DFT Study on the mechanism and kinetics of the gas-phase reaction between methylene blue and OH radicals

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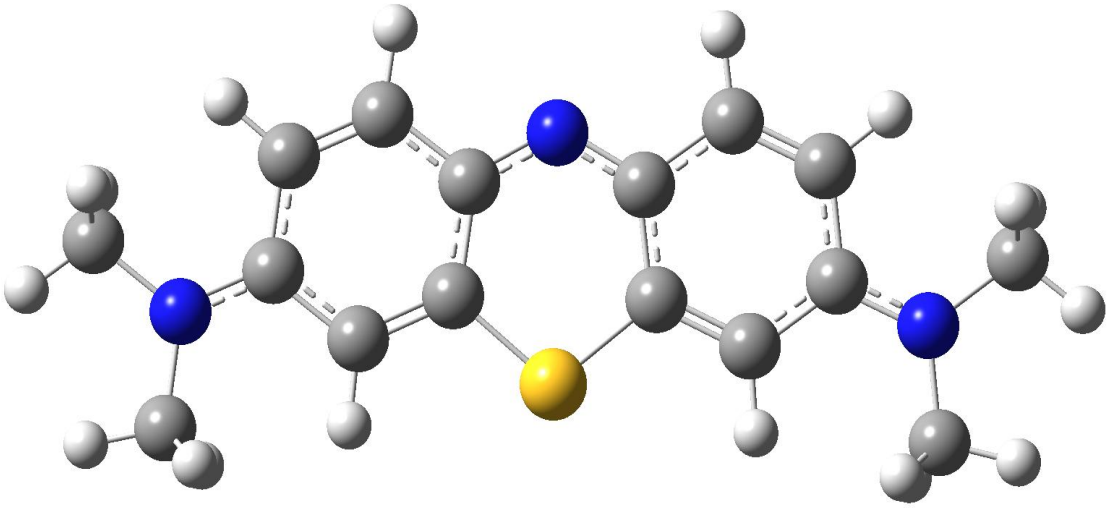

Figure S1. The optimized structure of MB for the calculations.

Table S1: The Cartesian coordinates and energies of TS the MB + HO• reaction in the gas phase at 298. 15 K

Cartesian Coordinates				**Energy**	
MBN-C1-TS					
Atom	X	Y	Z	Electronic Energy (EE)	-1258.338607
C	3.587632	1.383041	0.027949	Zero-point Energy Correction	0.326557
C	3.759156	-0.04192	0.014952	Thermal Correction to Energy	0.347549
C	2.601637	-0.860441	0.040967	Thermal Correction to Enthalpy	0.348493
C	2.32752	1.940549	0.155479	Thermal Correction to Free Energy	0.275724
C	1.336919	-0.299778	0.061157		
S	-0.02435	-1.371114	0.047683		
N	-0.017834	1.746821	0.043736		
C	1.142198	1.119314	0.078072		
C	-1.388297	-0.293488	0.018594		
C	-2.649994	-0.850061	0.006365		
C	-3.800779	-0.022866	-0.024795		
C	-3.613728	1.401789	-0.041349		
C	-2.366379	1.937286	-0.026065		
C	-1.195088	1.124001	0.006795		
N	-5.035401	-0.551222	-0.037826		
C	-5.215466	-1.999179	-0.01623		
C	-6.215797	0.310815	-0.0716		
N	4.990537	-0.574537	-0.032078		
C	6.17926	0.278889	-0.011724		
C	5.161025	-2.021687	-0.118326		
H	4.442549	2.040612	-0.011582		
H	2.18073	3.00482	0.034369		
H	2.696609	-1.937131	0.029084		
H	-2.751073	-1.92629	0.018377		
H	-4.470638	2.058805	-0.062953		
H	-2.214501	3.009805	-0.032323		
H	-6.277705	-2.224114	-0.027445		
H	-4.755779	-2.461928	-0.893437		
H	-4.781049	-2.432068	0.888615		
H	-6.257289	0.952451	0.811507		
H	-6.221126	0.93163	-0.970302		
H	-7.104152	-0.313627	-0.082586		
H	6.165723	0.939377	0.857127		
H	7.059901	-0.353041	0.054724		
H	6.25021	0.878116	-0.922811		
H	4.647274	-2.418967	-0.997062		
H	6.219069	-2.248478	-0.208204		
H	4.775039	-2.514417	0.778187		

