4	-25.3	-56.6	-20.6
ΔE_{oi}^{π}	-3.5	-4.4	-5.4	-5.5	-14.6	-12.3
ΔE_{oi}	-25.3	-28.2	-29.8	-30.8	-71.2	-32.9
ΔE_{Pauli}	46.8	45.6	45.4	45.2	93.0	-4.7
ΔV_{elstat}	-44.5	-50.1	-52.4	-56.4	-109.0	-28.6
ΔE_{disp}	-6.4	-6.4	-6.4	-6.4	-12.8	0.0

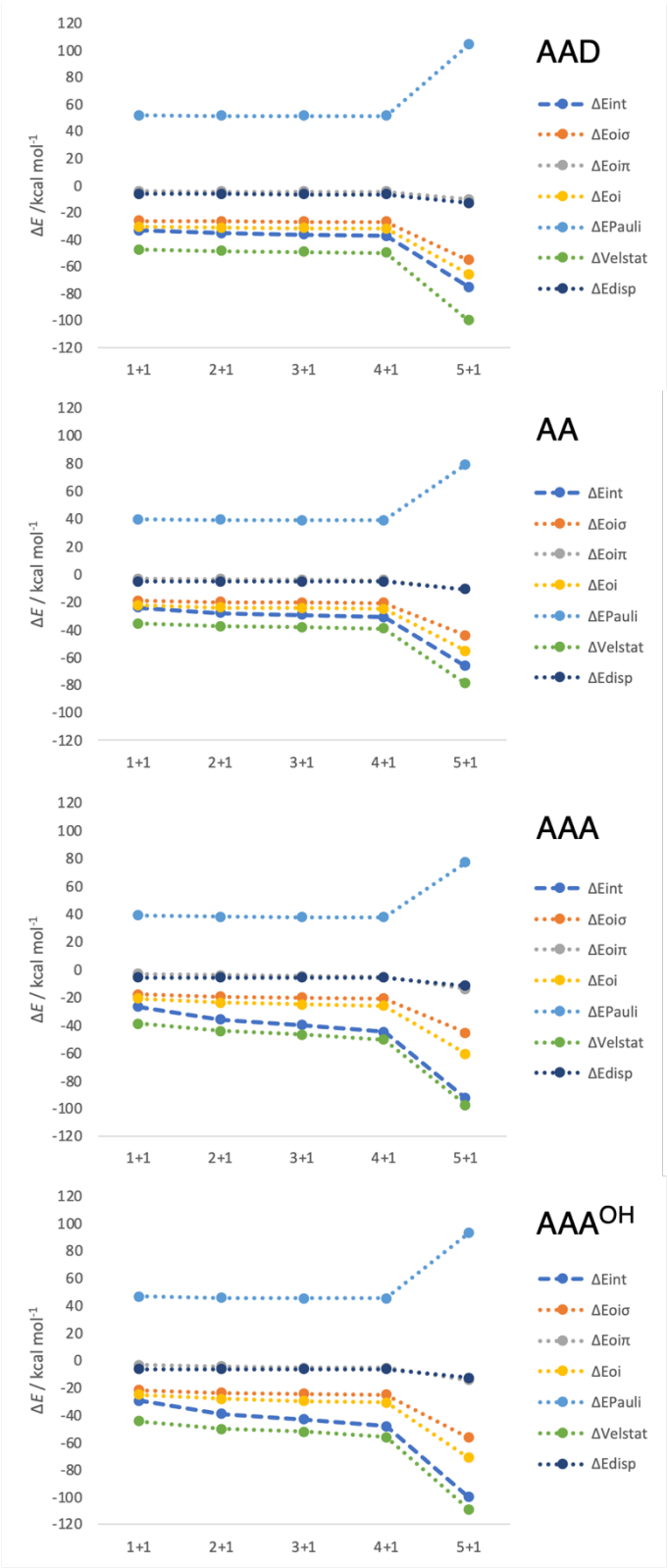

Figure S2. Schematic representation of the energy decomposition analysis (in kcal mol^{-1}) for the formation in a stepwise one-way direction of **AAD**, **AA**, **AAA** and **AAA^{OH}** rosettes. Computed at ZORA-BLYP-D3(BJ)/TZ2P level.

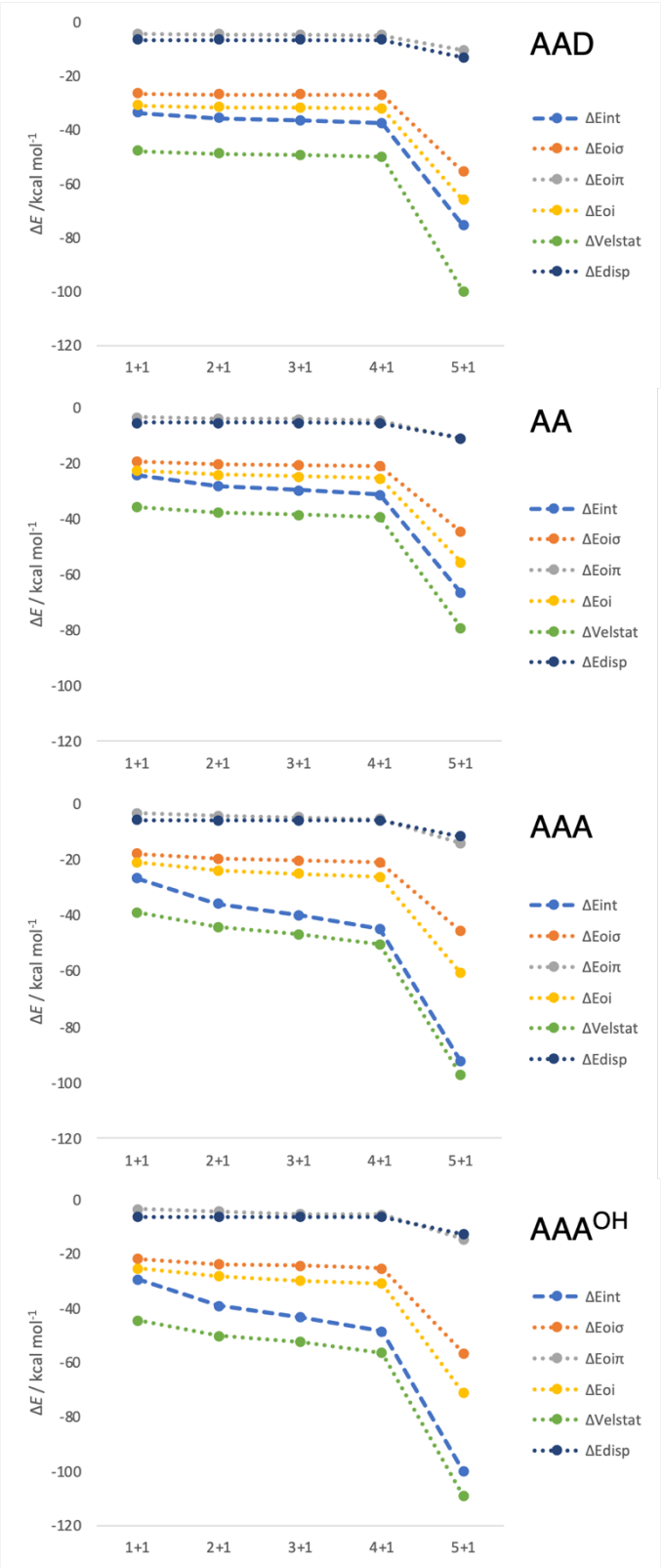

Figure S3. Schematic representation of the attractive terms of the energy decomposition analysis (in kcal mol^{-1}) for the formation in a stepwise one-way direction of **AAD**, **AA**, **AAA** and **AAA^{OH}** rosettes. Computed at ZORA-BLYP-D3(BJ)/TZ2P level.

