

Electronic Supplementary Information

On the Mechanism of Catalytic Hydrogenation of Thiophene on Hydrogen Tungsten Bronze

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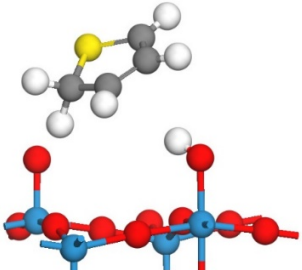
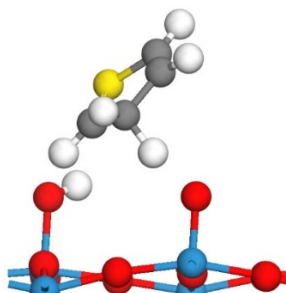
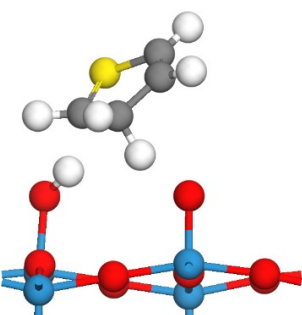
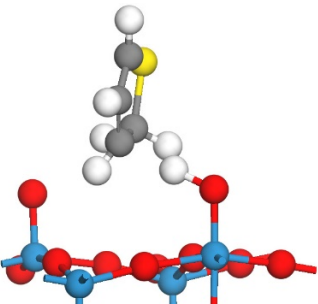
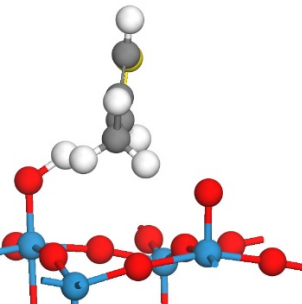
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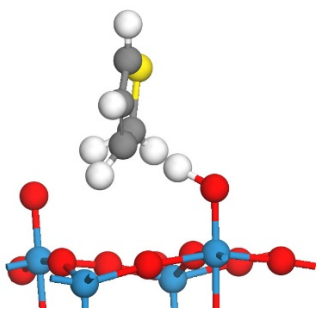
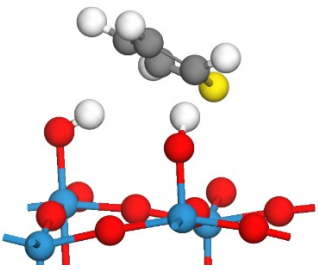
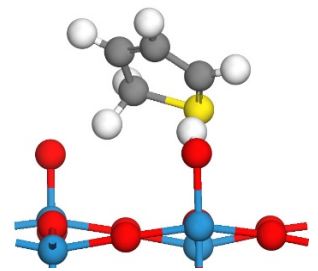
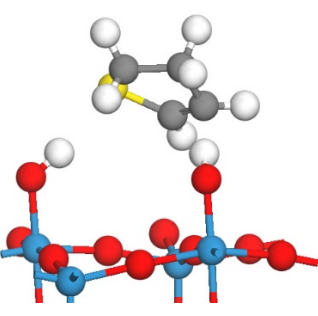
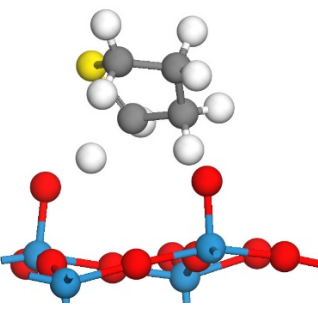
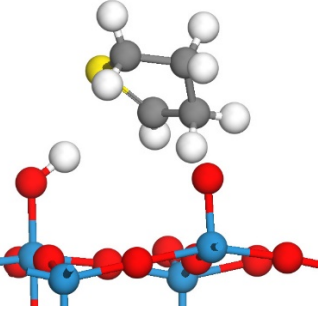
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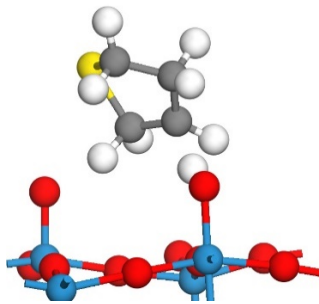
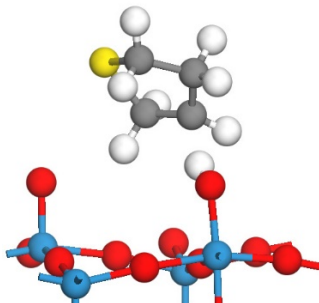
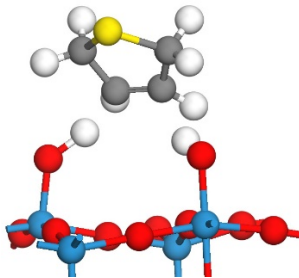
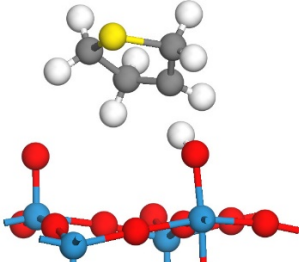
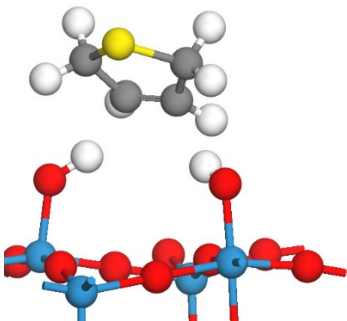
