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# Theoretical study of the catalytic hydrodeoxygenation of furan, methylfuran and benzofurane on $MoS_2$: Electronic Supporting Information

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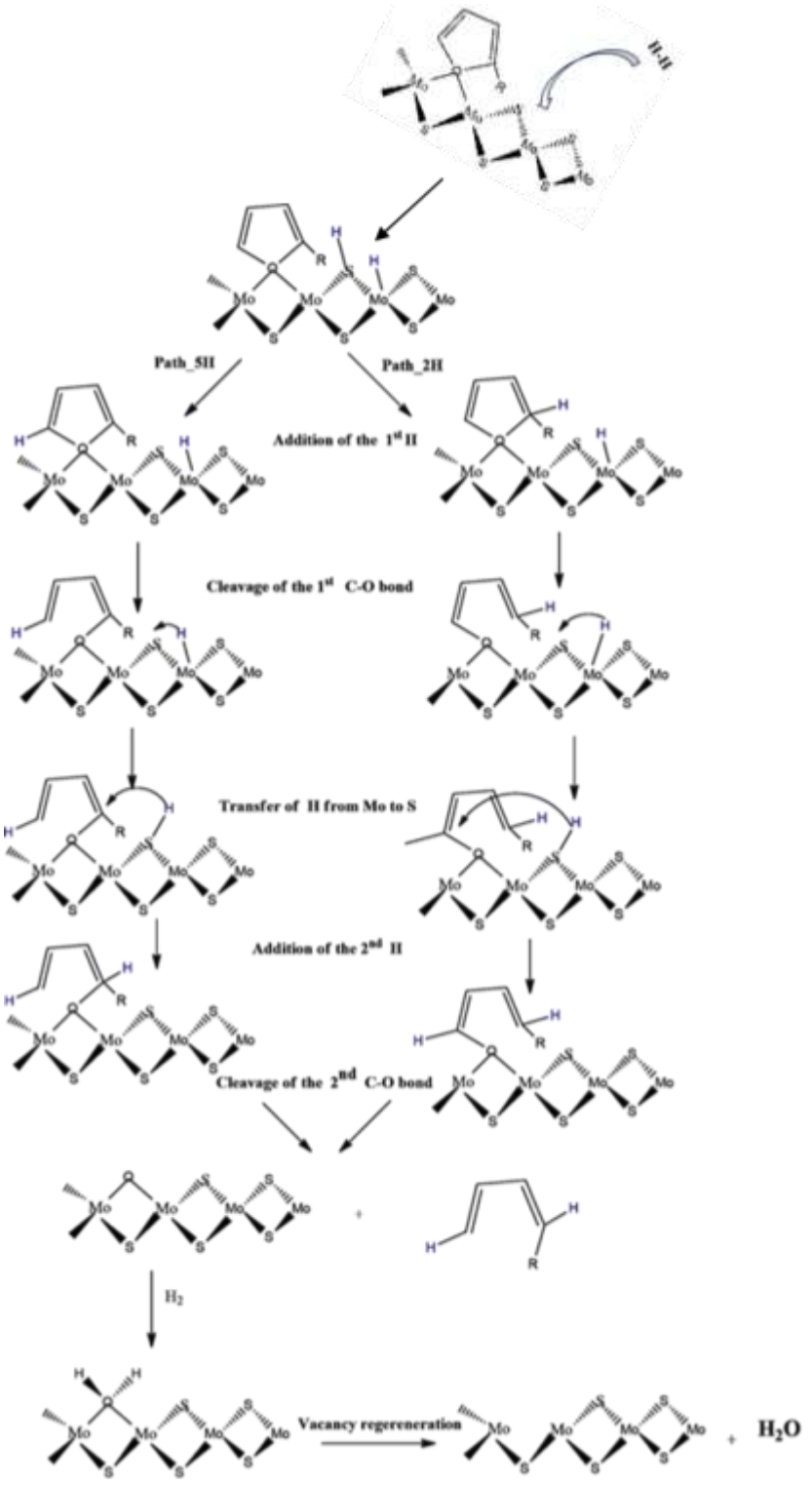


FIG. S1. Reaction scheme for the DDO mechanism of furan [1] and 2-methylfuran, R = H or -CH3, R= H corresponds to the case of furan where the two routes are equivalent.

[1] In this work, the DDO mechanism utilized is based on the well-established experimental and theoretical studies of the hydrodesulfurization mechanism of thiophene, with furan serving as its oxygen counterpart where the sulfur atom is substituted by an oxygen atom. (https://doi.org/10.1016/j.cattod.2018.02.013, https://doi.org/10.1021/acs.jpcc.6b02769).

