**ELECTRONIC SUPPLEMENTARY MATERIAL**

**DFT and TD-DFT study on quadratic NLO response and optoelectronic activity in novel Y-Shaped imidazole-based push-pull chromophores**

Lamia Kara Zaitri and Sidi Mohamed Mekelleche\*

Laboratory of Applied Thermodynamics and Molecular Modeling, Department of Chemistry,

Faculty of Science, University of Tlemcen, BP 119, Tlemcen, 13000, Algeria

\*email of the corresponding author: sm\_mekelleche@mail.univ-tlemcen.dz

**S2-17** Cartesian coordinates of the CAM-B3LYP/6-31G (d,p) optimized ground-states of derivatives D1-D8**.**

**S18-32** Cartesian coordinates of the TD-CAM-B3LYP/6-31G(d,p) optimized singlet excited states of derivatives D1-D8.

Derivative D1 (CAM-B3LYP/6-31G (d,p) optimized ground-state )

 O 8.19105400 0.95875200 -0.54470200

 O 8.25795300 -0.92627600 0.51656900

 N 1.13007700 -1.20556200 0.02178300

 N 1.26864900 1.00618100 0.00185200

 N 7.65549600 -0.00016600 -0.00809400

 N -4.67844700 -4.19517700 -0.25707200

 N -3.99889100 4.77700900 0.08661100

 C -0.16967500 -0.72280700 0.01926600

 C -0.05346500 0.65621700 0.01900800

 C 1.95821300 -0.11355100 0.01082000

 C 3.42469900 -0.14008800 0.01769600

 C 4.09888300 0.93838800 -0.57246300

 C 5.47990200 0.99258000 -0.58223800

 C 6.19316100 -0.04384100 0.00604000

 C 5.56026400 -1.11511300 0.61521000

 C 4.17480700 -1.15553400 0.62324600

 C -1.33616300 -1.61704900 -0.03909300

 C -1.55865700 -2.60408500 0.92452000

 C -2.65439200 -3.44915700 0.86575400

 C -3.59400400 -3.34309400 -0.17669000

 C -3.38067400 -2.33535400 -1.13710900

 C -2.27598200 -1.50531900 -1.06768000

 C -1.09469100 1.69516300 0.04907600

 C -2.37541600 1.48005800 0.56102900

 C -3.32671200 2.48725800 0.58639600

 C -3.03966000 3.77202300 0.09398000

 C -1.73991200 3.99509300 -0.39439600

 C -0.80060000 2.97910200 -0.41481400

 C -4.96215200 -5.09067800 0.84299900

 C -5.71908500 -3.93322400 -1.22776800

 C -5.22301200 4.57961100 0.83096900

 C -3.58253600 6.13772700 -0.17465100

 H 3.50983900 1.73227400 -1.01458200

 H 6.01551200 1.81471900 -1.03827400

 H 6.15552500 -1.88884800 1.08172200

 H 3.68000900 -1.97141500 1.13483600

 H -0.86576100 -2.70408500 1.75491000

 H -2.78111400 -4.18846700 1.64549000

 H -4.07969800 -2.19847500 -1.95147300

 H -2.13940600 -0.74113000 -1.82571400

 H -2.63760500 0.50947300 0.96621500

 H -4.29905100 2.26624800 1.00665900

 H -1.45306000 4.97147700 -0.76234300

 H 0.19750800 3.17877400 -0.78822000

 H -4.12931700 -5.77989800 1.01725000

 H -5.83714500 -5.69211900 0.59807700

 H -5.16428200 -4.55943100 1.78402700

 H -6.20535800 -2.95886400 -1.07805100

 H -5.32447700 -3.95982700 -2.24870100

 H -6.48117100 -4.70838800 -1.15232700

 H -5.77681900 3.71503500 0.45253700

 H -5.05445900 4.42792900 1.90782800

 H -5.86202900 5.45409000 0.70582200

 H -3.13705500 6.22737600 -1.16995700

 H -2.85233800 6.51374600 0.55750100

 H -4.45645300 6.78916300 -0.15057300

 C 1.49588000 -2.59679400 -0.17951300

 H 2.41583500 -2.65310900 -0.76014300

 H 1.64002400 -3.12269400 0.76853400

 H 0.69797500 -3.09455700 -0.72908200

Derivative D2 (CAM-B3LYP/6-31G(d,p) optimized ground-state)

 N 0.93020700 -1.16489500 -0.02340000

 N 1.04800300 1.04719200 -0.03663400

 C -0.37525700 -0.69725400 -0.02700000

 C -0.27031700 0.68027000 -0.04213600

 C 1.75003700 -0.06410800 -0.02801900

 C 3.21601500 -0.10333900 -0.00538700

 C 3.90611600 0.90417100 0.67507900

 C 5.28608900 0.94376100 0.70408300

 C 6.05546500 -0.03690800 0.04531600

 C 5.35910800 -1.03337100 -0.66415800

 C 3.97481200 -1.05840800 -0.68484600

 C -1.53385000 -1.59955300 0.02961500

 C -1.67493100 -2.65239100 -0.88380600

 C -2.76160400 -3.50981700 -0.82069200

 C -3.71512300 -3.30045100 0.16333200

 C -3.61411900 -2.26447800 1.08001500

 C -2.51777800 -1.42103100 1.01086500

 C -1.31223800 1.71608600 -0.09889100

 C -2.58203600 1.48269300 -0.64057100

 C -3.53277900 2.48910100 -0.68084500

 C -3.20159900 3.74068500 -0.18422500

 C -1.94573500 4.01283900 0.33947800

 C -1.00632600 2.99776700 0.37609500

 H 3.33368200 1.67320100 1.18136100

 H 5.77041600 1.74620500 1.24420700

 H 5.89870700 -1.78853800 -1.21969000

 H 3.48409500 -1.82478500 -1.27563100

 H -0.93313500 -2.78785500 -1.66316800

 H -2.88888400 -4.32571800 -1.51992400

 H -4.38210900 -2.14262100 1.83250800

 H -2.82594800 0.51092500 -1.05129000

 H -4.51764700 2.32644900 -1.09834100

 H -1.72716700 5.00678900 0.70702500

 H -0.01263700 3.18057200 0.76595200

 C 1.33137000 -2.54184500 0.21376000

 H 2.28452700 -2.54790200 0.74004800

 H 0.58143800 -3.03646700 0.83058500

 H 1.44010700 -3.10201300 -0.71867100

 N 7.43300700 -0.01845300 0.09244400

 N -4.20252700 4.80706300 -0.22360200

 O -3.88482200 5.90281200 0.21621800

 O -5.30010300 4.54129000 -0.69284100

 N -4.86665100 -4.20505100 0.23741100

 O -5.69518100 -3.99661900 1.11025600

 O -4.92622300 -5.11339800 -0.57773500

 C 8.11380300 1.11374000 0.68405200

 H 9.18943400 0.94600100 0.64105200

 H 7.89397600 2.05753800 0.16634400

 H 7.84168900 1.23440300 1.73781300

 C 8.18889700 -0.94245400 -0.72499600

 H 9.25254700 -0.79581600 -0.54032700

 H 7.95155400 -1.98126200 -0.47220300

 H 8.00665200 -0.80459500 -1.79995000

 H -2.41305900 -0.61239500 1.72488200

Derivative D3 (CAM-B3LYP/6-31G(d,p) optimized ground-state)

