# Electronic Supplementary Material

## Reaction mechanism of formate dehydrogenase studied by computational methods

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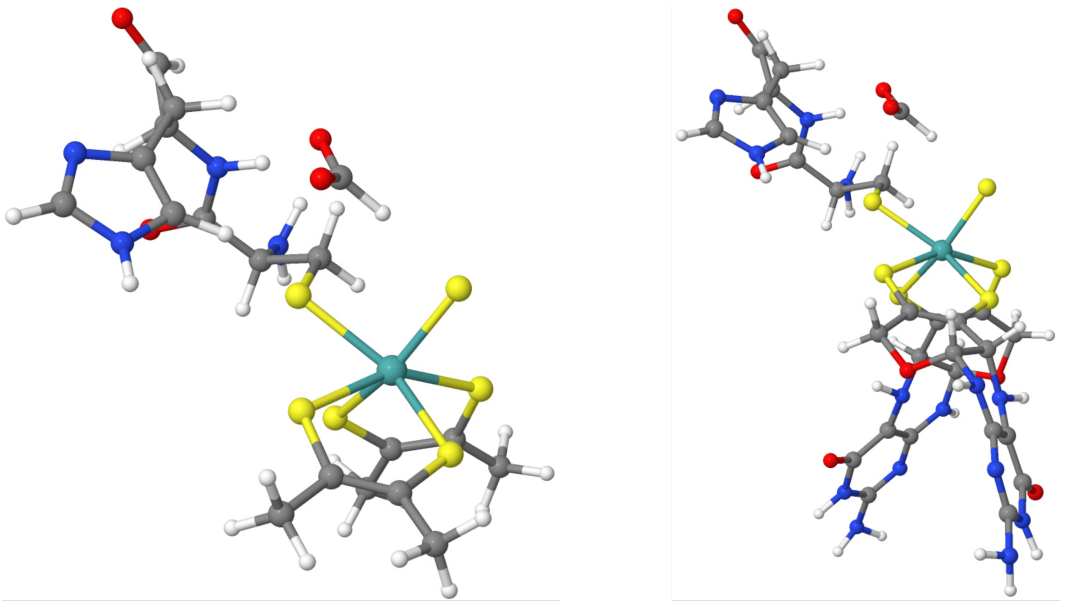


**Figure S1**. Models used to make a comparison between the S-shift and RS species.

**Table S1.** Energy difference with different methods and models at TPSS/def2-TZVP level of theory.

| Model | Method | $\Delta E$[a] (kJ/mol) |
|---|---|---|
| Small MPT model | Opt-vacuum | 26.9 |
| Large MPT model | Opt-vacuum | 0.3 |
| QM/MM with large MPT model in QM region | QM/MM | 176.4 |
| | QM-ptch | 104.4 |
| | QM-vacuum | 76.4 |

[a] $\Delta E = E$(S-shift species) – $E$(RS)