Supplementary Materials:

Article

DFT Study on Two Mechanisms of the N_2O Direct Catalytic Decomposition over Cu-ZSM-5

Congru Gao, Jianwei Li * and Jie Zhang * and Xiuliang Sun

State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing 100029, China; gaocr@mail.buct.edu.cn (C.G.); sunxl@mail.buct.edu.cn (X.S.)

* Correspondence: lijw@mail.buct.edu.cn (J.L.); zhangjie@mail.buct.edu.cn (J.Z.); Tel: +86-1361-105-3831 (J.L.); +86-1800-113-7991 (J.Z.)

Received: 23 April 2020; Accepted: 6 June 2020; Published: date

Abstract: Nitrous oxide (N_2O) is an industrial emission that causes the greenhouse effect a

Table S1. Structural parameters (diameter in Å, angle in o) of optimized models.

	Model	Cu-O1	O1-N1	N1-N2			∠O1-N1-N2
Part A1	**Cu-Z-N_2O**	**2.05**	**1.21**	**1.13**	**-**	**-**	**177.9**
	Cu-Z-N_2O-TS	**1.75**	**1.80**	**1.11**	**-**	**-**	**143.7**
	Cu-O-Z-N_2	**1.70**	**2.65**	**1.10**	**-**	**-**	**-**
	Cu-O-Z	**1.70**	**-**	**-**	**-**	**-**	**-**
	N_2O	**-**	**1.19**	**1.13**	**-**	**-**	**180.0**
	N_2	**-**	**-**	**1.11**	**-**	**-**	**-**
	Model	**Cu-O1**	**Cu-O2**	**O1-O2**	**O2-N3**	**N3-N4**	**∠O2-N3-N4**
Part A2	Cu-O-Z-N_2O	1.71	3.36	2.28	1.20	1.13	179.8
	Cu-O-Z-N_2O-TS	1.73	1.90	2.00	1.47	1.12	149.6
	Cu-O_2-Z-N_2	1.87	1.87	1.33	3.30	1.10	140.8
	Cu-O_2-Z	1.86	1.86	1.33	-	-	-
	O_2	-	-	1.22	-	-	-
	Model	**Cu-O1**	**O1-N4**	**N4-N3**	**N3-O2**		**∠O2-N3-N4**
Part B1	Cu-O-Z-N_2O'	1.71	2.32	1.14	1.19	-	179.9
	Cu-O-Z-N_2O'-TS1	1.76	1.74	1.15	1.18	-	179.7
	Cu-Z-$(NO)_2$	1.94	1.25	1.21	1.20	-	145.3
Part B2	Cu-O-Z-N_2O'-TS2	1.91	1.24	1.34	1.19	-	125.8
	Cu-Z-NO-NO	1.92	1.20	1.75	1.16	-	108.6
	Model	**Cu-O1**	**O1-N1**	**-**	**-**	**-**	**-**
Part B3	Cu-Z-NO	1.96	1.17	-	-	-	-
	NO	-	1.16	-	-	-	-

Table S2. Energy results of each step for O_2 formation mechanism and NO formation mechanism.

	Reaction steps	ΔE / kcal·mol^{-1}	*ΔH$_r$/ kcal·mol^{-1}
O_2 formation mechanism (Part A)	A1	-10.12	-8.67
	A2	33.08	33.40
	A3	-2.81	-1.81
	A4	0.45	-0.96
	A5	-3.17	-0.65
	A6	28.61	26.09
	A7	-80.45	-78.92
	A8	1.31	-0.52
	A9	33.59	38.32
NO formation mechanism (Part B)	B1	-2.82	-0.32
	B2	0.79	0.35
	B3	-14.39	-15.00
	B4	2.43	1.89
	B5	-9.12	-7.29
	B6	-3.93	-2.95

*The enthalpy values were calculated under the condition of 1.0 atm and 298.15K.