Supporting Information for

"Catalytic Reduction of Nitrous Oxide by the Low-Symmetry Pt_8 Cluster."

Erendida Hernández[1], Virineya Bertin[1*], Jorge R. Soto[2], Alan Miralrio[3] and Miguel Castro[3]*

[1]Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, San Rafael Atlixco 186, Col. Vicentina, México, D. F. 09340, México.
[2]Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México (UNAM), CP 04510, México, D. F, México.
[3]Departamento de Física y Química Teórica, DEPg. Facultad de Química, UNAM, Del. Coyoacán, México D.F., 04510, México

Figure S1. Optimized *atop* adsorption configurations of the N_2O molecule on the different non-equivalent sites of Pt_8 cluster.

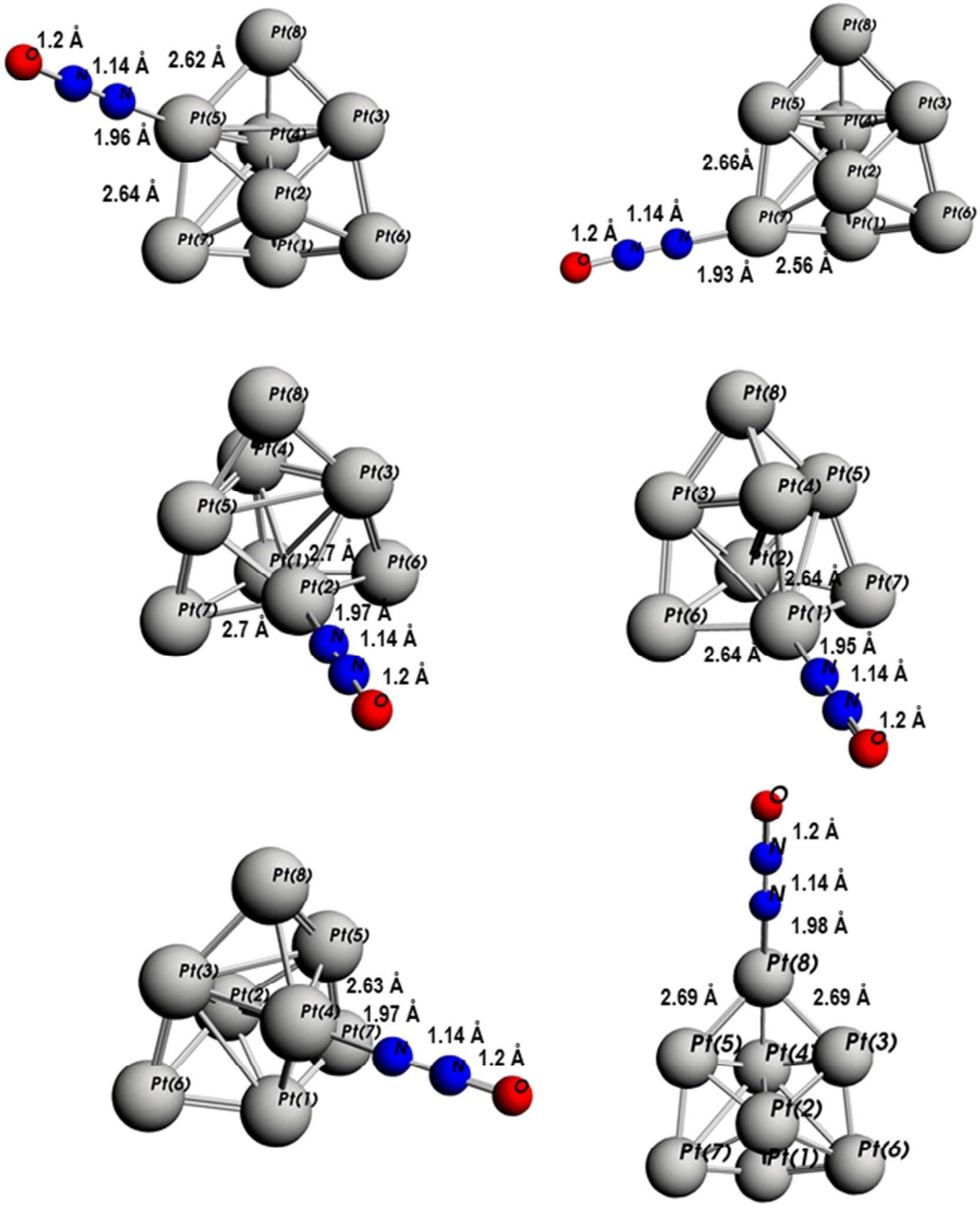

Figure S2. Transition structures (TS1), *bridge* local minima, and transition structures (TS2) for the reaction pathways starting from the site **5**. Only non-desorption configurations are presented.

