Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

Influence of Dispersive Forces in the Final Shape of a Micelle

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Figure S1. Calculated structures for ciclohexanol$_2$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

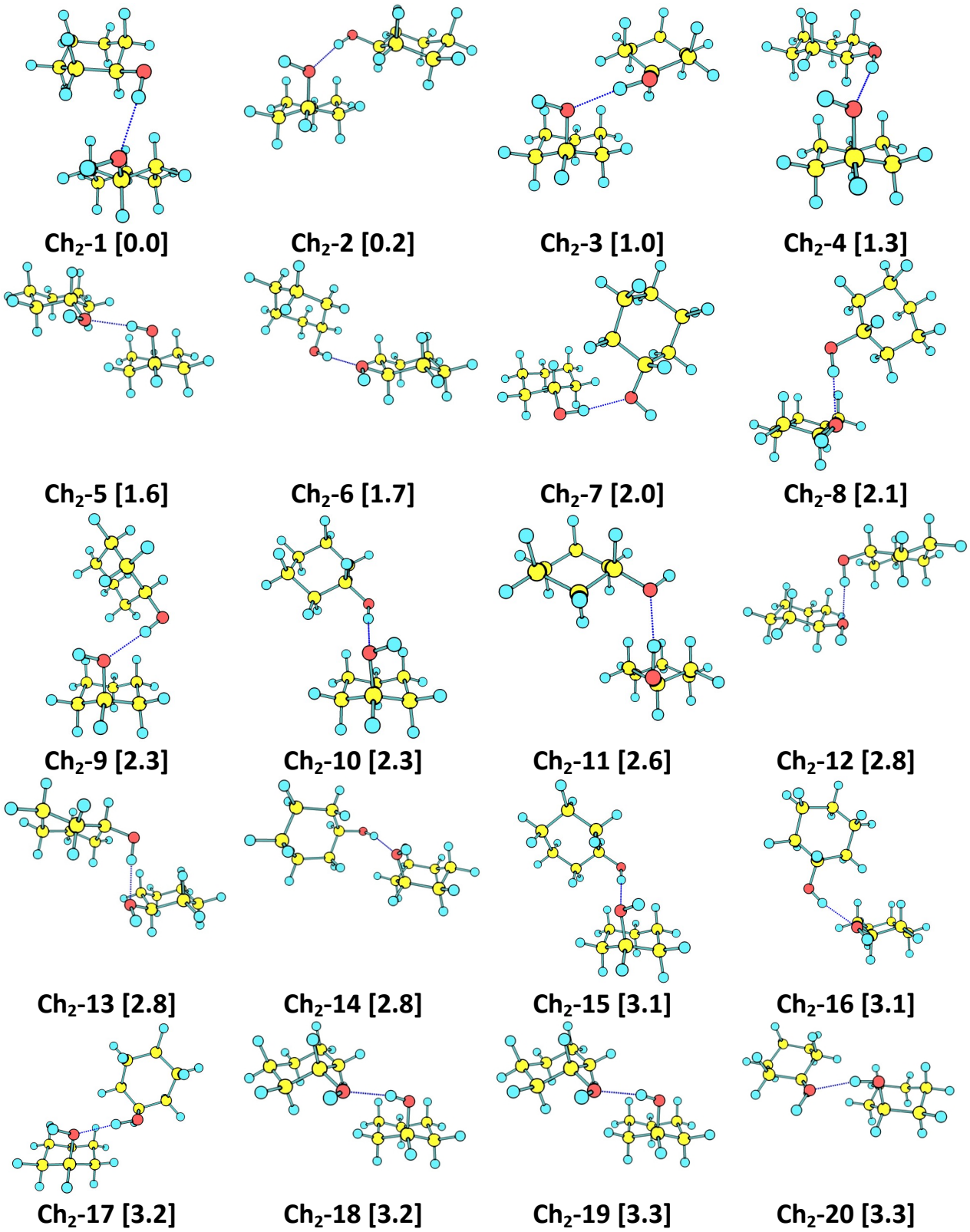

Figure S1. Cont.

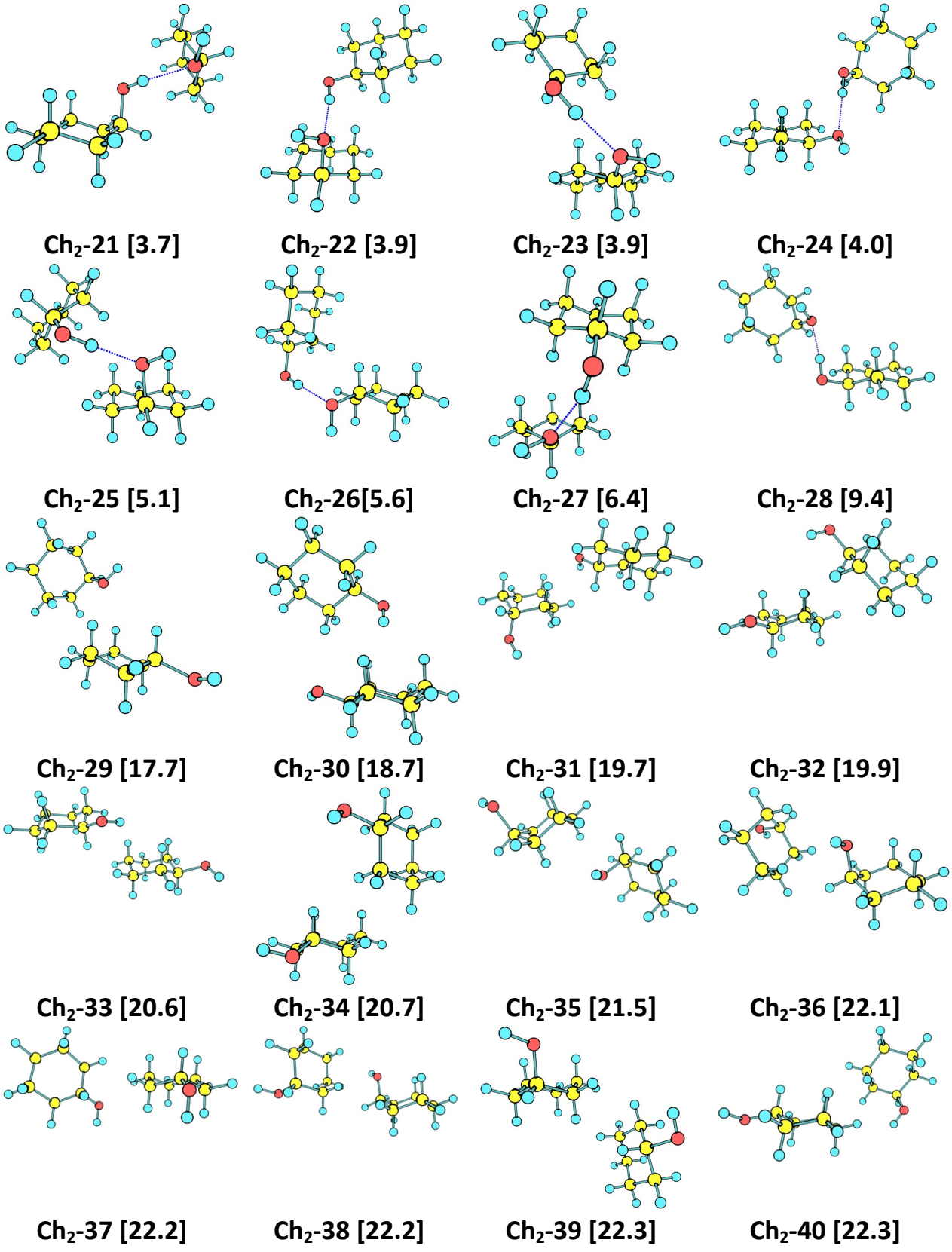

Figure S1. Cont.

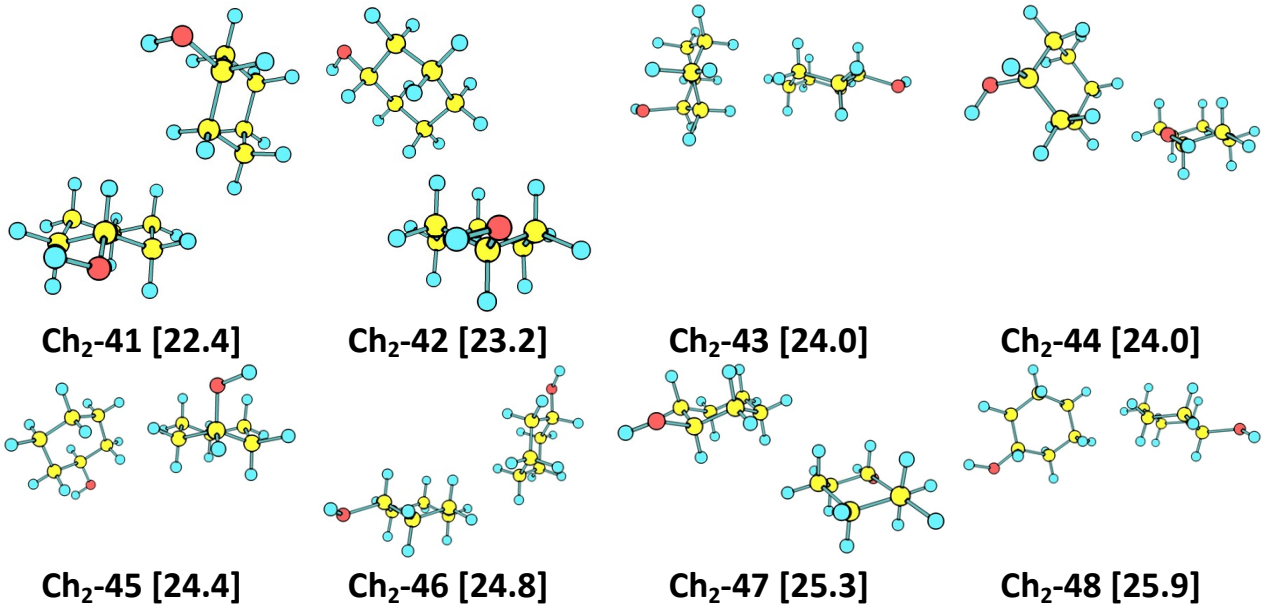

Table S1. Calculated structures for ciclohexanol$_2$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

Structure Ch_2-n n=	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*D_0 (kJ/mol)*	*BSSE (kJ/mol)*
1	0.00	0.00	-25.47	3.73
2	-0.10	0.20	-27.05	3.60
3	-1.20	1.05	-25.89	3.90
4	0.42	1.30	-25.66	3.89
5	1.29	1.57	-25.50	3.77
6	2.13	1.75	-25.74	3.34
7	0.27	1.97	-23.85	3.38
8	-0.35	2.12	-23.19	3.89
9	2.10	2.31	-29.62	3.72
10	1.02	2.33	-24.71	3.79
11	2.18	2.65	-27.70	3.67
12	-0.29	2.77	-27.26	3.99
13	-0.29	2.78	-27.84	3.40
14	2.29	2.80	-29.76	3.11
15	0.43	3.08	-28.56	4.03
16	2.10	3.11	-22.68	3.41
17	0.81	3.16	-25.62	3.70
18	2.32	3.22	-24.15	3.46
19	1.57	3.28	-24.09	3.49
20	2.52	3.28	-25.20	2.35
21	2.27	3.66	-25.06	2.11
22	1.75	3.90	-23.54	3.40
23	2.07	3.93	-21.79	3.48
24	0.85	4.04	-23.20	3.60
25	2.29	5.11	-26.68	3.87
26	2.50	5.56	-29.15	4.14
27	5.01	6.40	-23.99	3.64
28	4.04	9.44	-25.52	3.88
29	20.07	17.75	-11.41	1.68
30	19.81	18.73	-12.79	2.50
31	20.89	19.74	-9.41	1.69
32	21.78	19.88	-7.54	1.78
33	21.19	20.56	-6.74	1.90
34	21.14	20.74	-6.64	1.82
35	22.65	21.54	-9.50	1.44
36	22.63	22.10	-8.63	1.75
37	22.85	22.20	-10.19	1.64
38	22.33	22.20	-8.83	1.44
39	23.65	22.30	-6.97	1.57

Table S1. Cont.

Structure Ch_2-n n=	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*D_0 (kJ/mol)*	*BSSE (kJ/mol)*
40	24.48	22.32	-6.87	1.65
41	23.79	22.36	-9.92	1.75
42	23.20	23.22	-4.56	1.42
43	25.75	24.01	-5.45	1.37
44	23.38	24.01	-5.24	1.58
45	25.15	24.41	-5.16	1.26
46	26.65	24.77	-3.21	1.22
47	26.65	25.33	-2.59	1.28
48	26.51	25.89	-1.84	1.47

Figure S2. Experimental IDIRS for cyclohexanol$_2$ (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-311++G(d,p) level. A correction factor of 0.935 was employed.

