

Supporting Information

A Theoretical Investigation on Boron-Ligand Cooperation to Activate Molecular Hydrogen by a Frustrated Lewis Pair and Subsequent Reduction of Carbon dioxide

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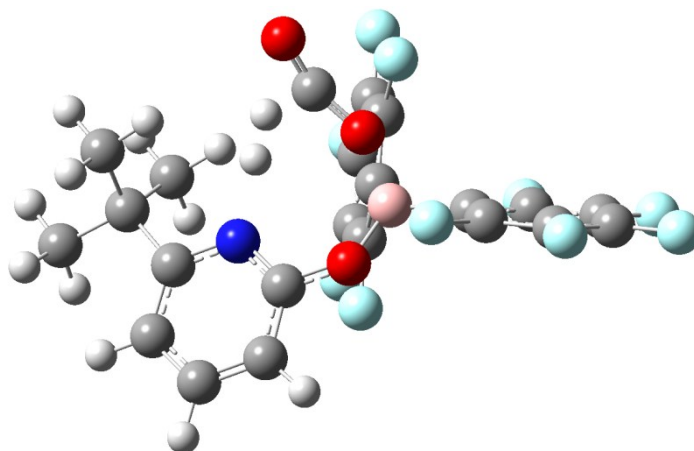
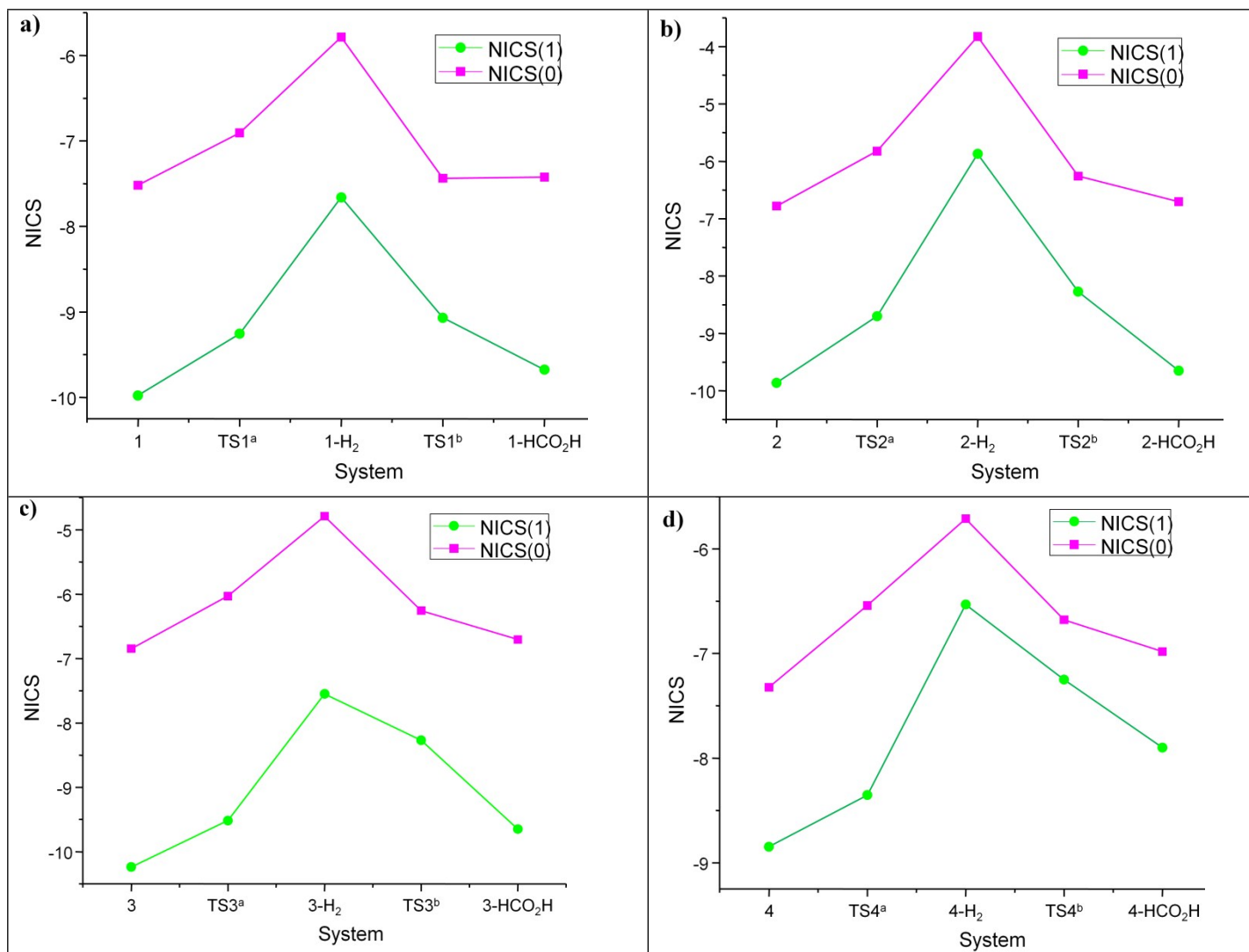


Fig. S1 Transition state geometry when the H₂ activation and CO₂ hydrogenation take place simultaneously with a barrier height of 50.8 kcal/mol.