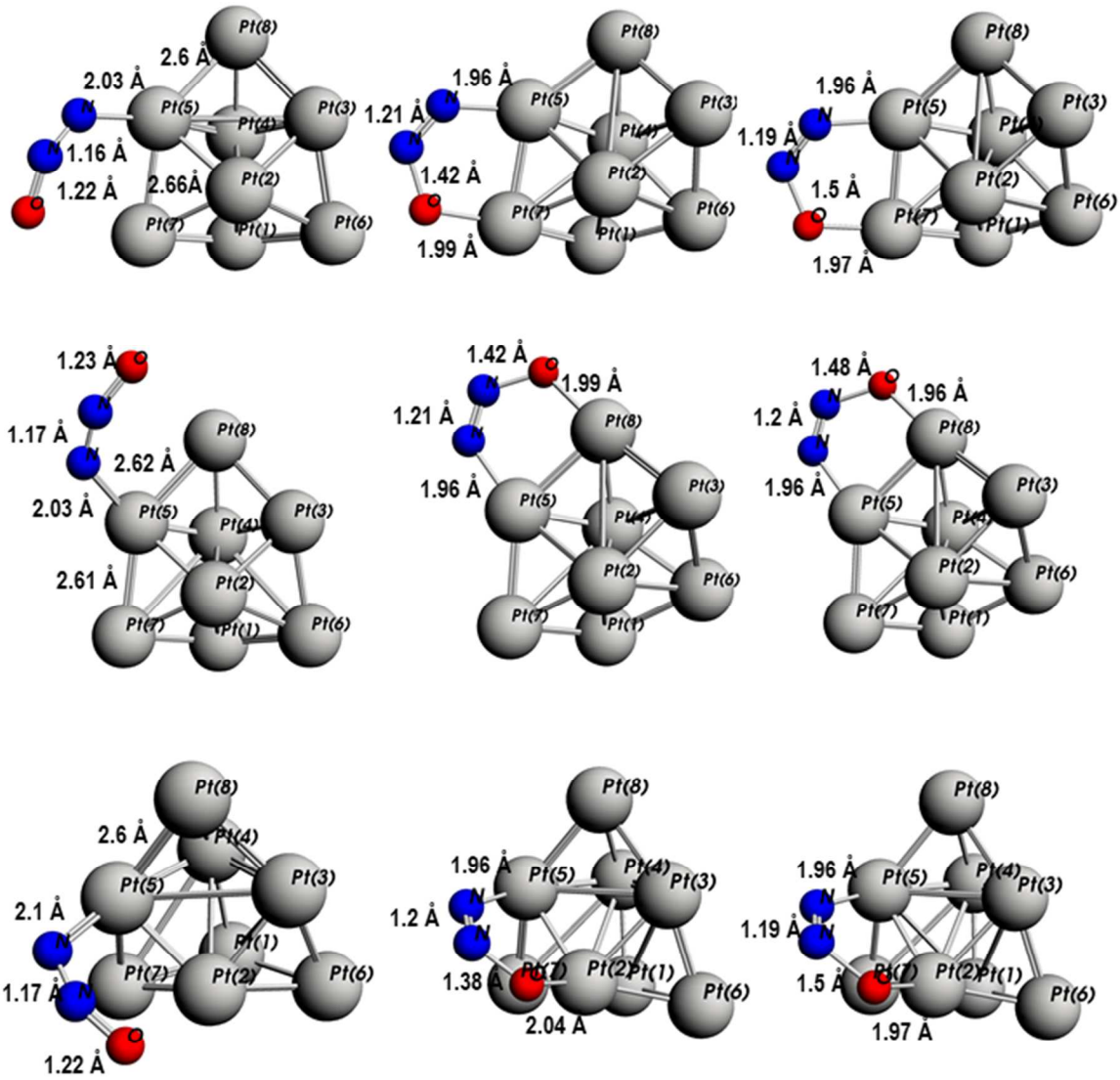

Figure S3. Transition structures (TS1), *bridge* local minima, and transition structures (TS2) for the reaction pathways starting from the site **7**. Only non-desorption configurations are presented.

