

## **Electronic Supplementary Information Part II**

### **Practical computation of electronic excitation in solution: vertical excitation model**

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**Contents:** Cartesian coordinates of solute molecules (in Å)

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acetone in gas  
8 0.000000 0.000000 1.389623  
6 0.000000 0.000000 0.185718  
6 0.000000 1.283709 -0.610247  
6 0.000000 -1.283709 -0.610247  
1 0.000000 2.136862 0.060961  
1 0.000000 -2.136862 0.060961  
1 0.877283 1.319182 -1.257563  
1 0.877283 -1.319182 -1.257563  
1 -0.877283 1.319182 -1.257563  
1 -0.877283 -1.319182 -1.257563

acetone in n-hexane  
8 0.000000 0.000000 1.391018  
6 0.000000 0.000000 0.184805  
6 0.000000 1.281337 -0.609856  
6 0.000000 -1.281337 -0.609856  
1 0.000000 2.138759 0.056941  
1 0.000000 -2.138759 0.056941  
1 0.877165 1.315998 -1.258147  
1 0.877165 -1.315998 -1.258147  
1 -0.877165 1.315998 -1.258147  
1 -0.877165 -1.315998 -1.258147

acetone in water  
8 0.000000 0.000000 1.393231  
6 0.000000 0.000000 0.175962  
6 0.000000 1.277595 -0.607353  
6 0.000000 -1.277595 -0.607353  
1 0.000000 2.138501 0.056265  
1 0.000000 -2.138501 0.056265  
1 0.877264 1.305459 -1.256477  
1 0.877264 -1.305459 -1.256477  
1 -0.877264 1.305459 -1.256477  
1 -0.877264 -1.305459 -1.256477

acrolein in gas  
6 -0.151176 -0.744097 0.000000  
6 0.000000 0.723075 0.000000  
6 1.207902 1.271620 0.000000  
8 -1.210139 -1.311458 0.000000  
1 0.800471 -1.310542 0.000000  
1 -0.911795 1.306957 0.000000  
1 1.356361 2.342250 0.000000  
1 2.095718 0.649410 0.000000

acrolein in n-hexane  
6 -0.152670 -0.739822 0.000000  
6 0.000000 0.724264 0.000000  
6 1.211953 1.264825 0.000000  
8 -1.213446 -1.309252 0.000000  
1 0.796624 -1.308587 0.000000  
1 -0.908176 1.314212 0.000000  
1 1.366754 2.335193 0.000000  
1 2.096667 0.637598 0.000000

acrolein in water  
6 -0.147500 -0.734358 0.000000  
6 0.000000 0.721333 0.000000  
6 1.216256 1.257348 0.000000  
8 -1.220846 -1.303210 0.000000  
1 0.791264 -1.312027 0.000000  
1 -0.905941 1.316034 0.000000  
1 1.369856 2.328723 0.000000  
1 2.099054 0.627012 0.000000

coumarin 153 in gas  
6 -0.929513 -0.143133 -0.011826  
6 -0.192930 1.046469 -0.016562  
6 1.195566 1.077383 -0.018403  
6 1.893012 -0.146803 -0.030000  
6 1.167408 -1.372101 -0.035640  
6 -0.207991 -1.346413 -0.016082  
6 1.907843 2.408875 -0.005740  
6 3.986689 1.076532 -0.320352

6	3.360667	2.245066	0.424215
6	3.994735	-1.391178	-0.269373
6	3.321266	-2.555764	0.438719
6	1.896250	-2.696418	-0.081551
1	1.341224	-3.437833	0.497082
1	3.889970	-3.471693	0.268449
1	1.858872	2.854610	-1.005278
1	-0.741742	-2.289562	-0.013835
1	3.924593	3.158431	0.226938
7	3.273415	-0.154042	-0.014892
1	3.979229	1.271480	-1.404179
1	5.026373	0.938819	-0.016696
1	3.414382	2.041549	1.496983
1	1.379935	3.095662	0.657503
1	5.014628	-1.257279	0.097663
1	4.056228	-1.593792	-1.350249
1	3.312574	-2.357212	1.513898
1	1.925862	-3.058299	-1.115523
6	-2.365211	-0.019630	-0.003089
6	-2.965778	1.183109	-0.002296
6	-2.181052	2.415996	-0.010112
6	-3.206983	-1.269980	0.004891
9	-2.960088	-2.026466	-1.073363
9	-2.945118	-2.023219	1.081769
9	-4.513449	-1.003054	0.013490
1	-4.039048	1.303176	0.004517
8	-0.812801	2.261857	-0.019294
8	-2.628819	3.523497	-0.009566

