Supporting information

Mass spectrometric and computational investigation of the protonated carnosine-carboplatin complex fragmentation

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Table S1. Cartesian coordinates (Å) and absolute energies, (Hartrees) of all optimized structures **S3**

Figure S1. Geometrical structures of stationary points intercepted along the fragmentation Pathways 1 and 2 for the elimination of the NH_3 molecule cis to the CBDCA ligand. Bond lengths are in Å. Gray, red, blue and white spheres represent carbon, oxygen, nitrogen and hydrogen atoms, respectively. **S38**

Figure S2. Free energy profile for the CO_2 release from the carnosine ligand. Structure labels are in bold and relative free energies in kcal mol^{-1}. **S39**

Figure S3. Geometrical structures of stationary points intercepted along the fragmentation Pathways 3 and 4 for the elimination of the NH_3 molecule cis to the CBDCA ligand. Bond lengths are in Å. Gray, red, blue and white spheres represent carbon, oxygen, nitrogen and hydrogen atoms, respectively. **S40**

Table S1. Cartesian coordinates (Å) and absolute energies, (Hartrees) of all optimized structures

1A: E(B3LYP)= = -1561.86139733
Gas-phase zero-point energy = -1561.402454
Gas-phase free energy = -1561.467547

Pt	2.34327700	-0.88412200	-0.26850700
N	2.90294600	-2.85315900	-0.77641300
H	2.50078800	-3.48798800	-0.07860700
H	2.54528500	-3.11216600	-1.70172400
N	3.66475100	-0.02583700	-1.65075800
H	3.74922500	-0.53445200	-2.53462600
H	3.20075200	0.91680200	-1.81421500
O	1.72802700	0.94115700	0.39490600
O	-1.57866700	3.79229100	0.08143700
C	1.60983400	2.03372600	-0.36388800
C	-0.73679300	2.77174600	-0.00533000
C	0.73706700	3.13051800	0.22988900
C	1.00344600	3.50132300	1.75167000
H	0.20700500	3.22861800	2.44924500
H	1.94612500	3.07489600	2.10738400
C	1.12655600	4.60179400	-0.15753900
H	0.41108900	5.11287400	-0.80273000
H	2.11991100	4.64482200	-0.61249200
C	1.10127200	5.00927700	1.35175800
H	0.20131300	5.57047200	1.61563200
H	1.98012000	5.54386700	1.72216800
O	-1.10372300	1.58083300	-0.23319200
O	2.18074900	2.17304700	-1.48904800
H	3.92208000	-2.96186900	-0.76680000
H	4.59752700	0.11839400	-1.25240600
N	0.97383500	-1.58332000	1.07431700
C	-0.36546100	-1.96325100	0.82132600
C	1.13953400	-1.49684500	2.40714800
C	-0.89373800	-2.12539900	-0.58616000
C	-0.98796900	-2.11374300	2.04910700
N	-0.03242600	-1.81773100	3.02138700
H	2.03734000	-1.18302200	2.91210800
C	-2.42273400	-1.92317100	-0.78436800
H	-0.64065300	-3.12068900	-0.97867800
H	-0.38457500	-1.38889900	-1.22093400
H	-2.00807700	-2.38088000	2.27518900
H	-0.19010900	-1.82801900	4.02161600
N	-2.82610900	-0.60730800	-0.30455100
C	-3.24383600	-3.04528200	-0.12199200
H	-2.62399400	-2.02548000	-1.85871500
C	-4.14574300	-0.22661600	-0.34736400
O	-3.47876500	-4.05392100	-1.03082800
O	-3.59642300	-3.11632700	1.06349800
C	-4.40861700	1.21139200	0.09898000
O	-5.05567900	-1.00563300	-0.73713400
C	-4.27422500	2.19902100	-1.08423200
H	-5.41881800	1.25507000	0.51985900

H	-3.68752500	1.48635000	0.87712000
N	-4.00198900	3.58993400	-0.56490800
H	-3.41857000	1.92758300	-1.70997600
H	-5.17963700	2.18294800	-1.70145100
H	-4.11416000	4.29077000	-1.30462600
H	-4.63465500	3.83166600	0.20396100
H	-4.03773800	-4.76720200	-0.64573700
H	-2.11216800	0.11490800	-0.15394300
H	-2.70627800	3.65559200	-0.16776900

TS$_{(1A \rightarrow 1B)}$: E(B3LYP)= -1561.83508632
Gas-phase zero-point energy = -1561.375830
Gas-phase free energy = -1561.442120

Pt	2.14132800	-1.29983800	-0.03075700
N	2.27523300	-3.39142700	-0.23640700
H	1.51842400	-3.81867000	0.30864000
H	2.16065800	-3.66592400	-1.21786900
N	3.85051600	-1.00006100	-1.20975500
H	3.78622700	-1.43446900	-2.13492900
H	3.87857400	0.05576500	-1.31918300
O	1.81893900	0.69000800	0.24745600
O	-0.64601500	3.70029200	0.25034800
C	2.36488000	1.70572600	-0.42206500
C	0.17065400	2.83285300	-0.45062500
C	1.64657000	3.02998200	-0.17977000
C	2.02195500	3.74551100	1.18093200
H	1.22174200	3.77156700	1.92182300
H	2.92031900	3.30868900	1.62893500
C	2.22611100	4.28927900	-0.94454900
H	1.58358100	4.70839400	-1.72324800
H	3.19992900	4.04564100	-1.37625400
C	2.30609200	5.07257200	0.40529000
H	1.50089800	5.80338600	0.52010400
H	3.26164500	5.55784000	0.61747000
O	-0.31096200	2.02085900	-1.26084000
O	3.39668500	1.61320900	-1.14878800
H	3.17149200	-3.74842200	0.11013600
H	4.70667200	-1.31565700	-0.74449500
N	0.47593500	-1.50533100	1.13297000
C	-0.86539000	-1.31956100	0.72888900
C	0.49143700	-1.69966700	2.46640800
C	-1.23394300	-1.03449800	-0.70541200
C	-1.65296600	-1.43118500	1.86313600
N	-0.78775200	-1.66400200	2.93378000
H	1.36844400	-1.82882300	3.07830800
C	-2.74960900	-0.97354600	-1.01942800
H	-0.79851000	-1.80871700	-1.35051100
H	-0.78904100	-0.07942500	-1.01198100
H	-2.72535200	-1.40783800	1.96480800
H	-1.06613500	-1.79293800	3.89888700
N	-3.42477900	0.15136400	-0.37671600

C	-3.44886600	-2.29718500	-0.66021000
H	-2.85053600	-0.88214500	-2.10702200
C	-4.73355300	0.40635100	-0.73102300
O	-3.22479500	-3.24167000	-1.64428300
O	-4.07952100	-2.54877600	0.37493700
C	-5.44653300	1.56917400	-0.04255200
O	-5.32842900	-0.32945000	-1.56337900
C	-4.59920400	2.79555600	0.34976600
H	-6.24437200	1.88474200	-0.72271200
H	-5.94935500	1.16568000	0.85094300
N	-3.56143100	2.44488400	1.36716300
H	-4.09063700	3.19049400	-0.53988600
H	-5.28447100	3.57950300	0.70973900
H	-3.05142600	3.25836200	1.71621100
H	-3.96680900	1.94604100	2.16238600
H	-3.72796400	-4.06947600	-1.46855400
H	-2.95778000	0.80065400	0.26325600
H	-1.58690200	3.53120200	0.01044800

1B: E(B3LYP)= -1561.83706472
Gas-phase zero-point energy = -1561.377791
Gas-phase free energy = -1561.445178

Pt	2.17583000	-1.22557200	-0.05253900
N	2.52186500	-3.29350200	-0.23808600
H	1.78063500	-3.79078700	0.26777700
H	2.48872000	-3.57948600	-1.22236400
N	3.84913700	-0.77605800	-1.23577300
H	3.77037500	-1.13939500	-2.19027000
H	3.83601000	0.28537100	-1.26450300
O	1.64041900	0.72653200	0.19989400
O	-0.85134200	3.94064100	-0.45854000
C	2.18554300	1.79938800	-0.36967700
C	0.03269100	2.92858900	-0.81868200
C	1.38017200	3.07660000	-0.14421700
C	1.34267100	3.58743800	1.35551300
H	0.36310300	3.54527400	1.83598600
H	2.06832000	3.05399600	1.97723000
C	2.10606600	4.42798300	-0.53608200
H	1.66207800	4.97590900	-1.37034700
H	3.16039700	4.24182000	-0.75285200
C	1.83037300	4.99796300	0.89243200
H	1.03231900	5.74456300	0.90488100
H	2.70105000	5.39624300	1.41910300
O	-0.29139600	2.06168300	-1.64575600
O	3.27565700	1.79549500	-1.01285000
H	3.42811100	-3.56158200	0.15921000
H	4.72867700	-1.09624800	-0.82053300
N	0.53960900	-1.58773500	1.11007400
C	-0.80906300	-1.46523300	0.70932500
C	0.56581300	-1.83806600	2.43425200
C	-1.19021400	-1.14845800	-0.71554600

C	-1.59054300	-1.67006200	1.83480600
N	-0.71439200	-1.89721400	2.89727400
H	1.44780000	-1.94080200	3.04402300
C	-2.71080500	-1.06566600	-1.00051400
H	-0.76813100	-1.91004400	-1.38455800
H	-0.73976900	-0.19069700	-1.00652300
H	-2.66329700	-1.70559600	1.93276100
H	-0.98713300	-2.08277600	3.85478600
N	-3.34922900	0.01569900	-0.26104000
C	-3.40988300	-2.40828200	-0.71928100
H	-2.83133000	-0.90011400	-2.07767500
C	-4.66489800	0.32284100	-0.53292100
O	-3.24875500	-3.26685400	-1.78974200
O	-3.99398300	-2.74047600	0.32070200
C	-5.25897900	1.49361700	0.24927100
O	-5.33371000	-0.34449600	-1.36644400
C	-4.30574500	2.68656400	0.48408500
H	-6.13900300	1.83078600	-0.30791000
H	-5.62523300	1.11447600	1.21564800
N	-3.15233800	2.31626400	1.35618500
H	-3.90298700	3.01667600	-0.48310200
H	-4.88799100	3.52557300	0.89644700
H	-2.39715500	3.00237600	1.32954700
H	-3.43807500	2.13719700	2.31981600
H	-3.74955200	-4.10423300	-1.65812800
H	-2.85162100	0.64308700	0.38774500
H	-1.65790700	3.90935400	-1.02332600

TS$_{(1B\rightarrow 2A)}$: E(B3LYP)= -1561.79329089
Gas-phase zero-point energy = -1561.335553
Gas-phase free energy = -1561.402506

Pt	0.89810600	-1.43718600	0.24248300
N	-0.20694000	-3.09125900	-0.34273900
H	-0.44586900	-3.73363400	0.41649900
H	-1.06369400	-2.73676500	-0.80261100
N	2.38634100	-3.21213500	-1.66494500
H	2.17792300	-3.47589800	-2.62936000
H	2.87268400	-2.31116000	-1.62520800
O	1.94696800	0.25739000	0.75448900
O	3.51417700	4.03074400	-0.05518000
C	2.91217200	0.38126500	-0.14539100
C	2.83628400	2.84871800	-0.28523700
C	3.74286300	1.64384200	-0.10502000
C	4.72989000	1.73648600	1.13939900
H	4.48814300	2.52508700	1.85372200
H	4.80179600	0.78078300	1.66805300
C	5.01125600	1.67566900	-1.04992500
H	4.97818300	2.41954000	-1.84887900
H	5.19262400	0.68979800	-1.48535100
C	5.92456200	2.01407800	0.17216900
H	6.24084200	3.05976100	0.18739000

H	6.79959500	1.37237500	0.30174100
O	1.64405300	2.83510500	-0.63385700
O	3.09688900	-0.57526400	-0.97128200
H	0.44912000	-3.53669800	-1.00444900
H	2.92785000	-3.94246300	-1.20102700
N	-0.53270800	-0.85375200	1.48948700
C	-1.33583500	0.30082300	1.36028400
C	-0.82786400	-1.46074200	2.65418300
C	-1.27737700	1.28575100	0.22294100
C	-2.12618200	0.35651100	2.49614900
N	-1.79956300	-0.74497200	3.28557500
H	-0.35310900	-2.34270300	3.04873500
C	-2.30685900	1.08090800	-0.93064700
H	-0.26771600	1.32914200	-0.19647000
H	-1.46693500	2.28431700	0.63589100
H	-2.87494300	1.07584800	2.78341500
H	-2.19713700	-0.97033100	4.18920500
N	-3.67815300	1.06271400	-0.42384300
C	-2.00927700	-0.18845600	-1.73837100
H	-2.16890200	1.91200300	-1.63303200
C	-4.71273400	0.72825900	-1.26390500
O	-1.41304300	0.12220900	-2.93047300
O	-2.15107900	-1.36196400	-1.34083100
C	-6.12044700	0.85635000	-0.68754700
O	-4.48995500	0.32264200	-2.43798500
C	-6.33467300	2.04799200	0.27125000
H	-6.80231600	0.94627500	-1.53933900
H	-6.37753700	-0.08590200	-0.17970300
N	-5.54737100	1.89589800	1.53724200
H	-6.00664100	2.97526100	-0.21341400
H	-7.41267500	2.14694600	0.47042400
H	-5.54662400	2.75642100	2.08764800
H	-5.90309300	1.12513800	2.10713500
H	-1.26704700	-0.66798000	-3.49775200
H	-3.93885700	1.40474400	0.51126300
H	2.94208300	4.81355000	-0.22469700