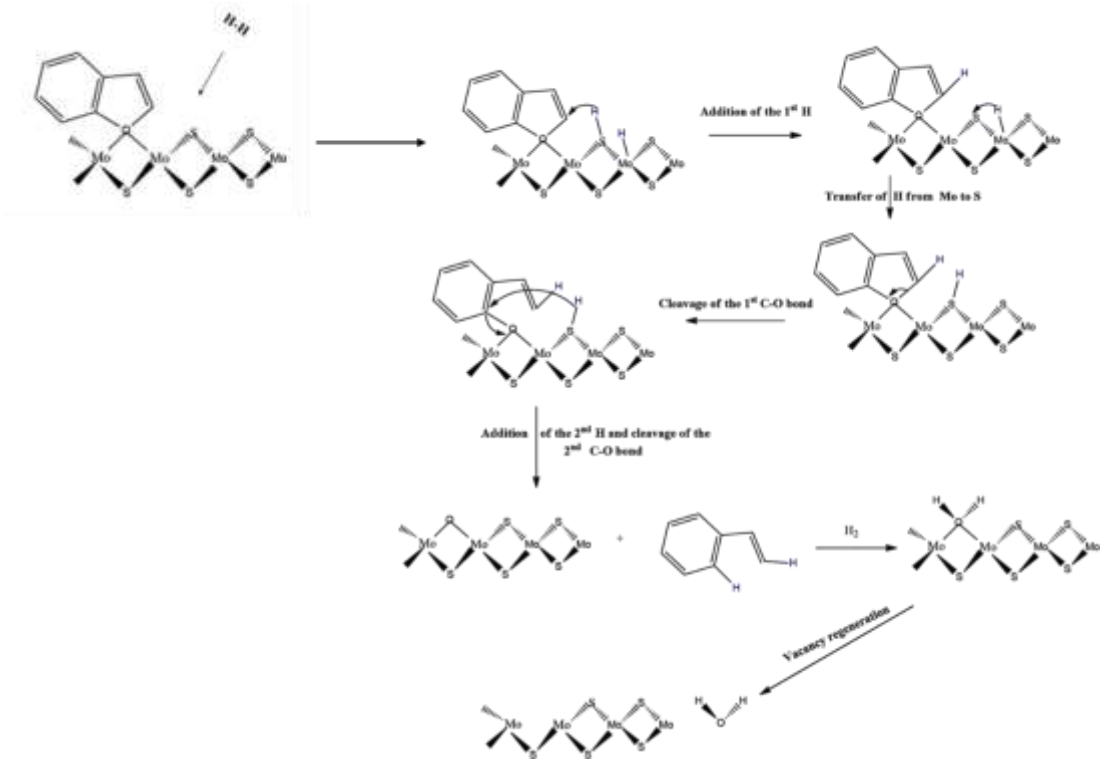


FIG. S2. Reaction scheme for the DDO mechanism of benzofuran.

