Supporting information for:

Mass resolved IR spectroscopy of aniline-water

aggregates

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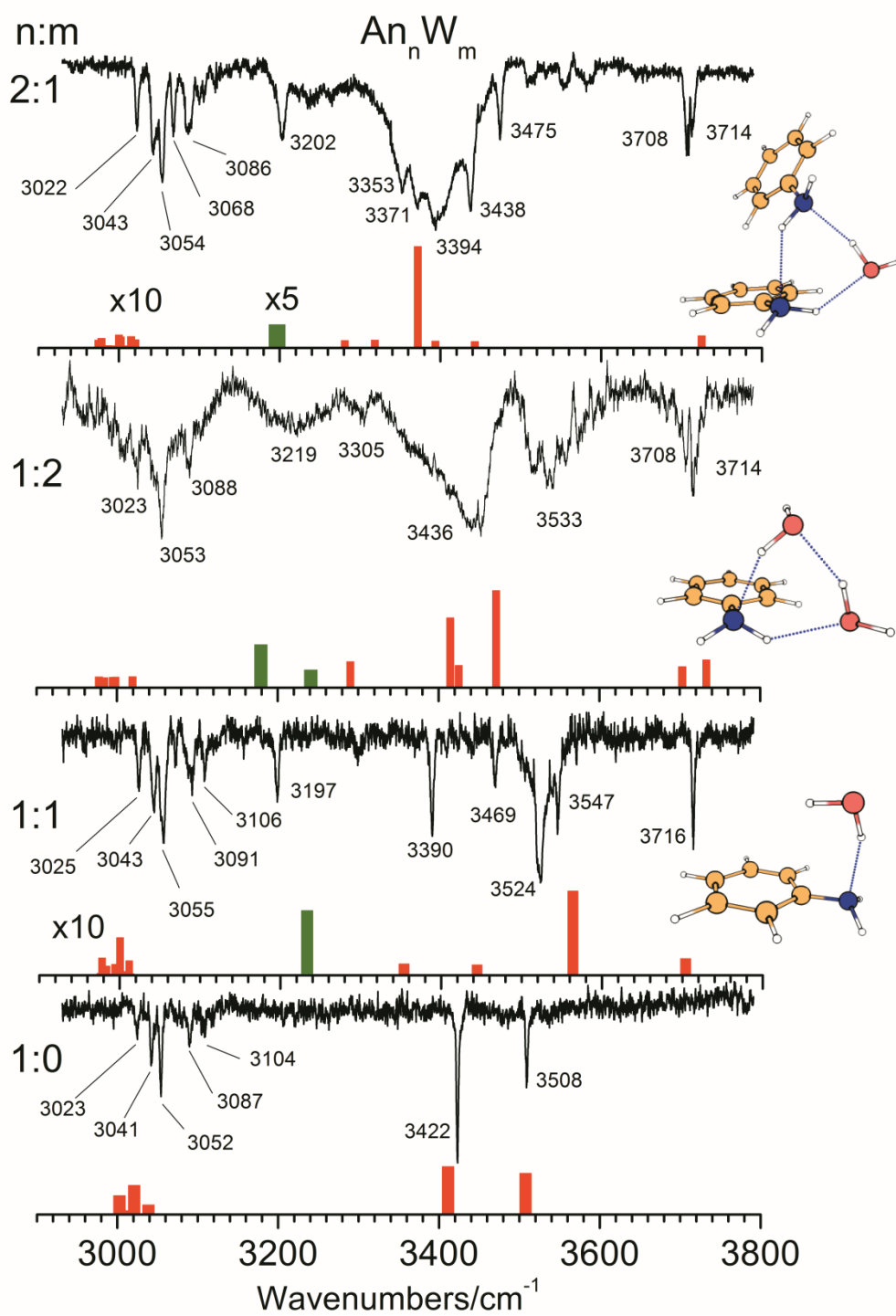
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Figure S1. Annotated version of Figure 1.

