

# Cleanbustion Computation Model Reference

## Basis description

The Cleanbustion Computation model combines a SNCR reaction model with a gaseous combustion reaction model. The SNCR reaction model handles the “N”-reactions while the combustion reaction model handles the “C”-reactions. As result, the Cleanbustion Computation model can handle any combined “N & C” reactions. Especially from the point of NO<sub>x</sub> reduction, C-components are able to support selective N-reducing agents and work as reactions enhancer.

## Definitions

NO<sub>x</sub> total of N<sub>x</sub>O<sub>y</sub> expressed as NO<sub>2</sub>

## Cleanbustion Database

The following input parameters are set for constant

Pressure	1013.25 hPa
CO	0.00 mg/Nm <sup>3</sup>
SO <sub>2</sub>	0.00 mg/Nm <sup>3</sup>
NO <sub>x</sub> -Ratio	$n\text{NO}_x = 0.95n \text{ NO} + 0.05n \text{ NO}_2$ n in mol/Nm <sup>3</sup>

## Input Parameters

N <sub>2</sub>	Nm <sup>3</sup> /Nm <sup>3</sup> dry gas
O <sub>2</sub>	Nm <sup>3</sup> /Nm <sup>3</sup> dry gas
CO <sub>2</sub>	Nm <sup>3</sup> /Nm <sup>3</sup> dry gas
H <sub>2</sub> O	Nm <sup>3</sup> /Nm <sup>3</sup> humid gas
NO <sub>x</sub>	mg/Nm <sup>3</sup> dry gas at present oxygen level
NH <sub>3</sub>	mg/Nm <sup>3</sup> dry gas
NH <sub>2</sub> CONH <sub>2</sub>	mg/Nm <sup>3</sup> dry gas
Reference Oxygen	equal to present oxygen level

## Partial Chemical Reactions

There are 428 partial chemical reactions included to attain the most accurate approximation of real SNCR-states.