O	2.654993	2.231906	2.113153
H	2.745573	1.331302	2.46601

MBN-C14-TS

Atom	X	Y	Z
C	3.636291	1.396979	0.042608
C	3.809244	-0.033614	-0.040265
C	2.651579	-0.860871	-0.077629
C	2.402482	1.929196	0.151997
C	1.400025	-0.316477	0.025757
S	0.036888	-1.375831	0.020063
N	0.04674	1.763485	0.059456
C	1.209953	1.113324	0.217675
C	-1.315432	-0.283901	0.032303
C	-2.578373	-0.831203	0.03774
C	-3.729386	-0.002022	-0.011856
C	-3.540159	1.421735	-0.092322
C	-2.293093	1.951717	-0.090827
C	-1.117071	1.137891	-0.007496
N	-4.963403	-0.528164	0.008142
C	-5.148393	-1.973434	0.110058
C	-6.144126	0.331769	-0.072259
N	5.032593	-0.5639	-0.094554
C	6.224406	0.287481	-0.054399
C	5.209675	-2.013263	-0.18534
H	4.496726	2.048452	0.011871
H	2.250245	3.000919	0.201391
H	2.752087	-1.931826	-0.1826
H	-2.684223	-1.906748	0.069384
H	-4.395571	2.079188	-0.143215
H	-2.137941	3.022872	-0.134985
H	-6.211049	-2.191433	0.155921
H	-4.727322	-2.482357	-0.760801
H	-4.677528	-2.359472	1.01706
H	-6.189265	1.012394	0.780776
H	-6.141558	0.910463	-0.998257
H	-7.032455	-0.292502	-0.061231
H	6.239695	0.886059	0.858032
H	7.10584	-0.346175	-0.06461
H	6.26178	0.946256	-0.924351
H	4.764675	-2.400589	-1.104657
H	6.271452	-2.238996	-0.194979
H	4.756623	-2.509541	0.6756

Electronic Energy (EE)	-1258.342667
Zero-point Energy Correction	0.327114
Thermal Correction to Energy	0.347923
Thermal Correction to Enthalpy	0.348867
Thermal Correction to Free Energy	0.276865

O	1.202468	0.841322	2.235554
H	0.933684	1.731232	2.515001

MBN-C16-TS

Atom	X	Y	Z
C	3.625278	1.368831	0.057536
C	3.789308	-0.054671	-0.016381
C	2.638257	-0.872635	-0.032909
C	2.383454	1.91473	0.084321
C	1.378156	-0.306783	-0.006519
S	0.009414	-1.370899	-0.047734
N	0.032972	1.747752	0.075356
C	1.20229	1.112807	0.045898
C	-1.343601	-0.288543	-0.006379
C	-2.61053	-0.832374	-0.030475
C	-3.75532	0.002571	0.004257
C	-3.559653	1.427832	0.064347
C	-2.311176	1.953555	0.087066
C	-1.139973	1.131901	0.052842
N	-4.992506	-0.514616	-0.017646
C	-5.184089	-1.96096	-0.075388
C	-6.16862	0.354665	0.017596
N	5.025859	-0.600346	-0.061382
C	6.192588	0.229506	-0.163383
C	5.19793	-2.043309	0.08459
H	4.491474	2.007921	0.150568
H	2.242056	2.986108	0.15637
H	2.73128	-1.948532	-0.087457
H	-2.720101	-1.906838	-0.075233
H	-4.413197	2.089006	0.092093
H	-2.151093	3.023915	0.132138
H	-6.248088	-2.177086	-0.083022
H	-4.740783	-2.375406	-0.984337
H	-4.739185	-2.446432	0.796882
H	-6.190963	0.944991	0.93622
H	-6.184737	1.024727	-0.844655
H	-7.06056	-0.263794	-0.013497
H	6.324443	0.809338	0.83077
H	7.076873	-0.379698	-0.325096
H	6.097299	0.980704	-0.947663
H	4.826902	-2.572215	-0.797422
H	6.256123	-2.260832	0.198016
H	4.674522	-2.402877	0.972582

Electronic Energy (EE)	-1258.339967
Zero-point Energy Correction	0.322207
Thermal Correction to Energy	0.343255
Thermal Correction to Enthalpy	0.344199
Thermal Correction to Free Energy	0.270627