Figure S2. Calculated structures of aniline·W_1 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.
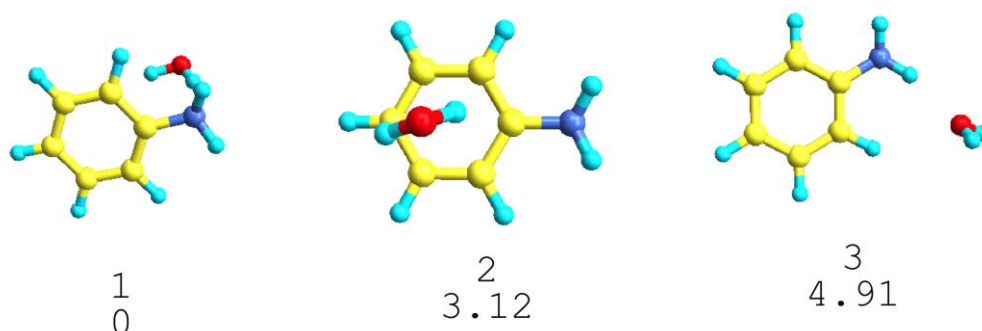

Table S1. Calculated structures for aniline·W_1 at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.

Structure	ΔE (kJ/mol)	ΔE_{ZPE} (kJ/mol)	D_0 (kJ/mol)	BSSE (kJ/mol)
1	0.00	0.00	-16.93	4.16
2	7.44	3.12	-14.85	3.12
3	6.86	4.91	-12.87	3.31