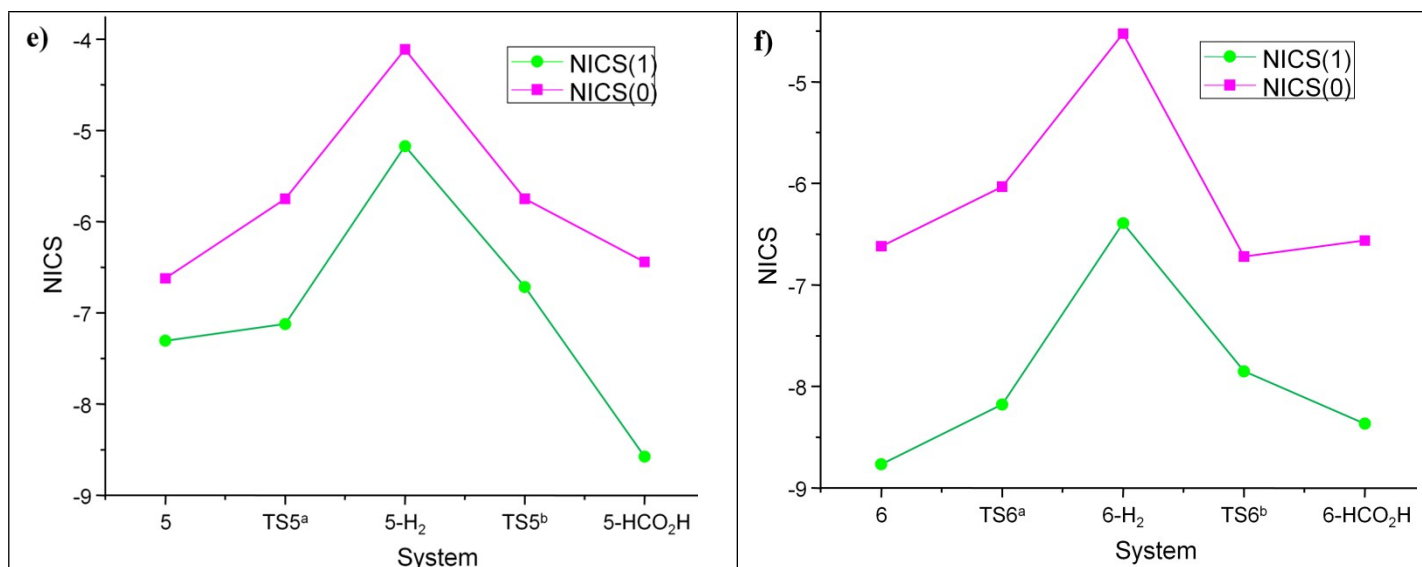
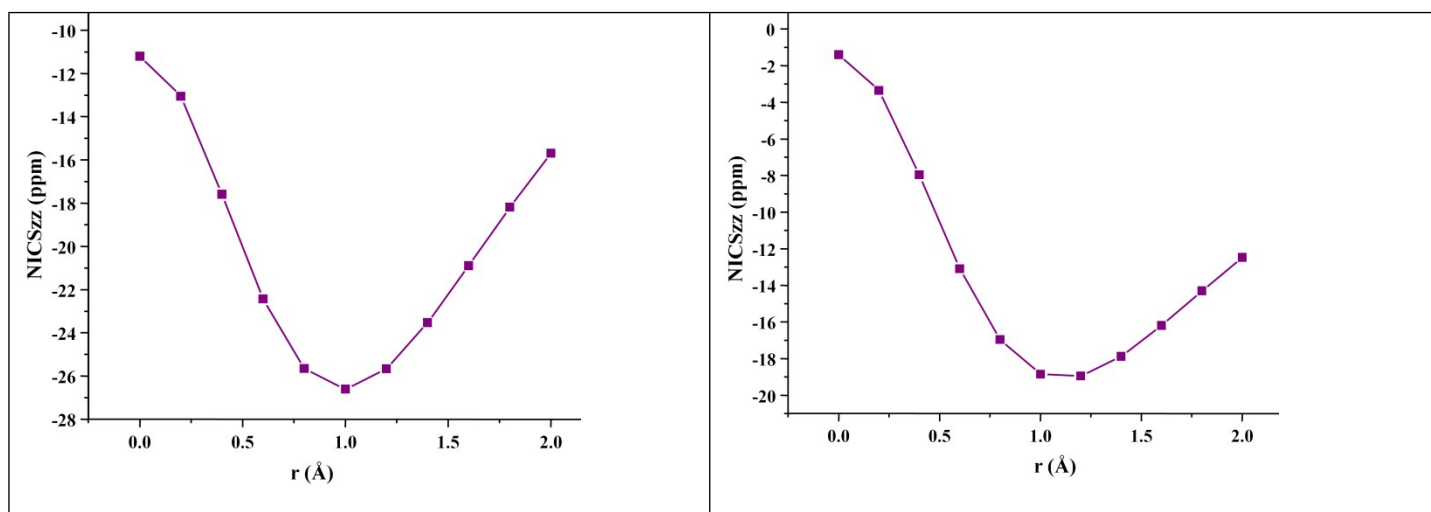
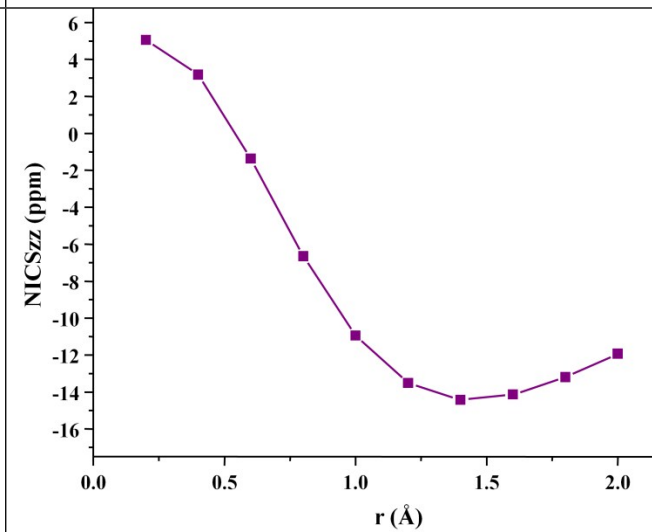
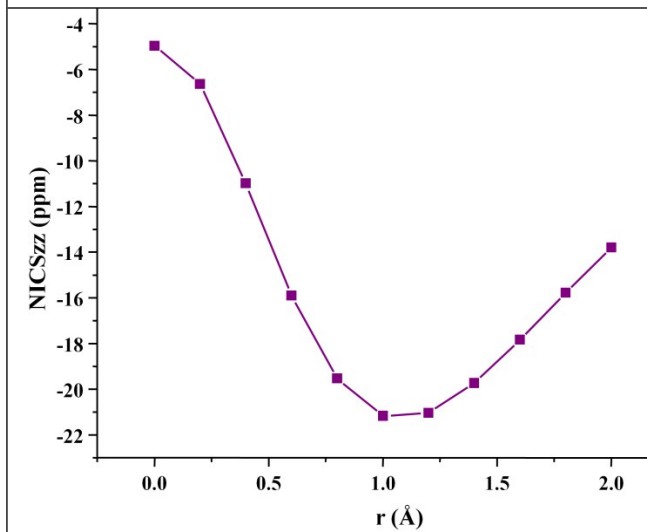