 N -1.35714500 0.98002500 -0.09823700

 N -1.42124000 -1.21631400 -0.01519400

 N -6.57793900 4.80022900 0.24671500

 N -7.02360700 -4.47040200 0.03667200

 C -2.69428100 0.64616800 -0.05052600

 C -2.70852300 -0.73893700 -0.01749500

 C -0.62661200 -0.17067200 -0.05999000

 C -3.72009100 1.69272900 -0.00130800

 C -3.61409600 2.84439400 -0.78525300

 C -4.54810300 3.86533100 -0.71596900

 C -5.64945000 3.77906400 0.15413700

 C -5.76506900 2.61045700 0.93170700

 C -4.81861500 1.60480200 0.85894300

 C -3.84142000 -1.67701300 -0.01190100

 C -5.07641200 -1.38133200 -0.59122600

 C -6.11882700 -2.29421000 -0.58792100

 C -5.97281600 -3.56194700 0.00156200

 C -4.71815400 -3.86986100 0.55713500

 C -3.68700500 -2.94660100 0.54844400

 C -6.53224700 5.88685300 -0.70676200

 C -7.79959100 4.58218200 0.99071300

 C -8.19530500 -4.21363400 -0.77136600

 C -6.74802700 -5.84226500 0.40407700

 H -2.79255500 2.93786900 -1.49029700

 H -4.42116300 4.72825900 -1.35615400

 H -6.59763200 2.48669200 1.61148900

 H -4.53919700 -4.84018400 1.00151200

 H -2.72596200 -3.21116300 0.97524300

 H -5.58080700 6.42533100 -0.64671100

 H -7.32429000 6.59886600 -0.47594500

 H -6.66565200 5.55039400 -1.74516300

 H -7.58923000 4.36930500 2.04376800

 H -8.40513100 5.48755300 0.95622100

 H -8.40021100 3.75251000 0.59110000

 H -8.67753800 -3.27687100 -0.47594300

 H -7.97370000 -4.15479000 -1.84768100

 H -8.91899200 -5.01406200 -0.61545600

 H -6.34909900 -5.90345600 1.42104500

 H -6.03114400 -6.33401300 -0.27041700

 H -7.67847900 -6.41027400 0.38609700

 C 0.83376900 -0.22239800 -0.07397900

 C 1.46999300 -1.45255800 0.11219100

 C 1.62603000 0.91327500 -0.27461000

 C 2.85022500 -1.53496200 0.10701300

 H 0.85511400 -2.33291700 0.25686400

 C 3.00664100 0.82628400 -0.27546800

 H 1.16622400 1.88046100 -0.45417600

 C 3.65155900 -0.40044400 -0.07565300

 H 3.32691500 -2.49978300 0.25444800

 H 3.58892800 1.72409100 -0.45188500

 C 5.10756000 -0.55041300 -0.05694600

 H 5.45193800 -1.58196600 -0.03712300

 C 6.01606400 0.43452100 -0.03667500

 H 5.67782600 1.46700600 -0.00237600

 C 7.47143200 0.26695100 -0.02195000

 C 8.27539600 1.38359000 0.24689700

 C 8.10515300 -0.96032600 -0.27104100

 C 9.65581100 1.28833600 0.28569700

 H 7.80292100 2.34239900 0.43461900

 C 9.48247100 -1.07363100 -0.23445900

 H 7.51458500 -1.83666000 -0.51106400

 C 10.24133800 0.05494400 0.04615300

 H 10.28359500 2.14400600 0.49653000

 H 9.98236000 -2.01400000 -0.42593400

 N 11.69871100 -0.05951200 0.08220800

 O 12.18872100 -1.15866700 -0.13435300

 O 12.34293400 0.95044600 0.32745600

 H -1.00727000 1.92148000 -0.02499900

 H -4.93238800 0.72575600 1.48383800

 H -7.04973000 -2.01472300 -1.06356200

 H -5.22771400 -0.42160200 -1.07290000

Derivative D4 (CAM-B3LYP/6-31G(d,p) optimized ground-state)

 O 8.38424800 1.18025100 -0.46959800

 O 8.47886300 -0.68809900 0.61899000

 N 1.39033400 -1.20027000 -0.08943700

 N 1.45575000 1.03426700 0.01909300

 N 7.86399300 0.21360600 0.06757800

 N -4.97749700 -3.31843500 -0.13592900

 N -4.50701300 3.79514500 -0.05009800

 C 0.07654200 -0.75900500 -0.05385400

 C 0.15493700 0.61731200 0.00596400

 C 2.17414100 -0.06442700 -0.03340600

 C 3.64140500 -0.04690300 -0.00575000

 C 4.29649500 1.04195400 -0.59607300

 C 5.67595200 1.13521400 -0.57343200

 C 6.40254200 0.12817200 0.04782500

 C 5.78685600 -0.95202100 0.65941200

 C 4.40333700 -1.03154100 0.63478400

 C -1.17876900 -1.45811200 -0.06173100

 C -1.32078000 -2.85588500 -0.01857900

 C -2.54914500 -3.47143500 -0.02850600

 C -3.73378700 -2.70645400 -0.08545500

 C -3.60149400 -1.31818100 -0.08411600

 C -2.36048600 -0.66516100 -0.07164200

 C -1.02061000 1.43693100 0.02254800

 C -2.28053000 0.80706200 -0.03906300

 C -3.42749200 1.61950900 -0.04947500

 C -3.35937700 3.01161900 -0.00674000

 C -2.07986700 3.61076100 0.07364100

 C -0.94782100 2.83479100 0.08272500

 C -5.07877000 -4.73612700 0.13652500

 C -6.16594300 -2.50956400 0.01805600

 C -5.79561700 3.15433700 0.08044100

 C -4.41332900 5.20044600 0.28368500

 H 3.69657400 1.81239900 -1.06458300

 H 6.19976300 1.96509200 -1.02912300

 H 6.39283700 -1.70009500 1.15313400

 H 3.91449300 -1.85037600 1.14915200

 H -0.44380500 -3.48553500 0.04833400

 H -2.59018900 -4.55146400 0.01659600

 H -4.49694600 -0.71776600 -0.08212000

 H -4.39931200 1.15396400 -0.09460000

 H -1.97897800 4.68659700 0.12640500

 H 0.03284800 3.29447600 0.13863200

 H -4.50515500 -5.32028100 -0.58971700

 H -6.12086800 -5.04229300 0.04593400

 H -4.72889300 -5.00743000 1.14337200

 H -6.21065800 -1.99088400 0.98737800

 H -6.23089300 -1.75428700 -0.77172100

 H -7.04594300 -3.14683700 -0.06837700

 H -5.96533400 2.44453500 -0.73588200

 H -5.91216200 2.61065000 1.03044800

 H -6.57923400 3.90978600 0.02162800

 H -3.76253100 5.73161400 -0.41749600

 H -4.03295800 5.37792300 1.30039400

 H -5.40324100 5.65065800 0.20844400

 C 1.83759600 -2.53219700 -0.45534000

 H 2.85991500 -2.48058200 -0.82413800

 H 1.80451000 -3.22074500 0.39404200

 H 1.20640200 -2.92310000 -1.25440200

Derivative D5 (CAM-B3LYP/6-31G(d,p) optimized ground-state)