Figure S3. Experimental IDIRS of ciclohexanol·W_1 (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-311++G(d,p) level. A correction factor of 0.938 was employed.
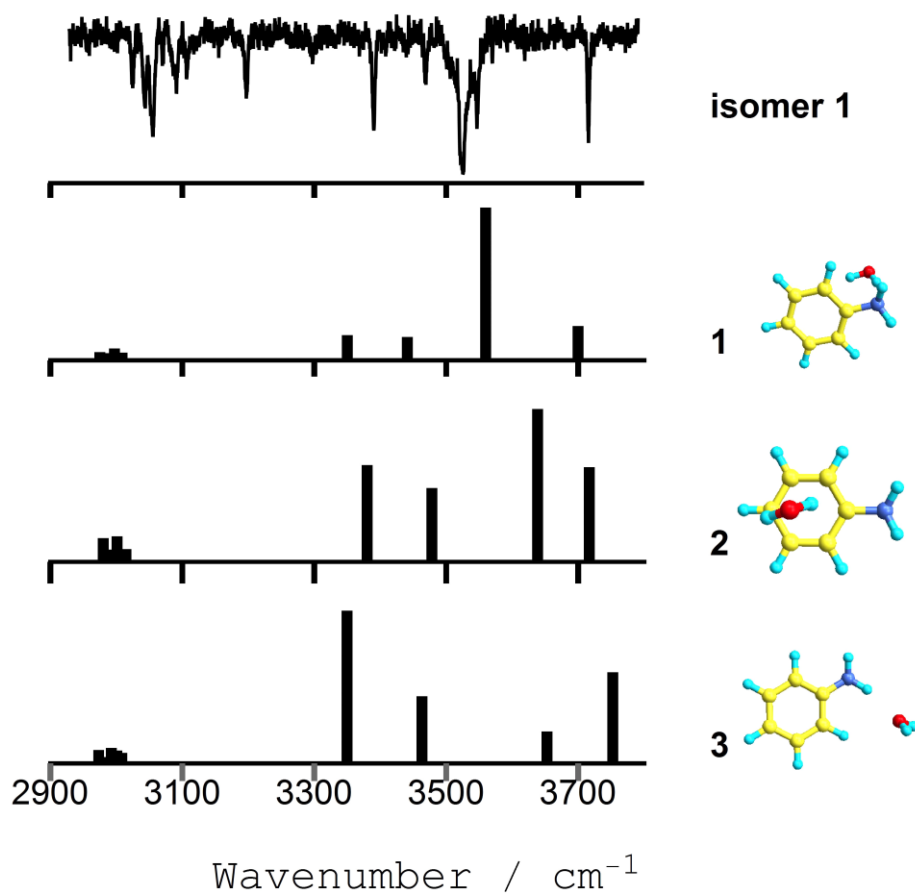
Figure S4. Calculated structures of aniline·W_2 at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.
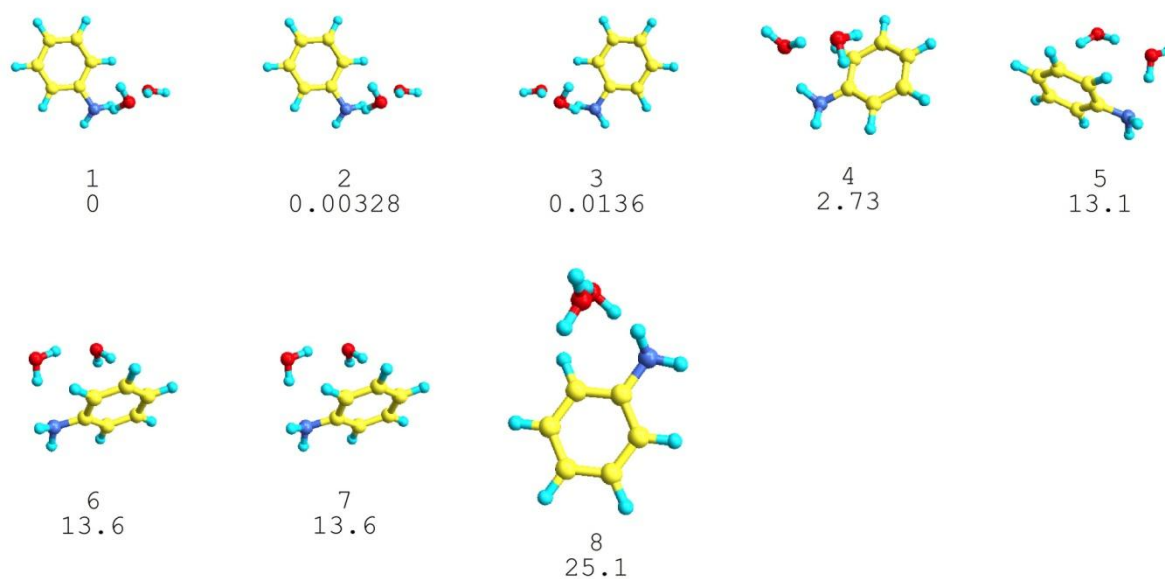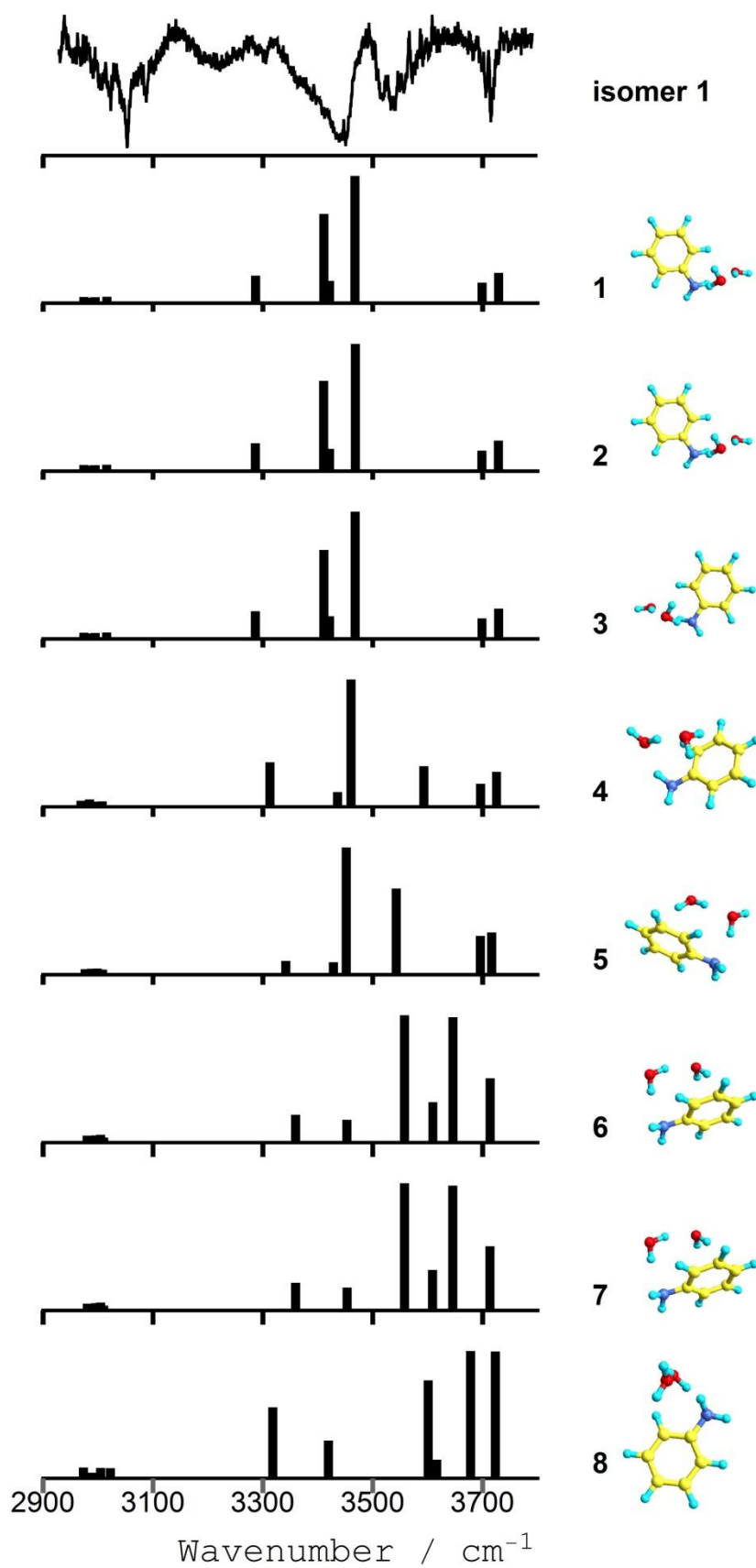