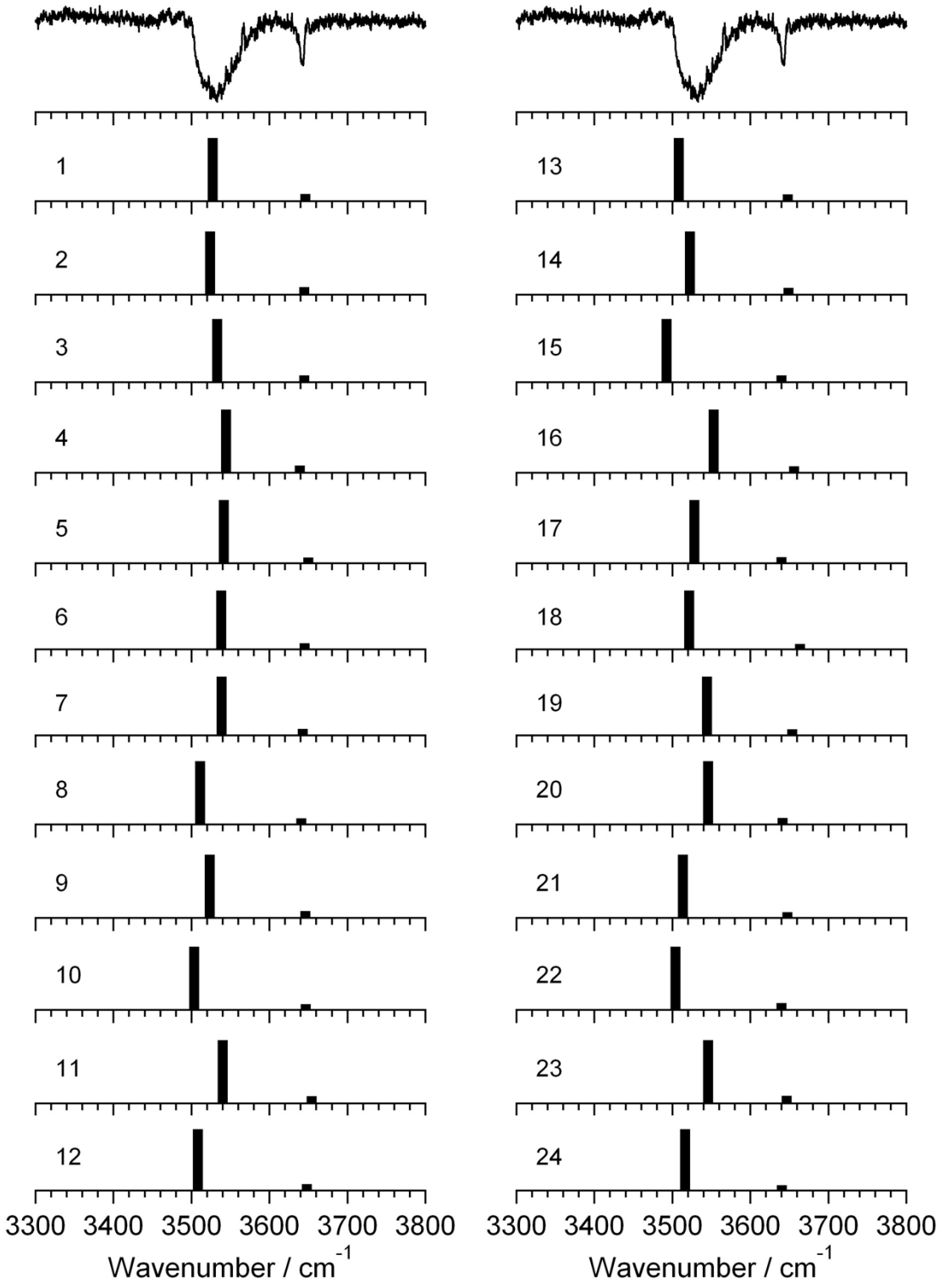

Figure S2. Cont.

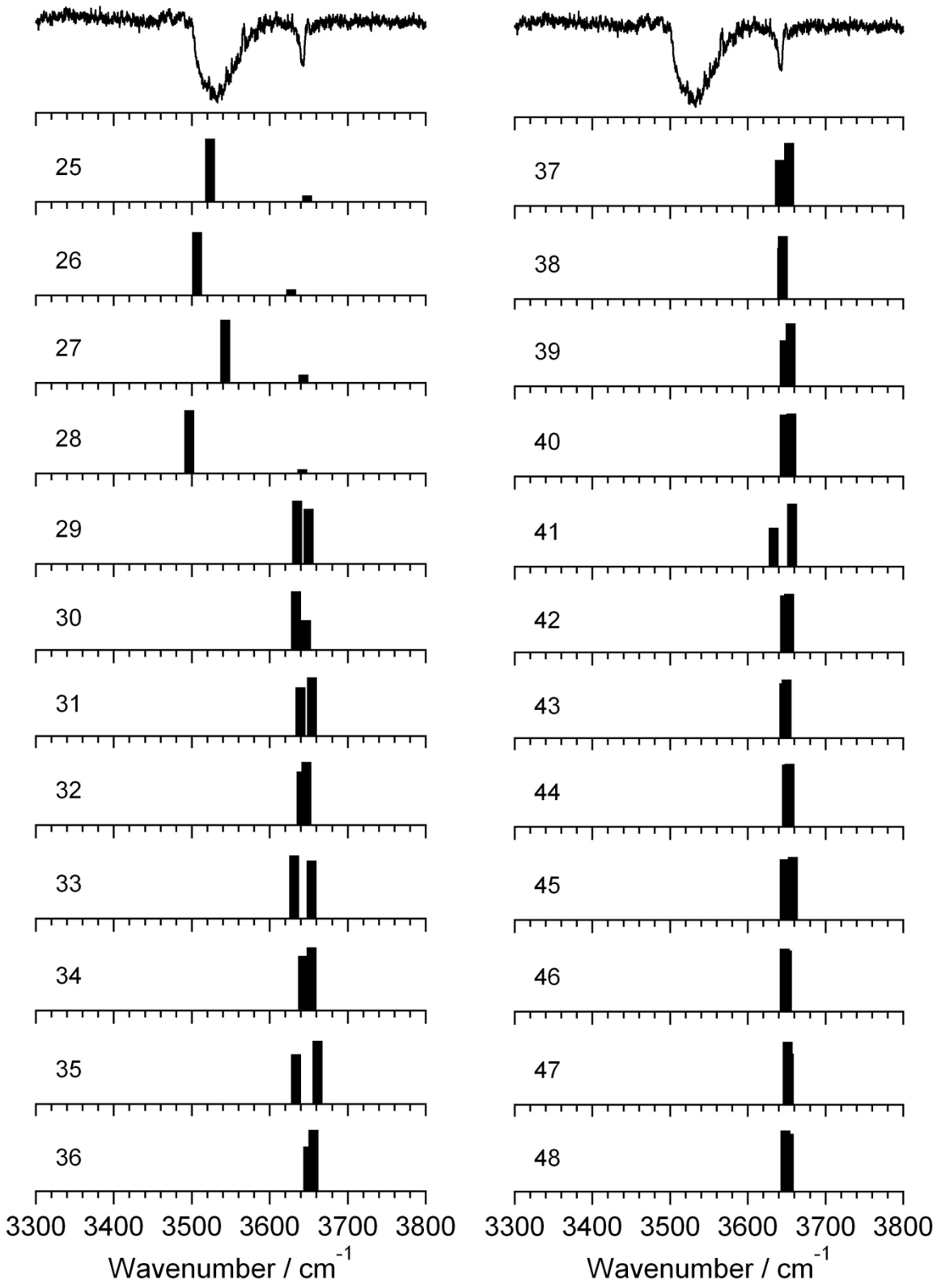

Figure S3. Calculated structures for ciclohexanol$_3$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

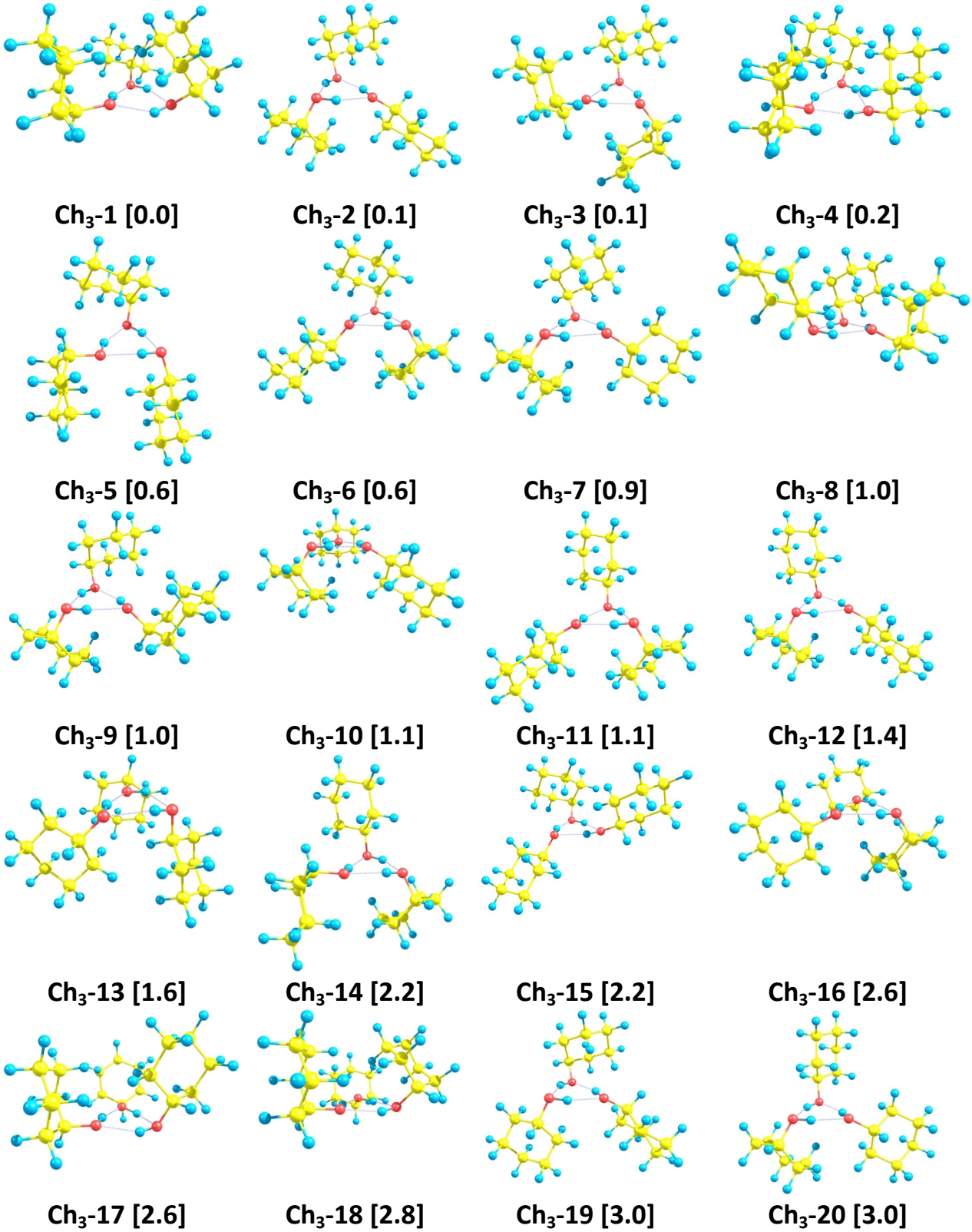

Figure S3. Cont.