2A: E(B3LYP)= -1505.25065272
Gas-phase zero-point energy = -1504.830529
Gas-phase free energy = -1504.892459

Pt	0.52449100	-1.06269300	-0.63996000
N	-0.63663400	-0.71661400	-2.31244500
H	-1.44360800	-1.34082900	-2.39744900
H	-0.95073600	0.26528500	-2.17062300
O	2.09379700	-0.91031500	0.82629000
O	5.04471000	2.67233400	0.05614700
C	2.82781300	-0.23216300	-0.02484300
C	3.87467800	1.97001300	0.09146900
C	4.09463100	0.48533100	0.32858400
C	4.71277300	0.17306400	1.75584900
H	4.71258600	1.01068500	2.45696800

H	4.20527800	-0.67718100	2.21855600
C	5.41289700	-0.12250900	-0.32056800
H	5.88748900	0.52041700	-1.06265200
H	5.22652000	-1.10645700	-0.76140800
C	6.08164800	-0.17811100	1.08979200
H	6.83364000	0.60236000	1.22810000
H	6.51011400	-1.14184700	1.37333500
O	2.76972200	2.53981800	-0.01200500
O	2.33355000	-0.18348600	-1.24608900
H	-0.05721700	-0.78505400	-3.15523300
N	-1.09642900	-1.81997000	0.29357500
C	-1.85971800	-1.14809000	1.27724700
C	-1.63756000	-3.03900200	0.09616600
C	-1.53663300	0.18656400	1.88555700
C	-2.87997500	-2.00551100	1.65162200
N	-2.72468200	-3.17500700	0.90953900
H	-1.25821500	-3.80322700	-0.56163000
C	-1.96090800	1.48263200	1.09036600
H	-0.46303400	0.26046700	2.09399500
H	-2.06942600	0.23045200	2.83659300
H	-3.67966000	-1.84201500	2.35529400
H	-3.30612700	-4.00160200	0.97779300
N	-3.25318300	1.40982000	0.41144300
C	-0.87402100	1.87305500	0.09032400
H	-1.97484400	2.27371200	1.85406500
C	-4.40996700	1.08099800	1.07457000
O	0.23084300	2.29669900	0.73437600
O	-0.98497200	1.78172900	-1.15511900
C	-5.71725000	1.31111200	0.30818500
O	-4.42093100	0.64046500	2.26130700
C	-5.65351700	1.23155900	-1.23279700
H	-6.44138400	0.58115500	0.68618900
H	-6.09826200	2.29897300	0.61091100
N	-4.71995900	2.24944300	-1.79135200
H	-5.28642400	0.24290200	-1.53846300
H	-6.67706000	1.33403300	-1.62704200
H	-4.52116700	2.11867100	-2.78250300
H	-5.02906000	3.20767200	-1.62081900
H	1.08215100	2.43910000	0.22258800
H	-3.37912300	1.81551500	-0.53708000
H	4.90037100	3.64157900	-0.04627600

TS$_{(2A \rightarrow 5A)}$: E(B3LYP)= -1505.17384522
Gas-phase zero-point energy = -1504.758692
Gas-phase free energy = -1504.821275

Pt	-0.44776600	-0.70437100	0.31929300
N	1.70679600	-1.18296800	2.75148100
H	1.84920900	-2.17287400	2.91153500
H	1.95336500	-0.82942100	1.83714400
O	-2.36976200	-1.36923600	-0.46586900

O	-5.07236800	2.38772400	-0.53343100
C	-2.93896400	-0.45655700	0.28955400
C	-3.93403000	1.66354800	-0.32745700
C	-4.24939500	0.20359100	-0.00382500
C	-5.19913100	-0.51212700	-1.04676200
H	-5.37720600	0.04913000	-1.96594600
H	-4.82439400	-1.50661200	-1.30294100
C	-5.38525600	0.00607700	1.09791700
H	-5.67528500	0.92189100	1.61528700
H	-5.10439800	-0.75023600	1.83676200
C	-6.36452800	-0.50744700	-0.00561000
H	-7.14784500	0.21513000	-0.24544300
H	-6.82281600	-1.47916600	0.19064100
O	-2.80192900	2.17941600	-0.42585700
O	-2.17549900	-0.00741000	1.26478600
H	0.90280000	-0.73692700	3.22661100
N	1.06175900	-1.44179300	-0.80589200
C	1.95359900	-0.74706400	-1.66376100
C	1.42909700	-2.73699100	-0.78174000
C	1.87946800	0.69405800	-2.08162600
C	2.86638000	-1.67539800	-2.13198100
N	2.52141600	-2.90659700	-1.57836900
H	0.94156900	-3.51905500	-0.22405300
C	2.14260100	1.77629100	-0.94566100
H	0.91366300	0.91954100	-2.55185900
H	2.66776100	0.85844100	-2.81907300
H	3.70690700	-1.53754300	-2.79215400
H	2.99503300	-3.78660500	-1.74405300
N	3.28434500	1.48448400	-0.09548900
C	0.87407200	1.78791900	-0.12990100
H	2.25072600	2.73350600	-1.47038500
C	4.54193900	1.25367100	-0.60340200
O	-0.09909800	2.55685700	-0.61318600
O	0.74658700	1.00848300	0.88263700
C	5.62641000	1.05432100	0.45930200
O	4.78730200	1.22042100	-1.84327700
C	5.18351600	0.26204800	1.71740100
H	6.46574600	0.54547200	-0.02637300
H	5.99123900	2.04723500	0.76201400
N	4.07292700	0.93714300	2.44697400
H	4.82466400	-0.73089500	1.41628600
H	6.06556900	0.10247700	2.35546200
H	3.46965600	0.28831100	2.96446900
H	4.39016900	1.70679900	3.03596200
H	-1.04825000	2.40526200	-0.31557000
H	3.22382300	1.43083200	0.95279100
H	-4.89316400	3.32866000	-0.76406500

5A: E(B3LYP)= -1448.61913717
Gas-phase zero-point energy = -1448.240633
Gas-phase free energy = -1448.300691

Pt	0.50628300	0.67599100	0.51751800
O	2.43015000	1.43280500	-0.08036200
O	4.86079000	-2.34416000	-1.11292000
C	2.96452800	0.34652600	0.44772400
C	3.78906500	-1.63744600	-0.65307200
C	4.22144000	-0.31267700	-0.01960100
C	5.22067600	0.55311300	-0.88348900
H	5.35568300	0.21003700	-1.91085200
H	4.92395500	1.60542800	-0.89456600
C	5.37197500	-0.46693300	1.07652600
H	5.59156300	-1.49816300	1.35755600
H	5.14848700	0.10877200	1.97925500
C	6.38418400	0.22014900	0.10531400
H	7.11158600	-0.47956800	-0.31256300
H	6.91357200	1.08260000	0.51594800
O	2.62219400	-2.06783400	-0.77433900
O	2.18484000	-0.26833600	1.30986200
N	-0.99016000	1.67081100	-0.42039700
C	-1.98586000	1.15569700	-1.29389300
C	-1.27399000	2.96409200	-0.18080400
C	-2.02473600	-0.20438900	-1.93353500
C	-2.86712300	2.19111500	-1.55086500
N	-2.40744100	3.30700000	-0.85442000
H	-0.70271400	3.62891400	0.44592900
C	-2.31644700	-1.45479800	-0.98220700
H	-1.09407100	-0.40723100	-2.47866800
H	-2.84947300	-0.21343900	-2.65027500
H	-3.75043100	2.20417300	-2.16837000
H	-2.83357200	4.22604700	-0.85402600
N	-3.48916900	-1.30654500	-0.14069000
C	-1.05204400	-1.54261900	-0.17145200
H	-2.39949800	-2.31838100	-1.65224800
C	-4.73609200	-1.09951800	-0.68535300
O	-0.08603000	-2.26171200	-0.72658200
O	-0.93099800	-0.80431400	0.87988200
C	-5.89836700	-1.11773200	0.31037000
O	-4.91577400	-0.93385900	-1.92520500
C	-5.58708000	-0.59023700	1.73023600
H	-6.71026400	-0.53134600	-0.13252600
H	-6.26515600	-2.15381100	0.37256600
N	-4.51885500	-1.39577400	2.39294900
H	-5.22789800	0.44489900	1.67043100
H	-6.52249100	-0.57761600	2.31020100
H	-4.12398900	-0.93956800	3.21505200
H	-4.82620600	-2.34028200	2.63081000
H	0.88650900	-2.14517800	-0.47982300
H	-3.46533900	-1.40824800	0.89840700
H	4.60690800	-3.20053500	-1.52880500

$TS_{(5A \rightarrow 5B)}$: E(B3LYP)= -1448.59728254
Gas-phase zero-point energy = -1448.220736
Gas-phase free energy = -1448.280482

Pt	0.50397200	0.65036500	0.52937200
O	2.42016700	1.43260200	-0.04171400
O	4.83651300	-2.34837300	-1.20923700
C	2.96474300	0.34856900	0.48115000
C	3.79426000	-1.63247400	-0.64678000
C	4.22069800	-0.29964500	-0.00584500
C	5.19094200	0.57057800	-0.90041700
H	5.28931400	0.23247200	-1.93325100
H	4.89506400	1.62302200	-0.89279200
C	5.39914800	-0.43915100	1.05629600
H	5.62595300	-1.45822100	1.38215500
H	5.20457200	0.16294100	1.94810600
C	6.38643700	0.23176100	0.04735700
H	7.09820000	-0.46843600	-0.39754500
H	6.93651300	1.09003600	0.43840000
O	2.62504400	-2.01916000	-0.77929100
O	2.19046700	-0.27974700	1.33836100
N	-0.98049600	1.65628500	-0.41580400
C	-1.98117900	1.16160900	-1.29625500
C	-1.24527500	2.95286000	-0.17033400
C	-2.04255200	-0.19208200	-1.94794300
C	-2.84490500	2.21240200	-1.55021900
N	-2.37028000	3.31708900	-0.84628600
H	-0.66587800	3.60530400	0.46193300
C	-2.34029600	-1.44749900	-1.00548500
H	-1.12097300	-0.40162300	-2.50566200
H	-2.87499600	-0.18442700	-2.65583500
H	-3.72560900	2.24270000	-2.17083600
H	-2.78193500	4.24270800	-0.84254500
N	-3.50443800	-1.29426500	-0.15342700
C	-1.07033400	-1.55265900	-0.20711500
H	-2.43697800	-2.30411300	-1.68258100
C	-4.75396600	-1.07412800	-0.68733700
O	-0.11218400	-2.26476800	-0.78534400
O	-0.93667800	-0.83436600	0.85559600
C	-5.90888100	-1.08982200	0.31686100
O	-4.94129100	-0.89879800	-1.92458700
C	-5.58333100	-0.57299100	1.73737500
H	-6.71979800	-0.49504000	-0.11649700
H	-6.28261000	-2.12361200	0.37578200
N	-4.51703300	-1.39090200	2.38784100
H	-5.21623400	0.45955800	1.68083800
H	-6.51450400	-0.55617900	2.32404800
H	-4.11320100	-0.94315400	3.21019600
H	-4.83000200	-2.33459400	2.62154200
H	0.85861300	-2.15624500	-0.54183500
H	-3.47317400	-1.40300500	0.88460700
H	5.37424900	-2.93906700	-0.64365700

5B: E(B3LYP)= -1448.60833760
Gas-phase zero-point energy = -1448.230077
Gas-phase free energy = -1448.289508