- (1)  $\text{OH} + \text{H}_2 = \text{H}_2\text{O} + \text{H}$
- (2)  $\text{O} + \text{OH} = \text{O}_2 + \text{H}$
- (3)  $\text{O} + \text{H}_2 = \text{OH} + \text{H}$
- (4)  $\text{H} + \text{O}_2 + \text{X} = \text{HO}_2 + \text{X}$
- (5)  $\text{H} + \text{O}_2 + \text{N}_2 = \text{HO}_2 + \text{N}_2$
- (6)  $\text{OH} + \text{HO}_2 = \text{H}_2\text{O} + \text{O}_2$
- (7)  $\text{H} + \text{HO}_2 = \text{OH} + \text{OH}$
- (8)  $\text{H} + \text{HO}_2 = \text{H}_2 + \text{O}_2$
- (9)  $\text{H} + \text{HO}_2 = \text{O} + \text{H}_2\text{O}$
- (10)  $\text{O} + \text{HO}_2 = \text{O}_2 + \text{OH}$
- (11)  $\text{OH} + \text{OH} = \text{O} + \text{H}_2\text{O}$
- (12)  $\text{H} + \text{H} + \text{X} = \text{H}_2 + \text{X}$
- (13)  $\text{H} + \text{OH} + \text{H}_2\text{O} = \text{H}_2\text{O} + \text{H}_2\text{O}$
- (14)  $\text{H} + \text{O} + \text{H}_2\text{O} = \text{OH} + \text{H}_2\text{O}$
- (15)  $\text{O} + \text{O} + \text{X} = \text{O}_2 + \text{X}$
- (16)  $\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$
- (17)  $\text{H}_2\text{O}_2 + \text{X} = \text{OH} + \text{OH} + \text{X}$
- (18)  $\text{H}_2\text{O}_2 + \text{H} = \text{HO}_2 + \text{H}_2$
- (19)  $\text{H}_2\text{O}_2 + \text{H} = \text{OH} + \text{H}_2\text{O}$
- (20)  $\text{H}_2\text{O}_2 + \text{O} = \text{OH} + \text{HO}_2$
- (21)  $\text{H}_2\text{O}_2 + \text{OH} = \text{H}_2\text{O} + \text{HO}_2$
- (22)  $\text{NO} + \text{HO}_2 = \text{NO}_2 + \text{OH}$
- (23)  $\text{NO}_2 + \text{NO}_2 = \text{NO} + \text{NO} + \text{O}_2$
- (24)  $\text{NO}_2 + \text{H} = \text{NO} + \text{OH}$
- (25)  $\text{NO}_2 + \text{O} = \text{NO} + \text{O}_2$
- (26)  $\text{NO} + \text{O} + \text{X} = \text{NO}_2 + \text{X}$
- (27)  $\text{NO}_2 + \text{NH} = \text{N}_2\text{O} + \text{OH}$
- (28)  $\text{NO}_2 + \text{NH}_2 = \text{N}_2\text{O} + \text{H}_2\text{O}$
- (29)  $\text{NH}_2 + \text{NO}_2 = \text{H}_2\text{NO} + \text{NO}$
- (30)  $\text{NO}_2 + \text{HNO} = \text{HONO} + \text{NO}$
- (31)  $\text{NO} + \text{OH} + \text{H}_2\text{O} = \text{HONO} + \text{H}_2\text{O}$
- (32)  $\text{HONO} + \text{O} = \text{OH} + \text{NO}_2$
- (33)  $\text{HONO} + \text{OH} = \text{H}_2\text{O} + \text{NO}_2$
- (34)  $\text{HONO} + \text{NH}_2 = \text{NO}_2 + \text{NH}_3$
- (35)  $\text{HONO} + \text{H} = \text{H}_2 + \text{NO}_2$
- (36)  $\text{NH} + \text{O}_2 = \text{HNO} + \text{O}$
- (37)  $\text{NH} + \text{O}_2 = \text{NO} + \text{OH}$
- (38)  $\text{NO} + \text{NH} = \text{N}_2\text{O} + \text{H}$
- (39)  $\text{NH} + \text{NO} = \text{N}_2 + \text{OH}$
- (40)  $\text{NH} + \text{OH} = \text{HNO} + \text{H}$
- (41)  $\text{NH} + \text{OH} = \text{N} + \text{H}_2\text{O}$
- (42)  $\text{NH} + \text{N} = \text{N}_2 + \text{H}$
- (43)  $\text{NH} + \text{H} = \text{N} + \text{H}_2$
- (44)  $\text{NH} + \text{O} = \text{NO} + \text{H}$
- (45)  $\text{N}_2\text{O} + \text{OH} = \text{N}_2 + \text{HO}_2$
- (46)  $\text{N}_2\text{O} + \text{OH} = \text{HNO} + \text{NO}$
- (47)  $\text{N}_2\text{O} + \text{NO} = \text{NO}_2 + \text{N}_2$
- (48)  $\text{N}_2\text{O} + \text{H} = \text{N}_2 + \text{OH}$
- (49)  $\text{N}_2\text{O} + \text{X} = \text{N}_2 + \text{O} + \text{X}$
- (50)  $\text{N}_2\text{O} + \text{O} = \text{N}_2 + \text{O}_2$
- (51)  $\text{N}_2\text{O} + \text{O} = \text{NO} + \text{NO}$
- (52)  $\text{NH}_2 + \text{O} = \text{HNO} + \text{H}$
- (53)  $\text{NH}_2 + \text{O} = \text{NH} + \text{OH}$
- (54)  $\text{NH}_2 + \text{OH} = \text{NH} + \text{H}_2\text{O}$
- (55)  $\text{NH}_2 + \text{H} = \text{NH} + \text{H}_2$
- (56)  $\text{NH}_2 + \text{HO}_2 = \text{NH}_3 + \text{O}_2$
- (57)  $\text{NH}_2 + \text{HO}_2 = \text{H}_2\text{NO} + \text{OH}$
- (58)  $\text{NH}_2 + \text{NH}_2 = \text{N}_2\text{H}_2 + \text{H}_2$
- (59)  $\text{NH}_2 + \text{NO} = \text{N}_2 + \text{H}_2\text{O}$
- (60)  $\text{NH}_2 + \text{NO} = \text{NNH} + \text{OH}$
- (61)  $\text{NH}_3 + \text{X} = \text{NH}_2 + \text{H} + \text{X}$
- (62)  $\text{NH}_3 + \text{OH} = \text{NH}_2 + \text{H}_2\text{O}$
- (63)  $\text{NH}_3 + \text{H} = \text{NH}_2 + \text{H}_2$
- (64)  $\text{NH}_3 + \text{O} = \text{NH}_2 + \text{OH}$
- (65)  $\text{NH}_3 + \text{HO}_2 = \text{NH}_2 + \text{H}_2\text{O}_2$
- (66)  $\text{NNH} = \text{N}_2 + \text{H}$
- (67)  $\text{NNH} + \text{O}_2 = \text{N}_2 + \text{HO}_2$
- (68)  $\text{NNH} + \text{O}_2 = \text{N}_2 + \text{O}_2 + \text{H}$
- (69)  $\text{NO} + \text{NNH} = \text{N}_2 + \text{HNO}$
- (70)  $\text{NNH} + \text{H} = \text{N}_2 + \text{H}_2$
- (71)  $\text{NNH} + \text{OH} = \text{N}_2 + \text{H}_2\text{O}$
- (72)  $\text{NNH} + \text{NH}_2 = \text{N}_2 + \text{NH}_3$
- (73)  $\text{NNH} + \text{NH} = \text{N}_2 + \text{NH}_2$
- (74)  $\text{NNH} + \text{O} = \text{N}_2 + \text{OH}$
- (75)  $\text{NNH} + \text{O} = \text{N}_2\text{O} + \text{H}$
- (76)  $\text{NNH} + \text{O} = \text{NH} + \text{NO}$
- (77)  $\text{NO} + \text{H} + \text{X} = \text{HNO} + \text{X}$
- (78)  $\text{HNO} + \text{NO} = \text{N}_2\text{O} + \text{OH}$
- (79)  $\text{HNO} + \text{X} = \text{NO} + \text{H} + \text{X}$
- (80)  $\text{HNO} + \text{OH} = \text{NO} + \text{H}_2\text{O}$
- (81)  $\text{HNO} + \text{H} = \text{H}_2 + \text{NO}$
- (82)  $\text{HNO} + \text{O} = \text{OH} + \text{NO}$
- (83)  $\text{HNO} + \text{NH}_2 = \text{NH}_3 + \text{NO}$
- (84)  $\text{HNO} + \text{HNO} = \text{N}_2\text{O} + \text{H}_2\text{O}$
- (85)  $\text{HNO} + \text{O}_2 = \text{HO}_2 + \text{NO}$
- (86)  $\text{H}_2\text{NO} + \text{O}_2 = \text{HNO} + \text{HO}_2$
- (87)  $\text{H}_2\text{NO} + \text{H}_2\text{O} = \text{HNOH} + \text{H}_2\text{O}$
- (88)  $\text{H}_2\text{NO} + \text{H}_2\text{O} = \text{HNO} + \text{H} + \text{H}_2\text{O}$
- (89)  $\text{H}_2\text{NO} + \text{NO}_2 = \text{HNO} + \text{HONO}$
- (90)  $\text{H}_2\text{NO} + \text{H} = \text{HNO} + \text{H}_2$

