Supplementary Material for PCCP
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The structure of host-guest complexes between dibenzo-18-crown-6 and water, ammonia, methanol, and acetylene -Evidence of molecular recognition on the complexation-

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Supporting Information

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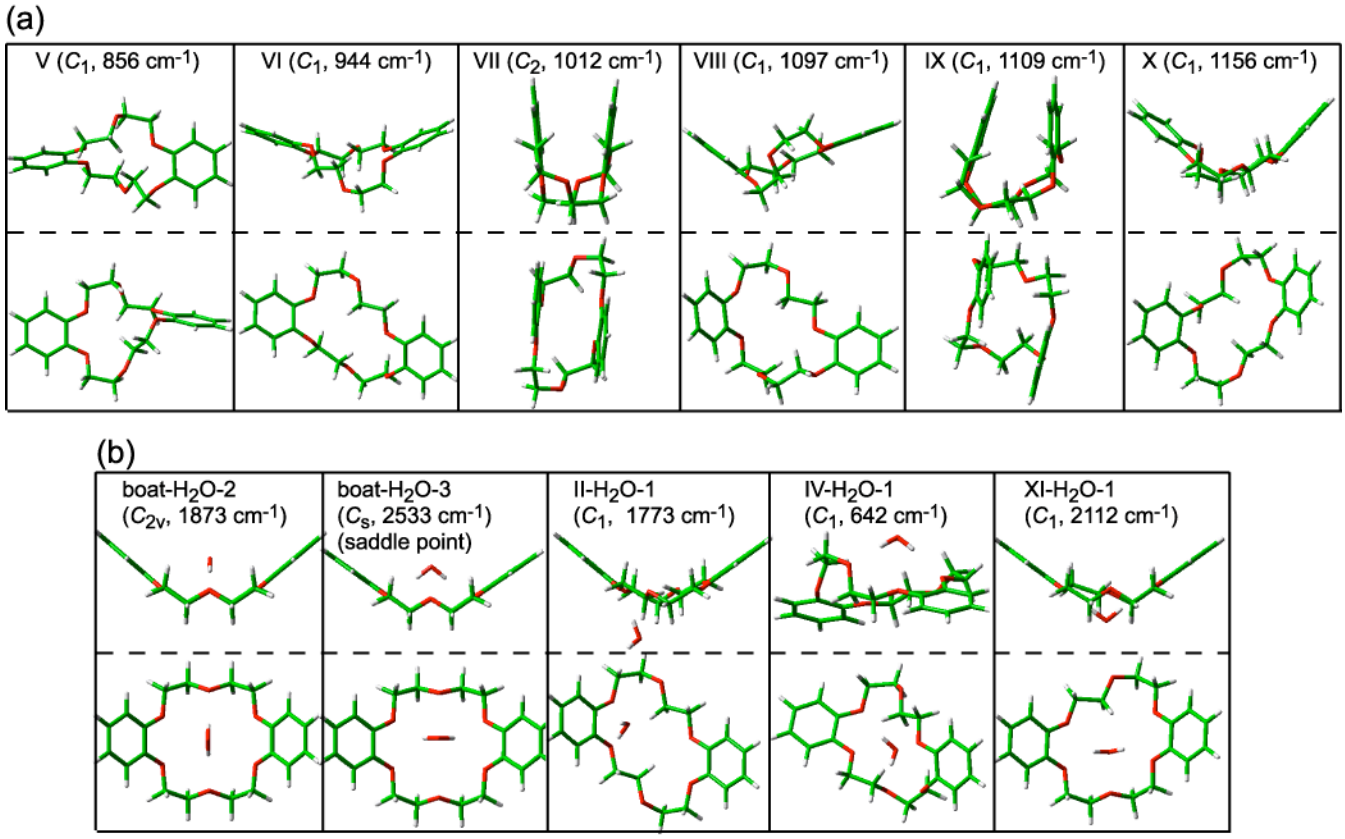

Fig. S1. Optimized structures of (a) DB18C6 and (b) DB18C6-H_2O at higher energy.

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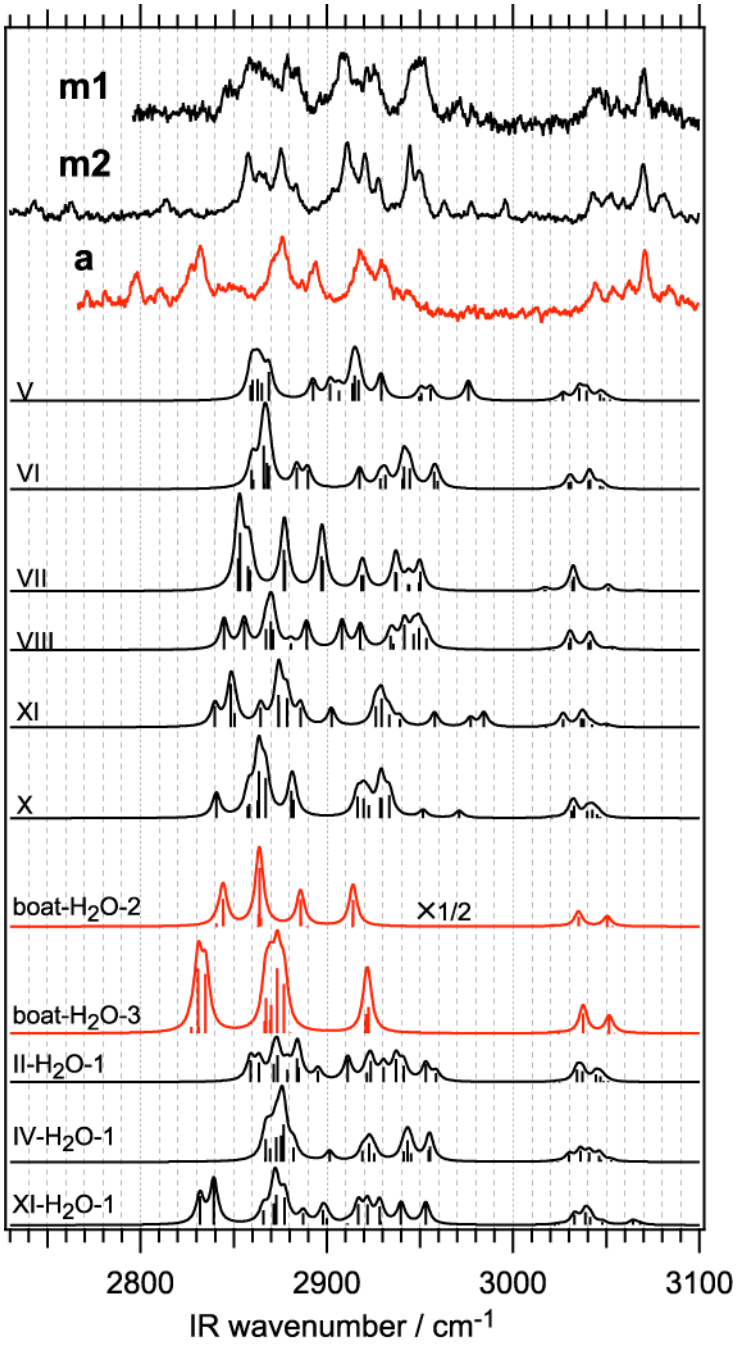