coumarin 153 in cyclohexane

6	-0.930433	-0.143124	-0.018281
6	-0.192200	1.046625	-0.023901
6	1.195320	1.079625	-0.027960
6	1.894463	-0.146419	-0.040725
6	1.166533	-1.373359	-0.047536
6	-0.207985	-1.347587	-0.024789
6	1.911331	2.409346	-0.011985
6	3.993434	1.077042	-0.308949
6	3.359512	2.242601	0.432289
6	4.001268	-1.394192	-0.250604
6	3.314164	-2.556615	0.446607
6	1.897747	-2.695884	-0.096163
1	1.334932	-3.444093	0.465765
1	3.884472	-3.472604	0.282042
1	1.875398	2.854045	-1.012551
1	-0.739177	-2.292292	-0.022108
1	3.925312	3.156102	0.241032
7	3.269786	-0.154786	-0.026847
1	4.005142	1.277797	-1.390859
1	5.026647	0.932458	0.011694
1	3.402252	2.038813	1.505596
1	1.381708	3.099089	0.646915
1	5.009944	-1.253455	0.142953
1	4.090898	-1.601708	-1.327644
1	3.288914	-2.361860	1.522381
1	1.944875	-3.046571	-1.133276
6	-2.364167	-0.018152	-0.002816
6	-2.966881	1.185032	0.001586
6	-2.180374	2.413320	-0.009301
6	-3.207256	-1.267588	0.008808
9	-2.969264	-2.026195	-1.070629
9	-2.943724	-2.023622	1.083999
9	-4.514346	-1.000993	0.023842
1	-4.040391	1.304815	0.013657
8	-0.815999	2.261244	-0.024527
8	-2.626537	3.524533	-0.006752

coumarin 153 in dimethyl sulfoxide

6	-0.932545	-0.142648	-0.019826
6	-0.192092	1.047529	-0.028939
6	1.194176	1.083706	-0.037462
6	1.896500	-0.144949	-0.052061
6	1.164982	-1.374108	-0.061215
6	-0.208425	-1.349014	-0.031380
6	1.915221	2.410873	-0.025465

6	3.999420	1.078798	-0.295675
6	3.355662	2.240608	0.440785
6	4.009706	-1.396643	-0.221820
6	3.302278	-2.556706	0.456246
6	1.900123	-2.692549	-0.121715
1	1.324587	-3.454038	0.408438
1	3.875380	-3.472232	0.300755
1	1.900921	2.843012	-1.032152
1	-0.735053	-2.296717	-0.028965
1	3.925534	3.153098	0.258185
7	3.263813	-0.154843	-0.041285
1	4.031736	1.285076	-1.374929
1	5.024033	0.925047	0.045284
1	3.381948	2.036347	1.514944
1	1.382363	3.110618	0.620347
1	5.000616	-1.244749	0.209807
1	4.140616	-1.608710	-1.292327
1	3.251294	-2.368084	1.532687
1	1.975853	-3.016774	-1.165683
6	-2.362895	-0.017048	0.001065
6	-2.970764	1.185591	0.008348
6	-2.184603	2.409123	-0.007443
6	-3.203955	-1.266969	0.013047
9	-2.971375	-2.021708	-1.071279
9	-2.934892	-2.028248	1.084087
9	-4.512554	-1.006089	0.036013
1	-4.044853	1.302516	0.024316
8	-0.822136	2.262026	-0.029201
8	-2.628989	3.525517	-0.004555