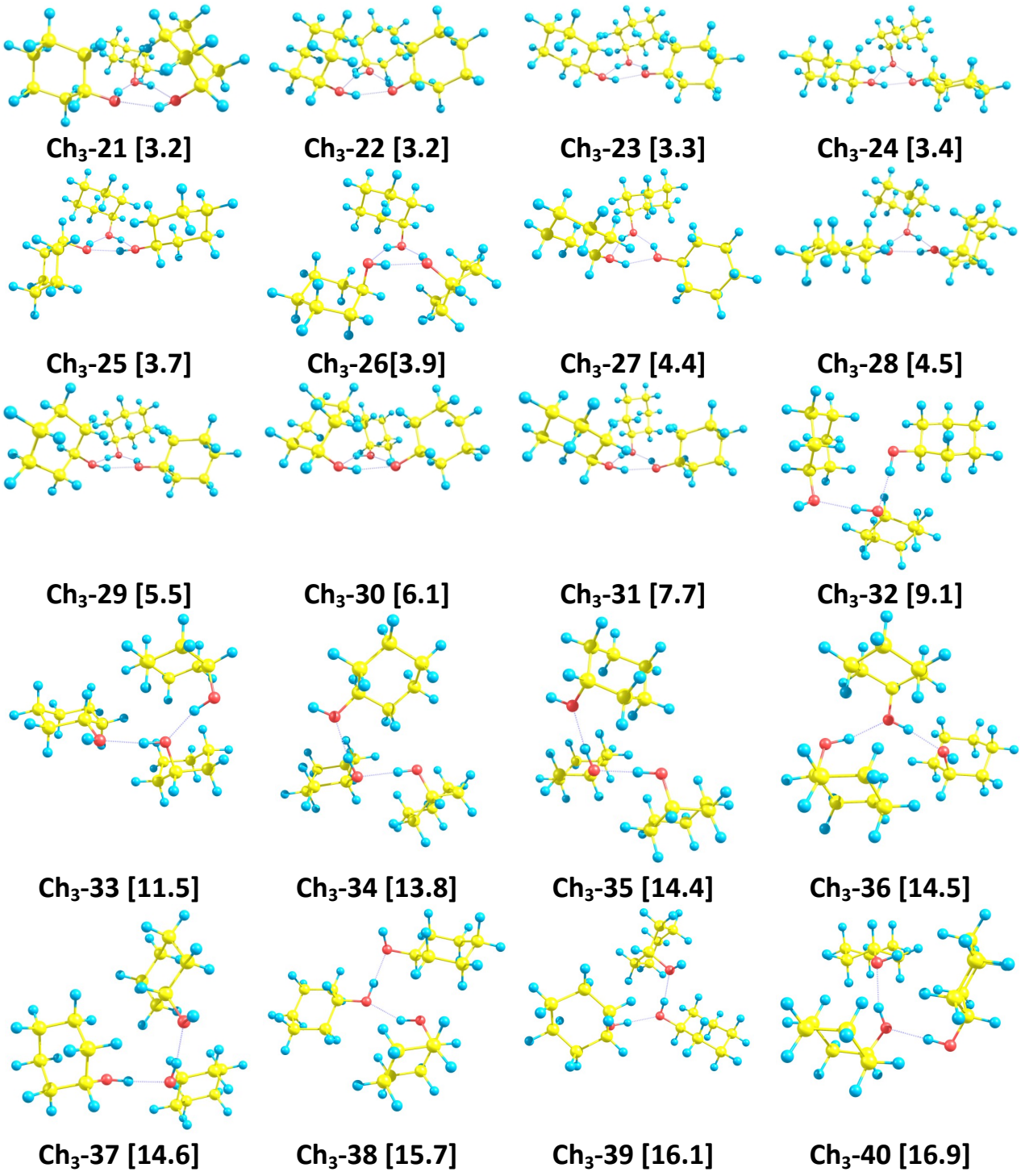

Figure S3. Cont.

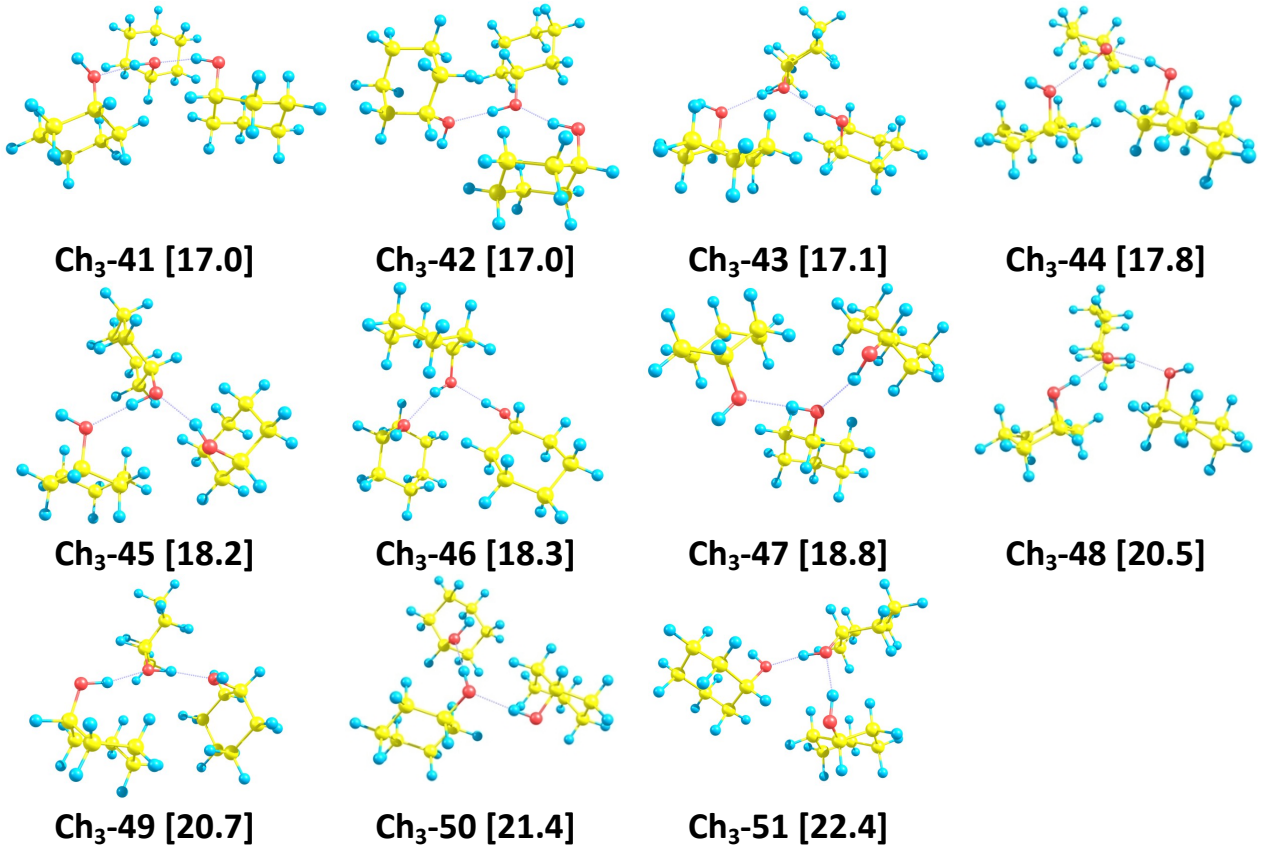

Table S2. Calculated structures for ciclohexanol$_3$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

Structure Ch_3-n n=	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*D_0 (kJ/mol)*	*BSSE (kJ/mol)*
1	0.00	0.00	-75.24	9.22
2	-0.40	0.12		
3	-0.86	0.12		
4	-0.17	0.17		
5	0.93	0.62		
6	-1.58	0.62		
7	0.94	0.90		
8	-0.76	0.96		
9	-2.27	1.00		
10	1.46	1.10		
11	1.64	1.10		
12	1.45	1.36		
13	1.78	1.61		
14	2.11	2.20		
15	3.09	2.24		
16	3.19	2.60		
17	4.96	2.64		
18	2.62	2.79		
19	4.01	3.00		
20	2.20	3.03		
21	3.12	3.18		
22	0.39	3.21		
23	3.61	3.34		
24	2.53	3.38		
25	4.03	3.75		
26	0.65	3.95		
27	3.15	4.43		
28	3.24	4.48		
29	5.08	5.47		
30	3.20	6.06		
31	8.50	7.70		
32	11.13	9.06		
33	12.95	11.50		
34	15.58	13.80		
35	16.08	14.40		
36	16.10	14.53		
37	14.76	14.58		
38	16.42	15.74		
39	18.88	16.06		

Table S2. Cont.

Structure Ch_3-n n=	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*D_0 (kJ/mol)*	*BSSE (kJ/mol)*
40	18.29	16.91		
41	19.31	17.00		
42	18.16	17.02		
43	19.86	17.10		
44	19.14	17.78		
45	17.92	18.16		
46	19.69	18.26		
47	19.66	18.78		
48	21.26	20.52		
49	22.15	20.66		
50	21.95	21.36		
51	22.74	22.38		

Figure S4. Experimental IDIRS for cyclohexanol$_3$ (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-311++G(d,p) level. A correction factor of 0.935 was employed.

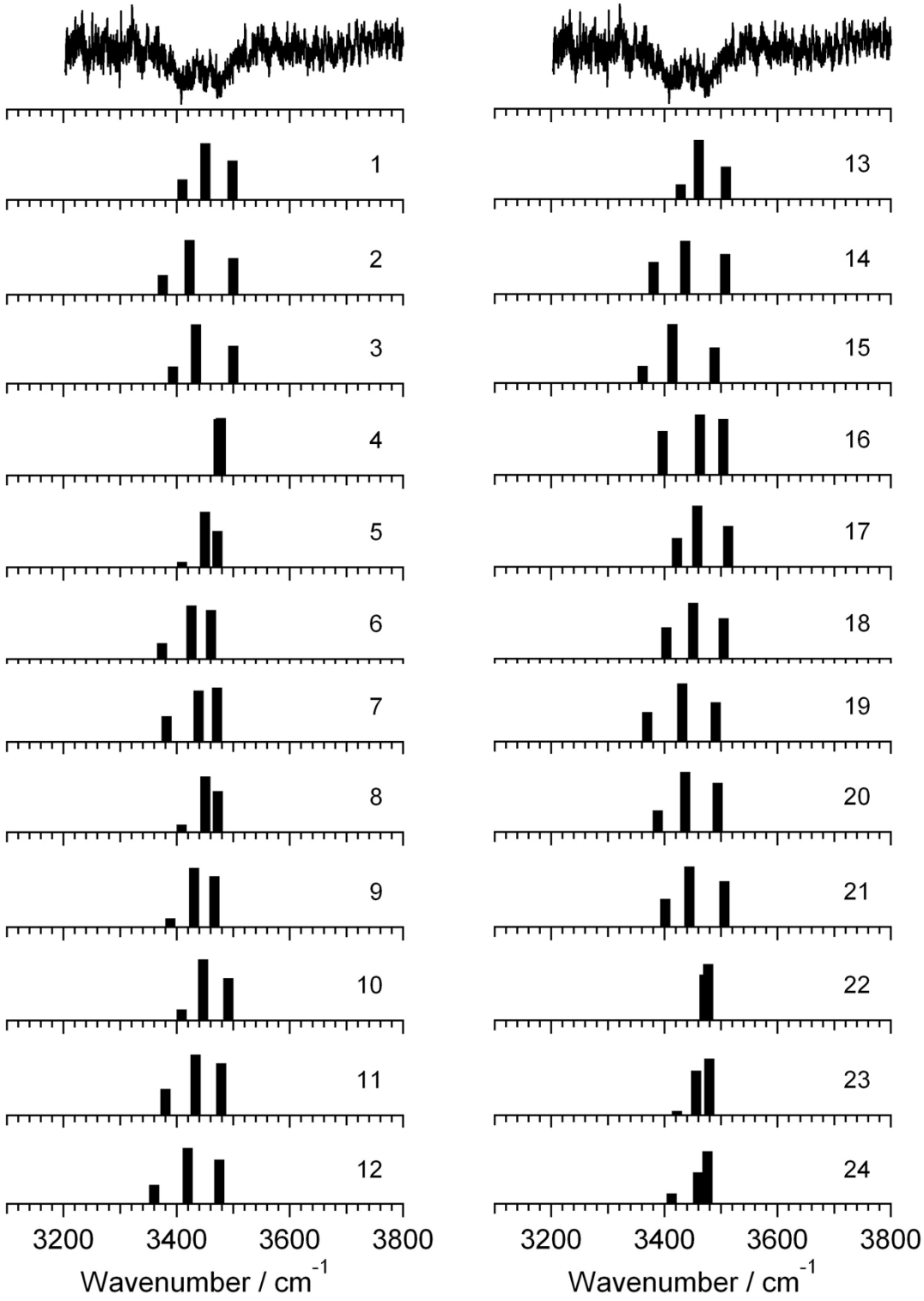

Figure S4. Cont.