 N -1.31119500 -1.73750500 0.08132100

 N -0.81021100 0.43649700 0.27111100

 N -7.95899400 -2.53278200 -0.39928700

 N -6.08262400 4.34003000 -0.10365600

 C -2.51028000 -1.04178500 0.04648100

 C -2.16270400 0.28974200 0.15214400

 C -0.32464000 -0.78480800 0.23160400

 C -3.87667200 -1.47404500 -0.05223800

 C -4.29746100 -2.81532200 -0.05364800

 C -5.62099200 -3.17131000 -0.15123400

 C -6.62320300 -2.18350500 -0.25819600

 C -6.21702600 -0.85046800 -0.21246100

 C -4.87370800 -0.46003500 -0.11052700

 C -3.14956600 1.32801200 0.11694100

 C -4.50339700 0.96514000 -0.03588800

 C -5.46169800 1.99197500 -0.09398500

 C -5.11937500 3.34106300 -0.01184700

 C -3.75355100 3.66964400 0.15915300

 C -2.80239300 2.68186400 0.21626300

 C -8.35786200 -3.90421200 -0.16730000

 C -8.96892900 -1.50432700 -0.28729700

 C -7.47856200 3.96957000 -0.05831500

 C -5.73064200 5.69383600 0.26828200

 H -3.56980100 -3.60914500 0.04862300

 H -5.87939600 -4.22168100 -0.13631500

 H -6.97304700 -0.08247800 -0.24673500

 H -6.50191600 1.73190800 -0.21013100

 H -3.44324000 4.70249500 0.24455100

 H -1.75493100 2.93345200 0.34146900

 H -7.86490600 -4.58311900 -0.86991500

 H -9.43166600 -3.99489600 -0.33089100

 H -8.13668700 -4.25150400 0.85278600

 H -8.83297300 -0.73666200 -1.05578100

 H -9.95159600 -1.94965400 -0.44282900

 H -8.96842500 -1.00548200 0.69350700

 H -7.73921100 3.31802200 -0.89887400

 H -7.75641900 3.44913600 0.87106800

 H -8.09068300 4.86765300 -0.14217300

 H -4.94225700 6.08985600 -0.37889700

 H -5.38928800 5.78074900 1.31038800

 H -6.60303600 6.33525100 0.14222700

 C -1.10500100 -3.13200900 -0.25711300

 H -0.07292700 -3.27123600 -0.57290500

 H -1.30809400 -3.79243200 0.59138400

 H -1.75665500 -3.40751700 -1.08695700

 C 1.09728500 -1.06325100 0.33631400

 C 1.77126700 -2.15768500 0.82368800

 S 2.20682300 0.17550700 -0.14451600

 C 3.17666000 -2.00403800 0.79909200

 H 1.27753400 -3.02923800 1.23323000

 C 3.58062800 -0.79139100 0.29673000

 H 3.86371200 -2.75620100 1.16673400

 C 4.91770500 -0.25755100 0.11741700

 H 4.96872300 0.78919800 -0.17099200

 C 6.05542200 -0.95305400 0.26847600

 H 5.99331200 -2.00961400 0.51716300

 C 7.41430100 -0.43409600 0.11069200

 C 8.48630000 -1.33749100 0.14277600

 C 7.70207400 0.92841300 -0.06769600

 C 9.79491500 -0.91242900 -0.00800300

 H 8.28333500 -2.39403500 0.28511500

 C 9.00291400 1.36938300 -0.22169200

 H 6.90028900 1.65744000 -0.07566700

 C 10.03482700 0.44042100 -0.19101500

 H 10.62766600 -1.60295500 0.01289700

 H 9.23691700 2.41685400 -0.35900200

 N 11.41263500 0.90328600 -0.35032200

 O 11.59534200 2.10178500 -0.50927500

 O 12.30208700 0.06490300 -0.31580000

Derivative D6 (CAM-B3LYP/6-31G(d,p) optimized ground-state)

 O -11.66967200 -0.89777600 0.09899400

 O -11.58264200 1.27585800 0.01869200

 N 1.48349400 -1.28119600 -0.10028100

 N 1.33071100 0.94877200 0.00395800

 N -11.06510000 0.16489600 0.05322700

 N 7.93150600 -3.15240400 -0.10612500

 N 7.18348900 3.93913200 -0.05163500

 C 2.78009800 -0.78960200 -0.06083700

 C 2.64775300 0.58184200 -0.00480800

 C 0.65566700 -0.17678000 -0.04956800

 C -0.81184000 -0.22049700 -0.03628200

 C -1.51148700 0.82395200 -0.65142900

 C -2.89330600 0.85300500 -0.64239400

 C -3.62966600 -0.15438600 -0.00564400

 C -2.93062700 -1.18750300 0.62372200

 C -1.54444100 -1.21891500 0.61165100

 C 4.06154000 -1.43942400 -0.06004300

 C 4.25769300 -2.83063500 -0.01418200

 C 5.50916400 -3.39802100 -0.01507400

 C 6.66377600 -2.58811400 -0.06519400

 C 6.47776700 -1.20649000 -0.06814500

 C 5.21200900 -0.60173500 -0.06522600

 C 3.79047000 1.44617300 0.01461100

 C 5.07450300 0.86586300 -0.03834300

 C 6.18903500 1.72281100 -0.04632300

 C 6.06643700 3.11102900 -0.00946700

 C 4.76413900 3.66003000 0.06284200

 C 3.66319200 2.84051400 0.06942500

 C 8.08427600 -4.56253700 0.18051600

 C 9.08523500 -2.29767100 0.06326100

 C 8.49458900 3.34888400 0.09217100

 C 7.03406900 5.33910700 0.28395600

 H -0.94422100 1.60769000 -1.13920400

 H -3.41448100 1.65288500 -1.15719200

 H -3.47455700 -1.95836900 1.16009500

 H -1.03161300 -2.00845300 1.14930200

 H 3.40519600 -3.49374600 0.04697000

 H 5.59134200 -4.47568700 0.03156700

 H 7.34905500 -0.57145200 -0.06201500

 H 7.17836600 1.29514500 -0.08527000

 H 4.62122600 4.73132800 0.11109700

 H 2.66480400 3.26115100 0.11884600

 H 9.13778600 -4.83014000 0.09924600

 H 7.53817400 -5.17433100 -0.54408800

 H 7.73790000 -4.83832900 1.18752600

 H 9.12982700 -1.53937400 -0.72494900

 H 9.09811800 -1.77872500 1.03354100

 H 9.99065400 -2.89974200 -0.01354800

 H 8.62559600 2.81630600 1.04670100

 H 8.69671500 2.64061700 -0.71799100

 H 9.24932100 4.13324100 0.03284800

 H 6.64793000 5.50094000 1.30125300

 H 6.36202600 5.84441200 -0.41618300

 H 8.00521900 5.82849200 0.20779800

 C 1.08722400 -2.63011700 -0.45967700

 H 1.14688700 -3.31349900 0.39257500

 H 0.06280600 -2.61743800 -0.82620100

 H 1.73156900 -3.00122600 -1.25794200

 C -7.51480100 -0.68958300 0.04257900

 C -7.26768400 0.67572200 -0.01221100

 C -5.09584400 -0.10477200 0.00415500

 S -6.03253700 -1.58748000 0.05629200

 C -5.88900300 1.00962900 -0.03240800

 H -5.49574900 2.01735800 -0.04110400

 C -9.63619200 0.11437600 0.03874400

 C -8.88699100 -1.02412000 0.07171100

 S -8.73240300 1.59951800 -0.02600400

 H -9.32157400 -2.01292900 0.11367500

Derivative D7 (CAM-B3LYP/6-31G(d,p) optimized ground-state)