indolinedimethine-malononitrile in gas

6	2.139370	1.149839	0.000000
6	2.298144	-0.234267	0.000000
6	3.562116	-0.789313	0.000000
6	4.672382	0.059102	0.000000
6	4.498820	1.438169	0.000000
6	3.226149	2.010725	0.000000
6	0.936620	-0.899751	0.000000
1	3.694373	-1.866090	0.000000
1	5.671076	-0.358371	0.000000
1	5.366114	2.086928	0.000000
1	3.111454	3.086677	0.000000
7	0.767516	1.448327	0.000000
6	0.207670	2.783410	0.000000
1	-0.408793	2.936865	0.889059
1	1.014052	3.511364	0.000000
1	-0.408793	2.936865	-0.889059
6	0.767516	-1.746074	1.272854
1	-0.206562	-2.234125	1.312493
1	1.537518	-2.520480	1.295442
1	0.879242	-1.126292	2.163991
6	0.767516	-1.746074	-1.272854
1	1.537518	-2.520480	-1.295442
1	-0.206562	-2.234125	-1.312493
1	0.879242	-1.126292	-2.163991
6	0.005751	0.317802	0.000000
6	-1.363604	0.362847	0.000000
6	-2.211962	-0.770878	0.000000
1	-1.780926	-1.764061	0.000000
6	-3.578134	-0.719855	0.000000
6	-4.262628	0.533903	0.000000
6	-4.354772	-1.917251	0.000000
7	-4.762619	1.571182	0.000000
7	-4.961465	-2.895861	0.000000
1	-1.848694	1.332073	0.000000

indolinedimethine-malononitrile in cyclohexane

6	2.142352	1.147882	0.000000
6	2.299288	-0.235936	0.000000
6	3.563088	-0.793011	0.000000
6	4.672888	0.055903	0.000000
6	4.500742	1.435826	0.000000
6	3.228657	2.009668	0.000000
6	0.937062	-0.898865	0.000000
1	3.694766	-1.869700	0.000000

1	5.671526	-0.362315	0.000000
1	5.368780	2.083850	0.000000
1	3.112774	3.085532	0.000000
7	0.768500	1.446736	0.000000
6	0.216683	2.787321	0.000000
1	-0.396364	2.944600	0.890251
1	1.028288	3.509602	0.000000
1	-0.396364	2.944600	-0.890251
6	0.768500	-1.747419	1.271070
1	-0.200523	-2.246163	1.306001
1	1.544106	-2.516424	1.293445
1	0.872392	-1.132399	2.166820
6	0.768500	-1.747419	-1.271070
1	1.544106	-2.516424	-1.293445
1	-0.200523	-2.246163	-1.306001
1	0.872392	-1.132399	-2.166820
6	0.010034	0.322129	0.000000
6	-1.366135	0.371457	0.000000
6	-2.208462	-0.756919	0.000000
1	-1.776095	-1.749423	0.000000
6	-3.581360	-0.714857	0.000000
6	-4.278364	0.528884	0.000000
6	-4.347854	-1.915859	0.000000
7	-4.793997	1.558872	0.000000
7	-4.952808	-2.896104	0.000000
1	-1.844836	1.343974	0.000000

indolinedimethine-malononitrile in acetonitrile

6	2.149394	1.141067	0.000000
6	2.303546	-0.242255	0.000000
6	3.567067	-0.802892	0.000000
6	4.676477	0.047687	0.000000
6	4.505782	1.429869	0.000000
6	3.233849	2.005735	0.000000
6	0.941736	-0.901318	0.000000
1	3.694594	-1.880203	0.000000
1	5.675737	-0.370512	0.000000
1	5.374653	2.077368	0.000000
1	3.115782	3.081491	0.000000
7	0.771772	1.439374	0.000000
6	0.224410	2.786953	0.000000
1	-0.386990	2.940222	0.891026
1	1.040085	3.503954	0.000000
1	-0.386990	2.940222	-0.891026
6	0.771772	-1.750199	1.271038
1	-0.193047	-2.257709	1.294114
1	1.555902	-2.510602	1.290912
1	0.865591	-1.132488	2.166599
6	0.771772	-1.750199	-1.271038
1	1.555902	-2.510602	-1.290912
1	-0.193047	-2.257709	-1.294114
1	0.865591	-1.132488	-2.166599
6	0.021564	0.322091	0.000000
6	-1.366188	0.376490	0.000000
6	-2.198819	-0.743615	0.000000
1	-1.770452	-1.738242	0.000000
6	-3.583865	-0.702475	0.000000
6	-4.290796	0.529907	0.000000
6	-4.350170	-1.897283	0.000000
7	-4.837788	1.545451	0.000000
7	-4.968833	-2.871158	0.000000
1	-1.834560	1.354252	0.000000

