

Electronic Supplementary Information for

**Supramolecular Light-switchable Triazole-hosts for
Photoadaptive Anion Binding**

Leon Hoppmann,^{a†} Leonard Wyszynski,^{b†} Marcus Böckmann,^c Pascal Steinforth,^b Lukas-Maximilian Entgelmeier,^a Nikos Doltsinis,^c Olga García Mancheño^{*a} and Monika Schönhoff^{*b}

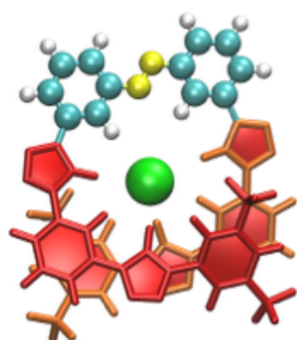
a. Organic Chemistry Institute, University of Münster, Corrensstraße 36, 48149 Münster, Germany. E-mail: olga.garcia@uni-muenster.de

b. Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany. E-mail: schoenho@uni-muenster.de

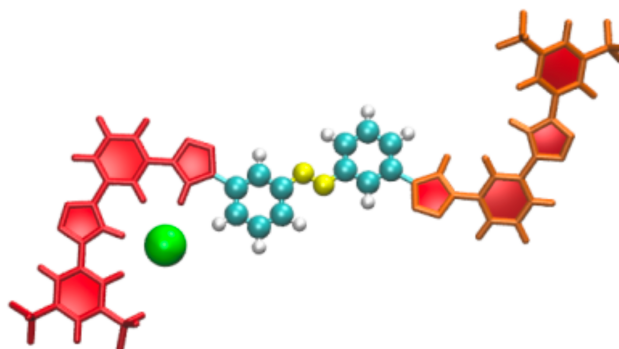
c. Institute of Solid State Theory and Center for Multiscale Theory and Computation, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany. E-mail: nikos.doltsinis@uni-muenster.de

[†] These authors contributed equally.

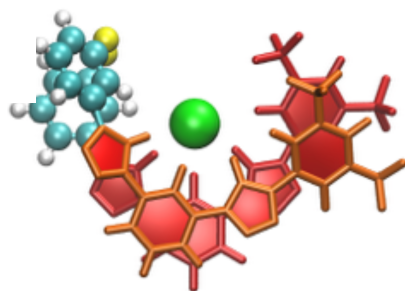
Cartesian Coordinates



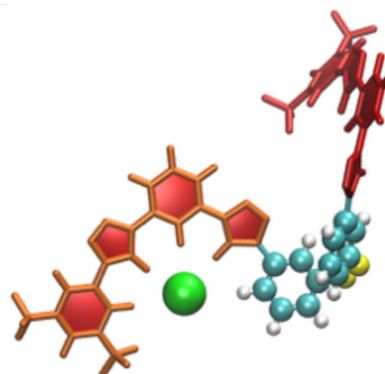
E-AB-mTTA-(1,3)Ph, close



E-AB-mTTA-(1,3)Ph, open



Z-AB-mTTA-(1,3)Ph, close



Z-AB-mTTA-(1,3)Ph, open

E-AB-mTTA-(1,3)Ph, close

C 0.23417600 6.21709400 0.38501500
N 1.51397400 5.67514100 0.12938600
N 2.45772800 6.49998300 -0.00165600
C 3.71124100 5.88516900 -0.27438700
C -0.09983800 7.58171900 0.41303000
C -0.74553100 5.25345600 0.63030500
C -1.41364200 7.94637600 0.69169800
C -2.06736800 5.61637800 0.91371200
C -2.39423500 6.97933300 0.94260600
H 0.66595100 8.32413600 0.22037800
H -0.43785900 4.21341600 0.61802700
H -1.68606300 8.99722800 0.71483800
C -3.04715500 4.56514200 1.19612000
H -3.41422500 7.27792300 1.16031400
C 3.86341800 4.51185700 -0.50552600
C 4.82499900 6.73136600 -0.32644700
C 5.12072700 3.97286700 -0.78161100
C 6.08477200 6.19596400 -0.59887000
C 6.23709000 4.82961000 -0.82576200
H 2.97868300 3.88774300 -0.48006400
H 4.68564000 7.79346000 -0.15271600
C 5.25544100 2.53800800 -1.05106300
H 6.95220300 6.84737900 -0.63722500
H 7.21470100 4.41388200 -1.04443300
C -2.90879600 3.20733400 0.99353400
N -4.26798400 4.77640600 1.78501300
N -4.04563800 2.66063800 1.48946700
N -4.86961100 3.63191800 1.96822200
H -2.14448600 2.62406200 0.51128900
C -4.34593800 1.27841200 1.62232200
C -3.28425200 0.38041300 1.66198200
C -5.66637500 0.83317900 1.70845000
C -3.52255600 -0.99443800 1.76288500
C -5.89937900 -0.53523000 1.84100000
C -4.84454700 -1.44797300 1.86404300
H -6.48184300 1.54427700 1.66322200
H -6.91996100 -0.89759700 1.90078200
H -5.03859100 -2.51144000 1.93439100
H -2.26845100 0.75286000 1.62799000
C -2.38549100 -1.91604200 1.74551800
C -1.03893400 -1.62232700 1.66254200
N -2.51154300 -3.28302400 1.77862400
N -0.41681900 -2.82895800 1.65597800
N -1.33409900 -3.83487900 1.72666500
H -0.50304800 -0.69252000 1.58668500
C 0.97376300 -3.10081600 1.60216400
C 1.88521000 -2.09043300 1.90260400
C 1.41421200 -4.36576400 1.21138500
C 3.25084500 -2.35139300 1.80318600
C 2.78276000 -4.60831200 1.13753700
C 3.71136500 -3.61106900 1.43541600
H 1.54860400 -1.10698200 2.20423000
H 0.69479700 -5.12585900 0.93889400