Fig. S2. IR spectra of **m1**, **m2** and **a** and calculated IR spectra of DB18C6 and DB18C6-H_2O in the CH stretching energy region.

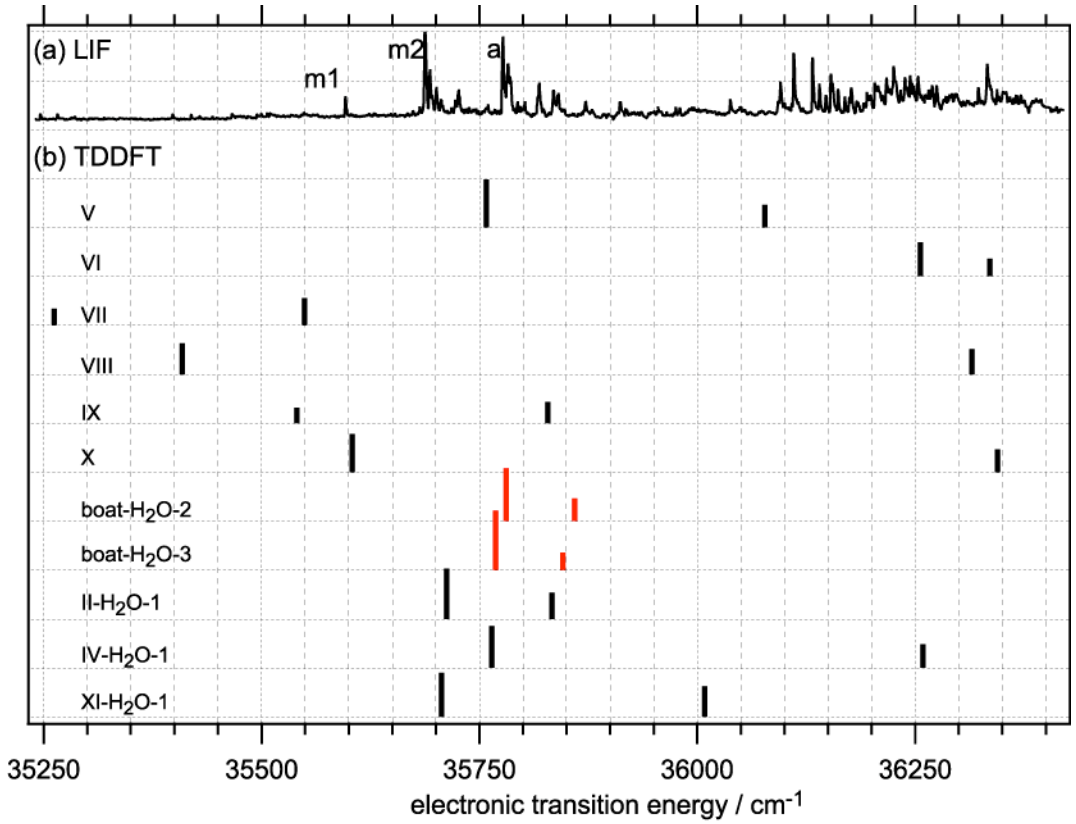

Fig. S3. (a) LIF spectrum of bare DB18C6 and DB18C6-H_2O. (b) Calculated S_1-S_0 and S_2-S_0 electronic transition energies of DB18C6 and DB18C6-H_2O.

