

Supplementary Information-II for Investigation of Nonadiabatic Dynamics in Photolysis of Methyl Nitrate (CH_3ONO_2) by On-the-fly Surface Hopping Simulation

Juanjuan Zhang^{†‡}, Jiawei Peng^{†‡}, Deping Hu^{†‡}, Zhenggang Lan^{†‡*}*

[†]SCNU Environmental Research Institute, Guangdong Provincial Key Laboratory of
Chemical Pollution and Environmental Safety & MOE Key Laboratory of
Environmental Theoretical Chemistry, South China Normal University, Guangzhou
510006, China

[‡]School of Environment, South China Normal University, Guangzhou 510006, China

*E-mail: zhenggang.lan@m.scnu.edu.cn; zhenggang.lan@gmail.com(ZL);

hudp1990@gmail.com(DH)

Cartesian coordinates of S₀-min (Unit: Å).

C	-1.77053800	0.00562000	0.00000000
H	-1.84735500	0.62329100	-0.89456400
H	-2.53979600	-0.76450300	0.00000000
H	-1.84735500	0.62329100	0.89456400
O	-0.54890000	-0.75276300	0.00000000
N	0.62555700	0.04878500	0.00000000
O	0.47701900	1.24768800	0.00000000
O	1.63173600	-0.60208800	0.00000000

Cartesian coordinates of S₁-min (Unit: Å).

C	0.08207046	-1.80025256	0.02671108
H	0.79971535	-1.75218294	0.85246196
H	-0.63728185	-2.60331412	0.19822494
H	0.60102794	-1.95122788	-0.92743691
O	-0.71658326	-0.60990212	-0.01701493
N	0.10364198	0.49555769	-0.22193907
O	1.07491557	0.73727217	0.55619251
O	-0.60772175	1.59136035	-0.37398064

Cartesian coordinates of CI₁₀-I (Unit: Å).

C	0.05755293	-2.34228766	0.11371655
H	0.21862838	-2.81533067	1.08538708
H	-0.36151674	-3.07444402	-0.58074497
H	1.01527926	-1.98903068	-0.27515951
O	-0.80423275	-1.26476429	0.24372368
N	0.10513251	1.62279463	-0.48766783
O	1.15889644	1.12207857	-0.44488724
O	-0.56136346	2.22642494	0.31901806

Cartesian coordinates of CI₁₀-II (Unit: Å).

C	0.11810513	-2.16626402	-0.17237466
H	0.34612132	-2.87513215	0.62740863
H	-0.31977136	-2.70380495	-1.01698740
H	1.04174747	-1.68180334	-0.49584306
O	-0.76466296	-1.20150047	0.28618638
N	0.13662569	1.85078315	0.42644072
O	1.25711930	1.30244777	-0.32161660
O	-0.76965954	2.01741383	-0.27376664

Cartesian coordinates of CI₁₀-III (Unit: Å).

C	0.03351298	-1.80441073	0.28496345
H	-0.38463267	-1.76052099	1.29037476
H	-0.44903493	-2.59350035	-0.28341777
H	1.10677333	-1.98348637	0.33219298
O	-0.24596616	-0.61261413	-0.42747181
N	0.25462105	0.46123989	0.21182169
O	1.02128946	1.19267422	-0.54420238
O	-0.76817418	1.46875142	0.37145791

Cartesian coordinates of Cl₂I-I (Unit: Å).

C	-0.02756020	-2.06603967	-0.08303863
H	0.98961785	-1.77775921	-0.35579156
H	0.00442699	-3.00486611	0.47606718
H	-0.62233088	-2.21289580	-0.98610120
O	-0.61711330	-1.10676924	0.72669809
N	0.84355264	1.28095652	0.24973759
O	0.54231202	2.11383695	0.96505046
O	-0.38767843	0.96152726	-0.76683917

Cartesian coordinates of Cl₂I-II (Unit: Å).