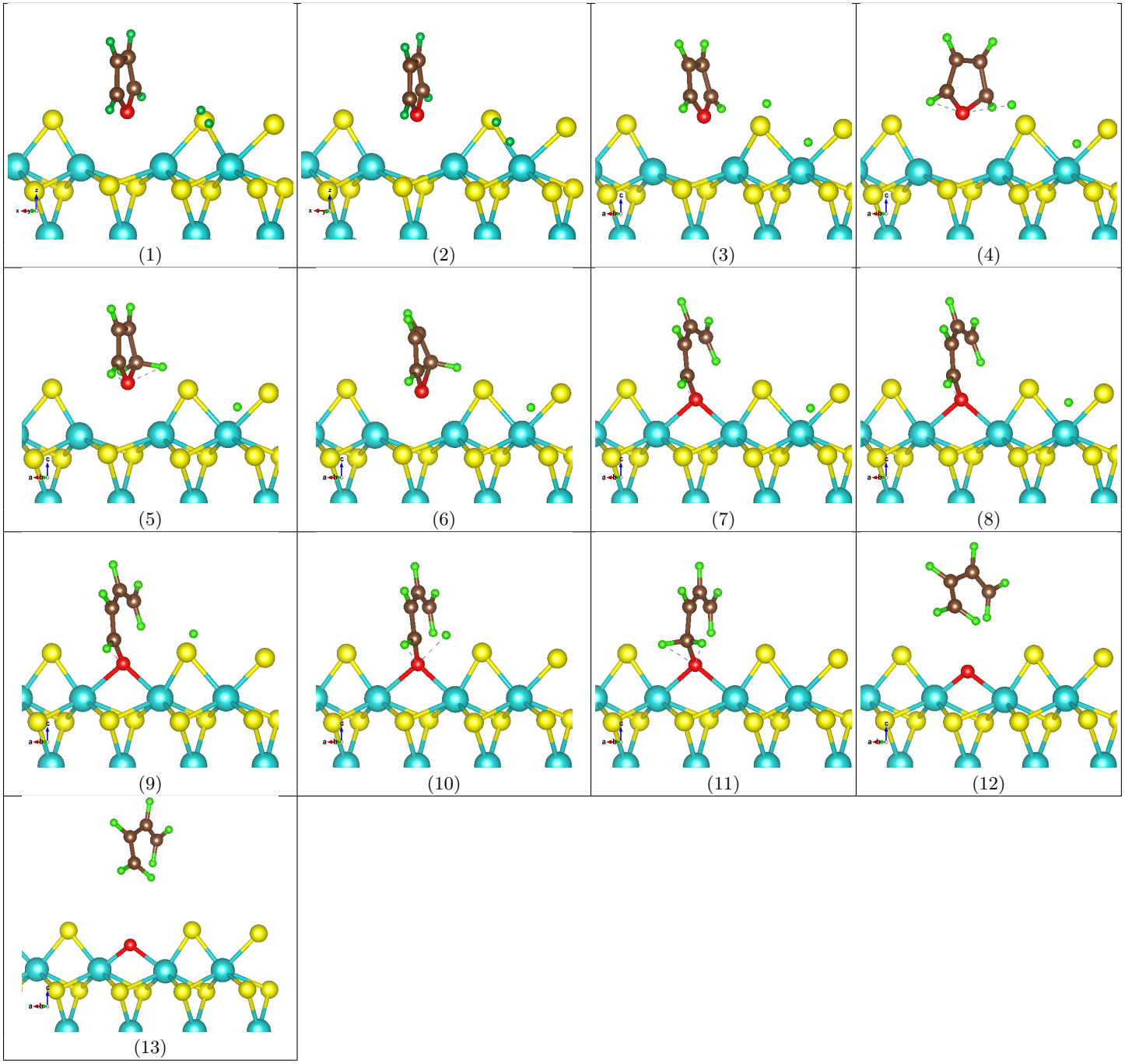


FIG. S3. Geometrical structures of the DDO route of furan on the metal edge of $MoS_2$ surface using the PBE+D2 approximation.