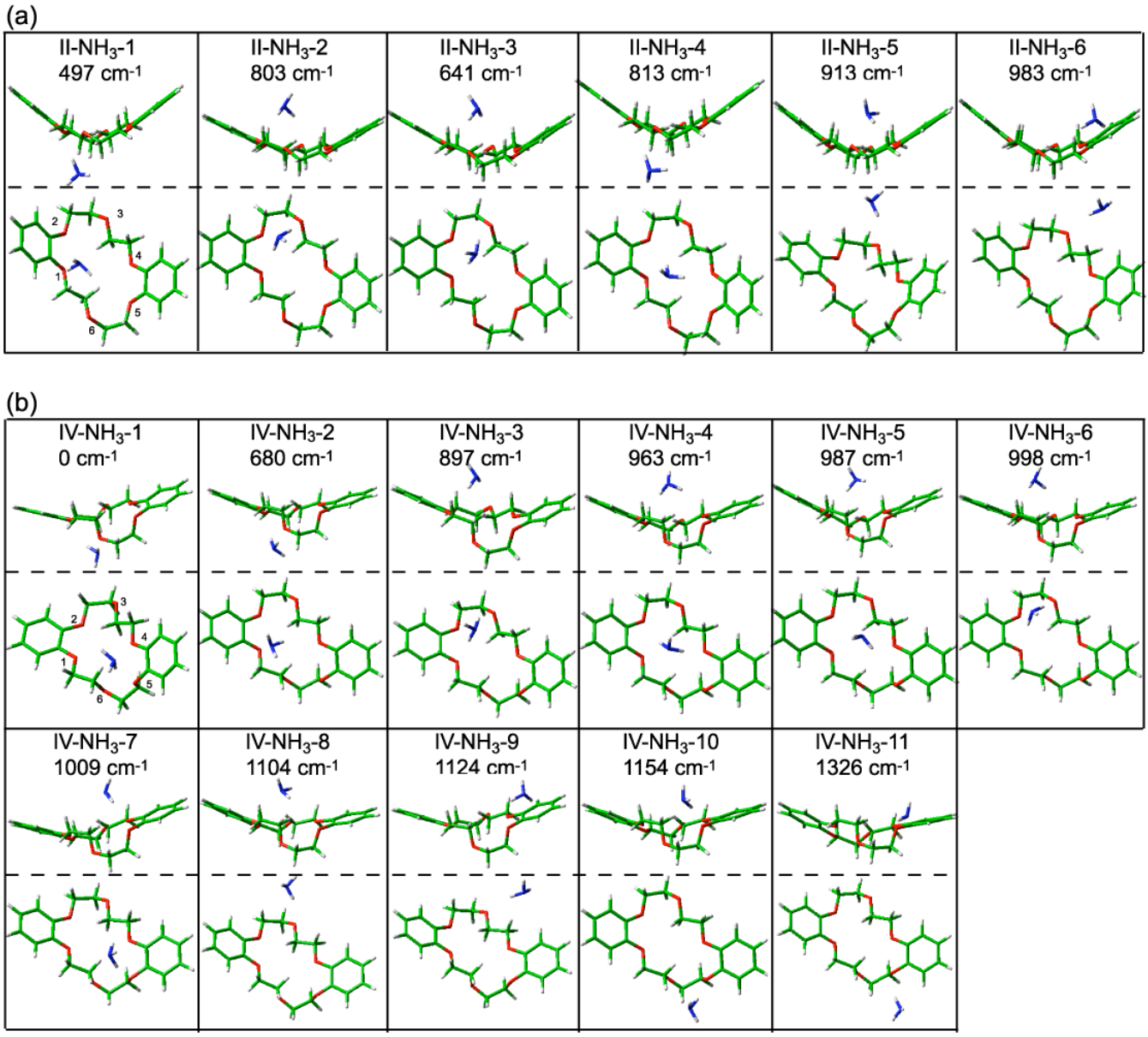

Fig. S4. Optimized structures of DB18C6-NH_3 built on (a) **II** and (b) **IV** conformations.