Table S2. Calculated structures of ciclohexanol·W_2 at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.
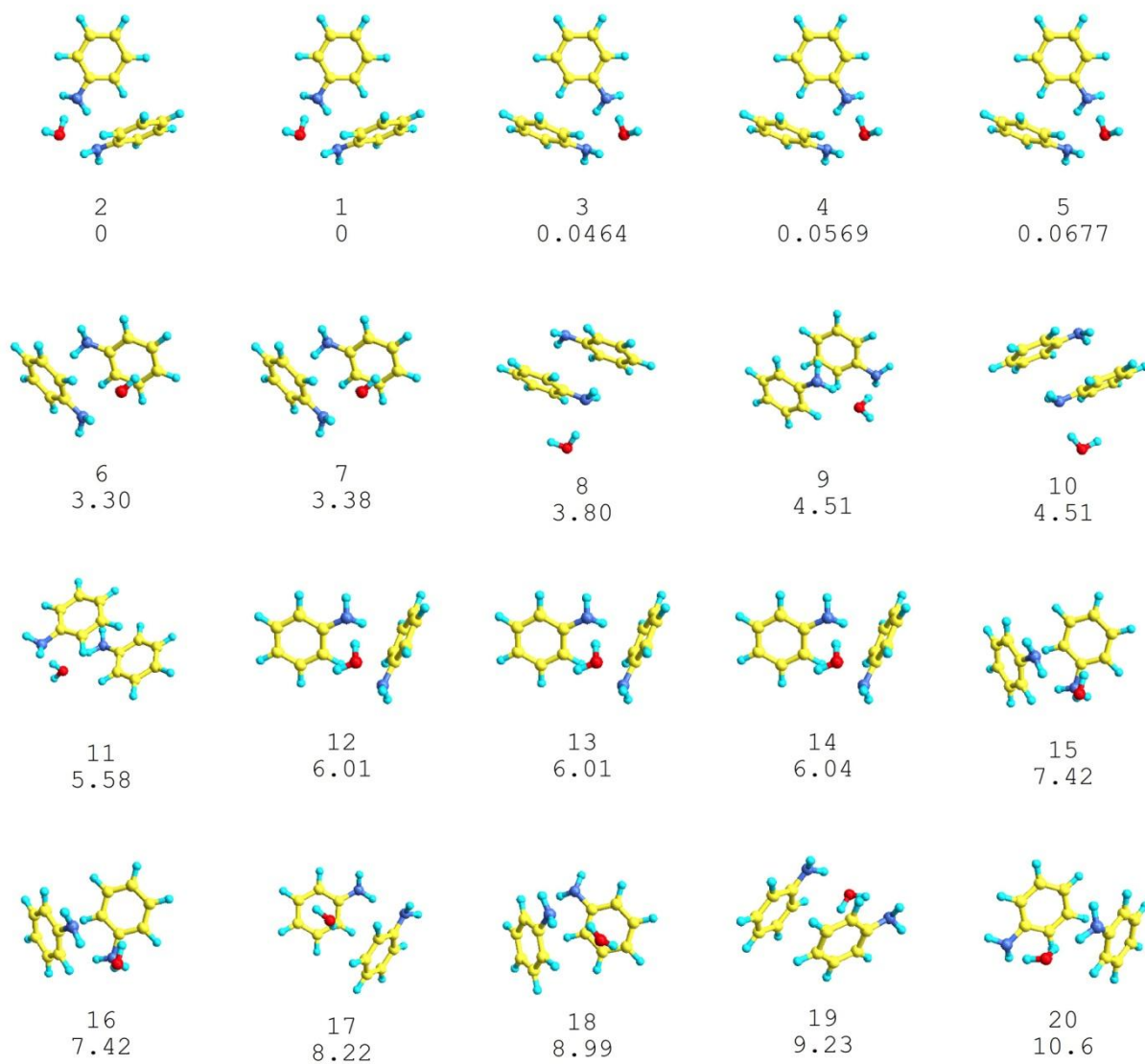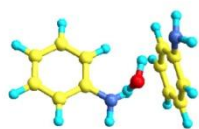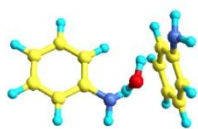
Structure	ΔE (kJ/mol)	ΔE_{ZPE} (kJ/mol)
1	0.00	0.00
2	0.00	0.00
3	0.00	0.01
4	6.52	2.73
5	15.53	13.10
6	16.72	13.63
7	16.72	13.64
8	27.51	25.11