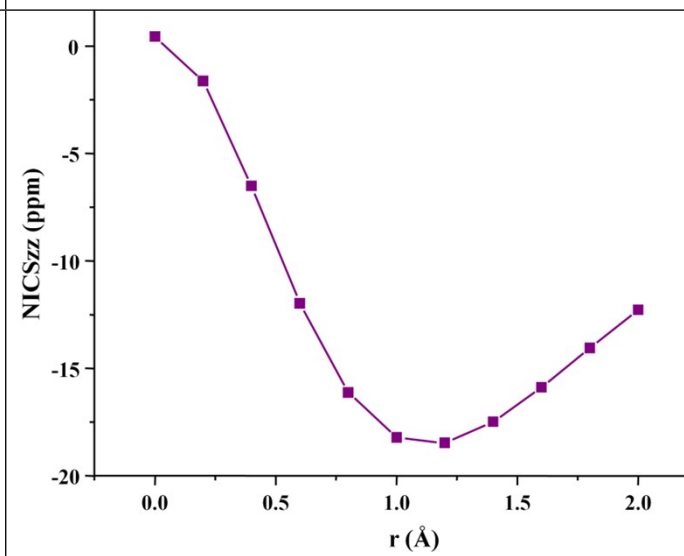
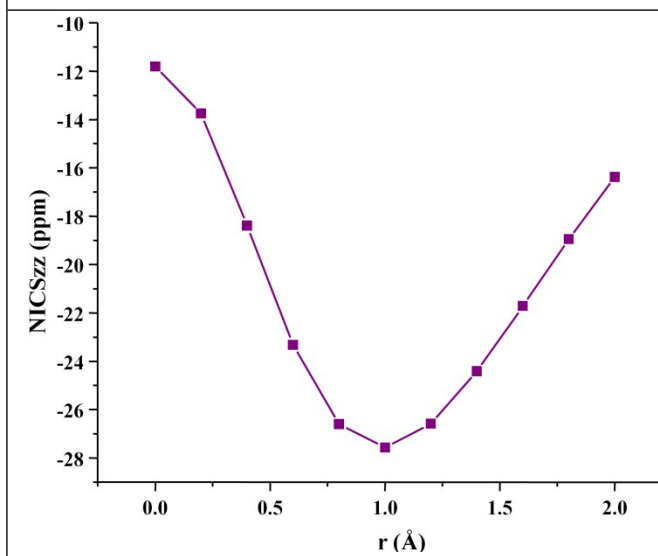
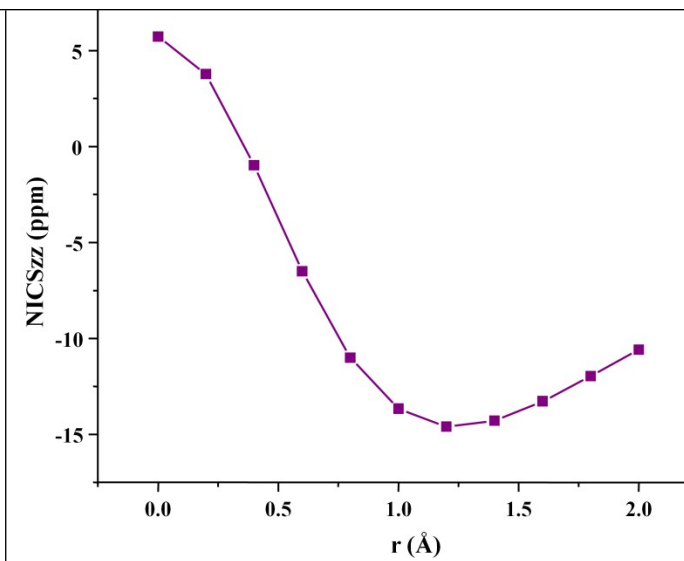
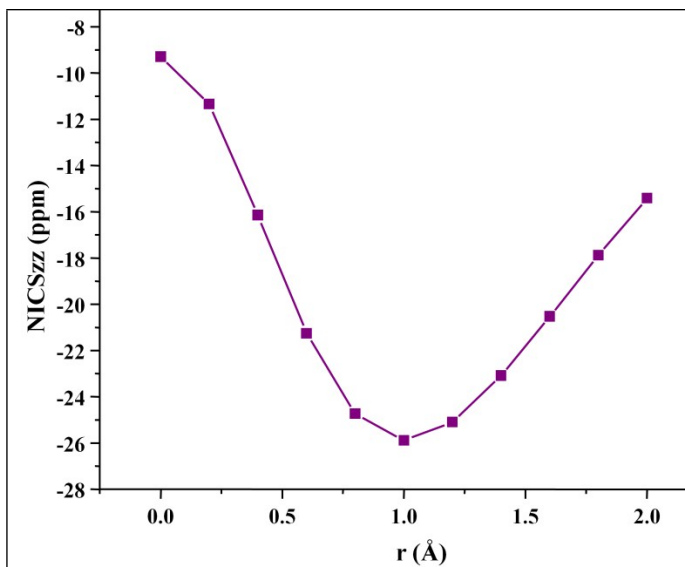