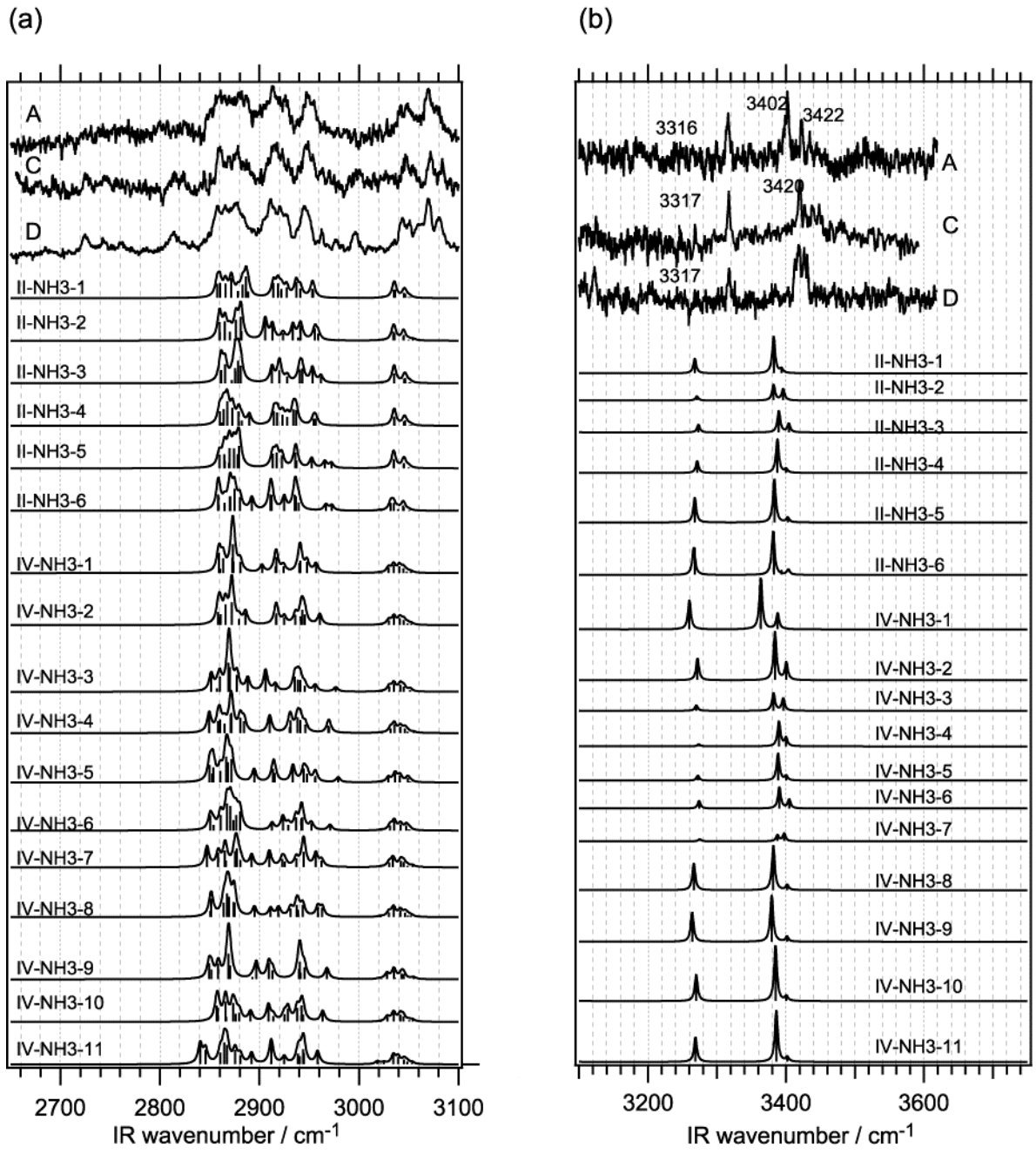

Fig. S5. Calculated IR spectra of DB18C6-NH_3 built on **II** and **IV** conformations in the region of (a) CH and (b) NH stretching vibrations.

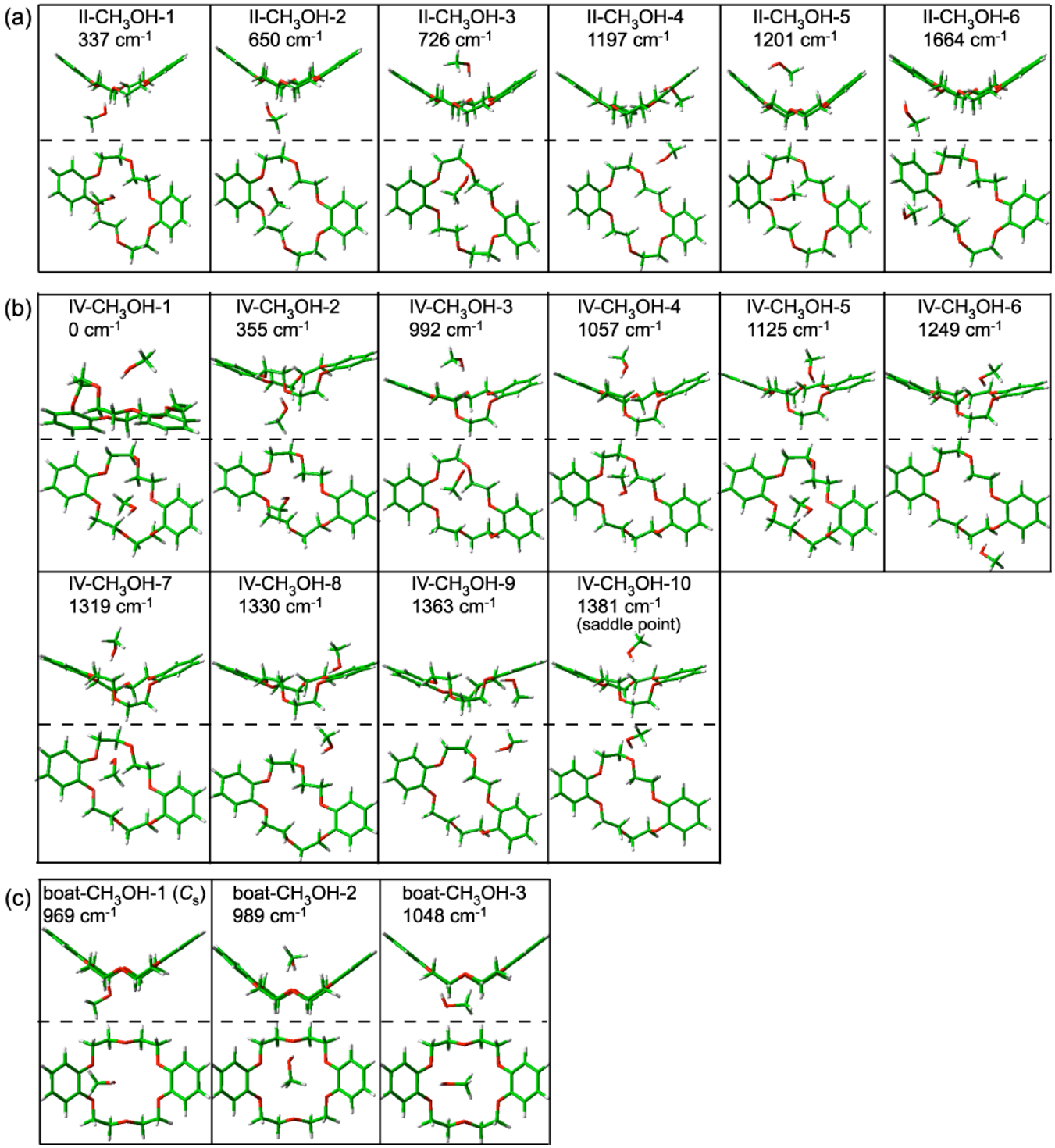

Fig. S6. Optimized structures of DB18C6-CH_3OH built on (a) **II**, (b) **IV**, and (c) boat conformations.