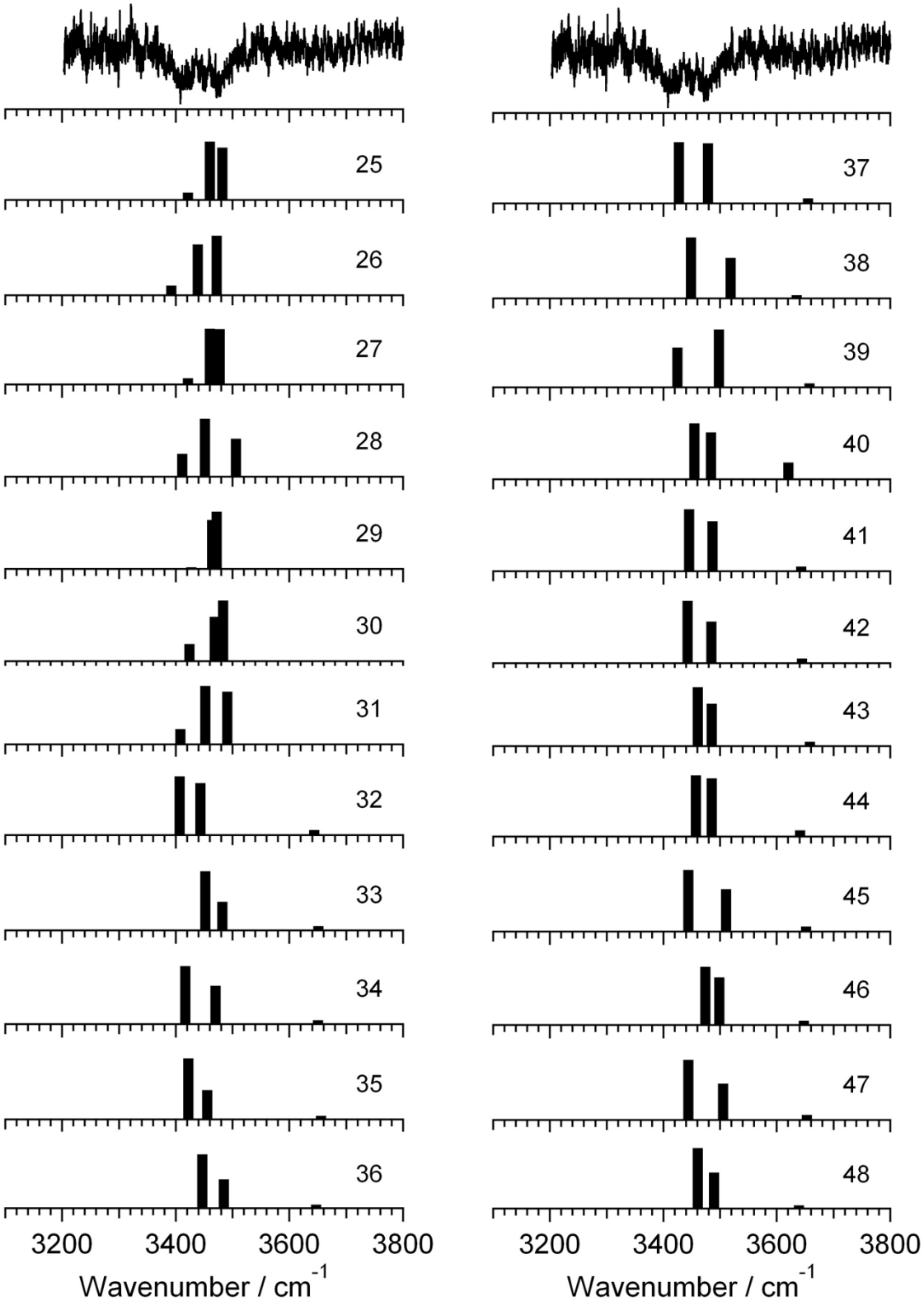

Figure S4. Cont.

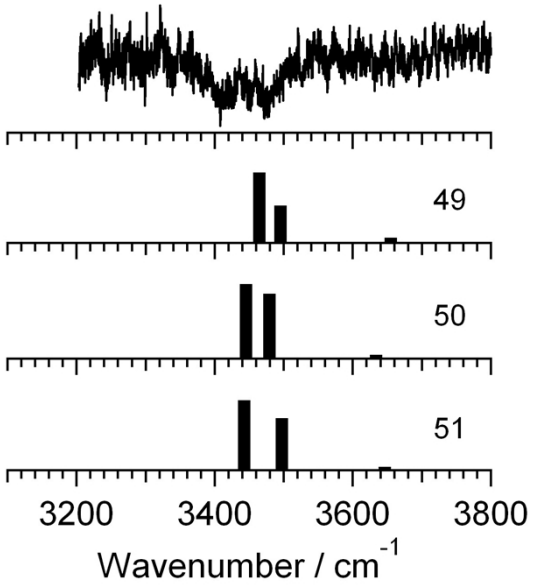

Figure S5. Calculated structures for ciclohexanol$_4$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

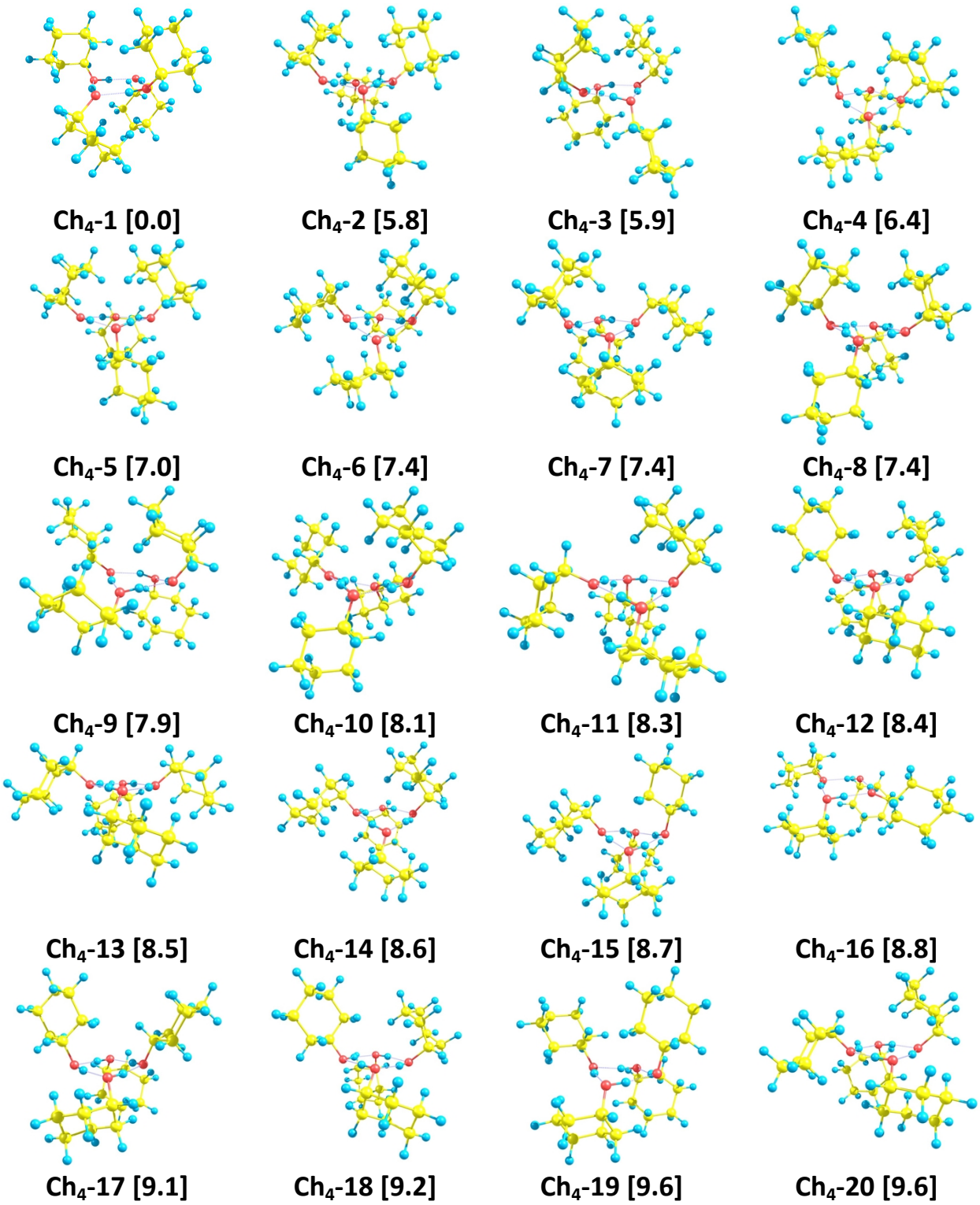

Figure S5. Cont.

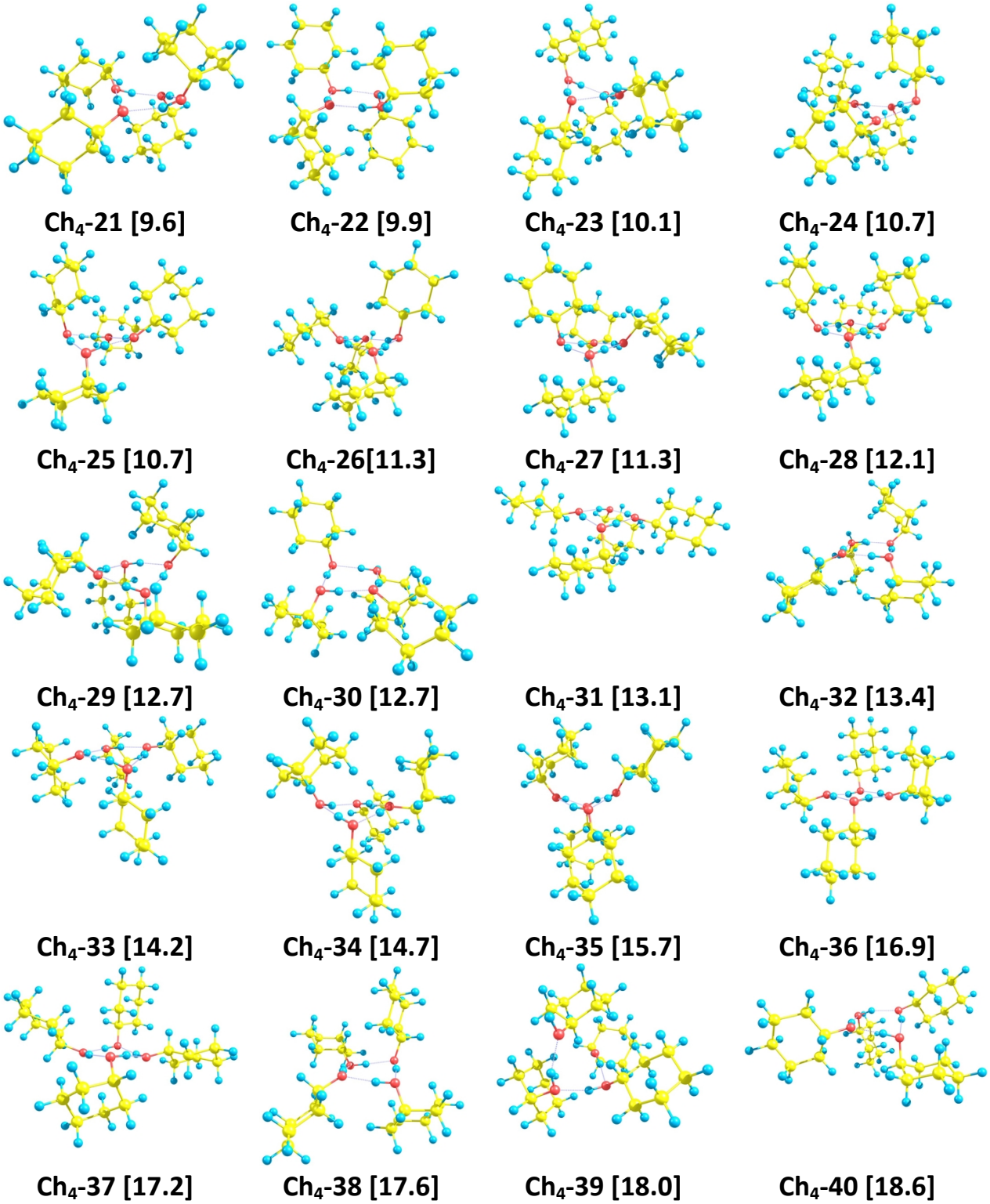

Figure S5. Cont.

