

Effects of Heavy Metal Ions on *N*-Nitrosodimethylamine (NDMA) Formation

Yameng Liu,^{ac} Yongdong Liu,^{*a} Rugang Zhong,^a Bin Peng,^{*bc}

Henry F. Schaefer, III^{*c}

^a Beijing Key Laboratory of Environmental and Viral Oncology, College of Life Science &

Bioengineering, Beijing University of Technology, Beijing 100124, P. R. China

^b Center for Computational Quantum Chemistry, MOE Key Laboratory of Theoretical

Chemistry of the Environment, South China Normal University, Guangzhou, Guangdong

510631, P. R. China

^c Center for Computational Quantum Chemistry, University of Georgia,

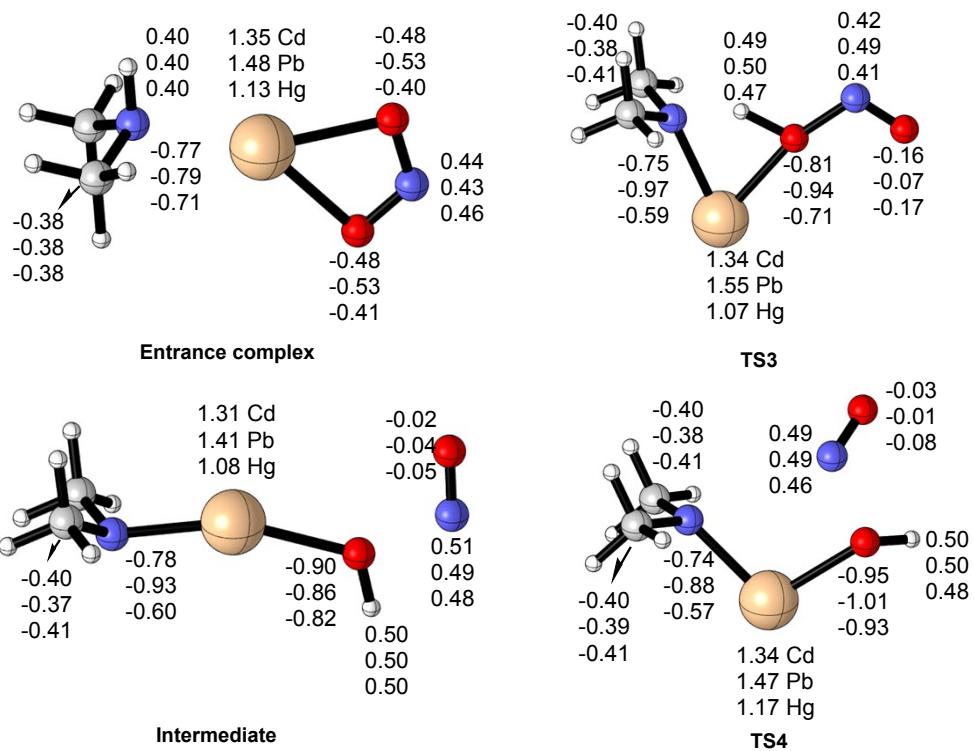
Athens, Georgia 30602, United States

^aCorresponding author. E-mail: ccq@uga.edu.

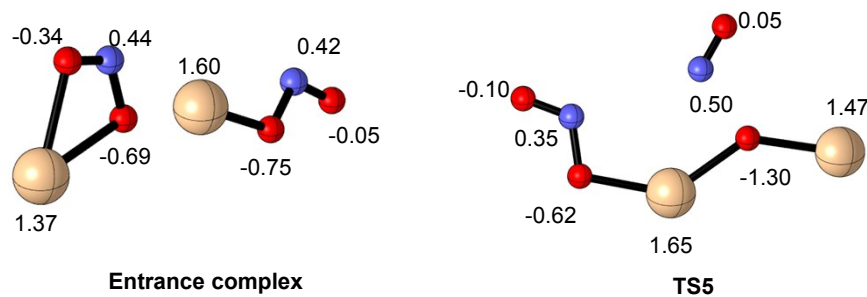
^bCorresponding author. E-mail: ydliu@bjut.edu.cn.

^cCorresponding author. E-mail: pengbin@scnu.edu.cn.