Pt	0.50680000	0.65987100	0.52097800
O	2.43656800	1.44369200	-0.04210800
O	4.71883000	-2.35566800	-1.29227200
C	2.96755000	0.35802000	0.48805600
C	3.74202600	-1.58928700	-0.72320400
C	4.21561300	-0.30564200	0.00242200
C	5.25094900	0.57683500	-0.79435600
H	5.35039100	0.35921900	-1.86143500
H	5.02284900	1.64012700	-0.68664100
C	5.34336000	-0.57481800	1.09347900
H	5.49482000	-1.62171500	1.36857200
H	5.15755100	-0.00620500	2.00829100
C	6.40138000	0.09240500	0.15195100
H	7.09773400	-0.61816200	-0.31113000
H	6.99871400	0.88378800	0.60786000
O	2.56258400	-1.95775200	-0.82189300
O	2.19176700	-0.26432100	1.34470800
N	-0.98079600	1.65751900	-0.42843400
C	-1.98620000	1.15842600	-1.30159400
C	-1.24753600	2.95410500	-0.18418800
C	-2.05149400	-0.19602900	-1.95221400
C	-2.85379800	2.20692200	-1.55205500
N	-2.37747600	3.31442000	-0.85380100
H	-0.66662900	3.60896500	0.44415800
C	-2.33602300	-1.45211000	-1.00738700
H	-1.13552800	-0.40400700	-2.51964000
H	-2.89127200	-0.18904300	-2.65136200
H	-3.73903700	2.23316900	-2.16635900
H	-2.79194200	4.23876500	-0.84869600
N	-3.49274200	-1.30309900	-0.14450600
C	-1.05642500	-1.54910200	-0.22209100
H	-2.43450900	-2.30987200	-1.68275200
C	-4.74716700	-1.07572600	-0.66283400
O	-0.10020800	-2.25052800	-0.80706800
O	-0.92459200	-0.82477900	0.83950600
C	-5.89092800	-1.09781000	0.35423500
O	-4.94892200	-0.88895900	-1.89632000
C	-5.54832100	-0.59466500	1.77569900
H	-6.70510900	-0.49713000	-0.06464200
H	-6.26655200	-2.13119300	0.40793000
N	-4.47675500	-1.42089900	2.40655300
H	-5.17930000	0.43748100	1.72424300
H	-6.47282300	-0.58090900	2.37295800
H	-4.06128500	-0.98144900	3.22755300
H	-4.78897300	-2.36597500	2.63549700
H	0.88205900	-2.13643900	-0.59140500
H	-3.45146600	-1.42153100	0.89214500
H	5.63818700	-2.02603800	-1.19208300

$TS_{(5B \rightarrow 4A)}$:: E(B3LYP)= -1448.51546292
Gas-phase zero-point energy = -1448.144465
Gas-phase free energy = -1448.208246

Pt	-0.64818500	-0.07964400	-0.12869100
O	-2.38862600	0.96120500	-0.42111700
O	-5.57767600	1.09202200	1.63654700
C	-3.16077200	-0.14635400	-0.31532500
C	-5.02223100	-0.05306700	1.81342700
C	-4.59714900	-0.11052800	-0.35949300
C	-5.28081500	0.81289800	-1.51026800
H	-5.91746600	1.64348300	-1.18272700
H	-4.52151900	1.21339400	-2.18825600
C	-5.38451700	-1.34651800	-0.89305800
H	-6.09138700	-1.79175000	-0.18649100
H	-4.73517300	-2.14202400	-1.26958400
C	-6.05016100	-0.45758400	-1.99734700
H	-7.13694300	-0.37382500	-1.91327800
H	-5.79854500	-0.75015700	-3.02039400
O	-4.69865200	-0.98095100	2.47565600
O	-2.42609900	-1.22986300	-0.11733500
N	0.73196700	1.38244300	-0.20065800
C	1.87520300	1.49122600	0.61293600
C	0.67980800	2.45823700	-1.00630500
C	2.20779900	0.51157100	1.69592300
C	2.51763300	2.66576500	0.26877600
N	1.75642000	3.25437800	-0.74284800
H	-0.09351600	2.66967400	-1.72580900
C	2.91753800	-0.79700800	1.24978600
H	1.29395900	0.23609100	2.23928300
H	2.88151600	1.00149400	2.39925800
H	3.42613700	3.09151800	0.66172900
H	1.95656300	4.13654200	-1.19837000
N	4.10223100	-0.62427100	0.39038900
C	1.97800100	-1.75879000	0.52610400
H	3.20816800	-1.31846800	2.17824300
C	5.09464800	0.29973900	0.64488000
O	2.51111400	-2.99220100	0.37780900
O	0.81576100	-1.54702200	0.09368500
C	6.34925800	0.15955800	-0.22635100
O	5.01518900	1.18748200	1.53815100
C	6.15626300	-0.44681600	-1.63365400
H	6.78917300	1.15892300	-0.31168300
H	7.07342900	-0.44303300	0.34347000
N	5.60504600	-1.83352900	-1.55845800
H	5.44320200	0.15960600	-2.20586000
H	7.11914900	-0.40806300	-2.16488300
H	5.28731800	-2.18172300	-2.46322300
H	6.26429600	-2.49643500	-1.14612000
H	1.91247900	-3.63303600	-0.07566700
H	4.37191000	-1.35154000	-0.31252800
H	-5.23506900	0.91904600	0.47443200

4A: E(B3LYP)= -1260.10446946
Gas-phase zero-point energy = -1259.738713
Gas-phase free energy = -1259.796622

Pt	1.04370300	0.05099300	-0.07097300
O	2.70118200	1.18063400	0.35509400
C	3.54702600	0.14991400	0.21919800
C	5.00708600	0.27892400	0.39665100
C	5.71859300	-0.77024000	1.34222600
H	5.98755500	-0.39902700	2.33420700
H	5.12754900	-1.68613800	1.43939000
C	5.92464900	-0.25002100	-0.77997900
H	6.35074900	0.52341400	-1.42337400
H	5.40244300	-0.99188100	-1.39196800
C	6.86085800	-0.91114900	0.28362600
H	7.72737700	-0.28557100	0.52101600
H	7.20552800	-1.92500400	0.06834700
O	2.92006400	-0.96201400	-0.09106100
N	-0.40446000	1.43443100	0.07060300
C	-1.59209000	1.51736600	-0.67935500
C	-0.34717800	2.49565000	0.89692400
C	-1.96094700	0.55554600	-1.76574500
C	-2.25643200	2.65946700	-0.27328500
N	-1.46384900	3.25524400	0.70941900
H	0.45795500	2.72060100	1.57672200
C	-2.54434100	-0.81246800	-1.30944100
H	-1.09088900	0.36401600	-2.40841500
H	-2.73150200	1.02533400	-2.37799200
H	-3.20094400	3.05936300	-0.60363900
H	-1.67009200	4.12038300	1.19424500
N	-3.58804300	-0.74422300	-0.27286700
C	-1.46964700	-1.76773800	-0.80247600
H	-2.95590200	-1.28683200	-2.21588400
C	-4.68654800	0.08215500	-0.38852300
O	-1.88186200	-3.05328300	-0.77689500
O	-0.29308800	-1.50162100	-0.44202600
C	-5.78155200	-0.14323900	0.66085400
O	-4.81191800	0.94565600	-1.29943800
C	-5.32858000	-0.70442900	2.02697500
H	-6.28775000	0.81714900	0.80553600
H	-6.52817900	-0.81513000	0.21009800
N	-4.66780200	-2.03795200	1.87952100
H	-4.59834100	-0.02582400	2.48493000
H	-6.20229700	-0.74427000	2.69448400
H	-4.19747600	-2.33900200	2.73359700
H	-5.31760500	-2.76397200	1.57099500
H	-1.19675500	-3.68799500	-0.45628900
H	-3.68138900	-1.47444000	0.47195400
H	5.23976800	1.31148100	0.66987700

TS$_{(2A \rightarrow 2B)}$: E(B3LYP)= -1505.22844968
Gas-phase zero-point energy = -1504.810449
Gas-phase free energy = -1504.872592

Pt	0.53306600	-1.04827900	-0.58624500
N	-0.63072900	-0.75635600	-2.26679700
H	-1.43233600	-1.38955900	-2.33483600
H	-0.95381000	0.22679400	-2.15736700
O	2.12520500	-0.86323700	0.85614100

O	4.99160500	2.77601400	0.35517700
C	2.86246200	-0.24195700	-0.03553400
C	3.86199800	1.97613300	0.25675900
C	4.14163400	0.47395900	0.27388500
C	4.93917200	-0.02265000	1.54747900
H	5.01779400	0.69259300	2.37182400
H	4.50915900	-0.94538300	1.94488500
C	5.38847400	0.04731000	-0.61894600
H	5.76629500	0.83663800	-1.27002800
H	5.17050300	-0.84029500	-1.21925200
C	6.21774900	-0.23897900	0.67399100
H	7.00299900	0.50088900	0.85098400
H	6.65862200	-1.23625100	0.73694800
O	2.74797600	2.48167400	0.08289300
O	2.34917000	-0.23008800	-1.24867100
H	-0.04865200	-0.84571900	-3.10590600
N	-1.08871700	-1.77390100	0.37513700
C	-1.87195400	-1.08165500	1.32851000
C	-1.60718900	-3.00915200	0.21864300
C	-1.58435000	0.28086900	1.88987400
C	-2.87935200	-1.94367300	1.72674800
N	-2.69766500	-3.13586100	1.02862200
H	-1.20950000	-3.78954800	-0.40861200
C	-2.03343100	1.53474100	1.04133000
H	-0.51480600	0.38802200	2.10437200
H	-2.12675800	0.34794100	2.83418200
H	-3.68735200	-1.76942200	2.41826400
H	-3.26457200	-3.97001600	1.12266200
N	-3.30908200	1.39719700	0.34238100
C	-0.93954300	1.91604000	0.04783100
H	-2.08536100	2.35261200	1.77436200
C	-4.46929400	1.07284500	1.00207800
O	0.14153200	2.39455600	0.69722400
O	-1.01959900	1.77336800	-1.19397200
C	-5.76742400	1.23020500	0.20267700
O	-4.48853600	0.69264100	2.20924500
C	-5.67324500	1.06297700	-1.32972900
H	-6.48319100	0.50796900	0.61013500
H	-6.17390800	2.22570100	0.44016600
N	-4.75337500	2.06924000	-1.93068600
H	-5.27770400	0.06730400	-1.57056400
H	-6.69128000	1.11748600	-1.74705300
H	-4.53622900	1.88783500	-2.90999500
H	-5.08719500	3.02801200	-1.81986900
H	0.99242100	2.52211200	0.19154800
H	-3.42666100	1.74798600	-0.62899800
H	5.36627300	2.95835100	1.24077700

2B: E(B3LYP)= -1505.23928689
Gas-phase zero-point energy = -1504.819443
Gas-phase free energy = -1504.881200

Pt	0.53215800	-1.04891200	-0.60780600

N	-0.64207800	-0.70641300	-2.26914600
H	-1.44890600	-1.33178900	-2.34666400
H	-0.95593000	0.27649300	-2.12483900
O	2.13322500	-0.89529900	0.83422400
O	4.91795300	2.82250600	0.26392300
C	2.86007800	-0.24882100	-0.04513700
C	3.84115900	1.97996800	0.19182300
C	4.13230800	0.47379300	0.28075300
C	4.86455100	0.05295400	1.61991200
H	4.86970500	0.80378700	2.41415000
H	4.44388900	-0.87173500	2.02209400
C	5.41153700	-0.01264700	-0.52138900
H	5.79717800	0.67839500	-1.27619400
H	5.23200100	-0.97404800	-1.00956000
C	6.19715200	-0.15661100	0.82577400
H	6.94517700	0.62695600	1.00039200
H	6.68994600	-1.11841700	0.97903900
O	2.70791100	2.46563500	0.09404400
O	2.35089600	-0.21781300	-1.25859600
H	-0.06949500	-0.77481200	-3.11659400
N	-1.08791100	-1.79171700	0.34080200
C	-1.87172400	-1.11898600	1.30804500
C	-1.60907400	-3.02186000	0.15443100
C	-1.58341200	0.22899100	1.90403600
C	-2.88227400	-1.98773900	1.68328200
N	-2.70167600	-3.16412500	0.95868000
H	-1.21208900	-3.78818700	-0.49033600
C	-2.02110700	1.50594100	1.08539200
H	-0.51510500	0.32748000	2.12889500
H	-2.13171900	0.27331500	2.84624200
H	-3.69272700	-1.82622100	2.37497500
H	-3.27147600	-3.99840600	1.03172600
N	-3.29302400	1.39326000	0.37435500
C	-0.91673900	1.90744800	0.11009400
H	-2.07367900	2.30493100	1.83882300
C	-4.45905300	1.04960600	1.01345200
O	0.15690400	2.36647600	0.77815500
O	-0.98987800	1.78924800	-1.13615000
C	-5.75147000	1.24437000	0.21257300
O	-4.48970700	0.62299600	2.20489800
C	-5.64805600	1.14724500	-1.32527800
H	-6.47069900	0.50529200	0.58208700
H	-6.15851000	2.22840000	0.49298400
N	-4.72053400	2.17614800	-1.87358900
H	-5.25472300	0.16210100	-1.60917200
H	-6.66325800	1.22487600	-1.74592200
H	-4.49794100	2.03960200	-2.85890700
H	-5.05023400	3.13036300	-1.71970100
H	1.02383800	2.49989800	0.29374500
H	-3.40406700	1.78613100	-0.58151600
H	5.79540000	2.38878200	0.33487900

TS$_{(2B\rightarrow 3A)}$: E(B3LYP)= -1505.12030438
Gas-phase zero-point energy = -1504.709375
Gas-phase free energy = -1504.773607

