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Supplementary material

Quantifying N-heterocyclic Carbenes as Umpolung Catalysts in the Benzoin Reaction: Balance between Nucleophilicity and Electrophilicity

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Table S1. Cartesien coordinates of benzaldehyde

C	1.99222300	0.46872900	0.00000400
O	2.84760800	-0.39586400	-0.00002300
H	2.27397300	1.54574100	0.00009800
C	0.53396300	0.21443500	-0.00000300
C	-0.36109000	1.29210900	0.00002700
C	0.04519700	-1.10111000	-0.00001200
C	-1.73590100	1.06061500	-0.00002900
H	0.02505600	2.30952000	0.00007500

C	-1.32631200	-1.33122100	0.00002800
H	0.75893200	-1.91937300	-0.00000600
C	-2.21683200	-0.25077500	-0.00000500
H	-2.43022500	1.89617800	-0.00008200
H	-1.70784300	-2.34856600	0.00006300
H	-3.28823500	-0.43328000	-0.00002400

Table S2. Cartesien coordinates of benzoin

C	-0.60655700	1.38147800	-0.08457600
H	0.82934400	3.05764200	-0.36455300
C	-1.64249100	0.31501000	-0.04448400
C	-2.76526200	0.52006700	0.77580300
C	-1.55441500	-0.86309200	-0.80264400
C	-3.77622000	-0.43280200	0.83821100
H	-2.82173000	1.43675700	1.35324000
C	-2.56892200	-1.81661100	-0.73877900
H	-0.69245800	-1.04649700	-1.43385000
C	-3.67965800	-1.60361000	0.07996100
H	-4.64022400	-0.26597000	1.47537800
H	-2.49159900	-2.72645000	-1.32719700
H	-4.46932900	-2.34873900	0.12743600
O	-0.73260600	2.41531800	0.56499800
C	0.67888200	1.24115400	-0.93341100
H	0.40304500	0.90726500	-1.94362100
C	1.61990200	0.20859100	-0.31609200
C	2.04633700	0.35529200	1.01055700
C	2.10778500	-0.86244300	-1.07040600
C	2.93232700	-0.56120700	1.57342300
H	1.68534700	1.19477000	1.59914700
C	2.99634500	-1.78225400	-0.50919900
H	1.80298800	-0.97037100	-2.10959300
C	3.40791500	-1.63479500	0.81543200
H	3.25344200	-0.43815600	2.60439400
H	3.37180000	-2.60685100	-1.10945500
H	4.09976500	-2.34847300	1.25466600
O	1.29433300	2.50548300	-1.02609300

Table S3. Cartesien coordinates of *t*-butanol

C	0.68958500	1.26617900	-0.50971300
C	-0.00543800	-0.00000700	0.01381600
H	0.20751500	2.15979500	-0.09981500
H	1.74650400	1.28148000	-0.21155600
H	0.65407300	1.32172600	-1.60402900
C	0.69189500	-1.26483100	-0.50992100
C	-1.49035800	-0.00131100	-0.35747600
H	0.21157700	-2.15939500	-0.10003500
H	0.65633300	-1.32035000	-1.60423500
H	1.74889300	-1.27815900	-0.21193400
H	-1.62221400	-0.00114300	-1.44477200
H	-1.98283900	-0.88834700	0.05430800
H	-1.98448000	0.88459100	0.05478200
O	0.01331400	-0.00010200	1.45232200
H	0.94402200	0.00044200	1.72846400

Table S4. Cartesien coordinates of imidazole-2-ylidene 1

C	0.00001400	0.98828300	-0.00002300
C	0.67827000	-1.21813700	0.00001900
C	-0.67825500	-1.21814600	-0.00001500
H	1.38344800	-2.03679100	0.00002500
H	-1.38342200	-2.03681400	-0.00003700
N	1.06265700	0.11945300	0.00001000
C	2.44197600	0.57374100	0.00000400
H	2.97288200	0.21951800	0.89125700
H	2.97307600	0.21891200	-0.89089300
H	2.42371100	1.66393400	-0.00036800
N	-1.06265600	0.11941000	-0.00002900
C	-2.44197700	0.57374900	0.00002400
H	-2.97302600	0.21888700	-0.89088000
H	-2.97280000	0.21941400	0.89127500
H	**-2.42404100**	**1.66395600**	**-0.00029900**

Table S5 Cartesien coordinates of imidazole-2-ylidene 1, TS-1

C	-1.26477200	0.04636000	0.12353700
C	-3.31613300	0.53851300	-0.71016600
C	-3.02861600	-0.74294200	-1.05184200
H	-4.18548400	1.14772800	-0.90573600
H	-3.60046300	-1.47395000	-1.60298500
N	-2.22419900	1.00249400	0.01582100
C	-2.10810400	2.35673300	0.54068800
H	-1.79568100	3.05416400	-0.24361500
H	-3.07271800	2.67721700	0.94339700
H	-1.36835700	2.36263100	1.34151100
N	-1.77482600	-1.02392100	-0.52919100
C	-1.08736300	-2.31234400	-0.63677200
H	-0.51993300	-2.45464200	0.28741200
H	-1.83487600	-3.10034000	-0.75497700
H	-0.41574500	-2.31367400	-1.50023000
C	0.18934200	-0.19401400	1.41348800
H	-0.07786500	0.72484600	1.99101800
C	1.42114700	0.06674700	0.54593900
C	2.32533400	-0.97611100	0.33156300
C	1.70647800	1.32998300	0.01551100
C	3.48199900	-0.76924800	-0.42323300
H	2.10748600	-1.93760100	0.78684900
C	2.86077100	1.54341400	-0.73634000

H	1.01844500	2.15561100	0.19332400
C	3.75162800	0.48954300	-0.96287800
H	4.17908000	-1.58883100	-0.58236500
H	3.07018400	2.52998200	-1.14341900
H	4.65345800	0.65379400	-1.54739900
O	**0.03067100**	**-1.31834300**	**1.95422900**

Table S6 Cartesien coordinates of imidazole-2-ylidene 1, IM-1

C	-1.22381900	-0.00223600	-0.18106900
C	-3.23440300	-0.33570500	0.76553000
C	-2.76899600	0.86795300	1.18657900
H	-4.15366600	-0.85712100	0.98106300
H	-3.20755300	1.60643600	1.83929300
N	-2.26794400	-0.86243100	-0.08364400
C	-2.36453600	-2.16379800	-0.73922400
H	-1.74894600	-2.90801100	-0.22578500
H	-3.40837600	-2.48301800	-0.71692300
H	-2.03559500	-2.07958800	-1.77597500
N	-1.53300300	1.05811100	0.59810400
C	-0.71757700	2.27377700	0.66530100
H	-0.31568600	2.40649100	-0.34793900
H	-1.35888000	3.10479300	0.96615300
H	0.09385600	2.14690600	1.38634000
C	-0.05016500	-0.01084900	-1.20824400
H	-0.18807700	-0.98435000	-1.76024800
C	1.29127100	-0.19131900	-0.43947000
C	2.33368900	0.68208700	-0.75031700
C	1.51164600	-1.20699800	0.49789600
C	3.57879700	0.54878100	-0.13155300
H	2.12686700	1.45138600	-1.48917900
C	2.75181800	-1.34176700	1.12395000
H	0.70896200	-1.90281700	0.74580500
C	3.79108900	-0.46135700	0.80919100
H	4.38623900	1.23286200	-0.38367400
H	2.90975300	-2.13224100	1.85444700
H	4.75912800	-0.56575900	1.29321300
O	**-0.16928500**	**1.08035700**	**-1.94490400**

Table S7 Cartesien coordinates of imidazole-2-ylidene 1, TS-2

C	1.28228600	-1.23427800	0.08909800
C	2.33213300	-2.99655200	-0.80916000
C	2.89947600	-2.75403200	0.40228700
H	2.54221800	-3.75213900	-1.54924500
H	3.69935300	-3.25803700	0.92183900
N	1.33057800	-2.05891800	-0.98609900
C	0.38662600	-2.02575400	-2.11121400
H	0.60876300	-1.17961500	-2.76666700
H	0.49709500	-2.95752800	-2.66873300
H	-0.62859600	-1.93167100	-1.70352600
N	2.24977700	-1.65982500	0.94142500
C	2.55468800	-1.03355200	2.22793500
H	3.52088200	-1.40853300	2.57032100
H	2.60108000	0.04868700	2.09776400
H	1.76731400	-1.26094700	2.94686000
C	0.30068300	-0.15460900	0.33039600
H	-0.84802200	-0.52042800	-0.23047600
C	0.75085700	1.21905600	-0.04213300
C	0.27401400	2.33048200	0.67740600
C	1.59883600	1.46400800	-1.14021900
C	0.62251500	3.62815900	0.30452000
H	-0.36225500	2.15483900	1.53769900
C	1.94257200	2.76284100	-1.51084200
H	2.00368100	0.63013700	-1.71095100
C	1.45594400	3.85708300	-0.79220600
H	0.23994200	4.46802000	0.88009600
H	2.59905100	2.91941800	-2.36382100
H	1.72494400	4.86957300	-1.08062900
O	-0.15275200	-0.26041900	1.69025900
H	-1.02820500	-0.69147200	1.56719400
O	-1.94882400	-1.18629600	-0.21250700
C	-3.13975500	-0.51416500	-0.55252400
C	-3.48475700	0.55077800	0.51076300
H	-2.69628600	1.31089200	0.56323900
H	-4.43244100	1.06092200	0.29375400
H	-3.57185800	0.08010000	1.49789500
C	-4.26203000	-1.56915300	-0.60352500
H	-5.23530300	-1.12829000	-0.85665900
H	-4.02278700	-2.33399500	-1.35169600
H	-4.34887700	-2.06764400	0.36875700
C	-3.00564600	0.16689600	-1.93191200
H	-2.19754100	0.90859600	-1.91502300
H	-2.76900000	-0.57906800	-2.70102100
H	**-3.92858100**	**0.68002600**	**-2.23222200**

Table S8 Cartesien coordinates of imidazole-2-ylidene 1, IM-2

C	1.23350100	0.06700600	0.09556000
C	2.76465000	-1.61396400	0.06013100
C	3.42622400	-0.46909100	-0.17955000
H	3.12537000	-2.62737900	0.14701000
H	4.47168400	-0.29419800	-0.38313700
N	1.40422700	-1.31723500	0.23067800
C	0.50886800	-2.15736000	1.00616900
H	-0.37517000	-2.45468900	0.43381900
H	1.05171500	-3.05188400	1.32042800
H	0.16275600	-1.61186500	1.89335900
N	2.51245800	0.59481300	-0.13637100

C	2.73462900	1.80833400	-0.91439300
H	3.78778700	2.09083400	-0.82776000
H	2.49226600	1.65287300	-1.97505700
H	2.10340400	2.60850700	-0.53032100
C	0.07272500	0.79592900	0.26953300
H	0.67920500	2.23397300	1.42269800
C	-1.29513000	0.35764700	0.04229200
C	-2.37204800	1.05122300	0.64195300
C	-1.62005600	-0.70647600	-0.83208700
C	-3.69032400	0.67173700	0.41388100
H	-2.15289300	1.89839900	1.28330900
C	-2.94254200	-1.08806300	-1.04695100
H	-0.82480100	-1.20453500	-1.38044600
C	-3.99064500	-0.40861800	-0.42221200
H	-4.49424100	1.22408800	0.89549100
H	-3.15586000	-1.90788800	-1.72941800
H	-5.02192800	-0.70303600	-0.59649600
O	**0.21935000**	**2.16924300**	**0.57004900**

Table S9 Cartesien coordinates of imidazole-2-ylidene 1, TS-3

C	-2.00822100	-0.17182000	0.08222600
C	-3.62976500	-0.35617600	1.62950900
C	-4.19078300	-0.56076000	0.41409700
H	-4.05629400	-0.35883500	2.62018500
H	-5.20925900	-0.77694200	0.13347600
N	-2.28273200	-0.11764800	1.41512500
C	-1.34106100	0.10001300	2.51414900
H	-1.74753600	0.86581600	3.18074200
H	-1.19650000	-0.83157400	3.06730000
H	-0.38911700	0.44456100	2.12116700
N	-3.18812400	-0.44085100	-0.53264200
C	-3.45240300	-0.59450800	-1.97349400
H	-4.53829500	-0.58300500	-2.09696000
H	-2.99299900	0.21851500	-2.52818600
H	-3.03666100	-1.53674900	-2.32659600
C	-0.66146100	-0.10894100	-0.59550500
H	-0.50610100	-1.57438700	-1.75976300
C	0.05321100	1.22219800	-0.45958900
C	1.21738800	1.41678100	-1.22443300
C	-0.40862300	2.30426900	0.30562400
C	1.91380400	2.61994300	-1.18142400
H	1.55885800	0.61330300	-1.86449600
C	0.28836600	3.51585200	0.34799800
H	-1.34454600	2.23275600	0.85310800
C	1.45956100	3.67737800	-0.38716300
H	2.81562100	2.73592000	-1.77721200
H	-0.10048200	4.33604700	0.94689800
H	2.00388100	4.61754600	-0.35676300
O	-0.79002200	-0.48417900	-1.90763600
C	0.18707800	-1.61547500	0.04767400
H	-0.29403900	-1.80545900	1.02656500
C	1.67214600	-1.38524100	0.25884000
C	2.56836300	-1.73366900	-0.76075000
C	2.19354000	-0.88366000	1.45800100
C	3.94133200	-1.55600900	-0.59764200
H	2.15789900	-2.16857100	-1.66643400
C	3.56733600	-0.70524900	1.62812800
H	1.52394800	-0.64738100	2.28274900
C	4.44755400	-1.03502900	0.59623900
H	4.62151500	-1.83404900	-1.39963700
H	3.95080700	-0.31679700	2.56883700
H	5.51847000	-0.90010100	0.72628500
O	**-0.12839800**	**-2.48088600**	**-0.91030600**

Table S10 Cartesien coordinates of imidazole-2-ylidene 1, IM-3

C	-2.01344800	-0.33669100	-0.03467900
C	-4.08682300	-0.91841000	0.61016600
C	-4.20044300	0.13906800	-0.22902000
H	-4.83439600	-1.49824500	1.12743100
H	-5.06795500	0.66728900	-0.59171200
N	-2.73379900	-1.20655600	0.72355300
C	-2.25305600	-2.33067800	1.53764200
H	-3.12058600	-2.93698500	1.80346600
H	-1.54900800	-2.91664400	0.94357400
H	-1.78122300	-1.96684400	2.45397700
N	-2.92345500	0.48488800	-0.61860300
C	-2.61968400	1.51687500	-1.61608600
H	-3.53704200	1.72993000	-2.16856800
H	-2.25846200	2.42336300	-1.12593400
H	-1.84429900	1.10225000	-2.26541200
C	-0.49292100	-0.25505600	-0.45984700
H	-0.30860600	-2.18659600	-1.34218500
C	0.03284900	1.12172700	0.00139200
C	0.79161700	1.87941800	-0.89493500
C	-0.19156200	1.62219600	1.28978400
C	1.32185800	3.11105600	-0.50985800
H	0.94652900	1.47583800	-1.89036900
C	0.33424800	2.85627000	1.67779200
H	-0.78608900	1.04937000	2.00085000
C	1.09502300	3.60462600	0.77722500
H	1.91401000	3.68843700	-1.21588800
H	0.14889800	3.23291900	2.68097800
H	1.50576200	4.56564800	1.07627100
O	-0.49578900	-0.47443500	-1.78700200
C	0.36266500	-1.41773200	0.21822100
H	0.12012600	-1.51593900	1.28303800
C	1.86091300	-1.19541200	0.10703400
C	2.51439600	-1.31898400	-1.12720200
C	2.62012700	-0.88495800	1.24017800

C	3.89194900	-1.12636500	-1.22024300
H	1.93021300	-1.55290200	-2.01001400
C	4.00007100	-0.69255200	1.15044500
H	2.12689600	-0.79236400	2.20592500
C	4.64083400	-0.81314800	-0.08268700
H	4.38484500	-1.22360100	-2.18469700
H	4.57270700	-0.45497100	2.04371200
H	5.71590900	-0.66916500	-0.15729300
O	**-0.04535300**	**-2.59264100**	**-0.46471500**

Table S11 Cartesien coordinates of imidazole-2-ylidene 1, TS-4

C	-2.13913500	-0.42389900	0.05078600
C	-4.19999200	-1.22561600	0.56420400
C	-4.36799100	-0.19724900	-0.30361600
H	-4.91720800	-1.87605800	1.04078200
H	-5.26112300	0.23040200	-0.73265300
N	-2.83188300	-1.35211000	0.76640300
C	-2.23732600	-2.38949200	1.60974500
H	-3.02335600	-3.08959000	1.90025000
H	-1.46719200	-2.91053100	1.03753600
H	-1.80647100	-1.94958900	2.51397000
N	-3.10056400	0.27407700	-0.60813000
C	-2.84436600	1.36789900	-1.54748200
H	-3.71760500	1.47754100	-2.19459100
H	-2.66991400	2.30323400	-1.00924600
H	-1.96575900	1.10921800	-2.13992400
C	-0.21052500	-0.14819800	-0.60150400
H	-0.18688600	-2.18581200	-1.39161500
C	0.07717400	1.24192100	-0.05192300
C	0.64528300	2.18183600	-0.91868400
C	-0.13633700	1.59844100	1.28573400
C	0.98803000	3.45534500	-0.46116300
H	0.81372500	1.89124700	-1.95072900
C	0.20498200	2.86941300	1.74603100
H	-0.59430500	0.88410400	1.96558400
C	0.76890900	3.80343700	0.87238400
H	1.43005800	4.17464100	-1.14620400
H	0.02716400	3.13404000	2.78550800
H	1.03402900	4.79483200	1.23079400
O	-0.29343600	-0.31307600	-1.85353700
C	0.51279500	-1.32120000	0.13434000
H	0.21745600	-1.35546400	1.18759500
C	2.02605200	-1.16002700	0.06811300
C	2.70680100	-1.28678300	-1.15055300
C	2.76309800	-0.88757800	1.22496100
C	4.09181600	-1.14219300	-1.20568400
H	2.14157900	-1.49113200	-2.05401000
C	4.15098200	-0.74176900	1.17327300
H	2.24671200	-0.79033200	2.17783300
C	4.81967200	-0.86944200	-0.04403300
H	4.60653700	-1.24293000	-2.15811600
H	4.70751700	-0.53402200	2.08383400
H	5.90035200	-0.76040900	-0.08872100
O	0.07997300	-2.51395200	-0.50088400

Table S12. Cartesien coordinates of phosphazole-2-ylidene 2

C	0.29181800	-1.07424800	0.30433700
C	-0.36256900	1.46966000	-0.06280400
C	0.94291900	1.17999200	-0.19911100
H	-0.76242600	2.47315500	-0.14815100
H	1.75851000	1.85847000	-0.43277200
C	-2.40396500	-0.61948300	-0.67267200
H	-3.30068100	0.00453200	-0.62283600
H	-2.00585600	-0.60539400	-1.68992600
H	-2.67996000	-1.64467300	-0.40965300
N	1.25878500	-0.20287800	0.00200300
C	2.65090400	-0.63010700	-0.18444600
H	3.01339800	-0.32802800	-1.17374100
H	3.29535800	-0.18331300	0.58099100
H	2.67069300	-1.71519000	-0.09420000
P	**-1.16767800**	**-0.02628700**	**0.59096300**

Table S13. Cartesien coordinates of phosphazole -2-ylidene 2, TS-1

C	0.99777400	0.09311000	0.03430600
C	3.37299000	0.02053700	-1.02936300
C	2.75472200	1.21394300	-1.06318000
H	4.34710500	-0.16396900	-1.46520500
H	3.11313100	2.14410800	-1.49140300
C	2.80132500	-1.86072900	1.20435400
H	3.61948300	-2.56095100	1.01372900
H	3.14357000	-1.06473300	1.86867400
H	1.98428400	-2.40704900	1.68363200
N	1.46081000	1.23002600	-0.46167400
C	0.70315000	2.49368700	-0.38462600
H	0.07230600	2.59944000	-1.27175300
H	0.09296200	2.45073800	0.52249000
H	1.40870100	3.32682700	-0.33582700
P	2.18003100	-1.20758800	-0.42938800
C	-0.46446200	0.11745200	1.41010100
O	-0.35905700	1.18673000	2.05796700
C	-1.68436000	-0.14633400	0.53811400
C	-1.88239300	-1.37526200	-0.10218700
C	-2.66506900	0.84295600	0.42793300
C	-3.02951600	-1.60468900	-0.85969600
H	-1.12929000	-2.15646200	-0.00791500
C	-3.81565000	0.61791500	-0.33045200

H	-2.51252700	1.77412000	0.96554800
C	-3.99966200	-0.60442800	-0.97934000
H	-3.17136000	-2.56254800	-1.35447200
H	-4.57439500	1.39329900	-0.40727500
H	-4.89645600	-0.78256400	-1.56745900
H	-0.08428400	-0.82939600	1.86025600

Table S14. Cartesien coordinates of phosphazole -2-ylidene 2, IM-1

C	0.97923700	-0.18339700	-0.00425100
C	3.12987500	1.13223800	-0.62215400
C	2.14105200	1.85785500	-0.06744300
H	4.05214000	1.56794900	-0.98536200
H	2.17942700	2.92863200	0.11773900
C	3.49874600	-1.48406700	0.54845600
H	4.55669700	-1.59034100	0.28459500
H	3.41621100	-0.94690500	1.49715100
H	3.07251500	-2.48545600	0.66354900
N	0.93666100	1.23573100	0.25748000
C	0.14972000	1.76398300	1.36998700
H	0.21122900	2.85573700	1.34184800
H	-0.89652700	1.47799800	1.26782900
H	0.51708000	1.41487900	2.34479100
P	2.62959300	-0.60070300	-0.85751700
C	-0.22064300	-1.02203800	-0.23405000
O	0.50700500	-1.07677800	1.01720600
C	-1.64321200	-0.56067800	-0.20504500
C	-2.22330500	-0.02714900	-1.36319300
C	-2.42747600	-0.71690300	0.94447700
C	-3.56516500	0.35438700	-1.36755500
H	-1.62046700	0.09286700	-2.26016500
C	-3.76979400	-0.33539400	0.93842700
H	-1.97311700	-1.13071100	1.83978600
C	-4.34170800	0.20170700	-0.21676400
H	-4.00375800	0.77357100	-2.26928500
H	-4.37008800	-0.46064200	1.83585700
H	-5.38702000	0.49881800	-0.22108400
H	-0.05485400	-1.90499600	-0.85986800

Table S15. Cartesien coordinates of phosphazole -2-ylidene 2, TS-2

C	-1.33045400	-0.68171900	0.25412800
C	-3.24048100	-2.31790700	0.61055200
C	-3.09949800	-1.38698600	1.57227700
H	-3.98065200	-3.10694600	0.65597200
H	-3.67857900	-1.26985300	2.48125800
C	-2.54361300	-1.71044300	-2.20052300
H	-2.98099100	-2.59288400	-2.67625000
H	-3.30209700	-0.92972200	-2.10995700
H	-1.69841700	-1.35207600	-2.79023100
N	-2.04110400	-0.47024700	1.37272800
C	-1.74934300	0.58215300	2.35255500
H	-2.32325900	0.38388100	3.25891400
H	-0.68352100	0.57610800	2.59071300
H	-2.01705400	1.56229800	1.95139800
P	-1.84532500	-2.22724200	-0.54722900
C	-0.13876200	0.03801300	-0.20790700
O	0.24341900	-0.50442200	-1.46105200
C	-0.23898300	1.55711300	-0.23193400
C	0.69106400	2.34490200	0.45558400
C	-1.23656200	2.19297100	-0.98526200
C	0.62260300	3.73884200	0.40138600
H	1.47791800	1.86093000	1.02810000
C	-1.30847700	3.58467800	-1.03971800
H	-1.95067100	1.59117000	-1.54197700
C	-0.37902400	4.36216700	-0.34380100
H	1.35520400	4.33595000	0.93807100
H	-2.08693200	4.06329000	-1.62850500
H	-0.43327900	5.44670900	-0.38756500
H	0.75549500	-0.28852600	0.45454800
H	1.13793100	-0.93221100	-1.17194900
O	2.05143800	-1.30493900	0.06038000
C	3.41481000	-1.03701500	0.12483800
C	3.80587100	-0.66545500	1.57386700
H	3.29533400	0.25788300	1.87942900
H	3.49133000	-1.46331600	2.25649800
H	4.88624600	-0.50918400	1.69392300
C	3.82136500	0.10867000	-0.83063200
H	4.89956100	0.31624400	-0.80028200
H	3.55312400	-0.14859300	-1.86247500
H	3.29025500	1.03233200	-0.57021200
C	4.17014500	-2.32634100	-0.28481800
H	3.89590500	-2.60723300	-1.30821000
H	5.26091800	-2.20363900	-0.23839800
H	**3.88101300**	**-3.14923000**	**0.37835500**

Table S16. Cartesien coordinates of phosphazole -2-ylidene 2, IM-2

C	0.99628400	-0.02273600	-0.23030100
C	3.41698700	0.81139800	-0.15312600
C	2.47274300	1.77147200	-0.16588200
H	4.47899300	1.01828600	-0.16980800
H	2.66186600	2.84095200	-0.19132700
C	2.70796500	-1.41515200	1.57953700
H	3.70719700	-1.80147900	1.80821200
H	2.46296200	-0.60758300	2.27522000
H	1.98777500	-2.23121900	1.70016300
N	1.13207300	1.38824400	-0.16494400
C	0.15015900	2.28729700	-0.76507500

H	0.59928600	3.27750000	-0.87208300
H	-0.15130900	1.92472000	-1.75743700
H	-0.74900600	2.37766100	-0.15152400
P	2.66665900	-0.84153900	-0.20935700
C	-0.14657300	-0.75340300	-0.34700100
O	-0.06043300	-2.10044500	-0.66976800
C	-1.54039800	-0.35487600	-0.08591100
C	-2.58841600	-0.92489400	-0.83279100
C	-1.86792000	0.52062200	0.96546600
C	-3.91370600	-0.59383600	-0.56439000
H	-2.34796700	-1.62912300	-1.62213100
C	-3.19667600	0.84874500	1.23275800
H	-1.07440800	0.91518200	1.59381400
C	-4.22495900	0.29853900	0.46556900
H	-4.70889100	-1.03600400	-1.15914400
H	-3.42903100	1.52206500	2.05385700
H	-5.26054000	0.55169400	0.67624600
H	**0.78920500**	**-2.25276900**	**-1.12407400**

Table S17. Cartesien coordinates of phosphazole -2-ylidene 2, TS-3

C	-1.79348200	-0.15518300	0.20768000
C	-4.22777200	-0.64732800	0.74919700
C	-3.42819900	-0.48287700	1.81851200
H	-5.27597400	-0.90721900	0.83403000
H	-3.68034000	-0.56412300	2.87055300
C	-3.73135400	0.74672900	-1.81730600
H	-4.68466300	0.50299100	-2.29477000
H	-3.83538000	1.66504200	-1.23617300
H	-2.94830400	0.86074800	-2.56722100
N	-2.06971900	-0.19777800	1.51760500
C	-1.10969700	-0.10154500	2.62280500
H	-1.46907400	0.63284900	3.34997900
H	-1.01769300	-1.07681900	3.11105000
H	-0.14075700	0.21302500	2.24617500
P	-3.22073300	-0.70298000	-0.76272300
C	-0.55248400	0.02535900	-0.57989300
O	-0.84152300	-0.16640200	-1.87280600
C	0.30775900	1.24926000	-0.31379200
C	1.38999100	1.47886100	-1.17913400
C	0.01624200	2.22983000	0.64457400
C	2.18825900	2.61002600	-1.04448000
H	1.57995300	0.76525400	-1.97093500
C	0.81238600	3.37205300	0.77715800
H	-0.86629700	2.14205300	1.27126200
C	1.91064900	3.56094600	-0.05758200
H	3.02707600	2.75668200	-1.72010500
H	0.55725100	4.11921800	1.52485300
H	2.53258600	4.44642400	0.04382300
H	-0.41258000	-1.57806800	-1.85856600
C	0.33766000	-1.63254400	-0.13973300
H	-0.15454600	-1.99253300	0.77482700
O	-0.01076200	-2.33255700	-1.24761900
C	1.80702900	-1.45537100	0.07478800
C	2.69928100	-1.60849500	-0.99833600
C	2.33542400	-1.17181500	1.34352900
C	4.07168900	-1.45754100	-0.81107100
H	2.29418900	-1.87290400	-1.96950200
C	3.70781700	-1.01786100	1.53302500
H	1.66927600	-1.09412500	2.19993500
C	4.58304700	-1.15456700	0.45347100
H	4.74744500	-1.58530200	-1.65335000
H	4.09579100	-0.80125800	2.52538000
H	5.65386900	-1.03872000	0.59929100

Table S18. Cartesien coordinates of phosphazole -2-ylidene 2, IM-3

C	-1.72495300	-0.32858100	0.40512200
C	-4.17231500	-0.77532200	0.13740000
C	-3.80385300	-0.35379300	1.37024700
H	-5.19710000	-1.04518900	-0.09244900
H	-4.40806500	-0.24015800	2.26335400
C	-3.06618900	-0.28336400	-2.51196000
H	-4.10103600	-0.52094800	-2.77807500
H	-2.94631500	0.80052000	-2.45725200
H	-2.37505500	-0.68670400	-3.25125900
N	-2.42163100	-0.07322800	1.50875600
C	-1.85720400	0.30661100	2.80594800
H	-1.06413300	1.03824400	2.65269900
H	-2.64703200	0.75587800	3.41144500
H	-1.45868400	-0.57190300	3.32255900
P	-2.68466600	-1.06570900	-0.87564700
C	-0.29478900	-0.26903600	-0.13509900
O	-0.53271600	-0.76165900	-1.40868500
C	0.17062600	1.20257400	-0.12795500
C	-0.05194800	1.98219200	-1.26867500
C	0.79062700	1.79803100	0.98024300
C	0.31421500	3.32784900	-1.29587000
H	-0.48630800	1.49795900	-2.13587400
C	1.15947300	3.14467600	0.95388900
H	1.03152300	1.20540400	1.85820800
C	0.91510500	3.91742800	-0.18197500
H	0.13796600	3.91591000	-2.19331100
H	1.65127200	3.58423200	1.81804600
H	1.20451900	4.96479500	-0.20376400
H	-0.10803600	-2.48371900	-0.56405900
C	0.66306400	-1.25498500	0.64107000
H	0.57240400	-1.10349000	1.72478700
O	0.17955600	-2.56100700	0.37393300
C	2.13201000	-1.11400700	0.26416400
C	2.54435200	-1.08294700	-1.07705900

C	3.10674200	-1.07281400	1.26708400
C	3.89908800	-1.00632900	-1.39626100
H	1.78939700	-1.10308000	-1.85668000
C	4.46467900	-0.99942100	0.94914800
H	2.80081900	-1.10826000	2.31150600
C	4.86453400	-0.96570900	-0.38647800
H	4.20426000	-0.97775300	-2.43955900
H	5.20658600	-0.97163000	1.74352500
H	**5.92011100**	**-0.90887600**	**-0.64028700**