E-AB-mTTA-(1,3)Ph, open

C -1.78901600 -0.07363000 -1.55703800
N -0.44577000 0.38053700 -1.53267500
N 0.41948700 -0.53484700 -1.48420300
C 1.76301700 -0.08211100 -1.45958800
C -2.17638100 -1.42396500 -1.52070500
C -2.75435500 0.93430500 -1.62332900
C -3.52914900 -1.74062000 -1.55078900
C -4.11875400 0.61713000 -1.65454000
C -4.49597200 -0.73364900 -1.61629700
H -1.41491800 -2.19284800 -1.46939400
H -2.43159300 1.96854400 -1.65146000
H -3.84215600 -2.77993500 -1.52168700
C -5.11882100 1.68574200 -1.72618400
H -5.54683700 -1.00559200 -1.63409900
C 2.72737500 -1.09245100 -1.42264000
C 2.15218800 1.26814700 -1.47235800
C 4.09243600 -0.77785400 -1.39878800
C 3.50571800 1.58226800 -1.44673200
C 4.47155000 0.57282300 -1.40900000
H 2.40338700 -2.12668600 -1.41520900
H 1.39153600 2.03903300 -1.50121300
C 5.09106700 -1.84956500 -1.36658200
H 3.81991500 2.62160900 -1.45361500
H 5.52289600 0.84233900 -1.38239400
C -6.49590900 1.61233300 -1.83084800
N -4.77467800 3.01373200 -1.70433000
N -6.91039200 2.90502300 -1.86539300
N -5.84720700 3.74840100 -1.78575700
H -7.18159400 0.78543400 -1.91374400
C -8.23534600 3.41246800 -1.96320900
C -9.28658800 2.69088300 -1.40247200
C -8.45636000 4.62422300 -2.62167600
C -10.59739400 3.17419800 -1.51059400
C -9.75993800 5.10794900 -2.71193800
C -10.82480800 4.39221900 -2.16946300
H -7.62177600 5.16267700 -3.05334500
H -9.94649400 6.04808700 -3.22094900
H -11.83825500 4.76810300 -2.24866300
H -9.08191300 1.76796500 -0.87177900
C -11.71863600 2.42862900 -0.93346600
C -11.73106600 1.24849200 -0.21465000
N -13.01733700 2.86085000 -1.04648400
N -13.04220800 1.03066200 0.06929800
N -13.81363300 2.02678300 -0.44879100
H -10.94735700 0.59263600 0.12632600
C -13.63748700 -0.03831500 0.78472800
C -12.99797100 -1.27561100 0.84927700
C -14.87100200 0.16403800 1.40519500
C -13.60037100 -2.31366300 1.55815900
C -15.46217900 -0.89186800 2.09356900
C -14.83377400 -2.13384900 2.18076300
H -12.05795800 -1.44179700 0.33806600
H -15.35528500 1.12918000 1.33835400

C 4.22364100	-1.24999400	2.12559800	C -12.88828800	-3.63454800	1.68028800
C 3.25739000	-5.96677100	0.69607300	C -16.76885500	-0.66762900	2.80740400
H 4.77160600	-3.80162500	1.34077200	H -15.30383700	-2.95070300	2.71392100
F 4.43066600	-1.13457500	3.45535900	F -12.08346000	-3.66148000	2.76748800
F 5.42571600	-1.44979700	1.54917900	F -13.75519400	-4.66082300	1.80522600
F 3.76305600	-0.04827200	1.69753600	F -12.10842000	-3.88501800	0.60675700
F 2.47682400	-6.46426000	-0.29082700	F -17.52504000	0.26369900	2.18937900
F 4.52321800	-5.92855800	0.22624000	F -17.49682300	-1.80168600	2.88424600
F 3.23260700	-6.86262200	1.70663400	F -16.57050700	-0.23848200	4.07517800
C 4.32153400	1.53277500	-0.89178800	C 6.47003800	-1.78599500	-1.44965600
N 6.38982000	1.97182200	-1.57571300	N 4.74260000	-3.17158900	-1.25189700
N 4.93465000	0.40963400	-1.34412100	N 6.88158900	-3.07841300	-1.37940400
N 6.19946200	0.69531600	-1.75817800	N 5.81427300	-3.91165600	-1.25710400
H 3.32957500	1.52650200	-0.47543300	H 7.15793800	-0.96758400	-1.58309400
C 4.39012100	-0.89520100	-1.49057600	C 8.20548200	-3.59662100	-1.41796400
C 3.00746300	-1.04669800	-1.54909800	C 9.25466800	-2.83513600	-0.90805400
C 5.23833000	-2.00104500	-1.59296500	C 8.42669100	-4.86286100	-1.96460300
C 2.44567800	-2.31983400	-1.70507600	C 10.56354800	-3.33336000	-0.95802600
C 4.67513900	-3.26243600	-1.77345100	C 9.72744900	-5.36124300	-1.99331700
C 3.29230600	-3.42932800	-1.83043400	C 10.79054700	-4.60648200	-1.50297700
H 6.31045400	-1.86542700	-1.52970600	H 7.59387200	-5.43255900	-2.35769900
H 5.32208200	-4.13007500	-1.84625100	H 9.91347700	-6.34377900	-2.41493400
H 2.86008500	-4.41595000	-1.94604100	H 11.80239800	-4.99331000	-1.53661000
C 0.99070300	-2.47769300	-1.72862300	C 11.68427500	-2.54571800	-0.43856400
H 2.36652000	-0.17590800	-1.49154800	H 9.04956300	-1.87215200	-0.45430400
C -0.00080900	-1.51974600	-1.64934900	C 11.71954400	-1.25065500	0.04234700
N 0.37845500	-3.70432400	-1.81221300	N 12.96034000	-3.04926600	-0.37259300
N -1.16566700	-2.21936500	-1.69456700	N 13.02076700	-1.04094200	0.37449800
N -0.91251500	-3.55446100	-1.79237500	N 13.76395400	-2.15256600	0.11440400
H 0.03269000	-0.44825200	-1.55027200	H 10.96583700	-0.48703500	0.13888400
C -2.49730300	-1.73506900	-1.65966600	C 13.63168200	0.11646700	0.91892200
C -2.75040300	-0.38401400	-1.89418300	C 12.87828000	1.01198600	1.67665500
C -3.53779400	-2.61595600	-1.36575500	C 14.98780100	0.34340800	0.67992400
C -4.05961500	0.08486900	-1.81765700	C 13.49429300	2.15401500	2.18554500
C -4.84030100	-2.12702200	-1.31147500	C 15.58631100	1.48237900	1.21194000
C -5.11450000	-0.77900300	-1.53383400	C 14.84762300	2.39802200	1.96080200
H -1.94904600	0.30251000	-2.13271100	H 11.83027300	0.82607200	1.87571100
H -3.32094400	-3.65354700	-1.15209500	H 15.55364100	-0.35711100	0.08040700
C -4.34813900	1.53600400	-2.09199400	C 12.70095600	3.10151200	3.04551400
C -5.96411000	-3.08263900	-1.01067700	C 17.06047700	1.70905400	1.00535600
H -6.12668300	-0.40406000	-1.45687900	H 15.31638200	3.29166300	2.35364600
F -5.59277900	-4.01810600	-0.10750700	F 17.49905900	1.15118400	-0.14255300
F -7.04642800	-2.44690200	-0.51319000	F 17.36200300	3.02422500	0.96290200
F -6.36470000	-3.74426200	-2.11888600	F 17.78705000	1.16943200	2.01081600
F -3.25117900	2.30875900	-1.91624100	F 11.39021300	3.09488600	2.72199200
F -4.77031800	1.73058900	-3.35972700	F 12.78685400	2.77004600	4.35417000
F -5.31399100	2.01427900	-1.27733700	F 13.14524100	4.37057400	2.92993900

