

Electronic Supplementary Information

Table S1. PBEs of (HF)₁₀ (eV) calculated by the NOMO/DC-PP2 method with various buffer regions. Deviations from the NOMO/PP2 results are shown in parentheses. The proton labeling scheme is defined in Fig. 2.

Proton	Buffer size										NOMO/PP2
	0 Å		1 Å		2 Å		3 Å		4 Å		
1	13.43	(0.13)	13.43	(0.13)	13.39	(0.09)	13.30	(0.01)	13.30	(0.01)	13.29
2	14.69	(0.55)	14.69	(0.55)	14.26	(0.12)	14.14	(0.01)	14.14	(0.01)	14.13
3	15.31	(0.60)	15.31	(0.60)	14.84	(0.14)	14.71	(0.00)	14.72	(0.01)	14.70
4	15.62	(0.61)	15.62	(0.61)	15.15	(0.14)	15.01	(0.00)	15.02	(0.01)	15.01
5	15.83	(0.62)	15.83	(0.62)	15.36	(0.14)	15.22	(0.01)	15.23	(0.01)	15.21
6	16.01	(0.62)	16.01	(0.62)	15.54	(0.14)	15.40	(0.01)	15.41	(0.01)	15.40
7	16.22	(0.62)	16.22	(0.62)	15.75	(0.14)	15.61	(0.01)	15.62	(0.01)	15.60
8	16.53	(0.61)	16.53	(0.61)	16.06	(0.14)	15.93	(0.00)	15.93	(0.01)	15.92
9	17.10	(0.58)	17.10	(0.58)	16.65	(0.13)	16.52	(-0.00)	16.53	(0.01)	16.52
10	18.74	(0.40)	18.74	(0.40)	18.39	(0.05)	18.33	(-0.01)	18.35	(0.01)	18.34

Table S2. PBEs of (Gly)₆ (eV) calculated by the NOMO/DC-PP2 method with various buffer regions. Deviations from the NOMO/PP2 results are shown in parentheses. The proton labeling scheme is defined in Fig. 2.

Proton	Buffer size										NOMO/PP2
	2 Å		3 Å		4 Å		5 Å		6 Å		
1	8.35	(-2.01)	10.07	(-0.29)	10.39	(0.03)	10.38	(0.01)	10.38	(0.01)	10.36
2	7.00	(-3.13)	9.65	(-0.48)	9.30	(-0.83)	10.15	(0.02)	10.14	(0.01)	10.13
3	7.00	(-3.13)	9.65	(-0.48)	9.30	(-0.83)	10.15	(0.02)	10.14	(0.01)	10.13
4	10.77	(-2.01)	12.40	(-0.38)	12.83	(0.05)	12.80	(0.02)	12.79	(0.01)	12.78
5	10.77	(-2.01)	12.40	(-0.38)	12.83	(0.05)	12.80	(0.02)	12.79	(0.01)	12.78
6	13.15	(-0.43)	13.29	(-0.28)	13.51	(-0.07)	13.59	(0.01)	13.59	(0.01)	13.58
7	16.18	(0.60)	15.50	(-0.08)	15.57	(-0.01)	15.60	(0.02)	15.59	(0.01)	15.58
8	16.18	(0.60)	15.29	(-0.29)	15.57	(-0.01)	15.61	(0.02)	15.59	(0.01)	15.58
9	14.76	(-0.49)	15.52	(0.26)	15.35	(0.10)	15.28	(0.03)	15.26	(0.01)	15.25
10	17.51	(0.61)	16.86	(-0.04)	16.97	(0.07)	16.93	(0.03)	16.92	(0.02)	16.90
11	17.51	(0.61)	16.86	(-0.04)	16.97	(0.07)	16.93	(0.03)	16.92	(0.02)	16.90
12	17.33	(1.04)	16.55	(0.26)	16.39	(0.10)	16.32	(0.03)	16.30	(0.01)	16.29
13	18.49	(0.61)	17.95	(0.07)	17.96	(0.07)	17.91	(0.03)	17.90	(0.02)	17.88
14	18.49	(0.61)	17.95	(0.07)	17.96	(0.07)	17.91	(0.03)	17.90	(0.02)	17.88
15	18.43	(1.05)	17.64	(0.27)	17.48	(0.10)	17.40	(0.03)	17.39	(0.01)	17.38
16	19.73	(0.61)	19.13	(0.00)	19.20	(0.07)	19.16	(0.03)	19.14	(0.01)	19.13
17	19.73	(0.61)	19.13	(0.00)	19.20	(0.07)	19.16	(0.03)	19.14	(0.01)	19.13
18	20.36	(1.07)	19.23	(-0.06)	19.33	(0.04)	19.31	(0.02)	19.29	(0.00)	19.29
19	22.17	(0.52)	21.67	(0.02)	21.67	(0.02)	21.66	(0.01)	21.66	(0.01)	21.65
20	22.17	(0.52)	21.67	(0.02)	21.67	(0.02)	21.66	(0.01)	21.66	(0.01)	21.65