Pt	0.66714900	-1.00469900	-0.53164200
N	-0.47082700	-0.96440400	-2.26320200
H	-1.19698800	-1.68587600	-2.29247100
H	-0.90681600	-0.02206300	-2.26968800
O	2.19655800	-0.69245900	0.92040000
O	4.03518500	2.60271700	1.70246500
C	2.98753900	-0.15307400	0.00077400
C	3.43938800	2.42421600	0.57937400
C	4.23015900	0.54734900	0.29152200
C	5.27018000	-0.28185500	1.27901500
H	5.70087800	0.28482600	2.11361200
H	4.79455100	-1.18290800	1.67249700
C	5.34166100	0.57745400	-0.79754500
H	5.80411800	1.56270800	-0.91455700
H	5.01619100	0.22542600	-1.77819700
C	6.21543800	-0.41181800	0.04289800
H	7.24552700	-0.09546400	0.22158400
H	6.22021400	-1.42728500	-0.36396300
O	2.68654100	2.86238500	-0.25014400
O	2.47834500	-0.20712500	-1.22380800
H	0.14790300	-1.07035700	-3.07366000
N	-0.93790600	-1.69956100	0.48388800
C	-1.75228000	-0.95351800	1.36664200
C	-1.38195400	-2.97259200	0.47500500
C	-1.54229900	0.48059800	1.75585300
C	-2.70093000	-1.82301300	1.87736100
N	-2.45460800	-3.07269000	1.31255000
H	-0.94237100	-3.79394600	-0.06601100
C	-2.14307100	1.58891800	0.80200400
H	-0.47433700	0.68867800	1.88786200
H	-2.03435400	0.62099300	2.71964600
H	-3.50664400	-1.62153300	2.56428700
H	-2.96756200	-3.92363500	1.50944700
N	-3.44232400	1.27600000	0.21213700
C	-1.15351700	1.92892300	-0.30503400
H	-2.21705800	2.48199800	1.43888400
C	-4.53223000	0.95382200	0.98343400
O	-0.09516000	2.62189500	0.19176400
O	-1.26453600	1.60376600	-1.50622300
C	-5.88112300	0.90708000	0.25790700
O	-4.45016500	0.73348000	2.22694800
C	-5.85698400	0.54778300	-1.24388800
H	-6.51053200	0.19240400	0.79925600
H	-6.35582000	1.89132300	0.39427800
N	-5.05518500	1.53182300	-2.02509400
H	-5.39551900	-0.43876100	-1.38226200
H	-6.89691800	0.47295000	-1.59893700
H	-4.86769900	1.23359200	-2.98170800

H	-5.46680600	2.46648300	-2.02584900
H	0.64348800	2.80282700	-0.44002000
H	-3.64529200	1.48363300	-0.78679200
H	4.36616000	1.36344500	1.39577200

3A: E(B3LYP)= -1316.70599144
Gas-phase zero-point energy = -1316.300039
Gas-phase free energy = -1316.361099

Pt	1.13416600	0.49802500	0.55232100
N	0.19936700	0.07030500	2.35961100
H	-0.29259500	0.88100700	2.74654700
H	-0.47636900	-0.69416500	2.17432200
O	2.45063700	0.63368500	-1.09304300
C	3.38241300	-0.06716500	-0.46854200
C	4.71063100	-0.36747900	-1.04702000
C	5.97026600	0.24620100	-0.30342200
H	6.40767200	1.12869500	-0.77631900
H	5.75328800	0.46176700	0.74769000
C	5.32537400	-1.79463100	-0.78858900
H	5.27296000	-2.49046700	-1.62979900
H	4.89185400	-2.26030700	0.10193200
C	6.70529000	-1.12141700	-0.48938800
H	7.36647700	-1.12104500	-1.36202000
H	7.25929900	-1.50012100	0.37261400
O	3.00280700	-0.45296200	0.74408600
H	0.90666400	-0.24352800	3.03209500
N	-0.50943400	1.52313300	-0.03741400
C	-1.45965900	1.11745900	-1.00223300
C	-0.80144000	2.78610600	0.33394100
C	-1.45083900	-0.18376700	-1.74772600
C	-2.32930500	2.17852700	-1.18965100
N	-1.90503700	3.20556300	-0.34958900
H	-0.23515000	3.39317300	1.02046400
C	-2.23424900	-1.39142600	-1.08839700
H	-0.42223200	-0.50713300	-1.94476900
H	-1.94033900	-0.00954200	-2.70746500
H	-3.18545900	2.24773000	-1.84097000
H	-2.32463800	4.12470200	-0.27791300
N	-3.50780300	-1.05084500	-0.46043400
C	-1.34625500	-2.08029600	-0.06700600
H	-2.38885100	-2.10072200	-1.91272200
C	-4.51355100	-0.41390000	-1.14455300
O	-0.44673400	-2.91535900	-0.66953700
O	-1.37395400	-1.90481400	1.16841800
C	-5.86534500	-0.34068800	-0.42676300
O	-4.35587300	0.06582400	-2.30491500
C	-5.82952900	-0.29304400	1.11729000
H	-6.38550200	0.54281800	-0.81221500
H	-6.45693500	-1.20904000	-0.75595600
N	-5.18089000	-1.51026000	1.68512700
H	-5.24612000	0.57573100	1.44852100

H	-6.85822000	-0.15369800	1.48447100
H	-4.95841400	-1.42316600	2.67625900
H	-5.72429900	-2.35967800	1.52288400
H	0.17185000	-3.33873800	-0.03033100
H	-3.76990300	-1.41662600	0.47892500
H	4.69869000	-0.09674700	-2.10610100

TS$_{(3A \rightarrow 4A)}$: E(B3LYP)= -1316.65179816
Gas-phase zero-point energy = -1316.249482
Gas-phase free energy = -1316.311047

Pt	1.11054200	0.14111900	0.31836900
N	0.95372600	-1.01381700	2.68902800
H	1.08802100	-0.35486600	3.45199200
H	0.08304100	-1.53312400	2.76302700
O	2.79124300	1.27594100	-0.23686500
C	3.58554600	0.21269100	-0.23645900
C	5.02405300	0.27375800	-0.58090300
C	6.03968700	-0.47216500	0.36951700
H	6.60754300	0.16866300	1.04882800
H	5.54572700	-1.26564000	0.93926200
C	5.52091300	-0.66598200	-1.75358300
H	5.68509600	-0.17199400	-2.71432200
H	4.85325000	-1.52256300	-1.88905900
C	6.77717800	-1.02520700	-0.89416200
H	7.65055900	-0.42212300	-1.16306700
H	7.06920600	-2.07772200	-0.87001300
O	2.94424900	-0.89493200	0.08732300
H	1.76103700	-1.61986400	2.55346700
N	-0.38932700	1.47646000	0.35700600
C	-1.47973000	1.48668800	-0.53496600
C	-0.48982300	2.54839500	1.16138500
C	-1.63992100	0.49294100	-1.64559600
C	-2.24406700	2.60115200	-0.24045200
N	-1.61177600	3.24976300	0.82113800
H	0.20843900	2.82959200	1.93134600
C	-2.37571300	-0.83376200	-1.31074900
H	-0.64824100	0.23553000	-2.04073200
H	-2.21051100	0.96871500	-2.44370400
H	-3.15068000	2.95074200	-0.70617100
H	-1.91733300	4.11170200	1.25578600
N	-3.69292500	-0.70117600	-0.65814400
C	-1.54096100	-1.76853600	-0.43331600
H	-2.49717800	-1.36255500	-2.27150000
C	-4.65236300	0.21167700	-1.03972900
O	-2.07748600	-3.02139700	-0.38885800
O	-0.48806200	-1.51460900	0.19440400
C	-6.03240500	0.01410700	-0.39792700
O	-4.45281400	1.13988700	-1.87198500
C	-6.06938400	-0.65608700	0.99246600
H	-6.49931600	1.00337900	-0.34381200
H	-6.63873800	-0.56860000	-1.10866200

N	-5.49012600	-2.03198500	0.94790800
H	-5.47314400	-0.07102700	1.70383600
H	-7.10888900	-0.65067300	1.35435500
H	-5.34007800	-2.42848400	1.87566300
H	-6.04848200	-2.67536000	0.38372300
H	-1.54661400	-3.65633700	0.14696000
H	-4.05734700	-1.46469600	-0.04515200
H	5.30025800	1.31818000	-0.74873700

TS$_{(1B\rightarrow 2C)}$: E(B3LYP)= -1561.79005726
Gas-phase zero-point energy = -1561.333329
Gas-phase free energy = -1561.401218

Pt	0.75536400	-1.40570500	0.17419500
N	-0.81470800	-3.47521400	1.27678000
H	-0.04862000	-3.40617300	1.94764100
H	-1.67860700	-3.07655800	1.65991500
N	1.67589900	-2.75212700	-1.12439000
H	1.03996200	-2.99000100	-1.89229200
H	2.50002500	-2.21724000	-1.49524000
O	2.34483400	-0.16414800	0.33111900
O	3.65022400	3.67728300	-0.32989300
C	3.26886400	-0.00112500	-0.63225000
C	3.05191100	2.46657000	-0.63102600
C	4.02816000	1.31361600	-0.47716100
C	4.96922900	1.40138000	0.79868900
H	4.66457100	2.14004100	1.54229200
H	5.08222800	0.42640500	1.28297900
C	5.31802900	1.46734300	-1.38005700
H	5.26385000	2.24819400	-2.14177700
H	5.56509700	0.51703500	-1.85896800
C	6.17471000	1.79341800	-0.11458800
H	6.43207800	2.85249000	-0.03770700
H	7.07977400	1.19393700	0.01051900
O	1.87150800	2.39927900	-1.01304600
O	3.51461200	-0.83671700	-1.54044300
H	-0.95258100	-4.45314200	1.00882200
H	1.99180700	-3.60878800	-0.66211000
N	-0.16641100	0.00811400	1.32111700
C	-1.00136400	1.02912900	0.81563500
C	0.03642900	0.24169800	2.62738200
C	-1.39743200	1.10031700	-0.63235300
C	-1.30474400	1.87061300	1.86889700
N	-0.64783200	1.36395000	2.99239400
H	0.66547700	-0.33462400	3.28444700
C	-2.63983500	0.23339700	-1.02374900
H	-0.54158800	0.79514700	-1.24158000
H	-1.62103100	2.13685400	-0.90406000
H	-1.90804300	2.76225200	1.90043800
H	-0.66738800	1.76234500	3.92298800
N	-3.88745600	0.88971500	-0.67959500
C	-2.54892700	-1.14251800	-0.35881300
H	-2.60923900	0.05288400	-2.10481500

C	-5.06805600	0.38801700	-1.18484000
O	-1.53876400	-1.93304200	-0.94124300
O	-3.17243700	-1.55178000	0.62553900
C	-6.34337100	1.11180700	-0.75814400
O	-5.08001600	-0.62234900	-1.93787800
C	-6.20143900	2.61934400	-0.45872400
H	-7.07429500	0.96556500	-1.56053400
H	-6.74602700	0.58966900	0.12370700
N	-5.30086300	2.87237700	0.71036200
H	-5.76729800	3.13025400	-1.32667400
H	-7.20736700	3.03853600	-0.30090500
H	-5.11093000	3.86743100	0.83722000
H	-5.68083200	2.48028800	1.57459800
H	-1.44946700	-2.78350200	-0.43068800
H	-3.96462200	1.66990900	-0.00902500
H	3.04158600	4.43184600	-0.49968300

2C: E(B3LYP)= -1505.26363912
Gas-phase zero-point energy = -1504.843444
Gas-phase free energy = -1504.906936

Pt	-0.26046800	-0.29125600	-1.03604000
H	3.81230300	-0.12728500	-2.86178500
N	-0.40376800	-2.32890600	-1.41406100
H	0.45853600	-2.79302100	-1.11087300
H	-1.22593200	-2.64859700	-0.85035000
O	-2.11722300	-0.08475400	-0.26641600
O	-4.86794400	1.16071300	2.44437200
C	-2.87228800	-1.06993800	0.24256000
C	-3.76973900	0.41471000	2.03634700
C	-4.13360200	-0.55451400	0.92925400
C	-5.25487000	-0.05528600	-0.07652000
H	-5.46550400	1.01489900	-0.03432600
H	-5.02765800	-0.34246600	-1.10845800
C	-5.14525400	-1.66742700	1.42504100
H	-5.28295800	-1.72642700	2.50735600
H	-4.84361400	-2.64725200	1.04776300
C	-6.29738200	-0.99217800	0.61368900
H	-6.99740900	-0.44241800	1.24771500
H	-6.85801200	-1.65323100	-0.05191200
O	-2.66685200	0.52864000	2.59259700
O	-2.62118300	-2.29814800	0.11566900
H	-0.55518200	-2.51372600	-2.40974400
N	-0.06010900	1.71257400	-0.62651200
C	1.03211300	2.47210900	-0.14711800
C	-1.08615100	2.55554100	-0.83788500
C	2.38453800	1.96800200	0.32465300
C	0.62192000	3.79343500	-0.09455600
N	-0.70203200	3.82423400	-0.52795600
H	-2.06550500	2.26001600	-1.17229800
C	2.63449100	0.44880200	0.18590200
H	2.48124000	2.20243000	1.39291000

