SUPPLEMENTARY MATERIAL

Supporting Information

"Three types of adsorptions of nitric oxide on the MgO surface"
by Yasunori Yanagisawa, Kei Kuramoto and Shinichi Yamabe

== Cartesian coordinates, frequencies and other key information obtained by *ab initio* calculations of GAUSSIAN94 ==

Coordinates are in Angstrom. Frequencies are in cm^{-1}.

(1) The geometry of $(MgO)_5NO$ in Figure 3

#N Geom=AllCheck Guess=Read Test UB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-0.398931	-0.097231	-0.052806
2	12	-0.555103	-0.079174	1.921043
3	12	-0.675323	1.863174	-0.092955
4	12	-0.249520	-0.117276	-2.026056
5	12	-0.126550	-2.059004	-0.012601
6	12	1.555772	0.181053	0.095839
7	8	1.404024	0.199709	2.070228
8	8	1.280348	2.141805	0.056108
9	8	1.707713	0.161397	-1.879228
10	8	1.831159	-1.779791	0.136233
11	7	-3.006095	-0.790966	-0.130720
12	8	-3.117895	0.383048	-0.044058

200 basis functions 456 primitive gaussians
58 alpha electrons 57 beta electrons

nuclear repulsion energy 1100.6757997366 Hartrees.

SCF Done: E(UB+HF-LYP) = -1506.46857462 A.U.
Convg = 0.6492D-08 -V/T = 2.0056
S**2 = 0.7520

	1	2	3
Frequencies --	25.0695	59.9301	83.8436
	4	5	6
Frequencies --	85.8187	101.5315	108.1161
	7	8	9
Frequencies --	123.1196	151.1667	163.1884
	10	11	12
Frequencies --	177.8363	200.6993	213.5461
	13	14	15
Frequencies --	254.0339	268.6573	301.2733
	16	17	18
Frequencies --	305.7901	319.2166	379.2824
	19	20	21

Frequencies --	384.9477	416.6182	448.0335
	22	23	24
Frequencies --	466.0929	484.9863	500.1420
	25	26	27
Frequencies --	529.4463	550.9950	564.2255
	28	29	30
Frequencies --	573.8272	610.2162	1630.5065

(2) The geometry of NO in Figure 4

#N Geom=AllCheck Guess=Read Test UB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.000000	0.000000	-0.617971
2	8	0.000000	0.000000	0.540725

30 basis functions 56 primitive gaussians
8 alpha electrons 7 beta electrons

nuclear repulsion energy 25.5752320521 Hartrees.

SCF Done: E(UB+HF-LYP) = -129.888155459 A.U.
Convg = 0.1200D-08 -V/T = 2.0088
S**2 = 0.7525

	1
Frequencies --	1991.6638

(3) The geometry of (MgO)NO in Figure 4

#N Geom=AllCheck Guess=Read Test UB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	12	-1.329208	-0.000083	0.000096
2	8	0.481039	-1.059687	-0.000258
3	7	1.179389	0.000028	0.000426
4	8	0.480809	1.059787	-0.000258

64 basis functions 136 primitive gaussians
18 alpha electrons 17 beta electrons

nuclear repulsion energy 128.8341250188 Hartrees.

SCF Done: E(UB+HF-LYP) = -405.226897377 A.U.
Convg = 0.2049D-08 -V/T = 2.0063
S**2 = 0.7507

	1	2	3
Frequencies --	235.2261	293.4060	397.5278
	4	5	6
Frequencies --	875.7921	1294.5995	1338.0748

(4) The geometry of $(MgO)_3NO$ in Figure 4

#N Geom=AllCheck Guess=Read Test UB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	12	0.239193	0.046565	1.124207
2	8	0.035037	-1.029021	2.738915
3	8	1.801617	0.480930	0.294588
4	12	3.158851	0.211745	1.507143
5	7	-0.626101	0.248336	3.119343
6	8	-0.032970	0.705768	4.188654
7	12	1.568648	-0.482401	3.938337
8	8	3.261535	-0.269367	3.268270

132 basis functions 296 primitive gaussians
38 alpha electrons 37 beta electrons

nuclear repulsion energy 502.3051966051 Hartrees.