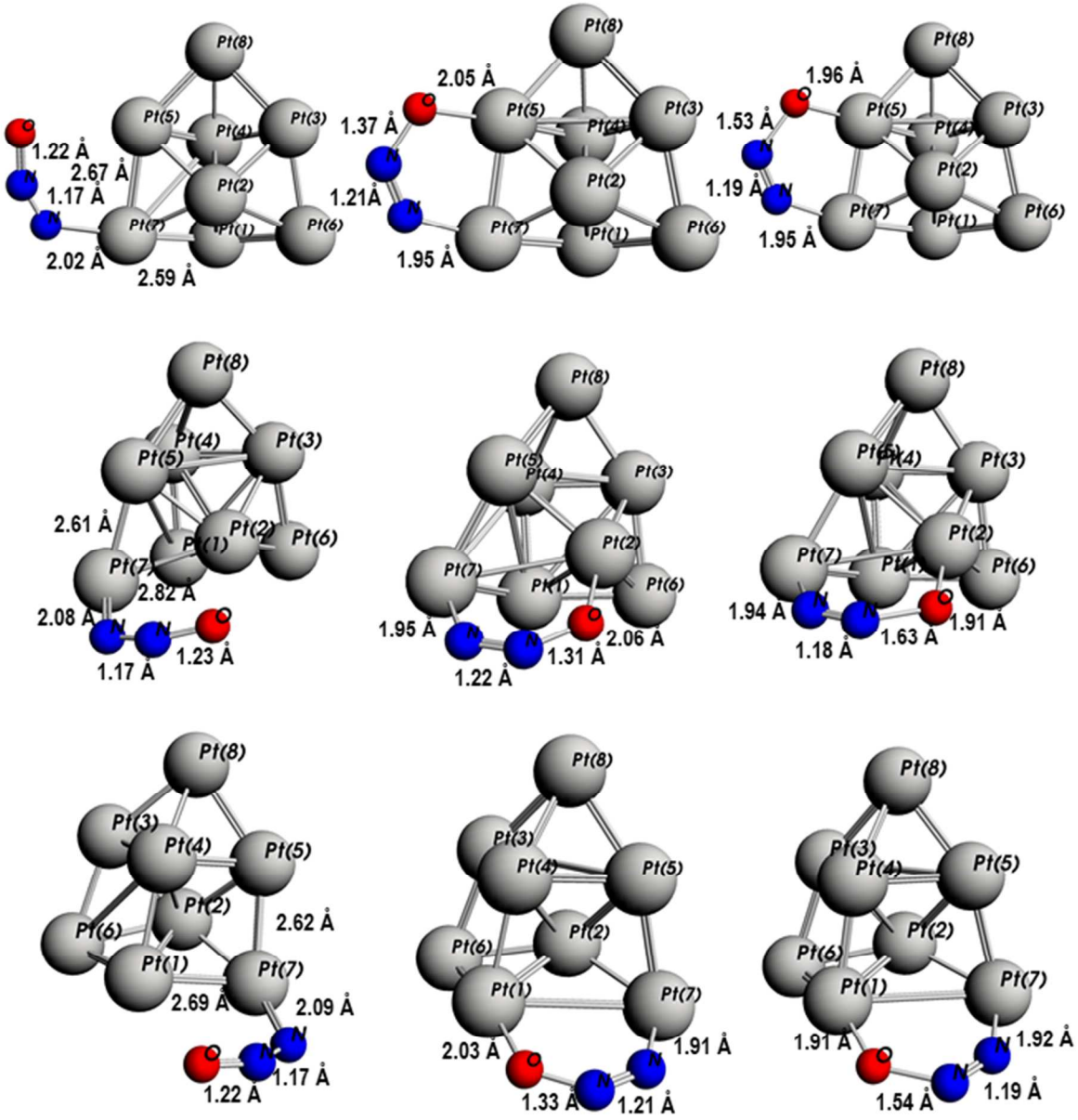

Figure S4. Transition structures (TS1), *bridge* local minima, and transition structures (TS2) for the reaction pathways starting from the sites **2** and **4**. Only non-desorption configurations are presented.