Table S19. Cartesien coordinates of phosphazole -2-ylidene 2, TS-4

C	-1.83754800	-0.43751400	0.35124500
C	-4.35404900	-1.04925900	0.30626600
C	-3.89714900	-0.59734800	1.48821200
H	-5.37656800	-1.36837100	0.14497100
H	-4.43449400	-0.48418300	2.42420100
C	-3.19587900	-0.21871100	-2.30127800
H	-3.98301500	-0.66408300	-2.91660500
H	-3.46875000	0.80553600	-2.03909000
H	-2.24838100	-0.22883100	-2.84148100
N	-2.51170900	-0.25638500	1.48084700
C	-1.89764900	0.23894900	2.72005600
H	-0.99806100	0.79635300	2.46616400
H	-2.60181900	0.90151900	3.23087200
H	-1.64629300	-0.59884200	3.37799600
P	-2.94614100	-1.29313000	-0.80295700
C	0.00148300	-0.20661500	-0.48458900
O	-0.20722600	-0.62881600	-1.66303300
C	0.21118600	1.28576100	-0.27624900
C	-0.17337200	2.15719300	-1.30343400
C	0.79622200	1.82857200	0.87712000
C	-0.01215700	3.53533900	-1.17010700
H	-0.58208300	1.72723800	-2.21167000
C	0.96348200	3.20821100	1.01129400
H	1.15797100	1.17519500	1.66545800
C	0.55225500	4.06780100	-0.00855700
H	-0.31774400	4.19593700	-1.97791600
H	1.42866500	3.60946500	1.90826600
H	0.68416800	5.14171900	0.09485300
H	0.08436600	-2.40302700	-0.86210700
C	0.80472900	-1.20202000	0.40849000
H	0.59237300	-1.04092200	1.47100800
O	0.34386300	-2.50194400	0.08042100
C	2.31233800	-1.07502000	0.19708100
C	2.87240500	-1.03437700	-1.08856200
C	3.17072700	-1.04477500	1.30214800
C	4.25432000	-0.96059200	-1.25666800
H	2.21373500	-1.04795100	-1.95113800
C	4.55538900	-0.97255700	1.13690700
H	2.75106100	-1.08909200	2.30578400
C	5.10154800	-0.92943400	-0.14586100
H	4.67250600	-0.92515300	-2.25969900
H	5.20487100	-0.95365900	2.00872600
H	6.17877600	-0.87275300	-0.28036500

Table S20. Cartesien coordinates of oxazole-2-ylidene 3

C	-0.08993000	-1.19253000	-0.00010400
C	-0.21228700	1.09912600	0.00007100
C	-1.46432400	0.61239100	-0.00009300
H	0.16382100	2.11063200	0.00019700
H	-2.44209500	1.06781100	-0.00015200
N	0.61457600	-0.03096500	0.00006200
C	2.06804100	0.00253600	0.00019600
H	2.44389300	0.51470600	-0.89175400
H	2.44373200	0.51457100	0.89229300
H	2.41540200	-1.03108800	0.00014900
O	-1.39197400	-0.76112700	-0.00019900

Table S21. Cartesien coordinates of oxazole-2-ylidene 3, TS-1

C	1.32787900	-0.28425500	0.23632200
C	3.31331100	-0.30177000	-0.80584700
C	3.15432500	-1.48276300	-0.18388100
H	4.11776500	0.08934500	-1.40869900
H	3.75336500	-2.37352100	-0.09019000
N	2.15899900	0.43528100	-0.52296400
C	1.87418900	1.80360500	-0.96874100
H	1.16888500	2.22368700	-0.24247500
H	2.80723900	2.37164600	-0.97681200
H	1.44371400	1.78572000	-1.97358000
O	1.93336300	-1.46632300	0.45827900
C	-0.02075900	0.45851000	1.29798300
H	0.15155400	-0.26635500	2.13040000
C	-1.29353000	0.08360100	0.53525900
C	-2.08427700	1.10323700	0.00289800
C	-1.70878500	-1.24601500	0.40033900
C	-3.26773300	0.79917400	-0.67345400
H	-1.75731200	2.12835000	0.15013600
C	-2.88945100	-1.55404000	-0.27444900
H	-1.10169000	-2.04349200	0.82721400
C	-3.67170900	-0.52954900	-0.81675500
H	-3.87984200	1.59966000	-1.08273200
H	-3.20422500	-2.59020700	-0.37417900
H	-4.59481700	-0.76753300	-1.33951700
O	0.26433800	1.67848800	1.48461300

Table S22. Cartesien coordinates of oxazole-2-ylidene 3, IM-1

C	1.38256000	0.24980000	-0.35711400
C	3.09470200	0.04205900	1.04653800
C	3.48350000	0.81383400	0.01785500
H	3.62640200	-0.30190600	1.91960500
H	4.39764400	1.31597400	-0.24928500
N	1.76071500	-0.28941700	0.81719800
C	0.98341200	-1.30469600	1.52783500
H	0.66052000	-2.02532900	0.77017400
H	1.62401000	-1.76990600	2.27873100
H	0.11419600	-0.85149400	2.00845200
O	2.41113200	0.95987600	-0.84227000
C	0.20408600	-0.13903900	-1.22975800
H	0.24353800	0.56401900	-2.09886800
C	-1.15779500	0.08710400	-0.54506600
C	-2.04109200	-0.99018800	-0.46969900
C	-1.55168800	1.33416600	-0.04660600
C	-3.30569500	-0.82754700	0.10061600
H	-1.70447500	-1.94200200	-0.87113900
C	-2.81058900	1.49821300	0.53294200
H	-0.87217600	2.18363800	-0.11431500
C	-3.69204700	0.41539600	0.60647900
H	-3.99097500	-1.67061300	0.15087400
H	-3.10716600	2.46940400	0.92217400
H	-4.67493900	0.54310700	1.05322300
O	0.56665300	-1.40532500	-1.48199800

Table S23. Cartesien coordinates of oxazole-2-ylidene 3, TS-2

C	-0.41632600	-1.67793800	-0.08167400
C	0.11984000	-3.77840800	0.39849500
C	-1.03641700	-3.48707100	1.01654500
H	0.70694700	-4.68260100	0.37650000
H	-1.71407600	-4.03097000	1.65244400
N	0.51242900	-2.63092800	-0.29070300
C	1.79008300	-2.46636800	-1.00277800
H	2.41007900	-3.33212900	-0.76199500
H	1.60745600	-2.41821400	-2.07650300
H	2.26149300	-1.53137500	-0.66262600
O	-1.37359400	-2.18495800	0.71525500
C	-0.35976100	-0.28582800	-0.49481700
H	0.63671600	0.15841400	0.09007500
C	-1.59580300	0.53936500	-0.23933700
C	-2.27470500	1.13330700	-1.31025900
C	-2.05506900	0.77141400	1.06569900
C	-3.40024400	1.92563400	-1.08184700
H	-1.90022600	0.97219800	-2.31520300
C	-3.18361500	1.55837700	1.29226300
H	-1.52234600	0.34072800	1.91011600
C	-3.86244500	2.13786600	0.21810100
H	-3.91700100	2.37994200	-1.92366100
H	-3.52523700	1.72933400	2.31006200
H	-4.73800900	2.75715700	0.39463600
O	0.15098800	-0.19867600	-1.81869600
H	1.02416400	0.24911600	-1.64465100
O	2.04759500	0.42408600	-0.18486000
C	2.69425100	1.55771100	0.33187700
C	4.08252200	1.65802500	-0.33399400
H	4.65231600	2.52592700	0.02303900
H	4.66527900	0.75318200	-0.12463900
H	3.96981300	1.74223200	-1.42121700
C	1.88254300	2.83318200	0.02312100
H	0.88513700	2.77103800	0.47505600
H	2.37286400	3.73798000	0.40545200
H	1.75470900	2.94582500	-1.06019700
C	2.86267600	1.40603000	1.85885800
H	3.41213900	2.24527100	2.30518100
H	1.88045900	1.34800000	2.34477600
H	3.40522800	0.48004100	2.08316900

Table S24. Cartesien coordinates of oxazole-2-ylidene 3, IM-2

C	1.26149600	-0.08728100	-0.09342200
C	3.36435500	-0.88855900	-0.16717400
C	2.52307400	-1.91901100	-0.28684400
H	4.44333700	-0.86203800	-0.16668600
H	2.65354300	-2.97858500	-0.42977400
N	2.60921300	0.28938200	-0.07503900
C	3.12905500	1.49520900	0.55433100
H	4.19497200	1.56936800	0.32283900
H	2.60855700	2.36628100	0.16148600
H	3.00598800	1.46849600	1.64720100
O	1.21482000	-1.45897900	-0.25097000
C	0.13850000	0.68381400	-0.05221800
C	-1.24950100	0.22667300	-0.01857100
C	-2.27455200	1.13976200	-0.35243900
C	-1.63935900	-1.07253300	0.37886400
C	-3.61761200	0.77388300	-0.29162300
H	-2.00553000	2.13488600	-0.69230800
C	-2.98275100	-1.42982000	0.43237600
H	-0.88450400	-1.79965900	0.65164700
C	-3.98515800	-0.51306900	0.10142400
H	-4.38018400	1.50029200	-0.56284100
H	-3.25047800	-2.43665100	0.74448500
H	-5.03232300	-0.79933600	0.14763300
O	0.35271800	2.06811500	-0.13673100
H	-0.16345300	2.48376100	0.57496600

Table S25. Cartesien coordinates of oxazole-2-ylidene 3, TS-3

C	-2.02316800	0.25834000	0.24425200
C	-4.00052800	-0.18273200	1.15933300
C	-3.23217800	0.40879100	2.08757000
H	-5.01514800	-0.54518800	1.20075200
H	-3.37115000	0.70246200	3.11426300
N	-3.23437100	-0.27269600	-0.00369000
C	-3.69670900	-0.92175600	-1.24528600
H	-4.72626500	-1.24374800	-1.07472100
H	-3.63437400	-0.21351500	-2.06735200
H	-3.05444500	-1.77637000	-1.46044800
O	-2.00780800	0.68327800	1.51811000
C	-0.86045900	0.26643200	-0.65728400
C	0.21019200	1.30031200	-0.35576800
C	0.71042000	2.01806800	-1.45057000
C	0.73002100	1.57424300	0.91830000
C	1.69665400	2.98849700	-1.27912200
H	0.30159000	1.79350300	-2.42924400
C	1.71337200	2.54910000	1.08935100
H	0.38532400	1.02154300	1.78448300
C	2.20068200	3.26221800	-0.00673000
H	2.06961300	3.53449300	-2.14241100
H	2.10643000	2.74336400	2.08432900
H	2.96894200	4.01912600	0.12991900
O	-1.23132300	0.14563300	-1.92796300
H	-0.89560000	-1.21936200	-2.00933900
C	-0.25105600	-1.54361600	-0.26668200
H	-0.85654100	-1.88689300	0.58624500
O	-0.61892600	-2.09300100	-1.45144900
C	1.20144400	-1.58056400	0.06097300
C	1.63373800	-1.65727600	1.39271000
C	2.16469800	-1.55574500	-0.95901500
C	2.99276000	-1.69852200	1.70291600
H	0.89538400	-1.70044200	2.19204200
C	3.52221400	-1.59512900	-0.65055900
H	1.83023700	-1.52373200	-1.99082100
C	3.94302900	-1.66426900	0.68074500
H	3.30983900	-1.76599600	2.74082400
H	4.25733600	-1.57670500	-1.45143200
H	5.00313100	-1.69929900	0.91835300

Table S26. Cartesien coordinates of oxazole-2-ylidene 3, IM-3

C	-1.98642300	-0.48271100	0.19851800
C	-4.18334900	-0.70084700	0.44932900
C	-3.60027800	-0.90880200	1.64193000
H	-5.21688200	-0.71969400	0.14225400
H	-3.95523700	-1.15861400	2.62770800
N	-3.14957700	-0.43570500	-0.45121500
C	-3.33469800	-0.11936500	-1.87667400
H	-3.69485000	0.90852900	-1.97031400
H	-2.34347500	-0.24475000	-2.32966900
H	-4.06943800	-0.81350200	-2.29104600
O	-2.24150400	-0.76917300	1.48081000
C	-0.55051000	-0.32691600	-0.39110300
C	-0.14507500	1.14193900	-0.12367600
C	0.21421800	1.92527800	-1.22311900
C	-0.12495700	1.71218000	1.15654300
C	0.59678400	3.25605400	-1.04853600
H	0.19278500	1.45450600	-2.20032400
C	0.25478800	3.04346700	1.33180700
H	-0.40006700	1.11865900	2.02567300
C	0.61646500	3.81998600	0.22851500
H	0.88179000	3.85404400	-1.91094600
H	0.27180800	3.47360000	2.33033300
H	0.91396800	4.85657600	0.36542000
O	-0.58687800	-0.69349700	-1.68006500
H	-0.30658700	-2.38019800	-1.02977600
C	0.33941100	-1.38496400	0.41421400
H	0.10688200	-1.35884100	1.48490800
O	-0.08679500	-2.63610700	-0.09545000
C	1.82872800	-1.15144100	0.24046300
C	2.63150500	-0.87307800	1.35183900
C	2.43454100	-1.23820300	-1.02204400
C	4.00810600	-0.68174000	1.21557500
H	2.17590600	-0.81225900	2.33842900
C	3.80784200	-1.04524100	-1.16114500
H	1.81344000	-1.43576000	-1.88878200
C	4.60079600	-0.76818300	-0.04387100
H	4.61518100	-0.47116000	2.09278300
H	4.26326600	-1.11194000	-2.14641000
H	5.67259800	-0.62352300	-0.15547900

Table S27. Cartesien coordinates of oxazole-2-ylidene 3, TS-4

C	2.11368000	-0.48246900	-0.26394400
C	4.29815600	-0.97556100	-0.42826400
C	3.74047300	-1.12758900	-1.64070200
H	5.30977400	-1.11318400	-0.08016500
H	4.10651400	-1.42687900	-2.60894500
N	3.25878500	-0.57076200	0.41852900
C	3.40905200	-0.26003700	1.84468000
H	3.97469500	0.66901000	1.95830200
H	2.40427300	-0.16162500	2.26139600
H	3.94485200	-1.07826600	2.33279600
O	2.40073600	-0.81989400	-1.53444700
C	0.33446100	-0.21439000	0.53705600
C	0.08391200	1.24597600	0.18726100
C	-0.14157800	2.14353300	1.23526900

C	0.04413700	1.71802900	-1.13192800
C	-0.39949000	3.49007800	0.97374400
H	-0.11757700	1.75915400	2.24966700
C	-0.21304900	3.06263300	-1.39516500
H	0.22500900	1.03626900	-1.95895200
C	-0.43562800	3.95393900	-0.34193600
H	-0.57677300	4.17665900	1.79800800
H	-0.24088200	3.41617300	-2.42290800
H	-0.63822500	5.00186900	-0.54803400
O	0.45486700	-0.53450700	1.76274400
H	0.24422700	-2.33267600	1.11766700
C	-0.41633800	-1.29635800	-0.31181600
H	-0.13722700	-1.23277700	-1.36832000
O	0.03430600	-2.54725400	0.18016400
C	-1.92725600	-1.13623900	-0.20213100
C	-2.69730900	-0.90558600	-1.34669400
C	-2.57673300	-1.23688100	1.03668700
C	-4.08543500	-0.77641500	-1.26463900
H	-2.20645000	-0.83267100	-2.31518400
C	-3.96174800	-1.10822000	1.12219600
H	-1.98604400	-1.40177700	1.93213900
C	-4.72199600	-0.87815900	-0.02792500
H	-4.66707200	-0.60140300	-2.16641200
H	-4.45120200	-1.18639000	2.08998900
H	-5.80252900	-0.78060800	0.04106700

Table S28. Cartesien coordinates of thiazole-2-ylidene 4

C	0.09789300	-1.16777300	0.00000000
C	0.32780000	1.19998900	0.00000000
C	-1.02058500	1.15658200	-0.00000200
H	0.96618300	2.07505100	0.00000600
H	-1.70364400	1.99466000	0.00000100
S	-1.51936300	-0.52366100	0.00000000
N	0.90121600	-0.07949600	0.00000000
C	2.35873900	-0.23612400	0.00000000
H	2.79277000	0.22692500	-0.89241000
H	2.79276000	0.22679300	0.89248300
H	2.57015000	-1.30442900	-0.00007700

Table S29. Cartesien coordinates of thiazole-2-ylidene 4, TS-1

C	-1.19557500	0.01638000	-0.33517800
C	-2.88118900	1.29612900	0.61515000
C	-3.40225500	0.06150100	0.79984600
H	-3.29573500	2.25650200	0.89824300
H	-4.34522500	-0.17428700	1.27354300
S	-2.34064700	-1.17147000	0.16947900
N	-1.64092100	1.24221300	-0.02301400
C	-0.88497500	2.45817100	-0.34643700
H	-0.91604300	3.14052300	0.50661200
H	0.14878900	2.18113200	-0.54902300
H	-1.31942600	2.94885400	-1.22265500
C	0.17446900	-0.96275400	-1.13457300
H	0.08374000	-0.50620000	-2.15182000
O	-0.18558200	-2.16420000	-0.95305300
C	1.43565500	-0.44454300	-0.44608200
C	2.19343800	0.59605200	-0.99333400
C	1.87470700	-1.06206400	0.72967900
C	3.35809300	1.03848300	-0.35964000
H	1.88305000	1.04479700	-1.93705000
C	3.03300000	-0.62107400	1.36711600
H	1.29882400	-1.90163900	1.10820600
C	3.77598600	0.43433200	0.82741500
H	3.94514400	1.84160300	-0.79905800
H	3.36666300	-1.10556900	2.28178700
H	4.68354200	0.77223500	1.32130200

Table S30. Cartesien coordinates of thiazole-2-ylidene 4, IM-1

C	1.17222700	0.01457200	0.35329100
C	2.74281300	1.24805800	-0.75858400
C	3.25515700	0.00453900	-0.91306700
H	3.12865000	2.19676200	-1.11245700
H	4.16922500	-0.24399500	-1.43499500
S	2.25504900	-1.21741800	-0.12676400
N	1.55288400	1.23954400	-0.02832200
C	0.79548200	2.45533900	0.28634500
H	1.36206600	3.31846300	-0.06551500
H	-0.18103600	2.42401800	-0.20034200
H	0.65398100	2.52901500	1.36747700
C	0.02182300	-0.64972600	1.14673600
H	0.01095100	-0.11751800	2.13888200
O	0.35096200	-1.93869700	1.16822700
C	-1.32525000	-0.31223000	0.45814800
C	-2.12693400	0.76356500	0.85255700
C	-1.77020300	-1.15110300	-0.56874200
C	-3.34248800	1.01947200	0.21048300
H	-1.81638100	1.39026500	1.68805600
C	-2.97824900	-0.89560400	-1.21541100
H	-1.16226400	-2.01752200	-0.81137400
C	-3.76634400	0.19442700	-0.83211700
H	-3.96311600	1.85140400	0.53534300
H	-3.31564900	-1.55437800	-2.01218700
H	-4.71329600	0.38709900	-1.33004900

Table S31. Cartesien coordinates of thiazole-2-ylidene 4, TS-2

C	1.30368400	-0.99934900	-0.05244700
C	2.93940100	-2.15499100	1.08145400

C	2.79767000	-2.96983100	0.01583900
H	3.60521400	-2.27103900	1.92621700
H	3.32957100	-3.89052200	-0.17512900
S	1.58255300	-2.36097700	-1.08494200
N	2.09409200	-1.04840100	1.04392500
C	2.03884900	-0.06145200	2.12743200
H	2.64820400	-0.42751900	2.95484800
H	2.41599700	0.90425900	1.78597600
H	1.00610300	0.05683200	2.46234600
C	0.23203600	-0.07153200	-0.39998300
H	-0.75037700	-0.36870700	0.23086900
O	-0.22950900	-0.43716800	-1.69290000
C	0.56065900	1.40692700	-0.28309400
C	-0.08387300	2.21967400	0.65624800
C	1.49232900	1.98872900	-1.15558800
C	0.20695800	3.58398100	0.73702600
H	-0.82468900	1.78227800	1.32053900
C	1.78240800	3.35019600	-1.07868700
H	1.97303000	1.36984300	-1.90866200
C	1.14257100	4.15127000	-0.12830400
H	-0.30507700	4.20256900	1.46948400
H	2.50504600	3.78857900	-1.76226400
H	1.36757700	5.21293700	-0.06958300
H	-1.15264700	-0.77729100	-1.43679600
O	-2.05500300	-1.11451700	-0.06346200
C	-3.32947800	-0.59629200	0.17034700
C	-4.35653900	-1.65867400	-0.28738500
H	-4.18957800	-2.59373700	0.25912200
H	-5.39364200	-1.33628300	-0.12257100
H	-4.22387400	-1.86600100	-1.35556300
C	-3.57073300	0.71114000	-0.61797600
H	-4.58162400	1.11175000	-0.46301300
H	-2.85129400	1.48210800	-0.31624200
H	-3.43627000	0.53338900	-1.69179800
C	-3.51939300	-0.33088900	1.68141000
H	-2.81605900	0.44008400	2.02486800
H	-4.53455100	0.00885900	1.92644500
H	-3.31374000	-1.24790700	2.24564300

Table S32. Cartesien coordinates of thiazole-2-ylidene 4, IM-2

C	-1.19503200	-0.21672400	0.00162600
C	-2.81831100	1.45250000	0.00939200
C	-3.61559600	0.41033300	-0.26544900
H	-3.11978800	2.48822800	0.10477200
H	-4.68063600	0.43233900	-0.44366800
S	-2.71743200	-1.11216700	-0.29939600
N	-1.46576400	1.14578200	0.19537200
C	-0.64349400	1.96967600	1.07760500
H	-1.22497100	2.84240100	1.38347100
H	-0.36032600	1.39793200	1.96973300
H	0.27336800	2.30807000	0.58673200
C	-0.00527900	-0.87631400	0.05434800
O	-0.13530700	-2.26519400	0.16088800
C	1.35601700	-0.34740700	-0.02111500
C	1.67985700	0.79435100	-0.78607300
C	2.41490000	-1.04796000	0.59660900
C	2.99674400	1.23628600	-0.89031500
H	0.89357800	1.30705400	-1.33298200
C	3.73003300	-0.60514100	0.48209400
H	2.18666800	-1.93335000	1.18262100
C	4.03047700	0.54350000	-0.25481700
H	3.21980900	2.11510100	-1.49040400
H	4.52544800	-1.15684300	0.97715600
H	5.05724600	0.88775600	-0.34210500
H	0.46941200	-2.67153800	-0.48313400

Table S33. Cartesien coordinates of thiazole-2-ylidene 4, TS-3

C	-0.02343800	1.24569500	-0.37349800
C	-1.54853500	1.69890300	-2.04057200
C	-1.87103300	2.68850900	-1.18508000
H	-1.99136200	1.47753400	-3.00278500
H	-2.64162000	3.43426500	-1.31700600
S	-0.85724100	2.64224700	0.23933200
N	-0.50289000	0.89154600	-1.59276800
C	0.01683300	-0.18996100	-2.43701400
H	-0.33290200	-0.01996600	-3.45665100
H	1.10548500	-0.18288700	-2.42449400
H	-0.35214800	-1.15536900	-2.08441200
C	0.95037900	0.72373600	0.58072400
O	1.12251200	1.59831600	1.55849600
C	2.18421400	-0.04303400	0.15402700
C	2.19183600	-1.34244600	-0.37386300
C	3.41958300	0.58796600	0.37656100
C	3.39118400	-1.97867300	-0.70209600
H	1.25777400	-1.87381600	-0.52006900
C	4.61699200	-0.04536400	0.04973500
H	3.41366700	1.57509600	0.82526800
C	4.60940100	-1.33104200	-0.49631600
H	3.37067200	-2.98865700	-1.10418500
H	5.56039300	0.46505000	0.22698800
H	5.54311100	-1.82779000	-0.74652100
H	0.25333100	0.94918100	2.52676200
C	-0.27834100	-0.61574500	1.63704700
H	0.54196300	-1.33485100	1.75885300
O	-0.50100600	0.21662500	2.65691300
C	-1.47283200	-1.15934900	0.96069300
C	-2.70529000	-0.48223800	1.01865500
C	-1.41770300	-2.38154500	0.26461400
C	-3.82646300	-0.98943000	0.36546100

H	-2.76564200	0.43052600	1.60129700
C	-2.54104000	-2.88861400	-0.38705700
H	-0.49187000	-2.95289400	0.26338300
C	-3.75059600	-2.18937300	-0.34779100
H	-4.77043100	-0.45287500	0.42359600
H	-2.47792400	-3.83979100	-0.91009000
H	-4.62936600	-2.58704000	-0.84851600

Table S34. Cartesien coordinates of thiazole-2-ylidene 4, IM-3

C	0.10263100	-1.27466100	0.21211700
C	-0.93898100	-2.33546000	1.95430800
C	-0.77610500	-3.38142400	1.11329700
H	-1.38625300	-2.31891000	2.94022800
H	-1.07531300	-4.40404600	1.29748400
S	0.04044400	-2.89413600	-0.35623400
N	-0.43156300	-1.14486100	1.43454600
C	-0.52433200	0.10315400	2.20758800
H	-0.47667800	-0.15318900	3.26784200
H	0.31600400	0.74592100	1.95547500
H	-1.46652900	0.60784900	1.98450500
C	0.76126200	-0.38240200	-0.86454300
O	1.20913200	-1.28286000	-1.76791200
C	1.90933000	0.45576700	-0.25448800
C	1.76929200	1.74219500	0.28385200
C	3.18789700	-0.11931100	-0.27809300
C	2.87402500	2.43017300	0.79634400
H	0.79990400	2.22746200	0.29675400
C	4.28877800	0.56166800	0.23859100
H	3.29249700	-1.09439400	-0.74072200
C	4.13708900	1.84047100	0.78085500
H	2.74285400	3.43171300	1.19887700
H	5.27154600	0.09742600	0.20799800
H	4.99658300	2.37520500	1.17685300
H	-0.05719600	-0.91153200	-2.77188700
C	-0.38079800	0.53489600	-1.64987800
H	0.20581400	1.38721300	-2.03329300
O	-0.83818200	-0.28234100	-2.68299600
C	-1.56549000	1.05871900	-0.86701100
C	-2.64553300	0.21109200	-0.56981400
C	-1.64905500	2.39872800	-0.46350700
C	-3.73738500	0.67206200	0.16450500
H	-2.62785800	-0.80533200	-0.95011100
C	-2.74123700	2.86605500	0.27151700
H	-0.86233800	3.09265000	-0.74971400
C	-3.78495900	2.00039300	0.60158500
H	-4.56322100	-0.00097600	0.38291700
H	-2.78290900	3.91047100	0.57039300
H	-4.63924800	2.36158400	1.16822700

Table S35. Cartesien coordinates of thiazole-2-ylidene 4, TS-4

C	0.07568000	1.32619300	-0.19692300
C	-0.62809200	2.74953200	-1.89826500
C	-0.35842700	3.67183700	-0.94748500
H	-0.98940600	2.90787600	-2.90675300
H	-0.45872400	4.74454300	-1.03647400
S	0.23032200	2.90217100	0.49758500
N	-0.37137600	1.45082500	-1.45582700
C	-0.62671700	0.29221100	-2.32521700
H	-0.48695600	0.59643700	-3.36483300
H	0.08443700	-0.49440300	-2.07990800
H	-1.64634700	-0.06939900	-2.17169400
C	0.80956700	0.08694400	1.18506200
O	1.25155700	0.91711200	2.03820400
C	1.85380800	-0.65928400	0.36068500
C	1.58538200	-1.77556800	-0.44442100
C	3.17724100	-0.20402200	0.44998800
C	2.61046600	-2.41003400	-1.15076900
H	0.57618400	-2.16171100	-0.52128400
C	4.19985200	-0.83334700	-0.25751200
H	3.37851700	0.64372800	1.09566700
C	3.92105500	-1.93962100	-1.06347200
H	2.38206200	-3.27810200	-1.76446700
H	5.21913700	-0.46421900	-0.17417900
H	4.71834800	-2.43483000	-1.61175600
H	-0.20798200	0.67259300	2.99765900
C	-0.45286300	-0.71627600	1.75466500
H	0.00096200	-1.64343000	2.15350700
O	-0.96995400	0.07277300	2.79750300
C	-1.59963700	-1.10917700	0.84258800
C	-2.60932400	-0.18144700	0.54381700
C	-1.73592500	-2.41406500	0.35113900
C	-3.68665200	-0.53256900	-0.26992900
H	-2.55522800	0.80513400	0.99092100
C	-2.80981700	-2.76983900	-0.46873400
H	-1.00545400	-3.16961400	0.63162300
C	-3.78614700	-1.82672800	-0.79132400
H	-4.46220300	0.19966300	-0.48261100
H	-2.89274700	-3.78960300	-0.83612900
H	-4.62965500	-2.10269700	-1.41888400

Table S36. Cartesien coordinates of imidazoline-2-ylidene 5

C	0.00000000	1.02668100	0.00000000
C	0.76893700	-1.23712800	-0.03080500
C	-0.76893700	-1.23712700	0.03080600
H	1.15419400	-1.67132800	-0.96453300
H	-1.15419400	-1.67132700	0.96453400

N	-1.07336800	0.20538600	-0.03786800
N	1.07336800	0.20538600	0.03786700
C	-2.44114400	0.66381900	-0.00126900
H	-3.01578300	0.27550900	-0.85455300
H	-2.95035000	0.34467300	0.92094000
H	-2.43127700	1.75395900	-0.04263100
C	2.44114400	0.66381900	0.00127000
H	3.01578200	0.27550800	0.85455400
H	2.95035100	0.34467300	-0.92093900
H	2.43127700	1.75395900	0.04263200
H	-1.23120400	-1.78070400	-0.80292500
H	1.23120400	-1.78070400	0.80292600

Table S37. Cartesien coordinates of imidazoline-2-ylidene 5, TS-1

C	1.22901300	-0.00660500	-0.39919100
C	2.61071600	1.79020700	0.19386500
C	3.43018900	0.49537500	0.18996800
H	2.88678400	2.46590800	-0.62873300
H	3.64683400	0.14787400	1.21066100
N	2.50404600	-0.44518100	-0.46660600
N	1.24427400	1.27909200	-0.01503400
C	2.86174600	-1.85625500	-0.50123800
H	3.92390300	-1.94425400	-0.74724100
H	2.64502300	-2.32959400	0.46337600
H	2.28604200	-2.36180000	-1.27860400
C	0.14470700	2.22294000	-0.08058900
H	-0.01583700	2.69263800	0.89720400
H	0.37057900	3.01300400	-0.81090000
H	-0.76502000	1.70903700	-0.38113000
H	4.37207000	0.57651300	-0.36094500
H	2.68384400	2.34611100	1.13441900
C	-0.03789300	-1.32685300	0.14025600
H	0.12866800	-2.02227400	-0.71414300
O	0.41672900	-1.61834800	1.28361300
C	-1.41626000	-0.69419100	0.01565100
C	-2.03815400	-0.53519700	-1.22753100
C	-2.09696200	-0.31665500	1.17599800
C	-3.31585600	0.01891600	-1.31389900
H	-1.51180100	-0.84207600	-2.13044200
C	-3.37577500	0.23664700	1.09401900
H	-1.59981000	-0.47887000	2.12773500
C	-3.98654500	0.41017300	-0.15069700
H	-3.79214100	0.14060000	-2.28390300
H	-3.90088700	0.52752100	2.00090600
H	-4.98388600	0.83806000	-0.21535500