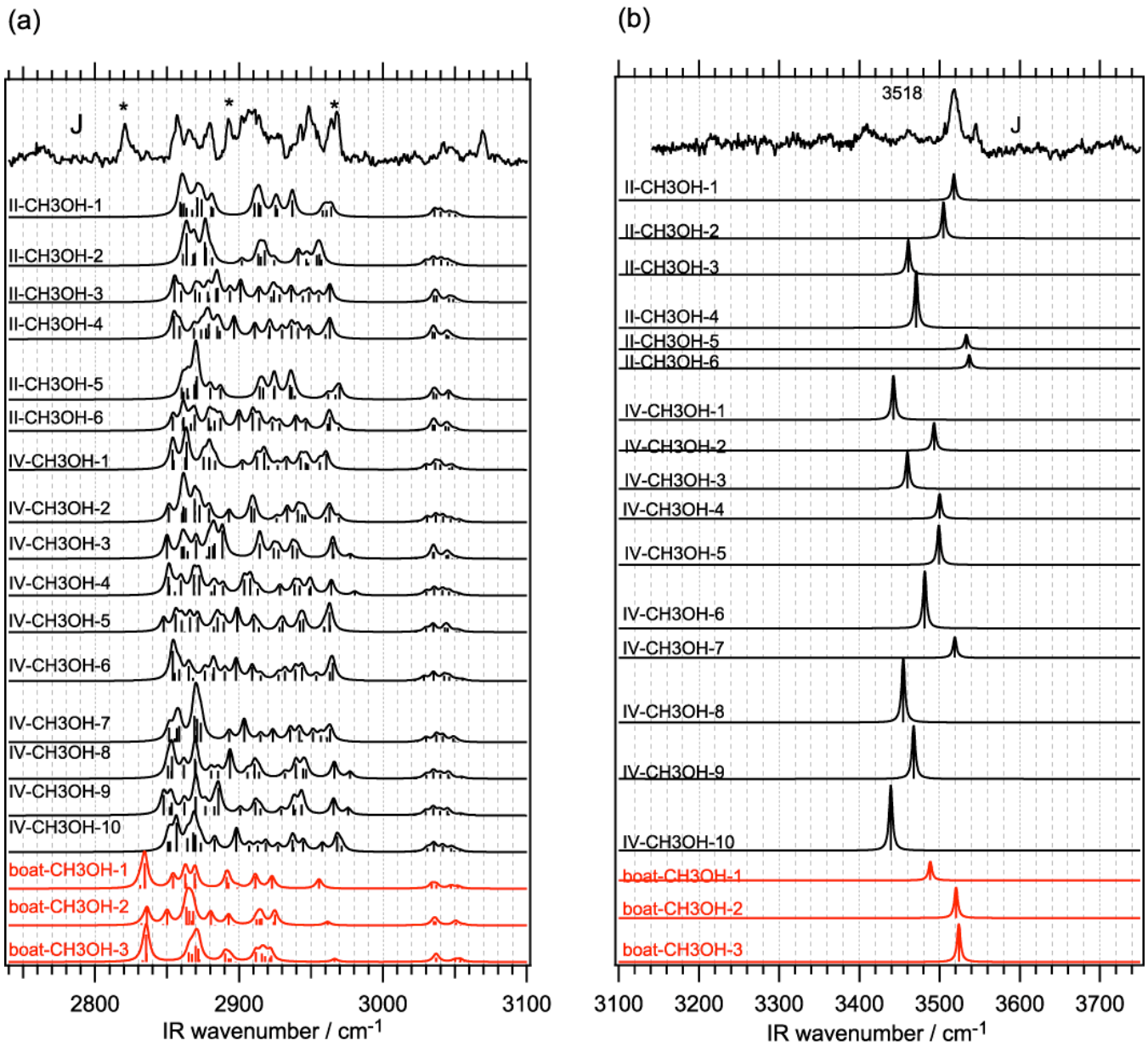

Fig. S7. Calculated IR spectra of DB18C6-CH_3OH in the region of (a) CH and (b) NH stretching vibrations.