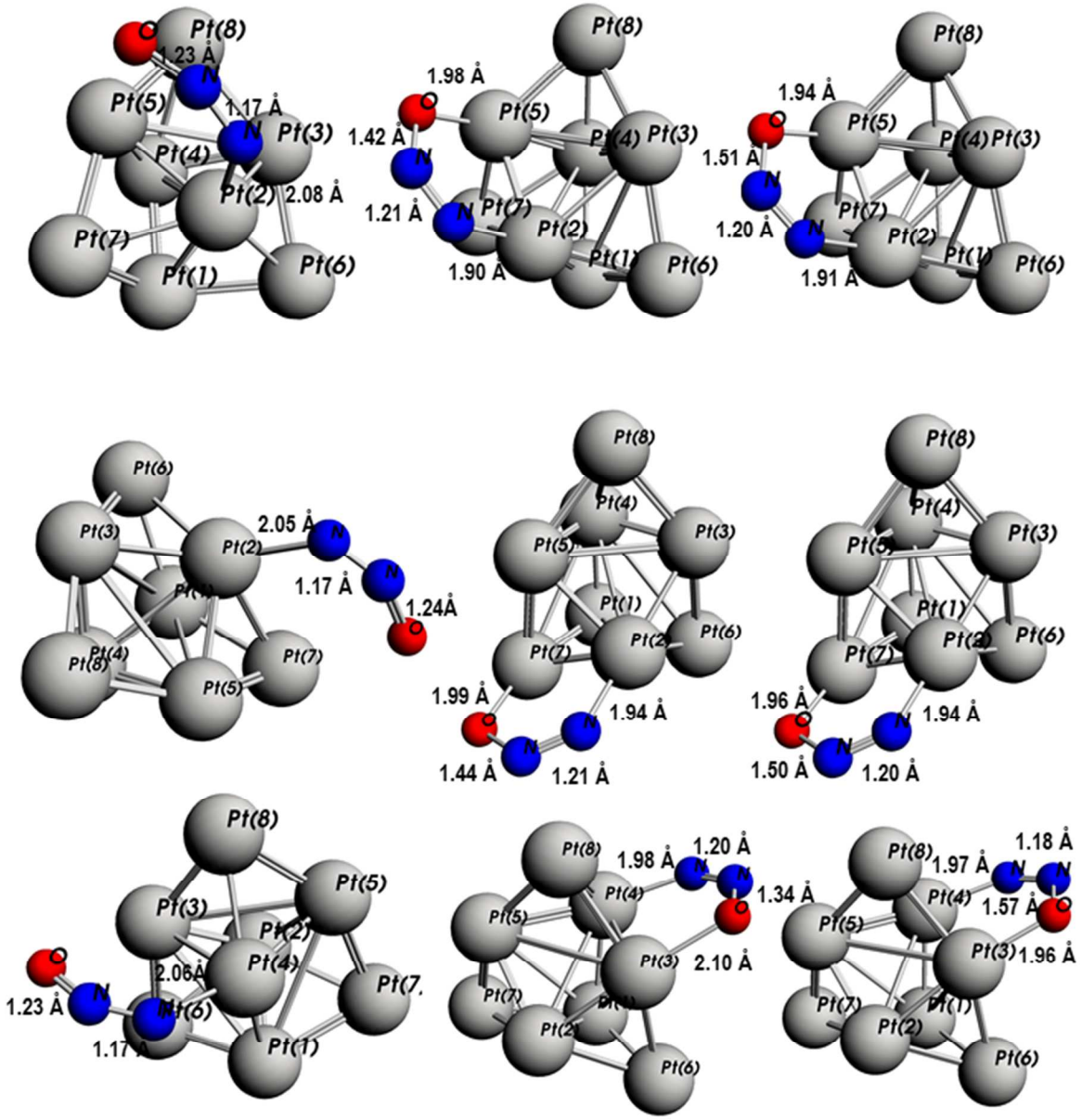

Figure S5. Transition structures (TS1) prior to spontaneous dissociation. Non-*bridge* formation cases.