Table S38. Cartesien coordinates of imidazoline-2-ylidene 5, IM-1

C	-1.18727300	-0.11161000	0.14281600
C	-2.62664700	1.70610000	0.18434800
C	-3.43003900	0.39796400	0.21195500
H	-2.71454600	2.26661500	1.12518500
H	-3.86267900	0.17294900	-0.77489200
N	-2.39897300	-0.59469800	0.54880500
N	-1.25326200	1.22671300	-0.00149900
C	-2.74353700	-2.00293300	0.38438400
H	-3.77589700	-2.14485300	0.71355000
H	-2.62927000	-2.30314200	-0.66458900
H	-2.10058700	-2.62733300	1.00790200
C	-0.21430300	2.05641300	-0.59361700
H	-0.66517200	3.00785800	-0.88726800
H	0.60189500	2.25405100	0.10737800
H	0.17907600	1.55118300	-1.47927200
H	-4.23006800	0.39925400	0.95739700
H	-2.92775500	2.36384000	-0.63763800
C	-0.05867000	-1.00238400	-0.27961600
H	-0.14641700	-1.97234700	0.26678200
O	-0.49424500	-1.01217200	-1.56563400
C	1.37143400	-0.52388900	-0.00875300
C	1.83899200	-0.26418800	1.28467000
C	2.25045500	-0.41791300	-1.08783100
C	3.16496400	0.11833400	1.49358100
H	1.16272800	-0.35948800	2.13372500
C	3.58073600	-0.04677600	-0.88107800
H	1.85731700	-0.63065300	-2.07801300
C	4.04037900	0.22702400	0.40891300
H	3.51756800	0.32689500	2.50100300
H	4.25995400	0.03090500	-1.72696100
H	5.07450600	0.52069000	0.57101700

Table S39. Cartesien coordinates of imidazoline-2-ylidene 5, TS-2

C	1.43929800	-0.93383500	0.14898100
C	3.35331700	-1.73144500	-0.90090900
C	2.63925700	-2.88997200	-0.19449700
H	3.25324700	-1.78732400	-1.99435300
H	3.18061100	-3.23150000	0.70043700
N	1.36211400	-2.28179500	0.17629000
N	2.63710200	-0.56433600	-0.37487100
C	0.28245300	-3.10063000	0.72002500
H	0.34593100	-4.08399700	0.24344800
H	0.39024400	-3.21779200	1.80419700
H	-0.68963800	-2.64620200	0.49005200
C	3.26094600	0.74822300	-0.41269100
H	4.33346500	0.61864300	-0.23090500
H	3.12355800	1.24301000	-1.38166200
H	2.84680100	1.38784600	0.36315300
H	2.47754300	-3.75181300	-0.84787300

H	4.41704900	-1.66887600	-0.65506100
C	0.31963500	-0.08197600	0.56825500
H	-0.71244300	-0.50663500	-0.00855900
O	-0.07507200	-0.41982000	1.89585000
C	0.38313800	1.39990400	0.30698500
C	0.35743400	1.88988400	-1.00966900
C	0.37113400	2.32138500	1.36373100
C	0.36852700	3.26135000	-1.26405600
H	0.31740000	1.18679600	-1.83946600
C	0.37678100	3.69372100	1.10896300
H	0.34717500	1.94235300	2.38003500
C	0.38345500	4.17079900	-0.20388200
H	0.34597800	3.62005700	-2.29020600
H	0.37143600	4.39422300	1.94063300
H	0.38264000	5.23988200	-0.39915000
H	-1.02261900	-0.67536300	1.74669300
O	-1.94776500	-1.15577400	0.22451000
C	-3.14371000	-0.68395500	-0.33649700
C	-2.99947100	-0.56234400	-1.86914900
H	-2.68616600	-1.52502600	-2.29034700
H	-3.93743700	-0.26142500	-2.35429500
H	-2.23557000	0.18442100	-2.12085700
C	-4.24833900	-1.70958300	-0.00583500
H	-4.33717500	-1.82291900	1.08076100
H	-5.22660400	-1.41003900	-0.40487500
H	-3.98743000	-2.68806000	-0.42591800
C	-3.52282100	0.68877700	0.25895400
H	-4.46752200	1.07177700	-0.14972800
H	-3.63001300	0.60780900	1.34742400
H	-2.73848600	1.42600400	0.05135500

Table S40. Cartesien coordinates of imidazoline-2-ylidene 5, IM-2

C	1.18336500	0.13527600	-0.11218200
C	2.62688400	-1.68405900	0.17771000
C	3.46409700	-0.39987500	0.02937200
H	2.65310500	-2.06641400	1.20900800
H	4.04634600	-0.39915100	-0.90327100
N	2.46669000	0.67450000	0.02410900
N	1.28342800	-1.25558000	-0.20230000
C	2.72157700	1.84187400	0.85224600
H	3.73569400	2.20301100	0.65407200
H	2.01690500	2.62923200	0.58762600
H	2.63396900	1.62592000	1.93111900
C	0.48901000	-2.04318000	-1.12886300
H	1.13984000	-2.72795300	-1.68693000
H	-0.28483200	-2.63721900	-0.62461700
H	-0.01282900	-1.37756200	-1.83716300
H	4.16531000	-0.27107400	0.86136000
H	2.97221300	-2.48734800	-0.48123700
C	0.01757200	0.84672500	-0.21559100
O	0.13658100	2.20502500	-0.55552800
C	-1.34574400	0.34803700	-0.03096500
C	-1.65635600	-0.75071200	0.80321900
C	-2.42755000	1.03846900	-0.62231700
C	-2.97365900	-1.14721900	1.00955200
H	-0.84996200	-1.27592300	1.30580400
C	-3.74541600	0.64005400	-0.40541000
H	-2.21942700	1.87881100	-1.27802600
C	-4.03134800	-0.45721600	0.40812000
H	-3.17907700	-1.99346000	1.66123800
H	-4.55377200	1.18841600	-0.88370600
H	-5.05889300	-0.76776200	0.57626400
H	-0.48265600	2.69679500	0.01067800

Table S41. Cartesien coordinates of imidazoline-2-ylidene 5, TS-3

C	1.99479900	-0.08417300	-0.05194100
C	3.81142200	0.59847300	-1.33626700
C	4.07524200	-0.80612900	-0.78994700
H	3.63172000	0.60174500	-2.41962100
H	4.85761700	-0.81855700	-0.01772200
N	2.78694400	-1.16520500	-0.18847000
N	2.58896200	0.98768000	-0.62030500
C	2.73763700	-2.43773200	0.53183600
H	3.52411300	-2.43276300	1.29836100
H	1.76950000	-2.59903200	1.01478900
H	2.94209400	-3.24719800	-0.17688600
C	2.25316500	2.40536500	-0.53610300
H	3.19568300	2.96035900	-0.48333400
H	1.68693600	2.74452700	-1.40929100
H	1.67200600	2.60864700	0.35906600
H	4.34898100	-1.52606600	-1.56637300
H	4.62009400	1.30254500	-1.12096600
C	0.67845700	-0.11704400	0.70169700
O	1.02963500	-0.32529800	2.01683900
C	-0.22222500	1.08351000	0.47778600
C	-0.66524300	1.46455800	-0.79827600
C	-0.67751100	1.80645600	1.58690200
C	-1.52064700	2.55275700	-0.96295300
H	-0.34754700	0.90040100	-1.67164900
C	-1.53636000	2.89532600	1.42357700
H	-0.33865000	1.49719700	2.56962300
C	-1.95791400	3.27681800	0.14904200
H	-1.85724600	2.82742900	-1.95958200
H	-1.87712500	3.44658100	2.29674200
H	-2.62804200	4.12307700	0.02204000
H	0.50847400	-1.33703400	2.12010000
C	-0.20288900	-1.62943500	0.32064900
H	0.37216100	-2.07814000	-0.51398900
O	-0.10281800	-2.28537000	1.49129500

C	-1.62554100	-1.42957200	-0.15720200
C	-1.94654300	-1.49777300	-1.51757900
C	-2.66150800	-1.24109500	0.76664200
C	-3.26536800	-1.35521900	-1.95407000
H	-1.15477900	-1.67913100	-2.24386300
C	-3.97833000	-1.09368600	0.33662700
H	-2.41507300	-1.23562300	1.82352600
C	-4.28632800	-1.14625100	-1.02635300
H	-3.49599300	-1.41816200	-3.01516300
H	-4.77123300	-0.94567800	1.06610200
H	-5.31545200	-1.03802400	-1.35996800

Table S42. Cartesien coordinates of imidazoline-2-ylidene 5, IM-3

C	1.97390800	-0.34465700	0.07350400
C	4.19540100	0.35458100	0.15257900
C	4.10298400	-0.94665100	-0.65501300
H	4.47845000	1.21589000	-0.46720500
H	4.59382000	-1.79122600	-0.15462300
N	2.65096900	-1.19084000	-0.72328800
N	2.82902100	0.51559000	0.64860400
C	2.19689100	-2.37557300	-1.45234600
H	3.06372300	-3.03038900	-1.57818900
H	1.43646100	-2.89966900	-0.87017500
H	1.82117700	-2.11251300	-2.44759400
C	2.52193800	1.52370000	1.65507800
H	3.38525500	1.60235300	2.32450500
H	2.33167500	2.50101400	1.19775400
H	1.65044800	1.17207900	2.21010900
H	4.52044200	-0.85550200	-1.66239300
H	4.90159000	0.28994100	0.98696400
C	0.44628400	-0.28345900	0.48074700
O	0.44838900	-0.51192900	1.80746700
C	-0.07554800	1.09448600	0.01652000
C	0.16269600	1.59261800	-1.27018800
C	-0.84735400	1.85103700	0.90210100
C	-0.36067000	2.82519900	-1.66627600
H	0.76330900	1.01773000	-1.97467200
C	-1.37645700	3.08020500	0.50827900
H	-1.01544400	1.44950100	1.89634600
C	-1.13454000	3.57275500	-0.77645800
H	-0.16491700	3.20039400	-2.66808000
H	-1.97968900	3.65654000	1.20571200
H	-1.54468100	4.53195100	-1.08209500
H	0.21854800	-2.20465700	1.37017500
C	-0.42119200	-1.43614400	-0.20269200
H	-0.16393300	-1.54549200	-1.26304800
O	-0.05347400	-2.61387000	0.49591500
C	-1.91724300	-1.18536900	-0.11549600
C	-2.65441900	-0.86290300	-1.25964200
C	-2.59078900	-1.29850400	1.10883200
C	-4.03229300	-0.64832000	-1.19000800
H	-2.14531800	-0.77852900	-2.21782200
C	-3.96614600	-1.08334100	1.18201000
H	-2.02337600	-1.54359200	1.99961900
C	-4.69303300	-0.75815400	0.03357700
H	-4.58794800	-0.40198300	-2.09160600
H	-4.47469900	-1.17281800	2.13907600
H	-5.76664600	-0.59691000	0.09232800

Table S43. Cartesien coordinates of imidazoline-2-ylidene 5, TS-4

C	-2.05915700	-0.52397200	-0.08501800
C	-4.34326600	0.00887800	-0.18239300
C	-4.15165300	-1.19386000	0.75386900
H	-4.69003000	0.90544800	0.34800500
H	-4.61675800	-2.11010600	0.36772100
N	-2.68147800	-1.34891400	0.77373800
N	-2.98152800	0.22429200	-0.70045700
C	-2.09953100	-2.48060000	1.48482400
H	-2.85527400	-3.27094400	1.54972200
H	-1.24703200	-2.86482700	0.92289300
H	-1.80378600	-2.21093000	2.50667300
C	-2.74756900	1.24573000	-1.70977000
H	-3.54205900	1.17856400	-2.46208100
H	-2.76308600	2.25142800	-1.27110200
H	-1.78567300	1.05123800	-2.18400800
H	-4.53787700	-1.01674700	1.76337000
H	-5.04057500	-0.18914400	-1.00399300
C	-0.14862800	-0.20057900	-0.66182300
O	-0.15149900	-0.33750300	-1.92436500
C	0.05802300	1.18897000	-0.06544500
C	-0.19601200	1.49042900	1.27917600
C	0.59249700	2.18453400	-0.89020100
C	0.06992100	2.76210500	1.78595800
H	-0.61909000	0.73067000	1.93261600
C	0.86186500	3.45758600	-0.38571700
H	0.79501400	1.93550200	-1.92697800
C	0.60078300	3.75116200	0.95359900
H	-0.13710300	2.98247200	2.83041100
H	1.28014800	4.21990700	-1.03845500
H	0.80994600	4.74213300	1.34838100
H	0.03602700	-2.21383600	-1.48923400
C	0.62117900	-1.34045500	0.07671800
H	0.30175100	-1.41527900	1.12080700
O	0.27615000	-2.54452800	-0.59126200
C	2.12481300	-1.09499500	0.06040600
C	2.82289000	-0.89403200	1.25536700
C	2.83796500	-1.08238200	-1.14654800
C	4.20377600	-0.68463100	1.25361400
H	2.28169000	-0.90484500	2.19942600

C	4.21590600	-0.87398400	-1.15183200
H	2.30031400	-1.22317700	-2.07833200
C	4.90484400	-0.67533500	0.04805600
H	4.72951700	-0.53412800	2.19332300
H	4.75565500	-0.86591200	-2.09571100
H	5.98025100	-0.51629800	0.04156400

Table S44. Cartesien coordinates of 1,2,4-triazole-5-ylidene 6

C	-0.00256800	-1.00637400	0.00000700
C	0.59217100	1.17756500	-0.00000100
H	1.22488100	2.05444800	-0.00001500
N	-1.03808300	-0.13521100	0.00001300
C	-2.44344600	-0.49458500	-0.00000900
H	-2.93741600	-0.09375800	0.89026000
H	-2.93738200	-0.09377300	-0.89030200
H	-2.50157700	-1.58291800	-0.00000100
N	1.05509300	-0.11819000	-0.00000300
C	2.45188800	-0.52291400	-0.00000200
H	2.96738800	-0.15066800	-0.89171400
H	2.96730600	-0.15098900	0.89189200
H	2.47172800	-1.61276000	-0.00019400
N	-0.70889500	1.21172500	0.00000500

Table S45. Cartesien coordinates of 1,2,4-triazole-5-ylidene 6, TS-1

C	1.24507100	-0.09244500	0.08655900
C	2.98927900	0.75741000	-0.98390100
H	3.59711400	1.47199100	-1.51979100
N	2.27812700	-0.94614200	0.01167100
C	2.33793700	-2.30779600	0.51794800
H	2.26912300	-3.02179200	-0.30782200
H	3.28525800	-2.44968100	1.04159500
H	1.50580100	-2.45736500	1.20635800
N	1.71050400	1.01195700	-0.55993800
C	0.97683800	2.27305600	-0.68360100
H	1.68616100	3.06823700	-0.92216500
H	0.22760700	2.19663500	-1.47545000
H	0.49088000	2.45098800	0.28049400
N	3.37733100	-0.44281500	-0.65414400
C	-0.14915100	0.08542300	1.35450300
H	0.09585200	-0.86109500	1.89803000
O	0.04625200	1.18699600	1.94134900
C	-1.41409900	-0.11376900	0.51482200
C	-2.34717300	0.92316000	0.45501400
C	-1.69465000	-1.31936100	-0.13802400
C	-3.53498400	0.76741300	-0.26369400
H	-2.12494200	1.83705800	0.99787100
C	-2.87854000	-1.48066800	-0.85602300
H	-0.97879800	-2.13904100	-0.08526100
C	-3.80253300	-0.43290300	-0.92367800
H	-4.25614800	1.58056800	-0.30176600
H	-3.08467500	-2.42161200	-1.36071400
H	-4.72746700	-0.55741800	-1.48116100

Table S46. Cartesien coordinates of 1,2,4-triazole-5-ylidene 6, IM-1

C	1.21393200	-0.04785000	0.15334700
C	2.73467300	0.91021400	-1.11175200
H	3.21052700	1.65144300	-1.73694400
N	2.31810600	-0.80329700	0.03330900
C	2.58807800	-2.11644500	0.59896500
H	2.52103300	-2.88205900	-0.17910200
H	3.59539600	-2.11082100	1.01883800
H	1.85709500	-2.31870800	1.38144500
N	1.47655300	1.05705400	-0.59856300
C	0.62633200	2.24884400	-0.64494900
H	1.22569600	3.08768500	-1.00388400
H	-0.22251800	2.08066700	-1.31100600
H	0.27957000	2.39676800	0.38425000
N	3.28437700	-0.21680700	-0.75443300
C	0.05306400	-0.12694000	1.19018800
H	0.19430900	-1.12672700	1.68841400
O	0.22783100	0.92961600	1.96529400
C	-1.30192100	-0.24281400	0.44333900
C	-2.32249200	0.63360400	0.81279200
C	-1.55332400	-1.21093800	-0.53556600
C	-3.57936900	0.55012700	0.20913900
H	-2.09381200	1.36478600	1.58308600
C	-2.80516100	-1.29373000	-1.14698000
H	-0.76734600	-1.90936100	-0.82467000
C	-3.82312900	-0.41098100	-0.77426000
H	-4.37074100	1.23455400	0.50640200
H	-2.98903800	-2.04637000	-1.91027600
H	-4.80016900	-0.47597800	-1.24667300

Table S47. Cartesien coordinates of 1,2,4-triazole-5-ylidene 6, TS-2

C	-1.16612500	-1.14578100	-0.06976200
C	-2.61126500	-2.80055300	-0.06241300
H	-3.40120900	-3.46012000	-0.39100200
N	-1.05909100	-1.89857000	1.03802300
C	-0.03525600	-1.78620000	2.08024500
H	-0.25108300	-0.93507300	2.73118700
H	-0.06938300	-2.71241600	2.65276200
H	0.93284400	-1.65497300	1.58046700
N	-2.16869300	-1.72951300	-0.78916300
C	-2.70411200	-1.24255200	-2.06262000
H	-3.28808700	-2.04310100	-2.52017700
H	-3.34115100	-0.37183300	-1.88664700

H	-1.86172400	-0.95687800	-2.69231600
N	-1.95953500	-2.92839800	1.06125100
C	-0.30452000	-0.01071100	-0.45844900
H	0.88918700	-0.28719100	-0.01942300
O	0.00842000	-0.14428700	-1.85163900
C	-0.80471600	1.34508200	-0.07481700
C	-0.44490900	2.45889400	-0.85342300
C	-1.57797300	1.56835700	1.07939700
C	-0.83655000	3.74479400	-0.48280200
H	0.13464500	2.29624300	-1.75527900
C	-1.96474400	2.85605900	1.44798300
H	-1.89098700	0.72923400	1.69812800
C	-1.59592000	3.95520400	0.66990500
H	-0.54608400	4.58937300	-1.10319300
H	-2.56230000	2.99862400	2.34530000
H	-1.89881700	4.95858100	0.95629300
H	0.91230100	-0.53919200	-1.79641700
O	2.02471100	-0.93822600	-0.18862800
C	3.24910000	-0.25852100	-0.04288200
C	4.37486700	-1.27429300	-0.32159700
H	4.29975500	-2.11405400	0.37884000
H	4.27272900	-1.67487700	-1.33681800
H	5.37273600	-0.82689800	-0.22327300
C	3.35297200	0.91037900	-1.04665400
H	2.56258200	1.64844400	-0.86356600
H	4.31904900	1.42744700	-0.97914700
H	3.24055000	0.53793400	-2.07252200
C	3.39389600	0.29077600	1.39304200
H	4.34975000	0.80909700	1.54486200
H	2.58703700	1.00103500	1.61315900
H	3.33537400	-0.52954600	2.11923300

Table S48. Cartesien coordinates of 1,2,4-triazole-5-ylidene 6, IM-2

C	1.21734300	0.05588600	0.07143900
C	3.34779100	-0.54537800	-0.18696500
H	4.40845800	-0.45473600	-0.37716100
N	1.39965000	-1.32482100	0.17843500
C	0.59094500	-2.20016900	1.00733400
H	-0.39204300	-2.37176300	0.56254500
H	1.12823100	-3.14511000	1.09115700
H	0.44590600	-1.76695300	2.00664500
N	2.51018800	0.54936900	-0.16591200
C	2.83221600	1.83961600	-0.75799400
H	3.90554500	1.86168800	-0.96278700
H	2.28123700	1.97951000	-1.69528200
H	2.56632400	2.65561400	-0.08682900
N	2.74942200	-1.66430800	0.04481500
C	0.07050600	0.80445900	0.20862000
O	0.24885600	2.18620300	0.45052800
C	-1.30592100	0.36269800	0.02155600
C	-2.36702000	1.09973700	0.59278000
C	-1.64888400	-0.74643000	-0.78512300
C	-3.69238200	0.72196800	0.40223900
H	-2.13554000	1.98317200	1.17879700
C	-2.97759800	-1.12485400	-0.96516200
H	-0.86531200	-1.28564600	-1.31040700
C	-4.01121900	-0.40015200	-0.36799400
H	-4.48512500	1.30901600	0.86030200
H	-3.20662800	-1.98013900	-1.59671000
H	-5.04706600	-0.69425300	-0.51297400
H	0.45568100	2.29401700	1.39274800

Table S49. Cartesien coordinates of 1,2,4-triazole-5-ylidene 6, TS-3

C	2.02473300	-0.11549000	-0.06917100
C	3.88354100	0.44407300	-1.11526000
H	4.61410400	1.05321500	-1.62702600
N	2.87037100	-1.15904000	-0.20376800
C	2.79323400	-2.51799500	0.34547800
H	2.92980400	-3.22133300	-0.47822300
H	3.61364800	-2.63006900	1.05858200
H	1.82667200	-2.67444400	0.84124800
N	2.68896600	0.93368800	-0.65449400
C	2.36515300	2.36647000	-0.66696500
H	1.99955900	2.67042800	0.31240600
H	3.28822500	2.90207200	-0.89785400
H	1.60395700	2.58987800	-1.41363800
N	4.02505400	-0.82009100	-0.85268000
C	0.71276000	-0.14622300	0.66834400
O	1.02964400	-0.40401300	1.99223000
C	-0.13921900	1.08594400	0.46741800
C	-0.52894100	1.84540700	1.57844700
C	-0.59975900	1.47222100	-0.80183200
C	-1.33695600	2.97312700	1.42196700
H	-0.18681400	1.53143100	2.55840700
C	-1.40431600	2.60019700	-0.95924000
H	-0.34227000	0.87609600	-1.67382000
C	-1.77339400	3.35973900	0.15363400
H	-1.62663100	3.55118700	2.29608000
H	-1.75789100	2.87543600	-1.94972800
H	-2.40511000	4.23579400	0.03315400
H	0.58327200	-1.36847900	2.07899900
C	-0.18670400	-1.67886400	0.22336100
H	0.36494600	-2.02953100	-0.67614700
C	-1.62538900	-1.42144900	-0.17475300
C	-2.60606300	-1.24629100	0.81001800
C	-2.01721700	-1.42971500	-1.51756200
C	-3.93977300	-1.05441800	0.45666100
H	-2.30505300	-1.28647500	1.85213200
C	-3.35413600	-1.24470800	-1.87740200

H	-1.26908500	-1.60063400	-2.29099400
C	-4.31954800	-1.04970800	-0.88933600
H	-4.68980600	-0.91678500	1.23197600
H	-3.64186300	-1.26341600	-2.92609700
H	-5.36200400	-0.90757800	-1.16334600
O	-0.03169700	-2.41131100	1.31872500

Table S50. Cartesien coordinates of 1,2,4-triazole-5-ylidene 6, IM-3

C	-1.99818100	-0.33161700	-0.01348200
C	-4.15847100	0.05222200	-0.19293600
H	-5.08236900	0.51095600	-0.51270100
N	-2.72611900	-1.20106000	0.71166100
C	-2.30750900	-2.33550700	1.54003300
H	-1.87236300	-1.97927200	2.47740500
H	-3.21215700	-2.90375200	1.75200600
H	-1.58849000	-2.93055700	0.97417100
N	-2.92773600	0.48190300	-0.59458800
C	-2.66516100	1.52842500	-1.58790600
H	-1.91310700	1.12213400	-2.26884300
H	-3.60325100	1.74867000	-2.10114200
H	-2.28422200	2.42574400	-1.09702100
N	-4.07890600	-0.97240400	0.60680000
C	-0.48372000	-0.24525700	-0.44518500
O	-0.52386800	-0.46469000	-1.77065500
C	0.04089900	1.13275500	0.00609000
C	0.76970200	1.89897500	-0.90742600
C	-0.16051000	1.62838900	1.30020500
C	1.29463500	3.13621200	-0.53287300
H	0.90713100	1.49830800	-1.90660900
C	0.35922300	2.86845500	1.67675100
H	-0.72936500	1.04678300	2.02499300
C	1.09073800	3.62582200	0.75950000
H	1.86430400	3.72083900	-1.25115600
H	0.19286100	3.24214600	2.68418500
H	1.49704500	4.59117200	1.05018400
H	-0.32444900	-2.19333000	-1.32515800
C	0.36371800	-1.41398100	0.22788500
H	0.12150400	-1.50603000	1.29403000
C	1.86241000	-1.20134300	0.10748500
C	2.50551200	-1.32467800	-1.13215100
C	2.63104400	-0.89760900	1.23597500
C	3.88317100	-1.13832200	-1.23523600
H	1.91478300	-1.55559200	-2.01160500
C	4.01115800	-0.71163400	1.13600500
H	2.14583500	-0.80654500	2.20584100
C	4.64178200	-0.83163600	-0.10238400
H	4.36831600	-1.23560200	-2.20351200
H	4.59182700	-0.47982100	2.02548800
H	5.71685800	-0.69252300	-0.18472300
O	-0.05913100	-2.58791400	-0.44622500

Table S51. Cartesien coordinates of 1,2,4-triazole-5-ylidene 6, TS-4

C	-2.10610000	-0.39004400	0.08096900
C	-4.29236300	-0.24367800	-0.27947900
H	-5.23002400	0.11423900	-0.67899900
N	-2.81106500	-1.31832500	0.75078300
C	-2.30523100	-2.38372400	1.61378000
H	-1.91020100	-1.96338800	2.54287600
H	-3.14897800	-3.03480200	1.84043200
H	-1.52661100	-2.92774500	1.07574100
N	-3.07424400	0.30289200	-0.58764200
C	-2.84947900	1.40372300	-1.52718300
H	-2.01704800	1.12446100	-2.17533400
H	-3.76178300	1.54942400	-2.10946300
H	-2.60785600	2.32060300	-0.98514900
N	-4.17301200	-1.24573600	0.54411400
C	-0.24890900	-0.15101900	-0.56572700
O	-0.35386000	-0.32550000	-1.82061300
C	0.08014800	1.24078300	-0.03835600
C	0.65558700	2.15735000	-0.92457200
C	-0.11254600	1.61875200	1.29647800
C	1.02694000	3.43020500	-0.48788200
H	0.80622500	1.84930700	-1.95427900
C	0.25658400	2.88970700	1.73563900
H	-0.57202300	0.92130800	1.99322100
C	0.82812300	3.80062100	0.84297600
H	1.47488300	4.13184900	-1.18714900
H	0.09552400	3.17148300	2.77323800
H	1.11537200	4.79168700	1.18463300
H	-0.22687300	-2.19011700	-1.35959600
C	0.48528100	-1.32656600	0.16115800
H	0.20352800	-1.35963000	1.21895500
C	1.99733300	-1.17274000	0.07318500
C	2.65903600	-1.29544000	-1.15644000
C	2.75293600	-0.91279500	1.22091000
C	4.04391000	-1.15843000	-1.23109800
H	2.07987700	-1.49057400	-2.05311600
C	4.14069100	-0.77478100	1.14948600
H	2.25172600	-0.82020600	2.18228500
C	4.79036000	-0.89781500	-0.07854300
H	4.54386500	-1.25592100	-2.19164700
H	4.71195000	-0.57704100	2.05306200
H	5.87085800	-0.79488700	-0.13853300
O	0.03411300	-2.51656500	-0.46610700

Table S52. Cartesien coordinates of tetrazole-5-ylidene 7

C	0.00000000	1.02221700	-0.00001400
N	-1.02871000	0.13718600	-0.00000100
C	-2.44889600	0.44504100	0.00000700

H	-2.92528800	0.02784200	-0.89125700
H	-2.92527000	0.02792700	0.89132300
H	-2.54463200	1.53021800	-0.00004200
N	1.02871000	0.13718600	-0.00001300
C	2.44889600	0.44504100	0.00001200
H	2.92521300	0.02811000	0.89144300
H	2.92533300	0.02764800	-0.89113700
H	2.54465100	1.53021700	-0.00025700
N	-0.63497200	-1.18331100	0.00000500
N	0.63497000	-1.18331200	-0.00000500

Table S53. Cartesien coordinates of tetrazole-5-ylidene 7, TS-1

C	1.23655800	0.01730700	0.30249500
N	2.55635000	-0.25469300	0.29713700
C	3.17311400	-1.56669400	0.46071600
H	4.20240600	-1.49121700	0.11099300
H	3.15608900	-1.86402700	1.51200500
H	2.58617000	-2.25861100	-0.15292500
N	1.21758300	1.30837100	-0.07636700
C	0.08395100	2.20563500	-0.28195800
H	0.48984900	3.21259300	-0.37978500
H	-0.45531100	1.92422000	-1.18824400
H	-0.59226800	2.14298600	0.57048300
N	3.29383300	0.82155500	-0.09681500
N	2.48546200	1.77880400	-0.32119900
C	0.10902600	-1.32964900	0.08393200
H	0.28329700	-1.85276700	1.05790500
O	0.51876000	-1.88312900	-0.99478100
C	-1.29296800	-0.71534700	0.11189300
C	-1.88410800	-0.28859200	1.30549900
C	-2.00630900	-0.61299700	-1.08408300
C	-3.16810500	0.25922700	1.30178800
H	-1.33702800	-0.39095200	2.24240200
C	-3.29168300	-0.06689700	-1.09163700
H	-1.53038700	-0.98442500	-1.98702400
C	-3.87313800	0.37479600	0.09959100
H	-3.62357200	0.58565400	2.23363200
H	-3.84444400	0.00722700	-2.02511500
H	-4.87549700	0.79536400	0.09522500