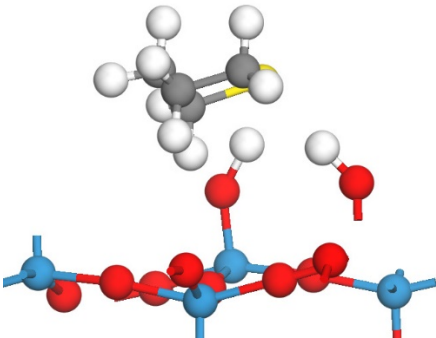
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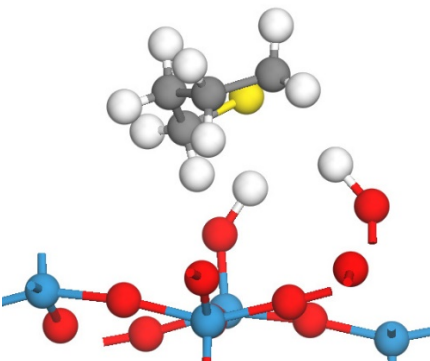
Table S1

Transition state configuration and imaginary vibrational frequency for each reaction step

	Reaction step	TS configuration	TS vibrational frequency
Figure 4a	$R_{(1-2)h}^s$		273.1i
	$R_{(2-1)h}^s$		384.3i
	$R_{(1,2)h}^c$		1149.6i
	$R_{(1-2)v}^s$		289.6i
	$R_{(2-1)v}^s$		898.6i

	$R_{(1,2)v}^c$		992.3i
Figure 4b	$R_{(1-4)h}^s$		989.1i
	$R_{(1,4)h}^c$		576.8i
Figure 5a	$R_{(3-4)}^s(\text{TS1})$		76.3i
	$R_{(3-4)}^s(\text{TS2})$		1584.5i
	$R_{(3,4)}^c$		389.9i

	$R_{(4-3)}^s(\text{TS1})$		488.1i
	$R_{(4-3)}^s(\text{TS2})$		76.6i
Figure 5b	$R_{(2-3)}^s(\text{TS1})$		1743.1i
	$R_{(2-3)}^s(\text{TS2})$		99.6i
	$R_{(2,3)}^c$		335.2i
Figure 7	S–C bond scission of 12-DTP		682.5i

	S-C bond scission of TTP		252.1i
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