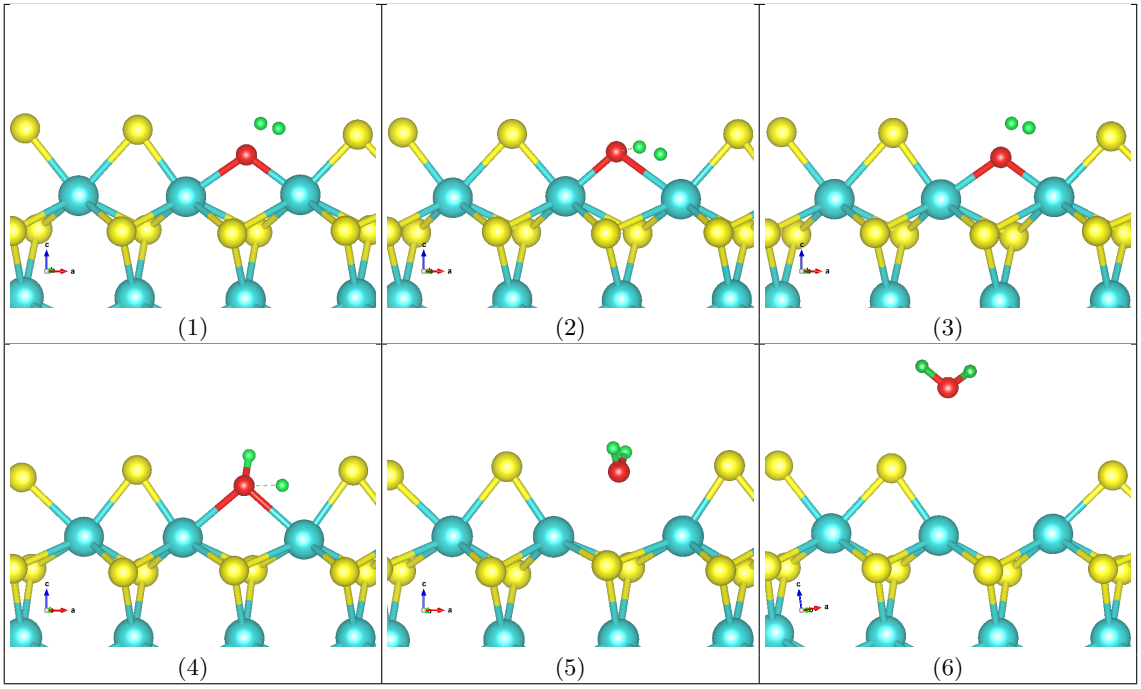


FIG. S4. Geometrical structures for vacancy regeneration on the metal edge of $MoS_2$ surface after oxygen atom removal from the studied molecules.

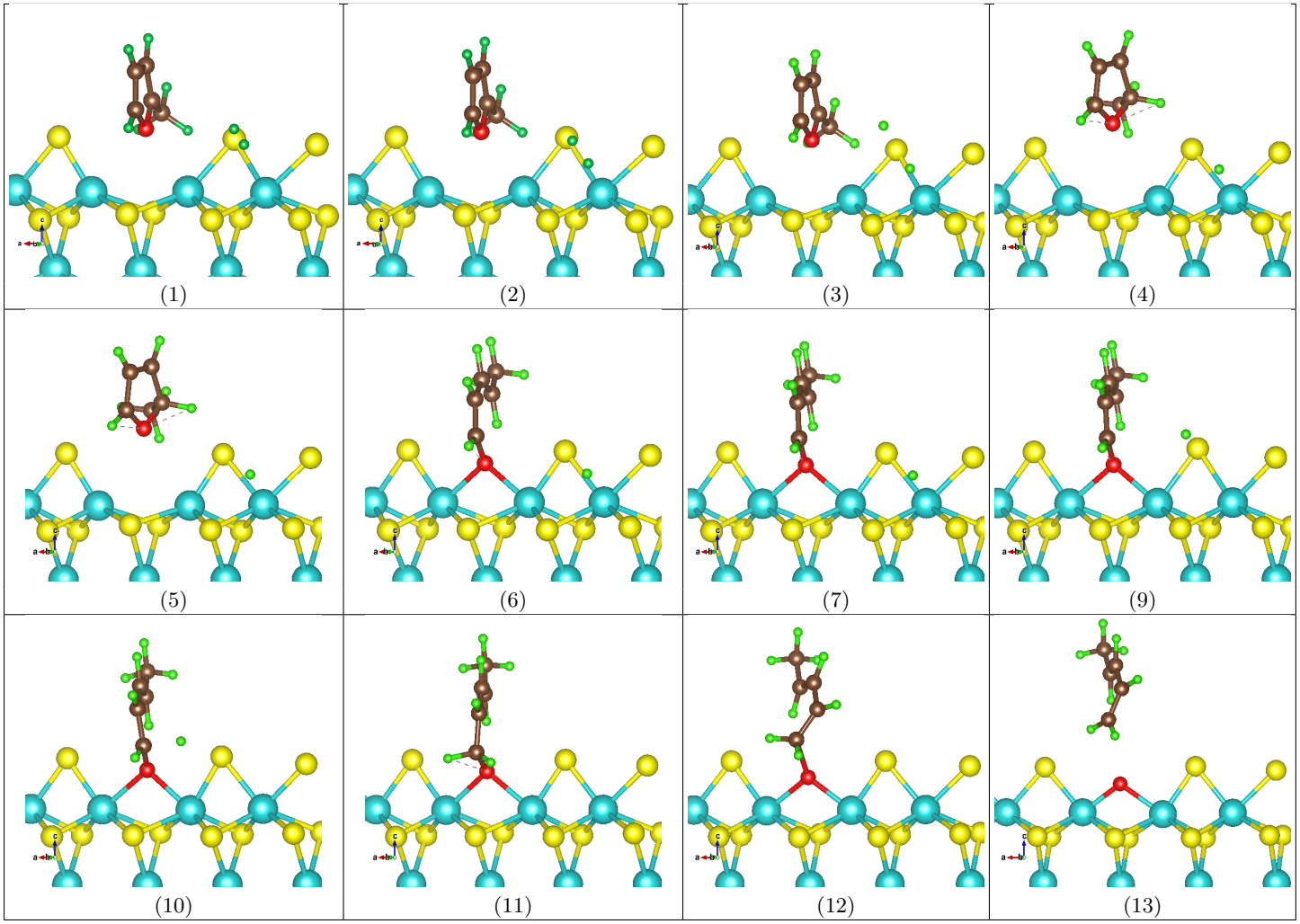


FIG. S5. Geometrical structures DDO (5H) route of the 2-methylfuran molecule on the metal edge of $MoS_2$ surface using the PBE+D2 approximation.