Table S54. Cartesien coordinates of tetrazole-5-ylidene 7, IM-1

C	1.21564800	-0.09285200	0.14548000
N	2.49409000	-0.43799500	0.41855500
C	3.03854200	-1.78771600	0.44484100
H	4.12471000	-1.69966900	0.45203700
H	2.70157000	-2.32015800	1.33687400
H	2.69460900	-2.29708200	-0.46017200
N	1.29304700	1.24512400	-0.01660800
C	0.26296700	2.16136100	-0.48639800
H	0.73068300	3.14092300	-0.58523200
H	-0.10035200	1.80485400	-1.45293400
H	-0.56144200	2.19897100	0.22670600
N	3.31694700	0.64883600	0.32412200
N	2.59464300	1.66234600	0.06625000
C	0.13210300	-1.06848100	-0.31114200
H	0.27155800	-1.99992600	0.29787800
O	0.52500500	-1.12469300	-1.58704200
C	-1.29830200	-0.58764800	-0.02014800
C	-1.76580500	-0.37544000	1.28186300
C	-2.16304300	-0.40460600	-1.09952000
C	-3.08151500	0.03576100	1.50052100
H	-1.10018900	-0.53422100	2.13024500
C	-3.48364700	-0.00386300	-0.88316100
H	-1.76769400	-0.58860800	-2.09440200
C	-3.94406100	0.22195700	0.41562400
H	-3.43688100	0.20416700	2.51423100
H	-4.15442500	0.13253000	-1.72807000
H	-4.97059600	0.53674500	0.58518400

Table S55. Cartesien coordinates of tetrazole-5-ylidene 7, TS-2

C	-0.92866200	-1.29106900	0.05796700
N	-0.74600500	-1.93005600	-1.11571600
C	0.13174200	-1.52999000	-2.21852900
H	0.18243200	-2.37491700	-2.90453600
H	-0.28252100	-0.65423500	-2.72267100
H	1.11041900	-1.29801600	-1.77859600
N	-1.63954400	-2.18085300	0.78119300
C	-2.17234500	-2.03906900	2.13416900
H	-2.29508500	-3.04120000	2.54508400
H	-1.45428200	-1.44966200	2.70460400
H	-3.13761400	-1.52744200	2.09664000
N	-1.32789100	-3.15744500	-1.08804800
N	-1.86637200	-3.31084600	0.05962900
C	-0.33188800	-0.00355300	0.46394300
H	0.83584800	-0.03446400	-0.02998900
O	0.05410900	-0.09454100	1.83635900
C	-1.11102700	1.22886700	0.12115500
C	-2.03687700	1.27912500	-0.93488000
C	-0.86691600	2.40639900	0.84755300
C	-2.68474600	2.46967400	-1.26459000
H	-2.27336200	0.38071900	-1.50204200
C	-1.52127300	3.59253200	0.51922100
H	-0.16922800	2.37193500	1.67676100
C	-2.43038500	3.63495000	-0.54017200
H	-3.39831400	2.48121200	-2.08475400
H	-1.31871000	4.49064400	1.09744500

H	-2.93806200	4.56137100	-0.79385000
O	2.09751100	-0.53998300	0.09025400
C	3.24572600	0.26699100	-0.00298900
H	1.00940500	-0.33545800	1.73104800
C	3.08998200	1.55147600	0.83972800
H	2.25198600	2.15577400	0.47066500
H	2.88782100	1.29583500	1.88750400
H	3.99281200	2.17534400	0.81347800
C	4.43778000	-0.55387000	0.53066400
H	4.54372600	-1.47668500	-0.05106100
H	5.38350800	0.00145400	0.47831400
H	4.25931900	-0.83529400	1.57517100
C	3.50584200	0.65436000	-1.47494400
H	4.41020600	1.26557800	-1.59296100
H	3.62577100	-0.24916500	-2.08555800
H	2.65793300	1.22632200	-1.87278600

Table S56. Cartesien coordinates of tetrazole-5-ylidene 7, IM-2

C	-1.21036600	0.06572300	0.06868800
N	-1.39511600	-1.31093600	0.20866700
C	-0.53989200	-2.24120000	0.92009900
H	-1.12962600	-3.13985600	1.10445500
H	0.35052100	-2.49100900	0.33856600
H	-0.21837200	-1.80319800	1.87309300
N	-2.51853400	0.50860900	-0.13247600
C	-2.94998000	1.74750900	-0.75625400
H	-4.04006100	1.72563900	-0.78971900
H	-2.59968800	2.60304900	-0.18021900
H	-2.54935200	1.82931800	-1.77402900
N	-2.73687100	-1.61583100	0.10092100
N	-3.38197100	-0.55900800	-0.13474800
C	-0.07643900	0.82853900	0.17975200
O	-0.26381000	2.21542800	0.36392000
C	1.30537700	0.38622200	0.01071000
C	1.65779000	-0.68946400	-0.83324700
C	2.35426700	1.09106800	0.63908300
C	2.98746300	-1.07702100	-0.99079700
H	0.88377800	-1.19157600	-1.40756500
C	3.68092900	0.70819000	0.46937700
H	2.11327300	1.95110500	1.25573600
C	4.00892700	-0.38668700	-0.33590400
H	3.22725600	-1.90658400	-1.65165300
H	4.46687000	1.26787000	0.97083900
H	5.04579300	-0.68419800	-0.46543400
H	-0.52091500	2.35890300	1.28898500

Table S57. Cartesien coordinates of tetrazole-5-ylidene 7, TS-3

C	-0.03603900	0.97427500	0.37790300
N	-0.11354900	1.64238200	-0.79706900
C	0.54559300	1.39550100	-2.07719800
H	-0.15694200	1.67897200	-2.86089900
H	1.45955400	1.98841500	-2.14847800
H	0.79566400	0.33964700	-2.15195800
N	-0.88849900	1.66010300	1.16883500
C	-1.27597900	1.44526200	2.56637000
H	-2.29735100	1.06037300	2.58759400
H	-0.57921600	0.71394900	2.97302700
H	-1.22343800	2.40650100	3.08006900
N	-0.98433700	2.68324800	-0.69985500
N	-1.45401400	2.68998300	0.48208100
C	0.71739900	-0.25815300	0.68817500
O	0.66126300	-0.60486000	2.00772800
C	2.15615300	-0.24933800	0.17050600
C	2.90457400	0.92953300	0.04373900
C	2.80322400	-1.47586800	-0.05250300
C	4.24691500	0.89404300	-0.34233200
H	2.44853500	1.89193300	0.26877200
C	4.14273400	-1.51215500	-0.43558500
H	2.25339900	-2.39739700	0.11394600
C	4.86859800	-0.32850300	-0.59276500
H	4.80631800	1.82182600	-0.43287100
H	4.62443200	-2.47163100	-0.60532100
H	5.91264100	-0.36070900	-0.89259300
H	0.32294400	-1.72353900	1.80147600
C	-0.20340400	-1.66014500	-0.04791200
O	-0.04934000	-2.54168700	0.93992500
H	0.36062500	-1.86927600	-0.97381700
C	-1.63914500	-1.30540600	-0.37433800
C	-2.04026100	-0.95429200	-1.66988200
C	-2.60883800	-1.34236900	0.63892000
C	-3.36802000	-0.61789400	-1.94506800
H	-1.31332700	-0.97655100	-2.48052900
C	-3.93419000	-1.00385200	0.36925300
H	-2.30316700	-1.67465000	1.62624100
C	-4.31810900	-0.63214400	-0.92302500
H	-3.66253500	-0.35816100	-2.95900700
H	-4.67551400	-1.04419800	1.16400200
H	-5.35243400	-0.37411000	-1.13435200

Table S58. Cartesien coordinates of tetrazole-5-ylidene 7, IM-3

C	-0.00463000	0.98298300	0.09204700
N	0.07336500	1.54466700	-1.12938000
C	0.64515700	1.02492300	-2.36855500
H	0.96000300	1.88080600	-2.96561400
H	1.49871200	0.39371100	-2.12354000
H	-0.11212700	0.45131000	-2.90696600

N	-0.65364500	1.91183700	0.81074400
C	-1.05359600	1.89334200	2.22298000
H	-2.13678600	1.76727500	2.27271000
H	-0.53198300	1.03545300	2.65729000
H	-0.76143900	2.84696600	2.66535500
N	-0.52300800	2.76794400	-1.13715700
N	-0.96286800	2.98941600	0.03834300
C	0.56145700	-0.37811700	0.61319000
O	0.42091100	-0.50751000	1.93268100
C	2.06615100	-0.40897100	0.21303900
C	2.88012700	0.67468200	0.57917000
C	2.67465300	-1.52871200	-0.37083000
C	4.25150000	0.66371200	0.33252100
H	2.43696700	1.53053400	1.08403700
C	4.05225500	-1.54539800	-0.60966500
H	2.08297200	-2.40876200	-0.59721500
C	4.84405000	-0.44887200	-0.27015900
H	4.85909200	1.51844800	0.61930100
H	4.50558700	-2.42627600	-1.05737300
H	5.91378800	-0.46382000	-0.46115800
H	0.17980900	-2.24969600	1.55639700
C	-0.28582000	-1.54924500	-0.11585600
O	-0.03765200	-2.67864600	0.68268900
H	0.09742800	-1.73426000	-1.12810900
C	-1.76856700	-1.23073200	-0.21457800
C	-2.38662300	-1.04756700	-1.45767000
C	-2.55152600	-1.11707300	0.94603900
C	-3.74582000	-0.73636400	-1.54957200
H	-1.80527200	-1.18053700	-2.36919200
C	-3.90765500	-0.80435000	0.85745200
H	-2.07941100	-1.27653800	1.90929300
C	-4.50966500	-0.60872700	-0.38954200
H	-4.20779100	-0.60739500	-2.52518600
H	-4.50253400	-0.72473600	1.76431500
H	-5.56867300	-0.37336200	-0.45522300

Table S59. Cartesien coordinates of tetrazole-5-ylidene 7, TS-4

C	0.00095200	1.07077400	0.04872600
N	0.30210200	1.84282300	-1.01221200
C	0.94643800	1.47245000	-2.26649000
H	1.31658400	2.38831000	-2.72741900
H	1.77065100	0.79038600	-2.05623300
H	0.22258600	0.99193600	-2.93000100
N	-0.60064500	1.94934300	0.86619800
C	-1.19850700	1.71491000	2.18155400
H	-2.28146900	1.62714300	2.07031700
H	-0.77719000	0.77986200	2.55540000
H	-0.95265500	2.56423500	2.82054000
N	-0.11308200	3.13614700	-0.83381400
N	-0.66337000	3.19912900	0.31170800
C	0.50813400	-0.67646800	0.60180300
O	0.24117600	-0.81901800	1.84004200
C	2.01112300	-0.62632600	0.26909100
C	2.82878800	0.17545400	1.07930600
C	2.61217600	-1.39992300	-0.73233700
C	4.20297900	0.24278800	0.86641600
H	2.36969600	0.72977400	1.89297600
C	3.99550100	-1.34491300	-0.93778900
H	2.01517100	-2.08266600	-1.32744100
C	4.79258200	-0.51657100	-0.14926600
H	4.81824900	0.87829200	1.49845600
H	4.44740000	-1.96176100	-1.71051600
H	5.86606600	-0.47213000	-0.31304400
H	-0.02623300	-2.83212000	1.04312600
C	-0.36680600	-1.56344100	-0.34787300
O	-0.13774200	-2.90331700	0.07554500
H	-0.01268800	-1.49300500	-1.38265000
C	-1.84079600	-1.19576900	-0.33269400
C	-2.45576200	-0.69951300	-1.48890000
C	-2.62066700	-1.35446700	0.82382500
C	-3.80769600	-0.34901900	-1.49559800
H	-1.87254400	-0.60215700	-2.40349500
C	-3.97141700	-1.00622900	0.82032200
H	-2.15748200	-1.74135700	1.72410200
C	-4.56977300	-0.49952700	-0.33703600
H	-4.26530000	0.02946700	-2.40614000
H	-4.56283000	-1.13774300	1.72324300
H	-5.62401900	-0.23513600	-0.33743400

Table S60. Cartesien coordinates of perhydrobenzimidazole-2-ylidene 8

C	-0.10977100	0.72314400	-0.23746400
C	-0.10976200	-0.72315100	0.23743000
C	-1.25257500	-1.49802900	-0.42610300
C	-2.50274700	-0.56749200	-0.52525500
C	-2.50273900	0.56749000	0.52526900
C	-1.25255800	1.49802000	0.42611200
C	2.12236400	0.00000100	-0.00006200
H	-0.95129100	-1.82312900	-1.42944000
H	-2.54288400	-0.12066300	-1.52672200
H	-3.41908000	1.15946900	0.42162100
H	-0.95125000	1.82308600	1.42945400
H	-1.48826200	2.40077900	-0.14937100
H	-2.54287400	0.12066200	1.52673700
H	-3.41909400	-1.15946300	-0.42160300
H	-1.48827400	-2.40077000	0.14941300
H	-0.26797000	-0.73417700	1.33195600
H	-0.26800900	0.73417800	-1.33198500
N	1.29389500	1.08361100	0.01629000
N	1.29389200	-1.08362800	-0.01636400

C	1.78094700	2.41541500	-0.27638700
H	1.58338800	2.70118700	-1.32180400
H	1.30727300	3.15993800	0.37510200
H	2.85912300	2.42250800	-0.10848800
C	1.78097500	-2.41538900	0.27647500
H	1.58351700	-2.70101200	1.32195300
H	1.30723800	-3.16000400	-0.37486200
H	2.85913500	-2.42251100	0.10847200

Table S61. Cartesien coordinates of perhydrobenzimidazole-2-ylidene 8, TS-1

C	-2.37485300	0.67794700	-0.34206400
C	-2.08740900	-0.77262100	0.01804200
C	-3.00503600	-1.71062000	-0.76867800
C	-4.41811100	-1.05595500	-0.87782000
C	-4.70834100	-0.04487100	0.25509100
C	-3.68803200	1.13574600	0.29957200
C	-0.09599600	0.40195500	0.02856300
H	-2.59454500	-1.88307800	-1.77093000
H	-4.50581200	-0.54092600	-1.84286200
H	-5.72506200	0.34735500	0.14369400
H	-3.51042500	1.43571800	1.33900500
H	-4.08651600	2.00960400	-0.22838000
H	-4.69098000	-0.57461700	1.21553400
H	-5.18924200	-1.83386800	-0.87923200
H	-3.06895000	-2.68504400	-0.27205600
H	-2.26894900	-0.90699500	1.09895400
H	-2.46184900	0.76231200	-1.44028400
N	-1.10338400	1.30595200	0.05344200
N	-0.62790400	-0.82061900	-0.18093100
C	-0.90512800	2.73343100	-0.11467400
H	-1.01522500	3.03206800	-1.16794200
H	-1.63681100	3.28831600	0.48153500
H	0.09702400	3.00061700	0.22296700
C	0.10010600	-2.05189100	0.08947500
H	-0.37295700	-2.87274000	-0.45767300
H	1.12847600	-1.94293100	-0.25373700
H	0.11544100	-2.26544000	1.16446900
C	1.45106700	0.57654200	1.24272700
H	1.32216700	1.67990200	1.34087500
O	1.12543900	-0.16537200	2.20139000
C	2.67640700	0.25832500	0.39643100
C	3.48284100	-0.82376700	0.75894200
C	3.06064700	1.06176200	-0.68267200
C	4.64708500	-1.11112400	0.04273400
H	3.17969600	-1.41760600	1.61635800
C	4.22214300	0.78015600	-1.39980200
H	2.43732900	1.90828400	-0.96713200
C	5.01895700	-0.31152500	-1.03932200
H	5.26902800	-1.95435000	0.33427200
H	4.50926800	1.40945900	-2.23899600
H	5.92631400	-0.53134300	-1.59640900

Table S62. Cartesien coordinates of perhydrobenzimidazole-2-ylidene 8, IM-1

C	-2.31005500	-0.53266800	0.43213500
C	-1.91934800	0.77411000	-0.24086100
C	-2.71002800	1.94220000	0.35377700
C	-4.15903500	1.46493000	0.67659900
C	-4.60957800	0.27500900	-0.19944200
C	-3.69932600	-0.98102700	-0.03498900
C	-0.07390600	-0.56211400	-0.12718600
H	-2.21798200	2.29641500	1.26726600
H	-4.21981400	1.17150400	1.73232200
H	-5.64665100	0.01487700	0.03846000
H	-3.61566600	-1.51056700	-0.99103000
H	-4.13664000	-1.67909300	0.68794700
H	-4.60818800	0.58846600	-1.25071100
H	-4.86016200	2.29731900	0.55332200
H	-2.73169600	2.78161700	-0.34975500
H	-2.14275400	0.68534200	-1.31908800
H	-2.32927800	-0.37665000	1.52575200
N	-1.14730000	-1.36260200	0.11022300
N	-0.45665100	0.75097800	-0.08720200
C	-1.07676000	-2.74236100	0.55692100
H	-0.88482400	-2.82201600	1.63755700
H	-2.02992500	-3.23071000	0.33678600
H	-0.29230300	-3.27174800	0.01529400
C	0.30608400	1.79065600	-0.77314900
H	-0.18756600	2.74926000	-0.59422200
H	1.31743000	1.83882100	-0.37235600
H	0.36422100	1.56753700	-1.84439800
C	1.24845100	-1.07728100	-0.63164300
H	1.35298800	-2.14457800	-0.31390300
O	0.92039700	-0.88994700	-1.92689400
C	2.51587800	-0.39185800	-0.09894800
C	3.43370700	0.10122100	-1.02813000
C	2.81545000	-0.31606600	1.26580400
C	4.63630800	0.66804300	-0.60133300
H	3.16868700	0.02858400	-2.07923300
C	4.01128300	0.26044100	1.69678200
H	2.10895200	-0.70634800	1.99796100
C	4.92690600	0.75261800	0.76223400
H	5.34746500	1.04632400	-1.33220600
H	4.23146600	0.32342400	2.76000100
H	5.86052700	1.19805700	1.09681200

Table S63. Cartesien coordinates of perhydrobenzimidazole-2-ylidene 8, TS-2

C	2.67421400	-0.28245400	-0.76856100
C	2.94143200	-0.11488700	0.72516100
C	4.27491000	0.60291700	0.94292100
C	5.29662700	0.09525800	-0.12227000
C	4.96056300	-1.31313400	-0.66265000
C	3.55720900	-1.39260800	-1.34200000
C	0.69971600	0.16436000	0.31717300
H	4.13894300	1.68629200	0.84253500
H	5.32696600	0.80019000	-0.96232600
H	5.73217700	-1.62535800	-1.37398800
H	3.10531900	-2.37234300	-1.14923500
H	3.64688400	-1.28324500	-2.42809100
H	5.00391900	-2.03104500	0.16549900
H	6.30446900	0.09170300	0.30563700
H	4.64597300	0.41462100	1.95602900
H	2.98462300	-1.11361800	1.19301000
H	2.91464000	0.66767700	-1.27557000
N	1.21278900	-0.43727300	-0.77369900
N	1.69303100	0.52841000	1.15920000
C	0.43915200	-0.96892800	-1.89265300
H	0.09789200	-0.17459300	-2.56742500
H	1.07923500	-1.65662600	-2.44967300
H	-0.41605600	-1.52059000	-1.48651400
C	1.52407900	1.07578900	2.49700600
H	2.38069900	1.71973400	2.71721800
H	0.60689900	1.65826400	2.54095000
H	1.46073900	0.28023500	3.24890700
C	-0.74889400	0.32538500	0.55404800
H	-1.32613500	-0.72541300	0.09906900
O	-1.04475100	0.08143800	1.93286000
C	-1.35744300	1.58350900	0.01593200
C	-2.55657300	2.05516200	0.57987700
C	-0.81476900	2.29974600	-1.06683600
C	-3.19041300	3.18724500	0.07027500
H	-2.97072000	1.52788400	1.43205200
C	-1.45454900	3.42858700	-1.57773300
H	0.12706500	1.98574400	-1.51109300
C	-2.64885600	3.88063100	-1.01437600
H	-4.11567300	3.53055000	0.52710500
H	-1.01008200	3.96227100	-2.41470500
H	-3.14578400	4.76221900	-1.41007800
H	-1.40040600	-0.83772000	1.88194600
O	-1.72085400	-1.99645400	0.26770000
C	-3.05341700	-2.37088300	0.02466900
C	-3.94664700	-1.99843400	1.22940100
H	-3.93830400	-0.91318800	1.38859600
H	-4.99003500	-2.31233100	1.09279900
H	-3.56293900	-2.47803200	2.13844100
C	-3.07633700	-3.90160400	-0.16979000
H	-4.08996500	-4.28617100	-0.34593800
H	-2.44761800	-4.17829600	-1.02441200
H	-2.66733800	-4.39472100	0.71962300
C	-3.60160400	-1.68497500	-1.24627800
H	-2.98385000	-1.94770400	-2.11431500
H	-4.63521900	-1.98432200	-1.46522900
H	-3.58261200	-0.59400200	-1.13371200

Table S64. Cartesien coordinates of perhydrobenzimidazole-2-ylidene 8, IM-2

C	1.88638900	-0.85530500	-0.09605600
C	2.37798300	0.57714100	0.10489900
C	3.64112400	0.82383100	-0.73050600
C	4.51064400	-0.46733000	-0.75352600
C	4.28626400	-1.36342900	0.48308500
C	2.80661800	-1.83113900	0.64425500
C	0.04918400	0.56931300	0.11049900
H	3.35830100	1.09955100	-1.75348400
H	4.28245000	-1.04576100	-1.65745100
H	4.94700800	-2.23572000	0.42911700
H	2.55082400	-1.85948300	1.70998800
H	2.67672000	-2.84747800	0.25509700
H	4.59022200	-0.80856100	1.37951100
H	5.57118700	-0.20145000	-0.82482900
H	4.21227100	1.66250100	-0.31616800
H	2.62536500	0.71243100	1.17697500
H	1.93207500	-1.08344300	-1.17598600
N	0.49357200	-0.73656500	0.32051000
N	1.17964100	1.33166000	-0.23440200
C	-0.26509000	-1.78796800	0.95336400
H	-0.87038400	-2.37996500	0.25227200
H	0.41909000	-2.46215600	1.47648300
H	-0.95130500	-1.34773600	1.68351500
C	1.22840700	2.77700800	-0.31759000
H	2.09500500	3.06156400	-0.92311900
H	0.32563200	3.15379900	-0.79335300
H	1.32952900	3.26464300	0.66768300
C	-1.24727600	1.01297400	0.24687900
O	-1.47110100	2.38967600	0.49872900
C	-2.46936100	0.24753300	0.00274200
C	-3.67967700	0.62351100	0.62679000
C	-2.52568300	-0.81884100	-0.92236200
C	-4.86547400	-0.05926100	0.37512100
H	-3.67544800	1.46897400	1.30724300
C	-3.71291200	-1.50748900	-1.16332600
H	-1.63187600	-1.07873600	-1.48277500
C	-4.89238700	-1.13876200	-0.51317600
H	-5.77842800	0.25277000	0.87752300
H	-3.72076800	-2.32154700	-1.88481200
H	-5.81986700	-1.67039800	-0.70826100
H	-1.18380400	2.57240100	1.40569700

Table S65. Cartesien coordinates of perhydrobenzimidazole-2-ylidene 8, TS-3

C	-1.44854100	-1.71458700	-0.53408900
C	-1.99280800	-1.13405900	0.75992800
C	-2.88545100	-2.15899800	1.46257700
C	-3.72059800	-2.91033200	0.37789100
C	-3.89749100	-2.09726500	-0.92521000
C	-2.54335100	-1.71968700	-1.60429500
C	0.16186500	-0.39920100	0.46549700
H	-2.27243000	-2.87462300	2.02320800
H	-3.23093800	-3.86237700	0.13849300
H	-4.51716000	-2.66447700	-1.62759500
H	-2.62145600	-0.72589600	-2.05922100
H	-2.29727300	-2.43146200	-2.39981100
H	-4.45530600	-1.18039400	-0.69949100
H	-4.70417600	-3.16977900	0.78309800
H	-3.54274800	-1.65994100	2.18220000
H	-2.58464600	-0.23349100	0.52791800
H	-1.11313800	-2.75130800	-0.35325300
N	-0.25191800	-0.88834700	-0.72865900
N	-0.75824800	-0.67042700	1.41350300
C	0.49136400	-0.96257000	-1.97588600
H	0.95189300	-1.95061300	-2.10326600
H	-0.19897300	-0.77666900	-2.80338400
H	1.27718200	-0.21227300	-1.99710700
C	-0.81997500	-0.19070700	2.79273800
H	-1.18782300	-1.00481600	3.42485700
H	0.17454600	0.12970000	3.09191400
H	-1.51470100	0.65606200	2.85985500
C	1.41736600	0.38709500	0.64890100
O	1.64749800	0.80852900	1.93142100
C	2.66599100	-0.32509000	0.11691600
C	3.78768200	0.44155800	-0.23873500
C	2.78864500	-1.72143300	0.11566900
C	4.97636600	-0.17606000	-0.62464600
H	3.72573200	1.52379900	-0.16995400
C	3.97958100	-2.34132100	-0.27038300
H	1.95145600	-2.33939600	0.43538800
C	5.07697200	-1.56950500	-0.65081700
H	5.83280200	0.43554000	-0.89757400
H	4.05031300	-3.42646300	-0.26211500
H	6.00578000	-2.04755400	-0.95114300
H	1.84853500	1.92390900	1.63612200
C	1.19474300	1.96981100	-0.17204200
O	1.81645000	2.77064500	0.70021200
H	1.70145700	1.84263500	-1.14607100
C	-0.26806000	2.31255700	-0.39826800
C	-0.87559700	2.20150100	-1.65495100
C	-1.04092200	2.77763300	0.67593000
C	-2.22660900	2.51262900	-1.83351200
H	-0.27816600	1.89216900	-2.51079100
C	-2.39263100	3.07753900	0.50735700
H	-0.55001700	2.92148300	1.63340200
C	-2.99473700	2.93973200	-0.74839400
H	-2.67395100	2.43901700	-2.82246000
H	-2.97588700	3.44046200	1.35084200
H	-4.04415500	3.18934000	-0.88409000

Table S66. Cartesien coordinates of perhydrobenzimidazole-2-ylidene 8, IM-3

C	-1.35861700	-1.85811100	-0.55046500
C	-1.99019900	-1.22509600	0.67614300
C	-2.78128200	-2.26992100	1.46478800
C	-3.50351700	-3.21033400	0.44842000
C	-3.74002100	-2.55128100	-0.93054700
C	-2.42045500	-2.09116600	-1.62786900
C	0.08552200	-0.30635200	0.34911000
H	-2.10636500	-2.85500600	2.10054000
H	-2.90685500	-4.12025700	0.30866600
H	-4.27745800	-3.24895200	-1.58123100
H	-2.59600400	-1.16253000	-2.18305600
H	-2.07839300	-2.84463600	-2.34554200
H	-4.40123600	-1.68570300	-0.80184100
H	-4.46159100	-3.53822400	0.86491800
H	-3.50523200	-1.77967200	2.12369200
H	-2.67139600	-0.42117700	0.35268700
H	-0.91178900	-2.82753300	-0.26673800
N	-0.24978400	-0.92815100	-0.80644400
N	-0.82874300	-0.56464800	1.29374900
C	0.58738900	-1.13791500	-1.97911900
H	1.10890600	-2.10172700	-1.91856400
H	-0.05090200	-1.12736400	-2.86758000
H	1.33171800	-0.35222600	-2.06770200
C	-0.97345700	0.07130500	2.60482300
H	-1.22287900	-0.70096900	3.33908600
H	-0.02307200	0.56123900	2.82685700
H	-1.78599600	0.80679800	2.56148200
C	1.34650900	0.58160100	0.55508600
O	1.51275800	1.02302300	1.80804800
C	2.58994800	-0.25586900	0.14643900
C	3.67514000	0.30536400	-0.54135400
C	2.71028800	-1.57460500	0.61056200
C	4.82800800	-0.44488800	-0.78549900
H	3.63384100	1.34503600	-0.84883000
C	3.85748900	-2.32778100	0.36125800
H	1.90104800	-2.01356900	1.19138100
C	4.92257700	-1.76596900	-0.34611600
H	5.65926000	0.01138500	-1.31782400
H	3.92336600	-3.34989000	0.72723300
H	5.81979900	-2.34774000	-0.54107200
H	2.09014900	2.46259700	1.10936900
C	1.15561300	1.90421300	-0.40272400

O	2.01883400	2.84243600	0.17881600
H	1.48307500	1.69188300	-1.42898100
C	-0.27744600	2.40542500	-0.44399800
C	-1.07577400	2.24674500	-1.58413300
C	-0.83389600	3.03862400	0.67801500
C	-2.40162400	2.68704100	-1.60377700
H	-0.64838500	1.79035700	-2.47532200
C	-2.15912800	3.47474800	0.66428700
H	-0.21077000	3.18585200	1.55310600
C	-2.95056900	3.29774000	-0.47474200
H	-2.99889400	2.56854300	-2.50506200
H	-2.57313200	3.96786700	1.54084500
H	-3.97886000	3.65043200	-0.48807200

Table S67. Cartesien coordinates of perhydrobenzimidazole-2-ylidene 8, TS-4

C	-2.05651700	-1.58441000	-0.50722100
C	-2.51341000	-0.57941500	0.53654100
C	-3.52921900	-1.22133900	1.48467300
C	-4.45270700	-2.17105800	0.65762900
C	-4.53824000	-1.78716100	-0.83758900
C	-3.15126600	-1.79584400	-1.55583700
C	-0.25442200	-0.25840700	0.12259500
H	-3.00882800	-1.79211000	2.26297000
H	-4.07974900	-3.19977100	0.73795700
H	-5.22632900	-2.46754300	-1.35080900
H	-3.11395800	-0.99436100	-2.30334200
H	-2.99614200	-2.74238000	-2.08549400
H	-4.98206100	-0.78730200	-0.92083500
H	-5.45907300	-2.17973700	1.08994900
H	-4.12019900	-0.44922300	1.98907800
H	-2.99000000	0.27418900	0.02294600
H	-1.84775700	-2.54725200	-0.00736100
N	-0.75774400	-1.00230900	-0.89220500
N	-1.21711300	-0.10178600	1.04856600
C	0.03604800	-1.64680800	-1.92423600
H	0.32770600	-2.66425000	-1.62923800
H	-0.54526500	-1.69925900	-2.85051000
H	0.94155600	-1.07192600	-2.10680200
C	-1.18309800	0.88240200	2.12596600
H	-1.65425700	0.45636300	3.01798800
H	-0.14395800	1.13427100	2.33483200
H	-1.73211200	1.78656300	1.83108300
C	1.71075500	0.33366600	0.55530400
O	1.76346000	0.74249600	1.74464900
C	2.38713800	-1.01132500	0.28621800
C	3.36180000	-1.18910300	-0.70388900
C	2.09101100	-2.08469200	1.13876700
C	3.99652700	-2.42554700	-0.86062100
H	3.65712500	-0.35293500	-1.32947500
C	2.71255500	-3.32032700	0.97499500
H	1.37084500	-1.92998000	1.93736500
C	3.66767300	-3.49722100	-0.03167000
H	4.75697100	-2.54421500	-1.62870300
H	2.46199300	-4.14470900	1.63851500
H	4.15918000	-4.45860900	-0.15734400
H	3.34936900	1.93040900	0.59527600
C	1.87547400	1.43037600	-0.54093900
O	3.19860700	1.94922000	-0.36702900
H	1.84944200	0.98524400	-1.54115700
C	0.82862600	2.52778200	-0.47569200
C	-0.17780700	2.61024000	-1.44580900
C	0.84926700	3.48512700	0.54840200
C	-1.15008000	3.61149900	-1.39285600
H	-0.19736400	1.88453200	-2.25610600
C	-0.11891200	4.48775900	0.60422400
H	1.62395800	3.43844600	1.30514800
C	-1.12397000	4.55450200	-0.36420300
H	-1.91728800	3.66233100	-2.16184000
H	-0.08678500	5.22250700	1.40506700
H	-1.87290900	5.34144600	-0.32316600

