

174. P. R. Watson and G. A. Somorjai, *J. Catal.* 74, 282-295 (1982).
175. S. Novak, R. J. Madon, and H. Suhl, *J. Catal.* 77, 141-151 (1982).
176. R. B. Pannell, C. L. Kibby, and T. P. Kobylinski, *Proc. Int. Congr. Catal.*, 7th, 1980 (Pub. 1981), 447-455.
177. R. J. Madon and W. F. Taylor, *J. Catal.* 69, 32-43 (1981).
178. S. Novak, R. J. Madon, and H. Suhl, *J. Chem. Phys.* 74, 6083-6091 (1981).
179. K. M. Doxsee and R. H. Grubbs, *J. Am. Chem. Soc.* 103, 7696-7698 (1981).
180. J. B. Benziger and R. J. Madix, *Surf. Sci.* 115, 279-289 (1982).
181. D. E. Peebles, J. A. Schrievels, and J. M. White, *Surf. Sci.* 116, 117-134 (1982).
182. S. E. Moore and J. H. Lunsford, *J. Catal.* 77, 297-300 (1982).
183. B. L. Gustafson and J. H. Lunsford, *J. Catal.* 74, 405-407 (1982).
184. a) H. H. Kung, *Catal. Rev.-Sci. Eng.* 22, 235-259 (1980). b) K. Klier, *Adv. Catal.* 31, 243-313 (1982).
185. K. Klier, V. Chelikavanil, R. G. Herman, and G. W. Simmons, *J. Catal.* 74, 343-360 (1982).

TABLE I

Mechanism Proposed by Masuda and Miyahara<sup>19</sup> for  
Water Gas Shift Reaction on Unsupported Platinum

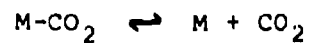
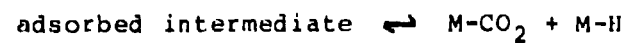


TABLE II

Mechanism Proposed by Grenoble, Estadt, and Ollis<sup>20</sup>



TABLE III

Proposed Mechanism of Water Gas Shift on Metals

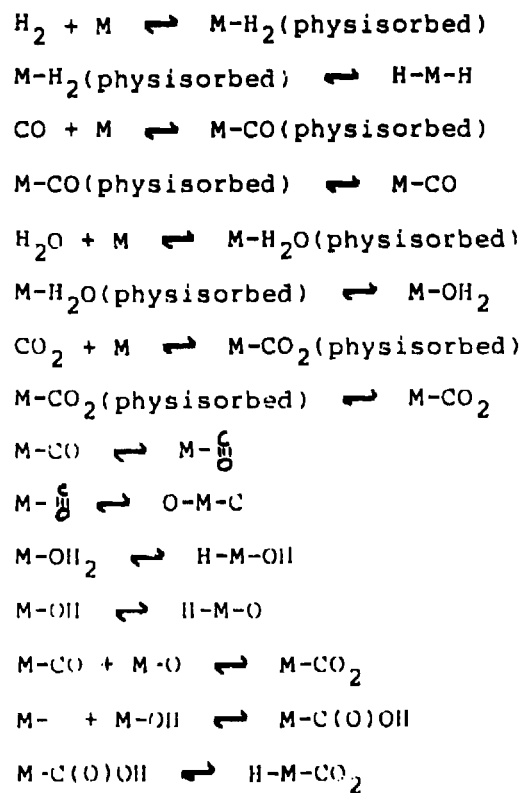


TABLE IV  
Proposed Mechanism for the Water Gas Shift Reaction on  
Metal Oxides

<u>Reaction</u>	<u>Number</u>
$H_2 + MO \rightleftharpoons MO-H_2(\text{physisorbed})$	(4)
$MO-H_2(\text{physisorbed}) \rightleftharpoons H-MO-H$	(5)
$H-MO-H + 2 MO \rightleftharpoons OM-H-MO-H-OM$	(6)
$H_2O + MO \rightleftharpoons H_2O-MO(\text{physisorbed})$	(7)
$H_2O-MO(\text{physisorbed}) \rightleftharpoons H_2O-MO$	(8)
$H_2O-MO(\text{physisorbed}) \rightarrow MO-HOH$	(9)
$H_2O-MO \rightleftharpoons HO-MO-H$	(10)
$MO-HOH \rightleftharpoons HO-MO-H$	(11)
$CO + MO \rightleftharpoons OM-CO(\text{physisorbed})$	(12)
$OM-CO(\text{physisorbed}) \rightleftharpoons OM-CO$	(13)
$CO + MOMO \rightleftharpoons M_2CO_3$	(14)
$CO_2 + MO \rightleftharpoons MO-CO_2(\text{physisorbed})$	(15)
$MO-CO_2(\text{physisorbed}) \rightleftharpoons OM-CO_2$	(16)
$MO-CO_2(\text{physisorbed}) \rightleftharpoons MO-CO_2$	(17)
$MO-CO_2(\text{physisorbed}) \rightleftharpoons OM-OCO$	(18)
$OM-OCO + OM-OH \rightleftharpoons OM-OC(O)OH + MO$	(19)
$MO-CO_2 + OM-OH \rightleftharpoons MO-C(O)OH + OM-O$	(20)
$OM-CO_2 + OM-OH \rightleftharpoons OM-OC(O)OH + MO$	(21)
$OM-CO + OM-OH \rightleftharpoons OM-C(O)OH + MO$	(22)
$OM-C(O)H \rightleftharpoons OM-OCOH$	(24)