Fig. S2 Plot of NICS(0) and NICS(1) throughout the stationary points for the activation of H₂ and transfer of it to CO₂. a) for FLP 1 b) for FLP 2 c) for FLP 3 d) for FLP 4 e) for FLP 5 and f) for FLP 6. In these figures 1-HCO₂H, 2-HCO₂H, 3-HCO₂H, 4-HCO₂H and 5-HCO₂H are the product complexes where the formic acid remains in weak van der Waals interaction with the FLPs.





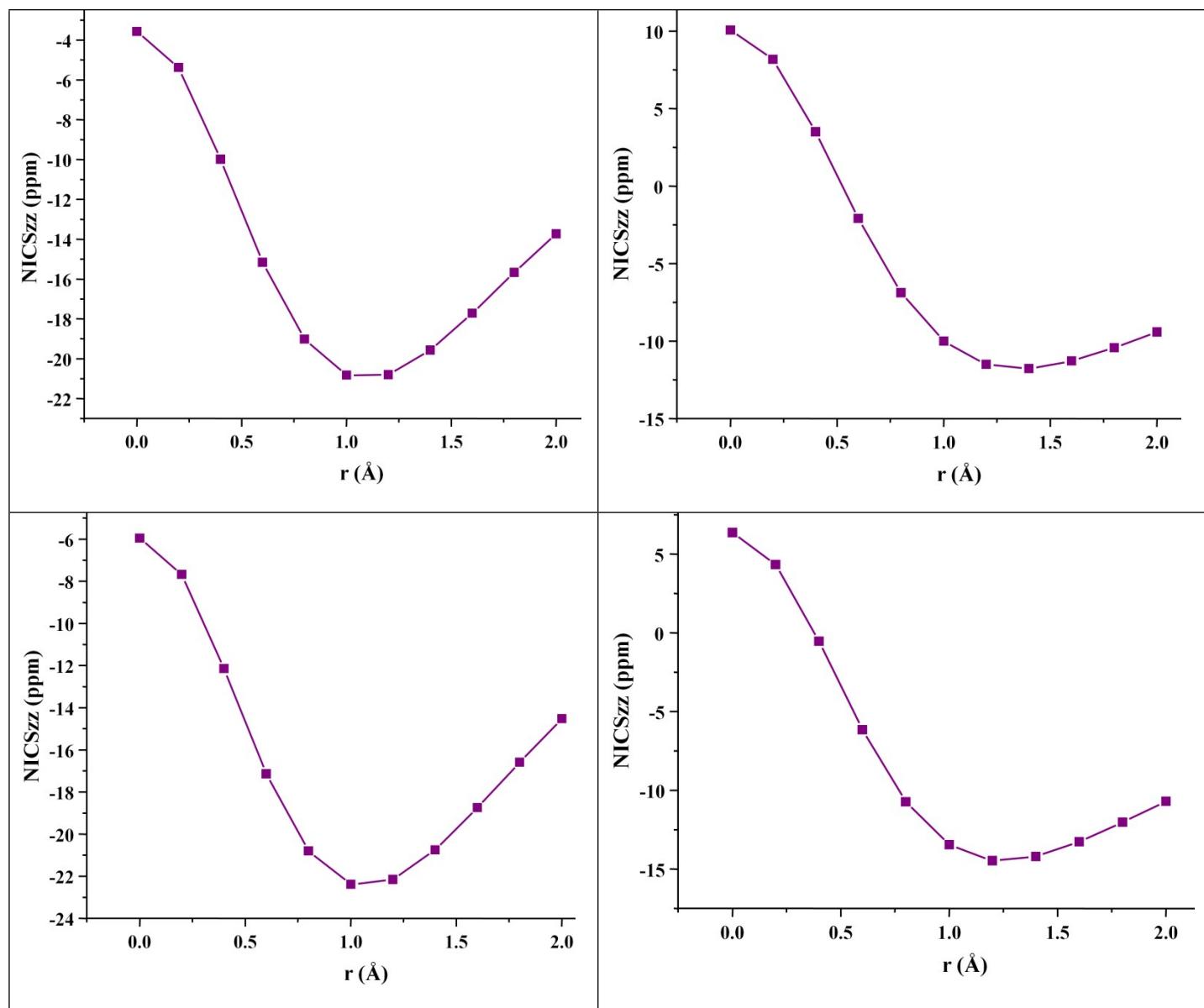


Fig. S3 Plot of NICS_{zz} as a function of distance (angstrom) from the center of the pyridine ring before (left-side) and after (right-side) the activation of H₂ for FLP systems **1**, **2**, **3**, **4**, **5** and **6** from top to bottom.

Table S1 The EDA results of the FLPs **1-6** using electron-shared neutral schemes at the BP86-D3(BJ)-TZ2P+/M06-2X-D3/6-31+G(d,p) level

Energy	1	2	3	4	5	6
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	[B(C ₆ F ₆) ₂] + [O-Py(tBu)]	[B(C ₆ F ₆) ₂] + [NH-Py(tBu)]	[B(C ₆ F ₆) ₂] + [S-Py(tBu)]	[B(C ₆ F ₆) ₂] + [O-Py(tBu)(NMe ₂)]	[B(C ₆ F ₆) ₂] + [NH-Py(tBu)(NMe ₂)]	[B(C ₆ F ₆) ₂] + [S-Py(tBu)(NMe ₂)]
ΔE_{int}	-147.0	-141.8	-112.6	-136.1	-142.9	-117.6
ΔE_{Pauli}	442.9	529.3	333.4	493.6	533.1	348.9
$\Delta E_{\text{disp}}^{[a]}$	-10.7 (1.8%)	-11.6 (1.7%)	-13.7 (3.1%)	-10.9 (1.7%)	-11.7 (1.7%)	-13.9 (3.0%)
$\Delta E_{\text{elstat}}^{[a]}$	-223.7 (37.9%)	-263.6 (39.3%)	-187.3 (42.0%)	-244.2 (38.8%)	-266.6 (39.4%)	-192.7 (41.3%)
$\Delta E_{\text{orb}}^{[a]}$	-355.5 (60.3%)	-396.0 (59.0%)	-244.9 (54.9%)	-374.6 (59.5%)	-397.6 (58.8%)	-260.0 (55.7%)

^[a]The values in parentheses give the percentage contribution to the total attractive interactions

$$\Delta E_{\text{elstat}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}.$$

Coordinates of Optimized Transition state (TS) geometries

TS1^a

C	2.96292700	-3.09278300	-2.03640400
C	1.68432400	-2.61531900	-2.24147700
C	3.65268800	-2.81401000	-0.84423400
C	1.12963500	-1.85136000	-1.20748500
B	-0.53200100	-0.37428700	-0.33820700
C	-2.11864700	-0.40941700	-0.14857400
C	-2.96487500	0.68104400	-0.31981000
C	-2.73766000	-1.61077100	0.18990900
C	-4.34410900	0.59329300	-0.17083300
C	-4.10899900	-1.74021600	0.35160100
C	-4.91700900	-0.62492100	0.16694400
C	0.25674800	1.02665500	-0.29274500
C	0.07514500	1.88888300	0.78596800
C	1.18574600	1.44068200	-1.24085900
C	0.75734300	3.08615900	0.93351900
C	1.89254100	2.63430200	-1.13343300
C	1.67676200	3.45996000	-0.04007400
F	-1.98741900	-2.70285300	0.39639000
F	-2.47173200	1.88052100	-0.65457400
F	-5.11836300	1.66197900	-0.35233700
F	-6.23431300	-0.72531900	0.31280600
F	-4.65541900	-2.90977700	0.68192300
F	1.45178700	0.68642600	-2.31684500
F	2.77695200	2.98667800	-2.06639100
F	2.34611600	4.60251200	0.07796000
F	0.54828600	3.87292400	1.98784000

F	-0.79340300	1.55139400	1.75245800
C	3.02644000	-2.06417800	0.13961600
H	4.66274100	-3.17607300	-0.70412900
H	3.44702600	-3.68320100	-2.80809400
H	1.11636800	-2.79245700	-3.14592600
N	1.77340200	-1.61005800	-0.07415800
O	-0.10183500	-1.33955500	-1.30947000
H	-0.20418900	-0.90865400	0.98506500
H	0.60720200	-1.12741200	0.74281400
C	3.64554000	-1.66183500	1.47109200
C	5.08820800	-2.15815000	1.59519800
H	5.72566200	-1.74512100	0.80667500
H	5.49939200	-1.83982800	2.55748800
H	5.14434800	-3.25089200	1.55474600
C	3.62559300	-0.12523100	1.56796600
H	4.20372100	0.32563100	0.75427000
H	2.60271100	0.26201700	1.51381200
H	4.06313100	0.19291600	2.51946600
C	2.80461400	-2.26126500	2.61153900
H	1.77270500	-1.89955800	2.58127500
H	2.78687700	-3.35421300	2.55379200
H	3.23301100	-1.97435200	3.57704800

TS2^a

C	3.03657400	-3.38016000	-1.76572900
C	1.75550400	-2.96012100	-2.04709900
C	3.72501300	-2.88731100	-0.64314900
C	1.17464600	-2.02335900	-1.16937700
B	-0.56142200	-0.45033100	-0.38929300
C	-2.15108900	-0.44465800	-0.18790100
C	-2.97102300	0.65415300	-0.43239800
C	-2.80317400	-1.59239900	0.26018800
C	-4.34822000	0.62475600	-0.24871700
C	-4.17442700	-1.66252200	0.46168300
C	-4.95181000	-0.54103200	0.20283900
C	0.23460200	0.95001100	-0.34505200
C	0.02811400	1.83158200	0.71411400
C	1.19928600	1.34422400	-1.26728500
C	0.71758600	3.02383700	0.86980300
C	1.91490200	2.53181700	-1.14982900
C	1.67453200	3.37446200	-0.07514600
F	-2.08951500	-2.69632300	0.53321400
F	-2.45079000	1.80554800	-0.87469100
F	-5.09264700	1.69898600	-0.50451700
F	-6.26775700	-0.58571400	0.38214600
F	-4.74776200	-2.78410700	0.89620700
F	1.50197700	0.57966200	-2.32493600
F	2.83842700	2.85985500	-2.05432100
F	2.35392300	4.51078300	0.05125400