Z-AB-mTTA-(1,3)Ph, close

C 6.49797400 -2.19888900 -2.63126600
N 5.88839200 -3.49700200 -2.83207000
N 5.91769600 -4.34450700 -1.90917700
C 6.41572000 -3.96504300 -0.61110800
C 7.89169700 -2.10046000 -2.60478700

Z-AB-mTTA-(1,3)Ph, open

C -1.53633300 5.27238800 -2.12002500
N -2.05699500 5.10330300 -3.44821100
N -1.42213700 4.50853200 -4.34752300
C -0.20616400 3.78938900 -4.09094200
C -0.28429100 5.85407400 -1.88138900

C 5.69809000 -1.06302200 -2.51854900	C -2.39146800 4.96796900 -1.06122600
C 8.47893700 -0.84908600 -2.42258500	C 0.10948100 6.09408700 -0.56721800
C 6.28950000 0.18163500 -2.26091800	C -1.97484200 5.16653600 0.26160400
C 7.69018600 0.28152400 -2.23011400	C -0.71580400 5.74066600 0.49918600
H 8.49892700 -2.99300100 -2.71014800	H 0.36162500 6.11534700 -2.71201900
H 4.61844000 -1.16560900 -2.56878200	H -3.37088600 4.55741500 -1.28504000
H 9.56093700 -0.76268200 -2.40074200	H 1.07452300 6.55160200 -0.37183400
C 5.47247400 1.36473600 -1.97618200	C -2.83845000 4.78953700 1.38321900
H 8.14557300 1.24697300 -2.04254100	H -0.39803600 5.91170000 1.52138800
C 5.82301700 -2.90429200 0.07140500	C -0.09360800 2.86429200 -3.04948800
C 7.45650300 -4.68971800 -0.02708500	C 0.82492500 3.93759900 -5.02452900
C 6.33315900 -2.47282600 1.29781100	C 1.07525600 2.10908800 -2.90564300
C 7.95308100 -4.27439700 1.21076100	C 2.00090100 3.20644700 -4.86405300
C 7.41346700 -3.16682900 1.86500800	C 2.12937700 2.29836100 -3.81500400
H 4.98699600 -2.38909600 -0.38000000	H -0.90514800 2.72225600 -2.34760600
H 7.89240700 -5.53177000 -0.55463600	H 0.70124600 4.63268400 -5.84862100
C 5.77670800 -1.26196200 1.90498300	C 1.18144100 1.14909400 -1.80382000
H 8.77980000 -4.81352000 1.66290100	H 2.81726300 3.33565100 -5.56769800
H 7.82250500 -2.83309800 2.81220000	H 3.04699700 1.72847900 -3.70957200
C 4.13191900 1.47222100 -1.65389800	C -4.03999000 4.10508900 1.38750400
N 6.00822800 2.62781700 -1.94494200	N -2.52769200 5.09089700 2.68506600
N 3.92609000 2.80097200 -1.45114500	N -4.39218700 4.03047000 2.69649600
N 5.08371900 3.48961800 -1.63595900	N -3.45714600 4.63599700 3.47630800
H 3.35458700 0.73684000 -1.53584700	H -4.65476400 3.70150200 0.60028500
C 2.72464500 3.49042200 -1.12549900	C -5.53754000 3.41837900 3.27622600
C 1.49560100 2.85899300 -1.30196800	C -6.09896300 2.30110200 2.66248700
C 2.79662400 4.80315100 -0.65324000	C -6.07540400 3.94763500 4.45151100
C 0.31136600 3.53930100 -0.99200500	C -7.23744100 1.70131400 3.21682800
C 1.61415900 5.47956900 -0.36411100	C -7.19641900 3.33549400 5.00860100
C 0.37839300 4.85868300 -0.52341500	C -7.78068600 2.22756000 4.39878300
H 3.76135800 5.27272500 -0.51450100	H -5.62173900 4.81925800 4.90683000
H 1.66185700 6.49825600 0.00690400	H -7.62490500 3.73613900 5.92164800
H 1.45142200 1.85484700 -1.70636700	H -8.65843600 1.76043200 4.83005200
H -0.53927300 5.38069200 -0.28047000	H -5.63919400 1.88890600 1.77150600
C -0.98514700 2.88341000 -1.16778300	C -7.84846200 0.53251900 2.57940400
C -1.28100700 1.55541000 -1.40726800	C -7.52614100 -0.10847900 1.39837100
N -2.17213600 3.57156200 -1.11238800	N -8.92430200 -0.12132100 3.12802300
N -2.63670100 1.51234400 -1.49135400	N -8.42873600 -1.11915200 1.29654900
N -3.16469400 2.75631800 -1.30374600	N -9.27517800 -1.11168300 2.36392300
H -0.66400500 0.68203300 -1.53629200	H -6.78253000 0.08295300 0.64281300
C -3.48716300 0.39716700 -1.68523200	C -8.56542000 -2.09703300 0.27970800
C -3.06863800 -0.86945300 -1.27719000	C -7.45819600 -2.47135800 -0.48029600
C -4.75490500 0.59330400 -2.22796300	C -9.81837300 -2.66772600 0.05140300
C -3.94220700 -1.94336700 -1.40755300	C -7.61912100 -3.41826500 -1.49043500
C -5.61611000 -0.49648500 -2.34342100	C -9.95243100 -3.62353300 -0.95191900
C -5.22211500 -1.76768500 -1.93463400	C -8.86093200 -4.00143700 -1.73366900
H -5.06732200 1.58587000 -2.52323500	H -6.48293200 -2.04103800 -0.28967500
H -2.09628500 -1.01361400 -0.82603300	H -10.66777400 -2.35717200 0.64502000
C -6.98014100 -0.28834000 -2.94733100	C -6.41966400 -3.86389600 -2.28381800
C -3.51388400 -3.31648900 -0.96729000	C -11.28679400 -4.28530500 -1.17260300
H -5.90702600 -2.60364700 -2.00511700	H -8.97880800 -4.73053200 -2.52571600
F -2.41384300 -3.27614200 -0.18637700	F -5.81785200 -4.93140100 -1.71094600
F -4.49157700 -3.92879100 -0.26165600	F -6.75875600 -4.22842800 -3.53820900
F -3.23143800 -4.11364300 -2.02019900	F -5.48976400 -2.88966500 -2.37716500