Table S68. Cartesien coordinates of 4,5-diphenyl-imidazole-2-ylidene 9

C	-0.00027200	3.12453600	-0.00006000
C	-0.68630200	0.91219900	-0.01658800
C	0.68601900	0.91230000	0.01654100
N	-1.06418600	2.26257500	-0.02884300
C	-2.42777100	2.75679700	-0.14834900
H	-2.94662000	2.26982500	-0.97996000
H	-3.00353800	2.58844100	0.76781500
H	-2.35752000	3.82876900	-0.33334200
N	1.06374300	2.26270400	0.02874100
C	2.42729100	2.75700600	0.14827500
H	2.94582300	2.27086300	0.98057900
H	3.00342400	2.58771600	-0.76747900
H	2.35695200	3.82915900	0.33218000
C	1.62625600	-0.22191500	0.07871800
C	1.47445700	-1.21466400	1.06246300
C	2.68626700	-0.34560900	-0.83667400
C	2.35397600	-2.29396400	1.12841900
H	0.66256000	-1.12941000	1.77821100
C	3.57059600	-1.42122100	-0.76383000
H	2.80483200	0.39538900	-1.62209400
C	3.40824500	-2.39944300	0.21893100
H	2.21950900	-3.05040100	1.89715700
H	4.38245600	-1.49925600	-1.48224300
H	4.09681300	-3.23829100	0.27428500
C	-1.62628900	-0.22221200	-0.07871100
C	-2.68692900	-0.34559000	0.83600200
C	-1.47359200	-1.21554300	-1.06174200

C	-3.57096100	-1.42144800	0.76319300
H	-2.80625100	0.39585400	1.62088000
C	-2.35281100	-2.29508500	-1.12764500
H	-0.66124500	-1.13054200	-1.77700400
C	-3.40769800	-2.40025000	-0.21883600
H	-4.38331400	-1.49921300	1.48107900
H	-2.21763200	-3.05195500	-1.89583200
H	-4.09603800	-3.23928600	-0.27415800

Table S69. Cartesien coordinates of 4,5-diphenyl-imidazole-2-ylidene 9, TS-1

C	-1.14431600	-0.48734700	0.48323200
C	0.83291900	0.59566200	0.18134100
C	1.09299800	-0.75161200	0.13696700
N	-0.54413000	0.72122000	0.40279100
C	-1.26867100	1.96910400	0.66287800
H	-0.56401300	2.72142500	1.01834800
H	-1.75584500	2.32847600	-0.24814700
H	-2.01562100	1.74945400	1.43068100
N	-0.14323600	-1.38789000	0.32562500
C	-0.35462800	-2.83111800	0.29014200
H	0.21414900	-3.27004000	-0.53281800
H	-0.04177400	-3.30000100	1.22789600
H	-1.41642800	-3.01970400	0.13920600
C	2.35788600	-1.46667800	-0.11511200
C	3.11495900	-1.17730600	-1.26323000
C	2.83731000	-2.43894500	0.77974200
C	4.31583000	-1.84109000	-1.50785000
H	2.75271400	-0.43027800	-1.96283900
C	4.03452100	-3.10810700	0.52805300
H	2.28004600	-2.65526200	1.68693000
C	4.77752300	-2.81137700	-0.61606500
H	4.88820000	-1.60471800	-2.40072600
H	4.39123600	-3.85494500	1.23214500
H	5.71149600	-3.33150100	-0.81023300
C	1.75898400	1.73402300	0.04623100
C	1.49331700	2.78437300	-0.84946500
C	2.94028100	1.77805300	0.80545300
C	2.38364400	3.84958500	-0.97816700
H	0.59273400	2.75756200	-1.45628700
C	3.83235200	2.84005600	0.66840200
H	3.15094900	0.97717400	1.50725800
C	3.55621900	3.88032500	-0.22108500
H	2.16329900	4.65278300	-1.67604800
H	4.74063800	2.85872600	1.26448700
H	4.24989000	4.71037800	-0.32309500
C	-2.86852400	-0.68620500	1.42105200
H	-2.73396200	-1.78391400	1.56625100
O	-2.82553200	0.07027800	2.42456700
C	-3.88041500	-0.41416500	0.30794000
C	-4.77029000	0.65200300	0.45934800
C	-3.99705500	-1.23708500	-0.81806700
C	-5.74539400	0.90709200	-0.50769200
H	-4.68664800	1.25740600	1.35693100
C	-4.96968700	-0.98968700	-1.78530500
H	-3.31617800	-2.07799200	-0.94327100
C	-5.84672600	0.08916100	-1.63405200
H	-6.43279400	1.73987600	-0.37752200
H	-5.04726200	-1.63622600	-2.65640700
H	-6.60721800	0.28349200	-2.38633600

Table S70. Cartesien coordinates of 4,5-diphenyl-imidazole-2-ylidene 9, IM-1

C	1.14329800	-0.67911700	-0.50535600
C	-0.72483400	0.54516100	-0.22368900
C	-1.07795900	-0.77701300	-0.10712000
N	0.64924500	0.57772100	-0.46613200
C	1.43799800	1.73580200	-0.90367700
H	0.75647000	2.50881400	-1.25830100
H	2.04287000	2.12217100	-0.07964800
H	2.07791700	1.35632300	-1.71047300
N	0.10459500	-1.51468900	-0.27669300
C	0.23693500	-2.96623500	-0.15482300
H	-0.67400600	-3.36293800	0.29185700
H	0.38984400	-3.41977000	-1.13823500
H	1.08623400	-3.20814200	0.48514200
C	-2.39329000	-1.38123800	0.17042500
C	-3.13541000	-0.97711400	1.29300800
C	-2.93844200	-2.35581100	-0.68443200
C	-4.38795200	-1.53109000	1.55128900
H	-2.72203300	-0.22791200	1.96117700
C	-4.18753600	-2.91520800	-0.41750100
H	-2.38838300	-2.66055600	-1.57072100
C	-4.91626300	-2.50410300	0.70017800
H	-4.94875900	-1.20716300	2.42369700
H	-4.59509500	-3.66546700	-1.08947000
H	-5.89074600	-2.93824700	0.90580800
C	-1.56280200	1.75364200	-0.13138800
C	-1.19321000	2.82465700	0.70031000
C	-2.75584100	1.84793400	-0.86640000
C	-1.99653100	3.96038000	0.79149700
H	-0.28036800	2.75973700	1.28558300
C	-3.56030800	2.98174200	-0.76674000
H	-3.04416000	1.03157500	-1.52106100
C	-3.18282300	4.04186900	0.05981100
H	-1.69733700	4.77940300	1.43974000
H	-4.47895600	3.04042200	-1.34388700
H	-3.80838800	4.92724400	0.13221800
C	2.54035300	-1.05473800	-1.07547300
H	2.58142500	-2.17496900	-0.98266900
O	2.55512300	-0.59163200	-2.31856500

C	3.65915600	-0.54629100	-0.12640900
C	4.74286000	0.11723100	-0.70308600
C	3.65673500	-0.77151700	1.25489300
C	5.80920400	0.55324600	0.08629500
H	4.71116800	0.27159300	-1.77815500
C	4.71642600	-0.33175900	2.05025300
H	2.81826400	-1.29205100	1.71929400
C	5.79833000	0.33265800	1.46549700
H	6.65087100	1.06655900	-0.37374100
H	4.70043300	-0.50728500	3.12376100
H	6.62630600	0.67397200	2.08220100

Table S71. Cartesien coordinates of 4,5-diphenyl-imidazole-2-ylidene 9, TS-2

C	-0.45022300	-0.41695800	-0.21892400
C	1.78667100	-0.63221900	-0.39138300
C	1.52697400	0.54418400	0.27111500
N	0.54949300	-1.20901900	-0.67918100
C	0.32317000	-2.47980000	-1.37459500
H	1.15333000	-2.65946500	-2.05813600
H	0.26043500	-3.29859400	-0.65190200
H	-0.61572300	-2.39217000	-1.92044800
N	0.13914200	0.65393000	0.36346600
C	-0.61804300	1.74934200	0.98719000
H	0.08528100	2.51612900	1.30630500
H	-1.33020800	2.13751500	0.25011800
H	-1.16084800	1.37143300	1.85695400
C	2.47716700	1.54173800	0.80427800
C	3.42082800	1.16591800	1.77282800
C	2.47240900	2.86758100	0.33811800
C	4.33617700	2.09482100	2.26614700
H	3.43074600	0.14324500	2.13763300
C	3.38441600	3.79608700	0.83903500
H	1.76104800	3.16524700	-0.42754900
C	4.31786400	3.41197500	1.80379100
H	5.06042200	1.79006100	3.01642900
H	3.36950500	4.81757500	0.46944800
H	5.02902700	4.13585400	2.19195800
C	3.08307100	-1.21712800	-0.78469400
C	3.42686500	-2.53169400	-0.42613600
C	4.00805600	-0.45010000	-1.51170900
C	4.66076300	-3.06663500	-0.79362600
H	2.73198700	-3.13044600	0.15579100
C	5.24401700	-0.98509700	-1.87069000
H	3.75034500	0.56501900	-1.79697300
C	5.57258200	-2.29495000	-1.51623900
H	4.91219400	-4.08417700	-0.50769400
H	5.94810400	-0.37957100	-2.43451700
H	6.53463700	-2.71206400	-1.80055500
C	-1.91332600	-0.61024500	-0.37658700
H	-2.47333300	0.60788300	-0.53409800
O	-2.19055200	-1.04113800	-1.72074900
C	-2.56127100	-1.46016500	0.66112200
C	-3.73678200	-2.17055900	0.34951600
C	-2.08068000	-1.54438700	1.98345000
C	-4.40446100	-2.91514500	1.32023600
H	-4.10525200	-2.13896700	-0.66984200
C	-2.75407500	-2.28692400	2.95242800
H	-1.16037600	-1.03329300	2.26099300
C	-3.92369600	-2.97797700	2.63026600
H	-5.30893000	-3.45459300	1.04791900
H	-2.35599900	-2.33097400	3.96384400
H	-4.44717200	-3.55883500	3.38482100
H	-2.48971300	-0.20057400	-2.13683100
O	-2.78250000	1.59721800	-1.26938400
C	-4.10063900	2.09325200	-1.20129100
C	-4.14559900	3.37975000	-2.04823600
H	-5.14429800	3.83579700	-2.05794000
H	-3.43323200	4.11286100	-1.65199800
H	-3.85596100	3.15572200	-3.08135300
C	-5.10062700	1.06611200	-1.77411000
H	-5.08630600	0.14422300	-1.18116500
H	-6.12941600	1.44954400	-1.77820100
H	-4.82911800	0.81294000	-2.80641300
C	-4.48579000	2.42001100	0.25789000
H	-3.79231400	3.15975700	0.67701200
H	-5.50183500	2.82876100	0.33456300
H	-4.43796700	1.51642400	0.87776000

Table S72. Cartesien coordinates of 4,5-diphenyl-imidazole-2-ylidene 9, IM-2

C	1.13325400	0.75260200	-0.16307500
C	-1.14647300	0.75917800	-0.00596800
C	-0.74896400	-0.53770600	-0.12579200
N	0.00507600	1.58899500	-0.04704800
C	0.09067600	2.75475600	0.84407400
H	-0.81802900	3.34978600	0.74973300
H	0.20600900	2.44159400	1.89079500
H	0.95535600	3.35377800	0.56107500
N	0.66289300	-0.56789800	-0.21579300
C	1.37810900	-1.58509800	-0.97826200
H	0.66514200	-2.31578800	-1.36079500
H	1.90192500	-1.10637800	-1.81444300
H	2.12690000	-2.09976400	-0.36862600
C	-1.54957000	-1.77064100	-0.17609700
C	-1.18343700	-2.88965600	0.59477000
C	-2.69210300	-1.86146100	-0.99030600
C	-1.94371000	-4.05694500	0.56068600
H	-0.30455800	-2.83212700	1.23096300
C	-3.45391700	-3.02815200	-1.01604100
H	-2.97560900	-1.01303400	-1.60491700

C	-3.08373500	-4.13071500	-0.24292500
H	-1.64742100	-4.90880400	1.16705000
H	-4.33402800	-3.07938900	-1.65155100
H	-3.67583500	-5.04137400	-0.26978000
C	-2.49526700	1.32507000	0.13743200
C	-3.42667900	0.77194200	1.03379600
C	-2.88061700	2.44575300	-0.62202800
C	-4.70613600	1.31113100	1.15153000
H	-3.13776500	-0.08015900	1.64085100
C	-4.15821900	2.98791700	-0.49483400
H	-2.17350100	2.87820100	-1.32478400
C	-5.07793900	2.42200700	0.39070800
H	-5.41143900	0.86883800	1.85018100
H	-4.43755400	3.85100300	-1.09353400
H	-6.07372000	2.84526400	0.49001900
C	2.42546400	1.19354100	-0.32658100
O	2.61097400	2.53817800	-0.70025000
C	3.66019400	0.47552000	-0.03766400
C	4.87089200	0.87486200	-0.64626000
C	3.72036100	-0.57929000	0.90077400
C	6.06680800	0.22397600	-0.36083800
H	4.85472400	1.70664500	-1.34225400
C	4.91961800	-1.23262100	1.17499900
H	2.82143800	-0.85845800	1.44380900
C	6.10262300	-0.84162500	0.54376100
H	6.98145300	0.55061100	-0.85040200
H	4.93298400	-2.03866200	1.90514900
H	7.03853300	-1.34800800	0.76352700
H	2.01401600	2.71706300	-1.44533900

Table S73. Cartesien coordinates of 4,5-diphenyl-imidazole-2-ylidene 9, TS-3

C	-0.07622200	-0.56444500	0.28520700
C	2.16929200	-0.72501200	0.13566000
C	1.84572300	0.60256400	0.05510900
N	0.96995100	-1.42637200	0.29831900
C	0.90909300	-2.86778000	0.60203900
H	0.69193200	-3.43547400	-0.30307600
H	1.87966900	-3.15522000	1.00749400
H	0.11300900	-3.05009800	1.31579400
N	0.45432100	0.68035300	0.15250500
C	-0.29294200	1.93034900	0.00616900
H	-0.07102400	2.37686900	-0.96608000
H	-1.35486900	1.72431500	0.08698500
H	-0.00845600	2.62875600	0.79566600
C	2.71335900	1.78058400	-0.15267300
C	2.80542800	2.79361300	0.81610600
C	3.47256400	1.89349900	-1.32786400
C	3.63032900	3.89829700	0.60849500
H	2.24341900	2.70531600	1.74222700
C	4.30197200	2.99614600	-1.52982700
H	3.40668900	1.11411500	-2.08095800
C	4.37974400	4.00222800	-0.56521700
H	3.69343500	4.67340300	1.36716800
H	4.88357800	3.07084200	-2.44432000
H	5.02351500	4.86256800	-0.72550200
C	3.49758700	-1.36129400	0.06438700
C	4.53999300	-0.91445200	0.89223600
C	3.75248300	-2.39815800	-0.84980700
C	5.80637600	-1.49103600	0.80755100
H	4.35120500	-0.11690200	1.60414000
C	5.01813100	-2.97678700	-0.92646300
H	2.96045500	-2.73952000	-1.51028200
C	6.04817600	-2.52493800	-0.09878500
H	6.60272300	-1.13628600	1.45585200
H	5.20084700	-3.77632300	-1.63890200
H	7.03448200	-2.97631500	-0.16071700
C	-1.53427200	-0.96379500	0.23051600
O	-1.65185900	-2.31629600	0.09823400
C	-2.38830200	-0.42503100	1.36151900
C	-3.70272300	-0.91215400	1.47525700
C	-1.93510700	0.45575700	2.35584000
C	-4.53946700	-0.49301500	2.50444000
H	-4.05075900	-1.63738200	0.75096700
C	-2.77269400	0.87497700	3.39369300
H	-0.90500900	0.80132100	2.35626900
C	-4.08356200	0.41125100	3.46845400
H	-5.55377000	-0.88040200	2.55893500
H	-2.38771600	1.55360800	4.15138700
H	-4.73752700	0.73498800	4.27394100
H	-1.73075300	-2.32990800	-1.06261400
C	-2.00800900	-0.48587700	-1.51688900
H	-1.29970800	0.31700100	-1.78958900
O	-1.79032000	-1.65223500	-2.12025700
C	-3.42919400	0.03120400	-1.59582900
C	-4.46777000	-0.86932600	-1.87303900
C	-3.74962700	1.38764600	-1.45337400
C	-5.78746700	-0.43231900	-1.97101900
H	-4.20511000	-1.90998300	-2.03366000
C	-5.06928400	1.83134200	-1.55208100
H	-2.95944900	2.11722000	-1.28873400
C	-6.09625700	0.92052400	-1.80450900
H	-6.57856100	-1.14662300	-2.18807000
H	-5.29396300	2.88970500	-1.44129800
H	-7.12485500	1.26342700	-1.88442700

Table S74. Cartesien coordinates of 4,5-diphenyl-imidazole-2-ylidene 9, IM-3

C	-0.10537400	0.09905900	-0.32809400
C	2.05394600	-0.55785000	-0.28263200
C	2.02668700	0.78532700	-0.02050200

N	0.73351000	-0.95612600	-0.46891800
C	0.29665300	-2.32696700	-0.76569000
H	1.13868600	-2.87612400	-1.18313600
H	-0.04311700	-2.81552900	0.15025300
H	-0.52642700	-2.23695800	-1.47845900
N	0.68033400	1.17605400	-0.06403200
C	0.26010700	2.58415400	0.00059500
H	-0.46861000	2.76242800	-0.79239600
H	-0.16513500	2.81666200	0.98073500
H	1.14273300	3.20227500	-0.15586500
C	3.15240100	1.69852100	0.25618500
C	3.18595000	2.47578000	1.42690200
C	4.23224900	1.77745400	-0.63791100
C	4.26725700	3.31481400	1.69073700
H	2.36706100	2.41118800	2.13826900
C	5.31653500	2.61107200	-0.36732100
H	4.21520400	1.18405200	-1.54670600
C	5.33595800	3.38429100	0.79464500
H	4.27801700	3.90845900	2.60063600
H	6.14362700	2.66132400	-1.06997200
H	6.17935600	4.03708400	1.00177500
C	3.21628400	-1.47020600	-0.34774100
C	3.98203300	-1.71514200	0.80173700
C	3.58665300	-2.08437100	-1.55564900
C	5.09120100	-2.55879300	0.74613100
H	3.70258900	-1.24145900	1.73807500
C	4.69186000	-2.93317300	-1.60694100
H	3.01302500	-1.88486300	-2.45693500
C	5.44598900	-3.17254500	-0.45627500
H	5.67518200	-2.73968200	1.64424900
H	4.96741300	-3.40158600	-2.54769200
H	6.30792400	-3.83269700	-0.49780100
C	-1.65847300	-0.09221700	-0.59976500
O	-1.75067500	-0.58424000	-1.84748100
C	-2.19140200	-0.99983100	0.53348400
C	-3.02826500	-2.06670100	0.19499400
C	-1.90014200	-0.77110400	1.88389500
C	-3.56724500	-2.88753700	1.18586200
H	-3.23599900	-2.22762800	-0.85788200
C	-2.43440200	-1.59284200	2.87863000
H	-1.24808500	0.05400500	2.16831200
C	-3.27174900	-2.65480700	2.53136000
H	-4.22008100	-3.71175000	0.90829000
H	-2.19695500	-1.40383400	3.92299400
H	-3.68931900	-3.29600700	3.30356000
H	-1.86283000	1.11503400	-2.34014900
C	-2.44454400	1.29627200	-0.58008100
H	-2.13631300	1.91767300	0.26826600
O	-2.05959700	1.92995900	-1.79004900
C	-3.95207200	1.12503300	-0.49737000
C	-4.67541400	0.60315700	-1.57926500
C	-4.65024700	1.51387400	0.65055600
C	-6.06087400	0.46876800	-1.50488200
H	-4.13681700	0.29026800	-2.46648400
C	-6.03825900	1.38192200	0.72776400
H	-4.10284900	1.92751400	1.49549400
C	-6.74872700	0.85838300	-0.35231600
H	-6.60795200	0.06016500	-2.35131700
H	-6.56241000	1.69372900	1.62801500
H	-7.83010100	0.75822800	-0.29948300

Table S75. Cartesien coordinates of 4,5-diphenyl-imidazole-2-ylidene 9, TS-4

C	0.01327500	-0.08574200	-0.18223200
C	-2.17519800	0.54098600	-0.25047300
C	-2.14187000	-0.79635400	0.04592200
N	-0.84263500	0.94572600	-0.38560800
C	-0.40544600	2.32529700	-0.62589900
H	-1.21402800	2.87754700	-1.10256600
H	-0.14962600	2.80884200	0.32074600
H	0.47004700	2.28950900	-1.27477400
N	-0.78592800	-1.15566300	0.07077400
C	-0.29835600	-2.53309400	0.19117700
H	0.45778300	-2.69789700	-0.57810500
H	0.12298700	-2.71047000	1.18579100
H	-1.13427400	-3.21525600	0.03865400
C	-3.26000100	-1.72638700	0.29047400
C	-3.30741600	-2.51332100	1.45453000
C	-4.31625000	-1.82357200	-0.63045600
C	-4.37666300	-3.37734000	1.68602500
H	-2.50893100	-2.43498600	2.18734500
C	-5.38872000	-2.68171500	-0.39242800
H	-4.28874200	-1.22454700	-1.53531700
C	-5.42119600	-3.46383100	0.76357100
H	-4.39710900	-3.97717600	2.59186000
H	-6.19675400	-2.74457400	-1.11614900
H	-6.25535600	-4.13593800	0.94512200
C	-3.34164100	1.43697900	-0.39500100
C	-4.19981500	1.66084600	0.69279600
C	-3.62581300	2.06338300	-1.62049400
C	-5.31176900	2.49192600	0.55989900
H	-3.98857200	1.17921700	1.64284100
C	-4.73333600	2.90101800	-1.74889100
H	-2.98291100	1.87958500	-2.47730600
C	-5.57885500	3.11784600	-0.65896500
H	-5.96668200	2.65450300	1.41156000
H	-4.93980700	3.37762700	-2.70329700
H	-6.44283800	3.76888100	-0.76036700
C	1.98199400	0.27190800	-0.61341100
O	1.95750300	0.78364800	-1.77265700
C	2.37088300	1.14105200	0.57583700
C	3.06361100	2.32938500	0.31973700
C	2.13077100	0.77265700	1.90584700

C	3.50171900	3.13773800	1.36992200
H	3.25059800	2.60102000	-0.71427300
C	2.56679500	1.57791100	2.95729600
H	1.58084800	-0.14063900	2.11981800
C	3.25463700	2.76520100	2.69195900
H	4.03988900	4.05774900	1.15521500
H	2.36750900	1.28162800	3.98429500
H	3.59437800	3.39379000	3.51116300
H	1.87327100	-1.06002700	-2.33996900
C	2.57299800	-1.17343600	-0.59122000
H	2.23359000	-1.71783300	0.29513100
O	2.06962300	-1.82409900	-1.74795100
C	4.09631900	-1.14542600	-0.57739400
C	4.81414300	-0.64079700	-1.67075400
C	4.80562000	-1.63682600	0.52305000
C	6.20757100	-0.62986100	-1.65822900
H	4.26987600	-0.24709500	-2.52286800
C	6.20209900	-1.62711200	0.53907300
H	4.26085700	-2.03609400	1.37625900
C	6.90747600	-1.12359300	-0.55359300
H	6.75088300	-0.23452100	-2.51309700
H	6.73611000	-2.01704700	1.40214000
H	7.99455600	-1.11699200	-0.54721000

Table S76. Cartesien coordinates of benzimidazole-2-ylidene 10

C	0.17232600	-0.70291800	-0.00006700
C	0.17232700	0.70291800	0.00000600
C	1.36294700	1.42820700	-0.00009000
C	2.55632400	0.70203900	-0.00022900
C	2.55632200	-0.70204000	-0.00028100
C	1.36294500	-1.42821000	-0.00019800
C	-2.02733600	0.00000000	0.00021100
H	1.36669300	2.51405900	-0.00006300
H	3.50302100	1.23483800	-0.00029600
H	3.50301800	-1.23484200	-0.00039000
H	1.36669300	-2.51406300	-0.00022900
N	-1.17175000	-1.07520600	0.00003200
N	-1.17174800	1.07520700	0.00019700
C	-1.63878700	-2.44848200	0.00017300
H	-1.28640900	-2.98225000	-0.89047400
H	-1.28720900	-2.98183000	0.89139200
H	-2.72870400	-2.42133700	-0.00031300
C	-1.63878500	2.44848400	0.00017700
H	-1.28610500	2.98226900	0.89069400
H	-1.28750600	2.98181400	-0.89117200
H	-2.72870200	2.42134000	0.00102900

Table S77. Cartesien coordinates of benzimidazole-2-ylidene 10, TS-1

C	-2.38228200	0.65395700	0.00287200
C	-2.17664300	-0.71821900	-0.20811800
C	-3.19938200	-1.54038400	-0.68025000
C	-4.43382100	-0.94084500	-0.92933400
C	-4.63872700	0.43335700	-0.71694800
C	-3.61475600	1.25601800	-0.24714900
C	-0.22913300	0.16763100	0.53377800
H	-3.04348800	-2.60033200	-0.85222400
H	-5.25386400	-1.54935600	-1.29885600
H	-5.61333200	0.86467300	-0.92521700
H	-3.77454600	2.31772300	-0.08765400
N	-1.16257200	1.15498000	0.46420400
N	-0.84866300	-0.96898000	0.13874700
C	-0.93415800	2.55385100	0.79184900
H	-0.94788900	3.17052900	-0.11337500
H	-1.71146500	2.90586900	1.47716600
H	0.03590400	2.64766100	1.27839500
C	-0.20830500	-2.28388400	0.11234100
H	-0.95165100	-3.04142500	0.37379200
H	0.19321400	-2.49534600	-0.88340400
H	0.58691900	-2.27075500	0.86217100
C	1.43623900	0.07124100	1.52858000
H	1.30922000	1.07906200	1.99460000
O	1.37464900	-0.94793100	2.26542200
C	2.47774000	0.13708900	0.40877000
C	3.33052200	-0.95359700	0.22356600
C	2.64890700	1.27373100	-0.38967900
C	4.32081800	-0.92158100	-0.76059200
H	3.20818400	-1.80985000	0.88014500
C	3.63726600	1.31252300	-1.37213000
H	2.00245000	2.13792700	-0.24239300
C	4.47507400	0.20950300	-1.56384400
H	4.97941600	-1.77664800	-0.89460100
H	3.75846600	2.20145400	-1.98680700
H	5.24775900	0.23792500	-2.32805100

Table S78. Cartesien coordinates of benzimidazole-2-ylidene 10, IM-1

C	2.45525300	0.45285400	0.24289900
C	1.98149100	-0.82886900	-0.08793700
C	2.84655200	-1.91623000	-0.18660000
C	4.20256400	-1.68088900	0.05012900
C	4.67461500	-0.40196800	0.37925400
C	3.80665600	0.68722500	0.48360200
C	0.22587800	0.57296000	-0.04499700
H	2.48639200	-2.90966600	-0.43278200
H	4.90314500	-2.50760300	-0.01874300
H	5.73471400	-0.25368800	0.56136700
H	4.17690300	1.67284600	0.74648900

N	1.33922700	1.28935200	0.27578500
N	0.60030200	-0.71906800	-0.24647000
C	1.36654700	2.74733400	0.33227700
H	0.93320300	3.12026800	1.26413800
H	2.40440400	3.07618500	0.26480200
H	0.81021000	3.13072500	-0.52714900
C	-0.26657100	-1.73247000	-0.84314800
H	0.36318800	-2.52259000	-1.25521000
H	-0.95203000	-2.15407400	-0.10491300
H	-0.82653800	-1.24941600	-1.64634000
C	-1.09223400	1.20742500	-0.42714500
H	-1.15630200	2.17207200	0.14194200
O	-0.85002800	1.32224200	-1.74552800
C	-2.34487500	0.42500800	0.00561700
C	-3.30368900	0.13356100	-0.96552700
C	-2.58282000	0.05963900	1.33549500
C	-4.48540000	-0.52354500	-0.61617200
H	-3.08779800	0.43548100	-1.98668300
C	-3.75804200	-0.60675500	1.68684300
H	-1.84581500	0.29622500	2.10287500
C	-4.71393800	-0.89930600	0.70940700
H	-5.22927300	-0.74408800	-1.37837200
H	-3.93121400	-0.89391900	2.72140800
H	-5.63158300	-1.41452100	0.98222200

Table S79. Cartesien coordinates of benzimidazole-2-ylidene 10, TS-2

C	2.92498500	-0.80293300	0.18984100
C	3.00217500	0.52688200	-0.24965800
C	4.19024800	1.06700400	-0.73928100
C	5.30691300	0.23064500	-0.76679700
C	5.23315800	-1.09835100	-0.32112400
C	4.04269600	-1.63724500	0.16714700
C	0.88787600	0.12695200	0.43041000
H	4.24967700	2.09088900	-1.09300600
H	6.24947400	0.61707800	-1.14237500
H	6.12112500	-1.72224400	-0.35556200
H	3.99454300	-2.66301900	0.51566200
N	1.61239500	-1.02035700	0.59167900
N	1.73757200	1.08476300	-0.06293300
C	1.10279800	-2.30837100	1.07503200
H	0.09849500	-2.48781100	0.66859700
H	1.78726300	-3.08435600	0.72736000
H	1.06494600	-2.30652300	2.16660300
C	1.49071500	2.51907000	-0.20030800
H	2.43383400	3.03799800	-0.01572100
H	1.12324900	2.76773700	-1.19942400
H	0.75692800	2.84177500	0.53424900
C	-0.55411800	0.19050800	0.68146600
H	-1.09568200	-0.75275200	0.04623300
O	-0.83485100	-0.30198800	1.99107800
C	-1.30601200	1.44790500	0.33123700
C	-1.90259000	2.23174100	1.32933700
C	-1.50165200	1.80919500	-1.01238500
C	-2.63724500	3.36977100	0.99363200
H	-1.78877900	1.92610100	2.36413900
C	-2.23236400	2.94964300	-1.34742600
H	-1.08652500	1.18262900	-1.79953500
C	-2.79908800	3.73894600	-0.34408100
H	-3.08933500	3.96885500	1.78036900
H	-2.37532600	3.21096400	-2.39304700
H	-3.37621700	4.62258500	-0.60314700
H	-1.45067400	-1.04999100	1.78002200
O	-1.74030200	-1.99408400	0.20599500
C	-2.89990900	-2.31767500	-0.51603700
C	-3.25686700	-3.78227900	-0.18671400
H	-4.16522500	-4.11438700	-0.70651800
H	-2.43128600	-4.44316200	-0.47560700
H	-3.41499800	-3.89306800	0.89221800
C	-2.63602900	-2.18124600	-2.03104800
H	-1.77556100	-2.79811200	-2.31594500
H	-3.49891300	-2.49164900	-2.63476400
H	-2.40580900	-1.13857200	-2.28458600
C	-4.07051200	-1.39903300	-0.10720100
H	-4.26079800	-1.49170100	0.96880400
H	-3.82685600	-0.35106200	-0.31760700
H	-4.99716400	-1.64725300	-0.64146700