F	0.47990800	3.82691900	1.90634300
F	-0.87650000	1.52124100	1.65764400
C	3.08311500	-1.99089900	0.19648100
H	4.74093300	-3.20333100	-0.44729500
H	3.52627400	-4.09136600	-2.42393500
H	1.20833300	-3.31048100	-2.91511400
N	1.82510600	-1.59003700	-0.08385000
H	-0.18925500	-0.96285000	0.97438700
H	0.63348900	-1.14151600	0.74146100
C	3.69693100	-1.37993100	1.45077600
C	5.15642200	-1.80596300	1.63092800
H	5.77430400	-1.49432500	0.78244300
H	5.56242500	-1.33532800	2.53107800
H	5.24962300	-2.89008900	1.75247200
C	3.62684800	0.15317400	1.33402000
H	4.16872800	0.50415400	0.44894900
H	2.58958700	0.49443400	1.25703600
H	4.07632500	0.61411900	2.21939200
C	2.88548400	-1.83898000	2.67498100
H	1.84257000	-1.51604000	2.60839200
H	2.90260800	-2.92939500	2.77066300
H	3.31301100	-1.40679700	3.58540400
N	-0.07842400	-1.49301000	-1.32164400
H	-0.72087900	-2.01394300	-1.90029100

TS3^a

C	-3.42831300	-2.94493300	2.27609400
C	-2.09155600	-2.69507800	2.53214600
C	-3.97824100	-2.59673300	1.03954600
C	-1.34307800	-2.09631800	1.51291500
B	0.66843400	-0.51598000	0.40734500
C	2.22599600	-0.41140300	0.06124400
C	2.98556300	0.68695900	0.45698300
C	2.92061000	-1.42164900	-0.60000400
C	4.34898800	0.78793400	0.21179400
C	4.27951300	-1.35404900	-0.87272000
C	4.99812900	-0.23958000	-0.45949400
C	-0.20544400	0.81983000	0.28885600
C	-0.07942500	1.59934500	-0.86185600
C	-1.12653300	1.28628900	1.22456700
C	-0.80302400	2.75926400	-1.09105600
C	-1.87007500	2.44633400	1.03379400
C	-1.70948300	3.18549200	-0.12894600
F	2.26241700	-2.50867100	-1.02700400
F	2.41004600	1.70186300	1.11462600
F	5.03601500	1.85449200	0.61549400
F	6.30152000	-0.15863100	-0.70319500
F	4.89622300	-2.34080200	-1.51980600
F	-1.35066300	0.63108600	2.36712000

F	-2.74337300	2.84818800	1.95624800
F	-2.41984700	4.29127800	-0.32281500
F	-0.64689400	3.45483700	-2.21590500
F	0.75922100	1.20601500	-1.83509200
C	-3.16341900	-2.00947400	0.07434400
H	-5.02642700	-2.77941500	0.84159100
H	-4.05250900	-3.40157900	3.03801500
H	-1.62965600	-2.93501200	3.48292700
N	-1.86206000	-1.77664900	0.33194000
H	0.34612100	-1.21108400	-0.95116000
H	-0.37809800	-1.34764700	-0.62870800
C	-3.65038300	-1.58530000	-1.30831800
C	-5.14759100	-1.84942100	-1.49248700
H	-5.74879500	-1.29455500	-0.76470800
H	-5.45133700	-1.52397900	-2.49171900
H	-5.38554000	-2.91455600	-1.40428100
C	-3.38123700	-0.08113400	-1.48271200
H	-3.90825200	0.50316600	-0.72007100
H	-2.31217700	0.13434400	-1.40091700
H	-3.72466800	0.24891600	-2.46845000
C	-2.86883300	-2.37456200	-2.37237300
H	-1.79411500	-2.19009800	-2.29353700
H	-3.03926200	-3.45070500	-2.26580900
H	-3.19405200	-2.07195200	-3.37294200
S	0.38745500	-1.77387100	1.75625600

TS4^a

C	3.59844200	-2.02263900	-0.72788500
C	2.24921600	-2.05250200	-1.11656200
C	3.95093700	-1.21491000	0.39345200
C	1.35351700	-1.29730800	-0.37327700
B	-0.81283400	-0.32691600	-0.10083000
C	-2.32285100	-0.84974800	-0.03588900
C	-3.41744900	-0.18153200	-0.57470000
C	-2.59811400	-2.07314500	0.57165700
C	-4.71004000	-0.68998100	-0.52302600
C	-3.87350800	-2.61313600	0.64872400
C	-4.93699200	-1.91272900	0.09292000
C	-0.51144600	1.23100100	-0.35984600
C	-1.13194500	2.20101800	0.42309100
C	0.39986300	1.70865700	-1.29517800
C	-0.87816200	3.55869400	0.30565600
C	0.68372300	3.06164000	-1.44835900
C	0.04162700	3.99050000	-0.64272100
F	-1.60192300	-2.76839000	1.13758700
F	-3.26100900	0.99848800	-1.18934200
F	-5.72854400	-0.01969700	-1.06077000
F	-6.16751600	-2.41297100	0.15079400
F	-4.08952900	-3.78458600	1.24679500

F	1.06333300	0.86652900	-2.09876900
F	1.57009200	3.47205700	-2.35642900
F	0.30443200	5.28739600	-0.77636200
F	-1.49698100	4.44558000	1.08426700
F	-2.01583800	1.81947600	1.35915900
C	2.97783600	-0.51318300	1.07460500
H	4.98121200	-1.13951100	0.70715700
H	1.87853300	-2.61059800	-1.96406600
N	1.68550900	-0.57052000	0.68718300
O	0.04784200	-1.28915100	-0.70163700
H	-0.58378400	-0.39092700	1.38291900
H	0.26519800	-0.36619400	1.27714000
C	3.24981200	0.39763400	2.26661900
C	4.73912800	0.46544900	2.61326100
H	5.32970400	0.85825100	1.77902000
H	4.88255300	1.13438700	3.46693100
H	5.13426500	-0.51734000	2.89126900
C	2.74749100	1.80984900	1.91447200
H	3.27182100	2.20260300	1.03649300
H	1.67499900	1.80213600	1.69470900
H	2.92354200	2.48924000	2.75471400
C	2.47482000	-0.13526700	3.48379000
H	1.39874800	-0.16045500	3.29091300
H	2.80034800	-1.14803800	3.74239700
H	2.64843700	0.51405300	4.34797500
N	4.54527600	-2.73201700	-1.40257000
C	4.16086100	-3.50370700	-2.57052000
H	3.74099600	-2.86105100	-3.35414100
H	5.03997700	-4.00630300	-2.97120600
H	3.41793600	-4.26647000	-2.31082700
C	5.94157400	-2.64792800	-1.01433000
H	6.08676800	-2.98045500	0.01967800
H	6.52798100	-3.29718700	-1.66291700
H	6.32802200	-1.62589000	-1.11132500