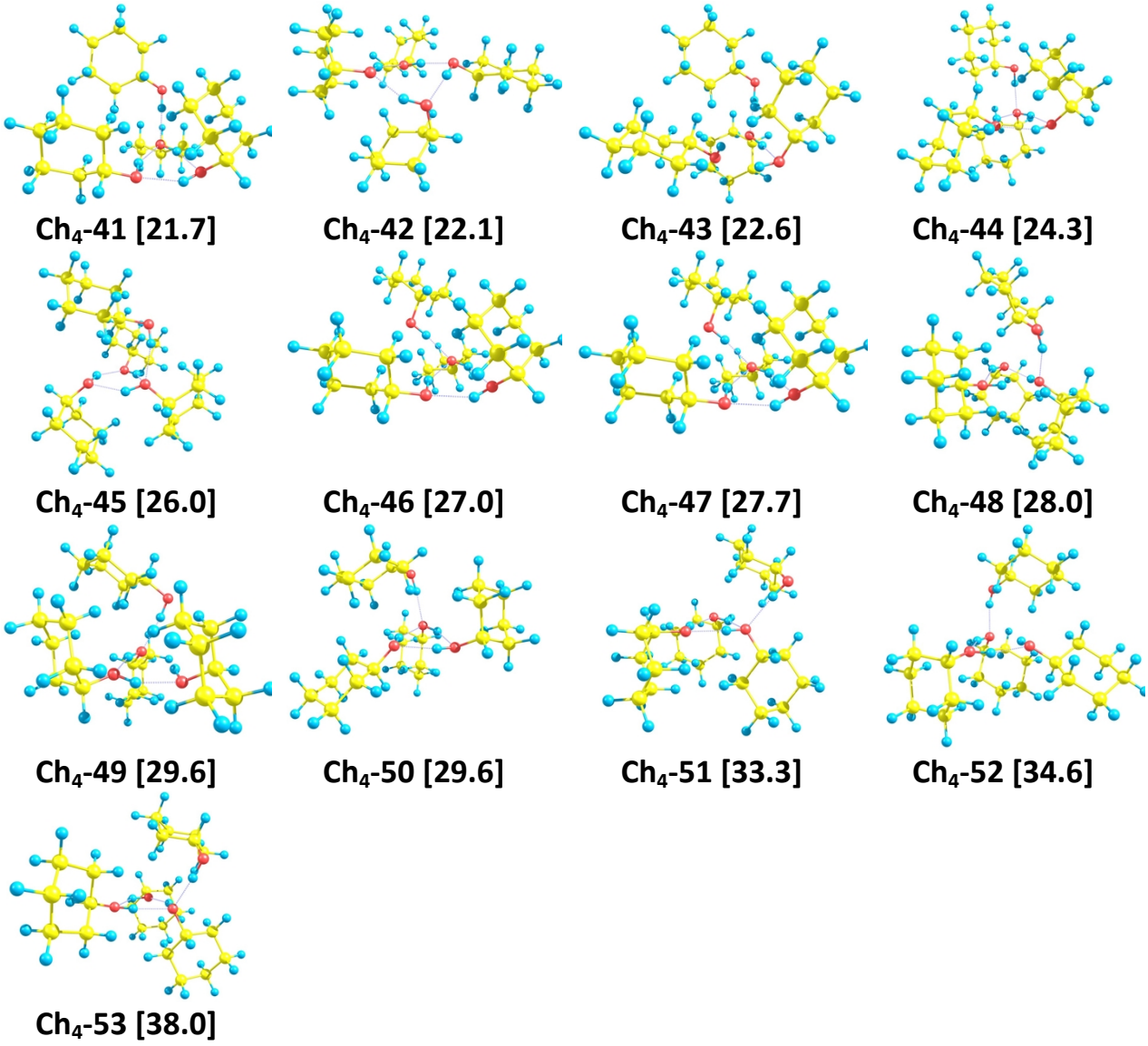

Table S3. Calculated structures for ciclohexanol$_4$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

Structure Ch_4-n n=	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*D_0 (kJ/mol)*	*BSSE (kJ/mol)*
1	0.00	0.00	-137.47	18.36
2	7.03	5.80		
3	7.77	5.90		
4	7.64	6.36		
5	7.05	7.00		
6	10.79	7.39		
7	5.58	7.40		
8	8.15	7.41		
9	11.25	7.87		
10	12.43	8.10		
11	9.98	8.26		
12	9.83	8.39		
13	9.65	8.53		
14	6.42	8.61		
15	10.51	8.69		
16	12.10	8.84		
17	10.78	9.08		
18	13.10	9.18		
19	9.14	9.59		
20	8.62	9.60		
21	11.98	9.61		
22	11.96	9.87		
23	11.82	10.12		
24	13.56	10.70		
25	13.02	10.75		
26	12.17	11.34		
27	13.14	11.35		
28	12.70	12.08		
29	12.87	12.70		
30	14.33	12.71		
31	14.72	13.12		
32	15.69	13.36		
33	17.83	14.17		
34	17.12	14.68		
35	16.88	15.68		
36	18.94	16.94		
37	19.18	17.22		
38	20.05	17.62		
39	21.69	18.01		

Table S3. Cont.

Structure Ch_4-n n=	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*D_0 (kJ/mol)*	*BSSE (kJ/mol)*
40	22.39	18.60		
41	25.62	21.74		
42	24.42	22.13		
43	25.44	22.64		
44	25.63	24.26		
45	27.68	25.98		
46	26.54	27.00		
47	30.55	27.66		
48	30.07	28.02		
49	30.26	29.56		
50	32.79	29.65		
51	34.76	33.33		
52	36.87	34.58		
53	40.84	38.05		

Figure S6. Experimental IDIRS for cyclohexanol$_4$ (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-311++G(d,p) level. A correction factor of 0.945 was employed.

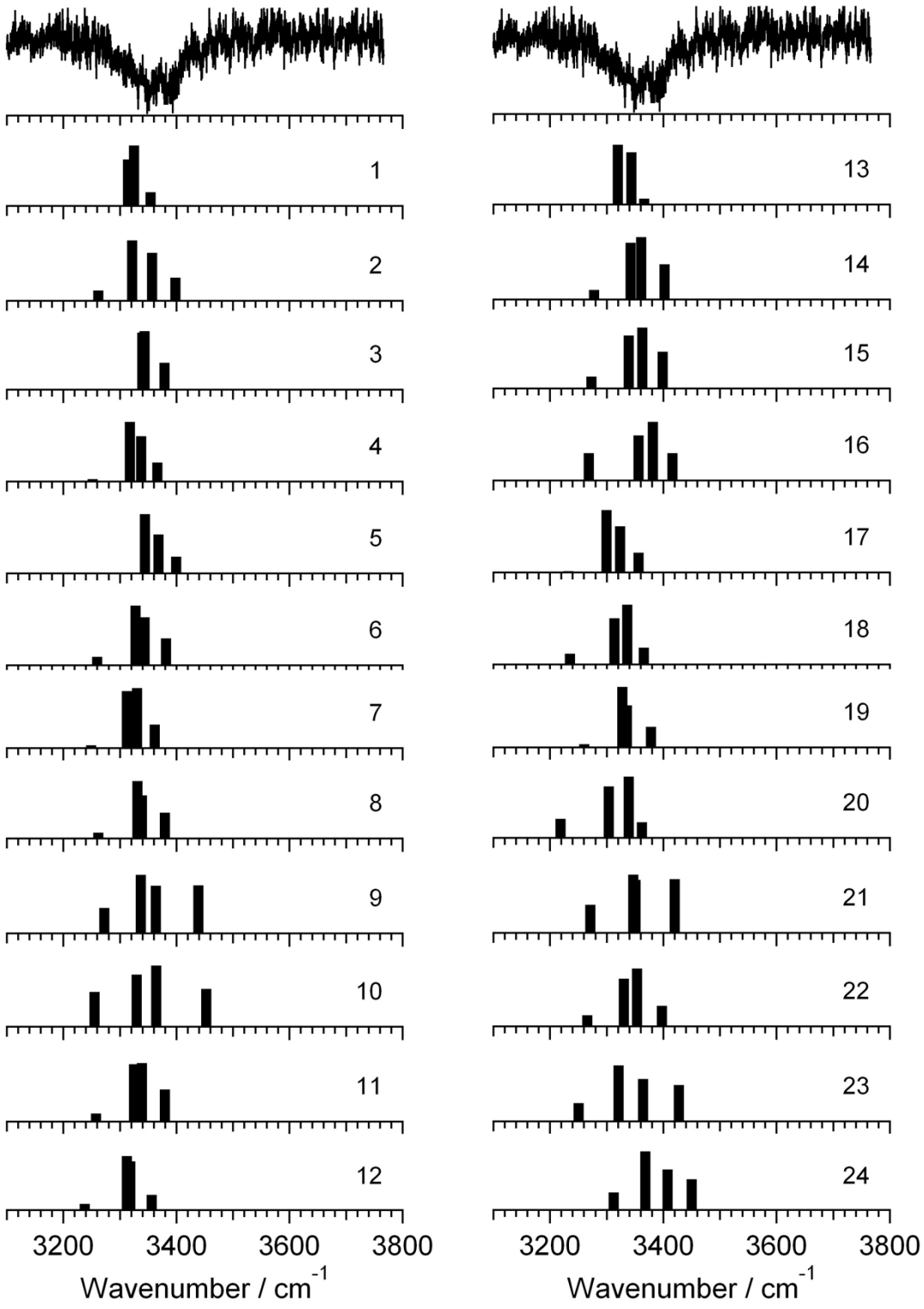

Figure S6. Cont.

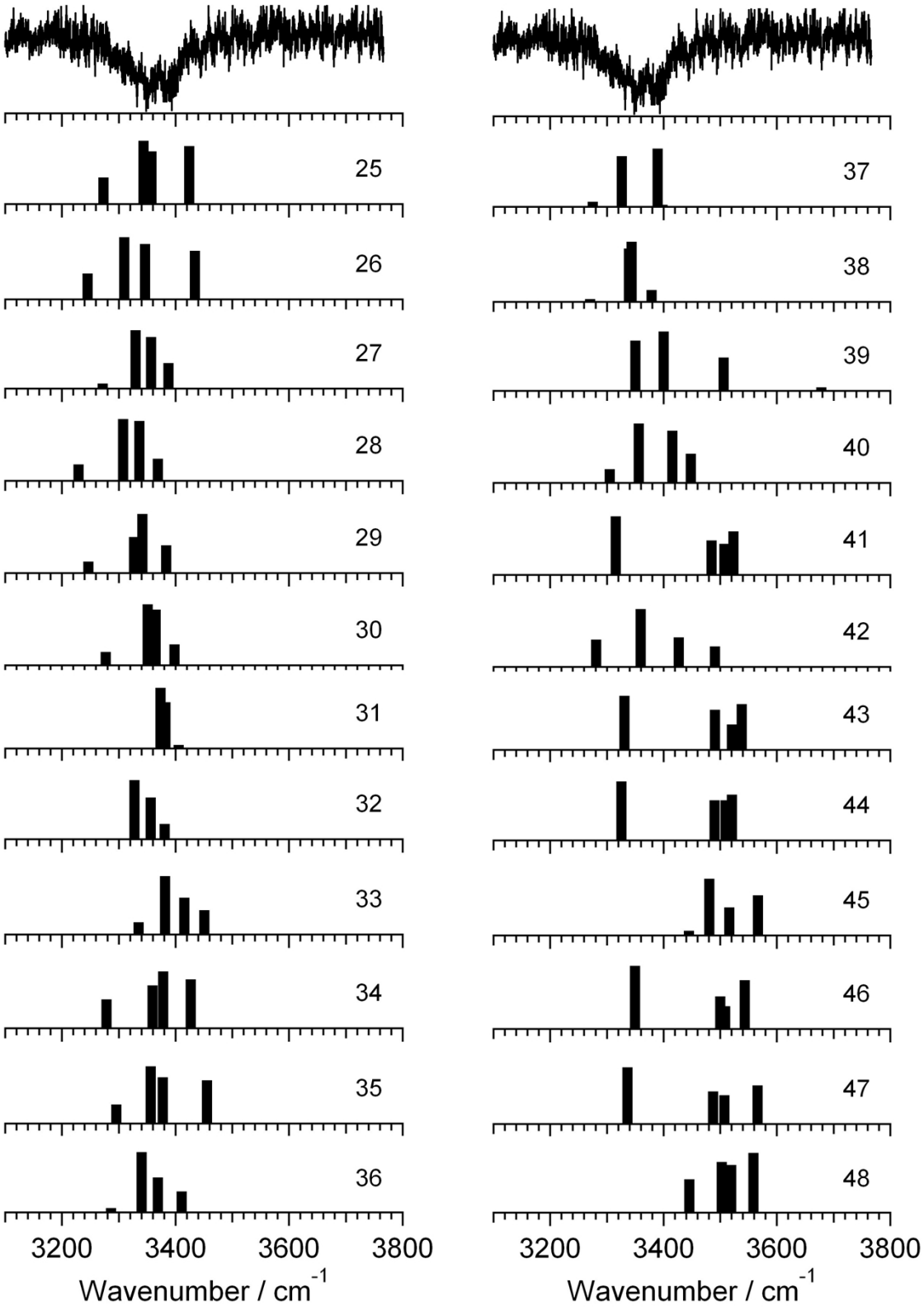

Figure S6. Cont.

