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&qmmm
!***** Geometry Optimization
maxcyc=0, ! Number of cycles for geometry optimization [0]
ntpr=1, ! Print results every ntp cycles [1]
grms_tol=0.001, ! Tolerance in eV/A (derivatives) [1.0d-2]

!***** Ground-State and Output Parameters
qm_theory='AM1', ! Integral type, check Amber's SQM for more options [AM1]
scfconv=1.0d-6, ! Ground-state SCF convergence criteria, eV [1.0d-6]
verbosity=1, ! QM/MM output verbosity (0-minimum, 5-maximum)
printcharges=0, ! Print (1) or do not print (0) Mulliken charges of QM atoms [0]
! [1 for dynamics and optimization, 5 for others]
printdipole=1, ! (0) Unrelaxed transitions, (1) Unrelaxed transitions plus
! total molecular, or (2) Unrelaxed/relaxed transitions plus
! total molecular [1 for dynamics, 2 for optimization and single-point]
itrmax=300, ! Max SCF iterations for ground state
! (negative to ignore convergence) [300]

!***** Excited-State Parameters
exst_method=1, ! CIS (1) or RPA (2) [1]
dav_guess=1, ! Restart Davidson from (0) Scratch, (1) Previous,
ftol=1.0d-7, ! Acceptance tolerance (|emin-eold|) [1.0d-5]
dav_maxcyc=200, ! Max cycles for Davidson diagonalization
! (negative to ignore convergence) [100]
calcxdens=.false., ! Print (.true.) or do not print (.false.)
! excited-to-excited transition dipole moments [.false.]

!***** Solvent Models and External Electric Fields
solvent_model=1, ! (0) None, (1) Linear response, (2) Vertical excitation,
! or (3) State-specific [0]
potential_type=1, ! (1) COSMO or (2) Onsager [1]
onsager_radius=14, ! Onsager radius, A (system dependent) [2]
ceps=30, ! Dielectric constant, unitless [10]
linmixparam=1, ! Linear mixing parameter for vertical excitation
! or state-specific SCF calculation [1]
cosmo_scf_ftol=1.0d-5, ! Vertical excitation or state-specific
! SCF tolerance, eV [1.0d-5]
doZ=.false., ! Use relaxed (.true.) or unrelaxed (.false) density for
! vertical excitation or state-specific COSMO or Onsager [.false.]
EF=0, ! (0) None or (1) Electric field in ground- and excited-state [0]
Ex=0, ! Electric field vector X, eV/A [0]
Ey=0, ! Electric field vector Y, eV/A [0]
Ez=0, ! Electric field vector Z, eV/A [0]
&endqmmm

&moldyn
!***** General Parameters
natoms=48, ! Number of atoms
! (must be equal to number of atoms in system)
rnd_seed=911702, ! seed for the random number generator
bo_dynamics_flag=0, ! (0) Non-BO or (1) BO [1]
exc_state_init=2, ! Initial excited state (0 - ground state) [0]
n_exc_states_propagate=4, ! Number of excited states [0]

!***** Dynamics Parameters
time_init=0.0, ! Initial time, fs [0.0]
time_step=0.1, ! Time step, fs [0.1]
n_class_steps=2000, ! Number of classical steps [1]
n_quant_steps=4, ! Number of quantum steps for each classical step [4]
moldyn_deriv_flag=1, ! (0) None, (1) Analytical, or (2) Numerical [1]
num_deriv_step=1.0d-3, ! Displacement for numerical derivatives, A [1.0d-3]
rk_tolerance=1.0d-7, ! Tolerance for the Runge-Kutta propagator [1.0d-7]

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!***** Non-Adiabatic Parameters
decoher_type=2, ! Type of decoherence: Reinitialize (0) Never,
! (1) At successful hops, (2) At successful plus frustrated hops...
dotrivial=1, ! Do unavoided (trivial) crossing routine (1) or not (0) [1]
quant_step_reduction_factor=2.5d-2, ! Quantum step reduction factor [2.5d-2]

!***** Thermostat Parameters
therm_type=1, ! Thermostat type: (0) Newtonian, (1) Langevin,
therm_temperature=300, ! Thermostat temperature, K [300]
therm_friction=20, ! Thermostat friction coefficient, 1/ps [20]

!***** Output & Log Parameters
verbosity=2, ! NEXMD output verbosity (0-minimum, 3-maximum)
! [2 for dynamics, 3 for optimization and single-point]
out_data_steps=1, ! Number of steps to write data [1]
out_coords_steps=1, ! Number of steps to write the restart file [10]
out_data_cube=0, ! Write (1) or do not write (0) view files to generate cubes [0]
out_count_init=0, ! Initial count for view files [0]
&endmoldyn