TS5^a

C	3.73643900	-2.06084700	-0.60696700
C	2.40720200	-2.16556400	-1.03802500
C	4.03109000	-1.12015700	0.42368900
C	1.44901700	-1.35214800	-0.42821900
B	-0.81519000	-0.39546000	-0.16854600
C	-2.32818100	-0.91866200	-0.07924100
C	-3.41948700	-0.26530800	-0.64638900
C	-2.62291700	-2.10074600	0.59808900
C	-4.72029000	-0.74511800	-0.55322200
C	-3.90782500	-2.61121500	0.72009500
C	-4.96458200	-1.92468000	0.13663000
C	-0.54962000	1.17719700	-0.39621300
C	-1.20648000	2.11674600	0.39553200

C	0.36466700	1.70151300	-1.30542200
C	-0.98714200	3.48308100	0.31274800
C	0.61518000	3.06517600	-1.42194700
C	-0.06240000	3.96019000	-0.60800700
F	-1.63490000	-2.79420600	1.18531900
F	-3.24974200	0.87402600	-1.32888500
F	-5.73147200	-0.08869500	-1.12025500
F	-6.20312100	-2.39787900	0.23399500
F	-4.13620300	-3.74370800	1.38496500
F	1.07298100	0.90493900	-2.11605200
F	1.51165700	3.51802600	-2.30052400
F	0.17088000	5.26649700	-0.70702200
F	-1.64387300	4.33551900	1.09988100
F	-2.09807700	1.69712600	1.30895500
C	3.01639300	-0.37417500	0.98573100
H	5.04725600	-0.98075800	0.75969200
H	2.10548900	-2.82301700	-1.84232700
N	1.74024100	-0.50248500	0.56487000
H	-0.50637500	-0.44750500	1.33042300
H	0.34609700	-0.37209500	1.20214900
C	3.22848400	0.65313400	2.09392000
C	4.70882100	0.82890200	2.44264500
H	5.28876300	1.16680600	1.57743700
H	4.80864500	1.58444000	3.22758100
H	5.14922800	-0.10020900	2.81951300
C	2.65748100	2.00253600	1.62305000
H	3.15462400	2.33911400	0.70649400
H	1.58491100	1.92377600	1.41984400
H	2.80837100	2.76189900	2.39727400
C	2.47167800	0.18708700	3.34990200
H	1.39961700	0.09127000	3.15669900
H	2.84644700	-0.78186600	3.69545400
H	2.60563700	0.91603100	4.15588500
N	0.11709700	-1.35797200	-0.77805100
H	-0.22457100	-2.20239600	-1.21269900
N	4.72641400	-2.82041400	-1.15953600
C	4.41055200	-3.71351600	-2.25774700
H	5.31310400	-4.24381900	-2.55841000
H	3.66327400	-4.45649700	-1.95618100
H	4.02462900	-3.16442800	-3.12642600
C	6.10822100	-2.63027400	-0.75708300
H	6.23728000	-2.81581100	0.31482900
H	6.73384300	-3.33887900	-1.29828100
H	6.46244100	-1.61637400	-0.98187900

TS6^a

C	-3.49265200	-3.12959400	1.99450100
C	-2.11360000	-2.95415100	2.21658400
C	-4.01623300	-2.65263700	0.76579600

C	-1.36397800	-2.34100000	1.22260700
B	0.67325400	-0.67259600	0.33042300
C	2.22771600	-0.49740800	0.00155600
C	2.96749600	0.55028900	0.54536100
C	2.94042600	-1.39322800	-0.79255600
C	4.32821900	0.71084100	0.31761000
C	4.29740500	-1.26132900	-1.05230000
C	4.99551000	-0.20127700	-0.48857600
C	-0.21884000	0.65429500	0.38910300
C	-0.14361100	1.56123200	-0.66786000
C	-1.09980300	1.00403200	1.41032400
C	-0.88240400	2.73256200	-0.73449500
C	-1.85511600	2.17156000	1.38423800
C	-1.74767100	3.03933600	0.30723400
F	2.30522400	-2.42357500	-1.36706700
F	2.37530800	1.45281800	1.33850600
F	4.99569300	1.72446500	0.86591700
F	6.29703700	-0.06245400	-0.71789200
F	4.93251500	-2.13643200	-1.82978200
F	-1.26466600	0.22519300	2.48286300
F	-2.68637900	2.46165400	2.38530500
F	-2.46976400	4.15480700	0.27154200
F	-0.77860600	3.55195100	-1.77981500
F	0.65640700	1.28859300	-1.71283700
C	-3.17708400	-2.06239000	-0.16564300
H	-5.07144400	-2.73976700	0.55409000
H	-1.63123800	-3.24936800	3.13860400
N	-1.85754300	-1.91494400	0.06301100
H	0.35638500	-1.15734400	-1.16229100
H	-0.35397800	-1.36662100	-0.86455100
C	-3.66345100	-1.54263100	-1.51713100
C	-5.18739400	-1.60769200	-1.65275800
H	-5.68688500	-1.01282200	-0.88063900
H	-5.48121000	-1.20571800	-2.62694600
H	-5.55693600	-2.63689400	-1.59680100
C	-3.20876200	-0.08271600	-1.67913700
H	-3.58932800	0.54195700	-0.86246200
H	-2.11804300	-0.01327700	-1.68130100
H	-3.57942000	0.32277500	-2.62617000
C	-3.02367800	-2.40067800	-2.62234700
H	-1.93249900	-2.36738600	-2.56028500
H	-3.33897500	-3.44569300	-2.53664000
H	-3.32569100	-2.02867100	-3.60706600
S	0.38969000	-2.11556400	1.46471200
N	-4.29550900	-3.71940500	2.92599100
C	-3.73594600	-4.11583100	4.20532800
H	-3.34096800	-3.25458800	4.75928900
H	-4.51558000	-4.58384800	4.80480900
H	-2.92820200	-4.84358100	4.07071100
C	-5.72898200	-3.78856000	2.71036000
H	-6.17467600	-2.78993100	2.61709900
H	-5.96542200	-4.36188000	1.80710100

H	-6.19040600	-4.29210500	3.55878900
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TS1^b

