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* Generated by FACSIMILE Reaction Wizard -
4. marts 2001 ;
*===== ;
* Model of Chemistry in Reaction Cell, Oslo. CO + OH, 760 torr
;
*===== ;

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EXECUTE OPEN 8 "C:\fac\karen\oslo\HOCO.out";

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PARAMETER

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P          1
T          296
R          0.0821
N          6.02214E23
PPM        2.461e13
PPB         2.461e10
;

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PARAMETER

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K1f 3e-2
K2f 2.2E-10
K4f 4E-11
K5f 2.6E-11
K7f 1.9E-12
K9f 1.2E-10
K10f 1.7E-12
K11f 1.2E-10
K12f 2E-15
K13f 6.8E-14
K14f 1.1E-10
K16f 7.1e-6
K17f 8e-15
K18f 2.9e-11
K19f 3.3e-11
K20f 5.9e-11
K21f 1.7e-15
K22f 1.7e-12
K23f 1.1e-10
K25f 6.3e-15
K27f 5.6e-12
K34f 1.0e-11
K35f 8.9e-13
K40f 5.5e-12
K41f 1.9e-15
K42f 2.03e-10
K43f 1.4e-10
K44f 1.5e-10
K45f 2e-3
k46f 2e-3
k47f 6.7e-15

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VARIABLE

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CO CO2 H H2 H2O H2O2 H02
M N2 O O2 O3 OH OP
via0 viaOH fromCH4 CH4via0 CH4viaOH X
K1f K3f K6f K8f K15f K16f K24f
CH4 CH3 CH3O2 CH3OOH CH3O HCHO CH3OH
CH3OOCH3 HCO CH2OH
K26f K28f K29f K30f K31f K32f
K36f K37f K38f K39f

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COMPILE INSTANT;
H2O = 100*PPM ;

CO = 2*PPM ;
CH4 = 0.165*PPM;
**;

COMPILE INITIAL ;
N2 = (0.8*(680/760)*1E-3*N)/(R*T) ;
O2 = (((0.2*(680/760))+(0.95*80/760))*1E-3*N)/(R*T) ;
O3 = ((0.05*80/760)*1E-3*N)/(R*T) ;
H2 = ((4/760)*1E-3*N)/(R*T) ;
M = (P*1E-3*N)/(R*T) ;
K3f = 1.5E-13*(1+0.6*P) ;
K6f = M*6.0E-34*((296/300)@(-2.3)) ;
K8f = M*6.2E-31*((296/300)@(-1.0)) ;
K15f = M*5.7E-32*((296/300)@(-1.6)) ;
K24f = M*1.0e-35;
K26f = M*4.5E-31*((296/300)@(-3.0)) ;
K28f = 4.7e-13*0.3;
K29f = 4.7e-13*0.6;
K30f = 4.7e-13*0.1;
K31f = 1.1e-10*0.6;
K32f = 1.1e-10*0.4;
K36f = 7.4e-12*0.7;
K37f = 7.4e-12*0.3;
K38f = 2.6e-12*0.1;
K39f = 2.6e-12*0.9;

**;

COMPILE EQUATIONS ;
* OH source ;

% K1f : O3 = O2 + O;
% K2f : O + H2O = OH + OH;

* H0x Chemistry ;
% K3f : OH + CO = CO2 + H ;
% K4f : O + O2 = OP + O2;
% K5f : O + N2 = OP + N2;
% K6f : OP + O2 = O3 ;*M
% K7f : OH + OH = H2O + OP;
% K8f : OH + OH = H2O2 ;*M
% K9f : O + O3 = O2 + O2;
% K10f : H2O + H2O = H2O2 + O2;
% K11f : O + O3 = O2 + O + OP;
% K12f : H2O + O3 = OH + O2 + O2;
% K13f : OH + O3 = H2O + O2;
% K14f : OH + H2O = H2O + O2;
% K15f : H + O2 = H2O ;*M
% K16f : H2O2 = OH + OH ;
% K17f : OP + O3 = O2 + O2 ;
% K18f : H + O3 = OH + O2 ;
% K19f : OP + OH = O2 + H ;
% K20f : OP + H2O = OH + O2 ;
% K21f : OP + H2O2 = OH + H2O ;
% K22f : OH + H2O2 = H2O + H2O ;
% K23f : O + H2 = OH + H ;* Hydrogen Source ;
% K24f : CO + O = CO2 + via0;

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* Methane Chemistry ;
% K25f : OH + CH4 = CH3 + H2O ;
% K26f : CH3 + O2 = CH3O2 ;*M
% K27f : CH3O2 + H2O = CH3OOH + O2 ;
% K28f : CH3O2 + CH3O2 = CH3O + CH3O + O2 ;
% K29f : CH3O2 + CH3O2 = HCHO+ CH3OH + O2 ;
% K30f : CH3O2 + CH3O2 = CH3OOCH3 + O2 ;
% K31f : CH3 + OP = HCHO+ H ;
% K32f : CH3 + OP = H + H2 + CO ;
% K34f : OH + HCHO= H2O + HCO ;
% K35f : OH + CH3OH = H2O + HCHO + H ;
% K36f : OH + CH3OOH = CH3O2 + H2O ;
% K37f : OH + CH3OOH = HCHO+ OH + H2O ;
% K38f : CH3 + O3 = CH3O + O2 ;
% K39f : CH3 + O3 = HCHO+ H2O ;
% K40f : HCO + O2 = CO + H2O ;
% K41f : CH3O + O2 = HCHO+ H2O ;
% K42f : CH3 + H = CH4 ;
% K43f : O + CH4 = CH3 + OH ;
% K44f : O + CH4 = HCHO+ H2;
% K45f : HCHO = CO + H2;
% K46f : HCHO = HCO + H;
% K47f : OH + H2 = H2O + H;

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** ;

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SETPSTREAM 1 8 ;
TIME CO ;
** ;

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COMPILE OUT ;
PSTREAM 1 ;
** ;

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WHENEVER TIME=
701 * (+8) 0 % CALL OUT;

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** ;

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BEGIN;
STOP;

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