 N -3.27886300 -1.82747800 0.04954900

 N -2.61601400 0.28579300 0.37755600

 N -9.96256200 -2.07321000 -0.54092100

 N -7.56364500 4.60484400 0.15419000

 C -4.41993300 -1.03946300 0.03697300

 C -3.97308900 0.25219400 0.22831900

 C -2.22505600 -0.96527400 0.27254000

 C -5.81354300 -1.35724800 -0.10680900

 C -6.33743700 -2.65927600 -0.18707900

 C -7.68321700 -2.90424700 -0.31710700

 C -8.60451500 -1.83685100 -0.37448600

 C -8.09637600 -0.54442800 -0.25150100

 C -6.72762200 -0.26641900 -0.12194800

 C -4.87516900 1.36538300 0.23258200

 C -6.24866500 1.11944800 0.03115700

 C -7.12002400 2.22194500 -0.01043700

 C -6.67790400 3.53229600 0.16620500

 C -5.29326100 3.74362900 0.36847500

 C -4.42453400 2.68162200 0.39955700

 C -10.46887700 -3.41841200 -0.37195100

 C -10.89010700 -0.97650100 -0.37519700

 C -8.92757600 4.37863300 -0.26602800

 C -7.03842800 5.94907800 0.04153700

 H -5.67533700 -3.51221000 -0.12091500

 H -8.02292700 -3.93024600 -0.36273500

 H -8.79013300 0.28078000 -0.23690200

 H -8.16913500 2.05319400 -0.19513000

 H -4.90318000 4.74461700 0.49573100

 H -3.36249000 2.84377900 0.54761900

 H -10.02631300 -4.10173700 -1.10315000

 H -11.54549300 -3.41738600 -0.54243100

 H -10.28167900 -3.82722900 0.63201600

 H -10.68350500 -0.17806800 -1.09477000

 H -11.90245100 -1.33255900 -0.56655300

 H -10.86422200 -0.53832800 0.63393600

 H -9.00533300 4.00265800 -1.29781300

 H -9.42531700 3.65907600 0.39208500

 H -9.48212600 5.31496600 -0.20166200

 H -6.44754400 6.10658100 -0.87284900

 H -6.40667100 6.20037900 0.89877800

 H -7.86859200 6.65560500 0.03543600

 C -3.17373200 -3.21155700 -0.36822600

 H -2.15070700 -3.41035100 -0.68175400

 H -3.43787900 -3.90276000 0.43790800

 H -3.83263900 -3.38797400 -1.21900100

 C -0.83118000 -1.36002900 0.38050200

 C -0.25276600 -2.53113600 0.80810300

 S 0.38015600 -0.18469500 -0.00708100

 C 1.16083500 -2.48673400 0.81245800

 H -0.81947300 -3.38466400 1.15675300

 C 1.66677600 -1.28161300 0.39130500

 H 1.78122500 -3.30995800 1.14462200

 C 3.04502300 -0.84621900 0.26228100

 H 3.18603200 0.21448800 0.07097500

 C 4.11870900 -1.64693100 0.34888900

 H 3.96358700 -2.71340500 0.49402800

 C 5.51791400 -1.23530500 0.24500000

 C 6.51158400 -2.22172900 0.18150300

 C 5.92722500 0.10599600 0.20948700

 C 7.85048500 -1.89422300 0.07410700

 H 6.21985500 -3.26702600 0.21314400

 C 7.26321500 0.43943800 0.10087800

 H 5.19364900 0.90089900 0.27966100

 C 8.24587500 -0.55415500 0.02991400

 H 8.61055600 -2.66450700 0.02262000

 H 7.54150500 1.48891600 0.07813000

 N 12.99542000 1.60787800 -0.36779900

 O 12.80058100 2.81766200 -0.36954500

 O 14.08742600 1.06276000 -0.44515600

 C 9.66954400 -0.23688900 -0.08367500

 C 11.83915500 -0.59769300 -0.24617900

 C 11.84848200 0.76365000 -0.26688900

 S 10.25380900 1.40882100 -0.15350700

 H 12.72692100 -1.21302700 -0.30551400

 N 10.60587200 -1.15351000 -0.14268800

Derivative D8 (CAM-B3LYP/6-31G(d,p) optimized ground-state)

 N 5.72395800 -1.66542200 0.09507600

 N 5.20536600 0.49210300 -0.20562500

 N 12.38998500 -2.41917800 0.28935600

 N 10.47214600 4.42075300 -0.28581400

 C 6.91963700 -0.96631100 0.03707500

 C 6.56205600 0.35627500 -0.13476800

 C 4.72908900 -0.72627600 -0.07255700

 C 8.29107600 -1.38973900 0.10072000

 C 8.71761500 -2.72800600 0.15497800

 C 10.04601600 -3.07516800 0.20586800

 C 11.04778000 -2.08089600 0.20379100

 C 10.63304800 -0.75296100 0.10542600

 C 9.28447200 -0.37165900 0.05662400

 C 7.54434400 1.39796600 -0.19518800

 C 8.90435900 1.04719300 -0.07361900

 C 9.85847900 2.07914100 -0.08735300

 C 9.50845500 3.42011700 -0.24253000

 C 8.13457900 3.73716000 -0.36404400

 C 7.18676800 2.74486000 -0.34029700

 C 12.78312500 -3.80094000 0.11470400

 C 13.38838200 -1.39555400 0.07498000

 C 11.84079500 4.08865100 0.03730200

 C 10.06073500 5.80206200 -0.15068600

 H 7.99009300 -3.52817200 0.13109200

 H 10.30844900 -4.12418500 0.23555800

 H 11.38576400 0.01663000 0.04505500

 H 10.90050600 1.83052800 0.03732900

 H 7.81555400 4.76512600 -0.47278300

 H 6.13365700 2.98886900 -0.42723100

 H 12.33533600 -4.43944300 0.88247100

 H 13.86502600 -3.87906400 0.22078600

 H 12.50583800 -4.20663400 -0.86926300

 H 13.28527800 -0.58894600 0.80782000

 H 14.37949900 -1.82974700 0.20611300

 H 13.33833900 -0.94941900 -0.92952900

 H 11.96175000 3.70295600 1.06121600

 H 12.23430000 3.33616800 -0.65386500

 H 12.45989500 4.97984800 -0.06641400

 H 9.53350000 6.00399600 0.79318200

 H 9.40605100 6.10340700 -0.97411500

 H 10.94296400 6.44105600 -0.18993200

 C 5.53661000 -3.04100400 0.51341700

 H 4.52394600 -3.16209200 0.89336100

 H 5.69335600 -3.74332200 -0.31067300

 H 6.23194400 -3.27541400 1.31970300

 C 3.30593300 -1.00759500 -0.10859700

 C 2.59496900 -2.12538400 -0.45586100

 S 2.19592800 0.27425900 0.26728700

 H 3.02983900 -3.06060900 -0.78219200

 C 0.87596500 -0.81357700 -0.05861200

 N -15.76269400 0.58513100 0.02683100

 O -16.00840400 1.73124100 0.38023900

 O -16.59002900 -0.26638900 -0.26223300

 C -12.01160100 0.04447000 -0.04535600

 C -13.89756600 -1.00709500 -0.42477600

 C -14.38304800 0.21142800 -0.05439200

 S -13.12318200 1.32429900 0.32806800

 H -14.51093300 -1.85207900 -0.70638200

 N -12.54187000 -1.09282500 -0.41657300

 C -0.51135500 -0.41364900 0.04828500

 C -1.05697600 0.78559300 0.41457700

 S -1.78149600 -1.53667700 -0.32206200

 H -0.48506100 1.66141000 0.69691500

 C -2.93849100 -0.28802800 0.04931900

 C -8.17475300 0.11773800 0.07225800

 C -8.70867300 1.32675800 0.44004300

 C -10.58057800 0.26028400 0.05872800

 S -9.44440600 -0.99540900 -0.30882200

 H -8.13151800 2.19715800 0.72804100

 C -4.36785000 -0.49640400 -0.04074700

 C -5.07582800 -1.61070000 -0.40008600

 C -6.78748700 -0.28724800 -0.02350800

 S -5.46773800 0.79042200 0.33658100

 H -4.63220300 -2.55713100 -0.68529300

 N -10.06528300 1.40061900 0.43036300

 N -6.43139200 -1.48950400 -0.38911000

 N -2.41737000 0.85257100 0.41363000

 N 1.23574200 -2.01411000 -0.42135800

Derivative D1 (TD-CAM-B3LYP/6-31G (d,p) optimized excited state)