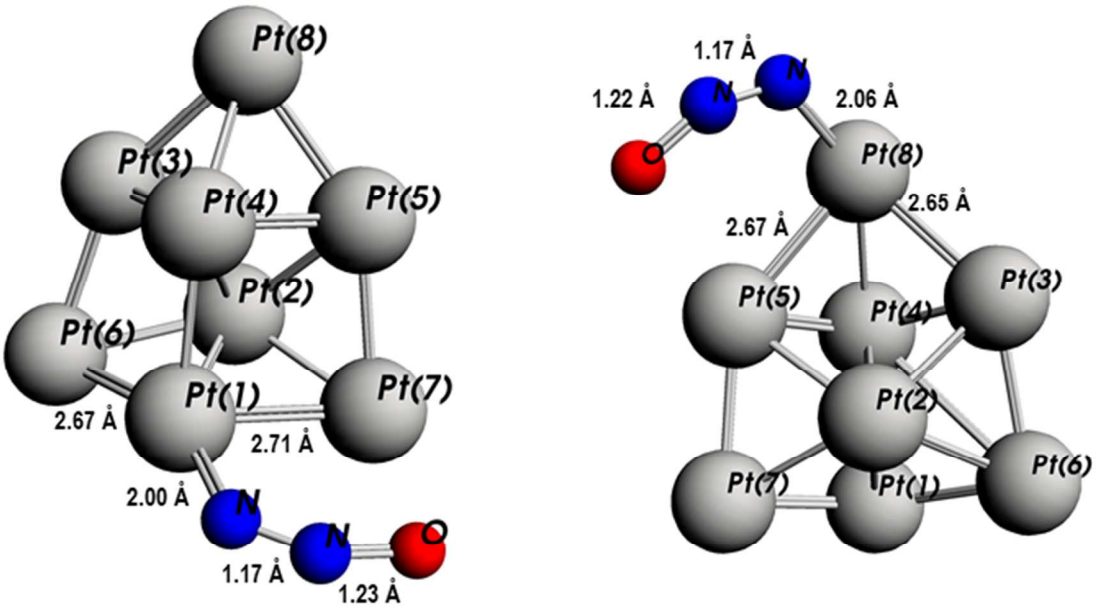

Figure S6. Evolution of the N-N-O structural parameters and Pt8 to N_2O charge transfer for the stages of the 7-2 reaction pathway.