SCF Done: E(UB+HF-LYP) = -956.021956327 A.U.
Convg = 0.2071D-08 -V/T = 2.0057
S**2 = 0.7542

	1	2	3
Frequencies --	107.5454	131.4772	158.8314
	4	5	6
Frequencies --	174.8610	192.9156	236.2251
	7	8	9
Frequencies --	294.6309	338.4658	365.4025
	10	11	12
Frequencies --	398.0211	486.8550	574.5140
	13	14	15
Frequencies --	646.0879	686.8659	774.9024
	16	17	18
Frequencies --	801.0833	817.1333	1249.1993

(5) The geometry of $(MgO)_4NO$ in Figure 4

#N Geom=AllCheck Guess=Read Test UB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	1.025830	-1.090285	0.007110
2	12	0.766807	1.223781	-0.000635
3	12	-0.422562	-0.914622	-1.361028
4	8	-0.560459	1.008059	-1.441130
5	12	-0.428301	-0.906204	1.366775
6	8	-0.566348	1.017005	1.434586
7	12	-1.868970	0.801732	-0.005593
8	8	-1.787997	-1.164094	0.000574
9	7	2.520794	-0.734680	-0.000824
10	8	2.612817	0.565129	0.000303

166 basis functions 376 primitive gaussians
48 alpha electrons 47 beta electrons

nuclear repulsion energy 829.4482525723 Hartrees.

SCF Done: E(UB+HF-LYP) = -1231.47720828 A.U.
Convg = 0.8322D-08 -V/T = 2.0057
S**2 = 0.7540

	1	2	3
Frequencies --	104.4150	119.2741	127.4693
	4	5	6
Frequencies --	243.8821	286.4953	291.2030
	7	8	9
Frequencies --	308.2124	334.5386	398.6398
	10	11	12
Frequencies --	420.8165	442.4109	460.1222
	13	14	15
Frequencies --	461.7157	474.3162	487.7036
	16	17	18
Frequencies --	540.9847	559.6162	564.4763
	19	20	21
Frequencies --	580.2094	586.2409	589.6684
	22	23	24
Frequencies --	614.2677	730.0549	1249.7451

(6) The geometry of $(MgO)_6NO$<a> in Figure 4

#N Geom=AllCheck Guess=Read Test UB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	8	0.452043	1.206773	0.000008
2	12	2.158218	-0.043644	0.001168
3	12	-0.280761	-0.303633	-1.519909
4	8	1.451571	-1.179688	-1.442403
5	12	-1.417865	1.803624	0.001907
6	8	-1.997208	0.655702	-1.445424
7	7	1.530735	2.425389	-0.000670
8	8	2.685684	1.883556	0.002183
9	12	-0.282510	-0.308383	1.520739
10	8	1.450332	-1.182798	1.441390
11	8	-1.997598	0.652366	1.446045
12	8	-1.007183	-1.638814	-0.001149
13	12	0.803390	-2.300400	-0.002304
14	12	-2.565162	-0.527105	-0.001644

234 basis functions 536 primitive gaussians
68 alpha electrons 67 beta electrons

nuclear repulsion energy 1534.9517678994 Hartrees.

SCF Done: E(UB+HF-LYP) = -1782.37453510 A.U.
Convg = 0.4373D-08 -V/T = 2.0057
S**2 = 0.7542

	1	2	3
Frequencies --	63.7778	120.6078	127.1034
	4	5	6
Frequencies --	170.1546	178.1266	224.5069
	7	8	9
Frequencies --	243.4224	251.0401	256.6798
	10	11	12
Frequencies --	265.0141	268.3745	285.7820
	13	14	15
Frequencies --	292.6117	307.2928	346.3119
	16	17	18
Frequencies --	363.5940	384.8370	427.0996
	19	20	21
Frequencies --	437.3904	448.1154	453.9126
	22	23	24
Frequencies --	477.2349	487.7501	493.9796
	25	26	27
Frequencies --	533.3001	543.3453	553.3168
	28	29	30
Frequencies --	580.0693	585.5963	590.7713
	31	32	33
Frequencies --	604.3334	617.7730	637.7970
	34	35	36
Frequencies --	721.6902	735.6568	1349.2450

(7) The geometry of $(MgO)_6NO$<b> in Figure 4

#N Geom=AllCheck Guess=Read Test UB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-0.243247	-0.125675	1.511382
2	12	1.465698	-0.985714	1.337935
3	12	0.119019	1.340043	-0.000206
4	8	2.487423	0.040193	-0.000070
5	12	-2.104152	0.450355	1.301815
6	8	-1.781229	1.839540	-0.000266
7	7	2.932052	1.475732	-0.000263
8	8	1.867905	2.228014	-0.000115
9	12	-0.826620	-1.563267	0.000158
10	8	0.968085	-2.299931	0.000324
11	8	-2.644352	-0.905131	0.000161
12	8	-0.243288	-0.126155	-1.511342
13	12	1.465699	-0.986141	-1.337699
14	12	-2.104205	0.449976	-1.301898

234 basis functions 536 primitive gaussians
68 alpha electrons 67 beta electrons

nuclear repulsion energy 1531.3084344873 Hartrees.