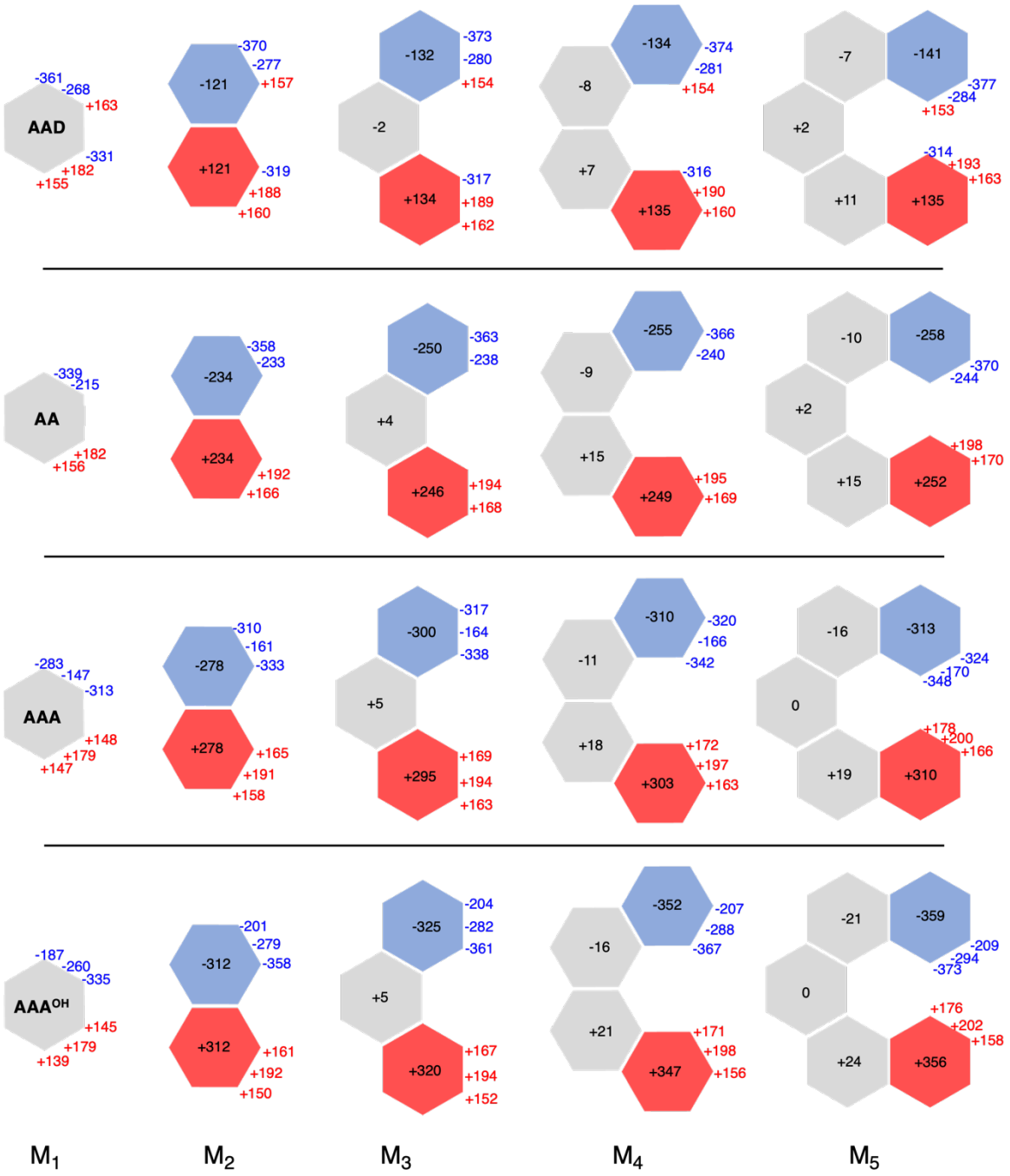

Figure S4. VDD charges (in milli-electrons) in the formation of **AAD**, **AA**, **AAA** and **AAA^{OH}** cyclic structures. Values in black are whole charges of the monomer, whereas values in blue and red correspond to charges of hydrogen-bond acceptor and donor atoms, respectively.

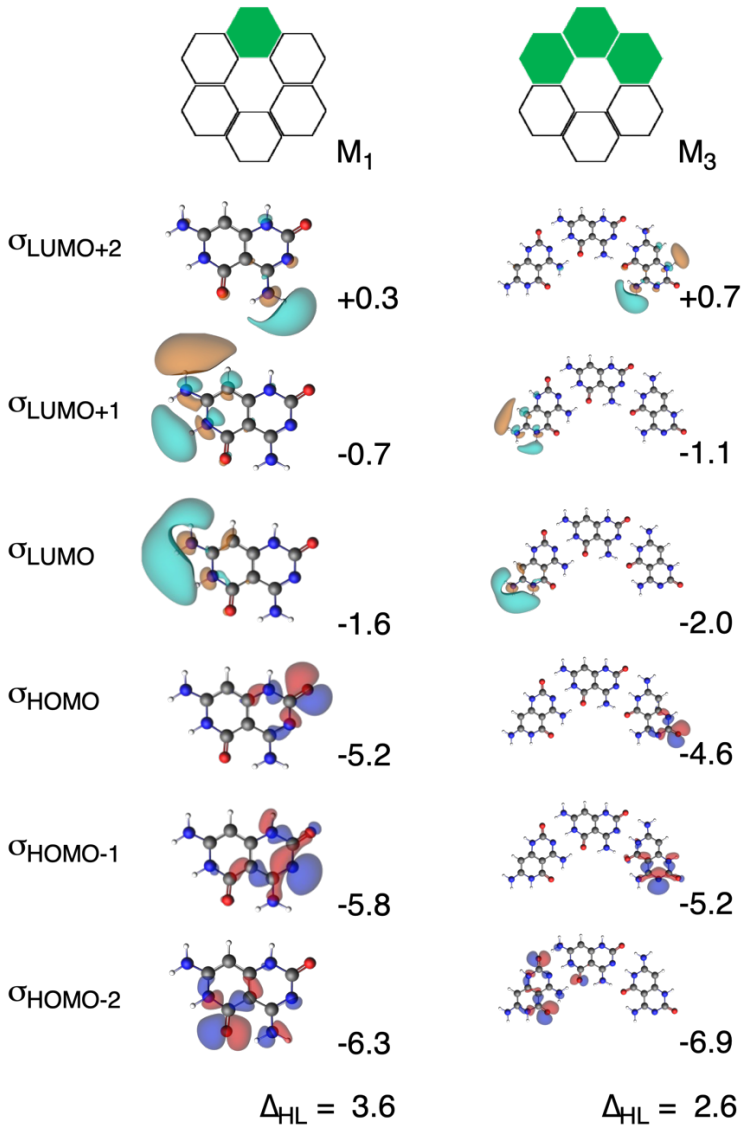

Figure S5. N-H unoccupied σ_{LUMO} orbitals and oxygen and nitrogen lone-pair σ_{HOMO} orbitals of the front atoms of **AAD** and their corresponding energies (in eV) for stepwise M_1 and M_3 states, computed at ZORA-BLYP-D3(BJ)/TZ2P level. HOMO LUMO gap (Δ_{HL}, in eV) also included.

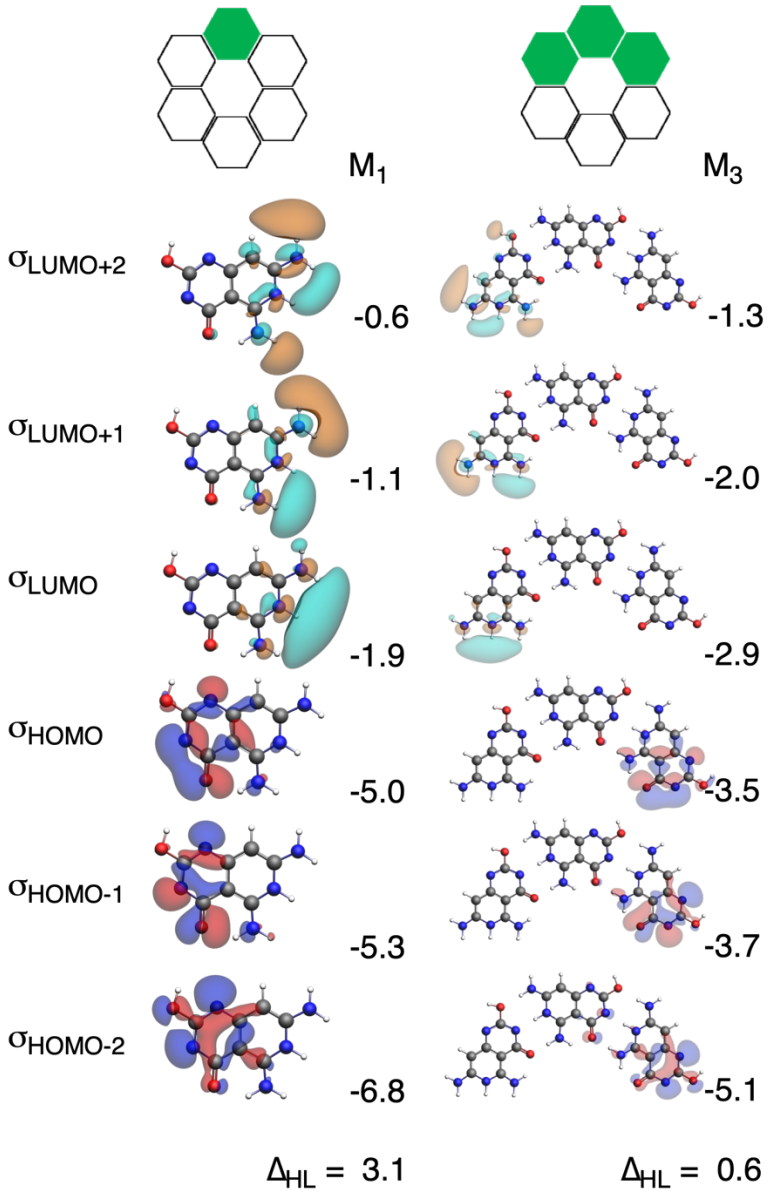

Figure S6. N-H unoccupied σ_{LUMO} orbitals and oxygen and nitrogen lone-pair σ_{HOMO} orbitals of the front atoms of **AAA^{OH}** and their corresponding energies (in eV) for stepwise M_1 and M_3 states, computed at ZORA-BLYP-D3(BJ)/TZ2P level. HOMO LUMO gap (Δ_{HL}, in eV) also included.