- S1.** Natural atomic charges of Entrance complex, TS1, Intermediate and TS2 on Pathway 1
- S2.** Natural atomic charges of Entrance complex, TS3, Intermediate and TS4 on Pathway 2
- S3.** Natural atomic charges of Entrance complex, TS5 on Pathway 3



S2. Natural atomic charges of Entrance complex, TS3, Intermediate and TS4 on Pathway 2



S3. Natural atomic charges of Entrance complex, TS5 on Pathway 3

Coordinates of Entrance complex in Pathway 1

N	0.4822	2.7114	0.0000
O	-0.5425	0.1906	1.0665
O	-0.5425	0.1906	-1.0665
H	1.4446	2.3844	0.0000
N	-0.6547	0.7808	0.0000
C	0.1096	3.3610	1.2493
H	0.3163	2.6924	2.0866
H	0.6703	4.2928	1.3974
H	-0.9555	3.5948	1.2307
C	0.1096	3.3610	-1.2493
H	0.6703	4.2928	-1.3974
H	0.3163	2.6924	-2.0866
H	-0.9555	3.5948	-1.2307
Cd	0.1844	-1.8776	0.0000
N	-0.4581	3.4776	0.0000
O	0.3904	1.1448	-1.0858
O	0.3904	1.1448	1.0858
H	-1.4469	3.2291	0.0000
N	0.3341	1.6131	0.0000
C	-0.0503	4.1071	-1.2576
H	-0.6016	5.0424	-1.4029
H	1.0176	4.3209	-1.2261
H	-0.2706	3.4358	-2.0884
C	-0.0503	4.1071	1.2576
H	-0.6016	5.0424	1.4029
H	-0.2706	3.4358	2.0884
H	1.0176	4.3209	1.2261
Hg	-0.0262	-1.6537	0.0000

Coordinates of TS1 in Pathway 1

N	2.4656	-0.3930	0.2972
O	1.2680	1.6892	-0.8201
O	-0.1801	-0.3570	-0.2566
H	1.6627	-0.8268	0.7506
N	1.2602	0.5713	-1.0076
C	3.1743	0.5589	1.1386
H	2.4883	1.3507	1.4531
H	3.5853	0.0813	2.0344
H	3.9941	1.0046	0.5729
C	3.2604	-1.3495	-0.4720
H	3.7949	-2.0436	0.1851
H	2.5978	-1.9167	-1.1262
H	3.9896	-0.8099	-1.0786
Cd	-2.0793	0.0554	0.1545

N	2.5180	-0.3923	0.2754
O	1.3193	1.7928	-0.5353
O	-0.1188	-0.4435	-0.3801
H	1.7178	-0.9012	0.6521
N	1.3573	0.7237	-0.8955
C	3.2049	0.4344	1.2584
H	2.5081	1.1707	1.6686
H	3.5973	-0.1679	2.0840
H	4.0345	0.9564	0.7793
C	3.3348	-1.2224	-0.6129
H	3.8683	-1.9942	-0.0494
H	2.6855	-1.7004	-1.3466
H	4.0636	-0.5944	-1.1276
Hg	-2.1201	-0.1939	0.0982

Coordinates of the Intermediate in Pathway 1

N	2.7469	-0.3723	0.2389
O	1.6962	1.8896	-0.4338
O	0.2037	-0.2834	0.1645
H	1.9081	-0.7990	0.6492
N	1.6726	0.8488	-0.8664
C	3.5365	0.3979	1.1885
H	2.9403	1.2389	1.5556
H	3.8290	-0.2128	2.0477
H	4.4335	0.7800	0.6993
C	3.4461	-1.2728	-0.6774
H	3.9236	-2.0923	-0.1314
H	2.7264	-1.6871	-1.3836
H	4.2112	-0.7181	-1.2230
Cd	-1.7334	-0.4130	-0.1787

N	2.9955	-0.4732	0.2289
O	2.0188	1.8469	-0.4631
O	0.4766	-0.2262	0.2896
H	2.2174	-0.9139	0.7256
N	1.9006	0.7995	-0.8570
C	3.8620	0.3082	1.1019
H	4.3013	-0.3178	1.8847
H	4.6643	0.7581	0.5150
H	3.2778	1.0977	1.5815
C	3.6216	-1.3763	-0.7385
H	4.1568	-2.1836	-0.2288
H	2.8485	-1.8071	-1.3748
H	4.3281	-0.8178	-1.3547
Hg	-1.5619	-0.0647	0.0202