 O -8.17859800 0.98855700 0.49610600

 O -8.22769300 -0.95311200 -0.54914500

 N -1.10730300 -1.20911700 -0.01824500

 N -1.23653000 1.02395300 0.08924200

 N -7.59131400 0.00103300 -0.02381000

 N 4.70035200 -4.14730500 0.18052800

 N 3.90938700 4.80427400 -0.23444900

 C 0.18599600 -0.74893600 0.00521600

 C 0.07203700 0.66945800 0.05274400

 C -1.94774700 -0.09624100 0.03294900

 C -3.38515700 -0.13211200 0.01710800

 C -4.09089500 0.96975900 0.57149700

 C -5.45973900 1.01764000 0.56645300

 C -6.19645800 -0.03786500 -0.01696800

 C -5.51634500 -1.12605900 -0.60596200

 C -4.14530800 -1.16864700 -0.58588000

 C 1.33967200 -1.61375900 0.03244200

 C 1.40982500 -2.79112600 -0.73960300

 C 2.50895100 -3.61797300 -0.70451000

 C 3.61489400 -3.32732300 0.13195900

 C 3.54330400 -2.15010800 0.91748500

 C 2.44424300 -1.32562200 0.86093900

 C 1.09419400 1.68579900 -0.01552100

 C 2.37266500 1.48332100 -0.57409800

 C 3.29511900 2.49946300 -0.65408600

 C 2.99613600 3.79896600 -0.17156100

 C 1.70162900 4.01164200 0.36766600

 C 0.78659300 2.98934800 0.42726400

 C 4.73815600 -5.35992600 -0.61781900

 C 5.82607700 -3.82123600 1.03804700

 C 5.22728900 4.56493300 -0.79718500

 C 3.56331800 6.13971600 0.22257600

 H -3.51970600 1.77799400 1.01288800

 H -5.99972600 1.84806600 1.00011100

 H -6.09845600 -1.90658100 -1.07600500

 H -3.64688200 -1.99431100 -1.07898800

 H 0.59689900 -3.03920100 -1.41283100

 H 2.51908500 -4.49503900 -1.33707800

 H 4.35150600 -1.89255700 1.58837100

 H 2.41566500 -0.44534900 1.49271000

 H 2.63226400 0.51616000 -0.98511500

 H 4.25296400 2.29710700 -1.11341300

 H 1.41999600 4.98755200 0.73890600

 H -0.20041400 3.17400300 0.83365700

 H 3.91430700 -6.03533000 -0.36324000

 H 5.67356400 -5.88212000 -0.42799400

 H 4.68344600 -5.13993900 -1.68965400

 H 6.26781800 -2.85505800 0.77155500

 H 5.53369000 -3.78592000 2.09335700

 H 6.59240300 -4.58534200 0.92562600

 H 5.75305600 3.77125600 -0.25693200

 H 5.17124800 4.28369300 -1.85460200

 H 5.81824900 5.47494300 -0.71918900

 H 3.29811500 6.14335200 1.28486800

 H 2.72274000 6.55401000 -0.34404800

 H 4.42038100 6.79561800 0.08613900

 C -1.51210600 -2.57761300 0.27518700

 H -2.42010700 -2.55475000 0.87508400

 H -1.70067800 -3.15239700 -0.63365100

 H -0.72129400 -3.06629500 0.84288500

Derivative D2 (TD-CAM-B3LYP/6-31G (d,p) optimized excited state)

 N 0.92174500 -1.25584600 -0.01164800

 N 1.07038400 0.97323600 0.16928000

 C -0.36895900 -0.78479000 0.01192900

 C -0.22882000 0.64886600 0.09034900

 C 1.76875200 -0.15890600 0.07920300

 C 3.19870500 -0.18023800 0.04016300

 C 3.89405500 0.95913800 0.51011700

 C 5.26079900 1.02961600 0.49101500

 C 6.03930000 -0.04366200 -0.02309900

 C 5.34210500 -1.17356400 -0.52815100

 C 3.97168300 -1.23580400 -0.49181800

 C -1.53169900 -1.61533800 0.04474400

 C -1.62900600 -2.80946900 -0.72800600

 C -2.75448400 -3.58884600 -0.69407900

 C -3.83574300 -3.21965000 0.13380200

 C -3.76639200 -2.04905500 0.91469400

 C -2.64594400 -1.26240700 0.86285500

 C -1.24227100 1.68160600 0.00347900

 C -2.49778400 1.46785700 -0.60040600

 C -3.41717000 2.49478400 -0.69859400

 C -3.08955000 3.74626900 -0.18923100

 C -1.85033300 3.99706500 0.40046000

 C -0.93545600 2.97107200 0.48569400

 H 3.31688000 1.78780300 0.90147600

 H 5.74395900 1.91707400 0.87535800

 H 5.88787700 -1.99871300 -0.96380000

 H 3.49162000 -2.10324600 -0.92476400

 H -0.81984200 -3.08309700 -1.39537600

 H -2.84138500 -4.48211100 -1.29726700

 H -4.60287200 -1.79701700 1.55220100

 H -2.74221800 0.50186900 -1.02009200

 H -4.37897600 2.34413200 -1.17010200

 H -1.62992400 4.98527000 0.78095000

 H 0.03450900 3.14245700 0.93533500

 C 1.29725900 -2.64261000 0.24378100

 H 2.18766400 -2.66145100 0.86910800

 H 0.48191700 -3.12988500 0.77569900

 H 1.48980700 -3.18749700 -0.68189900

 N 7.39123900 0.01304300 -0.03919500

 N -4.05649200 4.82114200 -0.28278600

 O -3.74183700 5.92361000 0.15835800

 O -5.14455600 4.58135000 -0.79934500

 N -4.98748900 -4.02330500 0.17931000

 O -5.94154500 -3.67063400 0.90734200

 O -5.02079200 -5.06777900 -0.50874900

 C 8.08554300 1.18969700 0.46255600

 H 9.15788900 1.03618800 0.36742100

 H 7.81612900 2.08531600 -0.10592000

 H 7.85805300 1.36566500 1.51841900

 C 8.16933100 -1.09368700 -0.57542600

 H 9.22768800 -0.86455500 -0.47581300

 H 7.96804600 -2.02124200 -0.03093200

 H 7.95320500 -1.25819700 -1.63592100

 H -2.58942500 -0.37670400 1.48417300

 Derivative D3 (TD-CAM-B3LYP/6-31G (d,p) optimized excited state)