julolidine-malononitrile in gas

6	1.188332	-0.549781	-0.044784
6	0.251366	-1.596551	-0.047886
6	-1.110227	-1.382427	-0.064600
6	-1.600493	-0.051115	-0.065053
6	-0.669715	1.023510	-0.079951
6	0.683338	0.762789	-0.061730
6	-2.067365	-2.552395	-0.089400
6	-3.903163	-0.888939	-0.220623
6	-3.424910	-2.153432	0.475954
6	-3.464110	1.544586	-0.226142
6	-2.564060	2.566264	0.450474

6	-1.158848	2.453242	-0.126737
1	-0.460115	3.094787	0.413401
1	-2.968281	3.568770	0.300108
1	-2.194023	-2.897886	-1.121574
1	0.610610	-2.621975	-0.037237
1	1.356141	1.610466	-0.065745
1	-4.156658	-2.950692	0.334405
7	-2.951087	0.195667	-0.031202
1	-4.057742	-1.084476	-1.292411
1	-4.859557	-0.563107	0.193685
1	-3.342156	-1.956821	1.548309
1	-1.641507	-3.385507	0.473704
1	-4.469233	1.577980	0.199675
1	-3.552570	1.772377	-1.298955
1	-2.546303	2.366857	1.525420
1	-1.166910	2.798722	-1.166600
6	2.581450	-0.912007	-0.021681
1	2.769188	-1.982346	-0.027461
6	3.708774	-0.151164	0.008717
6	3.730026	1.278411	0.028504
6	4.988269	-0.795572	0.026042
7	3.752160	2.429043	0.045166
7	6.008517	-1.327519	0.039556

julolidine-malononitrile in cyclohexane

6	1.188610	-0.547555	-0.026737
6	0.249905	-1.596596	-0.043460
6	-1.109823	-1.383573	-0.073226
6	-1.602444	-0.049445	-0.070116
6	-0.669239	1.028541	-0.070323
6	0.681609	0.767059	-0.040003
6	-2.068284	-2.551334	-0.115404
6	-3.906201	-0.888225	-0.226552
6	-3.423812	-2.157306	0.456961
6	-3.468476	1.549225	-0.204610
6	-2.562585	2.560779	0.477516
6	-1.163120	2.455987	-0.113872
1	-0.461075	3.100591	0.418120
1	-2.969333	3.564108	0.341448
1	-2.197147	-2.879403	-1.152845
1	0.609630	-2.621804	-0.035699
1	1.352718	1.616186	-0.029868
1	-4.156431	-2.952368	0.308058
7	-2.946456	0.195479	-0.051683
1	-4.076023	-1.075633	-1.296463
1	-4.853839	-0.559301	0.203979
1	-3.339582	-1.973439	1.531666
1	-1.642546	-3.393221	0.434388
1	-4.465696	1.567210	0.239234
1	-3.575632	1.796203	-1.270464
1	-2.534865	2.350277	1.550313
1	-1.185303	2.800057	-1.153986
6	2.575425	-0.910382	0.003781
1	2.760544	-1.981184	0.021869
6	3.709710	-0.150796	0.012722
6	3.740538	1.276500	-0.011353
6	4.984451	-0.799891	0.042873
7	3.770678	2.427056	-0.030365
7	6.003920	-1.333424	0.067917

julolidine-malononitrile in acetonitrile

6	1.185966	-0.549944	-0.033608
6	0.241688	-1.601353	-0.053545
6	-1.114576	-1.387054	-0.089649
6	-1.608257	-0.046506	-0.085069
6	-0.667823	1.034714	-0.089837
6	0.678951	0.770008	-0.053576
6	-2.079194	-2.548223	-0.137764
6	-3.915763	-0.883832	-0.199058
6	-3.418476	-2.153335	0.470170
6	-3.475149	1.557774	-0.166713
6	-2.546854	2.563053	0.491160
6	-1.167152	2.458550	-0.144283
1	-0.449504	3.115375	0.350763
1	-2.958494	3.565739	0.366817