SCF Done: E(UB+HF-LYP) = -1782.37442222 A.U.
Convg = 0.6619D-08 -V/T = 2.0057
S**2 = 0.7540

	1	2	3
Frequencies --	77.1347	78.7989	104.6866
	4	5	6
Frequencies --	212.0951	221.8901	225.8353
	7	8	9
Frequencies --	247.0144	253.0840	259.8002
	10	11	12
Frequencies --	266.3202	283.5557	306.3567
	13	14	15
Frequencies --	314.5276	342.9976	367.0942
	16	17	18
Frequencies --	391.4154	406.0821	416.6785
	19	20	21
Frequencies --	420.5302	463.2002	463.3391
	22	23	24
Frequencies --	465.6398	478.7889	523.2131
	25	26	27
Frequencies --	529.0571	537.7631	568.6545
	28	29	30
Frequencies --	572.0007	587.1552	602.8125
	31	32	33
Frequencies --	610.3853	657.5981	674.7218
	34	35	36
Frequencies --	705.1525	746.2099	1254.6453

(8) The geometry of $(MgO)_6NO^-$ in Figure 5

#N Geom=AllCheck Guess=Read Test RB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-1.674769	-1.389774	-0.317683
2	12	-1.747813	0.795531	-0.098294
3	12	0.913474	0.442152	-1.667925
4	8	-0.608491	1.594502	-1.460464
5	12	0.218888	-2.106001	-0.043339
6	8	1.379237	-1.403180	-1.420028
7	7	-2.933919	-1.502633	0.082227
8	8	-3.480092	-0.352153	0.128191
9	12	0.758369	0.379131	1.725407
10	8	-0.740384	1.527449	1.401635
11	8	1.249459	-1.457927	1.453615
12	8	1.836304	1.075372	0.077919
13	12	0.365929	2.451477	0.041552
14	12	2.561763	-0.815281	0.085842

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234 basis functions 536 primitive gaussians
68 alpha electrons 68 beta electrons

nuclear repulsion energy 1486.2651174248 Hartrees.

SCF Done: E(RB+HF-LYP) = -1782.39662606 A.U.
Convg = 0.5320D-08 -V/T = 2.0057
S**2 = 0.0000

	1	2	3
Frequencies --	71.9148	103.7008	121.3171
	4	5	6
Frequencies --	147.6843	170.3519	200.9640
	7	8	9
Frequencies --	202.2895	222.4699	226.8614
	10	11	12
Frequencies --	244.7568	267.7306	270.6134
	13	14	15
Frequencies --	286.0544	297.6246	320.0965
	16	17	18
Frequencies --	322.4138	364.2471	366.7488
	19	20	21
Frequencies --	415.1876	418.5070	423.4694
	22	23	24
Frequencies --	430.4218	439.5697	451.7871
	25	26	27
Frequencies --	501.3966	519.5243	526.0236
	28	29	30
Frequencies --	540.3997	553.7664	562.2526
	31	32	33
Frequencies --	576.2815	639.6215	657.5096
	34	35	36
Frequencies --	831.7981	1020.5449	1266.5421

(9) The geometry of $(MgO)_4NO^+$ in Figure 6

#N Geom=AllCheck Guess=Read Test RB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-1.221991	-1.191433	0.005069
2	12	-0.633311	1.529048	-0.004009
3	12	0.407055	-0.923079	1.433706
4	8	0.542191	0.984503	1.412158
5	12	0.405182	-0.933976	-1.427675
6	8	0.537589	0.973018	-1.419122
7	12	1.902698	0.694747	-0.003842
8	8	1.629789	-1.254697	0.003486
9	7	-2.441877	-0.691049	0.001327
10	8	-2.473372	0.543168	-0.000023

166 basis functions 376 primitive gaussians
47 alpha electrons 47 beta electrons

nuclear repulsion energy 822.3372660367 Hartrees.

SCF Done: E(RB+HF-LYP) = -1231.26692969 A.U.
Convg = 0.5189D-08 -V/T = 2.0058
S**2 = 0.0000

	1	2	3
Frequencies --	103.2799	127.7332	152.6065
	4	5	6
Frequencies --	205.4779	230.2583	253.9561
	7	8	9
Frequencies --	285.5195	304.6221	327.6784
	10	11	12
Frequencies --	334.8990	387.6642	441.0145
	13	14	15
Frequencies --	455.8488	461.9679	540.5098
	16	17	18
Frequencies --	560.7510	575.4129	577.8084
	19	20	21
Frequencies --	593.3127	631.6140	637.9759
	22	23	24
Frequencies --	800.0474	1113.5726	1476.1409