&coord
6 3.2335139553 8.3884849832 0.4296289066
6 2.0451051193 7.6799490184 0.1048419746
6 2.0936887226 6.3508355975 -0.2658880152
6 3.2989838533 5.6988597499 -0.2441093318
6 4.5246504645 6.3190402874 0.2331806665
6 4.4115259195 7.6446060263 0.6352500572
6 9.2775344897 5.0390092339 0.2138018908
6 8.0485066622 4.3515196254 0.2042294270
6 7.9603581212 2.9406258819 0.1296133412
6 9.1119958718 2.2798612282 -0.0046693370
6 10.3829417511 2.9020765241 0.0242917022
6 10.5318336620 4.2839614246 0.1064485325
6 5.7819827770 5.6656003582 0.2441944500
6 6.8821468767 5.1628217830 0.2565121937
6 11.7693716875 4.9332200048 0.1038455594
6 12.8598725967 5.4546230687 0.1168404527
6 15.1538213416 8.2527510682 -0.3725749594
6 13.9847852186 7.4898059978 -0.2544815675
6 14.1102470620 6.1138147030 -0.0133942990
6 15.4025137575 5.5435682493 0.0597521147
6 16.5197192441 6.3538442242 0.0687827431
6 16.4472883182 7.7527510742 -0.2493725195
6 17.5725500227 8.5520026866 -0.0991388737
6 18.6045985931 9.0435098940 0.2961405851
6 21.0502192459 11.8294485848 0.0335540419
6 19.8483167511 11.1697469022 0.0849063610
6 19.8306995318 9.7447733126 0.2455834842
6 21.0118635439 9.0192874731 0.4738344289
6 22.2149157928 9.7383715364 0.3565301993
6 22.2194593558 11.0584086570 0.0517088118
1 3.1749517410 9.4373930044 0.7220600683
1 1.0916773150 8.2115747202 0.2682213433
1 1.1713098281 5.7583179267 -0.4486754234
1 3.3063992178 4.6452311970 -0.4410805876
1 5.2547659597 8.1471274703 1.1165165804
1 9.3561226272 6.1020869302 0.2083609982
1 7.0146722933 2.3187979684 0.1506406277
1 9.2012679051 1.2001804226 -0.0020359664
1 11.2458569560 2.2653954044 0.0475581581
1 15.1154000027 9.3123278239 -0.6722503208
1 13.0301654988 7.9523337634 -0.4521624080
1 15.5539192507 4.4618968029 0.2942752146

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1 17.4708412871 5.8475298917 0.2982939965
1 21.0407777074 12.9206764640 -0.0995346068
1 18.8539712972 11.7082482982 0.1683484126
1 21.0742899579 7.9251889935 0.4329564310
1 23.1016898068 8.9964933748 0.6085801658
1 23.1808826483 11.6336934015 0.0610173450
&endcoord
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```
&veloc
1.6641412237 -0.9005444764 -0.4231083823
-0.4456776725 0.2636742562 -4.2605108637
-0.9346932194 10.5057862812 1.7013238936
-1.3645373032 -2.2595310369 4.9541498886
-5.6876544606 -3.3297416475 -6.6827474956
-5.6850079331 2.1561342699 2.0845529312
2.5866719557 -1.2826102208 -0.0252563104
-1.1385834787 0.3307591098 -1.9352531695
-1.5378409505 0.3997575308 -5.7355834363
-0.5277608886 -5.1626244423 4.9919822394
2.9736969555 -2.4890202762 -1.8761459098
-4.9126827910 -1.4428448268 -4.5854681724
-2.0824118948 -2.2720043273 1.5500751863
2.0555147476 1.4235435154 4.4927640640
-1.9995722009 2.7751078843 -3.7960654000
-1.3631246120 5.7600628396 3.1753440022
2.2727537198 2.9034425074 2.5379817114
-1.7808060366 -9.4369897846 8.8695743770
4.4915771810 6.6735588491 -3.2439615026
-2.7094346453 -5.1325910865 -1.6946742561
13.1542887450 -2.6057497830 3.9062191623
3.1001412765 -3.6513930814 1.9147794972
0.6646512040 -0.5800537956 -2.7879990230
0.4584037101 5.0105907093 4.7868364896
1.9206173324 -0.2500541746 -4.2328649076
-4.3797535586 -5.2454895582 -0.5821597447
0.7801273217 -0.1197128517 -5.6048143755
0.4400116406 -0.2474433368 0.0102348506
0.1469904344 0.2268372154 -7.6887975220
-2.6166625828 1.5712564320 7.0925500233
15.0105794907 -8.1580832354 -20.4908589368
5.3521114043 -10.8734235419 -7.0904631644
12.1056380533 -21.0994075697 28.1942100483
1.6903173925 2.7433357666 14.7823949844
-0.1763305616 5.5198361730 -0.2460250589
12.6571343733 18.8651516683 5.9547671169
2.1616926047 13.1620175067 -8.6554343833
21.6181161789 16.7964378469 -11.2387109247
-0.8677581786 -4.3546611127 13.9957399420
-23.6723766650 10.3738886641 -3.0620997027
14.1532876230 17.7611720182 -10.5015010609
13.9427376186 -9.4659174873 18.6049622268
-5.2756397074 26.9235336428 -11.2020179845
-4.8077738857 17.8134795637 7.7146402788
-19.6104825455 -8.6429178527 1.6094179848
-11.0392983872 -10.2142466930 -21.7259690821
-5.2299655489 -1.0301789700 21.5760141163
1.4944348928 20.8451180486 18.8593969193
&endveloc
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&coeff
0.000 0.000
1.000 0.000
0.000 0.000
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