H	3.18245000	2.51441900	-0.19431700
H	1.14953200	4.67769800	0.22335400
H	-1.28750300	4.64750000	-0.59591100
N	3.85590600	0.04137700	0.86071100
C	2.67006300	0.02495000	-1.28109900
H	1.77828100	-0.09656200	0.60719700
C	4.21765400	-1.27439600	0.73891400
O	1.63330900	-0.33918000	-1.91800300
O	3.83568100	0.18176100	-1.92606900
C	5.45937500	-1.72394900	1.49465400
O	3.54074200	-2.04452200	-0.01148300
C	5.73710500	-0.97149600	2.81644200
H	5.35011300	-2.79496800	1.69508000
H	6.32014000	-1.62316700	0.81577400
N	5.92577000	0.49486400	2.58936600
H	4.88458900	-1.09266900	3.49551300
H	6.60956500	-1.43336200	3.30207900
H	5.90510700	1.02804000	3.45944300
H	6.78725400	0.70255900	2.08020900
H	4.46347300	0.64000600	1.45821400
H	-4.64725800	1.71030900	3.23063700

TS$_{(2C\rightarrow 5C)}$: E(B3LYP)= -1505.19853658
Gas-phase zero-point energy = -1504.782399
Gas-phase free energy = -1504.847165

Pt	0.62153700	-0.12401600	-0.05138700
H	-2.35561600	-3.30374400	-0.60851600
N	1.43216700	-1.71982400	2.15656400
H	0.85545700	-1.70913300	2.99334800
H	1.50280400	-2.64084600	1.73164000
O	2.45641600	0.75281900	-0.10775900
O	4.51473700	-0.33151500	2.03343700
C	3.16364600	-0.36324000	-0.34241900
C	5.19670400	0.22661200	0.94891400
C	4.65922800	-0.29639900	-0.37417600
C	5.40889000	-1.61869300	-0.81955700
H	5.95169500	-2.14324000	-0.02950400
H	4.71201700	-2.31434100	-1.29446000
C	5.29369100	0.43640500	-1.62125000
H	5.75921200	1.39429300	-1.38294400
H	4.57179600	0.56688100	-2.43346100
C	6.25351700	-0.77976600	-1.83316000
H	7.26630400	-0.57641300	-1.47456300
H	6.30800500	-1.17683700	-2.84901700
O	6.15197700	0.99069400	1.10202800
O	2.45660500	-1.42532100	-0.52521500
H	2.34739700	-1.29414400	2.29760300
N	-0.37700800	1.61512300	0.05713900
C	-1.69444500	1.86974500	0.48035300
C	0.19270300	2.78788100	-0.28155500
C	-2.64478400	0.80648700	0.93171100

C	-1.90950200	3.23028000	0.36909200
N	-0.71854400	3.78561400	-0.09957400
H	1.20686100	2.91137600	-0.62366000
C	-3.13786000	-0.11802000	-0.24698400
H	-3.53303500	1.29614700	1.33140000
H	-2.20173800	0.20379600	1.73444800
H	-2.79721000	3.80968800	0.56006000
H	-0.55342800	4.76779400	-0.28360100
N	-4.55687400	-0.43260900	-0.17278700
C	-2.28529000	-1.36266600	-0.32291400
H	-2.95976800	0.44928900	-1.17750400
C	-5.45574000	0.57742200	-0.43424200
O	-1.03096200	-1.39482100	-0.19312700
O	-2.94918600	-2.51878000	-0.53538200
C	-6.92992900	0.17799100	-0.45549700
O	-5.06666600	1.75854500	-0.66592000
C	-7.32804600	-0.98303500	0.48331700
H	-7.50971400	1.07223100	-0.20368000
H	-7.19160600	-0.07664800	-1.49418000
N	-6.59761200	-2.23860100	0.13861200
H	-7.07252300	-0.72611700	1.51871600
H	-8.42074000	-1.10756300	0.43863800
H	-6.67882100	-2.95491600	0.86024300
H	-6.87957100	-2.62247700	-0.76505700
H	-4.95607100	-1.38549500	-0.03550300
H	4.91345700	-0.03326500	2.88378800

5C: E(B3LYP)= -1448.64291246
Gas-phase zero-point energy = -1448.263709
Gas-phase free energy = -1448.325876

Pt	0.70356900	-0.03410500	-0.11579400
H	-2.14738200	-3.32126100	-0.52965600
O	2.59158200	0.75947500	-0.01728300
O	4.69180100	0.30511600	2.22823100
C	3.18756400	-0.43728500	0.00676900
C	5.31883200	0.37587300	0.99567500
C	4.66850900	-0.58627800	0.00900100
C	5.22504600	-2.06010400	0.16555900
H	5.72024900	-2.27026000	1.11608900
H	4.43085100	-2.79392400	0.00506200
C	5.33986300	-0.53394500	-1.42690500
H	5.92423500	0.37191800	-1.59711400
H	4.61188200	-0.66758000	-2.23314800
C	6.13290400	-1.83742700	-1.08746500
H	7.17477400	-1.63279700	-0.82602300
H	6.10278800	-2.62592000	-1.84222000
O	6.30790700	1.08210900	0.78104800
O	2.33545700	-1.42704600	-0.05446700
N	-0.36200800	1.66745900	-0.15099200
C	-1.68149700	1.90267000	0.27720300
C	0.14953300	2.82833300	-0.60584100

C	-2.57367100	0.84905500	0.85392200
C	-1.95781100	3.23734100	0.04821300
N	-0.80164300	3.79715500	-0.49683500
H	1.15120100	2.96974000	-0.97760200
C	-3.09799200	-0.17633400	-0.22111700
H	-3.45801000	1.34449400	1.25541400
H	-2.07823800	0.32417600	1.68030600
H	-2.86420000	3.79599800	0.21240500
H	-0.68326200	4.76559100	-0.77009000
N	-4.47976600	-0.57323300	0.00006300
C	-2.17674800	-1.37075000	-0.31223700
H	-3.04410000	0.34498900	-1.19361700
C	-5.46451000	0.35492100	-0.25857000
O	-0.91458600	-1.33285400	-0.26267600
O	-2.77956200	-2.56653000	-0.45357000
C	-6.90337400	-0.13501800	-0.11169100
O	-5.17607400	1.53273400	-0.61862200
C	-7.13390300	-1.23753900	0.94683600
H	-7.52001000	0.73869000	0.12398000
H	-7.23673800	-0.49037200	-1.09894100
N	-6.34483500	-2.46696400	0.63550800
H	-6.81091300	-0.87876200	1.93178400
H	-8.21400700	-1.43809300	1.01101200
H	-6.31372900	-3.12387600	1.41542100
H	-6.67595400	-2.94322300	-0.20544100
H	-4.80289000	-1.53391800	0.24940500
H	5.12418800	0.88852000	2.89327900

TS$_{(5C \rightarrow 5D)}$: E(B3LYP)= -1448.62126286
Gas-phase zero-point energy = -1448.244133
Gas-phase free energy = -1448.306044

Pt	0.69378300	-0.07674100	-0.00304800
H	-2.17372900	-3.38612600	0.01784400
O	2.56719200	0.74240100	-0.12648100
O	4.75123300	0.24745100	2.16709100
C	3.18853900	-0.43870300	-0.07305200
C	5.31041500	0.39527600	0.87952900
C	4.67408200	-0.54526200	-0.15144800
C	5.27520700	-2.00842700	-0.09000800
H	5.82971100	-2.26354800	0.81835800
H	4.49869000	-2.76052800	-0.25264700
C	5.28154700	-0.39726800	-1.60406200
H	5.83407100	0.53282000	-1.74808500
H	4.52691800	-0.50565700	-2.38928400
C	6.12090500	-1.69512700	-1.36768700
H	7.16879600	-1.47809300	-1.14222300
H	6.07567600	-2.44539900	-2.15950300
O	6.17184800	1.23147400	0.63978200
O	2.36131600	-1.44775400	-0.00259500
N	-0.35886800	1.63253900	-0.03314700
C	-1.68362600	1.90097600	0.35894400

C	0.19756300	2.78337000	-0.46301800
C	-2.62175500	0.87295500	0.90828900
C	-1.91509300	3.24436500	0.13377100
N	-0.72866800	3.77643300	-0.37208300
H	1.21423000	2.89749800	-0.80278700
C	-3.05705200	-0.20969200	-0.15499000
H	-3.53500100	1.38424100	1.21382400
H	-2.19665300	0.39134200	1.79828000
H	-2.81043100	3.82678200	0.27321600
H	-0.57501200	4.74359100	-0.63211700
N	-4.46649500	-0.55683000	-0.07197700
C	-2.16735400	-1.42421000	-0.04517200
H	-2.87217900	0.24033200	-1.14608000
C	-5.38393600	0.37726500	-0.50171700
O	-0.90760100	-1.39768700	0.06359900
O	-2.78985400	-2.61703700	-0.04444500
C	-6.84531700	-0.06482500	-0.49581600
O	-5.01611400	1.52086800	-0.89713300
C	-7.23859600	-1.06968000	0.61087600
H	-7.45613600	0.83971200	-0.40763600
H	-7.06907800	-0.49345800	-1.48485900
N	-6.46133200	-2.33999100	0.49892400
H	-7.02440200	-0.63763400	1.59610300
H	-8.32492600	-1.23738500	0.55823000
H	-6.53793900	-2.92386100	1.33193200
H	-6.71283200	-2.88336200	-0.32882700
H	-4.84735100	-1.48517300	0.21408200
H	5.06270400	-0.51915500	2.69269700

5D: E(B3LYP)= -1448.62849689
Gas-phase zero-point energy = -1448.249926
Gas-phase free energy = -1448.312591

Pt	0.68481200	-0.10163200	0.07915600
H	-2.20679400	-3.38971000	0.02737500
O	2.56234200	0.71150500	-0.00244100
O	5.30229600	0.97947700	1.68247200
C	3.18336700	-0.47240200	0.01184600
C	5.35759900	0.71144100	0.32033000
C	4.66246600	-0.59396300	-0.11975600
C	5.31751600	-1.91148100	0.46987000
H	5.95584000	-1.77173600	1.34735300
H	4.55956600	-2.66965700	0.68618700
C	5.12967700	-1.07214000	-1.56269200
H	5.62097600	-0.27962200	-2.12973700
H	4.30961200	-1.50197900	-2.14511600
C	6.04050600	-2.15101200	-0.89476400
H	7.09307200	-1.85447700	-0.87720100
H	5.96103100	-3.16105700	-1.30109500
O	5.94981000	1.47634100	-0.43457000
O	2.35491600	-1.48116500	0.08759800
N	-0.35193500	1.61538000	0.02880100

C	-1.68344900	1.89360100	0.39015300
C	0.22095500	2.76038300	-0.39719000
C	-2.63944300	0.87168900	0.91936500
C	-1.90188800	3.23668400	0.15085100
N	-0.70155500	3.75839300	-0.33261800
H	1.24463200	2.86710300	-0.71854000
C	-3.05941300	-0.20517300	-0.15646900
H	-3.55541300	1.38818400	1.20722100
H	-2.23588900	0.38516000	1.81667100
H	-2.79694700	3.82489400	0.26573000
H	-0.53684200	4.72263300	-0.59738600
N	-4.47329400	-0.53946700	-0.10850200
C	-2.18278800	-1.42722300	-0.02939900
H	-2.84669100	0.24568400	-1.14170100
C	-5.37045000	0.40634100	-0.55594900
O	-0.92477800	-1.41113000	0.10795600
O	-2.81391400	-2.61432000	-0.04556000
C	-6.83571800	-0.02075600	-0.58871100
O	-4.98047800	1.54790200	-0.93575600
C	-7.26601600	-1.02742600	0.50255000
H	-7.43964200	0.88932900	-0.51089500
H	-7.03906100	-0.44199600	-1.58530300
N	-6.49720900	-2.30423900	0.40425800
H	-7.07367700	-0.60203400	1.49514800
H	-8.35195900	-1.18537000	0.42110400
H	-6.60066300	-2.89081600	1.23251500
H	-6.73376800	-2.84196600	-0.43161900
H	-4.87120400	-1.46543300	0.16339000
H	4.85737100	0.28938400	2.22036900

TS$_{(5D \rightarrow 4A)}$: E(B3LYP)= -1448.52049133
Gas-phase zero-point energy = -1448.149496
Gas-phase free energy = -1448.212746

Pt	0.73537100	-0.00204200	-0.20952100
H	-2.10497300	-3.28808000	-0.75977400
O	2.60967500	0.81357100	-0.13361500
O	5.37767300	-1.57999800	2.05675600
C	3.22611800	-0.38671100	-0.20628100
C	4.92387900	-0.37853400	2.05634100
C	4.65345500	-0.54306400	-0.13054700
C	5.31626400	-1.65920700	-1.10942100
H	5.83597400	-2.50358500	-0.64106300
H	4.56574300	-2.06179900	-1.79589300
C	5.59863200	0.54047600	-0.73655600
H	6.29407400	1.00374300	-0.03018500
H	5.06413100	1.33893100	-1.25927500
C	6.24819800	-0.53665800	-1.66986700
H	7.31090900	-0.71125900	-1.48200300
H	6.10632200	-0.34993000	-2.73777700
O	4.64834900	0.64800100	2.58195100
O	2.35177400	-1.37937600	-0.30534400