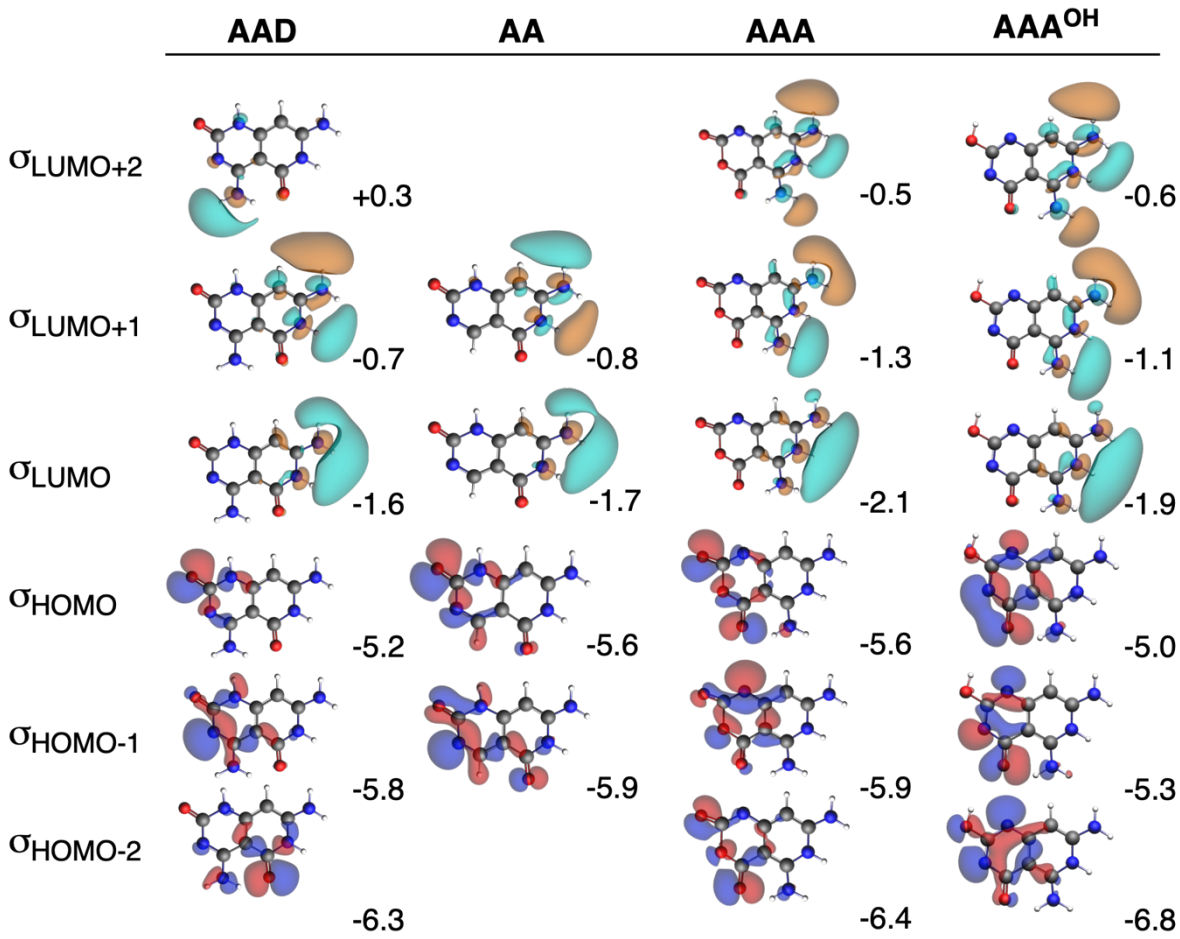

Figure S7. N-H unoccupied σ_{LUMO} orbitals and oxygen and nitrogen lone-pair σ_{HOMO} orbitals of the front atoms of the **AAD**, **AA**, **AAA** and **AAA^{OH}** monomers (equilibrium geometries) and their corresponding energies (in eV).

Table S2. Cartesian coordinates (in Å) and total ADF electronic energies (in kcal mol^{-1}) of all monomers optimized at ZORA-BLYP-D3(BJ)/TZ2P with restricted C_s symmetry.

AAD monomer

E (ZORA-BLYP-D3(BJ)/TZ2P): −3195.59

1	C	−2.454168	−8.412086	0.000000
2	N	2.419636	−7.125619	0.000000
3	H	−0.408487	−4.566700	−0.000000
4	O	1.367836	−5.098198	0.000000
5	C	−1.263726	−6.382974	0.000000
6	N	3.657781	−9.077517	0.000000
7	C	2.436966	−8.496170	0.000000
8	H	1.226938	−10.285825	−0.000000
9	H	3.721420	−10.085226	−0.000000
10	H	3.331324	−6.594845	0.000000
11	H	−2.213714	−4.559654	0.000000
12	O	−3.501556	−9.093993	−0.000000
13	C	1.222115	−9.200470	0.000000
14	N	−1.213150	−9.098062	0.000000
15	N	−2.439968	−7.056282	−0.000000
16	C	0.010626	−7.063818	0.000000
17	H	−1.278202	−10.111100	0.000000
18	N	−1.306548	−5.050806	0.000000
19	C	1.259001	−6.353908	0.000000
20	H	4.535309	−8.525292	0.000000
21	C	0.018731	−8.476631	0.000000

AA monomer

E (ZORA-BLYP-D3(BJ)/TZ2P): −2912.94

1	N	4.836674	−5.612949	0.000000
2	O	4.983636	−1.343331	0.000000
3	O	6.088086	−7.553877	0.000000
4	H	3.888009	−3.779473	0.000000
5	C	4.858291	−4.277278	0.000000
6	C	7.279737	−4.186005	0.000000
7	N	7.212620	−5.565337	0.000000
8	H	9.444287	−4.025279	0.000000
9	C	6.021239	−6.309012	0.000000
10	N	7.271060	−1.433061	0.000000
11	C	8.465123	−2.092997	0.000000
12	H	7.266475	−0.376871	0.000000
13	H	10.482777	−1.800985	0.000000
14	C	6.027590	−3.508429	0.000000
15	H	8.067263	−6.115953	0.000000
16	C	5.996511	−2.042911	0.000000
17	N	9.584178	−1.339593	0.000000
18	C	8.493145	−3.502242	0.000000
19	H	9.560912	−0.302860	0.000000

AAA monomer

E (ZORA-BLYP-D3(BJ)/TZ2P): −3058.14

1	N	−3.701184	−3.708097	0.000000
2	H	−2.825987	−4.258128	0.000000
3	N	−6.038848	−7.70016	0.000000
4	H	−4.078805	−6.174802	0.000000
5	O	−9.596642	−1.516165	0.000000
6	C	−6.104044	−2.114149	0.000000
7	C	−4.905651	−4.278540	0.000000
8	O	−7.306611	−1.483007	0.000000
9	C	−8.650189	−2.286728	0.000000
10	H	−3.701688	−2.688751	0.000000
11	C	−6.158036	−6.354580	0.000000
12	H	−6.877108	−8.263635	0.000000
13	H	−8.305105	−6.195416	0.000000
14	H	−5.126365	−8.177909	0.000000
15	C	−7.363763	−5.656913	0.000000
16	N	−4.965156	−5.650636	0.000000
17	C	−7.377219	−4.245866	0.000000
18	C	−6.122029	−3.547442	0.000000
19	O	−5.073752	−1.404277	0.000000
20	N	−8.574824	−3.599648	0.000000

AAA-OH monomer

E (ZORA-BLYP-D3(BJ)/TZ2P): -3173.11

1	C	7.359614	5.634709	0.000000
2	H	2.825872	4.220124	0.000000
3	O	9.658463	1.549524	0.000000
4	H	8.300846	6.173913	0.000000
5	H	5.158664	8.162170	0.000000
6	O	5.088373	1.361333	0.000000
7	C	6.153429	6.319518	0.000000
8	C	6.149636	2.055805	0.000000
9	H	10.341815	2.249784	0.000000
10	H	6.899236	8.224967	0.000000
11	C	6.126573	3.510501	0.000000
12	H	3.735494	2.645163	0.000000
13	H	4.057636	6.161073	0.000000
14	C	4.906110	4.247007	0.000000
15	N	8.551961	3.546837	0.000000
16	N	6.052963	7.675991	0.000000
17	C	7.360967	4.222836	0.000000
18	N	4.962409	5.622546	0.000000
19	C	8.453105	2.224847	0.000000
20	N	7.382844	1.428992	0.000000
21	N	3.708294	3.668207	0.000000

Table S3. Cartesian coordinates (in Å) and total ADF electronic energies (in kcal mol^{-1}) of all monomers optimized at ZORA-BLYP-D3(BJ)/TZ2P with C_1 symmetry, confirmed by frequency analysis.