Figure S5. Experimental IDIRS of aniline·W$_2$ (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-311++G(d,p) level. A correction factor of 0.938 was employed.

Figure S6. Calculated structures of anilina$_2 \cdot$W$_1$ 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.
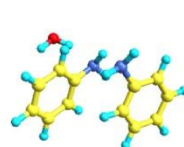

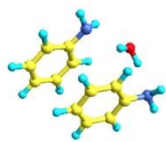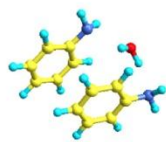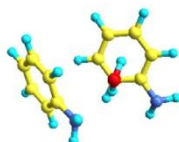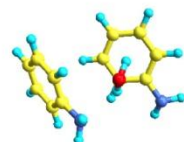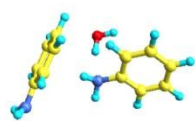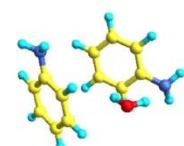|				
2 0	1 0	3 0.0464	4 0.0569	5 0.0677
6 3.30	7 3.38	8 3.80	9 4.51	10 4.51
11 5.58	12 6.01	13 6.01	14 6.04	15 7.42
16 7.42	17 8.22	18 8.99	19 9.23	20 10.6

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11.6

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11.6

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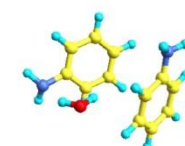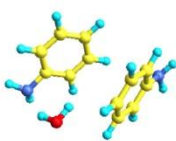11.7