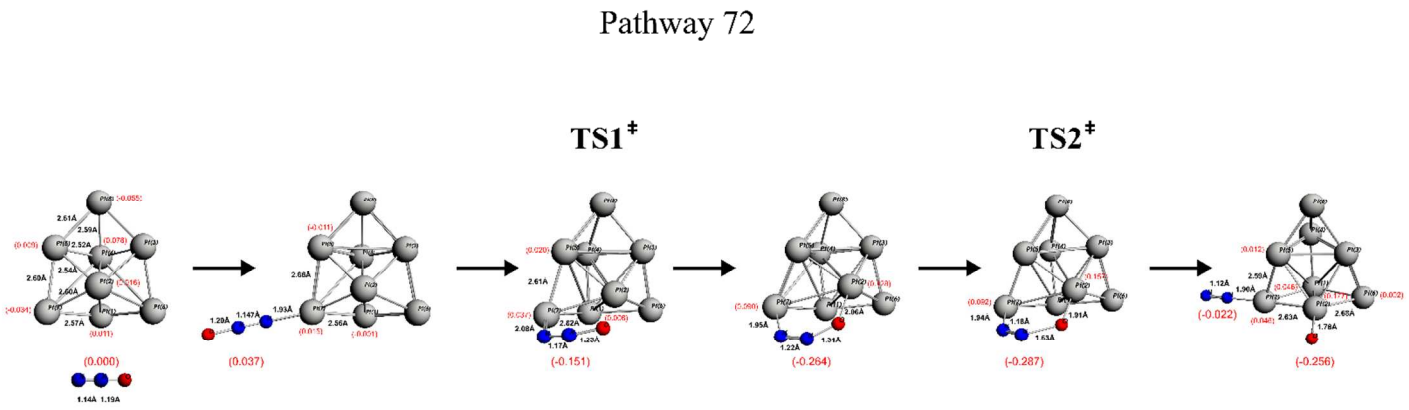

Table S1. Reaction released energy E_r, computed for O adsorbed on Pt_8 with different adsorption configuration and non-equivalent sites

adsorption configuration	Sites	E_r(kcal/mol)
Atop	**8**	-38.79
	4	-34.30
	2	-28.27
	5	-34.95
	7	-40.65
Bridge	**4-8**	-32.57
	5-8	-35.73
	2-5	-44.28
	1-4	-44.28
	2-7	-34.06
	3-6	-43.70

Table S2. Hirshfeld charges of the complex $Pt_8 + N_2O$ as a function of the reaction stage corresponding to the B57 reaction pathway.

stage	# atom	Hirshfeld q	stage	# atom	Hirshfeld q
1	Pt1	0.0109	4	Pt1	-0.0068
1	Pt2	0.0161	4	Pt2	0.0476
1	Pt3	0.0090	4	Pt3	0.0074
1	Pt4	0.0777	4	Pt4	0.0403
1	Pt5	0.0090	4	Pt5	0.1274
1	Pt6	-0.0339	4	Pt6	-0.0057
1	Pt7	-0.0339	4	Pt7	0.1054
1	Pt8	-0.0549	4	Pt8	-0.0144
1	N9	-0.0840	4	N9	-0.1207
1	N10	0.1960	4	N10	0.0021
1	O11	-0.1120	4	O11	-0.1827
2	Pt1	0.0035	5	Pt1	-0.0094
2	Pt2	-0.0044	5	Pt2	0.0464
2	Pt3	-0.0094	5	Pt3	0.0095
2	Pt4	0.0249	5	Pt4	0.0407
2	Pt5	0.0695	5	Pt5	0.1259
2	Pt6	-0.0254	5	Pt6	-0.0050
2	Pt7	-0.0324	5	Pt7	0.1119
2	Pt8	-0.0579	5	Pt8	-0.0150
2	N9	-0.0554	5	N9	-0.1131
2	N10	0.1935	5	N10	0.0001
2	O11	-0.1064	5	O11	-0.1920
3	Pt1	0.0170	6	Pt1	0.0203
3	Pt2	0.0195	6	Pt2	0.0290
3	Pt3	0.0043	6	Pt3	0.0101
3	Pt4	0.0532	6	Pt4	0.0305
3	Pt5	0.0849	6	Pt5	0.0754
3	Pt6	-0.0274	6	Pt6	-0.0120
3	Pt7	-0.0045	6	Pt7	0.1515
3	Pt8	-0.0455	6	Pt8	-0.0315
3	N9	-0.1010	6	N9	0.0091
3	N10	0.1311	6	N10	-0.0131
3	O11	-0.1316	6	O11	-0.2692

Table S3. Hirshfeld charges of the complex $Pt_8 + N_2O$ as a function of the reaction stage corresponding to the B72 reaction pathway. .