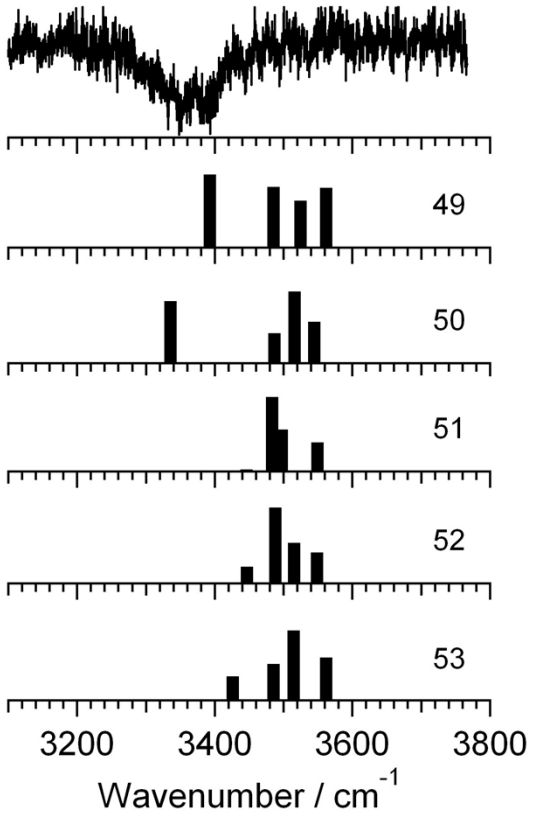

Figure S7. Calculated structures for ciclohexanol$_5$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

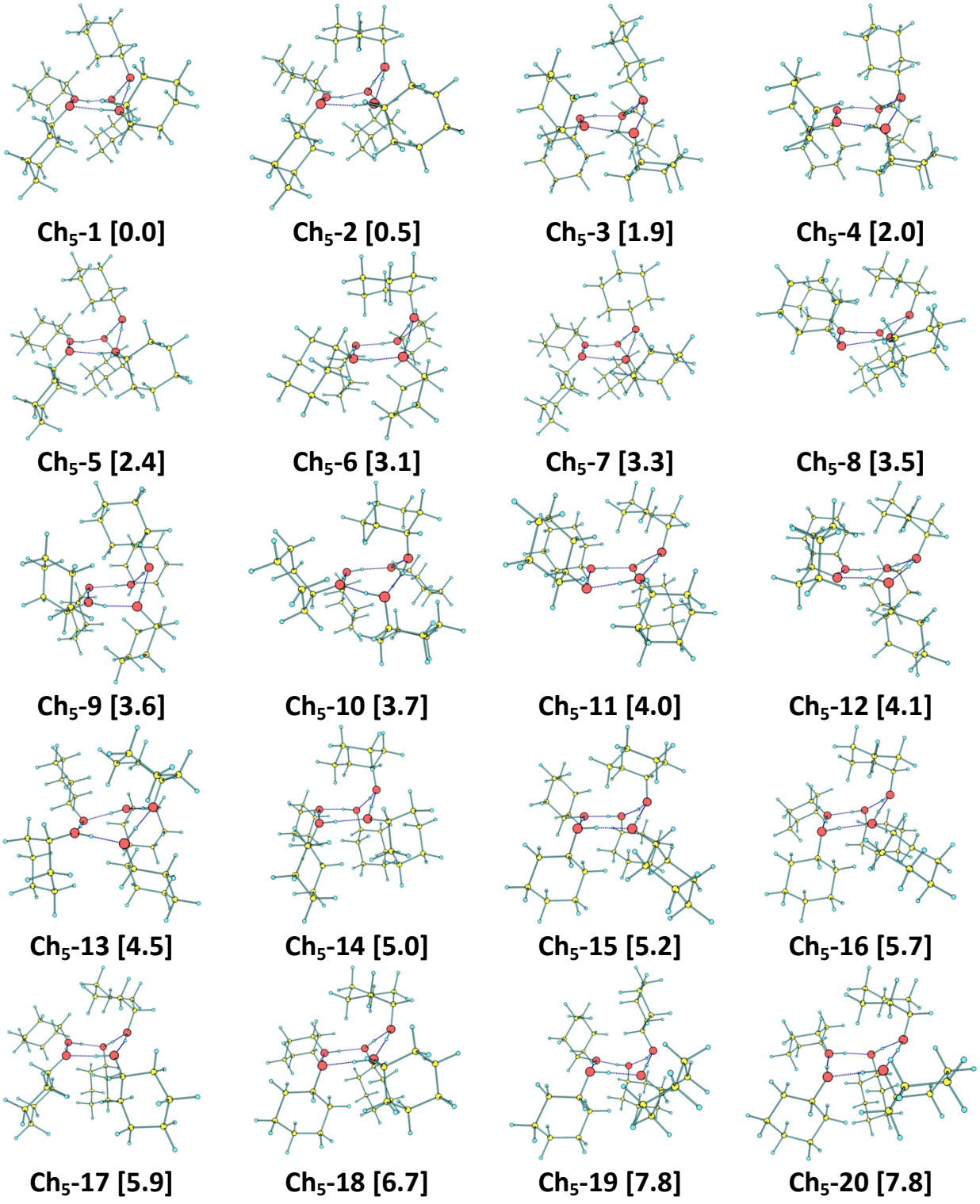

Figure S7. Cont.

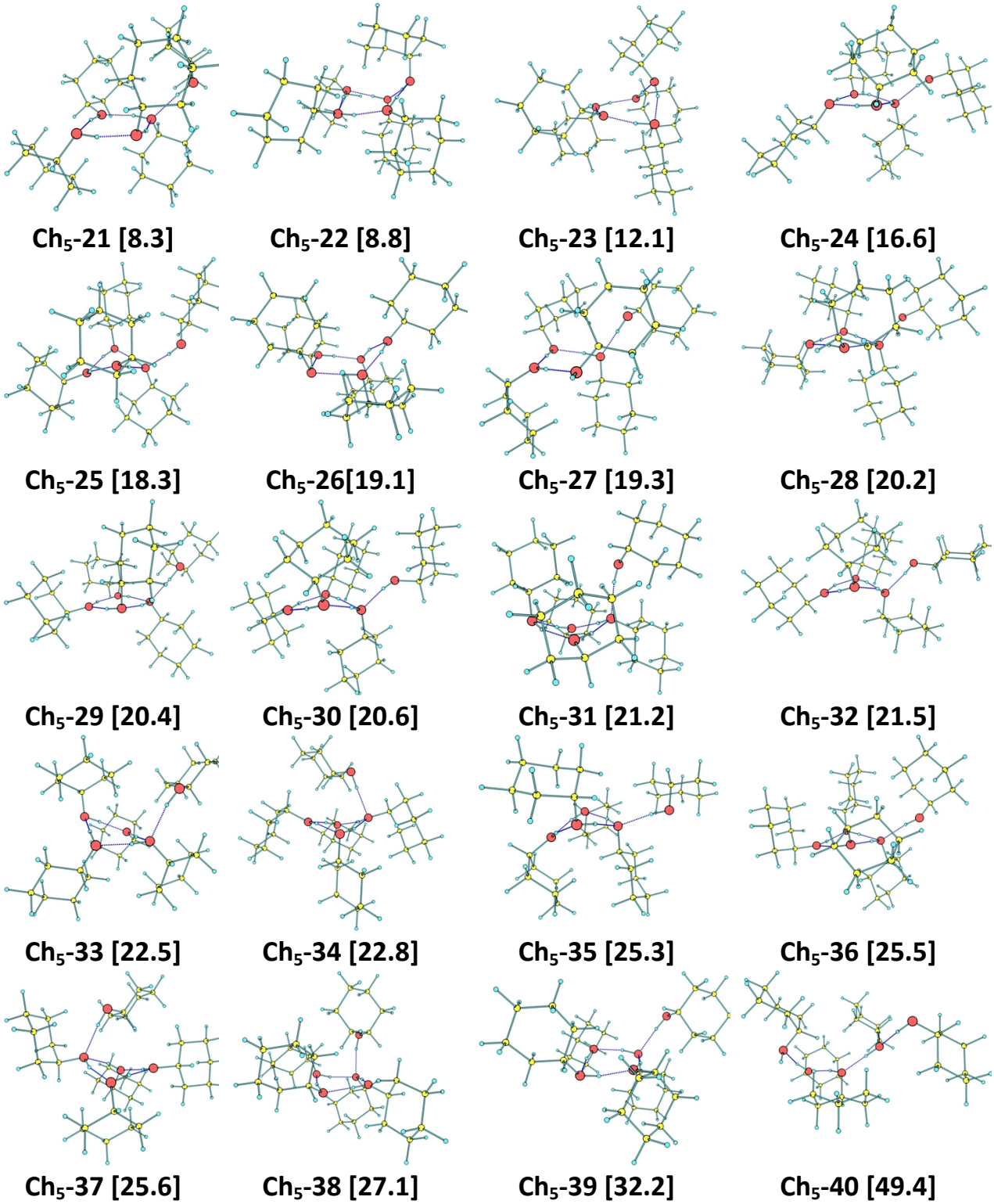

Table S4. Calculated structures for ciclohexanol$_5$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

Structure Ch_5-n n=	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*D_0 (kJ/mol)*	*BSSE (kJ/mol)*
1	0.00	0.00	-179.39	24.64
2	0.12	0.55		
3	0.47	1.95		
4	1.84	1.97		
5	0.44	2.40		
6	1.03	3.13		
7	2.60	3.34		
8	1.62	3.50		
9	-0.36	3.59		
10	4.22	3.66		
11	1.65	4.03		
12	2.64	4.14		
13	2.12	4.46		
14	2.64	4.96		
15	3.25	5.24		
16	3.81	5.69		
17	4.50	5.86		
18	3.66	6.72		
19	5.84	7.83		
20	2.81	7.84		
21	4.87	8.34		
22	5.48	8.79		
23	14.89	12.12		
24	13.71	16.64		
25	18.48	18.27		
26	17.50	19.13		
27	20.48	19.26		
28	17.41	20.24		
29	17.90	20.36		
30	16.43	20.55		
31	20.87	21.17		
32	20.42	21.53		
33	19.66	22.53		
34	21.78	22.82		
35	23.54	25.27		
36	23.90	25.54		
37	24.85	25.62		
38	26.80	27.10		
39	32.28	32.22		
40	49.09	49.41		

Figure S8. Experimental IDIRS for cyclohexanol$_5$ (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-311++G(d,p) level. A correction factor of 0.945 was employed.