AAD monomer

E (ZORA–BLYP–D3(BJ)/TZ2P): –3200.07

1.C	–2.458225	–8.415793	0.006271
2.N	2.426024	–7.127990	0.093722
3.H	–0.454076	–4.519313	0.130623
4.O	1.418050	–5.077529	0.131860
5.C	–1.284335	–6.390468	0.074255
6.N	3.679855	–9.103506	–0.020420
7.C	2.438059	–8.497780	0.050203
8.H	1.237345	–10.271328	0.001224
9.H	3.689505	–10.105445	0.133569
10.H	3.294937	–6.600992	0.054394
11.H	–2.238438	–4.595594	0.114933
12.O	–3.458533	–9.126648	–0.020828
13.C	1.243296	–9.186611	0.022414
14.N	–1.173991	–9.083299	–0.006374
15.N	–2.439547	–7.049649	0.046523
16.C	0.018594	–7.040455	0.068957
17.H	–1.226207	–10.097247	–0.039725
18.N	–1.329290	–5.040151	0.111083
19.C	1.258672	–6.311739	0.101799
20.H	4.457257	–8.623133	0.421020
21.C	0.029212	–8.450503	0.024496

AA monomer

E (ZORA–BLYP–D3(BJ)/TZ2P): –2916.55

1.C	2.422676	–8.388224	0.058738
2.H	–1.321135	–5.255931	0.009803
3.C	–0.018734	–6.973620	0.024684
4.N	2.392743	–7.018621	0.068389
5.H	–1.238266	–10.033689	–0.015117
6.N	3.666607	–8.981479	0.016083
7.O	1.337213	–4.981790	0.044651
8.H	1.253445	–10.188507	0.041797
9.H	3.698725	–9.977819	0.197130
10.C	1.210910	–6.205247	0.046297
11.C	0.019225	–8.385151	0.016586
12.H	3.257329	–6.483856	0.030752
13.O	–3.476425	–9.056961	–0.038724
14.N	–2.456035	–6.968793	–0.014718
15.C	1.237389	–9.103628	0.039579
16.N	–1.190062	–9.017750	–0.006910
17.C	–1.297590	–6.347382	0.005863
18.H	4.453592	–8.467485	0.396487
19.C	–2.469641	–8.362686	–0.021371

AAA monomer

E (ZORA–BLYP–D3(BJ)/TZ2P): –3063.11

1.C	–6.131201	3.501209	0.035522
2.C	–4.861524	4.224220	0.058541
3.N	–5.032199	1.347616	0.044517
4.H	–10.585794	1.832391	0.035035
5.N	–9.707077	1.323892	0.007522
6.H	–5.049354	0.378318	0.333974
7.H	–9.526938	4.061592	0.045007
8.N	–7.416651	5.577704	–0.023889
9.N	–7.373949	1.455694	0.095772
10.C	–8.584487	2.146785	0.065487
11.H	–4.165864	1.904568	0.108661
12.C	–8.592267	3.510594	0.033190
13.H	–7.395402	0.462097	–0.111713
14.H	–9.711279	0.539317	0.656195
15.O	–4.951385	5.575556	0.037127
16.O	–3.748207	3.685530	0.098808
17.O	–6.150728	7.507529	–0.066374
18.C	–7.359445	4.249493	0.002909
19.C	–6.153939	2.104073	0.069377
20.C	–6.272254	6.310649	–0.025666

AAA-OH monomer

E (ZORA-BLYP-D3(BJ)/TZ2P): −3178.52

1.N	−7.362997	1.481227	0.092122
2.H	−7.384034	0.478551	−0.066850
3.C	−4.846961	4.278457	0.061005
4.C	−6.131911	6.187187	−0.004732
5.O	−6.165029	7.548752	−0.036061
6.C	−6.142524	2.129606	0.081768
7.H	−7.114755	7.782358	−0.061990
8.N	−9.698015	1.335102	−0.001229
9.N	−7.362788	5.601478	−0.017583
10.H	−4.987221	0.415882	0.239101
11.H	−10.574743	1.848195	0.011513
12.C	−8.586944	3.530590	0.032701
13.H	−4.159880	2.042000	0.113940
14.H	−9.524082	4.077763	0.041797
15.N	−4.927190	5.648795	0.035239
16.O	−3.738411	3.678140	0.095093
17.C	−7.349305	4.259505	0.010319
18.C	−6.121846	3.532832	0.048701
19.H	−9.712153	0.577348	0.679478
20.C	−8.575606	2.165962	0.062013
21.N	−5.004316	1.414768	0.083652

Table S4. Cartesian coordinates (in Å) and total ADF electronic energies (in kcal mol^{-1}) of all dimers optimized at ZORA-BLYP-D3(BJ)/TZ2P with restricted C_s symmetry.

[AAD]$_2$

E (ZORA–BLYP–D3(BJ)/TZ2P): –6429.35

1	C	–2.466459	–8.499681	0.000000
2	O	5.187356	–1.252838	0.000000
3	H	–0.554055	–4.557614	0.000000
4	O	1.315493	–5.070398	0.000000
5	C	–1.335322	–6.449700	0.000000
6	C	7.334876	–4.196188	0.000000
7	H	9.514790	–4.128506	0.000000
8	H	1.263603	–10.271413	0.000000
9	H	3.736493	–10.036405	0.000000
10	H	3.277466	–6.552702	0.000000
11	H	–2.337906	–4.679817	0.000000
12	N	7.461701	–1.465540	0.000000
13	H	10.688223	–1.924662	0.000000
14	H	9.800925	–0.440291	0.000000
15	H	8.092019	–6.132794	0.000000
16	C	–0.020591	–7.067847	0.000000
17	C	6.124267	–3.473301	0.000000
18	C	8.594315	–3.554541	0.000000
19	H	2.823784	–4.138504	0.000000
20	N	4.873058	–5.579699	0.000000
21	C	0.021751	–8.484909	0.000000
22	N	2.385144	–7.091378	0.000000
23	N	3.664741	–9.029656	0.000000
24	C	2.432652	–8.463419	0.000000
25	N	9.797605	–1.449779	0.000000
26	O	6.101036	–7.528007	0.000000
27	H	3.727587	–2.576656	0.000000
28	C	8.636566	–2.169721	0.000000
29	C	6.153063	–2.032432	0.000000
30	H	7.462071	–0.448355	0.000000
31	C	4.882049	–4.228825	0.000000
32	H	4.532347	–8.473167	0.000000
33	O	–3.458164	–9.227749	0.000000
34	C	1.241544	–9.186252	0.000000
35	N	7.252121	–5.562056	0.000000
36	N	–2.478809	–7.131564	0.000000
37	C	6.028854	–6.285701	0.000000
38	N	–1.416692	–5.097761	0.000000
39	C	1.209144	–6.332610	0.000000
40	N	3.709033	–3.595327	0.000000
41	H	–1.208045	–10.153930	0.000000
42	N	–1.176495	–9.138972	0.000000

[AA]$_2$

E (ZORA–BLYP–D3(BJ)/TZ2P): –5854.06

1.	C	2.399430	–8.457711	0.000000
2.	O	4.928527	–1.382927	0.000000
3.	O	6.210396	–7.564515	0.000000
4.	H	3.877692	–3.884418	0.000000
5.	H	–1.331155	–9.976479	0.000000
6.	C	7.289867	–4.166846	0.000000
7.	O	1.436539	–5.022094	0.000000
8.	H	1.160574	–10.225281	0.000000
9.	H	3.648335	–10.086151	0.000000
10.	N	7.220693	–1.427634	0.000000
11.	C	8.437334	–2.054126	0.000000
12.	H	3.324180	–6.590677	0.000000
13.	H	10.467785	–1.682782	0.000000
14.	C	6.024604	–3.528929	0.000000
15.	H	8.152188	–6.058917	0.000000
16.	N	–1.243009	–8.963648	0.000000
17.	C	–1.241199	–6.295351	0.000000
18.	C	8.497088	–3.444539	0.000000
19.	H	9.488512	–0.257024	0.000000
20.	N	4.898019	–5.665264	0.000000
21.	C	4.868578	–4.343168	0.000000
22.	N	2.413661	–7.090925	0.000000
23.	N	3.610704	–9.077737	0.000000
24.	C	1.274235	–6.250972	0.000000

25.C	−0.002898	−8.381338	0.000000
26.C	5.938463	−2.075483	0.000000
27.N	9.548354	−1.265282	0.000000
28.C	1.181254	−9.140042	0.000000
29.H	4.491606	−8.557022	0.000000
30.C	−2.491768	−8.260991	0.000000
31.H	7.159654	−0.411807	0.000000
32.C	0.009349	−6.964252	0.000000
33.O	−3.528053	−8.918364	0.000000
34.C	6.105941	−6.333628	0.000000
35.N	7.277762	−5.539100	0.000000
36.N	−2.428592	−6.870635	0.000000
37.H	9.458375	−3.947344	0.000000
38.H	−1.223446	−5.203659	0.000000

