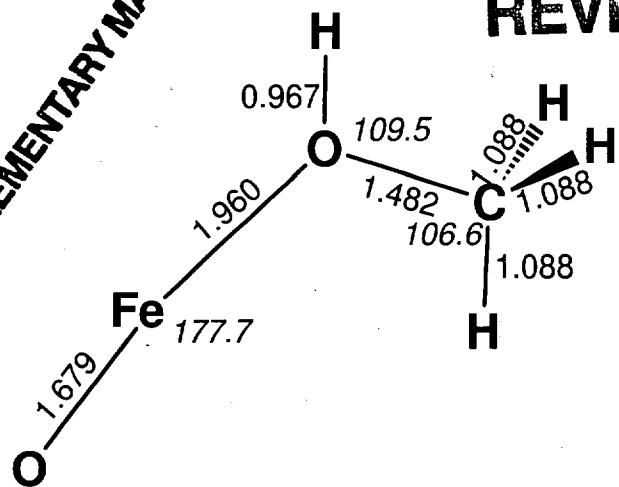


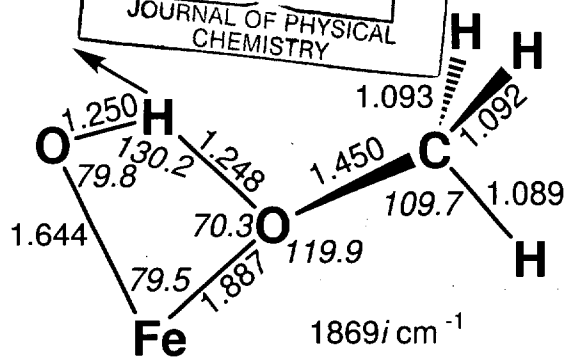
SUPPLEMENTARY MATERIAL

REVISED

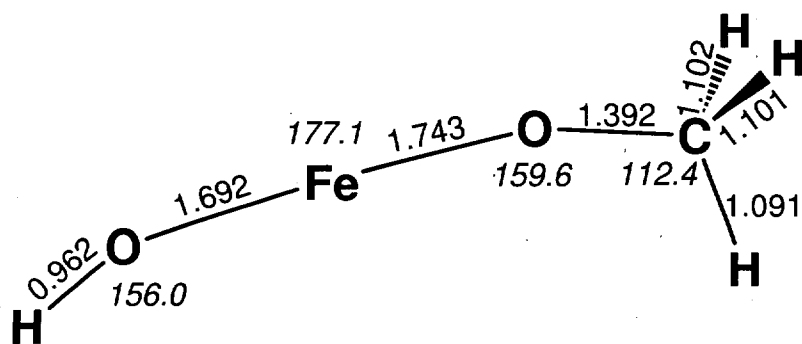
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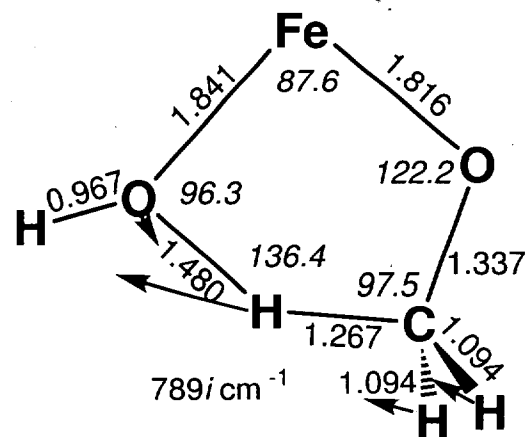
Reactant complex (q)



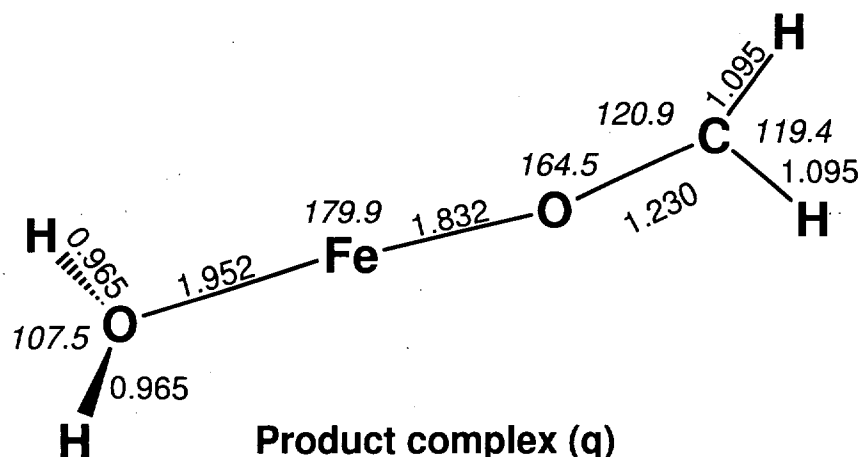
TS₁₋₁ (q)



Intermediate complex (q)