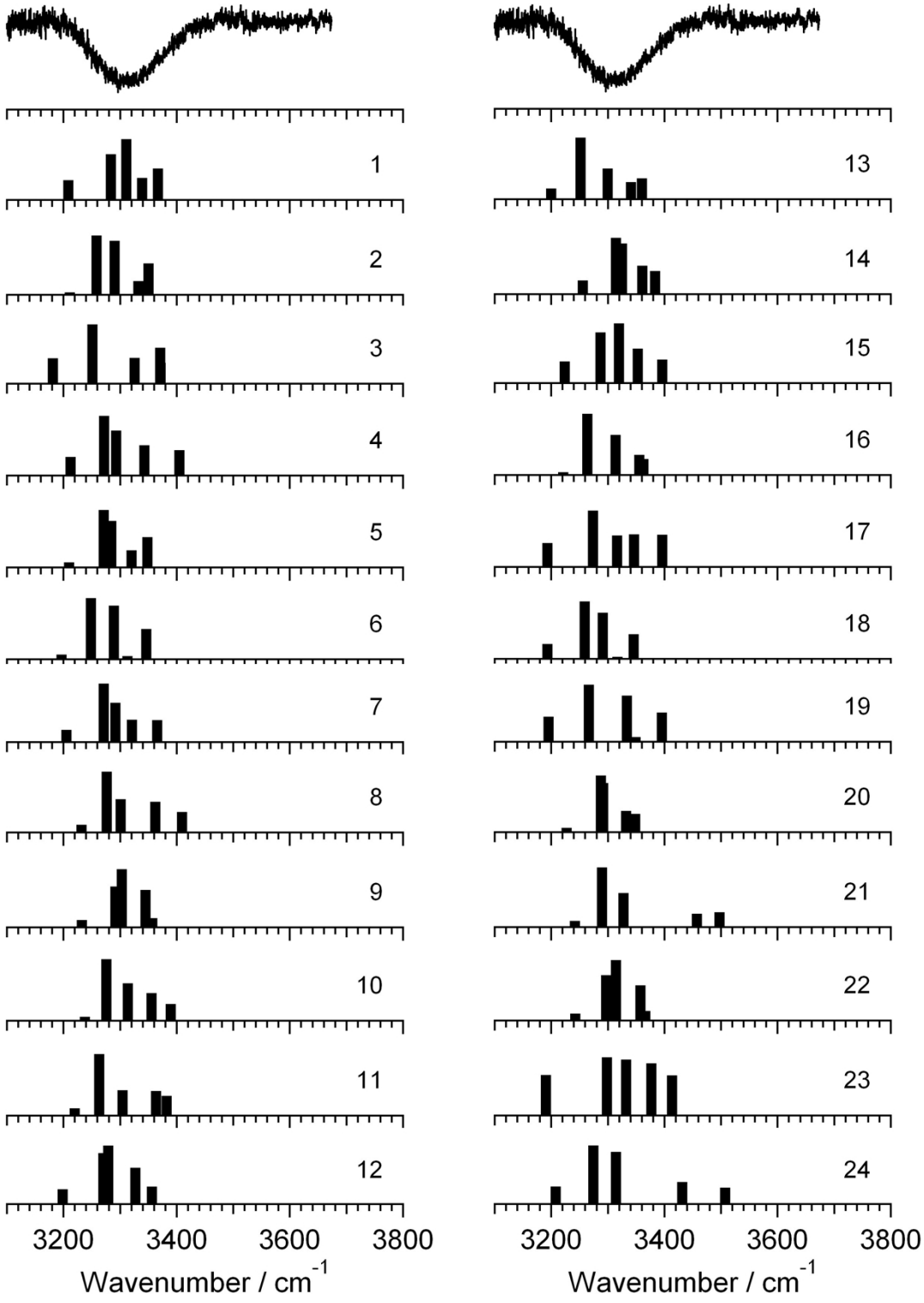

Figure S8. Cont.

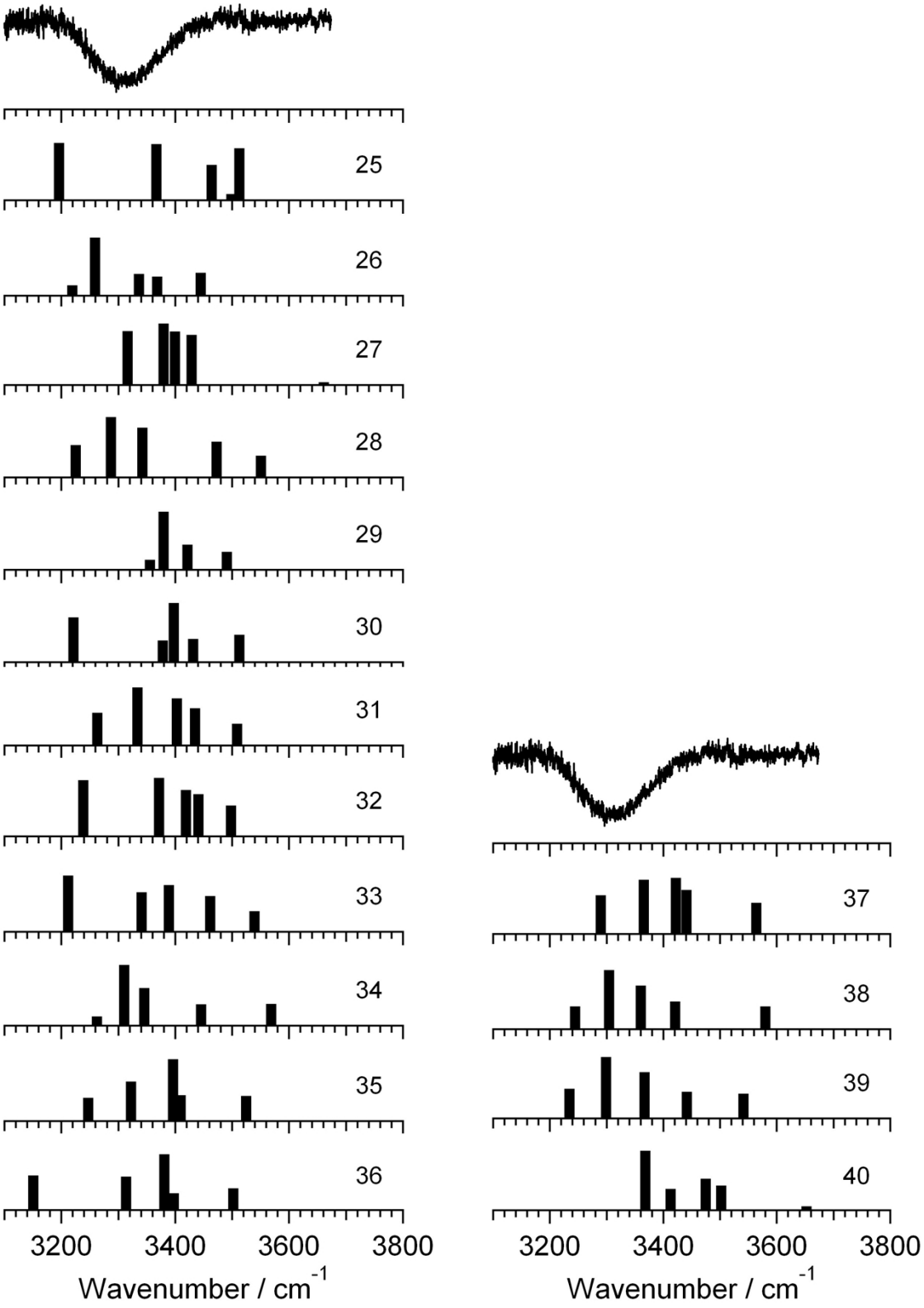

Figure S9. Calculated structures for ciclohexanol$_6$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

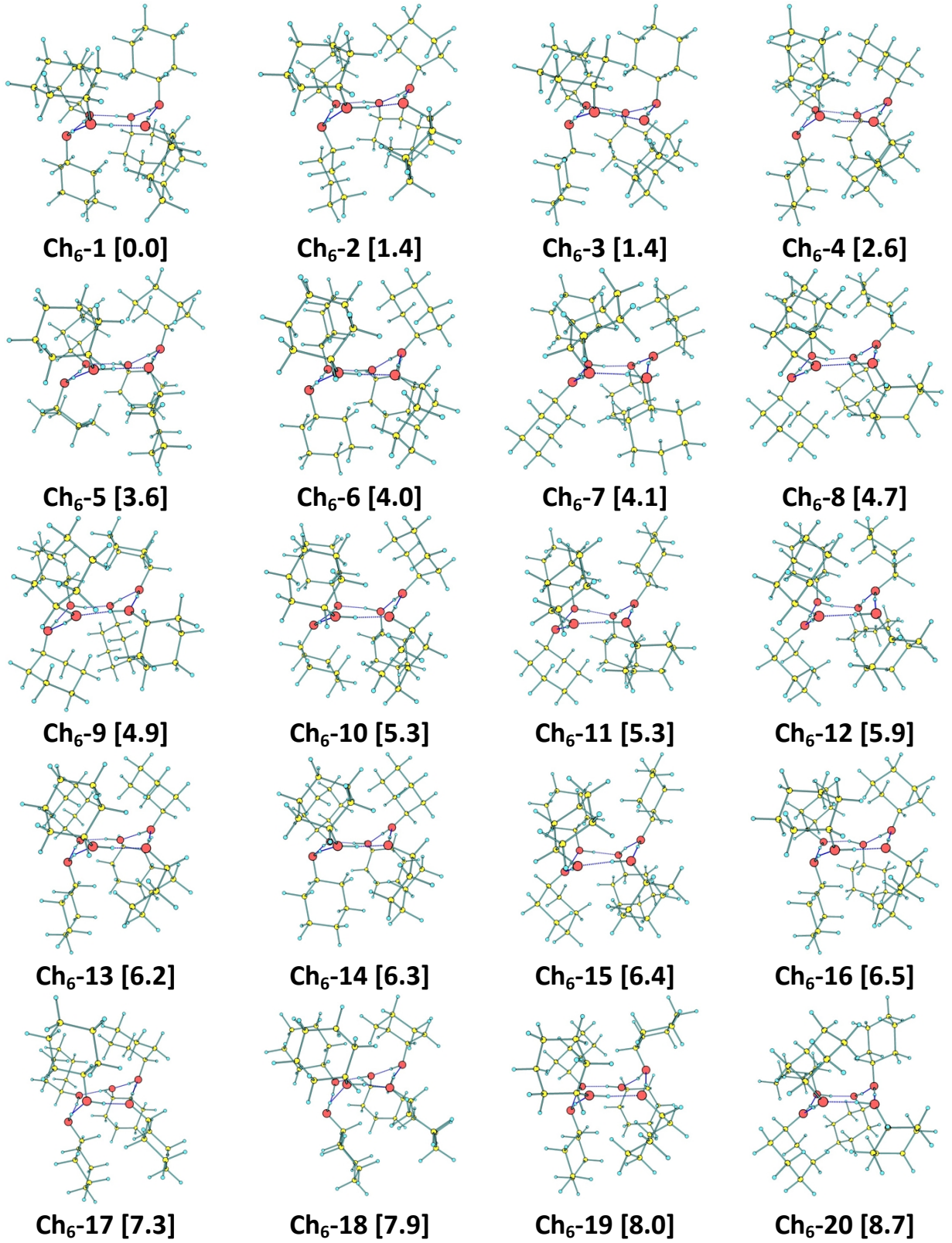

Figure S9. Cont.

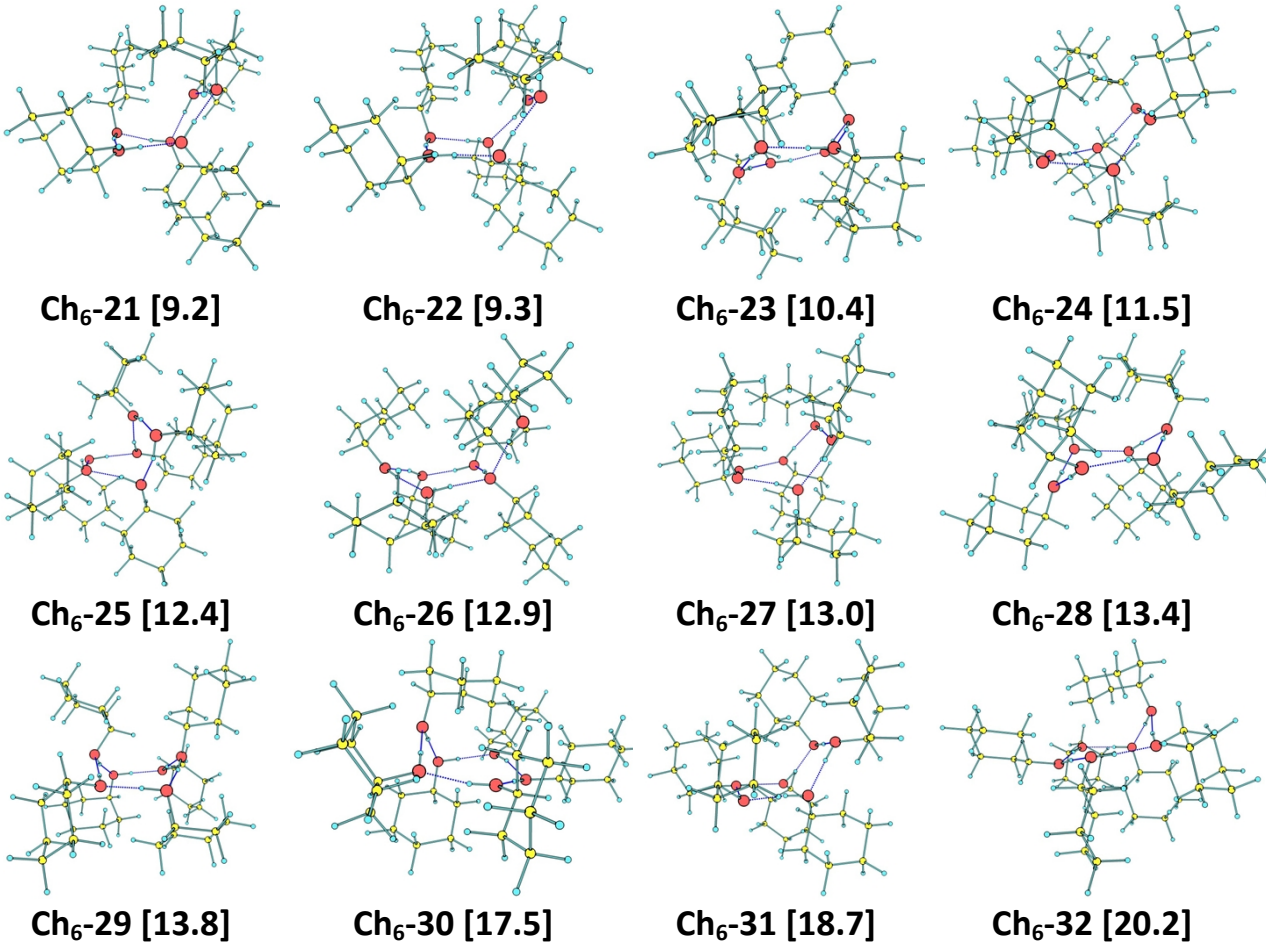

Table S5. Calculated structures for ciclohexanol$_6$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