C	0.11077204	-1.67418130	0.22448240
H	-0.70627538	-2.12957521	0.78415332
H	0.32570855	-2.26923549	-0.65786097
H	0.99978297	-1.61520994	0.85256212
O	-0.25510479	-0.39731065	-0.25185824
N	-0.55620935	0.42825227	0.77054157
O	1.96079386	0.78880438	-1.99666150
O	-0.85392898	1.50803601	0.35508165

Cartesian coordinates of Cl₂₁-III (Unit: Å).

C	0.16271155	-2.13006215	0.03027895
H	0.87017394	-2.13960708	0.86662610
H	-0.25343523	-3.13563904	-0.06183705
H	0.70497158	-1.82317628	-0.86635374
O	-0.77243556	-1.21070522	0.45270329
N	-0.07580816	1.38172286	-0.66085370
O	1.35303157	0.85551634	0.35151253
O	-0.69634747	2.11056316	-0.06240874

Cartesian coordinates of Cl₂I-IV (Unit: Å).

C	0.04769472	-1.79505690	-0.12886375
H	0.99131818	-1.98281655	0.37964415
H	-0.70305851	-2.51828830	0.17505307
H	0.19774699	-1.85009143	-1.23106569
O	-0.48938727	-0.51295832	0.25222648
N	0.41409281	0.46452040	-0.00738047
O	0.45471701	1.21964932	1.13712590
O	-0.26933479	1.39798246	-0.74392760

Cartesian coordinates of Cl₃₂-I (Unit: Å).

C	0.01805517	-1.77905288	0.08130175
H	-0.38611067	-1.63824864	1.07801248
H	-0.44561579	-2.62531189	-0.41412445
H	1.09947170	-1.90210514	0.11288754
O	-0.32321862	-0.66197740	-0.74427610
N	0.15490871	0.47745421	-0.27489609
O	0.87119182	1.19685544	-1.04724312
O	-0.15398892	0.85321332	1.19836680

Cartesian coordinates of Cl₃₂-II (Unit: Å).

C	0.15850524	-2.12184140	0.02906573
H	0.80407553	-1.73338897	0.81871504
H	-0.40143977	-2.98309041	0.40091625
H	0.78128391	-2.43024900	-0.81375905
O	-0.70986114	-1.12220898	-0.38374273
N	-0.12185201	1.87260105	-0.41072071
O	1.32832770	0.98522860	-0.19359671
O	-0.72020536	1.85352458	0.55064613

Cartesian coordinates of CI₃₂-III (Unit: Å).

C	0.14170307	-2.04812089	0.12687198
H	-0.45470588	-2.43538307	0.95617840
H	-0.52662751	-1.56722090	-0.59017213
H	0.66958992	-2.86906788	-0.36368021
O	1.03591458	-1.09589366	0.59081631
N	0.32061056	1.87812049	-0.01370774
O	0.46195910	1.45042848	-1.14436675
O	-0.67777689	1.20643028	0.59351762

Cartesian coordinates of CI₃₂-IV (Unit: Å).

C	0.10502495	-2.14967693	-0.15377162
H	1.13585832	-1.81223011	-0.02279722
H	-0.27749388	-2.47498560	0.81819115
H	0.06319656	-2.99821315	-0.84128671
O	-0.72637302	-1.12249650	-0.56340123
N	0.42438022	1.72342020	0.06006919
O	0.90013950	1.04391234	0.97496679
O	-0.72493093	2.10114598	-0.16951592

Cartesian coordinates of Cl₃₂-V (Unit: Å).

C	0.11210718	-2.25911190	-0.01319575
H	0.22057492	-2.87276782	0.88431798
H	-0.88750030	-1.81935945	-0.02673969
H	0.23944857	-2.88502139	-0.89974337
O	1.04754040	-1.23639294	-0.01092299
N	0.05019251	1.68902703	-0.02927303
O	1.04127567	2.36180680	-0.01991963
O	-1.03577692	1.22082560	-0.03891197