- (91)  $\text{H}_2\text{NO} + \text{H} = \text{NH}_2 + \text{OH}$   
 (92)  $\text{H}_2\text{NO} + \text{O} = \text{HNO} + \text{OH}$   
 (93)  $\text{H}_2\text{NO} + \text{O} = \text{NH}_2 + \text{O}_2$   
 (94)  $\text{H}_2\text{NO} + \text{OH} = \text{HNO} + \text{H}_2\text{O}$   
 (95)  $\text{H}_2\text{NO} + \text{NO} = \text{HNO} + \text{HNO}$   
 (96)  $\text{H}_2\text{NO} + \text{NH}_2 = \text{NH}_3 + \text{HNO}$   
 (97)  $\text{H}_2\text{NO} + \text{HO}_2 = \text{HNO} + \text{H}_2\text{O}_2$   
 (98)  $\text{HNOH} + \text{H} = \text{NH}_2 + \text{OH}$   
 (99)  $\text{HNOH} + \text{H} = \text{HNO} + \text{H}_2$   
 (100)  $\text{HNOH} + \text{O} = \text{HNO} + \text{OH}$   
 (101)  $\text{HNOH} + \text{OH} = \text{HNO} + \text{H}_2\text{O}$   
 (102)  $\text{HNOH} + \text{NH}_2 = \text{NH}_3 + \text{HNO}$   
 (103)  $\text{HNOH} + \text{HO}_2 = \text{HNO} + \text{H}_2\text{O}_2$   
 (104)  $\text{HNOH} + \text{H}_2\text{O} = \text{HNO} + \text{H} + \text{H}_2\text{O}$   
 (105)  $\text{HNOH} + \text{O}_2 = \text{HNO} + \text{HO}_2$   
 (106)  $\text{HNOH} + \text{NO}_2 = \text{HONO} + \text{HNO}$   
 (107)  $\text{NO} + \text{N} = \text{N}_2 + \text{O}$   
 (108)  $\text{N} + \text{O}_2 = \text{NO} + \text{O}$   
 (109)  $\text{N} + \text{OH} = \text{NO} + \text{H}$   
 (110)  $\text{NH}_2 + \text{NH} = \text{N}_2\text{H}_2 + \text{H}$   
 (111)  $\text{NH} + \text{NH} = \text{N}_2 + \text{H} + \text{H}$   
 (112)  $\text{NH}_2 + \text{N} = \text{N}_2 + \text{H} + \text{H}$   
 (113)  $\text{N}_2\text{H}_2 + \text{X} = \text{NNH} + \text{H} + \text{X}$   
 (114)  $\text{N}_2\text{H}_2 + \text{H} = \text{NNH} + \text{H}_2$   
 (115)  $\text{N}_2\text{H}_2 + \text{O} = \text{NH}_2 + \text{NO}$   
 (116)  $\text{N}_2\text{H}_2 + \text{O} = \text{NNH} + \text{OH}$   
 (117)  $\text{N}_2\text{H}_2 + \text{OH} = \text{NNH} + \text{H}_2\text{O}$   
 (118)  $\text{N}_2\text{H}_2 + \text{NO} = \text{N}_2\text{O} + \text{NH}_2$   
 (119)  $\text{N}_2\text{H}_2 + \text{NH} = \text{NNH} + \text{NH}_2$   
 (120)  $\text{N}_2\text{H}_2 + \text{NH}_2 = \text{NH}_3 + \text{NNH}$   
 (121)  $\text{NO}_2 + \text{O} + \text{X} = \text{NO}_3 + \text{X}$   
 (122)  $\text{NO}_2 + \text{NO}_2 = \text{NO}_3 + \text{NO}$   
 (123)  $\text{NO}_3 + \text{H} = \text{NO}_2 + \text{OH}$   
 (124)  $\text{NO}_3 + \text{O} = \text{NO}_2 + \text{O}_2$   
 (125)  $\text{NO}_3 + \text{OH} = \text{NO}_2 + \text{HO}_2$   
 (126)  $\text{NO}_3 + \text{HO}_2 = \text{NO}_2 + \text{O}_2 + \text{OH}$   
 (127)  $\text{NO}_3 + \text{NO}_2 = \text{NO} + \text{NO}_2 + \text{O}_2$   
 (128)  $\text{H}_2 + \text{O}_2 = \text{OH} + \text{OH}$   
 (129)  $\text{NH}_2 + \text{NH}_2 = \text{NH}_3 + \text{NH}$   
 (130)  $\text{NH}_2 + \text{NH}_2 + \text{X} = \text{N}_2\text{H}_4 + \text{X}$   
 (131)  $\text{N}_2\text{H}_4 + \text{H} = \text{N}_2\text{H}_3 + \text{H}_2$   
 (132)  $\text{N}_2\text{H}_4 + \text{O} = \text{N}_2\text{H}_2 + \text{H}_2\text{O}$   
 (133)  $\text{N}_2\text{H}_4 + \text{OH} = \text{N}_2\text{H}_3 + \text{H}_2\text{O}$   
 (134)  $\text{N}_2\text{H}_4 + \text{NH}_2 = \text{N}_2\text{H}_3 + \text{NH}_3$   
 (135)  $\text{N}_2\text{H}_3 = \text{N}_2\text{H}_2 + \text{H}$   
 (136)  $\text{N}_2\text{H}_3 + \text{H} = \text{NH}_2 + \text{NH}_2$   
 (137)  $\text{N}_2\text{H}_3 + \text{O} = \text{N}_2\text{H}_2 + \text{OH}$   
 (138)  $\text{N}_2\text{H}_3 + \text{O} = \text{NH}_2 + \text{HNO}$   
 (139)  $\text{N}_2\text{H}_3 + \text{OH} = \text{N}_2\text{H}_2 + \text{H}_2\text{O}$   