TABLE IV (continued)

<u>Reaction</u>	<u>Number</u>
$OM-OCOH \rightleftharpoons OM-OC(H)O$	(25)
$M-OCO + M-H \rightleftharpoons M-OC(H)O + M$	(26)
$OM-CO + OM-O \rightleftharpoons OM-CO_2 + MO$	(27)
$OM-CO_2 + OM-O \rightleftharpoons OM-OCO_2 + MO$	(28)

TABLE V  
 Previously Proposed Elementary Reactions  
 for Homogeneous Water Gas Shift Reaction

<u>Reaction</u>	<u>Reference</u>
$M-CO + OH^- \rightleftharpoons M-C(O)OH^-$	126,128,130,131
$M-CO + OH^- \rightleftharpoons M-H + CO_2$	137
$M-CO + OH^- \rightleftharpoons M-H^- + CO_2$	133
$[M-CO]OH \rightleftharpoons M-C(O)OH$	138
$M-CO + H_2O \rightleftharpoons H-M-C(O)OH$	128,131
$M-CO + Me_3N \rightleftharpoons M-C(O)NMe_3$	132
$M-C(O)NMe_3 + H_2O \rightleftharpoons M-H^- + CO_2 + Me_3NH^+$	132
$M-CO^+ + H_2O \rightleftharpoons H-M-C(O)OH^+$	129
$M-C(O)OH \rightleftharpoons M-H + CO_2$	128,131,138
$H-M-C(O)OH \rightleftharpoons M + HC(O)OH$	138
$M-C(O)OH^- + H_2O \rightleftharpoons H-M-C(O)OH + OH^-$	128,131
$M-C(O)OH^- \rightleftharpoons M-H^- + CO_2$	126
$M-C(O)OH^- + B \rightleftharpoons M-C(O)O^{2-} + BH^+$	130
$M-C(O)O^{2-} + H_2O \rightleftharpoons M-H^- + HCO_3^-$	130
$M-(Cl)C(O)OH^+ \rightleftharpoons M^+ + CO_2 + H^+ + Cl^-$	129
$M-OC(H)O \rightleftharpoons M-H + CO_2$	138
$M-OC(H)O^- \rightleftharpoons M-H^- + CO_2$	124,126,132
$H-M-H \rightleftharpoons M + H_2$	124,126, 28,131, 132,136,137,138
$H-M-H + CO \rightleftharpoons M-CO + H_2$	128,131,136

TABLE V (continued)

<u>Reaction</u>	<u>Reference</u>
$M-H^- + CO \rightleftharpoons M-CO + H^-$	126,133
$M-H^- + H_2O \rightleftharpoons M + H_2 + OH^-$	133
$M + CO \rightleftharpoons M-CO$	125,126,128,131, 132,136,137
$M^+ + CO \rightleftharpoons M-CO^+$	129
$M^- + CO \rightleftharpoons M-CO^-$	133
$M + H_2O \rightleftharpoons H-M-OH$	136,138
$M^- + H_2O \rightleftharpoons M-H + OH^-$	125,126,132,137
$M + HC(O)OH \rightleftharpoons H-M-OC(H)O$	138
$M + HCOO^- \rightleftharpoons M-OC(O)H^-$	125,126,132
$H-M-OH + S \rightleftharpoons [H-M-S]OH$	136,138
$[H-M-S]OH + CO \rightleftharpoons [H-M-CO]OH + S$	136,138
$CO + OH^- \rightleftharpoons HCO_2^-$	126,128,131,132
$CO_2 + OH^- \rightleftharpoons HCO_3^-$	128,131
$HCO_2^- + H_2O \rightleftharpoons H_2 + CO_2 + OH^-$	128,131
$H^- + H_2O \rightleftharpoons H_2 + OH^-$	126,133



TABLE VI  
Proposed Mechanism for the Homogeneous  
Water Gas Shift Reaction

<u>Reaction</u>	<u>Number</u>
$M-CO + OH \rightleftharpoons M-C(O)OH$	(29)
$M-CO + H_2O \rightleftharpoons H-M-C(O)OH$	(30)
$M-C(O)OH \rightleftharpoons M-H + CO_2$	(31)
$CO_2 + M-H \rightleftharpoons M-OC(H)O$	(32)
$CO + OH^- \rightleftharpoons HCO_2^-$	(33)
$M + HCO_2^- \rightleftharpoons M-OC(H)O^-$	(34)
$H_2O + M \rightleftharpoons H-M-OH$	(35)
$H-M-H \rightleftharpoons M + H_2$	(36)
$CO + M \rightleftharpoons M-CO$	(37)
$H-M-H + CO \rightleftharpoons M-CO + H_2$	(38)
$M-H + CO \rightleftharpoons M-CO + H$	(39)