N	-0.35399600	1.68653900	-0.06866900
C	-1.66086900	1.87154800	0.41828800
C	0.13498600	2.88813000	-0.43091000
C	-2.52678800	0.76101700	0.92352700
C	-1.95350000	3.21872700	0.32003300
N	-0.81808100	3.83615100	-0.20612500
H	1.12480500	3.07044300	-0.81600300
C	-3.06333900	-0.17627700	-0.22425300
H	-3.40575100	1.20638800	1.39012100
H	-2.00217300	0.17415100	1.68798600
H	-2.85846600	3.75166200	0.55980200
H	-0.71389600	4.82621900	-0.39300800
N	-4.44222900	-0.59317400	-0.02125700
C	-2.13931300	-1.35679300	-0.41514000
H	-3.01943900	0.41975100	-1.15295300
C	-5.43197700	0.34942800	-0.19028000
O	-0.87809500	-1.31314900	-0.38765200
O	-2.74095000	-2.54557800	-0.62208700
C	-6.86811900	-0.15572200	-0.06779500
O	-5.15202900	1.55435000	-0.45487800
C	-7.08490600	-1.33790000	0.90403400
H	-7.48412000	0.69497800	0.24206500
H	-7.21133100	-0.43425600	-1.07610400
N	-6.29899100	-2.53812900	0.48992600
H	-6.75038800	-1.05580600	1.90990000
H	-8.16418900	-1.54439400	0.96546300
H	-6.25402600	-3.25131300	1.21786200
H	-6.63995400	-2.95121500	-0.37991800
H	-4.75829500	-1.57157400	0.15345500
H	5.13170500	-1.51682800	0.85472000

TS$_{(2C \rightarrow 2D)}$: E(B3LYP)= -1505.24487280
Gas-phase zero-point energy = -1504.826383
Gas-phase free energy = -1504.889781

Pt	-0.24874200	-0.45670000	-0.93270900
H	3.77388200	-0.69022400	-2.83293200
N	-0.44938000	-2.52578000	-0.97643100
H	0.46128000	-2.96635300	-0.81326900
H	-1.11163800	-2.72734300	-0.19654400
O	-2.14646700	-0.16732400	-0.30435600
O	-5.44822700	1.61018700	1.51701000
C	-2.81075700	-0.95759400	0.54677500
C	-4.15487800	1.06952000	1.32561000
C	-4.17554700	-0.40731800	0.95863800
C	-5.31584400	-0.76766800	-0.10355900
H	-5.75781300	0.09463300	-0.60552800
H	-4.95602900	-1.48102400	-0.85141400
C	-4.96297900	-1.29305900	2.00727500
H	-5.15888900	-0.82996500	2.97978800
H	-4.43247100	-2.23317900	2.17108400

C	-6.17048700	-1.42594000	1.02467400
H	-7.03736400	-0.82109100	1.30434300
H	-6.50281900	-2.44839800	0.83016000
O	-3.16969400	1.80613900	1.39611100
O	-2.41672800	-2.10286100	0.90276400
H	-0.83290400	-2.85732500	-1.86605800
N	-0.03855500	1.58500100	-0.74386700
C	1.06089700	2.40839800	-0.39550700
C	-1.12051300	2.37887000	-0.85698400
C	2.49052400	1.99297700	-0.09883300
C	0.59334700	3.70843600	-0.31958100
N	-0.76729700	3.66702600	-0.61481300
H	-2.11970400	2.02879500	-1.04182200
C	2.72566100	0.47449000	0.08837500
H	2.78876900	2.48176100	0.83690000
H	3.16732400	2.36912900	-0.87749300
H	1.10744800	4.62256700	-0.07208100
H	-1.40908000	4.44987800	-0.59577800
N	3.97554800	0.19450100	0.77642100
C	2.69933900	-0.23083300	-1.26397900
H	1.88552000	0.03925300	0.64763600
C	4.34065400	-1.12162400	0.88416100
O	1.63524800	-0.68426100	-1.78678900
O	3.83967600	-0.21669900	-1.97105300
C	5.61628400	-1.42569100	1.65563300
O	3.63783200	-2.01648700	0.31868300
C	5.93917500	-0.44832700	2.80947200
H	5.52688700	-2.44433000	2.04735400
H	6.44826700	-1.44291300	0.93504400
N	6.10979900	0.95240900	2.31416400
H	5.11374400	-0.44485200	3.53149600
H	6.83236300	-0.81605500	3.33621000
H	6.12330200	1.63444400	3.07335600
H	6.94721600	1.06275600	1.73871500
H	4.60026600	0.89204500	1.23074200
H	-5.84889100	1.48088100	2.40109900

2D: E(B3LYP)= -1505.26090942
Gas-phase zero-point energy = -1504.841015
Gas-phase free energy = -1504.904117

Pt	-0.28213000	-0.38321500	-0.64922400
H	3.46346300	-0.23098700	-3.05523700
N	-0.50839500	-2.39871900	-1.11570700
H	0.19041300	-2.95491100	-0.61315900
H	-1.47423500	-2.65893700	-0.81740100
O	-2.04020300	-0.20964500	0.32160500
O	-5.63621500	0.38838100	-1.09377900
C	-3.07586100	-1.04998100	0.31025600
C	-4.72447700	0.72554300	-0.11281900
C	-4.34986900	-0.38881000	0.87357900

C	-5.45238300	-1.41731500	1.30914400
H	-6.47142800	-1.05984300	1.11717300
H	-5.32861700	-2.42417300	0.90469200
C	-4.19088000	0.05059700	2.37847500
H	-4.69816300	0.99988400	2.57555400
H	-3.16382600	0.11777400	2.74211500
C	-5.02991300	-1.19991700	2.80245100
H	-5.84503100	-1.01361100	3.50499700
H	-4.41351000	-2.01900700	3.18524100
O	-4.23556100	1.86194900	-0.10022400
O	-3.05234000	-2.23508300	-0.11967400
H	-0.38940200	-2.54454200	-2.12244900
N	-0.06109600	1.61732400	-0.20189800
C	1.07745000	2.41911600	0.05862000
C	-1.14547600	2.42213200	-0.17426300
C	2.52142300	1.97855200	0.22151400
C	0.63552300	3.71972100	0.22691800
N	-0.74889800	3.69741000	0.07773300
H	-2.17522000	2.11337100	-0.28014000
C	2.78925300	0.45903100	0.11798400
H	2.85718800	2.28718100	1.22000400
H	3.15709300	2.50646200	-0.50120700
H	1.18371700	4.62095500	0.44757200
H	-1.37646700	4.48911000	0.15093000
N	4.11995500	0.11604900	0.59149600
C	2.59248800	-0.02811700	-1.31457700
H	2.03292100	-0.08542900	0.70065600
C	4.50654000	-1.19277400	0.46521700
O	1.47280800	-0.42713100	-1.76091200
O	3.63458900	0.11040100	-2.14654100
C	5.88266300	-1.56217000	0.99994500
O	3.73856900	-2.02197800	-0.11382200
C	6.37537700	-0.72457300	2.20224800
H	5.85329000	-2.62191900	1.27451600
H	6.59737400	-1.47965500	0.16668400
N	6.46230500	0.72966900	1.86367100
H	5.67114200	-0.82714700	3.03670300
H	7.34043500	-1.13282400	2.53763400
H	6.59348500	1.31402200	2.69017200
H	7.19917200	0.92772700	1.18360500
H	4.80534400	0.76539000	1.03066100
H	-5.97441000	-0.53159600	-1.02832400

TS$_{(2D \rightarrow 3B)}$: E(B3LYP)= -1505.14026563
Gas-phase zero-point energy = -1504.728035
Gas-phase free energy = -1504.791272

Pt	-0.27740600	-0.47437800	-0.86354700
H	3.68588400	-0.64834400	-2.88982700
N	-0.44688400	-2.54590400	-0.96056300

H	0.39841900	-2.97330300	-0.56820500
H	-1.28824300	-2.78940500	-0.39293300
O	-2.11732600	-0.16643700	-0.10349700
O	-4.19536200	2.02723400	0.39804400
C	-2.97478400	-1.06065700	0.40665600
C	-3.75850900	1.33205800	1.41619500
C	-4.26105000	-0.41429300	0.89174800
C	-5.61696800	-0.85930200	0.00673500
H	-6.02776100	-0.13527700	-0.70425500
H	-5.35259700	-1.78624400	-0.51016200
C	-4.99792500	-1.06846500	2.10647200
H	-4.93809500	-0.49917500	3.03670900
H	-4.61060300	-2.07828000	2.27229800
C	-6.36024900	-1.07996400	1.35088900
H	-7.00085700	-0.23305900	1.61494400
H	-6.94451600	-2.00031900	1.41468300
O	-3.19474300	1.46413800	2.47870900
O	-2.77264900	-2.30341600	0.46267300
H	-0.56479300	-2.86174600	-1.92772400
N	-0.07967100	1.57198900	-0.69980200
C	1.02839900	2.40067300	-0.39600600
C	-1.15707900	2.36971600	-0.84711600
C	2.45238900	1.98487700	-0.07008900
C	0.57255300	3.70752500	-0.37972800
N	-0.78969500	3.66445200	-0.66381300
H	-2.16586600	2.03641400	-1.01955900
C	2.69759500	0.46447200	0.07383500
H	2.72149800	2.44165800	0.89065600
H	3.14532000	2.39320000	-0.81738600
H	1.09585500	4.62750500	-0.17710900
H	-1.42493300	4.45311300	-0.68953900
N	3.96217200	0.17532500	0.73012300
C	2.64435100	-0.21824200	-1.29005600
H	1.87182900	0.01445700	0.64275000
C	4.32568900	-1.14293100	0.81123600
O	1.57093500	-0.67460900	-1.79330300
O	3.76656200	-0.18567900	-2.02325500
C	5.61736600	-1.46189900	1.54862900
O	3.60615600	-2.02698800	0.24862100
C	5.97154800	-0.49913200	2.70571700
H	5.53294500	-2.48468800	1.93052700
H	6.43190500	-1.47428900	0.80827600
N	6.13176800	0.90750600	2.22336500
H	5.16515600	-0.50327000	3.44885700
H	6.87733600	-0.87454400	3.20451700
H	6.16297300	1.58010400	2.99046900
H	6.95646000	1.02459600	1.63105800
H	4.60052200	0.86528500	1.17890500
H	-4.54251300	0.69292500	0.22891300

3B: E(B3LYP)= -1316.72670796
Gas-phase zero-point energy = -1316.320040

Gas-phase free energy = -1316.379041

Pt	-0.66530900	0.04718100	-0.79936300
H	3.24663900	0.46853500	-2.93075400
N	-0.99513100	-1.79312300	-1.69994600
H	-0.19721000	-2.41206600	-1.52559400
H	-1.87152900	-2.15589800	-1.24735900
O	-2.43815000	0.15093900	0.16930700
C	-3.35229500	-0.83655100	0.28231000
C	-4.55348500	-0.47022500	1.11993000
C	-5.97061800	-0.73492800	0.48518400
H	-6.50086700	0.14213600	0.10286000
H	-5.91444800	-1.49971800	-0.29566500
C	-4.94247600	-1.47229200	2.27254700
H	-4.66719700	-1.17058600	3.28719700
H	-4.55431000	-2.47493300	2.06837400
C	-6.44358100	-1.33028500	1.85318600
H	-6.97981100	-0.59613300	2.46446700
H	-7.03096500	-2.25105800	1.81133800
O	-3.22798400	-1.97171100	-0.25963600
H	-1.12627300	-1.68802700	-2.71002200
N	-0.28437000	1.86623500	0.08762500
C	0.90031700	2.43642100	0.60927200
C	-1.26084700	2.78632200	0.18631000
C	2.25105400	1.77008100	0.80228200
C	0.59464400	3.72655000	1.00904900
N	-0.75778700	3.92492400	0.73816100
H	-2.28467200	2.62745600	-0.10552000
C	2.38603400	0.32462000	0.26980400
H	2.45972100	1.72448400	1.87934800
H	3.03456500	2.39425000	0.35391300
H	1.21337600	4.48395200	1.46179000
H	-1.28434500	4.77022500	0.92118200
N	3.63437700	-0.28554900	0.69622900
C	2.25990100	0.28087200	-1.25154800
H	1.53643100	-0.27294600	0.62943400
C	3.90137000	-1.54534700	0.22611800
O	1.14826300	0.13516600	-1.84524400
O	3.37367800	0.53437100	-1.95545600
C	5.18499000	-2.20562300	0.70833000
O	3.10770000	-2.08830900	-0.60303100
C	5.64575900	-1.80193400	2.12753600
H	5.03212800	-3.28905700	0.66330100
H	5.97480400	-1.97492400	-0.02302300
N	5.90094000	-0.33135900	2.22822500
H	4.86316600	-2.05118000	2.85423200
H	6.53378400	-2.39732500	2.38701500
H	6.01014000	-0.02156800	3.19461900
H	6.71327600	-0.03908100	1.68107300
H	4.33783900	0.13127100	1.34085300
H	-4.44902500	0.55440900	1.48579200