[AAA]$_2$

E (ZORA–BLYP–D3(BJ)/TZ2P): −6148.37

1.N	−3.661375	−3.846608	0.000000
2.H	−2.811862	−4.394118	0.000000
3.N	−6.135058	−7.809628	0.000000
4.H	−4.129414	−6.317585	0.000000
5.O	−9.497190	−1.552963	0.000000
6.H	−5.019603	0.476475	0.000000
7.H	−9.556308	4.112939	0.000000
8.O	−7.213789	−1.553448	0.000000
9.N	−7.352143	1.550148	0.000000
10.C	−8.577020	2.209121	0.000000
11.C	−6.206539	−6.445873	0.000000
12.C	−8.608213	3.585263	0.000000
13.H	−7.339632	0.531026	0.000000
14.H	−9.613533	0.384898	0.000000
15.C	−7.376287	−5.725007	0.000000
16.O	−3.771650	3.863041	0.000000
17.C	−7.350017	−4.301505	0.000000
18.C	−7.400095	4.344056	0.000000
19.O	−4.976597	−1.518198	0.000000
20.N	−8.518519	−3.644674	0.000000
21.C	−6.152956	3.626966	0.000000
22.C	−4.903341	4.373335	0.000000
23.C	−8.554157	−2.310920	0.000000
24.H	−3.641831	−2.820171	0.000000
25.N	−9.676638	1.401085	0.000000
26.N	−7.482147	5.680994	0.000000
27.H	−4.158647	2.057985	0.000000
28.N	−4.986493	−5.774468	0.000000
29.C	−6.071160	−3.642605	0.000000
30.C	−6.018352	−2.192536	0.000000
31.C	−6.361271	6.433513	0.000000
32.H	−6.987028	−8.351966	0.000000
33.H	−10.590771	1.827607	0.000000
34.H	−5.259981	−8.312818	0.000000
35.C	−4.888516	−4.398352	0.000000
36.C	−6.148244	2.223280	0.000000
37.H	−8.335924	−6.230315	0.000000
38.O	−5.018027	5.725241	0.000000
39.O	−6.255545	7.637555	0.000000
40.N	−5.017076	1.493200	0.000000

[AAA–OH]$_2$

E (ZORA–BLYP–D3(BJ)/TZ2P): −6381.04

1.N	−7.344761	1.557625	0.000000
2.H	−7.350845	0.527008	0.000000
3.C	−4.839464	4.375931	0.000000
4.H	−4.107437	−6.199252	0.000000
5.O	−9.657549	−1.638372	0.000000
6.C	−6.130027	2.214593	0.000000
7.H	−3.818580	−2.655331	0.000000
8.N	−4.984204	−5.687744	0.000000
9.C	−8.462861	−2.299839	0.000000
10.H	−6.881569	−8.344024	0.000000
11.H	−10.580965	1.890365	0.000000
12.C	−8.569220	3.612382	0.000000
13.N	−6.052361	−7.768449	0.000000
14.H	−9.510357	4.153220	0.000000
15.N	−4.927464	5.750827	0.000000
16.O	−3.721793	3.789972	0.000000

17.C	−7.382208	−4.303573	0.000000
18.C	−6.176990	−6.405184	0.000000
19.O	−5.096808	−1.449955	0.000000
20.C	−8.552231	2.236936	0.000000
21.H	−10.349380	−2.330540	0.000000
22.C	−6.138288	6.278242	0.000000
23.C	−7.372477	−5.727688	0.000000
24.H	−7.134559	7.863125	0.000000
25.N	−9.675636	1.447339	0.000000
26.N	−7.360882	5.692742	0.000000
27.H	−5.013479	0.469086	0.000000
28.H	−4.154551	2.089215	0.000000
29.C	−6.144165	−3.592232	0.000000
30.C	−6.163551	−2.124525	0.000000
31.H	−9.630872	0.436644	0.000000
32.H	−2.860348	−4.186382	0.000000
33.N	−8.559913	−3.640339	0.000000
34.H	−5.157831	−8.235467	0.000000
35.C	−6.108435	3.624095	0.000000
36.H	−8.313192	−6.267584	0.000000
37.N	−3.742001	−3.691892	0.000000
38.C	−4.933946	−4.307933	0.000000
39.N	−5.003371	1.488797	0.000000
40.O	−6.180007	7.649589	0.000000
41.N	−7.393830	−1.510916	0.000000
42.C	−7.341915	4.341135	0.000000

Table S5. Cartesian coordinates (in Å) and total ADF electronic energies (in kcal mol^{-1}) of all dimers optimized at ZORA-BLYP-D3(BJ)/TZ2P with C_1 symmetry, confirmed by frequency analysis.

[AAD]$_2$

E (ZORA–BLYP–D3(BJ)/TZ2P): –6429.65

1.C	–2.465486	–8.498145	0.006287
2.O	5.185055	–1.251779	–0.005581
3.H	–0.551504	–4.556745	–0.003382
4.O	1.318381	–5.070732	–0.004970
5.C	–1.333442	–6.448645	0.001237
6.C	7.334147	–4.193475	0.000662
7.H	9.515330	–4.122013	0.021441
8.H	1.263683	–10.271794	0.002685
9.H	3.737004	–10.038041	–0.000468
10.H	3.278845	–6.554130	–0.004528
11.H	–2.335258	–4.678349	–0.000461
12.N	7.460276	–1.462131	0.011080
13.H	10.660179	–1.938587	0.140156
14.H	9.789749	–0.488866	0.320629
15.H	8.094687	–6.128435	–0.003095
16.C	–0.018896	–7.067459	0.000092
17.C	6.124788	–3.470908	0.000281
18.C	8.594316	–3.548862	0.011971
19.H	2.824203	–4.138697	–0.008666
20.N	4.874931	–5.578144	–0.003885
21.C	0.022739	–8.484583	0.002070
22.N	2.386688	–7.092421	–0.003263
23.N	3.665567	–9.031275	–0.002424
24.C	2.433611	–8.464487	–0.001406
25.N	9.800391	–1.435197	–0.043384
26.O	6.103763	–7.525900	–0.001588
27.H	3.727472	–2.575975	–0.009673
28.C	8.634207	–2.166761	0.010988
29.C	6.152488	–2.028742	0.002256
30.H	7.464614	–0.445934	–0.037633
31.C	4.882382	–4.227532	–0.004733
32.H	4.533074	–8.475189	–0.002759
33.O	–3.457425	–9.225730	0.009292
34.C	1.242233	–9.186628	0.001223
35.N	7.253890	–5.558923	–0.001750
36.N	–2.477138	–7.130002	0.004165
37.C	6.030851	–6.284006	–0.002262
38.N	–1.414208	–5.096690	–0.000664
39.C	1.211120	–6.332951	–0.002824
40.N	3.709341	–3.594739	–0.008500
41.H	–1.207793	–10.153016	0.006466
42.N	–1.175706	–9.138066	0.004917

[AA]$_2$

E (ZORA–BLYP–D3(BJ)/TZ2P): –5854.06

1.C	2.400961	–8.460169	–0.054128
2.O	4.932062	–1.385441	–0.158862
3.O	6.209403	–7.564332	0.046652
4.H	3.881743	–3.887058	–0.161457
5.H	–1.328669	–9.971497	0.106254
6.C	7.287325	–4.166566	0.044628
7.O	1.443439	–5.023227	–0.081074
8.H	1.160899	–10.224860	0.021716
9.H	3.647709	–10.085331	0.013509
10.N	7.219238	–1.427687	0.000166
11.C	8.432717	–2.053665	0.083916
12.H	3.327623	–6.594824	–0.105031
13.H	10.435483	–1.688826	0.319348
14.C	6.025516	–3.529599	–0.042936
15.H	8.148940	–6.056771	0.130327
16.N	–1.239507	–8.958996	0.083717
17.C	–1.234824	–6.291109	0.030681
18.C	8.492788	–3.441968	0.112144
19.H	9.462684	–0.281362	0.346766
20.N	4.900604	–5.666501	–0.075727
21.C	4.871011	–4.344985	–0.098832
22.N	2.416899	–7.093863	–0.082653
23.N	3.611361	–9.083392	–0.105510
24.C	1.279341	–6.251600	–0.056839

25.C	0.000328	−8.378947	0.028286
26.C	5.939856	−2.075915	−0.075380
27.N	9.547992	−1.258092	0.092895
28.C	1.183136	−9.139811	0.003129
29.H	4.489507	−8.561409	−0.042134
30.C	−2.486701	−8.254236	0.114022
31.H	7.163180	−0.413071	−0.057034
32.C	0.014312	−6.962342	−0.000714
33.O	−3.523088	−8.909431	0.163378
34.C	6.106058	−6.334144	0.012436
35.N	7.275959	−5.538253	0.067213
36.N	−2.421891	−6.864148	0.084654
37.H	9.451858	−3.943970	0.183811
38.H	−1.215673	−5.199661	0.008661