O	6.127786	1.616019	2.04712
H	7.048033	1.834562	2.270445

MBN-C17-TS

Atom	X	Y	Z
C	3.618593	1.43384	-0.037212
C	3.80014	0.011813	-0.031549
C	2.660906	-0.820965	-0.027699
C	2.370123	1.968515	-0.054016
C	1.396048	-0.267204	-0.032528
S	0.042703	-1.350898	0.012546
N	0.022928	1.771991	-0.06082
C	1.201212	1.15055	-0.052197
C	-1.322959	-0.285773	-0.000782
C	-2.582748	-0.845934	0.029582
C	-3.738859	-0.026519	0.01751
C	-3.563612	1.402668	-0.026741
C	-2.323175	1.945618	-0.054118
C	-1.139931	1.139419	-0.041915
N	-4.968339	-0.560587	0.046418
C	-5.139443	-2.010128	0.092236
C	-6.156944	0.292354	0.032983
N	5.045592	-0.518636	-0.026655
C	6.214881	0.328796	0.205258
C	5.227925	-1.933169	-0.167653
H	4.477245	2.089484	-0.048162
H	2.215695	3.040397	-0.072286
H	2.768446	-1.894482	0.052442
H	-2.677338	-1.922267	0.061803
H	-4.426513	2.052101	-0.036841
H	-2.178055	3.018597	-0.085171
H	-6.200196	-2.240899	0.111877
H	-4.699475	-2.480799	-0.790556
H	-4.678238	-2.426986	0.99105
H	-6.17571	0.949745	0.904885
H	-6.194939	0.895136	-0.876924
H	-7.039713	-0.339204	0.061934
H	6.06928	0.951982	1.0887
H	7.077743	-0.309245	0.37494
H	6.417459	0.963691	-0.660935
H	4.678171	-2.332475	-1.021727
H	6.283391	-2.175943	-0.246742
H	4.796691	-2.468589	0.76175

Electronic Energy (EE)	-1258.340951
Zero-point Energy Correction	0.322395
Thermal Correction to Energy	0.343466
Thermal Correction to Enthalpy	0.34441
Thermal Correction to Free Energy	0.270868

O	3.926672	-3.060336	1.821923
H	4.47148	-3.825136	2.071899

MBN-C2-TS

Atom	X	Y	Z
C	3.570427	1.396271	0.080953
C	3.74463	-0.046516	-0.01113
C	2.586098	-0.86206	-0.044468
C	2.305754	1.937352	0.00643
C	1.330888	-0.299611	-0.018573
S	-0.032802	-1.369978	-0.00481
N	-0.034043	1.755213	-0.002095
C	1.138986	1.130378	0.005974
C	-1.395837	-0.291476	-0.010035
C	-2.656192	-0.847772	-0.011401
C	-3.81038	-0.022631	-0.016153
C	-3.627431	1.403486	-0.021174
C	-2.381775	1.939963	-0.018756
C	-1.204691	1.128914	-0.012146
N	-5.042367	-0.554422	-0.017223
C	-5.219405	-2.003669	-0.009842
C	-6.226413	0.30404	-0.025721
N	4.967339	-0.565503	-0.029151
C	6.156704	0.277493	0.140911
C	5.158388	-2.008914	-0.159262
H	4.422558	2.03973	-0.075723
H	2.163111	3.010885	-0.0248
H	2.680521	-1.93872	-0.06148
H	-2.755848	-1.924274	-0.010086
H	-4.486015	2.058618	-0.02546
H	-2.231976	3.012792	-0.020959
H	-6.281253	-2.230373	-0.00745
H	-4.772105	-2.454444	-0.899381
H	-4.770192	-2.445303	0.88323
H	-6.255632	0.93768	0.863457
H	-6.246636	0.9322	-0.918981
H	-7.112724	-0.323263	-0.028376
H	5.99934	0.974895	0.962267
H	6.998083	-0.364104	0.38759
H	6.38615	0.816512	-0.781968
H	4.606243	-2.390834	-1.019284
H	6.214188	-2.20939	-0.316012
H	4.83033	-2.525992	0.746421

Electronic Energy (EE)	-1258.346503
Zero-point Energy Correction	0.326701
Thermal Correction to Energy	0.347598
Thermal Correction to Enthalpy	0.348542
Thermal Correction to Free Energy	0.276358