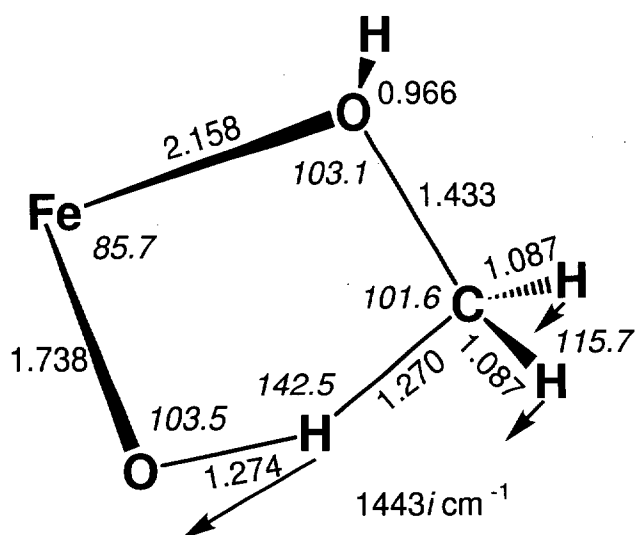


TS₁₋₂ (q)

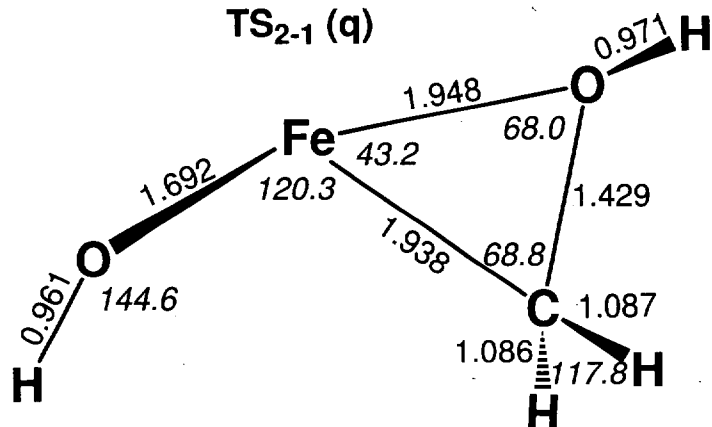


Product complex (q)

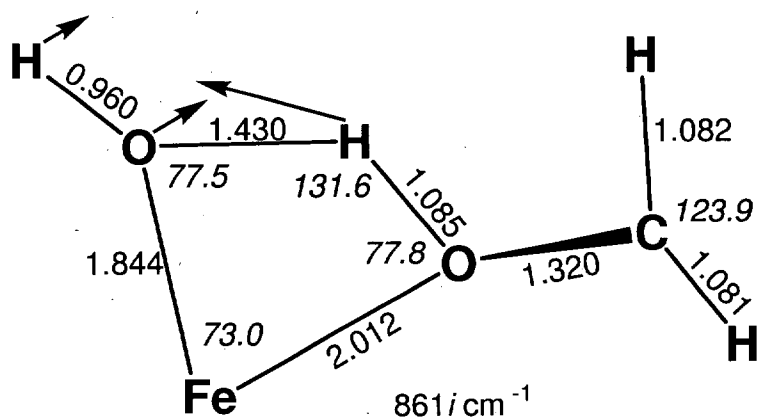
SI 1. Optimized structures for the reaction species of the quartet state for the conversion of methanol to formaldehyde by FeO⁺ via Path 1. Bond distances and angles (indicated in italic) are in units of Å and degree respectively.



$TS_{2-1}(q)$

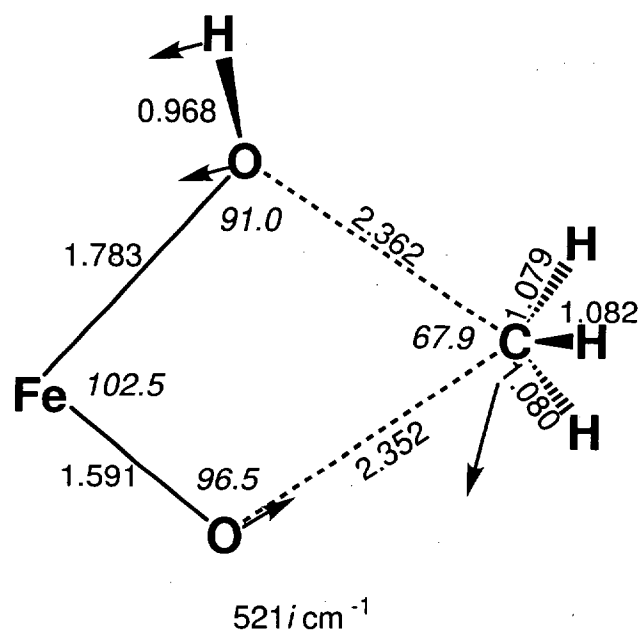


Intermediate complex (q)



$TS_{2-2}(q)$

SI 2. Optimized structures for the reaction species of the quartet state for the conversion of methanol to formaldehyde by FeO^+ via Path 2. Bond distances and angles (indicated in italic) are in units of Å and degree, respectively.



TS₃₋₁ (q)

SI 3. An optimized structure for **TS₃₋₁** of the quartet state for the conversion of methanol to formaldehyde by FeO^+ via Path 3. Bond distances and angles (indicated in *italic*) are in units of Å and degree, respectively.