C	1.75288400	-4.92180700	1.82806200
C	0.40347400	-4.96600500	1.55021600
C	2.61865300	-5.90264100	1.32357100
C	-0.06508700	-6.01903000	0.76055500
B	-1.90644800	-6.52653600	-0.80997600
C	-0.99372600	-6.51729400	-2.12113900
C	-1.17042700	-7.46748600	-3.12641900
C	0.00825500	-5.58077300	-2.35593900
C	-0.38796600	-7.51824900	-4.27119100
C	0.81141300	-5.59126600	-3.48811400
C	0.61472000	-6.57253500	-4.44940200
C	-3.47371700	-6.31304900	-0.89039800
C	-4.27826700	-6.63804000	0.20371300
C	-4.14172000	-5.85315100	-2.02320200
C	-5.65897200	-6.50839000	0.18932300
C	-5.52175500	-5.70643700	-2.07381500
C	-6.28188100	-6.03664400	-0.95993900
F	0.23778400	-4.59902300	-1.46582400
F	-2.13636600	-8.38158300	-3.00462400
F	-0.59001600	-8.45106600	-5.19669400
F	1.37652600	-6.60305800	-5.53672300
F	1.77021800	-4.67945100	-3.65102700
F	-3.45984800	-5.51205700	-3.12507800
F	-6.11895500	-5.24869700	-3.17265200
F	-7.60221000	-5.90014600	-0.99212900
F	-6.38926000	-6.82860800	1.25491000
F	-3.71751600	-7.11334000	1.31898800
C	2.10937500	-6.95436800	0.58420500
H	3.68053400	-5.84094300	1.51590100
H	2.15387300	-4.10685800	2.42213400
H	-0.29947200	-4.21067100	1.87646000
N	0.76645900	-6.99092900	0.35450300
O	-1.34242900	-6.05417000	0.41558700
H	-2.02171600	-8.00477600	-0.55838200
H	0.29630800	-7.90833300	-0.08215700
O	-0.35372900	-9.14943500	-0.39817700
C	-1.60871200	-9.13932600	-0.39858100
C	2.93716700	-8.08887200	-0.00333700
C	2.59914500	-8.23831400	-1.50032700
H	3.21434400	-9.03579400	-1.92718600
H	1.55182300	-8.50724100	-1.66679700
H	2.82163600	-7.31110200	-2.04053300
C	2.61915400	-9.39277400	0.75534700
H	2.85832300	-9.28673300	1.81845000
H	1.57222100	-9.68479600	0.65168100
H	3.23543500	-10.19954200	0.34649800

C	4.43472600	-7.79079300	0.13181600
H	4.71044000	-6.85466800	-0.36480500
H	4.74923200	-7.74390000	1.17918800
H	4.99748100	-8.59940600	-0.34200600
O	-2.49481600	-9.93693700	-0.29122100

TS2^b

C	1.83119700	-4.99315700	1.96727100
C	0.47519700	-5.02390700	1.73510000
C	2.68667700	-5.92846500	1.36316500
C	-0.03625200	-6.01562100	0.88016000
B	-1.93754200	-6.54849700	-0.75409600
C	-1.00479700	-6.56670300	-2.05419500
C	-1.17039400	-7.52659000	-3.05279700
C	-0.01118300	-5.62244300	-2.29931200
C	-0.38950600	-7.57971100	-4.19825400
C	0.78778500	-5.63408000	-3.43522600
C	0.60170400	-6.62463400	-4.38790500
C	-3.50622300	-6.30357000	-0.90188900
C	-4.36865900	-6.56053500	0.16610500
C	-4.12691100	-5.89998200	-2.08435300
C	-5.74681500	-6.43226300	0.08692600
C	-5.50369900	-5.75659500	-2.20434700
C	-6.31762600	-6.02705100	-1.11301400
F	0.22118000	-4.62921200	-1.42253600
F	-2.13457900	-8.44387500	-2.93311200
F	-0.58541700	-8.52196300	-5.11642300
F	1.36391900	-6.65732700	-5.47577900
F	1.74123600	-4.71664200	-3.60459300
F	-3.40482900	-5.61272400	-3.17444900
F	-6.04691400	-5.35724800	-3.35209300
F	-7.63427300	-5.89059500	-1.21239700
F	-6.52027500	-6.68608400	1.13969100
F	-3.86183700	-6.95138000	1.34636700
C	2.15134500	-6.92863700	0.57552500
H	3.75399900	-5.87497300	1.52429900
H	2.24863100	-4.21893500	2.60323600
H	-0.19584400	-4.27830900	2.14476600
N	0.80254700	-6.95146100	0.39062000
H	-2.09341300	-8.03780700	-0.53708400
H	0.32787700	-7.83122500	-0.04966100
O	-0.38523600	-9.11824600	-0.33371400
C	-1.63686500	-9.13984600	-0.29418700
C	2.95206800	-8.04500300	-0.08030500
C	2.54977100	-8.16779200	-1.56243300
H	3.13889700	-8.96424600	-2.02642200
H	1.49363200	-8.42625800	-1.68797900
H	2.75852700	-7.23476500	-2.09735600
C	2.66340500	-9.36508900	0.66326200
H	2.94177000	-9.28069300	1.71880200

H	1.61260500	-9.65425500	0.59163400
H	3.26462000	-10.16228000	0.21488500
C	4.45409700	-7.74909400	-0.00306000
H	4.70583300	-6.79542000	-0.47860100
H	4.81596500	-7.73769500	1.02982700
H	4.99535100	-8.53983300	-0.52934800
O	-2.49782900	-9.94953100	-0.08411200
N	-1.34648100	-6.05980500	0.50834100
H	-1.96543300	-5.58948500	1.15602500

TS3^b

C	2.26258000	-4.80620500	1.63704400
C	0.87908700	-4.78254600	1.64126000
C	2.94052300	-5.88004600	1.05980000
C	0.19668700	-5.85867600	1.07467000
B	-2.04593700	-6.43251500	-0.65833900
C	-1.02946400	-6.39316400	-1.88240700
C	-1.10478500	-7.36157900	-2.88664200
C	-0.07931800	-5.39443900	-2.09361700
C	-0.27743200	-7.37442900	-4.00096000
C	0.76283100	-5.36845100	-3.19757100
C	0.66612100	-6.36774800	-4.15559600
C	-3.60509400	-6.34769700	-0.93111600
C	-4.53528800	-6.88296000	-0.03587800
C	-4.13760500	-5.79117800	-2.09522800
C	-5.90253100	-6.87643700	-0.27083400
C	-5.49943200	-5.76066200	-2.36123800
C	-6.38537100	-6.30945900	-1.44336100
F	0.04811700	-4.37633200	-1.23101500
F	-2.01754200	-8.33363700	-2.80227400
F	-0.38519700	-8.33014000	-4.91935800
F	1.47173100	-6.36072800	-5.21115400
F	1.66150600	-4.39450700	-3.34106600
F	-3.33510800	-5.23967300	-3.01514000
F	-5.96186700	-5.20973500	-3.48164700
F	-7.69030500	-6.28611200	-1.68364700
F	-6.74980300	-7.39896500	0.61096000
F	-4.11378600	-7.43804700	1.10279200
C	2.22589900	-6.94868900	0.53085300
H	4.02115000	-5.88456500	1.02797400
H	2.82148800	-3.97676300	2.05853400
H	0.31733100	-3.94263900	2.03149400
N	0.87008400	-6.91148800	0.58024400
H	-2.09183200	-7.96330600	-0.41701900
H	0.22405400	-7.86250400	0.30565100
O	-0.45060900	-8.99231700	0.17324700
C	-1.68389100	-9.03726700	-0.11054600
C	2.87666300	-8.17793000	-0.09343600
C	2.27553500	-8.41954000	-1.49071400
H	2.76349200	-9.28588100	-1.94715800