Coordinates of the TS2 in Pathway 1

N	0.0031	0.0526	-0.1190
O	0.1701	-0.0746	2.3383
O	2.4204	-0.0773	0.2499
H	1.0606	0.1557	-0.2925
N	0.3157	-0.7775	1.4660
C	-0.6855	1.3244	0.0675
H	-0.2783	1.8279	0.9477
H	-0.5234	1.9690	-0.8000
H	-1.7559	1.1589	0.2014
C	-0.6091	-0.9421	-1.0045
H	-0.5999	-0.5792	-2.0353
H	-0.0324	-1.8652	-0.9462
H	-1.6403	-1.1303	-0.7001
Cd	4.3774	-0.2024	0.1675
N	2.2731	-0.4556	0.0981
O	2.2952	1.9951	-0.1839
O	-0.1421	0.0459	0.1172
H	1.2164	-0.5646	0.2623
N	2.0706	1.0976	-0.8280
C	3.0348	-0.2510	1.3264
H	2.7356	0.6960	1.7826
H	2.8208	-1.0532	2.0369
H	4.1036	-0.2336	1.1078
C	2.7632	-1.4497	-0.8640
H	2.6793	-2.4524	-0.4378
H	2.1549	-1.3930	-1.7670
H	3.8076	-1.2498	-1.1089
Hg	-2.1522	-0.3270	-0.0194

Coordinates of Exit complex in Pathway 1

N	-0.3557	0.3517	-0.0347
O	0.7123	1.6015	1.3824
O	2.5781	-0.8039	0.3801
H	2.8972	0.1098	0.4295
N	0.7407	0.7366	0.5409
C	-1.6292	0.9977	0.3233
H	-1.6111	2.0465	0.0196
H	-2.4286	0.4702	-0.1908
H	-1.7689	0.9452	1.4042
C	-0.2718	-0.6755	-1.0710
H	-0.5964	-0.2597	-2.0269
H	0.7631	-1.0036	-1.1306
H	-0.9161	-1.5138	-0.7999
Cd	4.1708	-2.1159	0.6521
N	3.4866	-0.4889	0.1113
O	3.1745	1.6735	0.2244
O	0.9231	0.2823	-0.3852
H	0.8771	0.9354	-1.1075
N	2.8213	0.5919	-0.1298
C	4.7583	-0.3802	0.8515
H	4.6212	0.3063	1.6870
H	5.0129	-1.3758	1.2070
H	5.5437	-0.0003	0.1947
C	3.0550	-1.7642	-0.4708
H	2.9215	-2.4904	0.3320
H	2.1178	-1.6088	-0.9961
H	3.8267	-2.1148	-1.1587
Hg	-1.3633	-0.0123	-0.0094

Coordinates of Entrance complex in Pathway 2

N	0.7662	0.0015	-0.1414
O	-1.6729	-0.0027	3.5142
N	-0.9389	-0.0002	4.5201
C	0.3502	-1.2405	-0.8678
H	0.7438	-2.1203	-0.3576
H	-0.7383	-1.2960	-0.9014
H	0.7320	-1.2238	-1.8913
C	0.3415	1.2388	-0.8709
H	-0.7474	1.2866	-0.9045
H	0.7289	2.1226	-0.3628
H	0.7233	1.2223	-1.8943
O	0.2861	0.0032	4.2904
Cd	0.0587	0.0017	2.0265
H	1.7858	0.0051	-0.1124
N	0.0000	0.0000	0.0000
O	0.0000	0.0000	3.1408
N	1.2574	0.0000	3.2086
C	0.4006	-0.5048	-1.3456
H	1.3532	-1.0324	-1.2767
H	-0.3656	-1.1831	-1.7245
H	0.5096	0.3247	-2.0481
C	-1.2387	0.8327	-0.0531
H	-2.0780	0.2184	-0.3844
H	-1.4492	1.2430	0.9352
H	-1.1136	1.6564	-0.7597
O	1.7792	-0.8658	2.4590
H	0.7557	0.5910	0.3467
Pb	-0.2136	-1.7578	1.6150
N	2.2098	-0.0255	-0.2898
O	-2.1814	0.1224	1.2220
N	-2.9321	0.0243	0.2537
C	2.8168	1.2654	0.1500
H	2.3994	2.0900	-0.4280
H	2.6123	1.4223	1.2092
H	3.8995	1.2383	0.0012
C	2.8191	-1.2018	0.3985
H	2.6147	-1.1447	1.4676
H	2.4033	-2.1258	-0.0035
H	3.9018	-1.2029	0.2470
O	-2.4296	-0.0877	-0.8638
H	2.3802	-0.1261	-1.2897
Hg	-0.1512	-0.0075	-0.0892