 (140)  $\text{N}_2\text{H}_3 + \text{OH} = \text{NH}_3 + \text{HNO}$   
 (141)  $\text{N}_2\text{H}_3 + \text{NH} = \text{N}_2\text{H}_2 + \text{NH}_2$   
 (142)  $\text{HONO} + \text{HONO} = \text{NO} + \text{NO}_2 + \text{H}_2\text{O}$   
 (143)  $\text{HNOH} + \text{NH}_2 = \text{N}_2\text{H}_3 + \text{OH}$   
 (144)  $\text{CO} + \text{O} + \text{X} = \text{CO}_2 + \text{X}$   
 (145)  $\text{CO} + \text{OH} = \text{CO}_2 + \text{H}$   
 (146)  $\text{CO} + \text{O}_2 = \text{CO}_2 + \text{O}$   
 (147)  $\text{CO} + \text{HO}_2 = \text{CO}_2 + \text{OH}$   
 (148)  $\text{HCO} + \text{H} = \text{CO} + \text{H}_2$   
 (149)  $\text{HCO} + \text{O} = \text{CO} + \text{OH}$   
 (150)  $\text{HCO} + \text{O} = \text{CO}_2 + \text{H}$   
 (151)  $\text{HCO} + \text{OH} = \text{CO} + \text{H}_2\text{O}$   
 (152)  $\text{HCO} + \text{O}_2 = \text{CO} + \text{HO}_2$   
 (153)  $\text{HCO} + \text{X} = \text{H} + \text{CO} + \text{X}$   
 (154)  $\text{HNCO} + \text{X} = \text{NH} + \text{CO} + \text{X}$   
 (155)  $\text{HNCO} + \text{H} = \text{NH}_2 + \text{CO}$   
 (156)  $\text{HNCO} + \text{O} = \text{NCO} + \text{OH}$   
 (157)  $\text{HNCO} + \text{O} = \text{NH} + \text{CO}_2$   
 (158)  $\text{HNCO} + \text{O} = \text{HNO} + \text{CO}$   
 (159)  $\text{HNCO} + \text{OH} = \text{H}_2\text{O} + \text{NCO}$   
 (160)  $\text{HNCO} + \text{HO}_2 = \text{NCO} + \text{H}_2\text{O}_2$   
 (161)  $\text{HNCO} + \text{O}_2 = \text{HNO} + \text{CO}_2$   
 (162)  $\text{HNCO} + \text{NH}_2 = \text{NH}_3 + \text{NCO}$   
 (163)  $\text{HNCO} + \text{NH} = \text{NH}_2 + \text{NCO}$   
 (164)  $\text{HNCO} + \text{NO}_2 = \text{HNNO} + \text{CO}_2$   
 (165)  $\text{NCO} + \text{X} = \text{N} + \text{CO} + \text{X}$   
 (166)  $\text{NCO} + \text{H} = \text{NH} + \text{CO}$   
 (167)  $\text{NCO} + \text{O} = \text{NO} + \text{CO}$   
 (168)  $\text{NCO} + \text{OH} = \text{NO} + \text{HCO}$   
 (169)  $\text{NCO} + \text{H}_2 = \text{HNCO} + \text{H}$   
 (170)  $\text{NCO} + \text{O}_2 = \text{NO} + \text{CO}_2$   
 (171)  $\text{NCO} + \text{HCO} = \text{HNCO} + \text{CO}$   
 (172)  $\text{NCO} + \text{N} = \text{N}_2 + \text{CO}$   
 (173)  $\text{NCO} + \text{NO} = \text{N}_2\text{O} + \text{CO}$   
 (174)  $\text{NCO} + \text{NO} = \text{N}_2 + \text{CO}_2$   
 (175)  $\text{NCO} + \text{NO}_2 = \text{NO} + \text{NO} + \text{CO}$   
 (176)  $\text{NCO} + \text{NO}_2 = \text{CO}_2 + \text{N}_2\text{O}$   
 (177)  $\text{NCO} + \text{HNO} = \text{HNCO} + \text{NO}$   
 (178)  $\text{NCO} + \text{HONO} = \text{HNCO} + \text{NO}_2$   
 (179)  $\text{NCO} + \text{NCO} = \text{CO} + \text{CO} + \text{N}_2$   
 (180)  $\text{NO} + \text{HCO} = \text{CO} + \text{HNO}$   
 (181)  $\text{NO}_2 + \text{HCO} = \text{CO} + \text{HONO}$   
 (182)  $\text{NO}_2 + \text{HCO} = \text{H} + \text{CO}_2 + \text{NO}$   
 (183)  $\text{NH}_2\text{CONH}_2 = \text{NH}_3 + \text{HNCO}$   
 (184)  $\text{NH}_2\text{CONH}_2 + \text{H}_2\text{O} = \text{NH}_3 + \text{NH}_3 + \text{CO}_2$   
 (185)  $\text{CO} + \text{NO}_2 = \text{CO}_2 + \text{NO}$   
 (186)  $\text{H}_2\text{O} = \text{H} + \text{OH}$   
 (187)  $\text{N}_2\text{H}_4 + \text{O}_2 = \text{N}_2 + \text{H}_2\text{O} + \text{H}_2\text{O}$   
 (188)  $2 \text{N}_2\text{H}_4 + 2 \text{NO} + 2 \text{O} = 3 \text{N}_2 + 4 \text{H}_2\text{O}$   
 (189)  $\text{N}_2\text{H}_4 + 2 \text{NO} = 2 \text{N}_2 + 2 \text{H}_2\text{O}$   
 (190)  $\text{N} + \text{CH} = \text{CN} + \text{H}$