Structure Ch_6-n n=	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*D_0 (kJ/mol)*	*BSSE (kJ/mol)*
1	0.00	0.00	-233.40	31.00
2	2.83	1.44		
3	5.24	1.45		
4	9.04	2.64		
5	3.60	3.58		
6	6.10	4.05		
7	4.54	4.09		
8	7.40	4.70		
9	6.25	4.92		
10	8.31	5.29		
11	6.40	5.35		
12	11.55	5.89		
13	9.81	6.19		
14	7.82	6.29		
15	10.59	6.43		
16	7.39	6.53		
17	12.41	7.28		
18	12.62	7.85		
19	9.29	8.03		
20	10.38	8.69		
21	12.72	9.25		
22	12.54	9.30		
23	10.48	10.37		
24	12.71	11.48		
25	11.46	12.44		
26	17.39	12.88		
27	15.44	13.03		
28	15.80	13.36		
29	14.66	13.85		
30	21.92	17.47		
31	23.21	18.69		
32	20.15	20.20		

Figure S10. Experimental IDIRS for cyclohexanol$_6$ (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-311++G(d,p) level. A correction factor of 0.945 was employed.

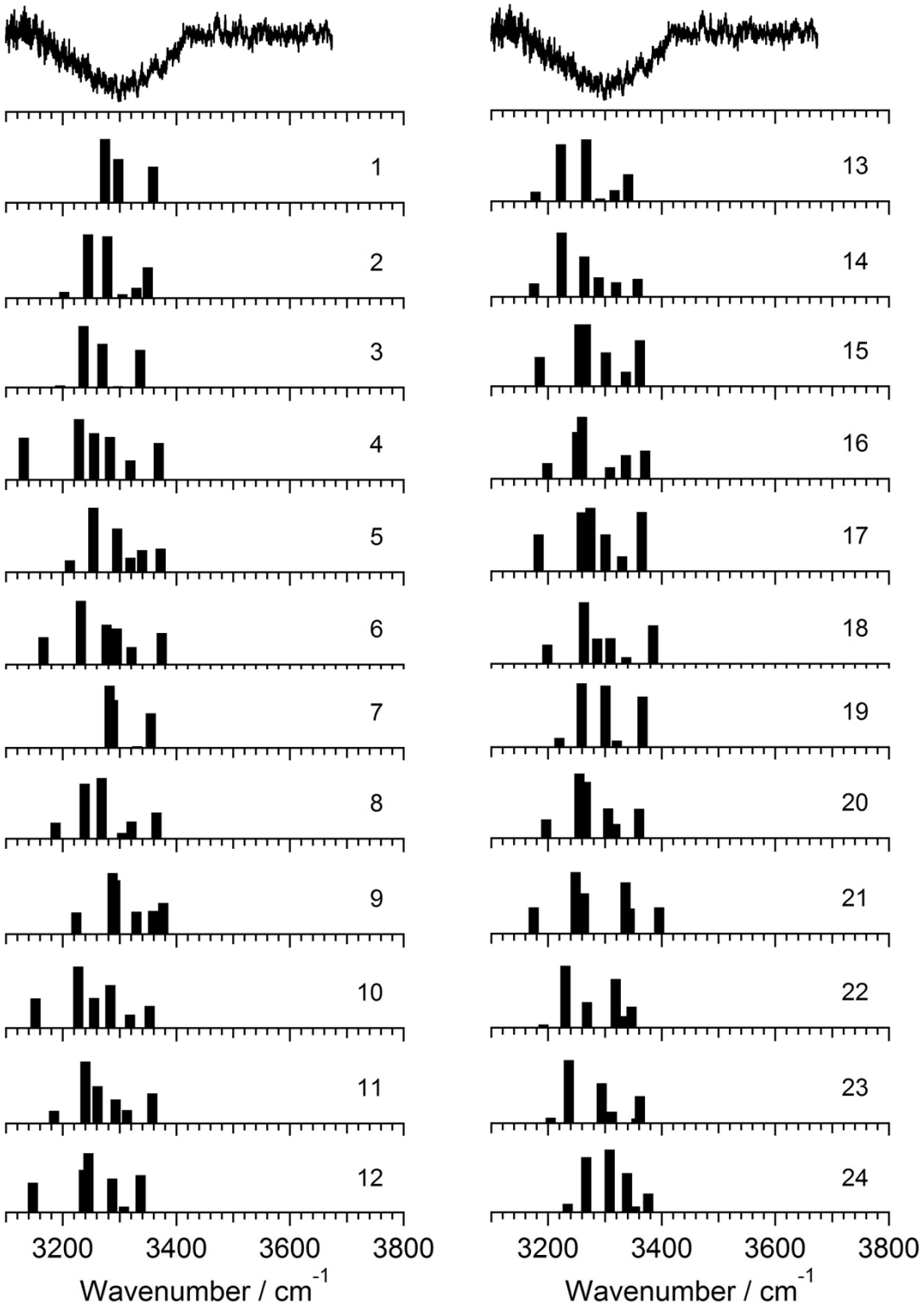

Figure S10. Cont.

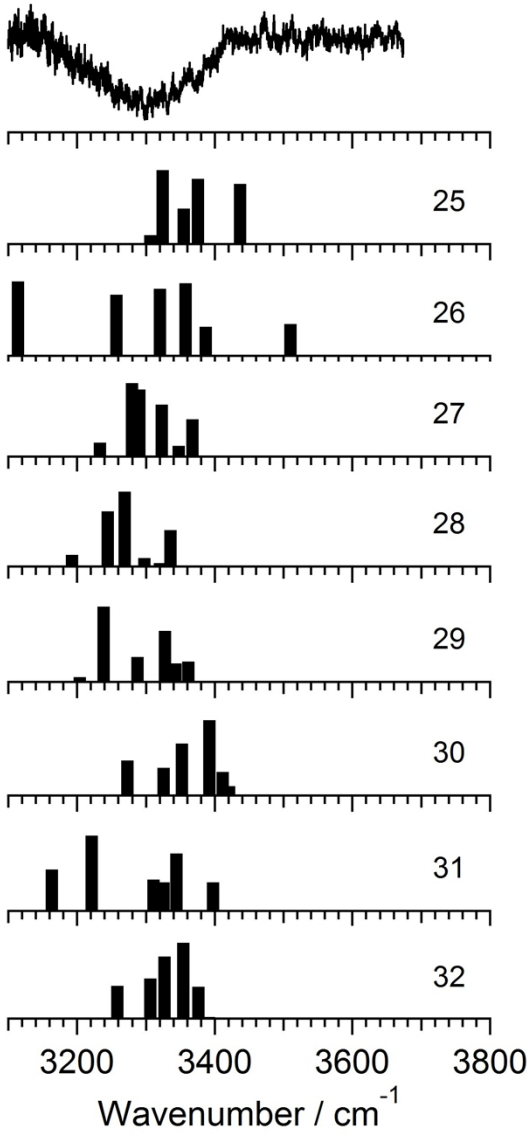

Table S6. Relative energies with the ZPE contributions for the first 20 ciclohexanol$_2$ structures, calculated at M06-2X/6-311++G(d,p) level. ΔG column indicates the sum of electronic and thermal Free Energies at 298.25K.

Structure Ch_2-n n=	ΔE_{ZPE} *(kJ/mol)*	*Relative position with* ΔG	ΔG *(kJ/mol)*
1	0.00	2	1.20
2	0.20	10	3.48
3	1.05	15	4.69
4	1.30	19	5.41
5	1.57	3	1.39
6	1.75	5	2.61
7	1.97	14	4.26
8	2.12	18	5.21
9	2.31	9	3.24
10	2.33	13	4.12
11	2.65	12	3.93
12	2.77	6	2.72
13	2.78	8	2.79
14	2.80	7	2.78
15	3.08	20	6.00
16	3.11	11	3.65
17	3.16	28	7.93
18	3.22	1	0.00
19	3.28	4	1.73
20	3.28	17	4.83

Table S7. Relative energies with the ZPE contributions for the first 20 ciclohexanol$_3$ structures, calculated at M06-2X/6-311++G(d,p) level. ΔG column indicates the sum of electronic and thermal Free Energies at 298.25K.

Structure Ch_3-n n=	ΔE_{ZPE} *(kJ/mol)*	*Relative position with* ΔG	ΔG *(kJ/mol)*
1	0.00	17	8.36
2	0.12	10	4.71
3	0.12	4	2.16
4	0.17	26	10.85
5	0.62	3	2.15
6	0.62	15	7.57
7	0.90	7	4.12
8	0.96	23	10.27
9	1.00	22	10.08
10	1.10	9	4.67
11	1.10	11	5.01
12	1.36	2	1.69
13	1.61	18	8.37
14	2.20	8	4.13
15	2.24	6	3.14
16	2.60	21	9.50
17	2.64	14	7.56
18	2.79	12	5.27
19	3.00	1	0.00
20	3.03	5	2.79

Table S8. Relative energies with the ZPE contributions for the first 20 ciclohexanol$_4$ structures, calculated at M06-2X/6-311++G(d,p) level. ΔG column indicates the sum of electronic and thermal Free Energies at 298.25K.

Structure Ch_4-n n=	ΔE_{ZPE} *(kJ/mol)*	*Relative position with* ΔG	ΔG *(kJ/mol)*
1	0.00	14	8.94
2	5.80	8	7.18
3	5.90	15	9.36
4	6.36	1	0.00
5	7.00	11	8.10
6	7.39	4	4.43
7	7.40	30	11.63
8	7.41	31	11.73
9	7.87	6	5.15
10	8.10	22	10.62
11	8.26	10	8.06
12	8.39	16	9.53
13	8.53	26	11.09
14	8.61	33	12.40
15	8.69	3	4.41
16	8.84	12	8.50
17	9.08	5	4.81
18	9.18	2	0.55
19	9.59	25	10.83
20	9.60	28	11.47

Table S9. Relative energies with the ZPE contributions for the first 20 ciclohexanol$_5$ structures, calculated at M06-2X/6-311++G(d,p) level. ΔG column indicates the sum of electronic and thermal Free Energies at 298.25K.

Structure Ch_5-n n=	ΔE_{ZPE} *(kJ/mol)*	*Relative position with* ΔG	ΔG *(kJ/mol)*
1	0.00	1	0.00
2	0.55	2	3.25
3	1.95	8	8.57
4	1.97	3	4.10
5	2.40	5	6.76
6	3.13	10	9.23
7	3.34	7	7.02
8	3.50	6	6.81
9	3.59	18	12.25
10	3.66	9	8.79
11	4.03	14	10.75
12	4.14	11	9.40
13	4.46	12	9.82
14	4.96	21	15.59
15	5.24	13	10.63
16	5.69	4	6.41
17	5.86	16	11.37
18	6.72	19	12.31
19	7.83	17	11.43
20	7.84	23	17.69

Table S10. Relative energies with the ZPE contributions for the first 20 ciclohexanol$_6$ structures, calculated at M06-2X/6-311++G(d,p) level. ΔG column indicates the sum of electronic and thermal Free Energies at 298.25K.

Structure Ch_6-n n=	ΔE_{ZPE} *(kJ/mol)*	*Relative position with* ΔG	ΔG *(kJ/mol)*
1	0.00	12	7.45
2	1.44	7	4.83
3	1.45	1	0.00
4	2.64	6	4.71
5	3.58	8	5.36
6	4.05	2	2.01
7	4.09	5	2.93
8	4.70	14	8.02
9	4.92	22	11.17
10	5.29	10	7.31
11	5.35	15	8.08
12	5.89	3	2.21
13	6.19	13	7.67
14	6.29	20	9.83
15	6.43	4	2.81
16	6.53	18	8.52
17	7.28	9	5.93
18	7.85	11	7.33
19	8.03	17	8.25
20	8.69	19	9.56