TS$_{(3B\rightarrow 4A)}$: E(B3LYP)= -1316.66694065
Gas-phase zero-point energy = -1316.263202
Gas-phase free energy = -1316.322317

Pt	0.93382900	0.26237300	0.29652900
H	-2.24902400	-1.02837100	3.12898800
N	0.21892700	-2.30553000	-0.58378900
H	-0.76921000	-2.55406600	-0.49450900
H	0.55558100	-2.38679300	-1.54055300
O	2.65956700	0.67562600	-0.71540400
C	3.36038300	-0.39379800	-0.29943500
C	4.76075900	-0.61136100	-0.74322400
C	5.86512400	-0.68661200	0.38810200
H	6.47518000	0.21144000	0.51482500
H	5.43141200	-0.97522200	1.35081300
C	5.17488400	-2.07245500	-1.16471800
H	5.25150900	-2.25315900	-2.24010300
H	4.51349900	-2.81828900	-0.71278600
C	6.50531200	-1.90208100	-0.35979700
H	7.34261100	-1.60215600	-0.99867700
H	6.81737100	-2.74795900	0.25733500
O	2.70290500	-1.16786800	0.50526400
H	0.82709600	-2.79687600	0.06728200
N	0.07188000	2.05574300	-0.10573800
C	-1.26506900	2.50490200	-0.18886700
C	0.87618300	3.08614200	-0.43767500
C	-2.53771800	1.72707800	0.07719300
C	-1.22613700	3.83449800	-0.57600600
N	0.11523000	4.17702700	-0.72399400
H	1.95101000	3.03411800	-0.49292700
C	-2.43473800	0.17691400	0.04417400
H	-3.25875900	2.00935700	-0.69903300
H	-2.97585500	2.03973100	1.03527400
H	-2.02743700	4.53199400	-0.75711400
H	0.47260900	5.08195800	-1.00534600
N	-3.73536300	-0.41851000	-0.20481800
C	-1.82741600	-0.31508600	1.35687000
H	-1.72324100	-0.13987000	-0.72916900
C	-3.81921800	-1.77459700	-0.39593300
O	-0.58935200	-0.30267400	1.59855400
O	-2.69201600	-0.70905600	2.30730700
C	-5.21569300	-2.34357500	-0.62396000
O	-2.78704800	-2.50521100	-0.35025800
C	-6.23497400	-1.38667700	-1.28221600
H	-5.10217300	-3.24181900	-1.24006500
H	-5.59640200	-2.68616800	0.35056100
N	-6.45139900	-0.15792200	-0.45673700
H	-5.86046900	-1.06430100	-2.26133300
H	-7.16928500	-1.94100000	-1.45636400
H	-6.97624600	0.55958200	-0.95818600
H	-6.91412000	-0.36290600	0.43128900
H	-4.64236900	0.09329800	-0.17790900

H	5.01060200	0.13042200	-1.50675600

TS$_{(1B \rightarrow CarH^+)}$: E(B3LYP)= -1561.805757
Gas-phase zero-point energy = -1561.347401
Gas-phase free energy = -1561.412328

Pt	1.85142500	-0.93720200	-0.53516400
N	0.73954300	-2.00854800	-1.95816800
H	-0.20979600	-2.14571700	-1.57207200
H	0.66845800	-1.46237400	-2.82258600
N	3.77620600	-1.46394700	-1.14917400
H	3.86180100	-1.78301400	-2.11724200
H	4.28788100	-0.56590700	-1.02613400
O	2.83965600	0.17572000	0.85222700
O	-0.16914200	2.96570600	0.17907300
C	3.16288900	1.33047000	0.19140700
C	0.73497600	1.99906100	0.05037900
C	2.15149000	2.45736700	0.37695700
C	2.32545400	3.13450800	1.81221400
H	1.35823000	3.45941400	2.20451100
H	2.83890800	2.51864600	2.55468000
C	2.60234000	3.82921500	-0.25488500
H	1.74650700	4.41127300	-0.60365900
H	3.34747800	3.72667000	-1.04597000
C	3.12028800	4.30053400	1.14292100
H	2.83444600	5.30944200	1.44848000
H	4.20354700	4.18811500	1.24654900
O	0.37313500	0.83231100	-0.32735500
O	4.21199400	1.42717500	-0.49291200
H	1.14369000	-2.92371100	-2.17514800
H	4.17877100	-2.16128300	-0.51588100
N	-0.00008100	-1.80505900	1.14873200
C	-1.26945600	-1.55990900	1.71291100
C	0.53472600	-2.81448400	1.85212500
C	-2.20284900	-0.45239100	1.30961800
C	-1.47561600	-2.45066500	2.75837900
N	-0.32696600	-3.23464000	2.83747200
H	1.51404800	-3.23813100	1.70036800
C	-2.65491300	-0.40389600	-0.19259900
H	-1.74051500	0.51941400	1.51469400
H	-3.10739700	-0.52602000	1.92468800
H	-2.31079600	-2.57054400	3.42909200
H	-0.14907000	-3.96616800	3.51364500
N	-3.79116800	0.51345200	-0.36267700
C	-3.11979200	-1.77403500	-0.65995800
H	-1.80309200	-0.06238700	-0.78724500
C	-3.66614900	1.85927200	-0.44531500
O	-2.11533100	-2.50689200	-1.30394400
O	-4.24921900	-2.24751200	-0.50627000
C	-4.95938200	2.64941800	-0.64874200
O	-2.55355500	2.47039700	-0.38846300
C	-6.21177600	2.07202400	0.05302900

H	-4.77116900	3.66725700	-0.29308500
H	-5.14129500	2.72478700	-1.73148800
N	-6.51437100	0.69470200	-0.42882900
H	-6.03302700	2.01430300	1.13363400
H	-7.04876300	2.76931500	-0.10080000
H	-7.12440700	0.16862500	0.19582200
H	-6.88369400	0.67280700	-1.38020900
H	-2.46225300	-3.39605000	-1.55384800
H	-4.78100700	0.16289100	-0.39006500
H	-1.14448300	2.72421300	-0.06890000

CarH$^+$ + CarbPt : E(B3LYP)= -1561.8615816
Gas-phase zero-point energy = -1561.401677
Gas-phase free energy = -1561.470295

Pt	-1.97803300	-1.14868700	-0.57818900
N	-0.66551300	-1.58530100	-2.14846400
H	-0.50259700	-0.70056600	-2.63943000
H	0.22918700	-1.90079900	-1.71868100
N	-3.06881400	-2.91975500	-0.49242200
H	-2.49018300	-3.75144900	-0.34713000
H	-3.64043500	-2.73908300	0.34821700
O	-3.15866700	-0.74144600	1.00977800
O	-0.66370400	2.64145400	0.47533300
C	-3.33546300	0.49513000	1.53447000
C	-1.43417400	1.65250300	0.23016800
C	-2.89683100	1.70280100	0.65463900
C	-3.91596900	1.88058500	-0.56343000
H	-3.41496700	2.24768500	-1.46638900
H	-4.50346800	0.99482200	-0.81808300
C	-3.40563400	3.06253200	1.22822000
H	-2.70695700	3.87445200	1.01430300
H	-3.63991500	3.03958600	2.29292300
C	-4.62221100	3.01661500	0.24554400
H	-4.83573200	3.93454100	-0.30835300
H	-5.53836800	2.67267500	0.73430200
O	-0.96191300	0.61582600	-0.44709100
O	-3.89755000	0.65782600	2.63126300
H	-1.00441900	-2.27791100	-2.81969500
H	-3.68138600	-3.05819600	-1.30083600
N	1.76365000	3.24030400	0.07654200
C	2.96269100	2.55205300	0.31510900
C	2.03716300	4.47995600	-0.35789100
C	3.00826900	1.15158400	0.86778500
C	3.98946100	3.42860600	0.00237400
N	3.38886500	4.61982300	-0.41422300
H	1.31189600	5.23579000	-0.60971700
C	3.25159000	0.03359800	-0.18321300
H	2.06090600	0.92696300	1.36939300
H	3.80339800	1.10051100	1.61959900
H	5.05532900	3.28079900	0.03782200
H	3.87926600	5.45677200	-0.70629500

N	3.28770000	-1.27966400	0.46971600
C	4.58679200	0.23693200	-0.91527000
H	2.44895900	0.01336900	-0.92672900
C	2.50235000	-2.33186300	0.09347600
O	4.62369400	-0.46062400	-2.09976400
O	5.54097700	0.91498800	-0.50186300
C	2.73720000	-3.63362800	0.86435000
O	1.64832500	-2.26800600	-0.83730900
C	3.13847500	-3.47933400	2.35052900
H	1.81419600	-4.21829000	0.79479600
H	3.50969900	-4.20500000	0.32710000
N	4.42558900	-2.73620100	2.49769500
H	2.36597500	-2.91186700	2.88328600
H	3.17920200	-4.48074400	2.80468100
H	4.58654500	-2.40984500	3.45080600
H	5.23200800	-3.27448300	2.17585800
H	5.49716400	-0.38197900	-2.54949100
H	3.94356200	-1.48642300	1.25723800
H	0.73580400	2.87324200	0.23339300

TS$_{(1B \rightarrow CarbPtH^+)}$: E(B3LYP)= -1561.7742863
Gas-phase zero-point energy = -1561.318179
Gas-phase free energy = -1561.388492

Pt	1.28931600	-1.67646600	-0.20174400
N	0.15768500	-3.38566900	-0.58660700
H	-0.42632700	-3.23023800	-1.41732300
H	0.66172800	-4.27214300	-0.65382800
N	3.08936400	-2.37853900	-0.88690700
H	2.98951400	-2.92231000	-1.74885100
H	3.61130400	-1.46227900	-1.07082500
O	2.07842100	0.09093700	0.36534500
O	2.09428000	4.14061300	0.93916200
C	3.07937200	0.73484300	-0.23300300
C	1.91280300	2.90141600	0.34247000
C	3.24378400	2.19410500	0.15711100
C	4.26972800	2.39563700	1.36363400
H	3.81848700	2.77452500	2.28200100
H	4.82118000	1.47489000	1.57868400
C	4.24735100	3.02531900	-0.74821600
H	3.79289600	3.84619200	-1.30743200
H	4.77486500	2.35964900	-1.43474200
C	5.08332700	3.41870500	0.51050400
H	4.91566000	4.45117300	0.82561900
H	6.15760000	3.23136300	0.44133900
O	0.78702100	2.52022200	-0.01121300
O	3.90140200	0.14995000	-1.00666500
H	-0.46407000	-3.34916000	0.25186900
H	3.57234500	-2.93349000	-0.17304600
N	-1.22804900	-2.12014100	1.59133600
C	-1.63025200	-0.79495100	1.32124300
C	-1.68638800	-2.41581700	2.81731200

C	-1.27276100	-0.12148700	0.02795800
C	-2.34030000	-0.31006300	2.40774300
N	-2.36872600	-1.34607600	3.34294200
H	-1.54883300	-3.34977800	3.33850300
C	-2.43896800	0.04430700	-1.00862600
H	-0.49031900	-0.73153000	-0.50258500
H	-0.81950100	0.86421400	0.17124800
H	-2.79404400	0.65012800	2.58630100
H	-2.80869700	-1.31246800	4.25405000
N	-3.36526200	1.09576300	-0.62796300
C	-3.20480300	-1.25152800	-1.24798400
H	-1.97458000	0.35130400	-1.95679500
C	-3.33437000	2.30942300	-1.29484200
O	-2.38779700	-2.27555200	-1.76183800
O	-4.40577100	-1.44787700	-1.05264900
C	-4.46268000	3.28765800	-0.95923700
O	-2.45987600	2.57683200	-2.15906800
C	-5.07976600	3.18904200	0.45214500
H	-4.06526900	4.29592300	-1.11715100
H	-5.24854200	3.14752200	-1.71786500
N	-5.68164800	1.84644100	0.69496600
H	-4.29988400	3.34525300	1.20868500
H	-5.81128800	4.00510300	0.56529000
H	-5.99788000	1.71629000	1.65546500
H	-6.43924700	1.62592500	0.04629700
H	-2.95917100	-3.04579600	-1.99329600
H	-4.18218400	0.93326700	-0.00984900
H	1.24617100	4.63772300	0.98603300

CarbPtH$^+$+Car: E(B3LYP)= -1561.8023796
Gas-phase zero-point energy = -1561.345244
Gas-phase free energy = -1561.411030

Pt	-1.13559100	-1.82937300	-0.12227700
N	-0.26387700	-3.69881800	-0.47063800
H	-0.48170100	-4.36562500	0.27706400
H	-0.55298300	-4.09936200	-1.36878700
N	-3.03008200	-2.55299500	-0.40514600
H	-3.28537100	-3.22919100	0.32130800
H	-3.63473600	-1.66635900	-0.32358300
O	-1.75227400	0.06693000	0.20832000
O	-1.44232900	2.35625100	-1.65019600
C	-2.97474400	0.58694900	0.03476500
C	-1.64351400	2.60576300	-0.32519900
C	-3.01204000	2.10390400	0.12529300
C	-4.23378000	2.81704000	-0.56182800
H	-3.99762400	3.36021500	-1.47924200
H	-5.03889300	2.10337000	-0.75700000
C	-3.49078200	2.69304200	1.50785100
H	-2.69045000	3.15257900	2.09162700
H	-4.01717300	1.95135000	2.11698000
C	-4.46335900	3.65109200	0.74209100