1	-2.235026	-2.848487	-1.179874
1	0.602788	-2.626019	-0.043060
1	1.350698	1.619316	-0.045110
1	-4.157291	-2.944557	0.333520
7	-2.940293	0.199006	-0.069007
1	-4.120402	-1.069250	-1.261453
1	-4.842748	-0.543055	0.263760
1	-3.308262	-1.974883	1.543814
1	-1.644661	-3.404041	0.382458
1	-4.450219	1.558023	0.322253
1	-3.629862	1.817419	-1.221978
1	-2.486016	2.352183	1.562856
1	-1.232077	2.780080	-1.189906
6	2.561164	-0.915440	0.004038
1	2.743477	-1.986864	0.024120
6	3.705180	-0.155490	0.018189
6	3.756921	1.267731	-0.008798
6	4.973558	-0.807801	0.056678
7	3.822266	2.417957	-0.030573
7	5.997527	-1.335262	0.088294

methanal (formaldehyde) in gas

8	0.000000	0.000000	0.670064
6	0.000000	0.000000	-0.525154
1	0.000000	0.938446	-1.104794
1	0.000000	-0.938446	-1.104794

methanal (formaldehyde) in n-hexane

8	0.000000	0.000000	0.670936
6	0.000000	0.000000	-0.525991
1	0.000000	0.938274	-1.105770
1	0.000000	-0.938274	-1.105770

methanal (formaldehyde) in water

8	0.000000	0.000000	0.674199
6	0.000000	0.000000	-0.531116
1	0.000000	0.938483	-1.103447
1	0.000000	-0.938483	-1.103447

methylenecyclopropene in gas

6	0.000000	0.655327	-1.013929
6	0.000000	-0.655327	-1.013929
1	0.000000	1.567170	-1.584575
1	0.000000	-1.567170	-1.584575
6	0.000000	0.000000	0.260147
6	0.000000	0.000000	1.583914
1	0.000000	-0.927546	2.135967
1	0.000000	0.927546	2.135967

methylenecyclopropene in n-pentane

6	0.000000	0.655638	-1.013409
6	0.000000	-0.655638	-1.013409
1	0.000000	1.570067	-1.580763
1	0.000000	-1.570067	-1.580763
6	0.000000	0.000000	0.257835
6	0.000000	0.000000	1.583841
1	0.000000	-0.928242	2.136190
1	0.000000	0.928242	2.136190

methylenecyclopropene in methanol

6	0.000000	0.656600	-1.012773
6	0.000000	-0.656600	-1.012773
1	0.000000	1.574566	-1.576973
1	0.000000	-1.574566	-1.576973
6	0.000000	0.000000	0.253562
6	0.000000	0.000000	1.584929
1	0.000000	-0.929536	2.138138
1	0.000000	0.929536	2.138138

pyridine in gas

6	0.000000	0.000000	-1.376382
6	0.000000	1.191369	-0.668626
6	0.000000	-1.191369	-0.668626
6	0.000000	1.136940	0.718258
6	0.000000	-1.136940	0.718258

7	0.000000	0.000000	1.409356
1	0.000000	2.146102	-1.174755
1	0.000000	-2.146102	-1.174755
1	0.000000	2.049771	1.302349
1	0.000000	-2.049771	1.302349
1	0.000000	0.000000	-2.457965

pyridine in cyclohexane

6	0.000000	0.000000	-1.375355
6	0.000000	1.192181	-0.668334
6	0.000000	-1.192181	-0.668334
6	0.000000	1.138763	0.718521
6	0.000000	-1.138763	0.718521
7	0.000000	0.000000	1.407618
1	0.000000	2.147034	-1.174802
1	0.000000	-2.147034	-1.174802
1	0.000000	2.052357	1.301730
1	0.000000	-2.052357	1.301730
1	0.000000	0.000000	-2.457300

pyridine in water

6	0.000000	0.000000	-1.376202
6	0.000000	1.192096	-0.668303
6	0.000000	-1.192096	-0.668303
6	0.000000	1.139865	0.717575
6	0.000000	-1.139865	0.717575
7	0.000000	0.000000	1.411601
1	0.000000	2.147660	-1.174452
1	0.000000	-2.147660	-1.174452
1	0.000000	2.056369	1.296186
1	0.000000	-2.056369	1.296186
1	0.000000	0.000000	-2.458724