Table S80. Cartesien coordinates of benzimidazole-2-ylidene 10, IM-2

C	2.48280200	0.49213500	0.08727100
C	2.03988000	-0.82564200	-0.13341500
C	2.92955900	-1.89088800	-0.17601400
C	4.29326600	-1.61204900	0.00733200
C	4.73398800	-0.30768900	0.23203000
C	3.83278400	0.76791500	0.27166400
C	0.21468000	0.54070600	-0.13930600
H	2.58448200	-2.90807400	-0.33329300
H	5.01008600	-2.42744200	-0.02124100
H	5.79278600	-0.11402600	0.37790100
H	4.18972300	1.78029800	0.43248300
N	1.36202600	1.32176000	0.06171300
N	0.65345100	-0.78460600	-0.29452100
C	1.33557500	2.66296500	0.62106700
H	0.70383600	2.69117900	1.51793300
H	2.35200500	2.94129800	0.90369800
H	0.94590700	3.38230400	-0.10029200
C	-0.07899800	-1.79652200	-1.03664500
H	0.63416700	-2.39995700	-1.60520700
H	-0.66627200	-2.45217000	-0.38463100
H	-0.76642500	-1.30454100	-1.73042800
C	-1.07696400	0.99718700	-0.22736100

O	-1.22862800	2.34846200	-0.58142300
C	-2.30571900	0.23846100	-0.01633100
C	-3.50411900	0.65367000	-0.64081100
C	-2.38440000	-0.84790500	0.88583700
C	-4.70783100	-0.00382300	-0.39847300
H	-3.47111800	1.48608700	-1.33758200
C	-3.58823500	-1.50758000	1.11355500
H	-1.49487500	-1.14788900	1.43289000
C	-4.76066900	-1.09355800	0.47353700
H	-5.61080400	0.33343700	-0.90206800
H	-3.61703400	-2.33745600	1.81582200
H	-5.70046100	-1.60553400	0.66059700
H	-1.89891600	2.73042300	0.01082500

Table S81. Cartesien coordinates of benzimidazole-2-ylidene 10, TS-3

C	-2.10656900	-1.30853100	0.69299200
C	-1.48921900	-1.97958200	-0.36866300
C	-2.17168000	-2.94326600	-1.11303200
C	-3.48903100	-3.21286400	-0.74909000
C	-4.10569800	-2.54324800	0.32206300
C	-3.42518700	-1.58043500	1.06232900
C	-0.00651800	-0.53259200	0.52020400
H	-1.71090000	-3.46481800	-1.94483100
H	-4.05024500	-3.95559400	-1.30774300
H	-5.13371900	-2.78086100	0.57784400
H	-3.90103900	-1.06720700	1.89027800
N	-1.17028900	-0.42428400	1.21093300
N	-0.18507800	-1.48361600	-0.44375900
C	-1.46846900	0.43769700	2.36379500
H	-2.50961000	0.75461000	2.27110000
H	-1.32541000	-0.13083100	3.28600600
H	-0.81881600	1.31021200	2.36356700
C	0.78009500	-1.99009200	-1.42305600
H	0.33496400	-2.86234000	-1.90095700
H	0.99771800	-1.23729100	-2.18196600
H	1.70542900	-2.28478800	-0.93289300
C	1.21520300	0.28851300	0.88069000
O	1.31601300	0.24396300	2.25299200
C	2.52051200	-0.17614900	0.21754100
C	3.32122200	-1.08340200	0.92827600
C	2.98294400	0.28229500	-1.02384300
C	4.52399700	-1.54914500	0.39778000
H	2.98712300	-1.39528900	1.91181000
C	4.19011900	-0.17830600	-1.55613800
H	2.40927500	1.01081600	-1.58823300
C	4.96209600	-1.10179100	-0.85157400
H	5.12630800	-2.25431600	0.96530700
H	4.53002100	0.19596400	-2.51861400
H	5.90288100	-1.45745500	-1.26368300
H	1.21170300	1.39585100	2.40032400
C	0.94227700	1.98034800	0.58475900
O	0.89617800	2.48728500	1.83473200
H	1.84764200	2.28408300	0.02860600
C	-0.27351100	2.30703000	-0.28138800
C	-1.24757300	3.18434100	0.21356800
C	-0.42875000	1.82307000	-1.58978100
C	-2.35171200	3.54543200	-0.56043500
H	-1.10383500	3.58465900	1.21164200
C	-1.53070600	2.18094500	-2.36815900
H	0.32133000	1.16086200	-2.01725700
C	-2.50210100	3.04203100	-1.85380100
H	-3.09253100	4.23124200	-0.15548300
H	-1.62852500	1.78997900	-3.37838000
H	-3.36016200	3.32404200	-2.45867600

Table S82. Cartesien coordinates of benzimidazole-2-ylidene 10, IM-3

C	-2.21319900	-1.27415700	0.60413400
C	-1.59026400	-1.90542300	-0.47853900
C	-2.25147600	-2.87260000	-1.23699500
C	-3.56106700	-3.17880400	-0.87349600
C	-4.18695600	-2.54401100	0.21363000
C	-3.52429000	-1.58285000	0.97239700
C	-0.12561600	-0.45650400	0.44006400
H	-1.77408100	-3.37748800	-2.06968400
H	-4.10699400	-3.92633700	-1.44088600
H	-5.20764700	-2.81090900	0.47018000
H	-4.00754400	-1.10215800	1.81553500
N	-1.28691200	-0.38904300	1.13865300
N	-0.30382900	-1.36698500	-0.55962800
C	-1.56098900	0.38712800	2.35262700
H	-2.61615800	0.67053200	2.32723300
H	-1.34543000	-0.22613800	3.22967200
H	-0.94032600	1.27681300	2.38051400
C	0.62911800	-1.76830900	-1.61488600
H	0.04253400	-2.19313500	-2.43048800
H	1.17661400	-0.90777800	-1.98731400
H	1.34227600	-2.50764500	-1.24479800
C	1.16690600	0.25829800	0.96066500
O	1.18101100	0.00963200	2.27921500
C	2.44378700	-0.30816800	0.27675300
C	3.00294700	-1.45373900	0.86235800
C	3.10157800	0.25531800	-0.82487100
C	4.15499700	-2.04122900	0.34132000
H	2.52322100	-1.84632600	1.75277100
C	4.26408700	-0.32364700	-1.34437400
H	2.72383300	1.15854700	-1.29440600
C	4.79068900	-1.47956300	-0.76979400
H	4.56740400	-2.93070600	0.81182300
H	4.76010500	0.13858100	-2.19441700

H	5.69519400	-1.92899900	-1.17162100
H	1.11721800	1.57231700	2.57291800
C	1.05568400	1.90484300	0.73955700
O	0.92402000	2.41712800	2.03349200
H	2.02024300	2.22153900	0.31846200
C	-0.04618000	2.40497700	-0.18107900
C	-1.03774700	3.27084400	0.30137000
C	-0.08205500	2.05806400	-1.54162900
C	-2.04247500	3.75247700	-0.53949600
H	-0.99323600	3.57292200	1.34170900
C	-1.08421800	2.53877100	-2.38516100
H	0.68853400	1.41314700	-1.95658700
C	-2.07487000	3.38615500	-1.88584200
H	-2.79787100	4.42633200	-0.14192200
H	-1.08766200	2.25418100	-3.43474100
H	-2.85562600	3.76360200	-2.54104800

Table S83. Cartesien coordinates of benzimidazole-2-ylidene 10, TS-4

C	2.86158400	-0.22917900	0.41735100
C	2.43122900	0.00071900	-0.89769200
C	3.33448300	0.09104700	-1.95707400
C	4.68683400	-0.05808500	-1.65301400
C	5.11937900	-0.28915200	-0.33540600
C	4.21514900	-0.37939400	0.72195200
C	0.60153100	-0.05855500	0.44370900
H	3.00392300	0.27626400	-2.97389800
H	5.42109600	0.00895600	-2.45029000
H	6.18136400	-0.39615300	-0.13534700
H	4.55585700	-0.55029000	1.73775100
N	1.70890600	-0.26699200	1.20210500
N	1.04081100	0.08877100	-0.83534700
C	1.72137600	-0.54897900	2.63858100
H	0.79800400	-1.05680600	2.90463300
H	2.57371200	-1.20045500	2.84784100
H	1.79779300	0.37639000	3.21229200
C	0.19270800	0.25364300	-2.01002100
H	0.62230100	-0.32181700	-2.83448700
H	-0.79922400	-0.13496400	-1.79076300
H	0.11849300	1.30728900	-2.29363700
C	-1.02033600	0.64092700	1.34654300
O	-0.61544200	1.01143300	2.49375400
C	-1.36689700	1.78909100	0.39481500
C	-0.61633400	2.96819600	0.52834900
C	-2.41294100	1.77193900	-0.53458100
C	-0.87977400	4.08164100	-0.26468700
H	0.16257200	2.99454800	1.28338000
C	-2.69081100	2.89385500	-1.32213500
H	-3.02148300	0.88553700	-0.65837500
C	-1.92187300	4.04942300	-1.19703700
H	-0.28157000	4.98199600	-0.14775900
H	-3.51421000	2.85997500	-2.03137600
H	-2.13667000	4.92056600	-1.81064700
H	-1.26244700	-0.49920100	3.16276800
C	-2.00340500	-0.61142500	1.44582300
O	-1.66459000	-1.25302900	2.65948900
H	-3.00881700	-0.15987500	1.52868700
C	-2.03928700	-1.63979400	0.33415200
C	-1.03596600	-2.61535100	0.22132900
C	-3.10762400	-1.69088100	-0.57197200
C	-1.07112200	-3.56701900	-0.79724600
H	-0.24260000	-2.64015000	0.95936800
C	-3.14656900	-2.63976000	-1.59648000
H	-3.93776400	-0.99718300	-0.46010400
C	-2.12095700	-3.57691700	-1.71935400
H	-0.28290500	-4.31306800	-0.86346000
H	-3.98798100	-2.65573000	-2.28457400
H	-2.14948300	-4.32146400	-2.51067500

Table S84. Cartesien coordinates of 1,3-diphenyl-imidazole-2-ylidene 11

C	-0.00000100	0.34323400	0.00002000
C	-0.67577800	-1.86475900	0.00240200
C	0.67578400	-1.86475600	-0.00248300
H	-1.37188000	-2.68780900	0.03215200
H	1.37189500	-2.68779800	-0.03229600
N	-1.06723600	-0.52160800	0.00400500
N	1.06723700	-0.52160400	-0.00401100
C	2.42001000	-0.07047000	-0.01587200
C	2.71711100	1.19397800	-0.53702200
C	3.44532200	-0.87696400	0.48799100
C	4.03603300	1.64047500	-0.55378700
H	1.90290700	1.80475400	-0.90908500
C	4.76495600	-0.42376800	0.45525600
H	3.21817900	-1.84309500	0.92752600
C	5.06741600	0.83415700	-0.06519800
H	4.25917900	2.62354100	-0.95964200
H	5.55494400	-1.05691900	0.84999600
H	6.09528300	1.18508200	-0.08680800
C	-2.42001300	-0.07047300	0.01588000
C	-2.71710000	1.19399900	0.53697900
C	-3.44533800	-0.87698600	-0.48792500
C	-4.03602000	1.64050200	0.55375200
H	-1.90288500	1.80478900	0.90899700
C	-4.76496900	-0.42378100	-0.45518900
H	-3.21821500	-1.84314400	-0.92741100
C	-5.06741500	0.83416800	0.06521400
H	-4.25915500	2.62358600	0.95956800
H	-5.55496800	-1.05694700	-0.84988400
H	-6.09528000	1.18509900	0.08682500

Table S85. Cartesien coordinates of 1,3-diphenyl-imidazole-2-ylidene 11, TS-1

C	0.55068600	-0.56673200	0.07973000
C	0.42670800	-2.82470900	0.35565700
C	1.73531200	-2.48783000	0.39902200
H	-0.06330900	-3.78370300	0.41136500
H	2.62335200	-3.09091800	0.50219900
N	-0.28445100	-1.64102400	0.15061300
N	1.79683600	-1.10529500	0.21783100
C	3.04457400	-0.40088600	0.10441700
C	3.29726100	0.38657700	-1.02334500
C	4.01021500	-0.56625900	1.09993000
C	4.53508600	1.02017800	-1.13585600
H	2.52270100	0.50972300	-1.77912600
C	5.24815200	0.06326500	0.96631900
H	3.78742800	-1.16941400	1.97562200
C	5.51202600	0.85724300	-0.15084900
H	4.73577000	1.64019400	-2.00495300
H	6.00028200	-0.06151600	1.74022000
H	6.47491900	1.35021400	-0.25182500
C	-1.70370300	-1.62372500	-0.06153400
C	-2.22139700	-0.97673500	-1.18509700
C	-2.53508900	-2.31216400	0.82497800
C	-3.59719400	-1.02241200	-1.41088100
H	-1.55005800	-0.43738100	-1.84953000
C	-3.90715000	-2.35806100	0.57984600
H	-2.11342200	-2.79199500	1.70367900
C	-4.43975100	-1.71426600	-0.53868100
H	-4.00929600	-0.51565700	-2.27875700
H	-4.55815600	-2.88942900	1.26835700
H	-5.50932100	-1.74809400	-0.72658400
C	0.28698200	1.22021000	-0.73294000
H	1.21388400	1.60204800	-0.25512500
O	0.27229600	1.03015700	-1.97989600
C	-0.92127500	1.81142500	-0.02079300
C	-0.97944600	1.91361900	1.37366200
C	-1.94130700	2.38021200	-0.78736400
C	-2.05259200	2.55060200	1.99434400
H	-0.17995700	1.48127000	1.97309400
C	-3.01597000	3.02363000	-0.17016300
H	-1.86314900	2.31590300	-1.86849100
C	-3.07687900	3.10708800	1.22172400
H	-2.09160800	2.61708800	3.07909300
H	-3.80369800	3.46550300	-0.77599700
H	-3.91291700	3.60752700	1.70407700

Table S86. Cartesien coordinates of 1,3-diphenyl-imidazole-2-ylidene 11, IM-1

C	-0.54303500	-0.48671600	-0.07924900
C	-0.35473000	-2.68785800	-0.51489000
C	-1.66935700	-2.37932300	-0.56336000
H	0.15983400	-3.62804000	-0.62725000
H	-2.53931900	-2.99413500	-0.72600100
N	0.33808600	-1.51573900	-0.21397000
N	-1.78094600	-1.01718900	-0.29266000
C	-3.04569700	-0.35590100	-0.11637400
C	-3.28357400	0.37831100	1.05064000
C	-4.03452800	-0.52244500	-1.08877200
C	-4.54080200	0.95626300	1.22552500
H	-2.47114500	0.49999800	1.77146000
C	-5.29006400	0.05162100	-0.88868300
H	-3.81894600	-1.07997400	-1.99604700
C	-5.54463300	0.79072400	0.26791800
H	-4.73607200	1.53619200	2.12318400
H	-6.06307000	-0.07229100	-1.64179500
H	-6.52198200	1.24040800	0.41987400
C	1.74933500	-1.51168700	0.06405300
C	2.20870800	-0.98146600	1.27117900
C	2.61627000	-2.11804200	-0.84749300
C	3.57157900	-1.06408200	1.55582100
H	1.49162200	-0.48938500	1.92879000
C	3.97428400	-2.19985100	-0.54158300
H	2.23566600	-2.50484300	-1.78870100
C	4.45257800	-1.67460900	0.66052800
H	3.94457100	-0.64857800	2.48767000
H	4.65674800	-2.66534000	-1.24700800
H	5.51175000	-1.73598800	0.89509400
C	-0.31633400	0.90992800	0.50302600
H	-1.19056600	1.49610800	0.12147900
O	-0.33150700	0.68590100	1.83043900
C	0.89917300	1.65138200	-0.08335000
C	1.14143800	1.72895200	-1.45927100
C	1.72362600	2.35878300	0.79302000
C	2.20667500	2.48435800	-1.95133800
H	0.49320900	1.19572300	-2.15442400
C	2.78402100	3.12381400	0.30431500
H	1.50505900	2.28797700	1.85431900
C	3.03241000	3.18537500	-1.06852400
H	2.39071700	2.52970700	-3.02233200
H	3.41917300	3.67319600	0.99564900
H	3.86077700	3.77738000	-1.44988900

Table S87. Cartesien coordinates of 1,3-diphenyl-imidazole-2-ylidene 11, TS-2

C	-0.31020200	-1.06206400	-0.25888200
C	0.00451300	-2.38031700	-2.06701700
C	-1.29843300	-2.46053700	-1.72983100
H	0.56347100	-2.82884900	-2.87195600
H	-2.12024300	-2.99435600	-2.17815300

N	0.61475300	-1.50419300	-1.16884200
N	-1.49992200	-1.63615100	-0.61948100
C	-2.83315200	-1.30460800	-0.18196100
C	-3.65274700	-2.31305200	0.32127200
C	-3.31309900	-0.00785000	-0.38758900
C	-4.97903600	-2.01571600	0.64129200
H	-3.25232100	-3.31070800	0.47630200
C	-4.63701100	0.27523800	-0.05482200
H	-2.63757800	0.75764400	-0.77070900
C	-5.47179300	-0.72376300	0.45525800
H	-5.62177000	-2.79450300	1.04197600
H	-5.01936000	1.28163800	-0.20209100
H	-6.50334000	-0.49464800	0.70796900
C	1.93440600	-0.97499400	-1.39271200
C	3.02052500	-1.85025200	-1.42987600
C	2.08557800	0.38917400	-1.65539400
C	4.28671000	-1.35103200	-1.73541400
H	2.87583400	-2.90350100	-1.20767800
C	3.36086900	0.87380800	-1.94575600
H	1.21910900	1.04989600	-1.61334700
C	4.45815500	0.01057300	-1.99163900
H	5.13787100	-2.02539700	-1.76323700
H	3.49210900	1.93378200	-2.14435300
H	5.44614700	0.39824800	-2.22423300
C	-0.07731400	-0.09254400	0.80585000
H	-0.16643600	1.03663500	0.16229300
O	-1.18268100	-0.06350200	1.71584900
C	1.20797500	-0.27481700	1.58619000
C	1.95839200	0.84180100	1.97625800
C	1.62298600	-1.53974800	2.02899800
C	3.09316000	0.70130100	2.77548700
H	1.64753200	1.82877000	1.64766900
C	2.76003400	-1.68716600	2.82347800
H	1.04216200	-2.41790400	1.75571900
C	3.50052500	-0.56483600	3.19910200
H	3.66204200	1.58168500	3.06389200
H	3.06276600	-2.67702200	3.15655200
H	4.38601600	-0.67615800	3.81967600
H	-1.65269700	0.76995000	1.54032100
O	-0.64502000	1.95131600	-0.66738900
C	-0.72353100	3.31778200	-0.35799600
C	-1.28200500	3.52815300	1.06834100
H	-2.28212500	3.08170200	1.14868700
H	-0.63305000	3.04974400	1.81300100
H	-1.36936300	4.58983800	1.33334400
C	-1.67625800	3.97831700	-1.37712400
H	-2.67750200	3.53761800	-1.29986000
H	-1.76501300	5.06195100	-1.22310800
H	-1.30976800	3.80052900	-2.39438600
C	0.66556900	3.98678700	-0.47051600
H	1.06138600	3.85100600	-1.48417000
H	0.62817400	5.06381600	-0.26001200
H	1.37485300	3.53066600	0.23048900

Table S88. Cartesien coordinates of 1,3-diphenyl-imidazole-2-ylidene 11, IM-2

C	0.48721100	-0.17483100	-0.54468500
C	0.37430200	-2.29565200	-1.37624700
C	1.66248900	-1.93513300	-1.41040100
H	-0.08474800	-3.21347200	-1.70590600
H	2.51986700	-2.47855300	-1.77427500
N	-0.39356200	-1.27905600	-0.75789900
N	1.80906700	-0.66126800	-0.81454800
C	2.99689200	-0.27488500	-0.16179700
C	4.23239100	-0.42201900	-0.82110800
C	2.97988600	0.25674200	1.14193800
C	5.41326200	-0.05089700	-0.18733600
H	4.25415800	-0.80576000	-1.83665900
C	4.17264100	0.64539800	1.75615600
H	2.03813000	0.32177400	1.67918300
C	5.39392600	0.49314800	1.10162900
H	6.35715800	-0.17009800	-0.71262000
H	4.13962100	1.05293500	2.76307500
H	6.31856100	0.79404400	1.58479200
C	-1.51343800	-1.61863200	0.04998000
C	-2.46774000	-2.51523800	-0.45597200
C	-1.69228000	-1.08566800	1.33336500
C	-3.56326200	-2.88825300	0.32015200
H	-2.36009000	-2.90720800	-1.46325600
C	-2.79762500	-1.45647200	2.09624700
H	-0.96803700	-0.38063000	1.72558600
C	-3.73743800	-2.36223200	1.60123000
H	-4.29060200	-3.58527200	-0.08794400
H	-2.91930600	-1.03421600	3.09033000
H	-4.59729800	-2.64647900	2.20080000
C	0.15123700	1.14183900	-0.40750300
O	1.11263700	2.12114700	-0.25333000
C	-1.20554200	1.71655200	-0.39067900
C	-1.44885100	2.87607000	0.37029300
C	-2.25562100	1.20522000	-1.17552600
C	-2.70210900	3.48397800	0.36595400
H	-0.64075400	3.29768500	0.95798100
C	-3.50585700	1.81829300	-1.17938100
H	-2.08420000	0.33498500	-1.79884000
C	-3.73970400	2.95714400	-0.40549100
H	-2.86766400	4.37478900	0.96684500
H	-4.29984600	1.40724800	-1.79757500
H	-4.71735800	3.43180400	-0.40927500
H	1.98415100	1.73268500	-0.07336700

Table S89. Cartesien coordinates of 1,3-diphenyl-imidazole-2-ylidene 11, TS-3

C	0.23847300	-1.30020300	-0.14716100
C	-0.20737700	-3.12370600	-1.41545300
C	1.13352800	-3.02403900	-1.30396100
H	-0.82962100	-3.86105300	-1.89533000
H	1.92581300	-3.65102800	-1.67804700
N	-0.75711700	-2.07827100	-0.68233600
N	1.41202400	-1.91123200	-0.51780200
C	2.78289300	-1.62196600	-0.16108300
C	3.73143600	-1.57260300	-1.18992800
C	3.16402000	-1.52402600	1.17655000
C	5.07693200	-1.41231300	-0.87151100
H	3.41230700	-1.63375800	-2.22644600
C	4.51658000	-1.36012900	1.47904200
H	2.41018400	-1.56588700	1.95131300
C	5.47163500	-1.30597900	0.46541000
H	5.81426200	-1.36189300	-1.66744500
H	4.81730100	-1.26973100	2.51832000
H	6.52129700	-1.17549500	0.71254300
C	-2.15591700	-2.09080300	-0.33763500
C	-3.10001100	-2.18955700	-1.35984000
C	-2.53683600	-2.11444600	1.00516900
C	-4.44985800	-2.31416000	-1.03221000
H	-2.78284000	-2.15073700	-2.39785500
C	-3.89018200	-2.22771700	1.31811100
H	-1.78399300	-2.02688800	1.78177300
C	-4.84629000	-2.33302000	0.30565000
H	-5.18948400	-2.38588800	-1.82426900
H	-4.19559400	-2.23683400	2.36014500
H	-5.89845800	-2.42478400	0.55921400
C	0.07101600	-0.08611900	0.69309500
O	0.35300300	-0.42592600	2.00840600
C	-1.20106900	0.68195000	0.49950000
C	-1.87637700	1.18566400	1.62132800
C	-1.69605300	1.01313800	-0.77327900
C	-3.01445000	1.97893300	1.47587100
H	-1.49308700	0.94025800	2.60552500
C	-2.83724500	1.79815500	-0.91826900
H	-1.17586100	0.66586200	-1.66294000
C	-3.50569000	2.28673500	0.20671100
H	-3.51983800	2.35775400	2.36137500
H	-3.19776200	2.04139700	-1.91488400
H	-4.39161700	2.90609200	0.09305000
H	1.14398500	0.26407000	2.20555800
C	1.57728200	1.18235000	0.43497500
O	2.04780700	1.19455400	1.64899500
H	2.15345000	0.62740000	-0.32752300
C	1.09329400	2.48044200	-0.14937600
C	0.70285800	3.53399200	0.68675400
C	1.08990700	2.68403100	-1.53461200
C	0.29780700	4.75308400	0.14750300
H	0.74515200	3.37785900	1.75986600
C	0.68905300	3.90462900	-2.07933000
H	1.41826500	1.87941300	-2.19182200
C	0.28655300	4.94317500	-1.23768600
H	-0.00433600	5.56276800	0.80778400
H	0.69836400	4.04845000	-3.15749100
H	-0.02419700	5.89719800	-1.65667100

Table S90. Cartesien coordinates of 1,3-diphenyl-imidazole-2-ylidene 11, IM-3

C	0.21996800	-1.36416700	-0.23652600
C	1.27989000	-3.35664000	-0.19213800
C	-0.04386400	-3.60392100	-0.08324000
H	2.13091600	-4.01722300	-0.22920500
H	-0.59947600	-4.52329500	0.00456600
N	1.43522600	-1.98111800	-0.28239200
N	-0.69138600	-2.36877200	-0.10422300
C	-2.11445400	-2.31263800	0.15735900
C	-2.54318800	-2.31788700	1.48648800
C	-3.02292900	-2.36723500	-0.89785100
C	-3.90975400	-2.34953300	1.76338700
H	-1.81157400	-2.29550300	2.28891400
C	-4.38762100	-2.40219100	-0.60850900
H	-2.66436400	-2.33571600	-1.91782100
C	-4.83139800	-2.39144000	0.71500500
H	-4.25069000	-2.34429300	2.79453600
H	-5.10424100	-2.42902500	-1.42381200
H	-5.89598500	-2.41476600	0.93011200
C	2.75565400	-1.39545500	-0.37901600
C	3.58354400	-1.47266700	0.74103400
C	3.21365500	-0.87427200	-1.58947900
C	4.89660600	-1.00890300	0.65351500
H	3.19483800	-1.87056200	1.67360700
C	4.52957900	-0.41909900	-1.66378000
H	2.52421800	-0.78668600	-2.41770200
C	5.37000600	-0.48437000	-0.54948600
H	5.54238700	-1.05447500	1.52560100
H	4.89688300	-0.00568300	-2.59873800
H	6.39209400	-0.12194400	-0.61825100
C	0.07903600	0.17565600	-0.54765800
O	0.62909100	0.30922500	-1.76757700
C	0.76966500	0.93575000	0.60095100
C	1.71350300	1.91553000	0.28709900
C	0.46337900	0.69458300	1.94580500
C	2.34012800	2.64393400	1.29853900
H	1.94087400	2.07823100	-0.76086500
C	1.09093600	1.41840000	2.96100900
H	-0.27502000	-0.06274500	2.20752300
C	2.03328800	2.39736900	2.63853600
H	3.07227000	3.40569900	1.04110400
H	0.84323100	1.22054800	4.00143900
H	2.52373900	2.96343400	3.42661700

H	-0.96731400	0.08178900	-2.39033600
C	-1.46117500	0.59663400	-0.67398700
O	-1.85770300	0.07636200	-1.92809100
H	-2.06699800	0.13925200	0.11468800
C	-1.66111500	2.10189100	-0.60379100
C	-1.22425200	2.93126300	-1.64646200
C	-2.30874700	2.68576100	0.48985000
C	-1.42542300	4.30927500	-1.58713600
H	-0.71500200	2.48380600	-2.49280700
C	-2.51449700	4.06566900	0.55146000
H	-2.65974600	2.05283400	1.30266000
C	-2.07253300	4.88275400	-0.48903900
H	-1.07833500	4.93983000	-2.40249900
H	-3.02415100	4.49945200	1.40862100
H	-2.23385700	5.95726200	-0.44793400

Table S91. Cartesien coordinates of 1,3-diphenyl-imidazole-2-ylidene 11, TS-4

C	-0.51128800	1.34908100	-0.28763600
C	-1.92599600	3.13025300	-0.33229700
C	-0.67655800	3.61957200	-0.17416000
H	-2.88284500	3.62119400	-0.41232500
H	-0.30535000	4.62958000	-0.10197000
N	-1.81034200	1.74462400	-0.40315600
N	0.18079700	2.51855800	-0.14971300
C	1.59601700	2.70689800	0.05808900
C	2.02276100	3.20776100	1.29098600
C	2.50127500	2.47707000	-0.97861200
C	3.37736400	3.47582500	1.49091700
H	1.29870700	3.37766000	2.08264400
C	3.85475400	2.74106400	-0.76303400
H	2.15045700	2.04178500	-1.90843300
C	4.29370300	3.24472200	0.46316600
H	3.71365400	3.86086600	2.44935500
H	4.56648400	2.55022600	-1.56089800
H	5.34860800	3.45201600	0.61978000
C	-3.00030000	0.92537200	-0.48775900
C	-3.76950200	0.75642100	0.66254800
C	-3.41831100	0.41407400	-1.71583200
C	-4.97677200	0.05923800	0.58421600
H	-3.41743000	1.15521900	1.60899200
C	-4.62568300	-0.27780600	-1.78513100
H	-2.78829500	0.53576200	-2.58778300
C	-5.40588400	-0.45512600	-0.63902500
H	-5.57551500	-0.08093600	1.47956600
H	-4.95401300	-0.68577100	-2.73669300
H	-6.34540300	-0.99751700	-0.70085200
C	-0.15128100	-0.54224000	-0.52290400
O	-0.89159500	-0.90120900	-1.49825400
C	-0.48712700	-1.06037200	0.87347300
C	-1.47242000	-2.04413100	0.99245600
C	0.17753700	-0.62208600	2.02664600
C	-1.79192300	-2.58095100	2.24083800
H	-1.97548600	-2.36970000	0.08815200
C	-0.13955600	-1.15631300	3.27492100
H	0.94372000	0.14669600	1.95151600
C	-1.12699600	-2.13952800	3.38574200
H	-2.55987400	-3.34686600	2.31908900
H	0.38447300	-0.80813000	4.16191200
H	-1.37311000	-2.55804700	4.35853400
H	0.52010600	-0.33901600	-2.56368700
C	1.36947800	-0.57309900	-0.90539100
O	1.42746600	-0.10399400	-2.24527500
H	1.95612500	0.09888100	-0.27512500
C	1.95190100	-1.97424500	-0.77349000
C	1.46875000	-3.03473300	-1.55349500
C	3.00368100	-2.22057600	0.11500400
C	2.02632500	-4.30709100	-1.44187700
H	0.64422300	-2.85380700	-2.23518500
C	3.56517900	-3.49433400	0.22908100
H	3.39320300	-1.40482900	0.72091600
C	3.07755400	-4.54240300	-0.55112600
H	1.63945300	-5.12004500	-2.05176100
H	4.38496300	-3.66456600	0.92290300
H	3.51289100	-5.53520300	-0.46820600