Table S3. PBEs of C₂₀H₂₂ (eV) calculated by the NOMO/DC-PP2 method with different buffer regions. Deviations from the NOMO/PP2 results are shown in parentheses. The proton labeling scheme is defined in Fig. 2.

Proton	Buffer size												NOMO/PP2
	1 unit		2 units		3 units		4 units		5 units		6 units		
1	18.56	(0.03)	18.53	(0.00)	18.53	(-0.00)	18.53	(-0.00)	18.53	(-0.00)	18.53	(-0.00)	18.53
2	18.44	(0.05)	18.41	(0.02)	18.40	(0.01)	18.40	(0.01)	18.40	(0.00)	18.40	(0.00)	18.39
3	18.31	(0.08)	18.25	(0.02)	18.24	(0.01)	18.24	(0.01)	18.23	(0.00)	18.23	(0.00)	18.23
4	18.09	(0.05)	18.06	(0.02)	18.05	(0.01)	18.05	(0.01)	18.05	(0.01)	18.03	(-0.01)	18.04
5	18.06	(0.07)	18.01	(0.02)	17.99	(0.01)	17.99	(0.00)	17.99	(-0.00)	17.99	(-0.00)	17.99
6	18.07	(0.11)	17.98	(0.02)	17.97	(0.01)	17.98	(0.02)	17.96	(-0.01)	17.96	(-0.00)	17.96
7	18.06	(0.11)	17.97	(0.02)	17.96	(0.01)	17.95	(-0.00)	17.95	(0.00)	17.95	(0.00)	17.95
8	18.07	(0.12)	17.98	(0.03)	17.96	(0.01)	17.94	(-0.00)	17.95	(-0.00)	17.95	(0.00)	17.95
9	18.06	(0.12)	17.98	(0.03)	17.96	(0.01)	17.95	(-0.00)	17.95	(0.00)	17.95	(0.00)	17.95
10	18.07	(0.12)	17.98	(0.03)	17.94	(-0.01)	17.95	(0.00)	17.95	(0.00)	17.95	(0.00)	17.95
11	18.07	(0.12)	17.98	(0.03)	17.93	(-0.01)	17.95	(0.00)	17.95	(0.00)	17.95	(0.00)	17.95
12	18.07	(0.12)	17.98	(0.03)	17.94	(-0.01)	17.95	(0.00)	17.95	(0.00)	17.95	(0.00)	17.95
13	18.07	(0.12)	17.98	(0.03)	17.93	(-0.01)	17.95	(0.00)	17.95	(0.00)	17.95	(0.00)	17.95
14	18.07	(0.12)	17.98	(0.03)	17.96	(0.01)	17.95	(-0.00)	17.95	(0.00)	17.95	(0.00)	17.95
15	18.07	(0.12)	17.98	(0.03)	17.97	(0.02)	17.95	(-0.00)	17.95	(-0.00)	17.95	(0.00)	17.95
16	18.07	(0.11)	17.98	(0.02)	17.97	(0.01)	17.96	(-0.00)	17.96	(0.00)	17.96	(0.00)	17.96
17	18.07	(0.11)	17.99	(0.02)	17.98	(0.01)	17.98	(0.02)	17.96	(-0.01)	17.97	(-0.00)	17.97
18	18.07	(0.07)	18.02	(0.02)	18.00	(0.01)	18.00	(0.00)	18.00	(-0.00)	18.00	(-0.00)	18.00
19	18.10	(0.05)	18.07	(0.02)	18.06	(0.01)	18.06	(0.01)	18.05	(0.01)	18.04	(-0.01)	18.05
20	18.33	(0.08)	18.27	(0.02)	18.26	(0.01)	18.25	(0.01)	18.25	(0.00)	18.25	(0.00)	18.25
21	18.46	(0.05)	18.42	(0.02)	18.42	(0.01)	18.41	(0.01)	18.41	(0.00)	18.41	(0.00)	18.41
22	18.57	(0.03)	18.54	(0.00)	18.54	(-0.00)	18.54	(-0.00)	18.54	(-0.00)	18.54	(-0.00)	18.54