Coordinates of TS3 in Pathway 2

Cd	0.3214	-1.0922	0.0000
N	1.1104	1.0249	0.0000
O	-3.4702	0.5330	0.0000
N	-2.5507	1.2227	0.0000
C	1.7867	1.4782	1.2208
H	1.2332	1.1659	2.1082
H	2.8182	1.1194	1.2896
H	1.8205	2.5758	1.2099
C	1.7867	1.4782	-1.2208
H	2.8182	1.1194	-1.2896
H	1.2332	1.1659	-2.1082
H	1.8205	2.5758	-1.2099
O	-1.2795	0.4770	0.0000
H	-0.2759	1.0839	0.0000
Pb	-0.2849	-0.7739	0.0000
N	-1.0049	1.3200	0.0000
O	3.6545	0.4905	0.0000
N	2.8948	1.3151	0.0000
C	-1.6603	1.8259	-1.2221
H	-1.1444	1.4648	-2.1174
H	-2.7142	1.5324	-1.2818
H	-1.6149	2.9199	-1.2399
C	-1.6603	1.8259	1.2221
H	-2.7142	1.5324	1.2818
H	-1.1444	1.4648	2.1174
H	-1.6149	2.9199	1.2399
O	1.3394	0.7204	0.0000
H	0.4811	1.4279	0.0000
Hg	-0.6064	-0.7174	0.0000
N	-0.2607	1.6783	0.0000
O	3.7281	-0.4964	0.0000
N	3.0402	0.4368	0.0000
C	-0.6919	2.3445	-1.2243
H	-0.3388	1.8053	-2.1034
H	-1.7766	2.4772	-1.2728
H	-0.2403	3.3481	-1.2348
C	-0.6919	2.3445	1.2243
H	-1.7766	2.4772	1.2728
H	-0.3388	1.8053	2.1034
H	-0.2403	3.3481	1.2348
O	1.6641	0.1543	0.0000
H	0.9329	1.1083	0.0000

Coordinates of the Intermediate in Pathway 2

N	2.2136	-0.0006	-0.2177
O	-3.6770	0.0090	1.0171
N	-3.6749	-0.0031	-0.0914
C	2.8766	1.2158	0.2604
H	2.3879	2.1095	-0.1340
H	2.9503	1.2990	1.3529
H	3.9029	1.2034	-0.1324
C	2.8781	-1.2053	0.2869
H	2.9519	-1.2644	1.3810
H	2.3905	-2.1081	-0.0877
H	3.9044	-1.2003	-0.1060
O	-2.0376	-0.0088	-0.7147
Cd	0.1070	-0.0005	-0.0861
H	-2.2093	-0.0193	-1.6703
N	0.2410	0.4596	-0.0563
O	-0.9064	-0.6292	5.0589
N	0.0247	-1.0442	4.6110
C	0.8502	-0.8550	-0.2310
H	0.7788	-1.4521	0.6802
H	0.3381	-1.4104	-1.0257
H	1.9069	-0.7676	-0.5125
C	0.1994	1.2242	-1.3077
H	-0.3759	0.6891	-2.0716
H	-0.2688	2.2048	-1.1635
H	1.2097	1.3947	-1.6970
O	0.3205	-0.3543	3.0664
H	1.1342	-0.8136	2.8035
Pb	-0.5285	1.3540	1.6353
N	2.3081	0.0003	-0.1950
O	-3.6786	0.0292	1.1581
N	-3.7618	-0.0007	0.0443
C	2.8687	1.2261	0.3739
H	2.4210	2.1089	-0.0834
H	2.8129	1.2993	1.4670
H	3.9349	1.2185	0.1040
C	2.8721	-1.1925	0.4370
H	2.8164	-1.2088	1.5324
H	2.4269	-2.0992	0.0263
H	3.9383	-1.1960	0.1670
O	-2.2373	-0.0179	-0.6663
H	-2.4559	-0.0434	-1.6127
Hg	0.0896	-0.0007	-0.1170

