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Title: New insight into the reaction mechanism of carbon disulfide hydrolysis and the impact of H_2S with density functional modeling

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Figure

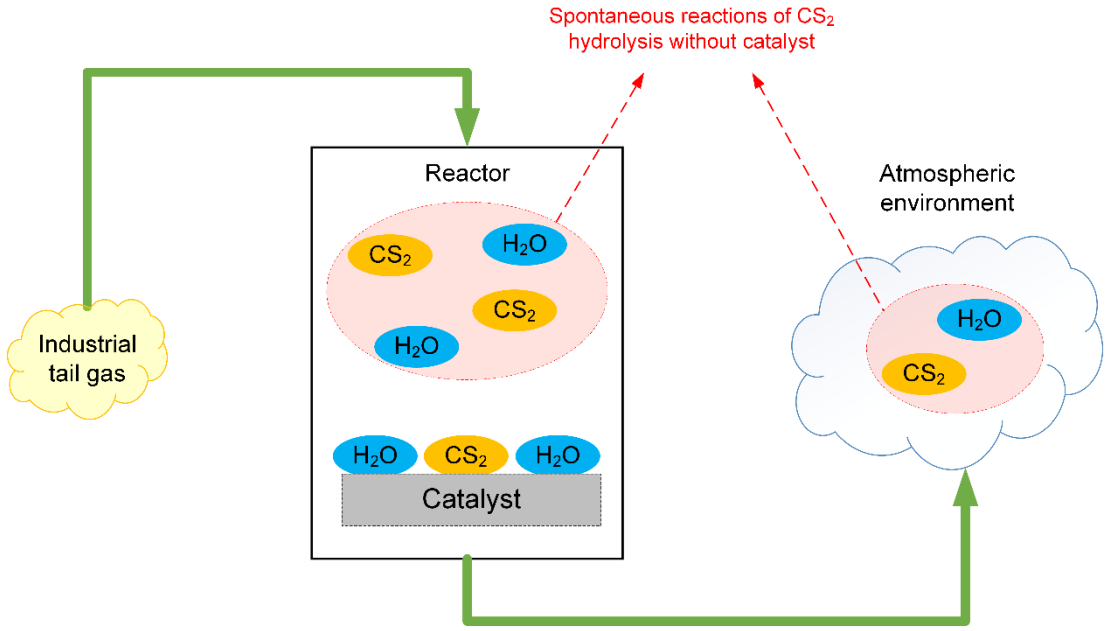

Fig. S1 Spontaneous reactions of CS_2 hydrolysis without catalyst

Tables

Table S1 Imaginary frequencies of the transition states and bonds corresponding to relative normal vibrations for the two-steps CS_2 hydrolysis

Transition States	Imaginary frequency (cm^{-1})	Bonds corresponding to relative normal vibrations
TS1	-1352.72	H5-O4
TS2	-1630.53	H6-O4
TS3	-526.82	H6-S2
TS4	-825.36	H6-S2
TS5	-1252.38	H9-O7
TS6	-1646.81	H9-O4
TS7	-759.05	H8-O7
TS8	-1575.38	H6-O4
TS9	-1420.75	H9-O7

Table S2 Imaginary frequency of the transition states and bonds corresponding to relative normal vibrations for the one-step CS_2 hydrolysis

Transition States	Imaginary frequency (cm^{-1})	Bonds corresponding to relative normal vibrations
TS1	-1352.72	H5-O4
TS2	-1630.53	H6-O4
TS10	-985.47	H9-O7
TS11	-764.38	H8-O7
TS12	-1039.72	H9-O7
TS13	-1659.89	H6-O7
TS14	-1208.14	H9-O7
TS15	-921.61	H8-O7