- (191)  $N + tCH_2 = HCN + H$   
 (192)  $N + CH_3 = H_2CN + H$   
 (193)  $N + HCCO = HCN + CO$   
 (194)  $N + C_2H_2 = HCN + CH$   
 (195)  $N + C_2H_3 = HCN + tCH_2$   
 (196)  $N_2 + CH = HCN + N$   
 (197)  $N_2 + tCH_2 = HCN + NH$   
 (198)  $NO + CH = HCN + O$   
 (199)  $NO + sCH_2 = HCN + OH$   
 (200)  $NO + tCH_2 = HCNO + H$   
 (201)  $NO + tCH_2 = HCN + OH$   
 (202)  $NO + CH_3 = HCN + H_2O$   
 (203)  $NO + CH_3 = H_2CN + OH$   
 (204)  $NO + C_2H = HCN + CO$   
 (205)  $NO + HCCO = HCNO + CO$   
 (206)  $N_2O + CH_3 = CH_3O + N_2$   
 (207)  $NO_2 + CH = HCO + NO$   
 (208)  $NO_2 + tCH_2 = H_2CO + NO$   
 (209)  $NO_2 + CH_3 = CH_3O + NO$   
 (210)  $NO_2 + HCO = CO_2 + H + NO$   
 (211)  $NO_2 + HCO = CO + HNO$   
 (212)  $NO_2 + HCCO = NCO + CO + OH$   
 (213)  $NO_2 + HCCO = HNCO + CO_2$   
 (214)  $NO_2 + HCCO = HCN + CO_2 + O$   
 (215)  $HCN + O = NCO + H$   
 (216)  $HCN + O = NH + CO$   
 (217)  $HCN + OH = HNCO + H$   
 (218)  $HCN + CN = C_2N_2 + H$   
 (219)  $CN + O = CO + N$   
 (220)  $CN + OH = NCO + H$   
 (221)  $CN + O_2 = NCO + O$   
 (222)  $CN + H_2 = HCN + H$   
 (223)  $CN + H_2O = HCN + OH$   
 (224)  $CN + N = N_2 + C$   
 (225)  $CN + NO = N_2 + CO$   
 (226)  $CN + NO = NCO + N$   
 (227)  $CN + N_2O = NCO + N_2$   
 (228)  $CN + NO_2 = NCO + NO$   
 (229)  $CN + CH_4 = HCN + CH_3$   
 (230)  $C_2N_2 + O = NCO + CN$   
 (231)  $HCNO + H = HCN + OH$   
 (232)  $HCNO + H = HNCO + H$   
 (233)  $CH + H = C + H_2$   
 (234)  $C + O_2 = CO + O$   
 (235)  $C + NO = CN + O$   
 (236)  $H_2CN + N = N_2 + tCH_2$   
 (237)  $H_2CN + X = HCN + H + X$   
 (238)  $HCO + HCO = H_2CO + CO$   
 (239)  $CH + O = CO + H$   
 (240)  $CH + OH = HCO + H$   
 (241)  $CH + O_2 = HCO + O$   
 (242)  $CH + CO = HCCO$   
 (243)  $CH + CO_2 = HCO + CO$   
 (244)  $CH + H_2O = H_2CO + H$   
 (245)  $CH + H_2O = tCH_2 + OH$   
 (246)  $tCH_2 + H = CH + H_2$   
 (247)  $tCH_2 + O = CO + H + H$   
 (248)  $tCH_2 + O = CO + H_2$   
 (249)  $tCH_2 + O_2 = CO + OH + H$   
 (250)  $tCH_2 + O_2 = CO_2 + H_2$   
 (251)  $tCH_2 + tCH_2 = C_2H_2 + H_2$   
 (252)  $tCH_2 + tCH_2 = C_2H_2 + H + H$   
 (253)  $tCH_2 + CH_3 = C_2H_4 + H$   
 (254)  $sCH_2 + X = tCH_2 + X$   
 (255)  $sCH_2 + H_2 = CH_3 + H$   
 (256)  $sCH_2 + O_2 = CO + OH + H$   
 (257)  $H_2CO + X = HCO + H + X$   
 (258)  $H_2CO + X = CO + H_2 + X$   
 (259)  $H_2CO + H = HCO + H_2$   
 (260)  $H_2CO + O = HCO + OH$   
 (261)  $H_2CO + OH = HCO + H_2O$   
 (262)  $H_2CO + HO_2 = HCO + H_2O_2$   
 (263)  $H_2CO + O_2 = HCO + HO_2$   
 (264)  $H_2CO + CH_3 = HCO + CH_4$   
 (265)  $CH_3 + X = tCH_2 + H + X$   
 (266)  $CH_3 + X = CH + H_2 + X$   
 (267)  $CH_3 + O = H_2CO + H$   
 (268)  $CH_3 + OH = CH_3O + H$   
 (269)  $CH_3 + OH = sCH_2 + H_2O$   
 (270)  $CH_3 + OH + X = CH_3OH + X$   
 (271)  $CH_3 + HO_2 = CH_3O + OH$   
 (272)  $CH_3 + O_2 = H_2CO + OH$   
 (273)  $CH_3 + O_2 = CH_3O + O$   
 (274)  $CH_3 + O_2 + X = CH_3O_2 + X$   
 (275)  $CH_3 + CO + X = CH_3CO + X$   
 (276)  $CH_3 + sCH_2 = C_2H_4 + H$   
 (277)  $CH_3 + CH_3 + X = C_2H_6 + X$   
 (278)  $CH_3O + H = CH_3 + OH$   
 (279)  $CH_3O + H = H_2CO + H_2$   
 (280)  $CH_3O + O = CH_3 + O_2$   
 (281)  $CH_3O + O = OH + H_2CO$   
 (282)  $CH_3O + OH = H_2CO + H_2O$   
 (283)  $CH_3O + O_2 = H_2CO + HO_2$   
 (284)  $CH_3O + H_2CO = HCO + CH_3OH$   
 (285)  $CH_2OH + H = H_2CO + H_2$   
 (286)  $CH_2OH + H = CH_3 + OH$   
 (287)  $CH_2OH + O_2 = H_2CO + HO_2$   
 (288)  $CH_3OH + H = CH_2OH + H_2$   
 (289)  $CH_3OH + H = CH_3O + H_2$   
 (290)  $CH_3OH + O = CH_2OH + OH$