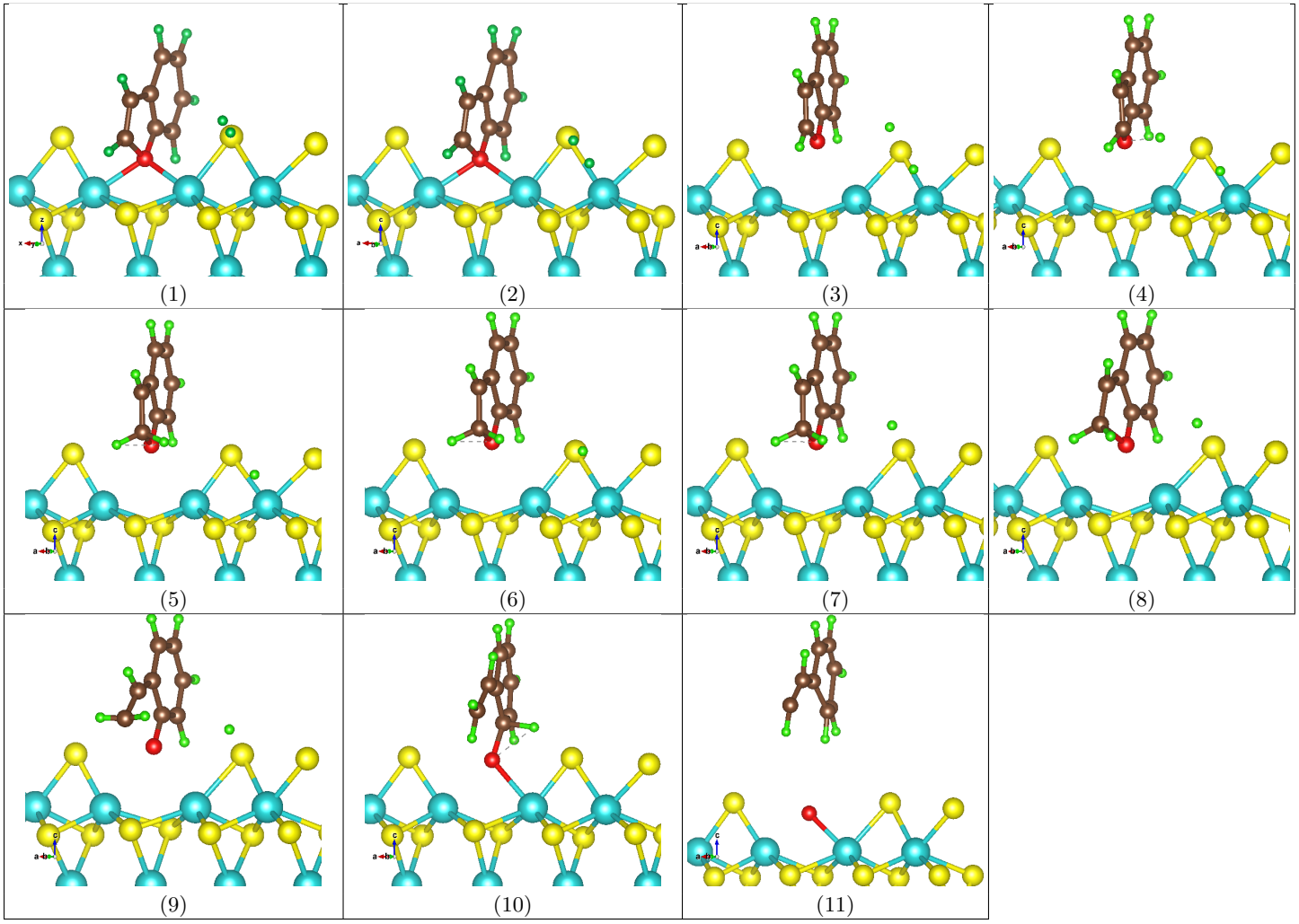


FIG. S6. Geometrical structures for DDO route of the benzofuran molecule on the metal edge of $MoS_2$ surface.