F -6.93136100 -0.33801400 -4.29875700	F -12.31134300 -3.48949400 -0.80124700
F -7.85591400 -1.23217600 -2.54658700	F -11.47218900 -4.61337100 -2.46903100
F -7.49283400 0.91513000 -2.61614800	F -11.39340400 -5.42857600 -0.45720400
C 4.67155900 -0.52683200 1.51367600	C 2.20305100 0.27827800 -1.47195100
N 6.36465700 -0.60303400 2.95251400	N 0.18080400 0.98657800 -0.87910300
N 4.65404400 0.54183000 2.34568500	N 1.76263600 -0.36517400 -0.35986700
N 5.69218000 0.48285400 3.22224800	N 0.52642400 0.08006700 -0.01050400
H 3.94248600 -0.65461000 0.73158100	H 3.15064400 0.05231500 -1.93212300
C 3.71602600 1.61108000 2.38293000	C 2.41793700 -1.36565000 0.40971900
C 2.36247300 1.33007300 2.21668500	C 3.80830900 -1.36181600 0.49590800
C 4.16988600 2.91392600 2.59503500	C 1.65263000 -2.32978600 1.06980400
C 1.42605300 2.37118700 2.26977000	C 4.46129600 -2.35386000 1.23958400
C 1.87534900 3.68094600 2.49130800	C 2.30658000 -3.30057800 1.82566300
C 3.23385400 3.94404600 2.64988200	C 3.69701800 -3.32244700 1.90807400
H 5.23044800 3.10343900 2.70907300	H 0.57322500 -2.31166800 0.98420000
H 3.56878800 4.96385300 2.80820600	H 1.72416900 -4.05529700 2.34424700
H 1.15184900 4.48536100 2.53138200	H 4.20248300 -4.08601800 2.48790600
H 2.04340600 0.30274400 2.07947100	C 5.92305000 -2.37617600 1.33180400
C -0.00687900 2.09597200 2.14620900	H 4.37614100 -0.57680300 0.00933200
C -0.67841500 0.89722200 2.00065200	C 6.87090100 -1.63437000 0.65312300
N -0.94743900 3.09624300 2.19404300	N 6.58871400 -3.22813700 2.17874600
N -1.99518700 1.23911400 1.97250700	N 8.06356600 -2.07919900 1.12959200
N -2.13793900 2.58990000 2.09166000	N 7.87056700 -3.05306900 2.06233000
H -0.34204200 -0.12156200 1.90205900	H 6.79673900 -0.88701300 -0.11924900
C -3.13901800 0.40540200 1.90166500	C 9.37475500 -1.66502100 0.78629000
C -3.07081400 -0.91244600 2.34848400	C 9.58828600 -0.38870800 0.26775400
C -4.32793000 0.92749600 1.38565500	C 10.43730400 -2.55119800 0.96990300
C -4.20618700 -1.71908700 2.26209200	C 10.88218200 -0.00802900 -0.08403400
C -5.44775600 0.10584200 1.31190000	C 11.72378000 -2.14329300 0.62815800
C -5.39647700 -1.22239100 1.73974900	C 11.95710200 -0.87647800 0.09337800
H -2.15601000 -1.30795400 2.77288700	H 8.76587400 0.30436800 0.14242700
H -4.35656300 1.94779400 1.02706300	H 10.25110000 -3.54102100 1.36453400
C -4.14241300 -3.11488100 2.82484300	C 11.12719900 1.38490500 -0.60010500
C -6.75133200 0.66400800 0.80544600	C 12.88499600 -3.06946300 0.87556900
H -6.26883500 -1.85865000 1.66402400	H 12.95802000 -0.57543100 -0.18963500
F -4.18173400 -3.09162700 4.17768000	F 12.51446600 -4.36607100 0.82547500
F -5.16992900 -3.87988200 2.40932700	F 13.86887100 -2.88923900 -0.03115400
F -2.99553300 -3.73927400 2.48058500	F 13.42986300 -2.85975000 2.09595500
F -6.56653100 1.72118000 -0.01228000	F 10.05373600 1.87106000 -1.25928800
F -7.45456000 -0.26644500 0.11885700	F 11.39432500 2.24554600 0.40874600
F -7.53919700 1.07887200 1.82116700	F 12.17958200 1.42681800 -1.44377600