H	-4.07360800	4.67142900	0.67029700
H	-5.49053600	3.68992300	1.11234200
O	-0.78511700	3.12206400	0.41845800
O	-4.00446000	-0.12685500	-0.15783300
H	0.79900500	-3.51993900	-0.48954800
H	-3.14240000	-2.97512100	-1.33232900
N	2.35075000	-2.88996900	-0.39930800
C	2.50642400	-1.52219100	-0.11167400
C	3.57884300	-3.42431500	-0.42150700
C	1.30690600	-0.61483000	-0.03306200
C	3.85692600	-1.24657500	0.04179200
N	4.51847900	-2.45885500	-0.15961600
H	3.81856300	-4.45797800	-0.61246100
C	1.49507300	0.74737100	0.70768500
H	0.54529600	-1.15778200	0.62309600
H	0.92218500	-0.37345700	-1.03101000
H	4.37625500	-0.33015500	0.26265300
H	5.52000700	-2.60074700	-0.11639200
N	2.42442300	1.65626500	0.03317100
C	1.97805700	0.54162200	2.14013100
H	0.49996300	1.21037200	0.75896100
C	2.12206300	2.24302200	-1.15687600
O	1.14518100	-0.32594700	2.81932100
O	2.97186000	1.06698500	2.65436500
C	3.03335400	3.37462200	-1.62695900
O	1.10909500	1.89846400	-1.84837400
C	4.49311700	3.35088400	-1.12171000
H	3.01906400	3.36818700	-2.72208100
H	2.54824000	4.31395200	-1.31868300
N	4.54666900	3.33930600	0.36615100
H	4.99411400	2.44224500	-1.47957200
H	5.02503300	4.20835600	-1.56195500
H	5.46838300	3.12213100	0.74290900
H	4.18905300	4.19677700	0.78987900
H	1.40994700	-0.42288500	3.76258400
H	3.23488300	2.08178900	0.54621800
H	-0.46385700	2.34495000	-1.89520900

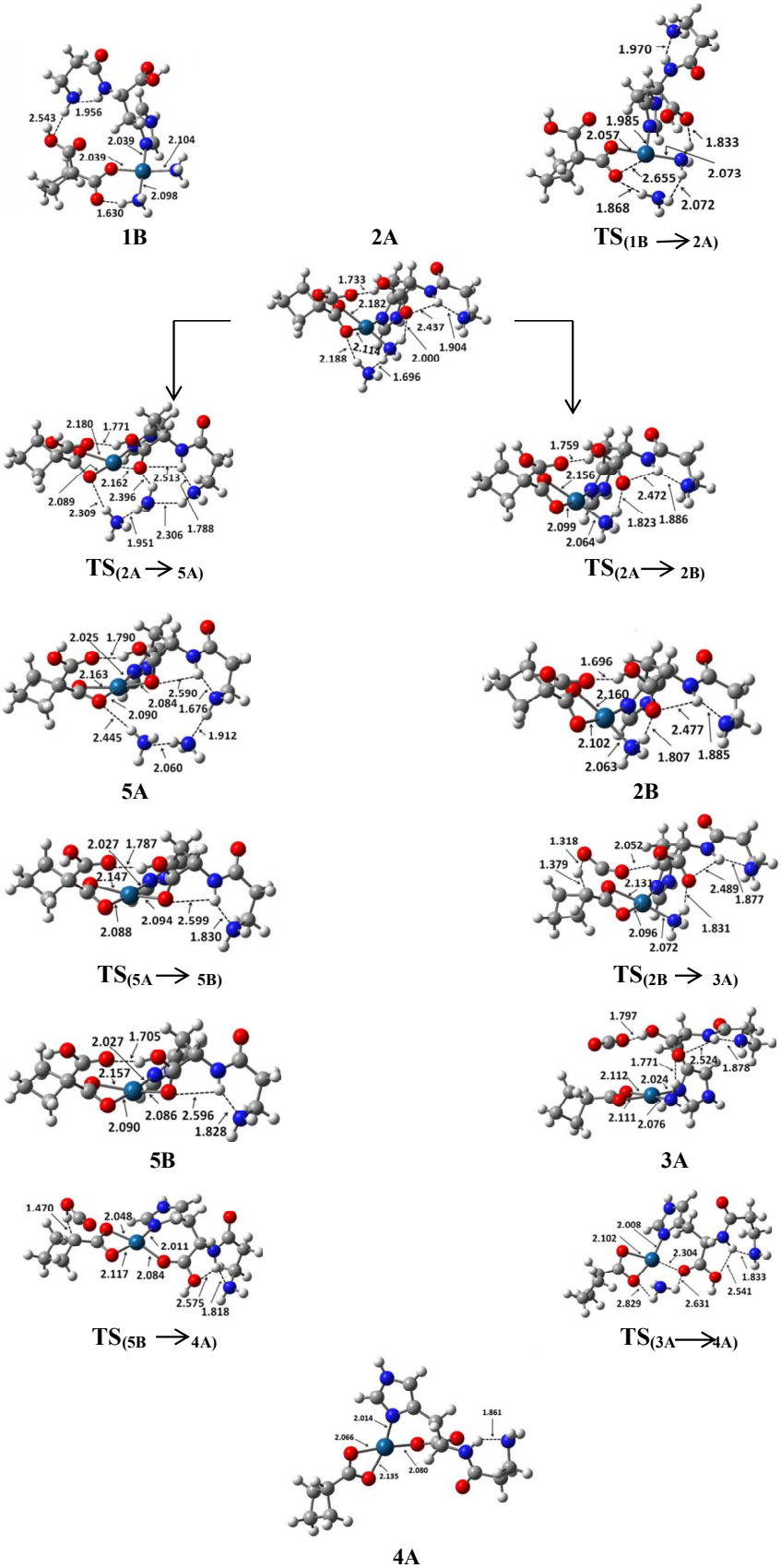


Figure S1. Geometrical structures of stationary points intercepted along the fragmentation Pathways 1 and 2 for the elimination of the NH_3 molecule cis to the CBDCA ligand. Bond lengths are in Å. Gray, red, blue and white spheres represent carbon, oxygen, nitrogen and hydrogen atoms, respectively.

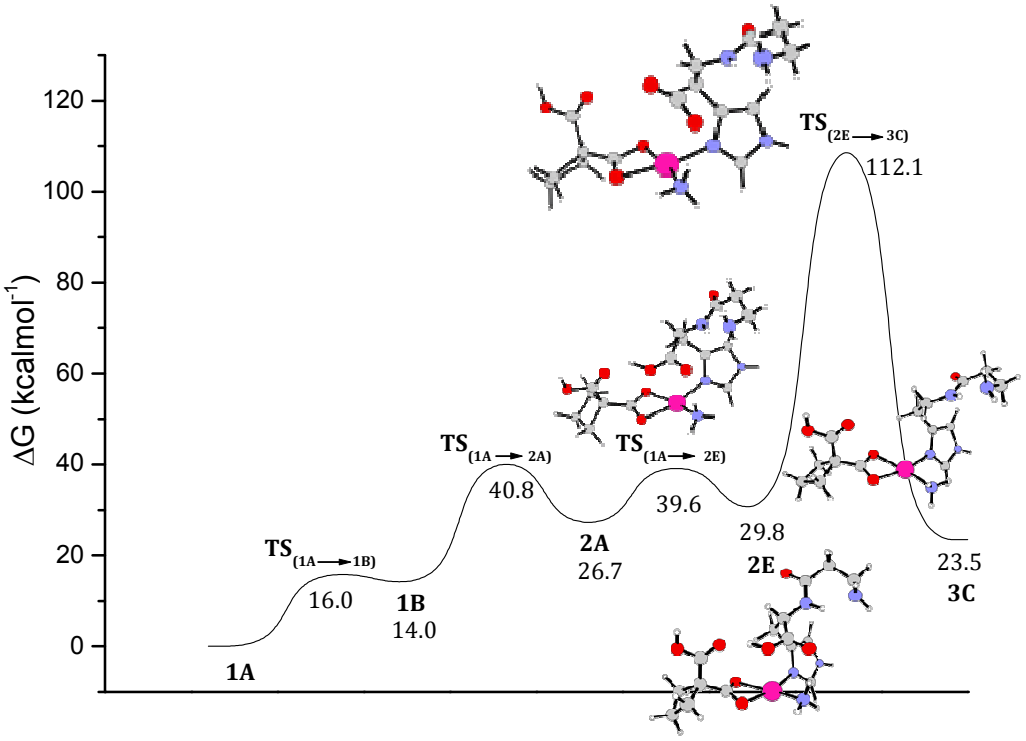


Figure S2. Free energy profile for the CO_2 release from the carnosine ligand. Structure labels are in bold and relative free energies in kcal mol^{-1}.

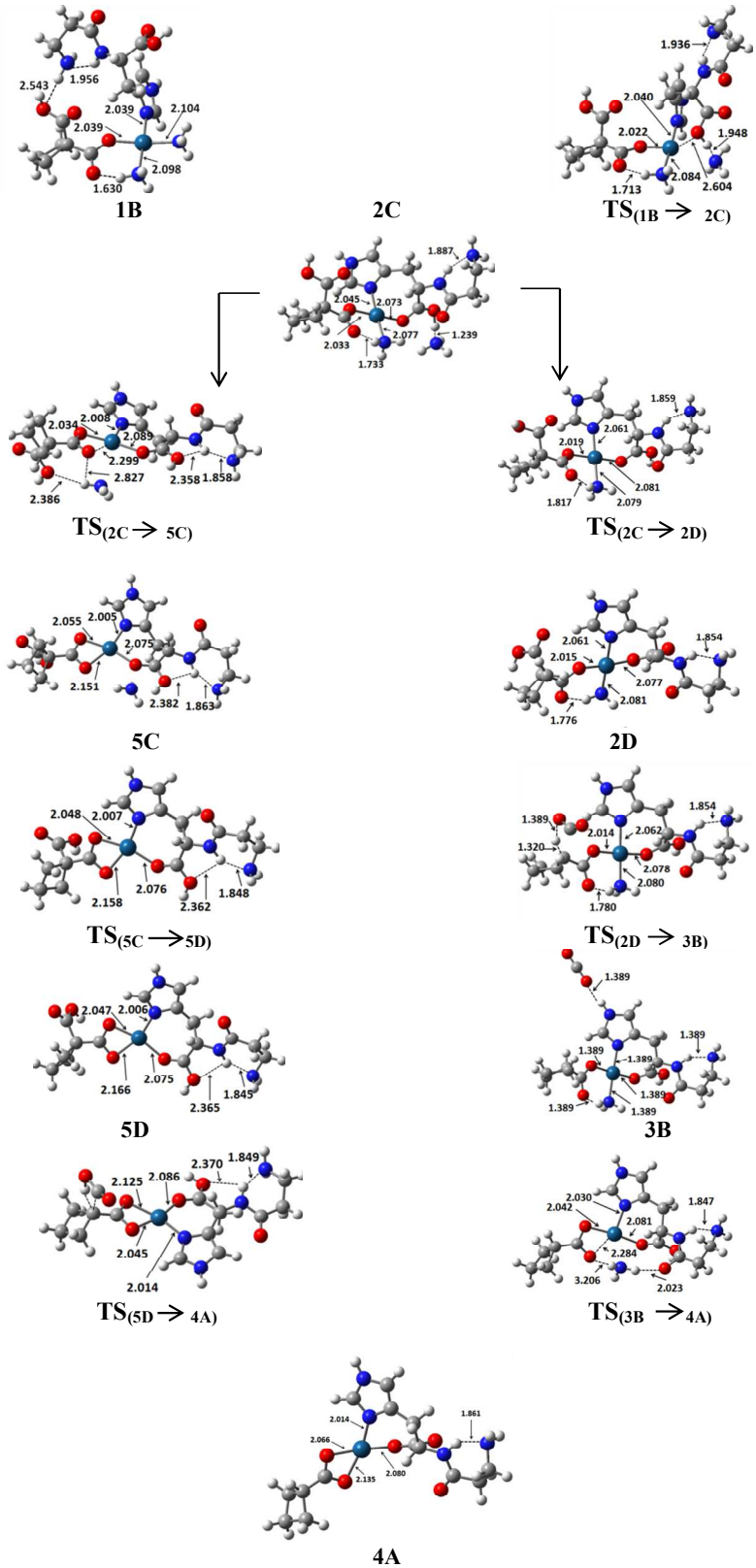


Figure S3. Geometrical structures of stationary points intercepted along the fragmentation Pathways 3 and 4 for the elimination of the NH_3 molecule cis to the CBDCA ligand. Bond lengths are in Å. Gray, red, blue and white spheres represent carbon, oxygen, nitrogen and hydrogen atoms, respectively.