O	3.959002	1.315672	2.106806
H	3.410146	2.043034	2.439377

MBN-C3-TS

Atom	X	Y	Z
C	3.601119	1.486797	0.152814
C	3.816126	0.031431	0.198474
C	2.616047	-0.798015	0.29314
C	2.362489	1.993034	0.086333
C	1.341665	-0.246665	0.194539
S	-0.010459	-1.328961	0.308156
N	0.011897	1.794063	-0.004752
C	1.162014	1.164446	0.087496
C	-1.368884	-0.256689	0.117054
C	-2.629789	-0.817731	0.109058
C	-3.779802	-0.002549	-0.024585
C	-3.589567	1.413183	-0.151513
C	-2.33968	1.953044	-0.140954
C	-1.173048	1.154039	-0.008261
N	-5.015453	-0.534475	-0.034457
C	-5.193425	-1.976027	0.0971
C	-6.192975	0.319127	-0.17556
N	4.984264	-0.473475	-0.220977
C	6.201016	0.33314	-0.062521
C	5.169186	-1.92592	-0.25371
H	4.458922	2.142485	0.154524
H	2.194028	3.061642	0.026561
H	2.728117	-1.872477	0.295931
H	-2.72787	-1.889973	0.206615
H	-4.443848	2.066027	-0.256088
H	-2.191295	3.021791	-0.235557
H	-6.25424	-2.206321	0.067451
H	-4.702784	-2.506045	-0.723665
H	-4.789627	-2.333646	1.048083
H	-6.260964	1.032738	0.648892
H	-6.171614	0.86274	-1.122978
H	-7.08128	-0.305426	-0.160415
H	6.348203	0.616864	0.983222
H	7.050519	-0.261878	-0.385485
H	6.162328	1.22167	-0.690653
H	4.413866	-2.391077	-0.885985
H	6.13947	-2.140753	-0.693043
H	5.128793	-2.348624	0.75455

Electronic Energy (EE)	-1258.338852
Zero-point Energy Correction	0.327535
Thermal Correction to Energy	0.348172
Thermal Correction to Enthalpy	0.349116
Thermal Correction to Free Energy	0.277314

O	3.583805	-0.490797	1.945688
H	3.081855	0.20363	2.396846

MBN-C4-TS

Atom	X	Y	Z
C	3.573929	1.478568	-0.03019
C	3.766296	0.052099	-0.001797
C	2.608778	-0.786184	0.10178
C	2.326068	2.007347	-0.022456
C	1.333922	-0.222593	0.036927
S	-0.009567	-1.303916	0.079175
N	-0.025298	1.817227	-0.012117
C	1.146614	1.190935	0.00677
C	-1.376329	-0.238384	0.014458
C	-2.634954	-0.8015	0.002844
C	-3.79157	0.017199	-0.025471
C	-3.615037	1.445674	-0.047942
C	-2.373721	1.990163	-0.040347
C	-1.192329	1.185208	-0.009576
N	-5.021125	-0.518324	-0.031459
C	-5.191554	-1.96837	-0.00779
C	-6.20931	0.334516	-0.057852
N	4.985675	-0.479995	-0.033341
C	6.171922	0.362071	-0.192861
C	5.177034	-1.921268	0.147966
H	4.429661	2.137504	-0.04742
H	2.170792	3.079457	-0.035777
H	2.709662	-1.85274	-0.030871
H	-2.728638	-1.878274	0.022103
H	-4.477469	2.095446	-0.071421
H	-2.229919	3.063627	-0.058892
H	-6.252216	-2.200271	-0.017211
H	-4.729808	-2.42788	-0.885357
H	-4.752297	-2.396354	0.896863
H	-6.246773	0.97962	0.822668
H	-6.228414	0.950202	-0.959753
H	-7.09235	-0.297353	-0.056557
H	6.367649	0.939047	0.714716
H	7.02629	-0.278499	-0.391638
H	6.050803	1.03961	-1.038383
H	4.882999	-2.467927	-0.752334
H	6.229528	-2.109219	0.340756
H	4.59501	-2.259868	1.005321

Electronic Energy (EE)	-1258.349862
Zero-point Energy Correction	0.327108
Thermal Correction to Energy	0.347937
Thermal Correction to Enthalpy	0.348881
Thermal Correction to Free Energy	0.276846