E-AB-mTTA-(1,3)Ph + Cl(-), close

C 0.04608900 6.18954200 0.26617500
N 1.34349700 5.68409600 0.04538600
N 2.28444100 6.51916200 -0.01852000
C 3.54837500 5.90241300 -0.24443100
C -0.33238400 7.54275900 0.29210800
C -0.90264500 5.18802700 0.47698500
C -1.66559900 7.85876800 0.53582100
C -2.23980900 5.50522200 0.74226100
C -2.61580600 6.85568600 0.76447400
H 0.41225800 8.31235800 0.12327300
H -0.55767400 4.15872700 0.44592600

E-AB-mTTA-(1,3)Ph + Cl(-), open

C -1.64566400 0.25654900 -0.89380300
N -0.28043700 0.61204200 -1.02928100
N 0.53078800 -0.34775500 -0.92847200
C 1.89487200 0.01240400 -1.07696700
C -2.11832200 -1.05768000 -0.73712900
C -2.54294800 1.32772200 -0.93129300
C -3.48608800 -1.27442200 -0.61650800
C -3.92081800 1.11045200 -0.80518100
C -4.38584900 -0.20531600 -0.64713500
H -1.40998400 -1.87722100 -0.71423900
H -2.15535800 2.33251500 -1.05621400

H -1.97699400	8.89904300	0.55447900	H -3.86418500	-2.28525100	-0.49563700
C -3.17791200	4.41702000	1.02102100	C -4.85440900	2.23845400	-0.83488400
H -3.64951600	7.11771200	0.96457200	H -5.45089600	-0.39770000	-0.54503700
C 3.69993900	4.52515300	-0.45339300	C 2.80712100	-1.03059900	-0.89741800
C 4.66650800	6.74308500	-0.26067800	C 2.35013200	1.30478100	-1.38872300
C 4.96225700	3.97839500	-0.68280600	C 4.18481100	-0.80474600	-1.01729600
C 5.93271800	6.19797200	-0.48053900	C 3.71600100	1.53005000	-1.51168100
C 6.08471900	4.82935200	-0.69180600	C 4.62994100	0.48930900	-1.32652700
H 2.81235600	3.90405000	-0.43994500	H 2.43255000	-2.01991400	-0.66112400
H 4.52665000	7.80739300	-0.10059100	H 1.62925300	2.10141800	-1.52837700
C 5.10184800	2.54293400	-0.94446500	C 5.12896000	-1.90804500	-0.82029600
H 6.80528400	6.84385000	-0.49118600	H 4.08062400	2.52414000	-1.75236800
H 7.06701200	4.40646300	-0.87197200	H 5.69247900	0.69107900	-1.42048100
C -2.91474700	3.06183200	1.00109600	C -6.23460400	2.22890600	-0.77469800
N -4.47957300	4.58987200	1.41607100	N -4.44360200	3.54472400	-0.92715300
N -4.07229800	2.48085500	1.40143500	N -6.58826300	3.54002100	-0.83112000
N -5.02172000	3.42472900	1.64797900	N -5.48379900	4.32986100	-0.92341300
H -2.03122200	2.50526800	0.72309000	H -6.94940200	1.41865600	-0.69974600
C -4.31472200	1.09724700	1.61249100	C -7.89472800	4.10273900	-0.79168400
C -3.22517200	0.23270000	1.61977700	C -8.97386200	3.27308100	-0.50140600
C -5.61270300	0.61770500	1.80509000	C -8.08149200	5.46539600	-1.04373100
C -3.41601300	-1.13970200	1.81171600	C -10.27226800	3.79851800	-0.47104100
C -5.79507900	-0.74895600	2.01268800	C -9.37520200	5.98313800	-0.99778200
C -4.71285500	-1.62879500	2.01692600	C -10.46862800	5.16436100	-0.71755900
H -6.45109400	1.30212900	1.78487200	H -7.23107000	6.09567900	-1.26983700
H -6.79909500	-1.13530900	2.15289400	H -9.53021700	7.04012500	-1.19062800
H -4.86728500	-2.69274900	2.15163700	H -11.47293700	5.57236000	-0.69153800
H -2.22348400	0.61630700	1.47065400	H -8.81576700	2.21938200	-0.29908700
C -2.24570700	-2.01648600	1.78014000	C -11.39153600	2.89855200	-0.18791100
C -0.92195200	-1.66378300	1.59605300	C -11.35773700	1.53224400	0.01054800
N -2.30551900	-3.38070000	1.91938500	N -12.69728800	3.31087800	-0.08785400
N -0.24775900	-2.84006100	1.64008700	N -12.65315900	1.18673700	0.22121100
N -1.10632500	-3.88225700	1.83816100	N -13.46061500	2.28649100	0.15798800
H -0.44167800	-0.71746400	1.38013900	H -10.53702900	0.82358500	0.00695300
C 1.14986500	-3.04651700	1.54664100	C -13.19016500	-0.10064200	0.46959600
C 2.01828100	-1.98981900	1.81685900	C -12.35785400	-1.22125100	0.42413300
C 1.63754800	-4.29380400	1.15912800	C -14.55212200	-0.23181600	0.74797900
C 3.39176300	-2.19553600	1.70383100	C -12.90895600	-2.47960900	0.66344500
C 3.01390000	-4.47558300	1.05638300	C -15.07741700	-1.49969100	0.98013300
C 3.90154200	-3.43709700	1.33466500	C -14.26550000	-2.63280500	0.94083700
H 1.63715400	-1.01433100	2.09151300	H -11.29957000	-1.12892400	0.19939700
H 0.94656600	-5.08746400	0.90845100	H -15.18296800	0.64618800	0.77160200
C 4.32941200	-1.06656900	2.03497400	C -12.00646000	-3.68455300	0.66872800
C 3.53691400	-5.81611700	0.61845800	C -16.53264900	-1.64224300	1.33511700
H 4.96777800	-3.58202600	1.22483800	H -14.68424700	-3.61646400	1.11139400
F 4.64057500	-1.04697700	3.35117800	F -11.44034800	-3.87209800	1.88379300
F 5.49372800	-1.16014600	1.35712200	F -12.67972600	-4.81691700	0.36964700
F 3.78411300	0.13574100	1.74288100	F -10.99862500	-3.56304400	-0.22004000
F 2.75982600	-6.35813200	-0.34811600	F -17.28381100	-0.66059500	0.79219400
F 4.79198600	-5.73353500	0.12676600	F -17.03741900	-2.82235500	0.91466300
F 3.56653400	-6.70302800	1.63861300	F -16.72261700	-1.58867100	2.67449200
C 4.13959600	1.54945900	-0.92472000	C 6.50191500	-1.94662000	-0.98219900
N 6.29042800	1.96943500	-1.31842400	N 4.72352700	-3.15590400	-0.41901300
N 4.80012600	0.42393200	-1.30275700	N 6.85291400	-3.22028400	-0.66699200