[AAA]$_2$

E (ZORA–BLYP–D3(BJ)/TZ2P): −6149.27

1.N	−3.688860	−3.860107	−0.434097
2.H	−2.833040	−4.394145	−0.366612
3.N	−6.090451	−7.768788	0.438129
4.H	−4.163976	−6.320207	−0.135070
5.O	−9.482257	−1.515767	0.101888
6.H	−5.022481	0.455939	−0.216260
7.H	−9.547180	4.097501	−0.140594
8.O	−7.223814	−1.544805	−0.226710
9.N	−7.350836	1.531856	−0.221768
10.C	−8.568865	2.199198	−0.269784
11.C	−6.185571	−6.395848	0.318292
12.C	−8.603460	3.562997	−0.107986
13.H	−7.341225	0.517059	−0.317223
14.H	−9.620231	0.414927	−0.290755
15.C	−7.347163	−5.673163	0.379069
16.O	−3.788065	3.793228	0.375002
17.C	−7.336324	−4.261990	0.158647
18.C	−7.400378	4.305934	0.098579
19.O	−5.008198	−1.529538	−0.535463
20.N	−8.497671	−3.601013	0.237559
21.C	−6.159745	3.580039	0.138385
22.C	−4.915198	4.310409	0.333608
23.C	−8.543059	−2.276142	0.065469
24.H	−3.674577	−2.840892	−0.554674
25.N	−9.659943	1.404633	−0.538767
26.N	−7.484826	5.633480	0.246083
27.H	−4.172783	2.000741	0.130996
28.N	−4.981118	−5.747766	0.053798
29.C	−6.074930	−3.626769	−0.109115
30.C	−6.033208	−2.189536	−0.306943
31.C	−6.369319	6.369988	0.442966
32.H	−6.949205	−8.236671	0.708591
33.H	−10.562172	1.840884	−0.394870
34.H	−5.273514	−8.142601	0.913040
35.C	−4.896161	−4.389328	−0.163581
36.C	−6.154304	2.185321	−0.021225
37.H	−8.289932	−6.157283	0.609822
38.O	−5.031505	5.654749	0.476353
39.O	−6.267623	7.563527	0.601016
40.N	−5.029785	1.443920	0.024205

[AAA–OH]$_2$

E (ZORA–BLYP–D3(BJ)/TZ2P): −6382.59

1.N	−0.692359	2.026960	−0.186466
2.H	−0.699157	0.995057	−0.205396
3.C	1.760112	4.829315	0.398015
4.H	2.477532	−5.722252	−0.282355
5.O	−2.960556	−1.072965	0.332304
6.C	0.498135	2.674869	0.067158
7.H	2.800270	−2.177940	−0.517302
8.N	1.647413	−5.180508	−0.060613
9.C	−1.785556	−1.752096	0.193106
10.H	−0.243786	−7.751087	0.487931
11.H	−3.872288	2.383227	−0.576295
12.C	−1.912368	4.078472	−0.276325
13.N	0.603397	−7.253942	0.232179
14.H	−2.842032	4.622591	−0.410619
15.N	1.664300	6.202494	0.457980
16.O	2.865563	4.240765	0.546674

17.C	−0.720462	−3.763092	0.187688
18.C	0.468014	−5.873579	0.198253
19.O	1.539512	−0.953468	−0.409855
20.C	−1.883803	2.708915	−0.358478
21.H	−3.646546	−1.750324	0.501108
22.C	0.467410	6.733477	0.287998
23.C	−0.707759	−5.184769	0.330592
24.H	−0.525027	8.319367	0.212827
25.N	−2.979481	1.913323	−0.674418
26.N	−0.734479	6.152062	0.048254
27.H	1.627598	0.944620	0.019160
28.H	2.448225	2.538239	0.374832
29.C	0.503290	−3.076672	−0.068472
30.C	0.487245	−1.613906	−0.188833
31.H	−2.984537	0.968257	−0.297929
32.H	3.750675	−3.712752	−0.491478
33.N	−1.881975	−3.088202	0.321445
34.H	1.419691	−7.620028	0.716006
35.C	0.511641	4.082295	0.151413
36.H	−1.632509	−5.704640	0.556994
37.N	2.873027	−3.212464	−0.450655
38.C	1.699525	−3.809171	−0.194714
39.N	1.609067	1.940865	0.236399
40.O	0.416975	8.101772	0.361367
41.N	−0.727783	−0.986718	−0.046780
42.C	−0.706155	4.803629	−0.022698

Table S6. Cartesian coordinates (in Å) and total ADF electronic energies (in kcal mol^{-1}) of all rosettes optimized at ZORA-BLYP-D3(BJ)/TZ2P with restricted C_s symmetry.

AAD rosette

E (ZORA-BLYP-D3(BJ)/TZ2P): -19391.85

1.H	-9.395109	-3.948772	0.000000
2.O	5.098834	-1.364267	0.000000
3.H	-0.408487	-4.566700	0.000000
4.H	-4.045173	-6.182429	0.000000
5.O	-9.626188	-1.514820	0.000000
6.C	7.350215	-4.221777	0.000000
7.C	6.138926	6.358612	0.000000
8.H	1.226938	-10.285825	0.000000
9.H	3.721420	-10.085226	0.000000
10.C	-2.436966	8.496170	0.000000
11.C	6.111728	3.541074	0.000000
12.C	-8.578689	3.541404	0.000000
13.H	10.594543	-1.819356	0.000000
14.N	-3.657781	9.077517	0.000000
15.H	8.117334	-6.162095	0.000000
16.N	-3.720811	3.656711	0.000000
17.C	-7.331148	-4.254567	0.000000
18.C	8.578689	-3.541404	0.000000
19.H	2.841941	-4.196791	0.000000
20.N	4.890922	-5.641029	0.000000
21.N	1.306548	5.050806	0.000000
22.N	2.419636	-7.125619	0.000000
23.N	3.657781	-9.077517	0.000000
24.H	5.055331	0.362737	0.000000
25.N	-9.690017	1.370624	0.000000
26.N	-7.272501	5.599303	0.000000
27.H	-3.721420	10.085226	0.000000
28.H	4.045173	6.182429	0.000000
29.C	-1.259001	6.353908	0.000000
30.C	-6.159406	-2.097076	0.000000
31.N	6.031810	7.706488	0.000000
32.C	8.511871	2.080789	0.000000
33.O	-3.501556	-9.093993	0.000000
34.H	-5.114694	-8.190231	0.000000
35.N	7.272501	-5.599303	0.000000
36.N	-2.439968	-7.056282	0.000000
37.C	2.454168	8.412086	0.000000
38.N	-1.306548	-5.050806	0.000000
39.C	1.263726	6.382974	0.000000
40.N	3.720811	-3.656711	0.000000
41.H	-1.278202	-10.111100	0.000000
42.N	-2.419636	7.125619	0.000000
43.N	-7.380562	1.466924	0.000000
44.H	-7.376748	0.411954	0.000000
45.C	-1.263726	-6.382974	0.000000
46.H	9.650508	-0.334538	0.000000
47.O	-1.367836	5.098198	0.000000
48.N	9.690017	-1.370624	0.000000
49.C	-8.511871	-2.080789	0.000000
50.N	7.330643	1.415063	0.000000
51.H	4.158865	1.929653	0.000000
52.H	6.872626	8.265563	0.000000
53.O	3.730815	3.733685	0.000000
54.N	-4.890922	5.641029	0.000000
55.H	1.278202	10.111100	0.000000
56.O	9.626188	1.514820	0.000000
57.O	3.501556	9.093993	0.000000
58.O	6.125002	-7.579236	0.000000
59.C	6.159406	2.097076	0.000000
60.H	-3.750555	2.636910	0.000000
61.N	5.027120	1.393922	0.000000
62.C	-0.010626	7.063818	0.000000
63.H	-5.055331	-0.362737	0.000000
64.H	-8.117334	6.162095	0.000000
65.C	0.010626	-7.063818	0.000000
66.C	2.436966	-8.496170	0.000000
67.N	-8.485292	-3.498535	0.000000
68.C	-6.122637	3.522382	0.000000
69.H	2.213714	4.559654	0.000000

70.H 0.408487 4.566700 0.000000
71.C −4.872741 −4.267273 0.000000
72.O −5.098834 1.364267 0.000000
73.C 6.131987 −2.086269 0.000000
74.N 4.960714 5.658233 0.000000
75.C 1.259001 −6.353908 0.000000
76.C 7.331148 4.254567 0.000000
77.C −6.131987 2.086269 0.000000
78.N 7.380562 −1.466924 0.000000
79.N 2.439968 7.056282 0.000000
80.H −6.872626 −8.265563 0.000000
81.N −6.031810 −7.706488 0.000000
82.H −9.521114 4.079805 0.000000
83.C −6.138926 −6.358612 0.000000
84.N −5.027120 −1.393922 0.000000
85.C −0.018731 8.476631 0.000000
86.H −2.213714 −4.559654 0.000000
87.C −6.057979 6.331238 0.000000
88.C 8.576152 −2.137192 0.000000
89.C 4.895935 −4.285706 0.000000
90.H 4.535309 −8.525292 0.000000
91.N −1.213150 −9.098062 0.000000
92.H −9.650508 0.334538 0.000000
93.H −2.841941 4.196791 0.000000
94.H −8.293835 −6.205421 0.000000
95.O −3.730815 −3.733685 0.000000
96.O 1.367836 −5.098198 0.000000
97.H −3.331324 6.594845 0.000000
98.H 9.395109 3.948772 0.000000
99.C 1.222115 −9.200470 0.000000
100.N 1.213150 9.098062 0.000000
101.C 4.872741 4.267273 0.000000
102.C −8.576152 2.137192 0.000000
103.C 6.057979 −6.331238 0.000000
104.C 7.356261 5.658621 0.000000
105.C 6.122637 −3.522382 0.000000
106.H 3.331324 −6.594845 0.000000
107.C −6.111728 −3.541074 0.000000
108.C 0.018731 −8.476631 0.000000
109.H 3.750555 −2.636910 0.000000
110.N −7.330643 −1.415063 0.000000
111.C −7.350215 4.221777 0.000000
112.C −4.895935 4.285706 0.000000
113.N 8.485292 3.498535 0.000000
114.N −4.960714 −5.658233 0.000000
115.H −1.226938 10.285825 0.000000
116.H −4.535309 8.525292 0.000000
117.H 5.114694 8.190231 0.000000
118.H −10.594543 1.819356 0.000000
119.C −7.356261 −5.658621 0.000000
120.H 8.293835 6.205421 0.000000
121.C −1.222115 9.200470 0.000000
122.H 7.376748 −0.411954 0.000000
123.H −4.158865 −1.929653 0.000000
124.C −2.454168 −8.412086 0.000000
125.O −6.125002 7.579236 0.000000
126.H 9.521114 −4.079805 0.000000