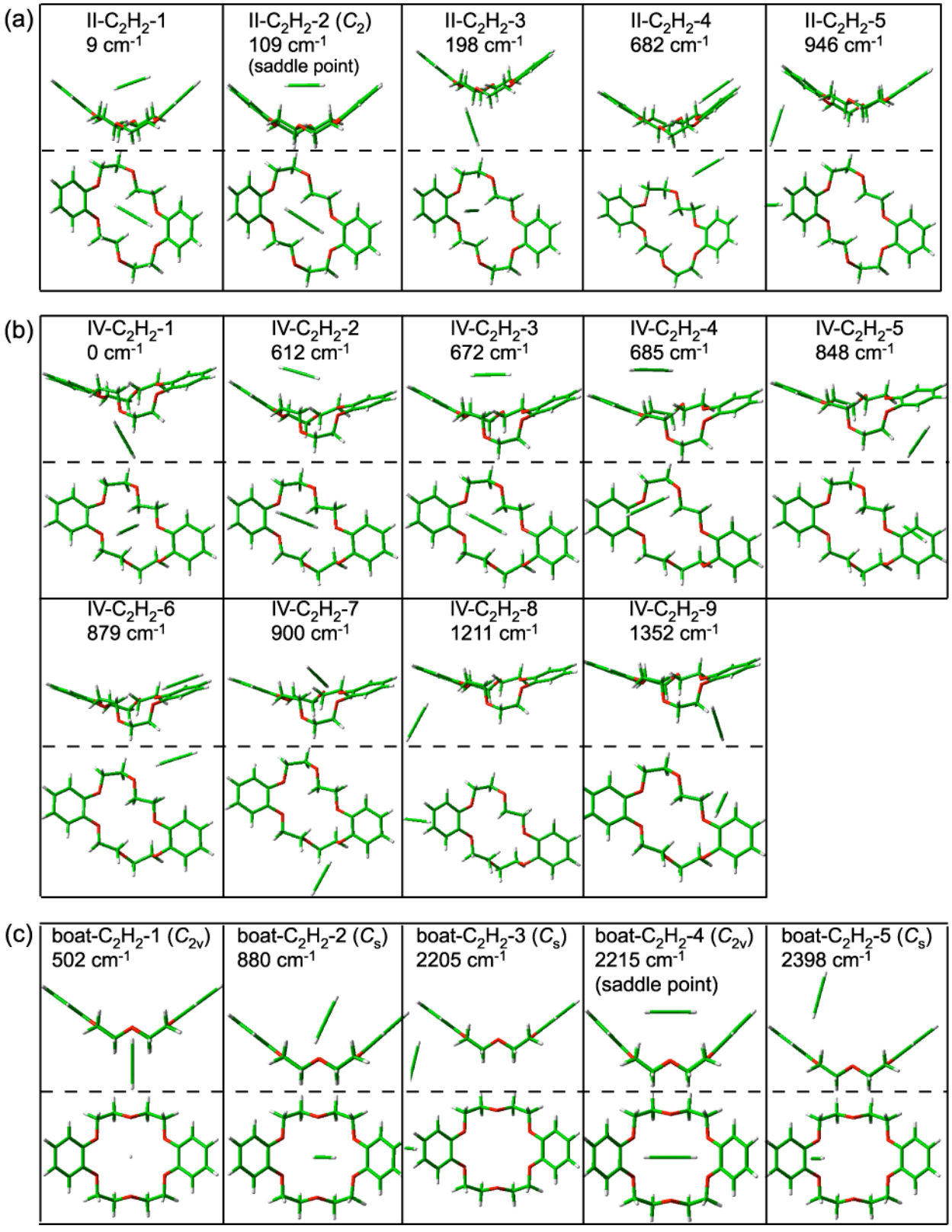

Fig. S8. Optimized structures of DB18C6-C_2H_2 built on (a) **II**, (b) **IV**, and (c) boat conformations.

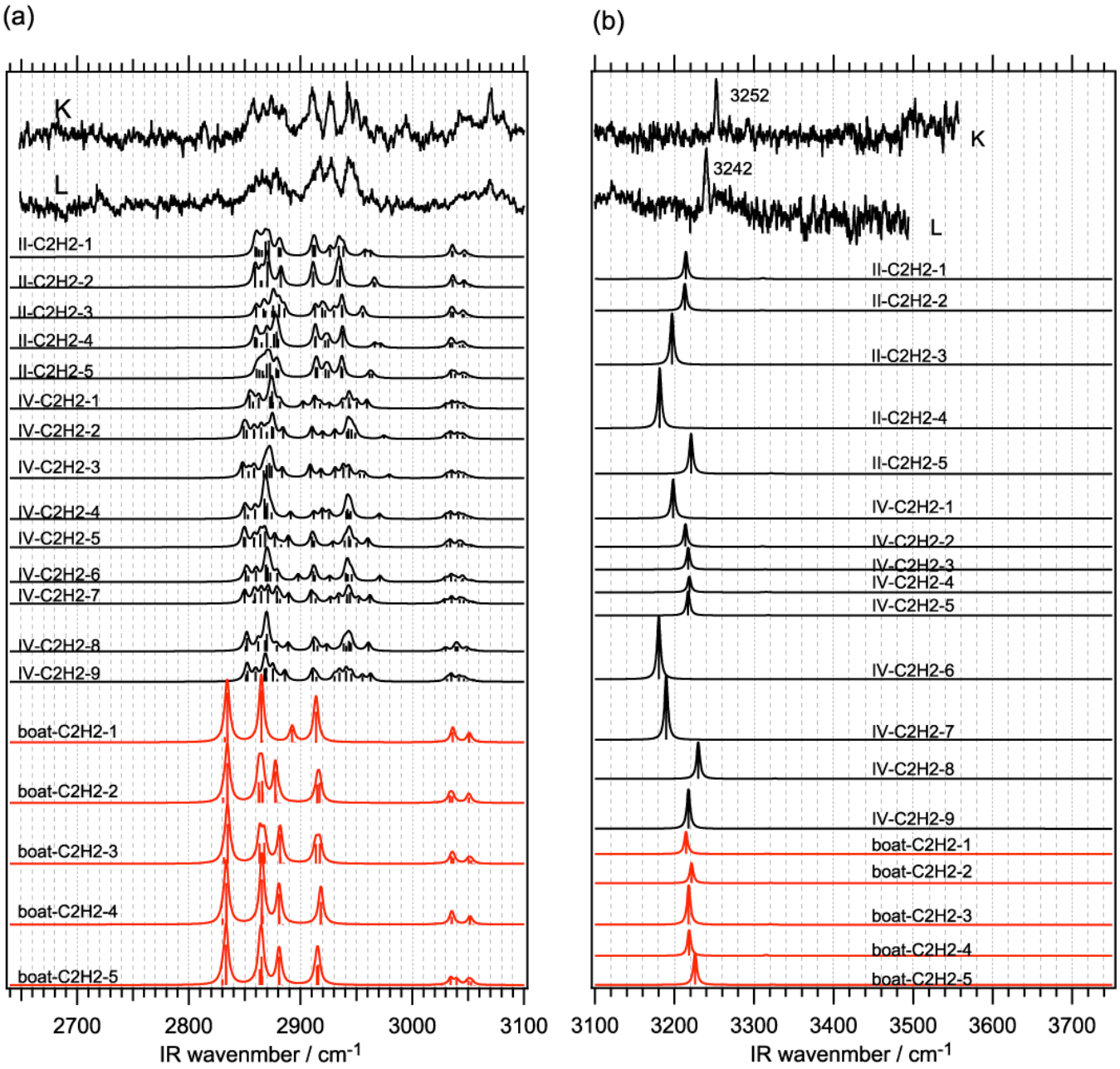

Fig. S9. Calculated IR spectra of DB18C6-C_2H_2 in the region of (a) methylene and (b) acetylene CH stretching vibrations.