Coordinates of TS4 in Pathway 2

N	-0.1904	-0.0002	-0.2554
O	1.1022	-0.0230	3.4709
N	1.4209	0.1640	2.4246
C	-1.6426	-0.1432	-0.3252
H	-2.1377	0.5073	0.3991
H	-2.0586	0.0558	-1.3221
H	-1.8978	-1.1833	-0.0774
C	0.4798	-0.8869	-1.2034
H	0.1850	-0.7201	-2.2482
H	1.5654	-0.7993	-1.1238
H	0.2050	-1.9225	-0.9581
O	1.4917	1.9351	1.9802
H	1.4522	2.5281	2.7477
Cd	0.6061	1.9906	-0.0253
Pb	0.0472	-0.9233	1.0828
N	1.1661	0.7109	0.3580
O	-2.5774	1.9598	-0.1068
N	-1.5700	1.5881	-0.3702
C	2.1570	1.3291	1.2386
H	2.1174	0.9024	2.2463
H	3.1722	1.1899	0.8474
H	1.9833	2.4081	1.3335
C	1.2593	1.1791	-1.0180
H	2.2699	1.0043	-1.4096
H	0.5526	0.6564	-1.6615
H	1.0693	2.2593	-1.0860
O	-1.4628	-0.3403	-0.4205
H	-2.2894	-0.7849	-0.6624
Hg	-0.7601	-0.3442	1.0744
N	0.4779	1.4562	0.3255
O	2.4007	-0.1235	-1.3208
N	2.2197	-0.0548	-0.2207
C	-0.0374	2.1415	-0.8492
H	-0.3364	1.4277	-1.6194
H	-0.8812	2.8072	-0.6283
H	0.7638	2.7778	-1.2540
C	0.9254	2.3755	1.3643
H	0.1295	3.0412	1.7202
H	1.3504	1.8288	2.2068
H	1.7072	3.0195	0.9373
O	1.1663	-1.4587	0.4422
H	1.2598	-2.2625	-0.0948

Coordinates of Exit complex in Pathway 2

N	-1.2661	0.3906	0.0589
O	-2.4620	-1.6086	-0.0796
N	-1.8620	-0.8912	-0.7501
C	-1.8168	0.4757	1.4286
H	-1.5883	-0.4319	1.9884
H	-1.3771	1.3345	1.9387
H	-2.9025	0.6049	1.3936
C	-1.6095	1.5612	-0.8004
H	-1.0749	2.4462	-0.4528
H	-1.3309	1.3460	-1.8334
H	-2.6832	1.7583	-0.7550
O	2.9183	-0.2458	0.2491
H	3.4541	-0.5201	-0.5050
Cd	0.9644	-0.0115	-0.0419
N	0.3995	-0.0537	-0.0838
O	0.7771	-0.2318	2.1318
N	1.3278	-0.1254	1.1046
C	-1.0123	-0.3475	0.2340
H	-1.3727	0.3680	0.9710
H	-1.5978	-0.2654	-0.6829
H	-1.1082	-1.3627	0.6294
C	0.9948	-0.8828	-1.1618
H	0.5459	-0.6195	-2.1206
H	2.0711	-0.7064	-1.1969
H	0.8175	-1.9432	-0.9683
O	-0.3190	2.6741	0.9828
H	-0.6171	3.4465	1.4752
Pb	0.7893	2.3962	-0.6331
N	0.0867	-0.2296	0.3356
O	-0.0431	-1.2604	2.4372
N	0.7469	-0.8894	1.6920
C	-1.3652	-0.4884	0.2571
H	-1.8695	-0.0985	1.1418
H	-1.7700	-0.0033	-0.6326
H	-1.5518	-1.5642	0.1875
C	0.8698	-0.8215	-0.7832
H	0.6481	-0.2951	-1.7123
H	1.9349	-0.7420	-0.5609
H	0.6068	-1.8754	-0.9039
O	0.7840	4.0685	0.7932
H	1.7147	4.3331	0.8356
Hg	0.6135	2.0151	0.5942

Coordinates of Entrance complex in Pathway 3

N	0.8156	1.8122	-0.0818
O	1.9882	2.0788	-0.1029
N	-4.7070	-0.0010	0.1826
O	-5.6561	-0.6326	0.0549
O	-3.5082	-0.7030	-0.1327
O	0.5496	0.5371	0.0116
Cd	2.9970	-0.0221	0.0411
Cd	-1.6929	0.2117	0.0186

Coordinates of TS5 in Pathway 3

N	0.3219	1.8194	0.1918
O	-0.2472	2.7541	0.2774
N	3.2742	0.8608	-0.1503
O	4.3481	1.3051	-0.2093
O	3.1252	-0.4777	-0.2139
O	-0.6981	0.2343	0.1073
Cd	-2.7764	-0.1406	0.1484
Cd	1.0806	-0.9322	-0.0812

Coordinates of Exit complex in Pathway 3

N	-4.8056	1.4705	-0.0526
O	-5.7844	0.9902	-0.0538
N	-3.5832	-0.3832	-0.0342
O	-4.4120	-1.2200	-0.0339
O	-2.3371	-0.7200	-0.0350
O	1.6072	0.3781	0.2068
Cd	3.5412	0.0414	-0.0265
Cd	-0.3300	-0.1123	0.0267