AA rosette

E (ZORA-BLYP-D3(BJ)/TZ2P): −17657.51

1.H −9.329467 −3.927922 0.000000
2.O 4.983636 −1.343331 0.000000
3.H −1.236227 10.190914 0.000000
4.H −3.958711 −6.102930 0.000000
5.O −9.585662 −1.495000 0.000000
6.C 7.279737 −4.186005 0.000000
7.C 6.044040 6.283267 0.000000
8.H 1.236227 −10.190914 0.000000
9.H 3.681953 −9.978135 0.000000
10.C −2.420225 8.376826 0.000000
11.C 6.051559 3.464516 0.000000
12.C −8.493145 3.502242 0.000000
13.H 10.482777 −1.800985 0.000000
14.N −3.632230 8.969227 0.000000
15.H 8.067263 −6.115953 0.000000
16.H −3.888009 3.779473 0.000000
17.C −7.264237 −4.210395 0.000000

18.C	8.493145	−3.502242	0.000000
19.H	−4.518478	8.430757	0.000000
20.N	4.836674	−5.612949	0.000000
21.H	1.328549	5.255896	0.000000
22.N	2.394745	−7.012747	0.000000
23.N	3.632230	−8.969227	0.000000
24.H	5.041126	8.127124	0.000000
25.N	−9.584178	1.339593	0.000000
26.N	−7.212620	5.565337	0.000000
27.H	−3.681953	9.978135	0.000000
28.H	3.958711	6.102930	0.000000
29.C	−1.229357	6.213804	0.000000
30.C	−6.133062	−2.067490	0.000000
31.N	5.950715	7.629035	0.000000
32.C	8.474043	2.059320	0.000000
33.O	−3.497539	−9.048221	0.000000
34.H	−5.041126	−8.127124	0.000000
35.N	7.212620	−5.565337	0.000000
36.N	−2.442280	−6.994109	0.000000
37.C	2.452806	8.368015	0.000000
38.H	−1.328549	−5.255896	0.000000
39.C	1.274709	6.345095	0.000000
40.H	3.888009	−3.779473	0.000000
41.H	−1.262751	−10.043497	0.000000
42.N	−2.394745	7.012747	0.000000
43.N	−7.271060	1.433061	0.000000
44.H	−7.266475	0.376871	0.000000
45.C	−1.274709	−6.345095	0.000000
46.H	9.560912	−0.302860	0.000000
47.O	−1.328880	4.986862	0.000000
48.N	9.584178	−1.339593	0.000000
49.C	−8.474043	−2.059320	0.000000
50.N	7.279111	1.381160	0.000000
51.H	−10.482777	1.800985	0.000000
52.H	6.799459	8.176765	0.000000
53.O	3.654496	3.642545	0.000000
54.N	−4.836674	5.612949	0.000000
55.H	1.262751	10.043497	0.000000
56.O	9.585662	1.495000	0.000000
57.O	3.497539	9.048221	0.000000
58.O	6.088086	−7.553877	0.000000
59.C	6.133062	2.067490	0.000000
60.C	−7.278601	−5.603096	0.000000
61.H	5.216908	1.475959	0.000000
62.C	0.024262	6.973410	0.000000
63.H	8.207109	6.165329	0.000000
64.H	−8.067263	6.115953	0.000000
65.C	−0.024262	−6.973410	0.000000
66.C	2.420225	−8.376826	0.000000
67.N	−8.425395	−3.462892	0.000000
68.C	−6.027590	3.508429	0.000000
69.C	−1.213757	9.105687	0.000000
70.H	7.266475	−0.376871	0.000000
71.C	−4.766719	−4.170088	0.000000
72.O	−4.983636	1.343331	0.000000
73.C	5.996511	−2.042911	0.000000
74.N	4.875637	5.578851	0.000000
75.C	1.229357	−6.213804	0.000000
76.C	7.264237	4.210395	0.000000
77.C	−5.996511	2.042911	0.000000
78.N	7.271060	−1.433061	0.000000
79.N	2.442280	6.994109	0.000000
80.H	−6.799459	−8.176765	0.000000
81.N	−5.950715	−7.629035	0.000000
82.H	−9.444287	4.025279	0.000000
83.C	−6.044040	−6.283267	0.000000
84.H	−5.216908	−1.475959	0.000000
85.C	−0.014996	8.396565	0.000000
86.H	9.444287	−4.025279	0.000000
87.C	−6.021239	6.309012	0.000000
88.C	8.465123	−2.092997	0.000000
89.C	4.858291	−4.277278	0.000000
90.H	4.518478	−8.430757	0.000000
91.N	−1.213156	−9.028049	0.000000
92.H	−9.560912	0.302860	0.000000
93.C	−2.452806	−8.368015	0.000000
94.H	−8.207109	−6.165329	0.000000

95.O -3.654496 -3.642545 0.000000
96.O 1.328880 -4.986862 0.000000
97.H -3.307169 6.480803 0.000000
98.H 9.329467 3.927922 0.000000
99.C 1.213757 -9.105687 0.000000
100.N 1.213156 9.028049 0.000000
101.C 4.766719 4.170088 0.000000
102.C -8.465123 2.092997 0.000000
103.C 6.021239 -6.309012 0.000000
104.C 7.278601 5.603096 0.000000
105.C 6.027590 -3.508429 0.000000
106.H 3.307169 -6.480803 0.000000
107.C -6.051559 -3.464516 0.000000
108.C 0.014996 -8.396565 0.000000
109.O -6.088086 7.553877 0.000000
110.N -7.279111 -1.381160 0.000000
111.C -7.279737 4.186005 0.000000
112.C -4.858291 4.277278 0.000000
113.N 8.425395 3.462892 0.000000
114.N -4.875637 -5.578851 0.000000

AAA rosette

E (ZORA-BLYP-D3(BJ)/TZ2P): -18588.50

1.H 4.175757 -1.861114 0.000000
2.N 5.058230 -1.350909 0.000000
3.H -1.214541 10.287483 0.000000
4.H -4.078805 -6.174802 0.000000
5.O -9.596642 -1.516165 0.000000
6.C 7.361964 -4.265666 0.000000
7.C 6.154460 6.352822 0.000000
8.H 1.210885 -10.289175 0.000000
9.H 3.716014 -10.086806 0.000000
10.C -2.426113 8.507771 0.000000
11.C 6.118344 3.545675 0.000000
12.C -8.581063 3.546650 0.000000
13.H 10.591455 -1.823900 0.000000
14.N -3.650959 9.077554 0.000000
15.H 0.476428 -4.548970 0.000000
16.O -3.753178 3.689748 0.000000
17.C -7.377219 -4.245866 0.000000
18.C 8.577236 -3.548451 0.000000
19.H -4.521016 8.526358 0.000000
20.O 4.933968 -5.585723 0.000000
21.O 1.318343 5.092982 0.000000
22.N 2.409411 -7.124376 0.000000
23.N 3.647267 -9.079115 0.000000
24.H 5.122688 8.176063 0.000000
25.N -9.688178 1.377705 0.000000
26.N -7.404873 5.624139 0.000000
27.H -3.719633 10.085250 0.000000
28.H 4.075317 6.173138 0.000000
29.C -1.254792 6.384918 0.000000
30.C -6.104044 -2.114149 0.000000
31.N 6.035203 7.698401 0.000000
32.C 8.646502 2.284948 0.000000
33.O -3.487062 -9.067310 0.000000
34.H -5.126365 -8.177909 0.000000
35.N 7.400985 -5.625918 0.000000
36.O -2.370554 -7.067749 0.000000
37.C 2.342773 8.631203 0.000000
38.O -1.322139 -5.094781 0.000000
39.C 1.218760 6.340181 0.000000
40.O 3.749369 -3.691401 0.000000
41.H 5.097039 -0.317948 0.000000
42.N -2.413179 7.122721 0.000000
43.N -7.376373 1.472422 0.000000
44.H -7.387156 0.442751 0.000000
45.C -1.222549 -6.341971 0.000000
46.H 9.642103 -0.350455 0.000000
47.N -1.363139 5.056603 0.000000
48.N 9.684415 -1.379551 0.000000
49.C -8.650189 -2.286728 0.000000
50.O 7.302961 1.481231 0.000000
51.H -10.595247 1.821992 0.000000
52.H 6.873428 8.261919 0.000000
53.N 3.697415 3.706525 0.000000
54.O -4.937840 5.584003 0.000000