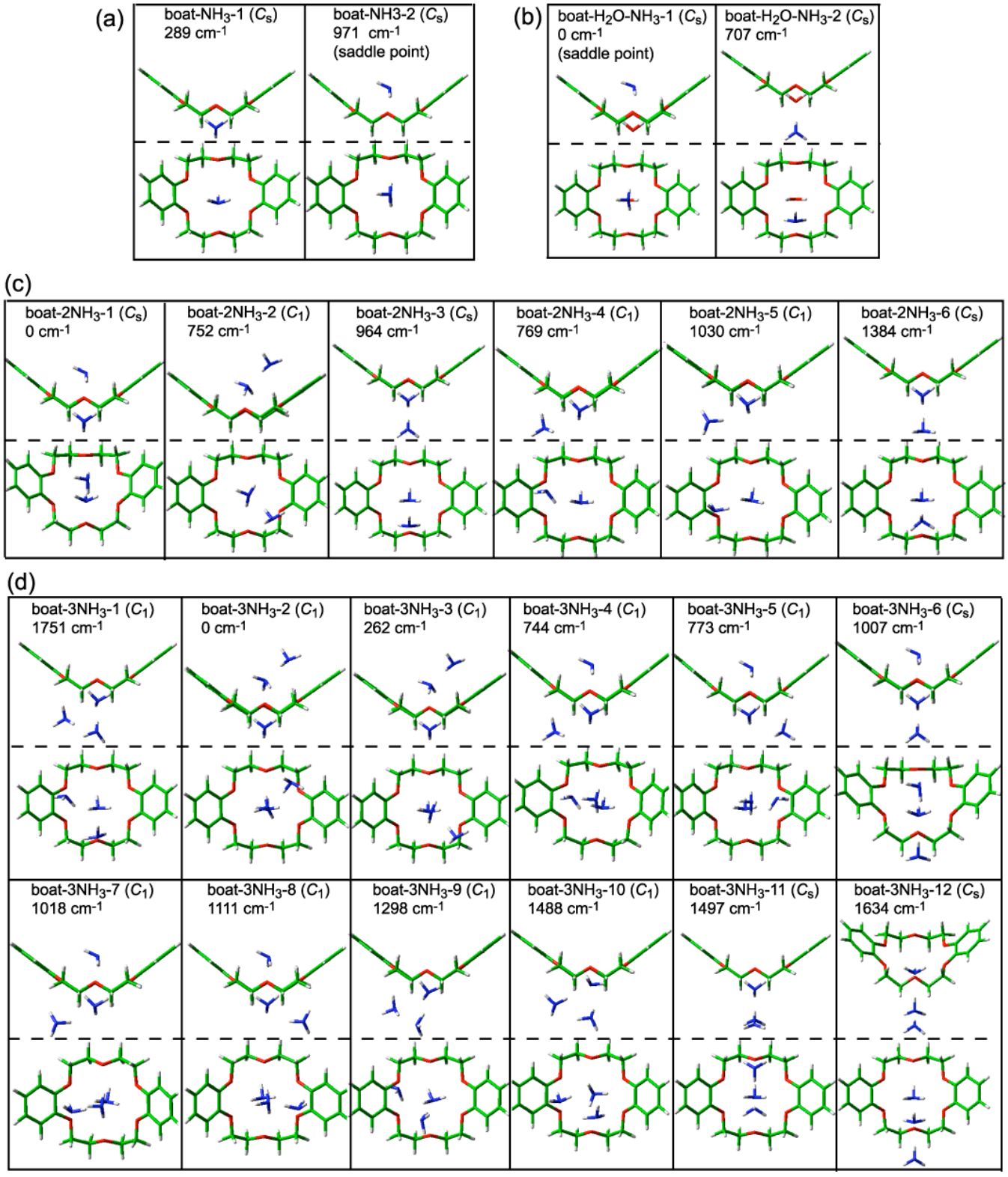

Fig. S10. Optimized structures of boat-$(NH_3)_n$ with (a) n=1, (c) n=2, (d) n=3, and (b) boat-H_2O-NH_3