stage	# atom	Hirshfeld q	stage	# atom	Hirshfeld q
1	Pt1	0.0109	4	Pt1	0.0068
1	Pt2	0.0161	4	Pt2	0.1281
1	Pt3	0.0090	4	Pt3	0.0238
1	Pt4	0.0777	4	Pt4	0.0788
1	Pt5	0.0090	4	Pt5	0.0213
1	Pt6	-0.0339	4	Pt6	-0.0350
1	Pt7	-0.0339	4	Pt7	0.0898
1	Pt8	-0.0549	4	Pt8	-0.0493
1	N9	-0.0840	4	N9	-0.1322
1	N10	0.1960	4	N10	0.0251
1	O11	-0.1120	4	O11	-0.1573
2	Pt1	-0.0014	5	Pt1	0.0046
2	Pt2	0.0127	5	Pt2	0.1574
2	Pt3	0.0092	5	Pt3	0.0126
2	Pt4	0.0056	5	Pt4	0.0577
2	Pt5	-0.0113	5	Pt5	0.0289
2	Pt6	-0.0282	5	Pt6	-0.0281
2	Pt7	0.0146	5	Pt7	0.0921
2	Pt8	-0.0374	5	Pt8	-0.0370
2	N9	-0.0560	5	N9	-0.0817
2	N10	0.1945	5	N10	0.0015
2	O11	-0.1022	5	O11	-0.2081
3	Pt1	0.0061	6	Pt1	-0.0093
3	Pt2	0.0854	6	Pt2	0.1773
3	Pt3	0.0222	6	Pt3	0.0273
3	Pt4	0.0826	6	Pt4	0.0427
3	Pt5	0.0202	6	Pt5	0.0117
3	Pt6	-0.0543	6	Pt6	0.0023
3	Pt7	0.0366	6	Pt7	0.0460
3	Pt8	-0.0484	6	Pt8	-0.0200
3	N9	-0.1156	6	N9	0.0020
3	N10	0.1119	6	N10	-0.0242
3	O11	-0.1456	6	O11	-0.2557

Table S4. Hirshfeld charges of the complex $Pt_8 + N_2O$ as a function of the reaction stage corresponding to the B85 reaction pathway (zero values for non-existent stage).

stage	# atom	Hirshfeld q	stage	# atom	Hirshfeld q
1	Pt1	0.0109	4	Pt1	0.0000
1	Pt2	0.0161	4	Pt2	0.0000
1	Pt3	0.0090	4	Pt3	0.0000
1	Pt4	0.0777	4	Pt4	0.0000
1	Pt5	0.0090	4	Pt5	0.0000
1	Pt6	-0.0339	4	Pt6	0.0000
1	Pt7	-0.0339	4	Pt7	0.0000
1	Pt8	-0.0549	4	Pt8	0.0000
1	N9	-0.0840	4	N9	0.0000
1	N10	0.1960	4	N10	0.0000
1	O11	-0.1120	4	O11	0.0000
2	Pt1	-0.0233	5	Pt1	0.0000
2	Pt2	0.0165	5	Pt2	0.0000
2	Pt3	0.0035	5	Pt3	0.0000
2	Pt4	0.0454	5	Pt4	0.0000
2	Pt5	0.0035	5	Pt5	0.0000
2	Pt6	-0.0256	5	Pt6	0.0000
2	Pt7	-0.0256	5	Pt7	0.0000
2	Pt8	-0.0155	5	Pt8	0.0000
2	N9	-0.0609	5	N9	0.0000
2	N10	0.1909	5	N10	0.0000
2	O11	-0.1090	5	O11	0.0000
3	Pt1	0.0012	6	Pt1	-0.0059
3	Pt2	0.0228	6	Pt2	0.0195
3	Pt3	0.0052	6	Pt3	0.0094
3	Pt4	0.0631	6	Pt4	0.0130
3	Pt5	0.0424	6	Pt5	0.1935
3	Pt6	-0.0236	6	Pt6	0.0055
3	Pt7	-0.0163	6	Pt7	0.0209
3	Pt8	0.0217	6	Pt8	0.0308
3	N9	-0.1052	6	N9	0.0024
3	N10	0.1253	6	N10	-0.0226
3	O11	-0.1367	6	O11	-0.2665