N 6.11246200	0.69793600	-1.53705900	N 5.75508800	-3.94521000	-0.32391200
H 3.09273900	1.55707300	-0.65757200	H 7.22045600	-1.21595700	-1.31464200
C 4.28471300	-0.88394900	-1.51976700	C 8.14566100	-3.81275100	-0.65744600
C 2.90711300	-1.08238700	-1.52517900	C 9.25834800	-3.02488500	-0.37121800
C 5.16580200	-1.94769900	-1.73995100	C 8.27378900	-5.17635200	-0.93200500
C 2.38850200	-2.36245700	-1.76446400	C 10.53674500	-3.59877800	-0.37659100
C 4.64227600	-3.21502300	-1.98160300	C 9.54531800	-5.74573400	-0.91511700
C 3.26526200	-3.42920700	-1.99982700	C 10.67040900	-4.96909700	-0.64776900
H 6.23367700	-1.77511000	-1.71775400	H 7.39308100	-5.76563500	-1.15508400
H 5.31760000	-4.04897700	-2.14129700	H 9.65896600	-6.80419700	-1.12607800
H 2.86251000	-4.42083900	-2.16816400	H 11.65898300	-5.41336500	-0.64661500
C 0.93974800	-2.56318300	-1.76446000	C 11.72197400	-2.78538500	-0.09425800
H 2.23084700	-0.25608300	-1.33711600	H 9.12712900	-1.97769800	-0.12333100
C -0.06406000	-1.63092100	-1.58735800	C 11.84531000	-1.42172400	0.09234000
N 0.35072100	-3.79100700	-1.94417800	N 12.97577200	-3.33548000	0.01366400
N -1.21331300	-2.34841300	-1.67393700	N 13.17286900	-1.22060900	0.30306400
N -0.94366000	-3.66826300	-1.89160700	N 13.84776100	-2.40279600	0.25240900
H -0.04122500	-0.57801300	-1.33666500	H 11.13466000	-0.61275200	0.05947100
C -2.54667000	-1.88072600	-1.59419100	C 13.86750100	-0.00927500	0.54608400
C -2.81859400	-0.53218700	-1.82560000	C 13.20146300	1.07395300	1.11795000
C -3.56718500	-2.77124200	-1.26518500	C 15.21633400	0.08030500	0.19952500
C -4.13224600	-0.08077900	-1.72699300	C 13.89787900	2.26264000	1.32841900
C -4.87316700	-2.29646700	-1.17519500	C 15.89654600	1.27239600	0.43398700
C -5.16903200	-0.95499600	-1.40807800	C 15.24563500	2.37232400	0.99167400
H -2.02331600	0.16189300	-2.06469500	H 12.15948500	0.99806400	1.40246500
H -3.33089300	-3.80456400	-1.04994200	H 15.71336300	-0.76730500	-0.25304800
C -4.44887000	1.35950600	-2.02496000	C 13.20093800	3.42192100	1.98949300
C -5.97439700	-3.25959900	-0.82466200	C 17.36513400	1.36115300	0.11384300
H -6.18342800	-0.59118300	-1.31014600	H 15.77684500	3.30239800	1.15123600
F -5.56228600	-4.18016400	0.07687100	F 17.70814400	0.54411900	-0.90410600
F -7.04789800	-2.63130000	-0.29914300	F 17.72673200	2.61591300	-0.22850600
F -6.40572200	-3.94183200	-1.91000500	F 18.12292200	1.00805600	1.17743500
F -3.37071700	2.15757500	-1.86876500	F 11.87225500	3.41120700	1.75086700
F -4.87872500	1.51893800	-3.29763800	F 13.36216400	3.39419000	3.33227900
F -5.42668800	1.83378700	-1.22101400	F 13.68527000	4.60568500	1.55860100
Cl 0.33042400	1.36630300	0.16030100	Cl -8.52555100	-0.48503500	-0.22756600