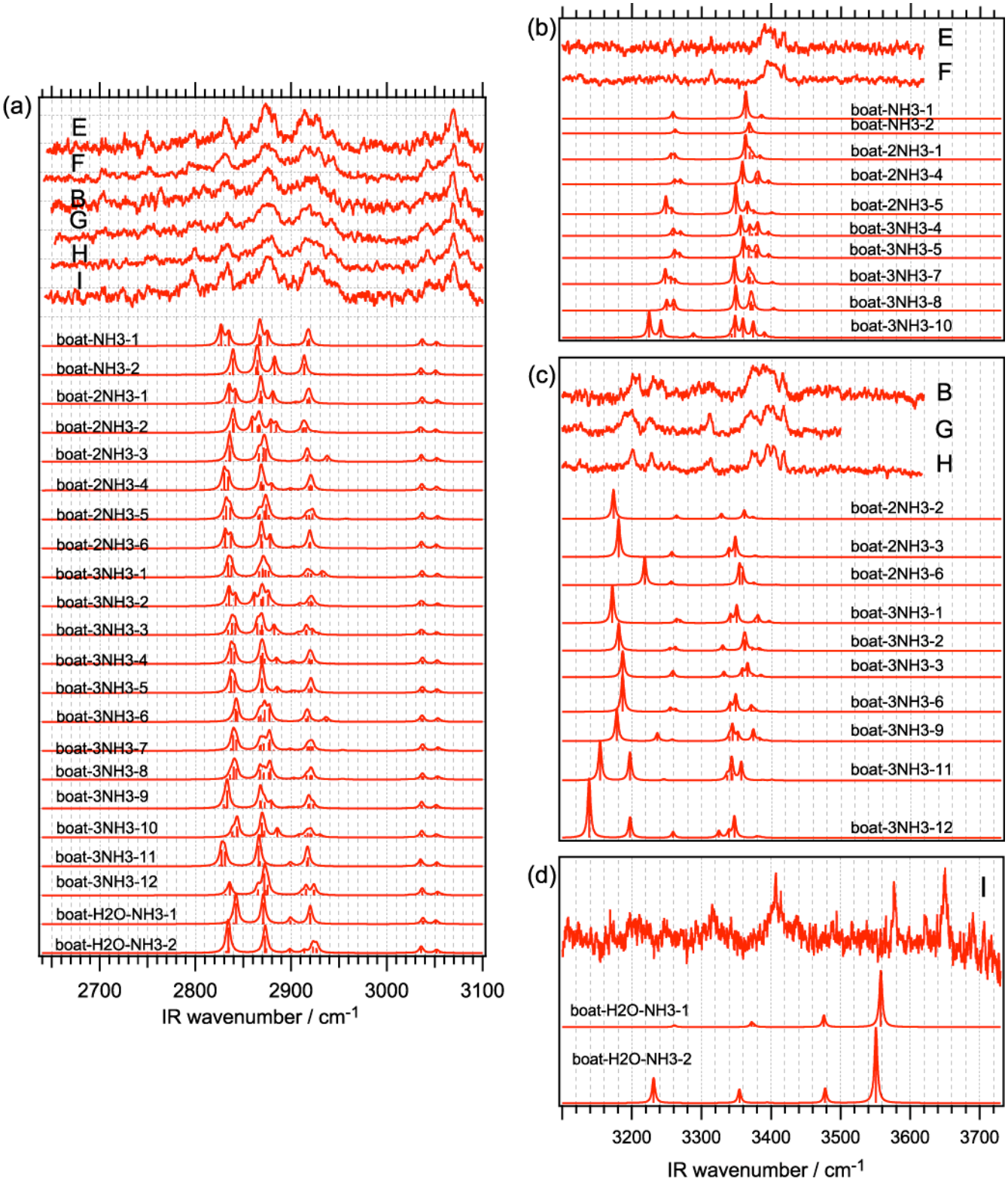

Fig. S11. Calculated IR spectra of boat-$(NH_3)_n$ with n=1-3 and boat-H_2O-NH_3 in the region of the (a) CH and (b)-(d) NH stretching vibrations.

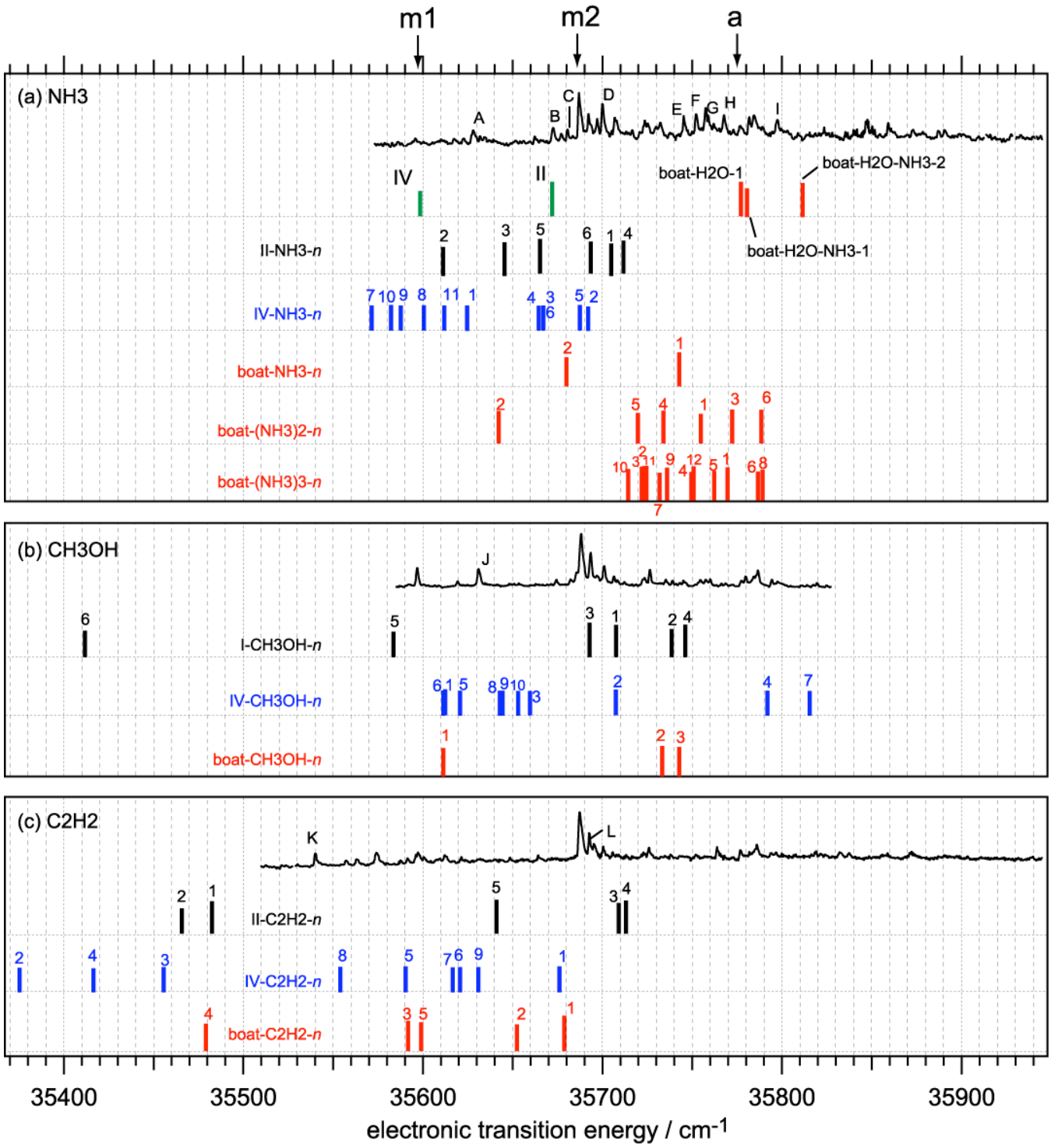

Fig. S12. Calculated S_1-S_0 electronic transition energies of DB18C6 complexes with (a) NH_3, (b) CH_3OH, and (c) C_2H_2.