(10) The geometry of $(MgO)_6NO^+$ in Figure 6

#N Geom=AllCheck Guess=Read Test RB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	1.420351	-1.390279	-0.000140
2	12	1.888548	0.800539	-0.000065
3	12	-0.718916	0.415716	1.736198
4	8	0.778922	1.540103	1.416218
5	12	-0.440478	-2.172011	-0.000044
6	8	-1.435591	-1.324751	1.416168
7	7	2.689622	-1.712445	0.000030
8	8	3.400446	-0.702641	0.000061
9	12	-0.718998	0.415770	-1.736167
10	8	0.778845	1.540175	-1.416243
11	8	-1.435674	-1.324696	-1.416166
12	8	-1.727691	1.188764	0.000065
13	12	-0.212151	2.432244	0.000037
14	12	-2.553358	-0.577782	0.000048

234 basis functions 536 primitive gaussians
67 alpha electrons 67 beta electrons

nuclear repulsion energy 1495.0312781535 Hartrees.

SCF Done: E(RB+HF-LYP) = -1782.18485333 A.U.
Convg = 0.3490D-08 -V/T = 2.0057
S**2 = 0.0000

	1	2	3
Frequencies --	48.7827	103.7337	134.3004
	4	5	6
Frequencies --	156.1444	185.6554	202.2809
	7	8	9
Frequencies --	211.8847	238.3573	250.7780
	10	11	12
Frequencies --	262.4818	282.9556	284.7062
	13	14	15
Frequencies --	290.0332	318.6478	339.8445
	16	17	18
Frequencies --	341.5741	359.8399	402.4162
	19	20	21
Frequencies --	434.6140	441.1088	458.6651
	22	23	24
Frequencies --	476.0030	510.1285	521.4024
	25	26	27
Frequencies --	535.8113	569.3929	573.2349
	28	29	30
Frequencies --	579.0914	616.0459	635.7860
	31	32	33
Frequencies --	653.9961	671.3059	712.3356
	34	35	36
Frequencies --	894.7800	1166.8440	1489.3103

(11) The geometry of $(MgO)_4NO$ in Figure 7

#N Geom=AllCheck Guess=Read Test UB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	2.367355	0.001538	-1.247645
2	12	1.052045	-0.000361	0.370657
3	12	-1.542019	1.577316	-0.806524
4	8	-0.298958	1.419588	0.635246
5	12	-1.542633	-1.576506	-0.808054
6	8	-0.299287	-1.420253	0.633647
7	12	-1.469093	-0.000551	1.274494
8	8	-2.572594	0.000419	-0.380919
9	7	3.388887	0.000281	-0.492229
10	8	3.090758	-0.001386	0.744514

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166 basis functions 376 primitive gaussians
48 alpha electrons 47 beta electrons

nuclear repulsion energy 760.9111789283 Hartrees.

SCF Done: E(UB+HF-LYP) = -1231.45349664 A.U.
Convg = 0.5561D-08 -V/T = 2.0057
S**2 = 0.7534

	1	2	3
Frequencies --	38.9735	67.9633	77.5200
	4	5	6
Frequencies --	150.9081	172.0984	196.1627
	7	8	9
Frequencies --	232.7311	305.9733	330.9943
	10	11	12
Frequencies --	331.0718	374.7082	410.0785
	13	14	15
Frequencies --	416.4832	424.5709	517.3425
	16	17	18
Frequencies --	521.0857	550.5203	556.5277
	19	20	21
Frequencies --	569.3642	591.0092	636.9480
	22	23	24
Frequencies --	879.2910	1297.8364	1351.2217

(12) The geometry of $(MgO)_3NO$ in Figure 8

#N Geom=AllCheck Guess=Read UB3LYP/6-31G(d) Freq

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	12	1.460245	-.628311	.495675
2	8	1.070152	.800583	-.870920
3	8	.004818	-.001739	1.640778
4	12	-.183384	1.576490	.502578
5	12	-1.271532	-.949279	.503607
6	8	-1.232182	.530481	-.863896
7	7	-.004715	.001188	-1.473103
8	8	.153345	-1.328715	-.869787

132 basis functions 296 primitive gaussians
38 alpha electrons 37 beta electrons

nuclear repulsion energy 561.7438668258 Hartrees.

SCF Done: E(UB+HF-LYP) = -955.974875456 A.U.
Convg = 0.1201D-08 -V/T = 2.0057
S**2 = 0.7538

	1	2	3
Frequencies --	254.6887	256.4694	272.2676
	4	5	6
Frequencies --	273.3906	357.4199	381.0762
	7	8	9
Frequencies --	403.5405	404.3890	458.5485
	10	11	12
Frequencies --	459.2017	490.8927	562.1463
	13	14	15
Frequencies --	593.4994	594.5002	679.0244
	16	17	18
Frequencies --	739.3883	739.4978	861.9218