 N -1.33978700 0.96530200 -0.09230900

 N -1.44152700 -1.24657800 0.04899000

 N -6.53059300 4.78028100 0.20696000

 N -7.01133600 -4.44159000 -0.16139300

 C -2.66805500 0.66163700 -0.04362700

 C -2.69843300 -0.76263200 0.01373000

 C -0.60801700 -0.19946800 -0.00943700

 C -3.67896600 1.68819300 -0.01178300

 C -3.44929700 2.94474800 -0.60472900

 C -4.37758000 3.95952200 -0.54207500

 C -5.60611000 3.78128900 0.13822800

 C -5.83346500 2.52241100 0.74621700

 C -4.89952600 1.51508100 0.66899800

 C -3.84031400 -1.66909500 -0.01623800

 C -5.03366600 -1.37763200 -0.69207100

 C -6.07452200 -2.28286700 -0.74946400

 C -5.97727300 -3.54552800 -0.12293800

 C -4.76576600 -3.84733000 0.53993800

 C -3.73247500 -2.93450400 0.57921700

 C -6.25719400 6.07173600 -0.39709400

 C -7.78929700 4.56568400 0.89767100

 C -8.22326600 -4.12206500 -0.88985900

 C -6.85719800 -5.75662700 0.42983400

 H -2.53419200 3.11863200 -1.16240100

 H -4.15702200 4.89713900 -1.03383000

 H -6.74565900 2.34165700 1.29843200

 H -4.63410400 -4.80452000 1.02657700

 H -2.80983200 -3.19348700 1.08635200

 H -5.35967600 6.53399600 0.02826500

 H -7.09823900 6.73688200 -0.21222000

 H -6.12032100 5.99111900 -1.48132700

 H -7.63839200 4.35920500 1.96337100

 H -8.40054100 5.46167200 0.81064700

 H -8.34904400 3.73071500 0.46274000

 H -8.69630000 -3.21303700 -0.50257600

 H -8.03469600 -3.97723300 -1.96076800

 H -8.93263700 -4.94029600 -0.77963300

 H -6.64848900 -5.69346400 1.50350000

 H -6.04708100 -6.32663400 -0.04089500

 H -7.78213700 -6.31602400 0.30182200

 C 0.80793200 -0.26526100 -0.00031500

 C 1.45147300 -1.52317800 0.16597600

 C 1.63104100 0.88349000 -0.15157300

 C 2.81261400 -1.61565900 0.18493000

 H 0.83309200 -2.40570300 0.27821400

 C 2.99334000 0.78834900 -0.13280200

 H 1.18300900 1.86147200 -0.29668700

 C 3.65308500 -0.46895900 0.03864600

 H 3.28305800 -2.58572300 0.31416800

 H 3.58176500 1.68988600 -0.25500800

 C 5.05659300 -0.62372700 0.06562200

 H 5.40759200 -1.64290900 0.20226500

 C 5.99870800 0.38400900 -0.06480900

 H 5.64655300 1.40279100 -0.20314500

 C 7.40733900 0.23395200 -0.03842100

 C 8.23567700 1.38395900 -0.19229800

 C 8.07007600 -1.01820700 0.13565600

 C 9.60329500 1.30253900 -0.17570600

 H 7.76063500 2.35105300 -0.32670100

 C 9.43695000 -1.10861600 0.15374400

 H 7.48712500 -1.92361400 0.25764300

 C 10.21825600 0.05003600 -0.00165800

 H 10.22427700 2.18052200 -0.29363100

 H 9.93569400 -2.05965200 0.28632300

 N 11.62913700 -0.04590100 0.01777100

 O 12.15352300 -1.16243300 0.17267300

 O 12.30211500 0.99013300 -0.12066100

 H -0.96829300 1.89992800 -0.01926400

 H -5.10054300 0.57674000 1.17145800

 H -6.96618200 -2.01377900 -1.29957300

 H -5.14154600 -0.43121000 -1.20940500

Derivative D4 (TD-CAM-B3LYP/6-31G (d,p) optimized excited state)

 O 8.36494000 1.27282000 -0.27590700

 O 8.46241000 -0.78880300 0.48843600

 N 1.36959600 -1.19303700 -0.14903000

 N 1.42890000 1.06233900 0.01328700

 N 7.80460100 0.20843800 0.09266400

 N -4.91834100 -3.33830800 0.02105700

 N -4.49577200 3.77678600 0.04884000

 C 0.06612200 -0.76497500 -0.07276100

 C 0.14652300 0.64934000 0.00167200

 C 2.17166800 -0.04703900 -0.06254300

 C 3.60396700 -0.04105400 -0.02861100

 C 4.28168600 1.14926800 -0.41348200

 C 5.64778500 1.23511100 -0.38144400

 C 6.40955100 0.13075600 0.06092700

 C 5.75873900 -1.04677000 0.48751100

 C 4.39081600 -1.12804800 0.44105300

 C -1.16212500 -1.45327300 -0.04062700

 C -1.28789600 -2.86493900 0.01689300

 C -2.50164700 -3.48990400 0.04525000

 C -3.70166800 -2.72971600 0.01672400

 C -3.58644100 -1.32414600 0.00025000

 C -2.36442200 -0.66686100 -0.02098200

 C -1.02216400 1.44711400 0.03952000

 C -2.29024000 0.80968300 0.00324800

 C -3.42885800 1.61050000 0.00411000

 C -3.36178600 3.01859000 0.04873300

 C -2.07892300 3.62754200 0.09438400

 C -0.95144800 2.85263200 0.08815300

 C -5.01243900 -4.78806400 0.06742100

 C -6.13744900 -2.54847600 0.01489100

 C -5.80257000 3.14659700 0.00734600

 C -4.40660500 5.22590500 0.09528900

 H 3.68975300 1.99307300 -0.74743200

 H 6.16597500 2.13343300 -0.68792400

 H 6.35991600 -1.86511500 0.85905300

 H 3.91291300 -2.02485400 0.81644600

 H -0.39972300 -3.47910300 0.06578200

 H -2.53538900 -4.56904900 0.09943800

 H -4.49353500 -0.74131500 0.01885000

 H -4.40314100 1.14928300 -0.03353300

 H -1.98288800 4.70366000 0.13198800

 H 0.02942200 3.31343800 0.11856100

 H -4.51089500 -5.24907900 -0.78953900

 H -6.06077000 -5.07705500 0.03967000

 H -4.57171800 -5.19313400 0.98482100

 H -6.21779500 -1.92136100 0.90980700

 H -6.18921700 -1.90083300 -0.86659600

 H -6.99481900 -3.21749100 -0.00750500

 H -5.93593900 2.55218900 -0.90341800

 H -5.96275600 2.49248900 0.87163100

 H -6.57053800 3.91709000 0.02166600

 H -3.86213600 5.62453600 -0.76739900

 H -3.90645000 5.57099700 1.00664700

 H -5.41076100 5.64442500 0.08255400

 C 1.80896700 -2.49113500 -0.64084100

 H 2.77698500 -2.37528800 -1.12269300

 H 1.89847700 -3.22560100 0.16322300

 H 1.09847600 -2.85280000 -1.38457200

Derivative D5 (TD-CAM-B3LYP/6-31G (d,p) optimized excited state)