- (291)  $\text{CH}_3\text{OH} + \text{O} = \text{CH}_3\text{O} + \text{OH}$   
(292)  $\text{CH}_3\text{OH} + \text{OH} = \text{CH}_2\text{OH} + \text{H}_2\text{O}$   
(293)  $\text{CH}_3\text{OH} + \text{OH} = \text{CH}_3\text{O} + \text{H}_2\text{O}$   
(294)  $\text{CH}_3\text{OH} + \text{HO}_2 = \text{CH}_2\text{OH} + \text{H}_2\text{O}_2$   
(295)  $\text{CH}_3\text{OH} + \text{O}_2 = \text{CH}_2\text{OH} + \text{HO}_2$   
(296)  $\text{CH}_3\text{OH} + \text{CH}_3 = \text{CH}_4 + \text{CH}_2\text{OH}$   
(297)  $\text{CH}_3\text{OH} + \text{CH}_3 = \text{CH}_4 + \text{CH}_3\text{O}$   
(298)  $\text{CH}_3\text{OH} + \text{CH}_3\text{O} = \text{CH}_2\text{OH} + \text{CH}_3\text{OH}$   
(299)  $\text{CH}_3\text{OH} + \text{H}_2\text{CO} = \text{CH}_3\text{O} + \text{CH}_3\text{O}$   
(300)  $\text{CH}_4 + \text{H} = \text{CH}_3 + \text{H}_2$   
(301)  $\text{CH}_4 + \text{O} = \text{CH}_3 + \text{OH}$   
(302)  $\text{CH}_4 + \text{OH} = \text{CH}_3 + \text{H}_2\text{O}$   
(303)  $\text{CH}_4 + \text{HO}_2 = \text{CH}_3 + \text{H}_2\text{O}_2$   
(304)  $\text{CH}_4 + \text{O}_2 = \text{CH}_3 + \text{HO}_2$   
(305)  $\text{CH}_4 + \text{CH} = \text{C}_2\text{H}_4 + \text{H}$   
(306)  $\text{CH}_4 + \text{tCH}_2 = \text{CH}_3 + \text{CH}_3$   
(307)  $\text{CH}_3\text{O}_2\text{H} = \text{CH}_3\text{O} + \text{OH}$   
(308)  $\text{CH}_3\text{O}_2\text{H} + \text{O} = \text{CH}_3\text{O}_2 + \text{OH}$   
(309)  $\text{CH}_3\text{O}_2\text{H} + \text{OH} = \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$   
(310)  $\text{C}_2\text{H} + \text{O} = \text{CO} + \text{CH}$   
(311)  $\text{C}_2\text{H} + \text{O}_2 = \text{HCCO} + \text{O}$   
(312)  $\text{C}_2\text{H} + \text{O}_2 = \text{CO}_2 + \text{CH}$   
(313)  $\text{C}_2\text{H} + \text{CH}_4 = \text{C}_2\text{H}_2 + \text{CH}_3$   
(314)  $\text{HCCO} + \text{H} = \text{tCH}_2 + \text{CO}$   
(315)  $\text{HCCO} + \text{O} = \text{CO} + \text{CO} + \text{H}$   
(316)  $\text{HCCO} + \text{tCH}_2 = \text{C}_2\text{H}_3 + \text{CO}$   
(317)  $\text{C}_2\text{H}_2 + \text{X} = \text{C}_2\text{H} + \text{H} + \text{X}$   
(318)  $\text{C}_2\text{H}_2 + \text{H} = \text{C}_2\text{H} + \text{H}_2$   
(319)  $\text{C}_2\text{H}_2 + \text{O} = \text{tCH}_2 + \text{CO}$   
(320)  $\text{C}_2\text{H}_2 + \text{O} = \text{HCCO} + \text{H}$   
(321)  $\text{C}_2\text{H}_2 + \text{OH} = \text{C}_2\text{H} + \text{H}_2\text{O}$   
(322)  $\text{C}_2\text{H}_2 + \text{O}_2 = \text{HCCO} + \text{OH}$   
(323)  $\text{CH}_2\text{CO} + \text{X} = \text{tCH}_2 + \text{CO} + \text{X}$   
(324)  $\text{CH}_2\text{CO} + \text{H} = \text{CH}_3 + \text{CO}$   
(325)  $\text{CH}_2\text{CO} + \text{O} = \text{H}_2\text{CO} + \text{CO}$   
(326)  $\text{CH}_2\text{CO} + \text{O} = \text{HCO} + \text{CO} + \text{H}$   
(327)  $\text{CH}_2\text{CO} + \text{O} = \text{HCO} + \text{HCO}$   
(328)  $\text{CH}_2\text{CO} + \text{OH} = \text{CH}_3 + \text{CO}_2$   
(329)  $\text{CH}_2\text{CO} + \text{OH} = \text{H}_2\text{CO} + \text{HCO}$   
(330)  $\text{C}_2\text{H}_3 + \text{X} = \text{C}_2\text{H}_2 + \text{H} + \text{X}$   
(331)  $\text{C}_2\text{H}_3 + \text{H} = \text{C}_2\text{H}_2 + \text{H}_2$   
(332)  $\text{C}_2\text{H}_3 + \text{O} = \text{C}_2\text{H}_2 + \text{OH}$   
(333)  $\text{C}_2\text{H}_3 + \text{O} = \text{CH}_3 + \text{CO}$   
(334)  $\text{C}_2\text{H}_3 + \text{O} = \text{HCO} + \text{tCH}_2$   
(335)  $\text{C}_2\text{H}_3 + \text{OH} = \text{C}_2\text{H}_2 + \text{H}_2\text{O}$   
(336)  $\text{C}_2\text{H}_3 + \text{O}_2 = \text{H}_2\text{CO} + \text{HCO}$   
(337)  $\text{C}_2\text{H}_3 + \text{O}_2 = \text{CH}_2\text{CHO} + \text{O}$   
(338)  $\text{CH}_3\text{CO} + \text{H} = \text{CH}_2\text{CO} + \text{H}_2$   
(339)  $\text{CH}_2\text{CHO} + \text{H} = \text{CH}_2\text{CO} + \text{H}_2$   
(340)  $\text{C}_2\text{H}_3 + \text{O}_2 = \text{C}_2\text{H}_2 + \text{HO}_2$   
(341)  $\text{C}_2\text{H}_4 + \text{X} = \text{C}_2\text{H}_2 + \text{H}_2 + \text{X}$   
(342)  $\text{C}_2\text{H}_4 + \text{X} = \text{C}_2\text{H}_3 + \text{H} + \text{X}$   