H	1.20416600	-8.62870200	-1.44809800
H	2.44770800	-7.55233300	-2.13828300
C	2.63352000	-9.39541600	0.82053600
H	3.06240400	-9.22204200	1.81299100
H	1.57196500	-9.62620300	0.92561500
H	3.12697700	-10.26993300	0.38496900
C	4.38909900	-7.97589200	-0.24778100
H	4.62393600	-7.10312700	-0.86621500
H	4.89063800	-7.87186500	0.71961000
H	4.81064000	-8.85618900	-0.74014800
O	-2.50808500	-9.90590500	-0.14322300
S	-1.56906000	-5.82047800	1.03577600

TS4^b

C	-3.31068600	-2.41743500	-0.71785100
C	-1.90356900	-2.43201800	-0.72273500
C	-3.95688900	-1.39832500	0.04133800
C	-1.22625600	-1.48542100	0.01855900
B	0.95972500	-0.33537800	0.00908100
C	0.40261300	1.09510500	-0.42645100
C	0.90222500	2.26547400	0.14456800
C	-0.58736800	1.27615400	-1.38740400
C	0.43052500	3.52996400	-0.17755000
C	-1.08380400	2.52221600	-1.74398200
C	-0.57493700	3.65662100	-1.12820500
C	2.49377500	-0.70437700	-0.13057200
C	3.02178200	-1.78743300	0.57588300
C	3.40195100	0.02510700	-0.89507000
C	4.36313000	-2.13721500	0.52622200
C	4.75029100	-0.29745000	-0.97251400
C	5.23076700	-1.38540100	-0.25653300
F	-1.10959500	0.21659100	-2.02861400
F	1.88480500	2.19169700	1.04495600
F	0.93312200	4.61591000	0.40283600
F	-1.04136700	4.85759500	-1.45239500
F	-2.04746200	2.63462000	-2.65968900
F	2.99434500	1.07963000	-1.61460300
F	5.58099000	0.41911900	-1.72837700
F	6.51733200	-1.70901400	-0.32208300
F	4.82614000	-3.17863000	1.21439600
F	2.22596300	-2.52371600	1.35473200
C	-3.22698600	-0.50943500	0.79205500
H	-5.03224700	-1.31574900	0.03646600
H	-1.31418500	-3.10909700	-1.32305300
N	-1.86552600	-0.58917500	0.79356400
O	0.10547200	-1.46328800	-0.03538900
H	1.09490000	-0.10574500	1.54940800
H	-1.26564400	-0.01434800	1.52992700
O	-0.48853300	0.54879800	2.62429800
C	0.72734000	0.22561800	2.64051900

C	-3.84032600	0.59271900	1.64737600
C	-3.16069300	1.93298800	1.30277600
H	-3.61889800	2.72976800	1.89625300
H	-2.09083000	1.92610100	1.53119700
H	-3.30036200	2.17434600	0.24278000
C	-3.62919300	0.24987600	3.13541500
H	-4.10741500	-0.70425800	3.38027100
H	-2.57076000	0.19796400	3.39863900
H	-4.09077000	1.03028000	3.74876200
C	-5.34352400	0.72671900	1.38057000
H	-5.55242800	0.94372300	0.32770400
H	-5.89294300	-0.17327600	1.67533500
H	-5.73342400	1.55590000	1.97702300
O	1.59788100	0.17521600	3.46757100
N	-4.02683400	-3.31828100	-1.42884300
C	-3.33500900	-4.32742900	-2.21640100
H	-4.07030800	-4.99046400	-2.66866500
H	-2.74009000	-3.87024800	-3.01567400
H	-2.67385700	-4.92824400	-1.58336000
C	-5.47952700	-3.24095100	-1.46526200
H	-5.85944800	-4.05119900	-2.08493900
H	-5.90591800	-3.34890200	-0.46230700
H	-5.81828600	-2.29151300	-1.89501400

TS5^b

C	1.93978800	-5.23220800	2.11702100
C	0.55938400	-5.25243700	1.85547500
C	2.76461900	-6.15928000	1.41230300
C	0.04661500	-6.17710200	0.95430900
B	-1.88761800	-6.58515600	-0.67848600
C	-0.98800800	-6.52528300	-2.00086000
C	-1.19519500	-7.40935600	-3.05985000
C	0.01976400	-5.58598800	-2.20312200
C	-0.43863600	-7.39948200	-4.22280600
C	0.79485700	-5.53571500	-3.35429800
C	0.56905000	-6.45439900	-4.36806100
C	-3.46210500	-6.34214600	-0.77865500
C	-4.30341200	-6.69530200	0.27836300
C	-4.10694000	-5.84715100	-1.91196800
C	-5.68401800	-6.57513700	0.23264300
C	-5.48683600	-5.70848900	-1.99714700
C	-6.27935000	-6.07760200	-0.91937100
F	0.29122100	-4.65942900	-1.26739300
F	-2.17747800	-8.31183400	-2.98510800
F	-0.67416000	-8.27179400	-5.19982700
F	1.30840900	-6.42682700	-5.47274600
F	1.76427600	-4.62670300	-3.48191100
F	-3.40626000	-5.46048800	-2.98584300
F	-6.05375900	-5.21949700	-3.09863100

F	-7.59948400	-5.94633100	-0.98515200
F	-6.43731600	-6.92302500	1.27382100
F	-3.77412100	-7.17581600	1.41459300
C	2.20830200	-7.08434400	0.56584600
H	3.83462000	-6.15006900	1.54626400
H	-0.11533800	-4.51638400	2.26956500
N	0.85900900	-7.09347700	0.37984200
H	-2.04594400	-8.10098700	-0.56818400
H	0.38436500	-7.92756200	-0.10578500
O	-0.36040800	-9.22708500	-0.50466000
C	-1.60878600	-9.22500100	-0.42615300
C	2.99920400	-8.15404400	-0.17687300
C	2.58542600	-8.15898600	-1.66103900
H	3.16762100	-8.91827800	-2.19162600
H	1.52705100	-8.40352000	-1.79612800
H	2.79195200	-7.18682200	-2.12232700
C	2.69799000	-9.52410700	0.46360300
H	2.98203900	-9.52415300	1.52111800
H	1.64303000	-9.79342700	0.37563900
H	3.28631300	-10.29231700	-0.04838200
C	4.50542400	-7.88557400	-0.08989200
H	4.76732800	-6.90334100	-0.49717800
H	4.87433800	-7.95512700	0.93855000
H	5.03218000	-8.64348100	-0.67595800
O	-2.48298900	-10.03262700	-0.24977400
N	-1.27632700	-6.19000200	0.59854000
H	-1.88637700	-5.79742300	1.30301100
N	2.48185900	-4.34242500	2.98277200
C	1.62348400	-3.39095100	3.66945100
H	2.22269200	-2.81198000	4.36994100
H	1.14777000	-2.69880700	2.96412700
H	0.84300300	-3.91076400	4.23513200
C	3.92393600	-4.27908200	3.16835200
H	4.31506400	-5.22629800	3.55453500
H	4.43731700	-4.03882400	2.23053700
H	4.15123600	-3.49789600	3.89157100