55.H 3.697815 2.687174 0.000000
56.O 9.592962 1.514413 0.000000
57.O 3.483414 9.065442 0.000000
58.O 6.107294 −7.552402 0.000000
59.C 6.100380 2.112372 0.000000
60.C −7.363763 −5.656913 0.000000
61.O 5.070111 1.402462 0.000000
62.C −0.013378 7.072655 0.000000
63.H 8.301525 6.193601 0.000000
64.H 2.822270 4.256648 0.000000
65.C 0.009603 −7.074397 0.000000
66.C 2.422389 −8.509411 0.000000
67.N −8.574824 −3.599648 0.000000
68.C −6.133416 3.525913 0.000000
69.C −1.218988 9.203016 0.000000
70.H 7.383367 −0.444521 0.000000
71.C −4.905651 −4.278540 0.000000
72.N −5.062044 1.349153 0.000000
73.C 6.154548 −2.108686 0.000000
74.N 4.961586 5.648904 0.000000
75.C 1.251004 −6.386619 0.000000
76.C 7.373553 4.244084 0.000000
77.C −6.158355 2.106932 0.000000
78.N 7.372574 −1.474195 0.000000
79.O 2.366742 7.065924 0.000000
80.H −6.877108 −8.263635 0.000000
81.N −6.038848 −7.700169 0.000000
82.H −9.518146 4.092533 0.000000
83.C −6.158036 −6.354580 0.000000
84.O −5.073752 −1.404277 0.000000
85.C 0.009631 8.508894 0.000000
86.H 9.514311 −4.094348 0.000000
87.C −6.305329 6.345672 0.000000
88.C 8.578571 −2.155432 0.000000
89.C 4.879334 −4.228635 0.000000
90.H 4.517282 −8.527855 0.000000
91.N −1.171883 −9.224495 0.000000
92.H −9.645785 0.348616 0.000000
93.C −2.346474 −8.632971 0.000000
94.H −8.305105 −6.195416 0.000000
95.N −3.701184 −3.708097 0.000000
96.N 1.359395 −5.058314 0.000000
97.H −3.310365 6.617376 0.000000
98.H 2.273416 −4.575510 0.000000
99.C 1.215293 −9.204707 0.000000
100.N 1.168188 9.222733 0.000000
101.C 4.901970 4.276823 0.000000
102.C −8.582368 2.153632 0.000000
103.C 6.301399 −6.347419 0.000000
104.C 7.360162 5.655136 0.000000
105.C 6.129594 −3.527657 0.000000
106.H 3.306555 −6.618960 0.000000
107.C −6.122029 −3.547442 0.000000
108.C −0.013354 −8.510635 0.000000
109.O −6.111247 7.550632 0.000000
110.O −7.306611 −1.483007 0.000000
111.C −7.365802 4.263889 0.000000
112.C −4.883165 4.226931 0.000000
113.N 8.571149 3.597864 0.000000
114.N −4.965156 −5.650636 0.000000
115.H −2.277148 4.573762 0.000000
116.H −0.480120 4.547335 0.000000
117.H −5.100822 0.316186 0.000000
118.H −4.179558 1.859329 0.000000
119.H −2.825987 −4.258128 0.000000
120.H −3.701688 −2.688751 0.000000

AAA-OH rosette

E (ZORA-BLYP-D3(BJ)/TZ2P): −19298.99

1.H 4.156026 −1.916207 0.000000
2.N 5.028308 −1.380973 0.000000
3.H −1.198293 10.279188 0.000000
4.H −4.065974 −6.160378 0.000000
5.O −9.666801 −1.548872 0.000000
6.C 7.335249 −4.266768 0.000000
7.C 6.153429 6.319518 0.000000
8.H 1.189723 −10.278898 0.000000

9.H	3.666577	−10.090583	0.000000
10.C	−2.397943	8.492159	0.000000
11.C	6.126573	3.510501	0.000000
12.C	−8.565608	3.560139	0.000000
13.H	10.570143	−1.865598	0.000000
14.N	−3.622961	9.083360	0.000000
15.H	0.416199	−4.560806	0.000000
16.O	−3.729148	3.730072	0.000000
17.C	−7.369405	−4.222298	0.000000
18.C	8.557203	−3.559500	0.000000
19.H	−4.491142	8.551963	0.000000
20.N	4.926694	−5.682611	0.000000
21.O	1.363417	5.090868	0.000000
22.N	2.381362	−7.111953	0.000000
23.N	3.614419	−9.083194	0.000000
24.H	5.158664	8.162170	0.000000
25.N	−9.680126	1.408027	0.000000
26.N	−7.353757	5.636768	0.000000
27.H	−3.675303	10.090736	0.000000
28.H	4.057636	6.161073	0.000000
29.C	−1.226708	6.375742	0.000000
30.C	−6.158064	−2.055250	0.000000
31.N	6.052963	7.675991	0.000000
32.C	8.453105	2.224847	0.000000
33.O	−3.493983	−9.142386	0.000000
34.H	−5.166524	−8.161203	0.000000
35.N	7.345375	−5.636205	0.000000
36.N	−2.460561	−7.111378	0.000000
37.C	2.297947	8.436559	0.000000
38.O	−1.371863	−5.090522	0.000000
39.C	1.292596	6.357176	0.000000
40.O	3.720811	−3.729446	0.000000
41.H	5.064989	−0.340842	0.000000
42.N	−2.389837	7.112201	0.000000
43.N	−7.356469	1.490094	0.000000
44.H	−7.370485	0.437266	0.000000
45.C	−1.301099	−6.356846	0.000000
46.H	9.645390	−0.389687	0.000000
47.N	−1.324257	5.049002	0.000000
48.N	9.671550	−1.407260	0.000000
49.C	−8.461518	−2.224286	0.000000
50.N	7.382844	1.428992	0.000000
51.H	−10.578669	1.866460	0.000000
52.H	6.899236	8.224967	0.000000
53.N	3.708294	3.668207	0.000000
54.N	−4.935088	5.683214	0.000000
55.H	3.735494	2.645163	0.000000
56.O	9.658463	1.549524	0.000000
57.O	3.485451	9.142727	0.000000
58.O	6.168723	−7.593084	0.000000
59.C	6.149636	2.055805	0.000000
60.C	−7.367983	−5.634185	0.000000
61.O	5.088373	1.361333	0.000000
62.C	0.021263	7.064546	0.000000
63.H	8.300846	6.173913	0.000000
64.H	2.825872	4.220124	0.000000
65.C	−0.029752	−7.064233	0.000000
66.C	2.389437	−8.491907	0.000000
67.N	−8.560398	−3.546281	0.000000
68.C	−6.109553	3.554414	0.000000
69.C	−1.201856	9.194464	0.000000
70.H	7.361935	−0.436694	0.000000
71.C	−4.914573	−4.246350	0.000000
72.N	−5.036850	1.381406	0.000000
73.C	6.128625	−2.128671	0.000000
74.N	4.962409	5.622546	0.000000
75.C	1.218255	−6.375452	0.000000
76.C	7.360967	4.222836	0.000000
77.C	−6.137104	2.129197	0.000000
78.N	7.347937	−1.489514	0.000000
79.N	2.452033	7.111740	0.000000
80.H	−6.907069	−8.224684	0.000000
81.N	−6.061018	−7.675371	0.000000
82.H	−9.503280	4.105514	0.000000
83.C	−6.161750	−6.318926	0.000000
84.O	−5.096770	−1.360843	0.000000
85.C	0.021557	8.489700	0.000000

86.H	9.494899	−4.104832	0.000000
87.C	−6.159450	6.212152	0.000000
88.C	8.547031	−2.172502	0.000000
89.C	4.852912	−4.301243	0.000000
90.H	4.482701	−8.551953	0.000000
91.N	−1.211004	−9.182816	0.000000
92.H	−9.654059	0.390454	0.000000
93.C	−2.306477	−8.436212	0.000000
94.H	−8.309180	−6.173449	0.000000
95.N	−3.716806	−3.667464	0.000000
96.N	1.315810	−5.048713	0.000000
97.H	−3.308600	6.597946	0.000000
98.H	2.234960	−4.560480	0.000000
99.C	1.193323	−9.194174	0.000000
100.N	1.202464	9.183168	0.000000
101.C	4.906110	4.247007	0.000000
102.C	−8.555521	2.173149	0.000000
103.C	6.151040	−6.211567	0.000000
104.C	7.359614	5.634709	0.000000
105.C	6.101165	−3.553865	0.000000
106.H	3.300102	−6.597705	0.000000
107.C	−6.135040	−3.509930	0.000000
108.C	−0.030073	−8.489374	0.000000
109.O	−6.177234	7.593663	0.000000
110.N	−7.391242	−1.428424	0.000000
111.C	−7.343628	4.267342	0.000000
112.C	−4.861291	4.301828	0.000000
113.N	8.551961	3.546837	0.000000
114.N	−4.970766	−5.621872	0.000000
115.H	−2.243466	4.560813	0.000000
116.H	−0.424697	4.561030	0.000000
117.H	−5.073573	0.341268	0.000000
118.H	−4.164521	1.916558	0.000000
119.H	−2.834446	−4.219399	0.000000
120.H	−3.743960	−2.644428	0.000000
121.H	3.220848	10.084699	0.000000
122.H	10.341815	2.249784	0.000000
123.H	7.116758	−7.835040	0.000000
124.H	−3.229376	−10.084358	0.000000
125.H	−10.350324	−2.248958	0.000000
126.H	−7.125296	7.835514	0.000000