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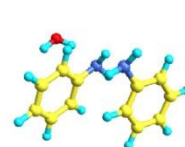
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12.1

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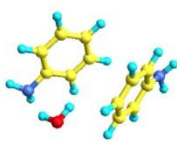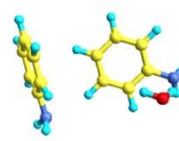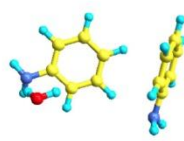30
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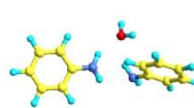18.0

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20.6

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20.6

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22.4

37
22.5

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26.4

39
26.4

40
28.5

Table S3. Calculated structures of aniline$_2 \cdot$W$_1$ 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	ΔE (kJ/mol)	ΔE$_{ZPE}$ (kJ/mol)
1	0.00	0.00
2	0.00	0.00
3	0.00	0.05
4	0.00	0.06
5	0.00	0.07
6	6.48	3.30
7	6.48	3.38
8	7.15	3.80
9	4.80	4.50
10	7.32	4.51
11	4.67	5.58
12	7.89	6.01
13	7.89	6.01
14	7.88	6.04
15	8.11	7.42
16	8.11	7.42
17	12.22	8.22
18	11.58	8.99
19	11.57	9.23

Table S3. Cont.

Structure	ΔE (kJ/mol)	ΔE_ZPE (kJ/mol)
20	12.93	10.57
21	12.47	11.56
22	12.47	11.57
23	13.38	11.73
24	13.74	12.08
25	13.74	12.09
26	12.65	12.30
27	12.65	12.31
28	16.68	12.92
29	16.68	12.97
30	17.27	13.50
31	17.26	13.60
32	18.70	15.13
33	20.43	17.99
34	23.15	20.63
35	23.14	20.63
36	25.37	22.43
37	25.38	22.46
38	30.86	26.43
39	30.86	26.44
40	30.79	28.51