Table S92. Cartesien coordinates of pyrazoline-3-ylidene 12

C	1.19572300	0.96140500	-0.09326100
C	1.89609600	-0.21394100	0.04280200
C	0.98706900	-1.32958200	0.10791200
H	1.51659600	1.99317900	-0.16735000
H	2.97524200	-0.29176700	0.07326100
N	-0.13518300	0.67682400	-0.14759100
N	-0.21219000	-0.71982200	0.03014600
C	-1.24067400	1.57942600	0.11195300
H	-1.53850400	1.57405300	1.16895200
H	-0.92591900	2.59012700	-0.15808500
H	-2.10535200	1.31614800	-0.50386100
C	-1.50744600	-1.36803700	-0.06051900
H	-1.97257300	-1.20164200	-1.03973300
H	-1.31185500	-2.43099700	0.07063800
H	-2.19063300	-1.02374400	0.72496800

Table S93. Cartesien coordinates of pyrazoline-3-ylidene 12, TS-1

C	-2.19736800	-1.89774200	0.01891200
C	-0.93253500	-1.52773800	-0.39120400
C	-0.88905700	-0.11330100	-0.47482000

H	-2.63810400	-2.86665800	0.21257800
H	-0.10761400	-2.19385800	-0.59971800
N	-2.94362800	-0.77937000	0.18647800
N	-2.11395500	0.29608200	-0.10878300
C	-4.29036400	-0.64124200	0.70653500
H	-4.90170900	-0.02462800	0.04129800
H	-4.72986500	-1.63867100	0.76010200
H	-4.28953000	-0.19974100	1.70920300
C	-2.61073000	1.66644000	-0.05080300
H	-3.06502800	1.86780800	0.92408600
H	-1.72642700	2.30334000	-0.18372400
H	-3.34475700	1.84501300	-0.84410600
C	0.57384500	1.34598600	-0.78156500
H	0.44414100	1.27047400	-1.88270200
O	0.23915400	2.39087100	-0.17658000
C	1.75640300	0.52812200	-0.30327100
C	2.34842100	-0.43969400	-1.12192700
C	2.30035500	0.77896200	0.96027000
C	3.45757000	-1.16212200	-0.67897300
H	1.93800200	-0.62117600	-2.11446200
C	3.40767800	0.05870600	1.40669000
H	1.84148900	1.55553800	1.56506800
C	3.98828800	-0.91612800	0.59000100
H	3.91352200	-1.90935300	-1.32448300
H	3.82585100	0.26057100	2.39029700
H	4.85484600	-1.47410200	0.93627100

Table S94. Cartesien coordinates of pyrazoline-3-ylidene 12, IM-1

C	2.69152400	-1.52105600	0.26652400
C	1.54859400	-1.44854400	1.03554700
C	0.93205000	-0.21429100	0.74709600
H	3.45202600	-2.28477600	0.18460900
H	1.18936600	-2.18663900	1.73655500
N	2.78788700	-0.39100500	-0.47129600
N	1.71278900	0.40604700	-0.15880400
C	3.85215400	0.03953600	-1.35931500
H	4.44578800	0.84277700	-0.91114600
H	4.49557700	-0.82266100	-1.54033100
H	3.43727800	0.38059600	-2.31136300
C	1.50214100	1.73460900	-0.72880200
H	1.10294200	1.65623700	-1.74441700
H	0.76169500	2.17155600	-0.01672900
H	2.44160200	2.29291100	-0.72626600
C	-0.32457600	0.48809300	1.36281800
H	-0.44094600	-0.07452400	2.33003800
O	-0.15274700	1.79494900	1.49540500
C	-1.55172000	0.05595600	0.49223900
C	-1.90450200	-1.27596700	0.24191300
C	-2.35465300	1.07455300	-0.02288500
C	-3.03153300	-1.58332200	-0.52206700
H	-1.30037100	-2.08623300	0.64868300
C	-3.48447500	0.77288600	-0.78670200
H	-2.06394900	2.09320600	0.21748900
C	-3.82497200	-0.55686500	-1.04246200
H	-3.29413400	-2.62257400	-0.70866900
H	-4.10472500	1.57623700	-1.17905500
H	-4.70510100	-0.79452500	-1.63536600

Table S95. Cartesien coordinates of pyrazoline-3-ylidene 12, TS-2

C	-2.89278600	-1.99596900	-0.97079000
C	-1.53465200	-2.01551300	-0.77432500
C	-1.21516000	-0.90743200	0.05158300
H	-3.54021400	-2.67702500	-1.50457100
H	-0.83090000	-2.74212300	-1.14634400
N	-3.42255100	-0.92747800	-0.32842100
N	-2.39244600	-0.26113600	0.30603300
C	-4.82005500	-0.60100000	-0.12987800
H	-5.07645500	0.36717800	-0.57171500
H	-5.40528400	-1.37574800	-0.62781100
H	-5.07392600	-0.59464900	0.93516800
C	-2.59718900	1.02541900	0.97562800
H	-3.54454300	1.44822400	0.63870100
H	-2.60908400	0.89002400	2.05892400
H	-1.77216800	1.69548400	0.69004700
C	0.06401600	-0.40157600	0.53510000
H	0.21380700	0.79018800	0.03010600
O	-0.04022200	0.02653700	1.89699100
C	1.25791400	-1.26894500	0.26024500
C	1.64419500	-1.57496600	-1.05726600
C	2.05551700	-1.74596900	1.31139200
C	2.76727000	-2.36219400	-1.31276500
H	1.06927200	-1.17576400	-1.89037900
C	3.18375600	-2.52507800	1.05468600
H	1.77559800	-1.48899800	2.32715300
C	3.54291900	-2.84465300	-0.25642700
H	3.04645200	-2.58362600	-2.34027300
H	3.78580800	-2.88641500	1.88530200
H	4.42309100	-3.45100000	-0.45394400
H	0.19771500	0.98006800	1.82426300
O	0.12706300	2.10618600	0.27190800
C	1.06126900	2.96688100	-0.33217800
C	2.49323600	2.60892900	0.11665500
H	2.74226000	1.58229400	-0.17643800
H	3.24315400	3.28014100	-0.32221000
H	2.57118800	2.67564500	1.20831500
C	0.72414900	4.40320500	0.11497700
H	1.41766600	5.14144400	-0.30867900
H	-0.29332500	4.66532000	-0.19834000
H	0.76910800	4.47368700	1.20786000

C	0.95505800	2.86417300	-1.86860000
H	1.63159800	3.56127800	-2.38011800
H	1.20375400	1.84816100	-2.20014200
H	-0.07105300	3.08285200	-2.18758600

Table S96. Cartesien coordinates of pyrazoline-3-ylidene 12, IM-2

C	2.34864500	-1.73476700	-0.19634800
C	1.03185100	-1.45049000	-0.24044000
C	0.88222600	-0.02157600	-0.04185900
H	2.84933400	-2.68101600	-0.35811200
H	0.22818900	-2.15004800	-0.41014900
N	3.11994600	-0.60727400	0.07966900
N	2.20194500	0.50879700	0.06399600
C	4.29205400	-0.37861700	-0.76893700
H	4.85498800	0.47770100	-0.38821600
H	4.93532600	-1.26200100	-0.71011400
H	4.01668100	-0.18967700	-1.81598400
C	2.48069600	1.44626700	1.15219700
H	3.53237600	1.74236400	1.10467000
H	1.85738000	2.32751400	1.00648000
H	2.27924400	1.00670400	2.14021200
C	-0.25682400	0.73390400	-0.03117800
O	-0.11353600	2.11965600	-0.14010700
C	-1.62944500	0.22349100	-0.02445400
C	-2.00667800	-0.94885100	0.66567000
C	-2.64801500	0.95461400	-0.67481700
C	-3.32765600	-1.38719800	0.66759900
H	-1.25942300	-1.49690300	1.23096500
C	-3.97079800	0.51767300	-0.65921500
H	-2.38308800	1.85472300	-1.22220400
C	-4.32075100	-0.65909100	0.00561000
H	-3.58888600	-2.29245900	1.21041100
H	-4.73094300	1.09595300	-1.17896000
H	-5.35243500	-0.99961000	0.01698200
H	-0.83553500	2.52667700	0.36625400

Table S97. Cartesien coordinates of pyrazoline-3-ylidene 12, TS-3

C	3.41517400	1.13832800	-1.41869800
C	2.10250400	1.36245000	-1.07532200
C	1.76029500	0.41329600	-0.08489100
H	4.06287300	1.64740300	-2.11819200
H	1.45660000	2.14142500	-1.44448700
N	3.88674400	0.10123600	-0.69253200
N	2.86423400	-0.36522000	0.10218500
C	5.18794600	-0.53632700	-0.76602000
H	5.11825400	-1.54047600	-1.19711700
H	5.81253400	0.08347500	-1.41088500
H	5.64878800	-0.59387200	0.22346700
C	3.09440300	-1.46336800	1.04474800
H	3.59768200	-1.09052200	1.94193800
H	2.12197300	-1.90022200	1.31242100
H	3.70627900	-2.22472000	0.55582900
C	0.51151300	0.21399700	0.68948200
O	0.82271600	0.07538900	2.03649000
C	-0.53620200	1.26711600	0.42397500
C	-1.00948200	1.55879300	-0.86687800
C	-1.08699800	1.97419200	1.50277300
C	-1.98105500	2.53815000	-1.07300900
H	-0.63968500	0.99632800	-1.71929000
C	-2.06435100	2.94811400	1.29787800
H	-0.72903300	1.74538100	2.49991400
C	-2.51296300	3.24128700	0.00912900
H	-2.33467700	2.73886500	-2.08150900
H	-2.47430400	3.48335600	2.15123500
H	-3.27408100	4.00074800	-0.15046900
H	0.52506000	-0.90480000	2.19888800
C	-0.07292500	-1.56181700	0.31760300
H	0.59255400	-1.82239900	-0.53339500
O	0.17779800	-2.16352200	1.46021600
C	-1.50837100	-1.57129400	-0.14795400
C	-1.82972900	-1.62514200	-1.50881900
C	-2.54908800	-1.58433900	0.78969500
C	-3.15980400	-1.67300900	-1.93090800
H	-1.02748000	-1.64624900	-2.24572700
C	-3.87781600	-1.62566900	0.37357100
H	-2.29200700	-1.58272600	1.84423500
C	-4.18944200	-1.66761400	-0.98898400
H	-3.39138000	-1.72263400	-2.99249800
H	-4.67574900	-1.63238300	1.11250500
H	-5.22680600	-1.70589400	-1.31231200

Table S98. Cartesien coordinates of pyrazoline-3-ylidene 12, IM-3

C	3.50362500	1.17529200	-1.24031900
C	2.16838600	1.35701800	-0.95026500
C	1.76677600	0.27645300	-0.13990400
H	4.19165000	1.76288300	-1.83154000
H	1.53865300	2.17444300	-1.26012800
N	3.92541700	0.04120000	-0.64278300
N	2.85437500	-0.52162100	0.00776500
C	5.23844700	-0.57698200	-0.69837400
H	5.20235700	-1.53643300	-1.22366300
H	5.89035500	0.10371500	-1.24731900
H	5.64325100	-0.72290100	0.30648200
C	3.04531000	-1.67438000	0.88972000
H	3.44532300	-1.33846700	1.85003400
H	2.07305800	-2.14578400	1.05520100

H	3.72372200	-2.38261300	0.40917500
C	0.46724300	0.03104800	0.66056200
O	0.82672500	-0.08972800	1.95349300
C	-0.49073900	1.20814000	0.38735200
C	-0.97314600	1.54164800	-0.88630300
C	-0.88208400	1.99154700	1.47663200
C	-1.82287700	2.63449900	-1.06580200
H	-0.69967800	0.93742200	-1.74780900
C	-1.73756700	3.08071300	1.30229800
H	-0.49372100	1.71482600	2.45097900
C	-2.20868400	3.40946000	0.03023900
H	-2.19250700	2.87302400	-2.06035200
H	-2.03443600	3.67679400	2.16235700
H	-2.87418200	4.25818100	-0.10748100
H	0.37626000	-1.53244700	1.96678300
C	-0.17966600	-1.45657500	0.18548600
H	0.38854000	-1.81077200	-0.69027500
O	0.07743700	-2.27054300	1.29732100
C	-1.64784200	-1.47148400	-0.17610100
C	-2.06345700	-1.61782500	-1.50425000
C	-2.62605700	-1.37149200	0.82311900
C	-3.41975200	-1.64258900	-1.83643200
H	-1.31507600	-1.72463500	-2.28853800
C	-3.98006700	-1.39363800	0.49668100
H	-2.31032500	-1.28743300	1.85825000
C	-4.38399200	-1.52635400	-0.83526700
H	-3.72135600	-1.76226600	-2.87450000
H	-4.72559300	-1.31120100	1.28403600
H	-5.44127600	-1.54819800	-1.08749500

Table S99. Cartesien coordinates of pyrazoline-3-ylidene 12, TS-4

C	3.92592900	0.98882600	-0.74222000
C	2.55951000	1.17059400	-0.77462000
C	1.93581400	-0.03035600	-0.34865400
H	4.74716800	1.64847100	-0.98860800
H	2.04332000	2.07765000	-1.05190500
N	4.18362300	-0.26653800	-0.30708000
N	2.95482300	-0.87533300	-0.09500600
C	5.45846100	-0.94500000	-0.17220600
H	5.56628900	-1.74643000	-0.91130100
H	6.24433100	-0.20622900	-0.33786700
H	5.57453500	-1.36095300	0.83271700
C	2.89768900	-2.23143900	0.43454200
H	3.16344300	-2.24355600	1.49678300
H	1.86845400	-2.57095800	0.30561400
H	3.57103900	-2.88599200	-0.12622300
C	0.05425600	-0.21600400	0.56897600
O	0.29616800	-0.58871800	1.75126600
C	-0.36465800	1.22159300	0.32767200
C	-0.71523600	1.71141900	-0.93777300
C	-0.41764500	2.08685400	1.42574800
C	-1.10939000	3.03948600	-1.10060900
H	-0.67499600	1.05581900	-1.80320600
C	-0.81041700	3.41595600	1.26538700
H	-0.14976000	1.68888900	2.39907000
C	-1.15783900	3.89730100	0.00174400
H	-1.38359600	3.40435300	-2.08745700
H	-0.84962700	4.07621100	2.12854400
H	-1.46801100	4.93153800	-0.12484700
H	-0.01960100	-2.29949900	1.18087600
C	-0.62931100	-1.32688700	-0.30741800
H	-0.28596500	-1.28151900	-1.34392000
O	-0.20880500	-2.57029300	0.24682000
C	-2.14946900	-1.22367600	-0.27924900
C	-2.88182500	-1.21943900	-1.47063600
C	-2.84517900	-1.17057000	0.93742100
C	-4.27734000	-1.16242600	-1.45599700
H	-2.35430200	-1.26961000	-2.42144900
C	-4.23725300	-1.11275100	0.95612600
H	-2.28398800	-1.16278500	1.86735800
C	-4.95944000	-1.10907700	-0.24068500
H	-4.82921000	-1.16360800	-2.39288300
H	-4.76196900	-1.06791600	1.90739400
H	-6.04552100	-1.06512000	-0.22406500

Table S100. Cartesien coordinates of imidazole-5-ylidene 13

C	0.02724500	-0.84600300	-0.00365400
C	-0.63006200	1.25813700	0.00695100
C	0.75257400	1.34964800	-0.00865700
N	1.09207800	-0.02493000	-0.01647900
H	0.02400600	-1.92662800	-0.00622800
H	-1.37593400	2.04241700	0.01135600
N	-1.06576700	-0.07334900	0.01026100
C	2.47198900	-0.48792300	0.00849100
H	2.88815800	-0.39184300	1.01652700
H	2.53285700	-1.53367700	-0.30927900
H	3.05375500	0.13985500	-0.66801100
C	-2.44152800	-0.54670700	-0.00174100
H	-2.98456500	-0.13444500	0.85400800
H	-2.94284100	-0.23364000	-0.92304900
H	-2.46092000	-1.63699900	0.05986300

Table S101. Cartesien coordinates of imidazole-5-ylidene 13, TS-1

C	-2.91389500	0.49241400	-0.80785700
C	-2.07142800	-1.01474300	0.56190700
C	-1.06106400	-0.10372800	0.35507100

N	-1.64910000	0.82282700	-0.51240000
H	-3.59059600	1.03676000	-1.44983400
H	-2.09524200	-1.90666300	1.17162300
N	-3.20650400	-0.64188200	-0.15914000
C	-0.95478600	2.00567900	-1.02734500
H	-0.28545400	1.71471300	-1.84160500
H	-1.68884000	2.72786000	-1.39367000
H	-0.36795700	2.42105200	-0.20363000
C	-4.48620700	-1.33729500	-0.19243200
H	-4.34739700	-2.35729500	-0.56192100
H	-4.91881000	-1.37479800	0.81146200
H	-5.17302400	-0.80911800	-0.85661000
C	0.62692000	0.56746400	1.45718500
H	0.34643800	-0.13224100	2.27262600
O	0.49290600	1.79811500	1.61630900
C	1.73982400	0.00959500	0.59049000
C	1.97460500	-1.36703700	0.49676500
C	2.59926700	0.89050400	-0.07169500
C	3.03533800	-1.85761500	-0.26175400
H	1.31092400	-2.05487500	1.01831600
C	3.66118800	0.40399800	-0.83700500
H	2.42541900	1.95627600	0.04502200
C	3.88146500	-0.97098200	-0.93647800
H	3.20712900	-2.92961600	-0.32774100
H	4.32488700	1.09839000	-1.34754000
H	4.71114800	-1.35150600	-1.52730600

Table S102. Cartesien coordinates of imidazole-5-ylidene 13, IM-1

C	-2.65210400	0.30875900	-0.98748700
C	-2.02159500	-0.71800000	0.86057400
C	-1.00412400	0.13203800	0.50857100
N	-1.43812700	0.75683600	-0.65897100
H	-3.23614700	0.63401400	-1.83472500
H	-2.11390200	-1.38150100	1.70615400
N	-3.03820500	-0.59678000	-0.07877100
C	-0.68386800	1.81393300	-1.34728200
H	0.05118100	1.36170000	-2.01735900
H	-1.38093300	2.43878900	-1.91043400
H	-0.17533700	2.34851500	-0.52579100
C	-4.31314000	-1.30296900	-0.06331100
H	-4.14016400	-2.38234800	-0.08097000
H	-4.87480600	-1.04051300	0.83743400
H	-4.89350200	-1.02005700	-0.94328700
C	0.28082700	0.60323400	1.24458200
H	0.21365200	0.05194600	2.22638300
O	0.27505600	1.92748500	1.33311100
C	1.51895100	-0.02409000	0.53074600
C	1.63938200	-1.38898600	0.24185500
C	2.57593200	0.82908600	0.20965300
C	2.79103600	-1.89049400	-0.36715400
H	0.82660500	-2.06950000	0.49563000
C	3.73270300	0.33281200	-0.39604100
H	2.44873700	1.87797400	0.46331700
C	3.84325500	-1.02810900	-0.68948900
H	2.87076900	-2.95287400	-0.58893700
H	4.55179100	1.00730900	-0.63760700
H	4.74240400	-1.41700100	-1.16181000

Table S103. Cartesien coordinates of imidazole-5-ylidene 13, TS-2

C	-3.23429600	1.52800000	-0.14578100
C	-1.12226900	1.84307400	0.43090300
C	-1.18827300	0.62279100	-0.18857300
N	-2.53742500	0.46027600	-0.54133400
H	-4.29363200	1.68497900	-0.28277800
H	-0.22964100	2.35319100	0.76598900
N	-2.39435200	2.38769100	0.45304000
C	-3.04882200	-0.68788000	-1.29114300
H	-2.99169200	-1.58227600	-0.66780400
H	-4.08168100	-0.49312700	-1.58669300
H	-2.41472600	-0.82143500	-2.16942500
C	-2.76062600	3.68081000	1.02126800
H	-2.57092300	3.68181700	2.09761500
H	-2.17040100	4.46929400	0.54814100
H	-3.82100300	3.86639700	0.84072300
C	-0.07552700	-0.28095500	-0.56691000
H	0.99248100	0.50319100	-0.20925100
O	0.06680200	-0.21764500	-2.00546800
C	-0.13976200	-1.66273300	-0.04969300
C	-0.65277100	-1.95444700	1.23441100
C	0.37397600	-2.74066200	-0.80096100
C	-0.64901400	-3.25336500	1.73869900
H	-1.04399100	-1.14618900	1.85014000
C	0.37795000	-4.03708700	-0.28948600
H	0.76414800	-2.53770000	-1.79240300
C	-0.13406800	-4.30931400	0.98181800
H	-1.04878700	-3.44120200	2.73324000
H	0.78293000	-4.84585800	-0.89441300
H	-0.13032600	-5.32189300	1.37631600
H	0.78333700	0.43807100	-2.11680500
O	1.72468400	1.50218700	-0.32077000
C	3.05811700	1.28304200	0.06819100
C	3.69605500	0.16594700	-0.78701800
H	4.74980400	-0.00555900	-0.52944300
H	3.15613700	-0.77865700	-0.64930900
H	3.64412200	0.43460400	-1.84933100
C	3.82483000	2.60111400	-0.15317000
H	3.37201100	3.40130000	0.44473700
H	4.88432600	2.51904600	0.12400600
H	3.76317800	2.89509400	-1.20745200

C	3.12471900	0.89068800	1.56122300
H	4.15598700	0.74853400	1.91132100
H	2.66148300	1.67500300	2.17292800
H	2.57608800	-0.04287800	1.73525000

Table S104. Cartesien coordinates of imidazole-5-ylidene 13, IM-2

C	3.21557600	0.06580100	0.05242300
C	1.35282200	-1.11835900	-0.17098700
C	0.94287100	0.23476700	-0.04982400
N	2.17929000	0.93840700	0.10725900
H	4.25623900	0.32276100	0.16160400
H	0.78850100	-1.98785100	-0.45643900
N	2.73183600	-1.16041300	-0.11524200
C	2.35202400	2.33445800	0.48782900
H	1.71829500	2.56025200	1.34863100
H	3.40178500	2.48879100	0.75401800
H	2.07156700	3.00662200	-0.32281900
C	3.53206300	-2.36720700	-0.24674900
H	3.25558300	-3.07816600	0.53688000
H	3.35702200	-2.82628400	-1.22436700
H	4.58971500	-2.11455500	-0.15242400
C	-0.30709700	0.85244300	-0.06515200
O	-0.30817000	2.25933100	-0.25126900
C	-1.59182600	0.20247000	0.00679000
C	-1.77944100	-1.16855800	0.33271000
C	-2.77400800	0.95220700	-0.24092700
C	-3.04602600	-1.74287300	0.36753900
H	-0.92940800	-1.77792300	0.61805100
C	-4.03380600	0.36548800	-0.20829200
H	-2.68630100	2.01590000	-0.43514900
C	-4.19054200	-0.99270100	0.08361800
H	-3.13944100	-2.79519700	0.63030200
H	-4.90844500	0.98154700	-0.40907100
H	-5.17604700	-1.44980700	0.10282300
H	-0.54723500	2.42570600	-1.17985400

Table S105. Cartesien coordinates of imidazole-5-ylidene 13, TS-3

C	-3.91941400	-0.30031400	-0.27164900
C	-1.88627900	-1.00862900	-0.73502100
C	-1.74160300	0.11669700	0.05136300
N	-3.05446200	0.53268800	0.32340400
H	-4.99427300	-0.22163600	-0.23167800
H	-1.13666200	-1.67588300	-1.12590800
N	-3.23519700	-1.24210500	-0.92588900
C	-3.49486100	1.70196000	1.10045000
H	-2.96247000	2.58558000	0.75565100
H	-4.57157300	1.81305700	0.94575800
H	-3.26206600	1.55556600	2.15277400
C	-3.81012900	-2.34532600	-1.68779100
H	-3.45949500	-2.30165100	-2.72196500
H	-3.51254900	-3.29814500	-1.24231900
H	-4.89819300	-2.26437700	-1.67205100
C	-0.53090400	0.74786100	0.62361400
O	-0.85755000	1.64689200	1.62170000
C	0.44591800	1.31631300	-0.38078500
C	0.65976900	0.80355000	-1.67039000
C	1.22248000	2.41800000	0.01860300
C	1.60474500	1.36874200	-2.52671700
H	0.08423600	-0.04342400	-2.02942300
C	2.16956100	2.98057200	-0.83530200
H	1.05794700	2.82845300	1.00770500
C	2.36782600	2.46191700	-2.11601500
H	1.74426500	0.94849800	-3.52022200
H	2.75362600	3.83359000	-0.49714500
H	3.10552000	2.90091500	-2.78283200
H	-0.32808400	1.18867800	2.43582900
C	0.26819000	-0.58409200	1.73396300
O	0.48160900	0.09806900	2.82693100
H	-0.56716900	-1.32411000	1.75882500
C	1.45705900	-1.19581500	1.03868500
C	2.72401900	-0.60876700	1.16232900
C	1.33894600	-2.37487600	0.29082700
C	3.83047800	-1.16548000	0.52574000
H	2.81533100	0.27897100	1.77923400
C	2.44575300	-2.93711400	-0.34995800
H	0.37448600	-2.88003300	0.24371400
C	3.69646700	-2.32856800	-0.23962200
H	4.80590200	-0.69559900	0.62915200
H	2.33542100	-3.85784900	-0.91917700
H	4.56281000	-2.76415200	-0.73150500

Table S106. Cartesien coordinates of imidazole-5-ylidene 13, IM-3

C	-3.99941400	-0.17598700	-0.28374700
C	-2.53363100	1.10789800	0.75210200
C	-1.81990100	0.24345600	-0.03842300
N	-2.77682300	-0.54827500	-0.67226600
H	-4.92764800	-0.61109800	-0.61975800
H	-2.19584300	1.93067000	1.35981500
N	-3.88329700	0.83439900	0.58718000
C	-2.47874400	-1.55297000	-1.70007600
H	-2.08786400	-2.45702700	-1.22892800
H	-3.39496600	-1.77532100	-2.25118900
H	-1.70677900	-1.09841900	-2.33130800
C	-4.98481400	1.54374300	1.22767000
H	-4.90298800	1.45489000	2.31413300
H	-4.95796200	2.59975700	0.94661300

H	-5.93139700	1.10882400	0.90228800
C	-0.33285600	0.19074400	-0.47050400
O	-0.32058500	0.41850400	-1.80239900
C	0.27449400	-1.15428100	-0.02186800
C	0.08201700	-1.68484300	1.26082300
C	1.06483300	-1.86335500	-0.93143900
C	0.67041200	-2.89669900	1.62844900
H	-0.53485300	-1.14968900	1.98107300
C	1.65712800	-3.07296100	-0.56672500
H	1.19192200	-1.43618600	-1.92091100
C	1.46199700	-3.59513500	0.71416800
H	0.51085600	-3.29528900	2.62791500
H	2.27379700	-3.61049900	-1.28353200
H	1.92145800	-4.53875300	0.99810900
H	-0.29418800	2.15849800	-1.31133400
C	0.39023500	1.42041700	0.25500000
O	-0.11252300	2.56193000	-0.41619100
H	0.09236300	1.47146700	1.31261500
C	1.90474900	1.34197800	0.19797200
C	2.58204600	1.50004900	-1.01992200
C	2.65529400	1.12430800	1.35814400
C	3.97353300	1.43404400	-1.06954900
H	2.00322600	1.65667000	-1.92322000
C	4.04958800	1.06034500	1.31236700
H	2.14275200	1.00495000	2.31101000
C	4.71390100	1.21573800	0.09575200
H	4.48458400	1.55557600	-2.02196500
H	4.61443800	0.89452600	2.22680600
H	5.79961100	1.17117500	0.05494200

Table S107. Cartesien coordinates of imidazole-5-ylidene 13, TS-4

C	4.28891500	-0.05492900	-0.33688600
C	2.82402600	-1.13696900	0.90406500
C	2.08992000	-0.17495200	0.24568500
N	3.06958600	0.47272400	-0.52228400
H	5.20991000	0.25682700	-0.80681300
H	2.50100600	-1.91268200	1.58331900
N	4.16997500	-1.05533700	0.54502500
C	2.77852300	1.56922300	-1.44413700
H	2.48351000	2.45776300	-0.88081800
H	3.66613500	1.79125300	-2.04233600
H	1.95167300	1.26271300	-2.08771500
C	5.25026400	-1.91280300	1.01332100
H	5.33956100	-1.84182000	2.10110700
H	5.04852100	-2.95184500	0.73765700
H	6.19190600	-1.59944500	0.55814100
C	-0.09363200	-0.04604400	-0.62119700
O	0.12173100	-0.21413300	-1.83648900
C	-0.47229200	1.31665100	-0.09887200
C	-0.38370900	1.67247800	1.25391600
C	-0.98714800	2.24564300	-1.01115700
C	-0.80199600	2.92979400	1.68340800
H	0.05296700	0.97336800	1.96022000
C	-1.40553300	3.50668500	-0.58268400
H	-1.05837400	1.95783300	-2.05533000
C	-1.31574500	3.85210400	0.76599000
H	-0.72100300	3.19597900	2.73445800
H	-1.80649900	4.21664500	-1.30194200
H	-1.64100800	4.83322200	1.10282000
H	0.27861700	-2.08906400	-1.33713800
C	-0.57071600	-1.30253600	0.16021600
O	0.00383800	-2.43426100	-0.46061000
H	-0.23155500	-1.25123800	1.19923200
C	-2.09679800	-1.36900200	0.14597900
C	-2.78130700	-1.66363400	-1.04058400
C	-2.83680000	-1.13927500	1.30990200
C	-4.17338500	-1.72453400	-1.05985100
H	-2.21251900	-1.84607400	-1.94712800
C	-4.23204600	-1.20011500	1.29501600
H	-2.31699300	-0.91539900	2.23914700
C	-4.90472900	-1.49284800	0.10863700
H	-4.69068900	-1.95437900	-1.98825500
H	-4.79098000	-1.02406400	2.21088600
H	-5.99054700	-1.54376900	0.09350200

Table S108. Cartesien coordinates of pyrrolidine-2-ylidene 14

C	-0.22898300	-1.03014800	-0.10100400
C	0.99588600	-0.11185300	-0.02252200
C	0.46975600	1.34000200	-0.27758500
C	-1.02476200	1.24494100	0.03469300
H	0.97779800	2.09531600	0.33096100
H	0.61598400	1.61255900	-1.32915700
H	-1.28531800	1.59089200	1.04423100
H	-1.66663800	1.78089000	-0.67439000
C	1.56270700	-0.25757400	1.40780300
H	1.79644800	-1.30469500	1.62544300
H	2.48053400	0.33353000	1.51771300
H	0.84646300	0.08757200	2.16371400
C	2.05762600	-0.53532000	-1.04806600
H	2.93576100	0.12162600	-0.99754100
H	2.38396000	-1.56385000	-0.86258200
H	1.66048700	-0.49147600	-2.06917200
N	-1.26707400	-0.22485300	-0.06008500
C	-2.64735800	-0.69229100	-0.03448700
H	-3.14259500	-0.37596300	0.89246900
H	-3.20895400	-0.27853100	-0.88147000
H	-2.63365200	-1.78044300	-0.09261900

