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&qmmm
!***** Geometry Optimization
maxcyc=0, ! Number of cycles for geometry optimization [0]
ntpr=1, ! Print results every ntpr 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-8, ! Ground-state SCF convergence criteria, eV [1.0d-6]
verbosity=5, ! 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=2, ! (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,
ftol0=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=0, ! (0) None, (1) Linear response, (2) Vertical excitation,
! or (3) State-specific [0]
potential_type=1, ! (1) COSMO or (2) Onsager [1]
onsager_radius=2, ! Onsager radius, A (system dependent) [2]
ceps=10, ! 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=19345, ! Seed for the random number generator
bo_dynamics_flag=1, ! (0) Non-BO or (1) BO [1]
exc_state_init=0, ! Initial excited state (0 - ground state) [0]
n_exc_states_propagate=11, ! 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=0, ! 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=3, ! 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=10, ! 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 3.2382494409 8.4391304456 0.1481165467
6 2.0825041799 7.6324792614 0.1841037864
6 2.0727699444 6.2084297599 0.2076345859
6 3.3284187743 5.6054864196 0.0856702772
6 4.5363245423 6.3558337363 0.1649473776
6 4.5059575694 7.7802339951 0.1347934451
6 9.3080908837 5.0221966350 0.1483496690
6 8.0552468165 4.4718864670 0.1686612864
6 7.9160784227 3.0532592794 0.0357965628
6 9.0253754223 2.2348174271 0.0262094963
6 10.2786545836 2.8215669614 -0.0152162266
6 10.4361325150 4.2160775165 0.0653731003
6 5.8001614357 5.7684592129 0.1474262416
6 6.8388899585 5.1918900805 0.3273900952
6 11.7479902537 4.8698672783 0.1255701031
6 12.7890089771 5.4681119394 -0.0274648085
6 15.2619908177 8.2469037222 -0.1397841439
6 14.0844962257 7.5863282678 -0.1611425103
6 14.0067806922 6.1866232727 -0.0657934336
6 15.2443113947 5.4509072852 0.0055335087
6 16.4374344747 6.1428278878 0.0651277807
6 16.4948584158 7.5391487628 0.0109680854
6 17.7046054164 8.2784959690 0.0657182581
6 18.7333257568 8.8923495537 0.0606564392
6 20.9556467053 11.9360668330 0.1427670451
6 19.8099821386 11.1485394638 0.0660685423
6 19.8614368183 9.7281378443 0.1667036245
6 21.1682414595 9.1370110132 0.2387406755
6 22.2832520394 9.9313922317 0.2555725838
6 22.2053900101 11.3492694169 0.3139389290
1 3.1700923305 9.5425723807 0.1838685039
1 1.1397797031 8.1239294863 0.3450759951
1 1.1912064951 5.5940347823 0.4181650710
1 3.2652893448 4.4657903304 0.1244908523
1 5.4968766174 8.2626960136 0.2063603177
1 9.4315926493 6.1266629444 0.3781039822
1 6.9116472861 2.6914159709 -0.0849428440
1 8.9465164482 1.1171825341 0.1035026374
1 11.1632451852 2.1863680151 -0.1940571844
1 15.2174596139 9.3800341090 -0.1144121929
1 13.2009773673 8.1867984627 -0.1809783396
1 15.2232014967 4.3268053441 -0.0457315313

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1 17.4080259817 5.5842120228 0.1979887702
1 20.8720337831 13.0116770957 -0.0027173173
1 18.7811692245 11.5392510442 -0.0074557744
1 21.1681027467 8.0358354981 0.4101710065
1 23.2312690355 9.4268937739 0.2884658252
1 23.1051189293 12.0125787527 0.4686192969
&endcoord
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&veloc
2.1351254570 -3.1322859594 -3.3221372695
-3.0261938429 -2.9524907855 1.0837643553
0.9864372938 -3.5689235029 4.1968814081
-1.4771642791 4.6363195034 0.6729707429
-0.6078126880 7.9483605865 0.3553665601
0.7538461137 3.7388448334 1.9710639972
-6.0356627059 -0.4512098998 -1.1021543160
-3.6039004191 -2.4738508103 3.5449482243
-6.8259304999 -3.1808652270 -2.2082866264
-0.8151983379 10.0867103317 5.1584130349
-1.8015069527 -0.5185448235 -4.4346747590
-1.3562648193 3.5531871280 0.4313255521
1.8140089856 -6.7728069026 -2.7940724098
0.3599059918 -2.0760276739 2.4247096940
0.5973986010 -0.0953433815 -7.4403212872
1.4648649017 -7.0645683979 -2.2401420453
3.8462353215 -2.4314546396 -0.9668975427
-2.0280802297 5.9891697267 -1.2629530578
2.2783844795 0.5609713082 4.4295281500
6.3679782629 1.7269762972 1.3722025484
1.9136508855 -1.9644153514 2.2823549354
-2.3827519551 4.5559141706 10.0418465191
4.5460910734 3.1818706953 5.2524444390
-2.1713619169 -2.6522066243 3.3762802052
1.7961958240 6.4586445653 -2.1576394960
-6.0309908817 1.7786007138 -0.3006062039
4.1451335165 -0.0515882270 -13.0173273182
4.7379427741 -6.0907847445 -2.1001157644
3.2565762223 -1.9491458616 -0.8744297629
-3.0466265936 0.2283682632 6.2147199998
6.1752762985 8.1569045012 0.4841897721
-0.9557429322 -16.3363675704 -32.5836841477
22.8282971068 7.7073804297 0.8088593147
-7.4277174808 -38.5371604184 -2.4703922305
7.7075581696 -3.7202549910 2.1842484997
-26.4161053886 -10.5484459404 -5.9636428464
7.3898371455 -17.5523914749 -39.6390667821
-0.4411664060 -15.0092592387 -7.9300336005
-10.3612856581 9.9811110240 -12.1454355010
23.4238044194 18.5390608139 25.6276386847
4.5997462396 21.1495358672 8.3961339131
8.4576721348 9.8219899858 1.3915994947
33.7952587369 -13.1902650866 10.1348833135
-11.3837074446 -13.1326733551 -31.9786931408
-9.1838511191 -11.0623769489 -13.7174007000
-24.4751153499 -10.7875663822 8.3997422214
-7.3024559441 23.0150309540 -36.6521385895
-13.9119511409 -32.7805475782 22.5139845571
&endveloc
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&coeff
0.00 0.00
0.00 0.00
0.00 0.00
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0.00 0.00
0.00 0.00
0.00 0.00
0.00 0.00
0.00 0.00
&endcoeff
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