 N -1.33650100 -1.76679300 -0.14332200

 N -0.80302400 0.42368600 0.02491000

 N -7.94878900 -2.51379500 0.05182900

 N -6.03174400 4.33981600 0.01094900

 C -2.51292800 -1.06897200 -0.05944000

 C -2.13540500 0.29184500 0.01948000

 C -0.30848800 -0.82580700 -0.05599500

 C -3.86957100 -1.48096800 -0.02142000

 C -4.29554500 -2.82696000 0.06001600

 C -5.61838500 -3.17602500 0.09197100

 C -6.62542100 -2.17862900 0.04684400

 C -6.20957300 -0.83557400 0.01745600

 C -4.87067600 -0.45660700 -0.01121500

 C -3.11775600 1.32730900 0.05125800

 C -4.48539300 0.97161300 0.00300100

 C -5.43567500 1.99608100 -0.01513500

 C -5.07878100 3.35412000 0.02700000

 C -3.69947300 3.67812400 0.08663800

 C -2.75608400 2.68268600 0.09562000

 C -8.34929900 -3.90680400 0.13412400

 C -8.96597700 -1.47946400 0.04298400

 C -7.43598400 3.99458000 -0.07593100

 C -5.63749400 5.73510200 0.03772500

 H -3.56420100 -3.62003000 0.13065300

 H -5.88207100 -4.22205100 0.16553400

 H -6.96762300 -0.06896700 0.03554200

 H -6.48354000 1.74627700 -0.06863500

 H -3.37874800 4.71041300 0.11951100

 H -1.70146000 2.93270500 0.13245400

 H -7.95382300 -4.48882000 -0.70506400

 H -9.43527700 -3.96713000 0.10097300

 H -8.01176700 -4.37547200 1.06579600

 H -8.86942700 -0.83098900 -0.83452200

 H -9.94860500 -1.94568800 0.00853700

 H -8.91869400 -0.85090400 0.94024300

 H -7.66537800 3.44280000 -0.99580600

 H -7.75734900 3.38284900 0.77545700

 H -8.02977100 4.90680300 -0.07507300

 H -5.02622100 6.00543700 -0.83148800

 H -5.06882000 5.97943700 0.94214300

 H -6.53018300 6.35778200 0.02666500

 C -1.17625900 -3.14923500 -0.56470100

 H -0.25332100 -3.24014200 -1.13305600

 H -1.14827700 -3.83549200 0.28550300

 H -1.99894300 -3.42088100 -1.22388900

 C 1.06891800 -1.08725100 -0.02567100

 C 1.80640400 -2.28061100 0.14086800

 S 2.16243700 0.28527500 -0.13121300

 C 3.16923400 -2.09877800 0.16138600

 H 1.34542800 -3.24799100 0.28233500

 C 3.57554900 -0.74834800 0.01456600

 H 3.87453000 -2.90881900 0.29362600

 C 4.86634200 -0.21005900 -0.01759400

 H 4.94090800 0.86805000 -0.12418900

 C 6.03328900 -0.95490900 0.07567400

 H 5.94166400 -2.03343900 0.17498200

 C 7.35803200 -0.45322300 0.05353100

 C 8.44942300 -1.36328100 0.15548900

 C 7.68129000 0.93069300 -0.06641200

 C 9.75290400 -0.93860100 0.14000200

 H 8.23509300 -2.42354400 0.24785300

 C 8.98220200 1.36299100 -0.08260800

 H 6.88853600 1.66534700 -0.14619600

 C 10.02865300 0.43272700 0.02046900

 H 10.57598700 -1.63648500 0.21779000

 H 9.22348500 2.41390400 -0.17345400

 N 11.37485700 0.88301000 0.00375200

 O 11.59735600 2.09803200 -0.10392200

 O 12.28474800 0.04604100 0.09748000

Derivative D6 (TD-CAM-B3LYP/6-31G (d,p) optimized excited state)

 O -11.64999100 -0.84033000 0.37922000

 O -11.54329400 1.27533500 -0.21621500

 N 1.50484800 -1.30908100 -0.20244300

 N 1.33351800 0.93359300 -0.02008100

 N -11.00302500 0.18373600 0.07593500

 N 7.90175700 -3.12673300 -0.00115300

 N 7.12202600 3.94699900 0.12953000

 C 2.78030400 -0.81578700 -0.10410200

 C 2.62909500 0.58785800 -0.01072400

 C 0.64395100 -0.21173500 -0.11639000

 C -0.78062400 -0.25887200 -0.08786700

 C -1.49661400 0.93720600 -0.37410000

 C -2.86045400 0.97855800 -0.34717600

 C -3.63637800 -0.17086000 -0.00876100

 C -2.91159300 -1.35279900 0.31850900

 C -1.54432900 -1.39819200 0.27847600

 C 4.04883400 -1.44343100 -0.07315700

 C 4.24902900 -2.84361500 -0.02958700

 C 5.49593400 -3.40431900 0.00063700

 C 6.65260400 -2.58257300 -0.00814800

 C 6.46128700 -1.18744600 -0.00571000

 C 5.20411700 -0.59563800 -0.03141800

 C 3.76185200 1.44859300 0.05439700

 C 5.05557500 0.87643600 0.01569200

 C 6.15777600 1.73213500 0.03743100

 C 6.02372800 3.13070600 0.10807100

 C 4.71369000 3.67340100 0.15673500

 C 3.62275500 2.84436800 0.12755500

 C 8.07144900 -4.56910100 0.02958100

 C 9.07534800 -2.27230500 0.02162200

 C 8.45553900 3.38072400 0.08089600

 C 6.95953700 5.38685300 0.20586400

 H -0.92889500 1.82340600 -0.62998000

 H -3.35971500 1.90845100 -0.59142600

 H -3.45110800 -2.24216600 0.62647700

 H -1.05170500 -2.31181000 0.58523200

 H 3.39672100 -3.50718600 0.00914500

 H 5.58534200 -4.48089100 0.04350100

 H 7.33433800 -0.55605200 0.03305000

 H 7.15264300 1.31779600 -0.00448100

 H 4.56432500 4.74284200 0.21324200

 H 2.62146100 3.25949300 0.15824600

 H 9.13371900 -4.80254700 0.00205400

 H 7.59815900 -5.04704900 -0.83437500

 H 7.65036300 -5.00931100 0.94040700

 H 9.10318800 -1.60695100 -0.84795700

 H 9.11222200 -1.65650200 0.92754500

 H 9.96832300 -2.89337200 -0.00132000

 H 8.64684500 2.71795900 0.93302500

 H 8.62099700 2.80890200 -0.83975200

 H 9.18696800 4.18592200 0.11144100

 H 6.43490300 5.68928500 1.11927300

 H 6.40343800 5.77946200 -0.65291800

 H 7.94152900 5.85595500 0.21230100

 C 1.14502100 -2.63331900 -0.69297300

 H 1.07293900 -3.36290600 0.11705500

 H 0.18889800 -2.57381100 -1.20692600

 H 1.89421100 -2.96297400 -1.41218700

 C -7.49746600 -0.67962300 0.22816300

 C -7.23103900 0.65776100 -0.15160700

 C -5.05041900 -0.12796700 0.01308500

 S -6.01067400 -1.56309600 0.43543600

 C -5.88814800 0.96650800 -0.27168300

 H -5.51083600 1.94023800 -0.55236900

 C -9.62545500 0.12181800 0.05837600

 C -8.84189700 -0.99198300 0.34919400

 S -8.71226500 1.55993500 -0.36581000

 H -9.26792600 -1.94541100 0.62587300

Derivative D7 (TD-CAM-B3LYP/6-31G (d,p) optimized excited state)