(343)  $\text{C}_2\text{H}_4 + \text{H} + \text{X} = \text{C}_2\text{H}_5 + \text{X}$   
(344)  $\text{C}_2\text{H}_4 + \text{H} = \text{C}_2\text{H}_3 + \text{H}_2$   
(345)  $\text{C}_2\text{H}_4 + \text{O} = \text{CH}_2\text{CHO} + \text{H}$   
(346)  $\text{C}_2\text{H}_4 + \text{O} = \text{HCO} + \text{CH}_3$   
(347)  $\text{C}_2\text{H}_4 + \text{O} = \text{CH}_2\text{CO} + \text{H}_2$   
(348)  $\text{C}_2\text{H}_4 + \text{OH} = \text{C}_2\text{H}_3 + \text{H}_2\text{O}$   
(349)  $\text{C}_2\text{H}_4 + \text{OH} = \text{CH}_3\text{CHO} + \text{H}$   
(350)  $\text{C}_2\text{H}_4 + \text{OH} = \text{H}_2\text{CO} + \text{CH}_3$   
(351)  $\text{C}_2\text{H}_4 + \text{CH}_3 = \text{C}_2\text{H}_3 + \text{CH}_4$   
(352)  $\text{CH}_3\text{CHO} + \text{X} = \text{CH}_3 + \text{HCO} + \text{X}$   
(353)  $\text{CH}_3\text{CHO} + \text{H} = \text{CH}_3\text{CO} + \text{H}_2$   
(354)  $\text{CH}_3\text{CHO} + \text{H} = \text{CH}_2\text{CHO} + \text{H}_2$   
(355)  $\text{CH}_3\text{CHO} + \text{O} = \text{CH}_3\text{CO} + \text{OH}$   
(356)  $\text{CH}_3\text{CHO} + \text{O} = \text{CH}_2\text{CHO} + \text{OH}$   
(357)  $\text{CH}_3\text{CHO} + \text{OH} = \text{CH}_2\text{CHO} + \text{H}_2\text{O}$   
(358)  $\text{CH}_3\text{CHO} + \text{OH} = \text{CH}_3\text{CO} + \text{H}_2\text{O}$   
(359)  $\text{CH}_3\text{CHO} + \text{HO}_2 = \text{CH}_3\text{CO} + \text{H}_2\text{O}_2$   
(360)  $\text{CH}_3\text{CHO} + \text{O}_2 = \text{CH}_3\text{CO} + \text{HO}_2$   
(361)  $\text{CH}_3\text{CHO} + \text{tCH}_2 = \text{CH}_3\text{CO} + \text{CH}_3$   
(362)  $\text{CH}_3\text{CHO} + \text{CH}_3 = \text{CH}_3\text{CO} + \text{CH}_4$   
(363)  $\text{C}_2\text{H}_5 + \text{X} = \text{C}_2\text{H}_4 + \text{H} + \text{X}$   
(364)  $\text{C}_2\text{H}_5 + \text{H} = \text{CH}_3 + \text{CH}_3$   
(365)  $\text{C}_2\text{H}_5 + \text{O} = \text{CH}_3\text{CHO} + \text{H}$   
(366)  $\text{C}_2\text{H}_5 + \text{O} = \text{H}_2\text{CO} + \text{CH}_3$   
(367)  $\text{C}_2\text{H}_5 + \text{OH} = \text{C}_2\text{H}_5\text{OH}$   
(368)  $\text{C}_2\text{H}_5 + \text{O}_2 = \text{C}_2\text{H}_4 + \text{HO}_2$   
(369)  $\text{C}_2\text{H}_5 + \text{CH}_3 = \text{C}_2\text{H}_4 + \text{CH}_4$   
(370)  $\text{C}_2\text{H}_5 + \text{C}_2\text{H}_5 = \text{C}_2\text{H}_4 + \text{C}_2\text{H}_6$   
(371)  $\text{C}_2\text{H}_5\text{O} = \text{CH}_3\text{CHO} + \text{H}$   
(372)  $\text{C}_2\text{H}_5\text{O} = \text{H}_2\text{CO} + \text{CH}_3$   
(373)  $\text{C}_2\text{H}_5\text{O} + \text{H} = \text{CH}_3\text{CHO} + \text{H}_2$   
(374)  $\text{C}_2\text{H}_5\text{O} + \text{O} = \text{CH}_3\text{CHO} + \text{OH}$   
(375)  $\text{C}_2\text{H}_5\text{O} + \text{OH} = \text{CH}_3\text{CHO} + \text{H}_2\text{O}$   
(376)  $\text{C}_2\text{H}_5\text{O} + \text{O}_2 = \text{CH}_3\text{CHO} + \text{HO}_2$   
(377)  $\text{CH}_3\text{CHOH} = \text{CH}_3\text{CHO} + \text{H}$   
(378)  $\text{CH}_3\text{CHOH} + \text{H} = \text{CH}_3\text{CHO} + \text{H}_2$   
(379)  $\text{CH}_3\text{CHOH} + \text{O} = \text{CH}_3\text{CHO} + \text{OH}$   
(380)  $\text{CH}_3\text{CHOH} + \text{OH} = \text{CH}_3\text{CHO} + \text{H}_2\text{O}$   
(381)  $\text{CH}_3\text{CHOH} + \text{O}_2 = \text{CH}_3\text{CHO} + \text{HO}_2$   
(382)  $\text{CH}_2\text{CH}_2\text{OH} = \text{C}_2\text{H}_4 + \text{OH}$   
(383)  $\text{CH}_2\text{CH}_2\text{OH} + \text{H} = \text{CH}_3\text{CHO} + \text{H}_2$   
(384)  $\text{C}_2\text{H}_5\text{OH} = \text{CH}_3 + \text{CH}_2\text{OH}$   
(385)  $\text{C}_2\text{H}_5\text{OH} = \text{C}_2\text{H}_4 + \text{H}_2\text{O}$   
(386)  $\text{C}_2\text{H}_5\text{OH} + \text{H} = \text{CH}_3\text{CHOH} + \text{H}_2$   
(387)  $\text{C}_2\text{H}_5\text{OH} + \text{H} = \text{C}_2\text{H}_5 + \text{H}_2\text{O}$   
(388)  $\text{C}_2\text{H}_5\text{OH} + \text{O} = \text{CH}_3\text{CHOH} + \text{OH}$   
(389)  $\text{C}_2\text{H}_5\text{OH} + \text{O} = \text{C}_2\text{H}_5\text{O} + \text{OH}$   
(390)  $\text{C}_2\text{H}_5\text{OH} + \text{O} = \text{CH}_2\text{CH}_2\text{OH} + \text{OH}$