Z-AB-mTTA-(1,3)Ph + Cl(-), close

C -6.05760300 2.74081800 -1.92415500
N -5.35273900 4.00533600 -1.83764300
N -5.29374200 4.60484000 -0.73833300
C -5.82085300 3.95907300 0.43834600
C -7.45490600 2.74056300 -1.93290200
C -5.34266900 1.55109100 -2.04069500
C -8.13160300 1.52358800 -2.01686100
C -6.02500500 0.32570000 -2.05403900
C -7.42874400 0.32211800 -2.05672100
H -7.99672600 3.67721800 -1.85650300
H -4.25741700 1.57871500 -2.05192400
H -9.21739500 1.51429200 -2.02154100
C -5.27774900 -0.93382400 -2.02932700
H -7.95498100 -0.62561400 -2.07813600
C -5.30800800 2.72689400 0.83958300
C -6.84159300 4.57621700 1.16332500

Z-AB-mTTA-(1,3)Ph + Cl(-), open

C 1.87228900 5.53795900 2.02076500
N 2.13220500 5.26870600 3.40793200
N 1.30126700 4.69578900 4.14788000
C 0.10038000 4.09434100 3.64143400
C 0.73443500 6.24074600 1.60298400
C 2.87621400 5.20807000 1.11058600
C 0.60414200 6.57860400 0.25818200
C 2.72198200 5.50765200 -0.24929400
C 1.57723900 6.20472100 -0.66727800
H -0.02770000 6.51869200 2.32221900
H 3.76496000 4.70285900 1.47517700
H -0.27090200 7.12896600 -0.07378100
C 3.74084000 5.10895500 -1.22350400
H 1.46350800 6.45275400 -1.71645100
C 0.10843000 3.22185000 2.54922300
C -1.06947700 4.29601400 4.38134900

C -5.90130100	2.02427700	1.89142200	C -1.06953300	2.57568400	2.16044700
C -7.40819600	3.89183500	2.24137400	C -2.25033100	3.67734000	3.97240300
C -6.96306100	2.61771200	2.59276500	C -2.25731600	2.82260500	2.87186600
H -4.48054200	2.29202500	0.29528900	H 1.02193700	3.03560100	1.99892900
H -7.21346700	5.54783900	0.85477600	H -1.04458100	4.94636100	5.24983200
C -5.46487400	0.65129600	2.15247500	C -1.05536600	1.66292600	1.01536900
H -8.21974600	4.34986700	2.79856700	H -3.16953700	3.85255200	4.52283700
H -7.43402600	2.07442200	3.40465500	H -3.18264600	2.33973200	2.56950500
C -3.95081600	-1.15210300	-1.71066000	C 4.82789000	4.26700300	-1.07619800
N -5.84420300	-2.14647800	-2.33411300	N 3.73524200	5.55721300	-2.52013600
N -3.77925400	-2.49219800	-1.85949300	N 5.42340500	4.25306700	-2.29623000
N -4.94316300	-3.08447100	-2.23961500	N 4.74319300	5.04513700	-3.16742700
H -3.16612600	-0.49164800	-1.36531600	H 5.21735200	3.71518000	-0.23679400
C -2.56923000	-3.23335900	-1.76852400	C 6.57906200	3.53757000	-2.71438600
C -1.36674700	-2.53560600	-1.76965900	C 6.85232700	2.29299300	-2.15167600
C -2.58928400	-4.62831800	-1.71248900	C 7.41514700	4.09578000	-3.68380800
C -0.15206500	-3.22625100	-1.70703400	C 7.99764100	1.58828200	-2.54546700
C -1.37471900	-5.31180700	-1.65873800	C 8.54287500	3.38225000	-4.08481800
C -0.16059300	-4.62623100	-1.65291900	C 8.84058400	2.14409300	-3.52016200
H -3.53367300	-5.15711500	-1.70600700	H 7.18084500	5.06669400	-4.10259000
H -1.37922600	-6.39609300	-1.60910600	H 9.20200500	3.80356100	-4.83702700
H -1.36684100	-1.45455400	-1.81694700	H 9.72393000	1.59676400	-3.82791900
H 0.77870900	-5.16473900	-1.59796400	H 6.16487000	1.86818000	-1.42909000
C 1.08676400	-2.44952400	-1.70158900	C 8.30929300	0.28193100	-1.96014000
C 1.22186200	-1.08054800	-1.57434300	C 7.66230900	-0.42902900	-0.96714900
N 2.34223400	-2.99085200	-1.81777600	N 9.39337000	-0.45844800	-2.36345900
N 2.55943400	-0.86256800	-1.62116600	N 8.39417400	-1.56513600	-0.82345100
N 3.23311500	-2.04248700	-1.77202200	N 9.44826700	-1.56569700	-1.68640000
H 0.49119600	-0.30037900	-1.40778300	H 6.79924100	-0.21426300	-0.35902200
C 3.25331600	0.36559700	-1.50284900	C 8.18810900	-2.65802400	0.05534500
C 2.57119600	1.51109300	-1.08461700	C 6.90317600	-2.95741100	0.50598600
C 4.61681800	0.40705400	-1.79011100	C 9.28570800	-3.41782500	0.46162300
C 3.27599900	2.70639100	-0.96538800	C 6.72540800	-4.02340100	1.38608500
C 5.30218700	1.61078400	-1.64612100	C 9.08254700	-4.48876900	1.32810400
C 4.64201200	2.76764100	-1.23755200	C 7.80760800	-4.79663200	1.80187600
H 5.12722400	-0.49326900	-2.09888300	H 6.05068100	-2.37739600	0.17521200
H 1.51586600	1.47772400	-0.83427600	H 10.27674200	-3.16328200	0.11014200
C 6.79042800	1.64537900	-1.86315200	C 5.33526800	-4.38325900	1.83881800
C 2.55049900	3.96649900	-0.57511700	C 10.25362300	-5.34604200	1.72888600
H 5.18266500	3.69873200	-1.12385300	H 7.66163600	-5.61826400	2.49187600
F 1.41377900	3.71085500	0.10208000	F 4.76026600	-5.27772000	1.00258300
F 3.32006000	4.76301400	0.19868400	F 5.33941300	-4.93866500	3.06880300
F 2.20916600	4.69293300	-1.66576900	F 4.52603000	-3.30367000	1.87888400
F 7.19844400	0.70587800	-2.73834400	F 11.40616400	-4.64370700	1.74975900
F 7.20142300	2.84502100	-2.32520800	F 10.08173300	-5.88689800	2.95360200
F 7.46628600	1.42442000	-0.70498100	F 10.43165800	-6.37183400	0.86496400
C -4.35434100	-0.01290400	1.66073200	C -2.07768900	0.88758600	0.50344200
N -6.20851300	-0.24464600	2.87583300	N 0.06177600	1.45271400	0.24590400
N -4.49292800	-1.28352200	2.11333100	N -1.52127400	0.24617700	-0.55804000
N -5.62519900	-1.41204100	2.85700300	N -0.21566400	0.60236900	-0.70156600
H -3.51329000	0.29759200	1.05331800	H -3.10851500	0.75671900	0.80876300
C -3.61030000	-2.38207500	1.92516700	C -2.13609000	-0.67351900	-1.45312700
C -2.24409600	-2.13606000	1.83430400	C -3.51386100	-0.85730800	-1.38383500
C -4.12236300	-3.67976900	1.85702600	C -1.36163200	-1.37681600	-2.38096200