 N -3.30078600 -1.85989100 -0.14989300

 N -2.58873300 0.27288400 0.03695600

 N -9.95955600 -2.05066600 0.02230400

 N -7.47384400 4.61511300 0.03487000

 C -4.41592700 -1.06752000 -0.06518400

 C -3.92923500 0.25329100 0.02699400

 C -2.20173200 -1.00919900 -0.05413700

 C -5.80591000 -1.36641800 -0.03693200

 C -6.34382400 -2.67071800 0.03264900

 C -7.69247000 -2.90723900 0.05932400

 C -8.61120600 -1.82883200 0.02132500

 C -8.08290200 -0.52677300 0.00311900

 C -6.71562000 -0.26222600 -0.02136300

 C -4.82107000 1.36914700 0.06414800

 C -6.21235600 1.12907700 0.00549100

 C -7.07443600 2.22988600 -0.00997000

 C -6.60617300 3.55225200 0.04654700

 C -5.20523400 3.75947900 0.11657700

 C -4.34780500 2.68870100 0.12227800

 C -10.47686300 -3.40423400 0.10496100

 C -10.88394500 -0.93302000 0.03449700

 C -8.90065600 4.38849700 -0.06791100

 C -6.96399300 5.97223200 0.05675700

 H -5.68276100 -3.52353800 0.09879600

 H -8.04341500 -3.92793600 0.12407800

 H -8.77252000 0.30161800 0.02810400

 H -8.13887900 2.06869500 -0.07385600

 H -4.80006700 4.76125900 0.15996600

 H -3.27624300 2.84985200 0.16682600

 H -10.12717000 -4.01962800 -0.73070600

 H -11.56389300 -3.37247300 0.06381000

 H -10.18686300 -3.89882200 1.03954300

 H -10.73530400 -0.28163400 -0.83352200

 H -11.90314800 -1.31267700 -0.00269000

 H -10.78017700 -0.32407500 0.94073800

 H -9.16940700 3.87518300 -0.99967700

 H -9.27680200 3.78910000 0.76952000

 H -9.41738900 5.34641100 -0.05109700

 H -6.33271900 6.18862200 -0.81347800

 H -6.37639800 6.17110300 0.96018800

 H -7.80157200 6.66734300 0.04456800

 C -3.25511000 -3.25324300 -0.56488700

 H -2.33819100 -3.42572200 -1.12373400

 H -3.29464700 -3.93457900 0.28867600

 H -4.09152300 -3.45626600 -1.23122900

 C -0.84467300 -1.38189900 -0.02463900

 C -0.20915800 -2.62882700 0.14119800

 S 0.35018700 -0.10502100 -0.13223400

 C 1.16611200 -2.55695600 0.16261700

 H -0.74650300 -3.55580300 0.28254400

 C 1.67629800 -1.24484100 0.01817600

 H 1.80383900 -3.42098900 0.29608000

 C 3.00364700 -0.80583800 -0.00802200

 H 3.16104500 0.26350100 -0.11003100

 C 4.10990500 -1.63987400 0.08549200

 H 3.93292300 -2.70837100 0.17836600

 C 5.46499400 -1.24507800 0.07166200

 C 6.48557700 -2.23634400 0.17226100

 C 5.89787800 0.11024100 -0.03762400

 C 7.81331600 -1.91135800 0.16451100

 H 6.18888900 -3.27757800 0.25702300

 C 7.22598700 0.43505900 -0.04518700

 H 5.16606600 0.90599800 -0.11520300

 C 8.23156300 -0.55975800 0.05494700

 H 8.57177500 -2.68093900 0.24186100

 H 7.50861500 1.48016200 -0.12936200

 N 12.95582500 1.58277800 -0.05963000

 O 12.77989400 2.80481500 -0.16821600

 O 14.07135600 1.05136000 0.00344800

 C 9.62068100 -0.24428100 0.04878300

 C 11.80280100 -0.60804300 0.11424800

 C 11.82703100 0.76472000 -0.00594700

 S 10.21980900 1.40985500 -0.08724800

 H 12.69628400 -1.21579600 0.18154900

 N 10.58756200 -1.16295300 0.14419600

Derivative D8 (TD-CAM-B3LYP/6-31G (d,p) optimized excited state)

 N 5.72666900 -1.68507700 0.15950800

 N 5.18513000 0.49593200 -0.02638000

 N 12.34432900 -2.41369100 -0.04670700

 N 10.40179700 4.43107800 -0.09356500

 C 6.90226700 -0.98580800 0.06379700

 C 6.52281200 0.36967800 -0.02755600

 C 4.70279500 -0.74835000 0.07196500

 C 8.26224500 -1.39629400 0.02669400

 C 8.69222900 -2.74060200 -0.03653600

 C 10.01678400 -3.08529400 -0.06765900

 C 11.01973400 -2.08395300 -0.04104300

 C 10.59857100 -0.74239000 -0.02873800

 C 9.25786900 -0.36881800 -0.00047200

 C 7.49866600 1.40917900 -0.07773500

 C 8.86764200 1.05861900 -0.03200700

 C 9.81447400 2.08605000 -0.03311600

 C 9.45259100 3.44238500 -0.09162600

 C 8.07172800 3.76094500 -0.14858000

 C 7.13171800 2.76276400 -0.13871500

 C 12.75004200 -3.80630800 -0.10928100

 C 13.35739900 -1.37522700 -0.05640600

 C 11.80826500 4.09193000 -0.01545900

 C 10.00291100 5.82464200 -0.14261300

 H 7.96441800 -3.53791500 -0.09229600

 H 10.28393400 -4.13136300 -0.12589900

 H 11.35333900 0.02694700 -0.05957100

 H 10.86345600 1.84065500 0.01757300

 H 7.74750300 4.79160800 -0.19442200

 H 6.07617200 3.00898300 -0.17362900

 H 12.36128100 -4.37661200 0.74098800

 H 13.83639200 -3.86181400 -0.08104000

 H 12.40942500 -4.29056900 -1.03173200

 H 13.26280700 -0.71575400 0.81305700

 H 14.34200100 -1.83711500 -0.02097200

 H 13.30301600 -0.75887400 -0.96161300

 H 12.04717400 3.55109300 0.90831600

 H 12.12446800 3.47237100 -0.86306500

 H 12.39840800 5.00631800 -0.03090900

 H 9.39162600 6.10621800 0.72282800

 H 9.43270900 6.05255900 -1.05034600

 H 10.89353800 6.45025900 -0.14181700

 C 5.56809500 -3.07273900 0.56616300

 H 4.63674900 -3.17448900 1.11863100

 H 5.55899400 -3.74968100 -0.29144300

 H 6.38074600 -3.34485000 1.23726300

 C 3.31589900 -1.01695800 0.06213000

 C 2.58157000 -2.19682500 -0.12779400

 S 2.19609600 0.31768000 0.20992000

 H 3.02716900 -3.16789400 -0.29885600

 C 0.86270100 -0.81992300 0.03279200

 N -15.72015200 0.57434900 -0.04844200

 O -15.97747100 1.76600000 0.11301800

 O -16.56086000 -0.30870900 -0.18779800

 C -11.97208900 0.03841100 -0.05318500

 C -13.86185200 -1.06605200 -0.24221400

 C -14.35413000 0.19930100 -0.07470400

 S -13.09024700 1.36310500 0.11124700

 H -14.47585500 -1.94654600 -0.37661800

 N -12.51342500 -1.15124000 -0.22914600

 C -0.48177200 -0.44096400 0.06594700

 C -1.04448500 0.83720400 0.23002300

 S -1.77515700 -1.60561600 -0.10725100

 H -0.45274500 1.73710900 0.35813000

 C -2.93435800 -0.28694700 0.05325700

 C -8.13354300 0.12379000 0.02710800

 C -8.68341700 1.38874200 0.19142800

 C -10.55748200 0.26349000 0.00359200

 S -9.41280700 -1.03883200 -0.15537700

 H -8.10300600 2.29363500 0.32589200

 C -4.32544900 -0.47428500 0.00725500

 C -5.05935400 -1.65157500 -0.16328200

 C -6.76883900 -0.26991200 -0.00349700

 S -5.43790000 0.86114700 0.17059100

 H -4.60800800 -2.62908900 -0.28820000

 N -10.02671900 1.45517900 0.17702400

 N -6.38985500 -1.53068000 -0.16804700

 N -2.36821200 0.91528200 0.22225600

 N 1.25725900 -2.09123200 -0.14188200