Figure S7. Experimental IDIRS of aniline$_2 \cdot$W$_1$ (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-311++G(d,p) level. A correction factor of 0.938 was employed.
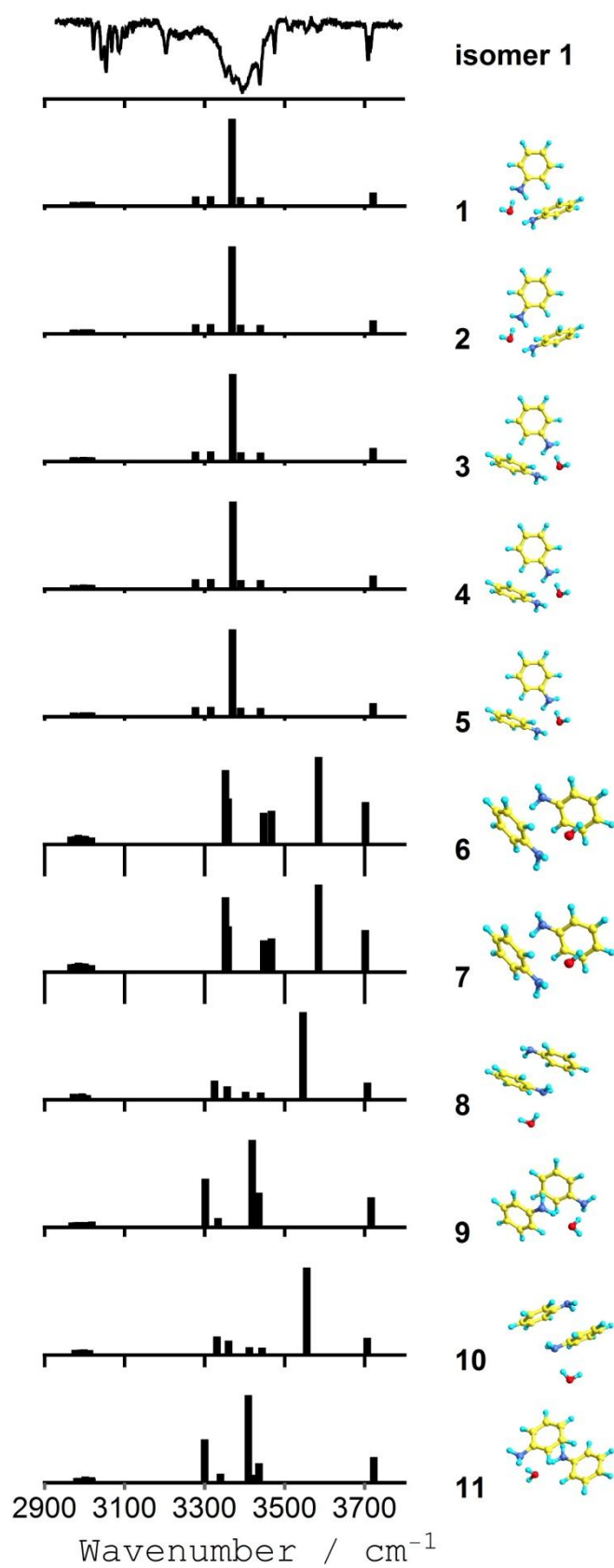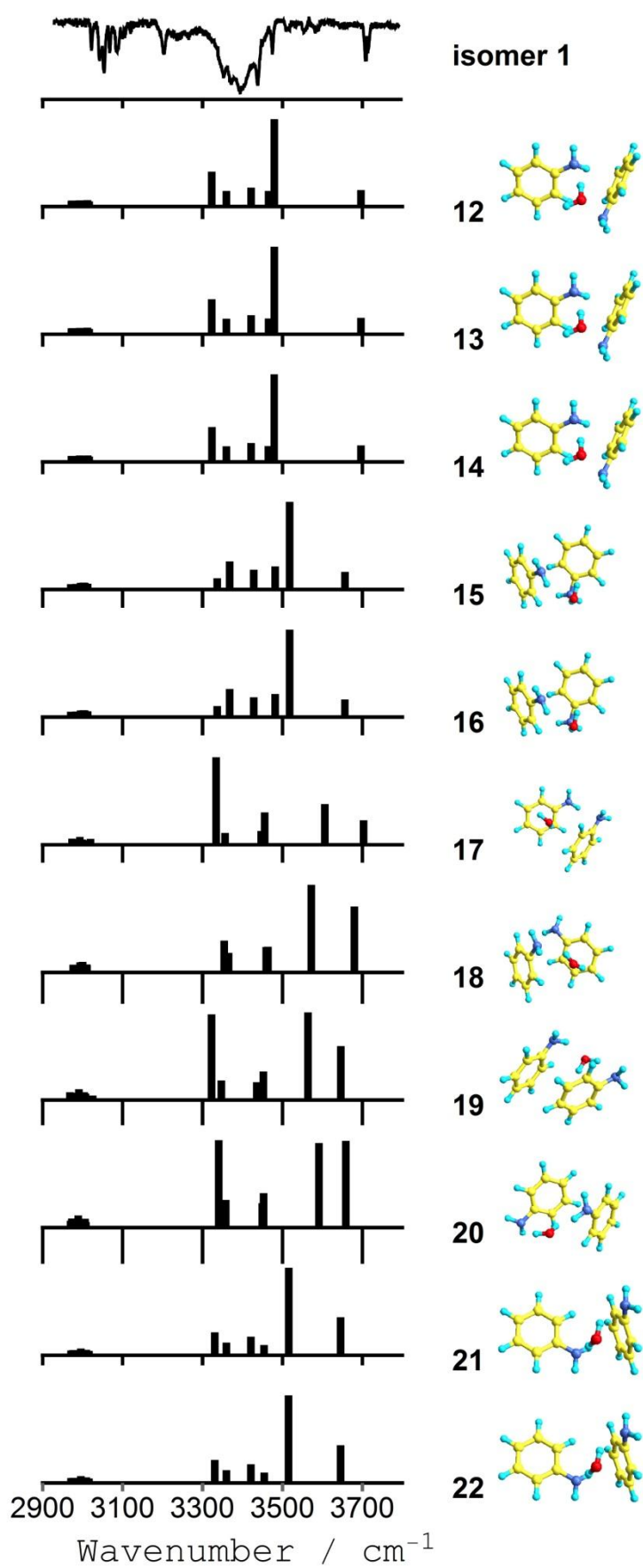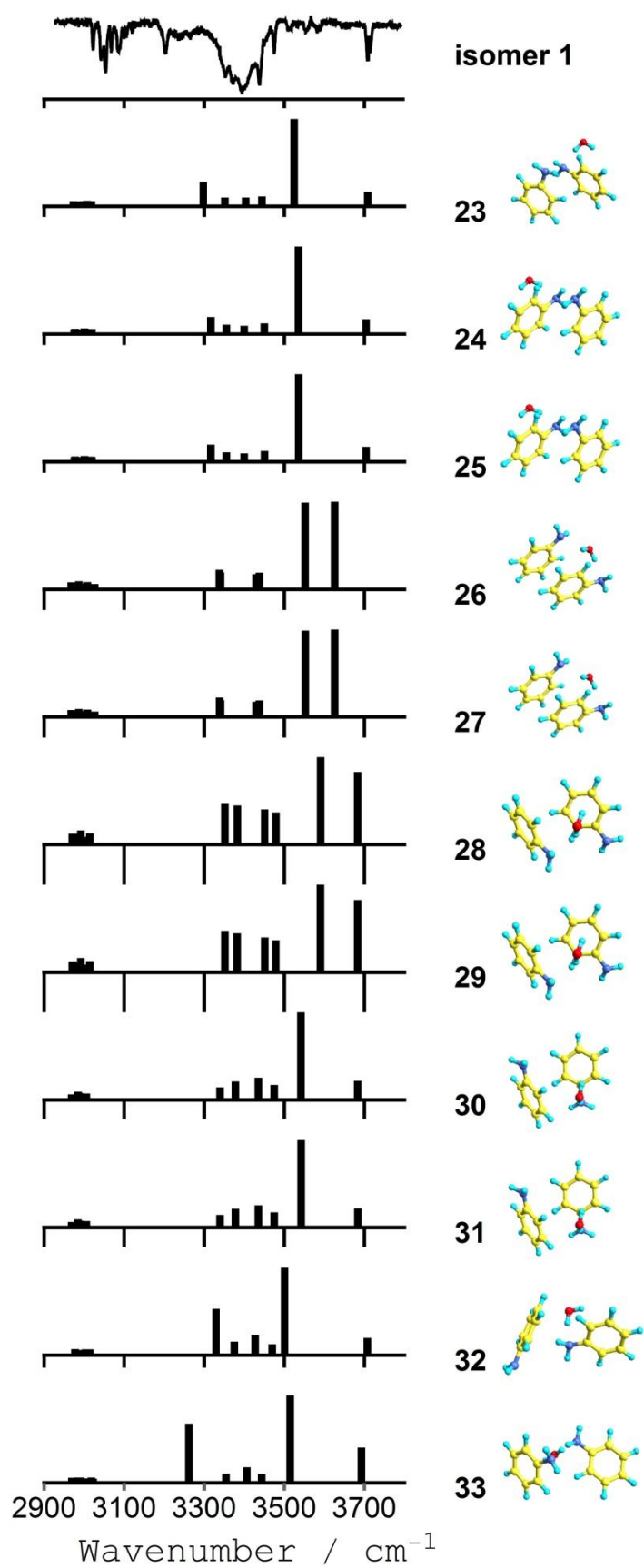

isomer 1

Wavenumber / cm^{-1}

Figure S7. Cont.

Wavenumber / cm⁻¹

Figure S7. Cont.

isomer 1

23

24

25

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33

2900 3100 3300 3500 3700

Wavenumber / cm^{-1}

Figure S7. Cont.

isomer 1

34

35

36

37

38

39

40

Wavenumber / cm^{-1}