**Los Alamos**  
NATIONAL LABORATORY

**Research Library Online Catalog**

<a href="#">New Search</a>	<a href="#">Comments</a>	
<a href="#">List Marks</a>	<a href="#">Help</a>	<a href="#">Databases</a>



**Full Record**

Records: 1 ... 71 81 91 101 111 121 131 141 151 161 171 181 191 201 211 221 ... 481

[Brief Records](#) [Mark](#)

[Previous](#)

Records: 1 ... 71 81 91 101 111 121 131 141 151 161 171 181 191 201 211 221 ... 481

[Next](#)

**Call No.:** DOE\PC\70020-T1  
**Title:** Methane suppression in the Fischer-Tropsch synthesis : Final report  
**Author:** Pittsburgh Univ., PA (USA). Dept. of Chemical and Petroleum Engineering  
**Published:** 31 January 1988  
**Description:** 50 p.  
**Tech. Rept. No.:** DOE\PC\70020-T1 ; DE88006658  
**Report type:** Progress report  
**Funding Info.:** AC22-84PC70020

**Abstract:** The objective of the project was to investigate the possibility of modifying methane formation during the F-T synthesis independent from other hydrocarbons by systematically changing catalyst characteristics. It would seem that the best way to decrease methane selectivity is still via the use of catalyst modifiers. In order to "tailor-make" catalyst surfaces which minimize "extraneous" methane synthesis without disrupting F-T synthesis, it is necessary for us to fully understand the mechanism(s) by which such modifiers operate. An investigation of Fischer-Tropsch synthesis on K- and Cl-modified Ru Catalysts was carried out. The steady-steady reaction results illustrate how chlorine enhances the selectivity of methane formation while potassium decreases it. In order to better understand methane selectivity changes, a detailed study of Cl-modification of Ru catalysts was made. A ammonia synthesis and methanation reaction results on the same series of catalysts (obtained by using the steady-state isotopic transient technique) in addition to the deactivation results for F-T suggest that structural rearrangements induced by the presence of chlorine, rather than selective site blocking or electronic interactions, may be the primary mechanism of chlorine modification of supported ruthenium catalysts. The results of this study indicate that catalyst modifiers may act to change the catalytic properties by inducing certain metal surface structures. This is a mechanism of modification which has, yet, not been addressed in detail. 49 refs., 16 figs., 7 tabs.

Location	Call Number	Status
REPT Mfiche	DOE\PC\70020-T1 c.0	In Library

[Previous](#)

Records: 1 ... 71 81 91 101 111 121 131 141 151 161 171 181 191 201 211 221 ... 481

[Next](#)

<a href="#">New Search</a>	<a href="#">Comments</a>
<a href="#">List Marks</a>	<a href="#">Help</a>
	<a href="#">Databases</a>



Full Record

Records: 1 ... 71 81 91 101 111 121 131 141 151 161 171 181 191 201 211 221 ... 481

<a href="#">Brief Records</a>	<a href="#">Mark</a>
-------------------------------	----------------------

[Previous](#)

Records: 1 ... 71 81 91 101 111 121 131 141 151 161 171 181 191 201 211 221 ... 481

[Next](#)

**Call No.:** DOE\PC\70023-T2  
**Title:** The development of a selective ruthenium Fischer-Tropsch catalyst Final report, October 1, 1984--February 28, 1989  
**Author:** UOP, Inc., Des Plaines, IL (United States). Technical Center  
**Published:** [1989]  
**Description:** 577 p.  
**Tech. Rept. No.:** DOE\PC\70023-T2 ; DE92002723  
**Report type:** Progress report  
**Funding Info.:** USDOE, Washington, DC (United States) AC22-84PC70023  
**Abstract:** A new stable Fischer-Tropsch catalyst with very high selectivity to distillate fuels and with low light ends production was developed. This catalyst, which was made by a reverse micelle technique, contains 2.8% (by weight) ruthenium in the form of 4--6 nm particles on alumina and a proprietary modifier. The new modified ruthenium catalyst did not noticeably deactivate during 814 hours at about 80% CO conversion, 2H<sub>2</sub>:1 CO feed ratio, 208[degree]C at inlet, 62 atm and 150 gas hourly space velocity. In order to determine the catalyst's tolerance, the operational severity was increased between 814 hours and 1700 hours by increasing the temperature and space velocity to 225[degree]C at inlet and to 205 hr<sup>-1</sup>, respectively. A deactivation rate of about 0.016%/hour was measured under these more severe conditions at about 70% conversion level. These results with the new modified ruthenium catalyst compare favorably with those reported for the two commercial Sasol processes. The Arge process makes approximately 38% distillate fuel with 14--18% light ends, while the Synthol process makes about 48% distillate with 38% light ends. 82 refs., 360 figs., 66 tabs.

Location	Call Number	Status
REPT	DOE\PC\70023-T2 c.0	In Library
Mfiche		

[Previous](#)

Records: 1 ... 71 81 91 101 111 121 131 141 151 161 171 181 191 201 211 221 ... 481

[Next](#)