- (391)  $C_2H_5OH + OH = CH_3CHOH + H_2O$   
(392)  $C_2H_5OH + OH = C_2H_5O + H_2O$   
(393)  $C_2H_5OH + OH = CH_2CH_2OH + H_2O$   
(394)  $C_2H_5OH + HO_2 = CH_3CHOH + H_2O_2$   
(395)  $C_2H_5OH + CH_3 = CH_3CHOH + CH_4$   
(396)  $C_2H_5OH + CH_3 = CH_2CH_2OH + CH_4$   
(397)  $C_2H_5OH + CH_3 = C_2H_5O + CH_4$   
(398)  $C_2H_5OH + CH_3O = CH_3CHOH + CH_3OH$   
(399)  $C_2H_5OH + H_2CO = C_2H_5O + CH_3O$   
(400)  $C_2H_5OH + C_2H_5O = C_2H_5OH + CH_3CHOH$   
(401)  $C_2H_6 + H = C_2H_5 + H_2$   
(402)  $C_2H_6 + O = C_2H_5 + OH$   
(403)  $C_2H_6 + OH = C_2H_5 + H_2O$   
(404)  $C_2H_6 + HO_2 = C_2H_5 + H_2O_2$   
(405)  $C_2H_6 + O_2 = C_2H_5 + HO_2$   
(406)  $C_2H_6 + tCH_2 = C_2H_5 + CH_3$   
(407)  $C_2H_6 + CH_3 = C_2H_5 + CH_4$   
(408)  $C_2H_6 + CH = C_2H_4 + CH_3$   
(409)  $CH_3O + X = H_2CO + H + X$   
(410)  $CH_2OH + X = H_2CO + H + X$   
(411)  $CH_3O_2 + HO_2 = O_2 + CH_3O_2H$   
(412)  $CH_3O_2 + CH_3 = CH_3O + CH_3O$   
(413)  $CH_3O_2 + CH_3O_2 = H_2CO + CH_3OH + O_2$   
(414)  $CH_3O_2 + CH_3O_2 = CH_3O + CH_3O + O_2$   
(415)  $CH_3O_2 + H_2O_2 = CH_3O_2H + HO_2$   
(416)  $CH_3O_2 + H_2CO = HCO + CH_3O_2H$   
(417)  $CH_3O_2 + CH_4 = CH_3 + CH_3O_2H$   
(418)  $CH_3O_2 + CH_3OH = CH_2OH + CH_3O_2H$   
(419)  $CH_4 + X = CH_3 + H + X$   
(420)  $SO_2 + NO_2 = SO_3 + NO$   
(421)  $SO_2 + CO = SO + CO_2$   
(422)  $SO + O_2 = SO_2 + O$   
(423)  $SO + SO_3 = SO_2 + SO_2$   
(424)  $SO + NO_2 = SO_2 + NO$   
(425)  $SO_2 + NO_3 = SO_3 + NO_2$   
(426)  $SO_3 + N_2 = SO_2 + O + N_2$   
(427)  $SO_2 + SO_2 = SO + SO_3$   
(428)  $SO_3 + NO_2 = SO_2 + NO_3$