C	-1.35479400	-3.20751200	1.68433600	C	-4.14255200	-1.76809300	-2.24297500
C	-1.85855700	-4.51429700	1.62999000	C	-1.99698000	-2.27029900	-3.24229700
C	-3.23106100	-4.74091100	1.71240400	C	-3.37515500	-2.47390000	-3.17978900
H	-5.19153600	-3.84204400	1.91859200	H	-0.29096800	-1.22256500	-2.42026300
H	-3.61341100	-5.75496800	1.65399300	H	-1.40450700	-2.81979200	-3.96718800
H	-1.16988400	-5.34200900	1.51188400	H	-3.86113600	-3.17690300	-3.84722800
H	-1.87454700	-1.11894600	1.88633100	C	-5.58971000	-1.95761200	-2.13140000
C	0.08482800	-2.95463700	1.63071600	H	-4.10626800	-0.29725100	-0.66856900
C	0.76387600	-1.75317100	1.56992800	C	-6.45012800	-1.40877600	-1.20112600
N	1.01573000	-3.96381000	1.65900700	N	-6.32580300	-2.75082500	-2.97625700
N	2.07847500	-2.10265700	1.57208000	N	-7.67045600	-1.89977200	-1.53478800
N	2.21246600	-3.45973000	1.62521700	N	-7.57765600	-2.71963600	-2.62323500
H	0.41654000	-0.73758500	1.45310300	H	-6.27528700	-0.74138800	-0.36450200
C	3.22548600	-1.27332600	1.56556100	C	-8.91748600	-1.65372000	-0.90882200
C	3.12764200	0.05393300	1.98003500	C	-8.98155900	-0.81757500	0.20759300
C	4.44664100	-1.80101700	1.14241900	C	-10.06902400	-2.26036500	-1.41516700
C	4.26669800	0.85782300	1.95917100	C	-10.21858500	-0.59495500	0.81245900
C	5.57250500	-0.98281600	1.13987800	C	-11.29075600	-2.02079900	-0.79331700
C	5.49447000	0.35042900	1.54359700	C	-11.37922400	-1.18873200	0.32281600
H	2.18320600	0.46167700	2.31746900	H	-8.09024800	-0.34713500	0.61264400
H	4.50031400	-2.82873800	0.81155900	H	-9.99911500	-2.91209100	-2.27534600
C	4.17685800	2.27442500	2.45787000	C	-10.29096900	0.34461200	1.98645700
C	6.87170400	-1.53327500	0.61623500	C	-12.54203100	-2.62700000	-1.36872700
H	6.36934700	0.98532200	1.51607500	H	-12.33184100	-1.01620900	0.80698700
F	4.43357600	2.35347700	3.78289200	F	-12.29500700	-3.79970900	-1.99058100
F	5.06337600	3.08252600	1.83661700	F	-13.47085300	-2.85817800	-0.41582900
F	2.94450300	2.79380800	2.26357100	F	-13.11312100	-1.80888100	-2.28383700
F	7.02008900	-2.83874700	0.92373300	F	-9.22655000	0.20577900	2.80502400
F	6.94444400	-1.44388000	-0.73707200	F	-10.31093100	1.63668600	1.58402500
F	7.93637800	-0.87057100	1.10936100	F	-11.40254000	0.14362100	2.72634600
Cl	-1.32458100	0.88219500	-0.18895400	Cl	-5.56527000	0.73298200	1.39769600