O	2.805498	-1.226184	2.163358
H	2.634583	-0.353045	2.550397

MBN-C5-TS

Atom	X	Y	Z
C	3.600447	1.427828	-0.051862
C	3.784426	0.002465	0.004474
C	2.630959	-0.825858	0.020653
C	2.35183	1.965643	-0.077277
C	1.335444	-0.262378	0.068215
S	0.008906	-1.3158	-0.327034
N	0.003772	1.796761	-0.062973
C	1.163893	1.171463	-0.055433
C	-1.355675	-0.253764	-0.11424
C	-2.61389	-0.815257	-0.116962
C	-3.769684	0.001327	-0.018261
C	-3.590906	1.422995	0.067297
C	-2.345228	1.964536	0.055336
C	-1.169862	1.161486	-0.026849
N	-5.000014	-0.538133	-0.00095
C	-5.170843	-1.984343	-0.093976
C	-6.183661	0.310826	0.117747
N	5.009407	-0.538137	0.037249
C	6.198779	0.304614	-0.08945
C	5.186626	-1.981529	0.196853
H	4.459439	2.082292	-0.063859
H	2.211002	3.039544	-0.114506
H	2.718654	-1.902518	0.01634
H	-2.709039	-1.890095	-0.180778
H	-4.450098	2.073593	0.136972
H	-2.199951	3.03639	0.11491
H	-6.231249	-2.217387	-0.073177
H	-4.752678	-2.366455	-1.028764
H	-4.689727	-2.488628	0.748151
H	-6.159782	0.886455	1.045834
H	-6.261102	0.995714	-0.729885
H	-7.067227	-0.320422	0.129571
H	6.316488	0.94777	0.786291
H	7.072524	-0.334812	-0.172494
H	6.137285	0.921724	-0.987251
H	4.880256	-2.517011	-0.705771
H	6.236845	-2.186388	0.382707
H	4.609249	-2.342282	1.049673

Electronic Energy (EE)	-1258.336009
Zero-point Energy Correction	0.327174
Thermal Correction to Energy	0.347744
Thermal Correction to Enthalpy	0.348688
Thermal Correction to Free Energy	0.277348

O	1.498572	-0.589919	1.988155
H	2.055223	0.128959	2.331116

MBN-N13-TS

Atom	X	Y	Z
C	3.605965	1.348386	0.188748
C	3.777557	-0.071352	0.05285
C	2.617104	-0.877531	-0.005116
C	2.366003	1.895569	0.260193
C	1.358569	-0.313086	0.074656
S	-0.004067	-1.387996	0.00311
N	-0.003201	1.712939	0.263607
C	1.190083	1.096249	0.201551
C	-1.36601	-0.311887	0.069335
C	-2.624734	-0.875196	-0.015283
C	-3.784678	-0.067962	0.038095
C	-3.612343	1.35166	0.174292
C	-2.372174	1.897727	0.25053
C	-1.196758	1.097318	0.196722
N	-5.013955	-0.60518	-0.034484
C	-5.175861	-2.050423	-0.151742
C	-6.203543	0.243086	0.010136
N	5.006623	-0.609654	-0.015182
C	6.196805	0.237478	0.034851
C	5.167682	-2.05503	-0.13196
H	4.469059	1.995326	0.243028
H	2.24126	2.962791	0.382656
H	2.70061	-1.950033	-0.110965
H	-2.7088	-1.947623	-0.121441
H	-4.475057	1.999397	0.224962
H	-2.246934	2.964866	0.37323
H	-6.235246	-2.287317	-0.178273
H	-4.715921	-2.420735	-1.071817
H	-4.729436	-2.561913	0.704944
H	-6.265056	0.783222	0.957828
H	-6.204164	0.958721	-0.815019
H	-7.084267	-0.385299	-0.083217
H	6.25506	0.776804	0.983188
H	7.077312	-0.391643	-0.05554
H	6.201349	0.95375	-0.789733
H	4.710089	-2.424929	-1.05336
H	6.226945	-2.292785	-0.155518
H	4.718383	-2.566193	0.723419

Electronic Energy (EE)	-1258.335087
Zero-point Energy Correction	0.327219
Thermal Correction to Energy	0.347936
Thermal Correction to Enthalpy	0.34888
Thermal Correction to Free Energy	0.277058

O	-0.005624	2.898422	1.654517	
H	-0.004327	3.726016	1.150677	