Table S109. Cartesien coordinates of pyrrolidine-2-ylidene 14, TS-1

C	-1.07598500	0.18068800	0.18567800
C	-1.85992400	-1.12171300	0.03143000
C	-3.28379900	-0.64667600	-0.39768000
C	-3.03986700	0.72945600	-1.01780400
H	-3.76866800	-1.34170400	-1.08946900
H	-3.92576400	-0.54887600	0.48483200
H	-2.92089700	0.70581400	-2.10843500
H	-3.80429200	1.47528600	-0.77779500
C	-1.18850900	-1.93258400	-1.10451500
H	-0.14296300	-2.14984100	-0.87014500
H	-1.72012400	-2.88147600	-1.24373000
H	-1.20958900	-1.38997400	-2.05687300
C	-1.90094300	-1.95737200	1.31960400
H	-2.54630700	-2.83239900	1.17516900
H	-0.90520500	-2.31634900	1.59665900
H	-2.29780900	-1.37865200	2.16096300
N	-1.74518600	1.13042600	-0.40224000
C	-1.27920000	2.51061500	-0.56909100
H	-0.89777600	2.64505800	-1.58733500
H	-2.12364200	3.18958900	-0.41549800
H	-0.49848000	2.69232200	0.17550200
C	0.43894100	0.65275000	1.40695500
H	0.13109900	-0.13890600	2.12839600
O	0.33251400	1.85888700	1.74494100
C	1.63152700	0.19297200	0.57695600
C	2.04035300	-1.14544700	0.55996100
C	2.38255300	1.13641000	-0.13171700
C	3.15293900	-1.54404100	-0.18293200
H	1.49133200	-1.87977700	1.14805500
C	3.49212600	0.74314200	-0.87984700
H	2.09179700	2.18046200	-0.06140100
C	3.87796000	-0.59957100	-0.91358100
H	3.46143300	-2.58689300	-0.18299900
H	4.06638900	1.48585500	-1.42900600
H	4.74661500	-0.90539200	-1.49124500

Table S110. Cartesien coordinates of pyrrolidine-2-ylidene 14, IM-1

C	-1.02661900	0.19812800	0.24736700
C	-1.79904100	-1.10597600	0.00215500
C	-3.18973100	-0.57747200	-0.44942500
C	-2.87846100	0.78520700	-1.06687700
H	-3.68856700	-1.25632900	-1.14670800
H	-3.83989300	-0.44878400	0.42316900
H	-2.69158000	0.74374300	-2.14724200
H	-3.64356300	1.54650700	-0.88661800
C	-1.12077800	-1.87006200	-1.16371500
H	-0.09168500	-2.14137100	-0.91982400
H	-1.68417400	-2.78727500	-1.37138000
H	-1.09632600	-1.27231600	-2.08211600
C	-1.91382600	-2.01563100	1.23399900
H	-2.59204800	-2.84795000	1.01020600
H	-0.94704200	-2.44003200	1.51905800
H	-2.31359300	-1.47412700	2.09786300
N	-1.63346000	1.17732600	-0.37413500
C	-1.15203900	2.55771500	-0.45261900
H	-0.52540900	2.67939600	-1.34225500
H	-2.01550000	3.22494800	-0.52222900
H	-0.55889900	2.70038400	0.47013000
C	0.16969900	0.44666400	1.25684400
H	-0.00015400	-0.39425700	1.98035400
O	0.12049100	1.64407400	1.80171800
C	1.48974200	0.08465000	0.50940900
C	1.98733200	-1.22086000	0.41962700
C	2.25075800	1.12873400	-0.02608600
C	3.19434100	-1.48635300	-0.23176500
H	1.44349800	-2.03988100	0.88896400
C	3.45319300	0.86974600	-0.68446000
H	1.89788400	2.14350300	0.13082900
C	3.92631300	-0.44031400	-0.79710700
H	3.57065400	-2.50555500	-0.28305200
H	4.03303500	1.69241200	-1.09714500
H	4.86834600	-0.64194200	-1.30088700

Table S111. Cartesien coordinates of pyrrolidine-2-ylidene 14, TS-2

C	0.81794200	-1.18861700	-0.20744500
C	1.34792900	-1.48206600	1.20589900
C	1.13549000	-3.01819200	1.29857100
C	1.22608700	-3.49718700	-0.14755700
H	1.86807000	-3.49868100	1.95300900
H	0.13528500	-3.22662800	1.69257500
H	2.24064900	-3.79106500	-0.44887600
H	0.55262100	-4.32796600	-0.38267600
C	2.85601100	-1.14241200	1.28353300
H	3.02985700	-0.07416800	1.13606500
H	3.23698700	-1.42085700	2.27288200
H	3.43945900	-1.68782200	0.53194400
C	0.57330800	-0.75494800	2.31592500
H	0.87174500	-1.16178300	3.28938500
H	0.78628000	0.31713000	2.32163100
H	-0.50628300	-0.89137700	2.19456300
N	0.81739900	-2.30789900	-0.91669700
C	0.54809900	-2.49036600	-2.34303600
H	1.45534300	-2.87399800	-2.82505100
H	-0.25187300	-3.22943200	-2.46144400
H	0.24525600	-1.53812000	-2.77078800
C	0.21072900	0.08793400	-0.58821000

H	-0.77625300	0.07301700	0.08948800
O	-0.41310300	0.12232400	-1.85879800
C	1.03813400	1.33639400	-0.34119700
C	0.55392100	2.37026200	0.46975600
C	2.26061300	1.52032800	-1.00399600
C	1.28114400	3.55124600	0.63084900
H	-0.40191200	2.24890100	0.97156400
C	2.98904300	2.69971700	-0.84735100
H	2.63674900	0.73568500	-1.65655400
C	2.50164600	3.71811800	-0.02502700
H	0.89070700	4.34226000	1.26577400
H	3.93450400	2.82509300	-1.36895900
H	3.06771600	4.63756300	0.09879800
H	-1.36968800	-0.03889600	-1.55911800
O	-2.25126600	-0.33349000	-0.14055100
C	-3.41082700	0.38806400	0.14451200
C	-4.62165000	-0.45286400	-0.32458800
H	-4.61329800	-1.42569000	0.18048400
H	-5.58160300	0.03961800	-0.11816000
H	-4.55178500	-0.63466800	-1.40361700
C	-3.42719200	1.74853700	-0.58968200
H	-4.34266200	2.32175200	-0.39022600
H	-2.57030600	2.36089200	-0.28280500
H	-3.35300500	1.59434900	-1.67318600
C	-3.52348700	0.62698300	1.66754600
H	-3.48751900	-0.33356800	2.19540500
H	-2.68094300	1.23657500	2.02013700
H	-4.45258800	1.14092700	1.94841300

Table S112. Cartesien coordinates of pyrrolidine-2-ylidene 14, IM-2

C	1.02920600	0.24802500	-0.00104900
C	1.36087800	-1.22706300	-0.23727100
C	2.68103700	-1.05537500	-1.04545600
C	3.36384300	0.15496800	-0.40772700
H	3.30525000	-1.95498600	-1.01972000
H	2.43785000	-0.84330900	-2.09343700
H	3.96219000	-0.14944800	0.46663000
H	4.03700400	0.68364800	-1.09380000
C	1.65623700	-1.96999000	1.08759500
H	0.75008800	-2.07175300	1.69342000
H	2.03739200	-2.97900100	0.88387600
H	2.40190600	-1.44572800	1.69513900
C	0.34439000	-2.02447100	-1.06733500
H	0.78714000	-2.98324600	-1.36524000
H	-0.57213900	-2.24021600	-0.51331200
H	0.06604500	-1.48101900	-1.97649900
N	2.24698500	1.01950900	0.00415400
C	2.52909000	1.81868100	1.19981300
H	2.74007800	1.19337000	2.08384000
H	3.40427900	2.45062100	1.01089000
H	1.67932400	2.46605100	1.42737500
C	-0.13770100	0.93954400	-0.07587400
O	-0.07942700	2.31188200	-0.24904600
C	-1.52224100	0.44745100	0.01822800
C	-2.51950100	1.01865400	-0.79365500
C	-1.90084900	-0.54126000	0.94129500
C	-3.83861200	0.58029800	-0.71531300
H	-2.24399200	1.80789500	-1.48534500
C	-3.22166900	-0.98357300	1.01490400
H	-1.15743900	-0.94103100	1.62356100
C	-4.19590300	-0.42825800	0.18402700
H	-4.59261100	1.02787100	-1.35792000
H	-3.49262100	-1.74956200	1.73708400
H	-5.22671400	-0.76679600	0.24630800
H	0.81425600	2.47923800	-0.61265500

Table S113. Cartesien coordinates of pyrrolidine-2-ylidene 4, TS-3

C	1.74503800	-0.22453300	-0.08894500
C	2.15023900	0.22343500	1.33512500
C	3.21073800	-0.84363000	1.71123400
C	3.80857600	-1.26038900	0.37486500
H	3.95606700	-0.45301100	2.40996000
H	2.71918400	-1.70014300	2.18625500
H	4.70847800	-0.69185500	0.10467000
H	4.05524200	-2.32552000	0.30827300
C	2.81431200	1.61808800	1.18708800
H	2.09628700	2.35449200	0.81680600
H	3.17888600	1.95199300	2.16546900
H	3.66509300	1.59671900	0.49662000
C	1.07881200	0.29296100	2.43183500
H	1.58728800	0.40273400	3.39748500
H	0.41451000	1.14717300	2.30689800
H	0.47234000	-0.61587000	2.47805300
N	2.74010300	-0.94741300	-0.58851500
C	2.97075500	-1.40796700	-1.96335600
H	3.99206600	-1.12535500	-2.24439400
H	2.87612500	-2.49782500	-1.99556500
H	2.23366900	-0.94117300	-2.61039500
C	0.47965600	0.03470900	-0.83308400
O	0.47859700	-0.19848100	-2.13265100
C	-0.23680400	1.34812300	-0.48645900
C	0.08419400	2.42628300	-1.33296500
C	-1.19029800	1.56918500	0.51475100
C	-0.49324200	3.68235700	-1.16100200
H	0.78104900	2.25218000	-2.14603000
C	-1.78120900	2.82626100	0.68185600
H	-1.50361300	0.76102500	1.16146900
C	-1.43168200	3.88987900	-0.14702200
H	-0.21882100	4.49679800	-1.82713000

H	-2.52750100	2.96301500	1.46057900
H	-1.89235000	4.86551500	-0.01432200
H	0.16478400	-1.67085900	-1.98256200
C	-0.29669600	-1.64725100	-0.17114400
O	0.03842500	-2.40107100	-1.25705100
H	0.22274300	-1.98705400	0.73158000
C	-1.76435400	-1.49248300	0.06362400
C	-2.62540000	-1.16450000	-0.99638500
C	-2.31472000	-1.71670200	1.33403600
C	-3.99633900	-1.04915400	-0.78122200
H	-2.20391700	-0.98538600	-1.98036400
C	-3.68937400	-1.60466000	1.54889400
H	-1.66149800	-1.99878400	2.15813500
C	-4.53494400	-1.26802700	0.49059800
H	-4.65043800	-0.78782200	-1.60926000
H	-4.09982300	-1.79168100	2.53821600
H	-5.60629800	-1.18290300	0.65282800

Table S114. Cartesien coordinates of pyrrolidine-2-ylidene 14, IM-3

C	1.74019000	-0.46526000	-0.06717400
C	2.40628200	0.16346400	1.18502200
C	3.62551700	-0.77101000	1.40466000
C	3.93635200	-1.29598500	0.01264400
H	4.46896500	-0.24782900	1.86309400
H	3.34366300	-1.60195200	2.06062400
H	4.66422600	-0.68751200	-0.53821600
H	4.27481900	-2.33574300	-0.01452000
C	2.89570800	1.58917900	0.81408000
H	2.05994900	2.26036500	0.61340700
H	3.47298300	1.99235900	1.65402500
H	3.54388000	1.58307000	-0.06985200
C	1.56575300	0.22888100	2.46834400
H	2.20566400	0.59868400	3.27865400
H	0.72173000	0.91169800	2.37451300
H	1.19527800	-0.75724400	2.76467100
N	2.63087100	-1.20140200	-0.67868600
C	2.53310800	-1.94280600	-1.94800900
H	3.47557500	-1.79882000	-2.48584100
H	2.40625400	-3.00407300	-1.71379100
H	1.66603500	-1.55394500	-2.48377600
C	0.25800300	-0.28601600	-0.62836100
O	0.14502700	-0.65595300	-1.90982500
C	-0.13645700	1.20509000	-0.44741700
C	0.23048000	2.06651300	-1.49293000
C	-0.85899800	1.73990700	0.62585700
C	-0.07186900	3.42588100	-1.44695100
H	0.72967100	1.63246300	-2.35294800
C	-1.17614300	3.10174700	0.66977000
H	-1.21929000	1.09608500	1.42050200
C	-0.77439100	3.95237200	-0.35907500
H	0.22785600	4.07420300	-2.26702200
H	-1.75152200	3.49048900	1.50639800
H	-1.02189400	5.01032800	-0.32435100
H	-0.17984600	-2.31740700	-1.27975300
C	-0.57429900	-1.35484500	0.26119800
O	-0.23592500	-2.60055800	-0.32731700
H	-0.24032400	-1.39066000	1.30349400
C	-2.08010700	-1.13550500	0.25368000
C	-2.78436700	-0.88153900	-0.93413700
C	-2.80063200	-1.25283300	1.44877600
C	-4.17097200	-0.74031100	-0.91398400
H	-2.22311900	-0.77939600	-1.85730200
C	-4.19036600	-1.11495900	1.46911200
H	-2.26891300	-1.46402300	2.37530500
C	-4.88028100	-0.85691600	0.28482100
H	-4.70254600	-0.53696800	-1.84056400
H	-4.73096000	-1.21351700	2.40748800
H	-5.96209300	-0.74904300	0.29413800

Table S115. Cartesien coordinates of pyrrolidine-2-ylidene 14, TS-4

C	1.82861600	-0.58166800	-0.03430500
C	2.57298400	-0.03112400	1.19619800
C	3.82690100	-0.95059200	1.29980100
C	4.03121900	-1.44898700	-0.12561200
H	4.69956800	-0.42247300	1.69452000
H	3.61635800	-1.79681000	1.96328900
H	4.73107200	-0.84084700	-0.71225900
H	4.34620500	-2.49445900	-0.19993500
C	3.00261600	1.42626900	0.89024100
H	2.13840400	2.07739400	0.74745300
H	3.59041500	1.81047400	1.73235500
H	3.62412900	1.48695900	-0.01082900
C	1.75984500	-0.06983200	2.49796500
H	2.39748200	0.24514700	3.33317500
H	0.90423900	0.60795900	2.45856700
H	1.39826500	-1.08054000	2.71578000
N	2.67132500	-1.30562000	-0.71404800
C	2.43610300	-1.99545200	-1.98832800
H	3.27905800	-1.78446600	-2.65461200
H	2.39400400	-3.07345000	-1.80035200
H	1.49822400	-1.63917600	-2.41206500
C	-0.03115000	-0.26361900	-0.73580700
O	-0.08095400	-0.66219400	-1.94818200
C	-0.14638600	1.24160200	-0.52065500
C	0.28030600	2.07675300	-1.56265400
C	-0.68671800	1.82971400	0.63018000
C	0.20903100	3.46295000	-1.44331400
H	0.65245200	1.60918000	-2.46864400
C	-0.76817700	3.21992100	0.74909200

H	-1.07545300	1.20913700	1.43098300
C	-0.31163400	4.04157600	-0.28209300
H	0.55015700	4.09489900	-2.25984600
H	-1.19962700	3.65841700	1.64547200
H	-0.37464200	5.12274500	-0.18890700
H	-0.40963200	-2.41877800	-1.16314800
C	-0.78216800	-1.22505800	0.24264400
O	-0.45751700	-2.54191500	-0.18872900
H	-0.41760200	-1.12827300	1.26847700
C	-2.29375900	-1.00664500	0.25275000
C	-3.02661900	-0.81597200	-0.92860000
C	-2.98608300	-1.04713500	1.46958900
C	-4.41235600	-0.66628300	-0.88536100
H	-2.49721300	-0.77251400	-1.87494900
C	-4.37357800	-0.89849200	1.51519700
H	-2.43218000	-1.20572000	2.39336000
C	-5.09182700	-0.70690700	0.33477000
H	-4.96475100	-0.51392700	-1.80944200
H	-4.89123400	-0.93505300	2.47070600
H	-6.17219900	-0.58970900	0.36428900

Table S116. Cartesien coordinates of 1,2,3-triazole-5-ylidene 15

C	0.64032900	1.26469000	-0.00530100
C	-0.75745300	1.35876100	0.01077700
N	-1.04988800	0.01001000	0.00754400
H	1.39624500	2.03799200	-0.01188000
N	1.01816900	-0.05035000	-0.02084400
C	-2.39066100	-0.56127200	0.00238200
H	-2.56579500	-1.11373700	-0.92550000
H	-2.51770900	-1.23734400	0.85248200
H	-3.08353800	0.27516100	0.07650600
C	2.35650300	-0.62381200	0.01373900
H	3.04881700	0.07829400	-0.45478100
H	2.66639300	-0.80820400	1.04664300
H	2.35306000	-1.56389400	-0.53919400
N	-0.02396500	-0.85944100	-0.01153700

Table S117. Cartesien coordinates of 1,2,3-triazole-5-ylidene 15, TS-1

C	-2.02305600	-0.92169600	-0.12330400
C	-1.00533600	-0.09312600	-0.55831700
N	-1.46858300	1.14499600	-0.20467500
H	-2.06966800	-1.99774500	-0.19516300
N	-2.98016100	-0.13488100	0.43178700
C	-0.81261800	2.42909600	-0.43508300
H	-1.30456400	3.18099000	0.18185700
H	0.23964100	2.33293800	-0.16375200
H	-0.89458700	2.69987700	-1.49108300
C	-4.23361400	-0.53348400	1.06398200
H	-4.76857000	-1.21689900	0.40140600
H	-4.02750600	-1.02953000	2.01591000
H	-4.82687000	0.36456800	1.23309500
N	-2.66212000	1.15018600	0.39599500
C	0.41425400	-0.99136400	-1.29739100
H	0.42107400	-0.48480900	-2.29699000
O	0.10890400	-2.21961400	-1.22142700
C	1.59465500	-0.46796600	-0.46646600
C	2.29893200	0.68787100	-0.81996700
C	2.00449100	-1.19452000	0.65538500
C	3.37694500	1.13126400	-0.04817000
H	2.01549500	1.23112900	-1.72183900
C	3.07688000	-0.75551900	1.43069400
H	1.47170200	-2.11456200	0.87893300
C	3.76389100	0.41269900	1.08513300
H	3.92338000	2.02591900	-0.33888100
H	3.38774100	-1.32786700	2.30205200
H	4.60500800	0.75125900	1.68516200

Table S118. Cartesien coordinates of 1,2,3-triazole-5-ylidene 15, IM-1

C	1.97945300	0.96610900	-0.11126700
C	0.98090400	0.10572400	-0.52184100
N	1.44478000	-1.12311000	-0.14237800
H	2.01423700	2.03492300	-0.24841100
N	2.93564100	0.20040800	0.47096600
C	0.80008300	-2.41917200	-0.33331500
H	1.43862500	-3.17977100	0.11484500
H	-0.18116500	-2.40162400	0.14409100
H	0.67812200	-2.60577900	-1.40283800
C	4.19034500	0.62542600	1.08297500
H	4.73474400	1.26254100	0.38290500
H	3.98406800	1.17898000	2.00240500
H	4.77262300	-0.26751800	1.30783500
N	2.63429100	-1.09062900	0.46018300
C	-0.27675300	0.67064400	-1.32516500
H	-0.32423600	-0.01449100	-2.22847200
O	-0.05078000	1.93914800	-1.53337800
C	-1.53465800	0.32526000	-0.47651900
C	-2.28258800	-0.84319400	-0.65282700
C	-1.95512200	1.25734300	0.47764400
C	-3.41208600	-1.09630000	0.13307000
H	-2.00230000	-1.54704700	-1.43689400
C	-3.07538800	1.00860900	1.26845000
H	-1.39369100	2.18524200	0.54484300
C	-3.80539100	-0.17373300	1.10350800
H	-3.99262300	-2.00294400	-0.02413600
H	-3.39241700	1.74092200	2.00804100

H	-4.68552500	-0.36360900	1.71312600

Table S119. Cartesien coordinates of 1,2,3-triazole-5-ylidene 15, TS-2

C	1.36679800	1.81107600	-0.16283600
C	0.06671900	1.33826000	-0.31787600
N	-0.70413500	2.45647400	-0.08462500
H	2.27924100	1.23070700	-0.22329100
N	1.26474100	3.11877200	0.15495900
C	-2.15751500	2.58437700	-0.15572800
H	-2.39280300	3.64830300	-0.16775500
H	-2.50445900	2.09991400	-1.06911900
H	-2.62036000	2.09027900	0.70117200
C	2.34141200	4.06976400	0.41611700
H	3.04404900	3.62989500	1.12635000
H	2.85756000	4.30630900	-0.51743700
H	1.89556800	4.97060100	0.83653300
N	0.00972100	3.53989700	0.22572200
C	-0.29650100	-0.04741900	-0.66530100
H	0.78798200	-0.67345500	-0.19599800
O	-0.00414300	-0.27567300	-2.05155700
C	-1.60630100	-0.57679200	-0.21260600
C	-2.01682900	-0.44524100	1.13139000
C	-2.43833400	-1.30386400	-1.08303800
C	-3.22110800	-0.98914800	1.57531700
H	-1.36782100	0.06602100	1.84142600
C	-3.63749600	-1.85549900	-0.63242800
H	-2.12142800	-1.42609300	-2.11298800
C	-4.04342300	-1.69760500	0.69480000
H	-3.50923200	-0.87549000	2.61805500
H	-4.26273200	-2.41216100	-1.32703000
H	-4.97837100	-2.12929200	1.04172400
H	0.83670600	-0.78196900	-2.00426800
O	2.02703700	-0.99182200	-0.39335900
C	2.44930600	-2.18787800	0.21575400
C	1.61023700	-3.37898200	-0.29336100
H	1.93412100	-4.33152200	0.14621000
H	0.55100900	-3.23554100	-0.04813700
H	1.69648500	-3.45884300	-1.38359100
C	3.92848900	-2.39913900	-0.16066900
H	4.53018200	-1.55352900	0.19369700
H	4.33929300	-3.32089300	0.27181800
H	4.03188000	-2.45138600	-1.25056100
C	2.31524300	-2.07783500	1.75018700
H	2.88248500	-1.21187500	2.11298600
H	1.26410700	-1.93792000	2.03206400
H	2.68691500	-2.97255700	2.26672800

Table S120. Cartesien coordinates of 1,2,3-triazole-5-ylidene 15, IM-2

C	2.29662300	0.98727600	-0.25734100
C	1.03661300	0.37399200	-0.00871400
N	1.40298500	-0.96360800	0.25813600
H	2.53709900	2.01080800	-0.48780900
N	3.22484700	0.02265800	-0.14483700
C	0.64600500	-1.90969900	1.05201000
H	1.33958200	-2.67054200	1.41236300
H	0.18881200	-1.38438900	1.90002100
H	-0.15596500	-2.37818100	0.47443000
C	4.65128100	0.14691400	-0.41651500
H	4.83741100	0.08807900	-1.49224300
H	4.99988800	1.10768100	-0.03291800
H	5.16246100	-0.66915900	0.09368300
N	2.75716200	-1.16996100	0.16326300
C	-0.20705800	0.97174900	0.04963700
O	-0.13185700	2.37732200	0.15795300
C	-1.52425900	0.37880500	-0.03109000
C	-1.78524200	-0.82838800	-0.72895800
C	-2.64447400	1.06717400	0.50016100
C	-3.07543000	-1.33930600	-0.83321600
H	-0.97042100	-1.33261000	-1.24134800
C	-3.93181600	0.55376900	0.38098700
H	-2.47848300	2.00014000	1.03076600
C	-4.16232300	-0.65928900	-0.27523400
H	-3.23785800	-2.26525100	-1.38083800
H	-4.76552200	1.10293000	0.81340800
H	-5.16889800	-1.05829700	-0.36405300
H	-0.72772900	2.74862000	-0.51538500

Table S121. Cartesien coordinates of 1,2,3-triazole-5-ylidene 15, TS-3

C	-2.34713300	0.94855700	0.74135900
C	-1.81270600	0.03373300	-0.15776400
N	-2.83303900	-0.88349000	-0.31437800
H	-1.92738200	1.85180600	1.15128600
N	-3.60221300	0.52148500	1.02859300
C	-2.87957800	-2.07724300	-1.17428700
H	-3.11003100	-1.76601300	-2.19452300
H	-1.89734100	-2.56404800	-1.15760300
H	-3.66634100	-2.71948300	-0.77810900
C	-4.57953600	1.12934800	1.92637100
H	-4.20640400	1.09861100	2.95291900
H	-4.75481500	2.16463900	1.62549600
H	-5.50202300	0.55547300	1.84645400
N	-3.91767500	-0.58861700	0.39187900
C	-0.50155900	-0.08027300	-0.82801400
O	-0.68643300	-0.46512600	-2.14675200
C	0.36255200	1.14275800	-0.66578200
C	0.68044100	1.68724600	0.59103100

C	0.88886500	1.76763400	-1.80637200
C	1.47549300	2.82831600	0.70124400
H	0.34184000	1.19360600	1.49772900
C	1.68994300	2.90374600	-1.69562400
H	0.65101800	1.34543800	-2.77595900
C	1.98256100	3.44600800	-0.44292900
H	1.71448400	3.22278800	1.68599700
H	2.08440000	3.37045100	-2.59517700
H	2.60623700	4.33206200	-0.35778100
H	-0.27954000	-1.42332600	-2.12142900
C	0.26801300	-1.70637800	-0.13980100
H	-0.42310100	-1.91055600	0.70643900
O	0.16752500	-2.49234600	-1.18369300
C	1.65446900	-1.44372500	0.39223900
C	2.75376700	-1.46358200	-0.47575700
C	1.87925900	-1.23102100	1.75698400
C	4.04276400	-1.25205200	0.00852900
H	2.57577800	-1.66926100	-1.52662100
C	3.16973000	-1.02381900	2.24801400
H	1.03464000	-1.24720800	2.44517400
C	4.25631100	-1.02828700	1.37231700
H	4.88718100	-1.26840300	-0.67660100
H	3.32774200	-0.86877700	3.31293900
H	5.26346900	-0.86946900	1.74974500

Table S122. Cartesien coordinates of 1,2,3-triazole-5-ylidene 15, IM-3

C	-2.71480300	0.72702100	-0.23726600
C	-1.81763500	-0.30637400	-0.00308000
N	-2.63119400	-1.33453000	0.40138300
H	-2.53325900	1.72943800	-0.58955300
N	-3.94989800	0.24424100	0.02098700
C	-2.28759900	-2.68763900	0.85554600
H	-3.15622600	-3.32048300	0.67450500
H	-1.41508000	-3.02299800	0.28550600
H	-2.06549200	-2.66313700	1.92610900
C	-5.23585200	0.91994700	-0.12459700
H	-5.18949000	1.89065700	0.37301100
H	-5.46280800	1.05586400	-1.18484600
H	-5.99560300	0.29469100	0.34294400
N	-3.92859700	-1.01589400	0.41456800
C	-0.32459700	-0.27368100	-0.50662000
O	-0.44154900	-0.51694000	-1.82007000
C	0.19457500	1.13207400	-0.14009200
C	0.27462700	1.58745000	1.18260200
C	0.57055000	1.99106700	-1.17494400
C	0.73502500	2.87333200	1.46600900
H	-0.02229800	0.93337500	2.00107800
C	1.03216600	3.27952600	-0.89509800
H	0.48959600	1.61516400	-2.18990600
C	1.11624600	3.72475100	0.42518400
H	0.79887700	3.21110100	2.49777200
H	1.32715900	3.93695700	-1.70973400
H	1.47617900	4.72692900	0.64444800
H	-0.04304800	-2.11158300	-1.47271900
C	0.56927300	-1.43373000	0.15266500
H	0.26088400	-1.61983500	1.19221700
O	0.27927300	-2.57803200	-0.63397500
C	2.05741500	-1.13902900	0.14227400
C	2.73964100	-0.99712000	-1.07498100
C	2.78187800	-1.03899400	1.33360800
C	4.11127400	-0.75342000	-1.09248200
H	2.17691000	-1.06768900	-2.00022200
C	4.15792700	-0.79805300	1.31956500
H	2.26685000	-1.15912300	2.28521700
C	4.82703800	-0.65454200	0.10451200
H	4.62638900	-0.64206200	-2.04368400
H	4.70516100	-0.72921000	2.25673600
H	5.89844000	-0.47051600	0.08809100

Table S123. Cartesien coordinates of 1,2,3-triazole-5-ylidene 15, TS-4

C	2.83260500	0.58227700	0.11744600
C	1.90570000	-0.41554600	-0.15262600
N	2.72621300	-1.48281800	-0.41602100
H	2.68161400	1.61265300	0.40124700
N	4.07642000	0.04602600	-0.00327700
C	2.33095300	-2.83138200	-0.82913500
H	3.09604600	-3.53091900	-0.49026100
H	1.36197000	-3.04710700	-0.37075300
H	2.25626500	-2.87094100	-1.91995000
C	5.36994800	0.67580400	0.23844100
H	5.37346400	1.66843100	-0.21616900
H	5.54836400	0.76174700	1.31364200
H	6.14064200	0.05420800	-0.21657300
N	4.03635600	-1.23162000	-0.33362600
C	0.05330900	-0.22443400	0.60347300
O	0.20285100	-0.46989800	1.83694800
C	-0.19299400	1.21543400	0.17545300
C	-0.29058000	1.60882600	-1.16593000
C	-0.33894900	2.18148300	1.17599200
C	-0.53603000	2.93992200	-1.49894500
H	-0.15913800	0.87297100	-1.95513600
C	-0.58067000	3.51675300	0.84531200
H	-0.26412900	1.85683400	2.20886000
C	-0.68165100	3.89986000	-0.49273700
H	-0.61282000	3.23060100	-2.54385400
H	-0.69605800	4.25676700	1.63369600
H	-0.87367200	4.93779800	-0.75285500
H	-0.15092100	-2.21061400	1.40143200
C	-0.75603800	-1.33722000	-0.15267200
H	-0.43147600	-1.41904800	-1.19543200
O	-0.44254900	-2.55220500	0.51685500

C	-2.25410900	-1.06903600	-0.12425900
C	-2.93928800	-0.96626600	1.09501700
C	-2.97861700	-0.94424800	-1.31371900
C	-4.31433400	-0.74194300	1.11779700
H	-2.38208100	-1.05328800	2.02271100
C	-4.35728100	-0.72041900	-1.29473200
H	-2.46066200	-1.03116200	-2.26703600
C	-5.02941500	-0.61880800	-0.07704500
H	-4.83141400	-0.66215800	2.07095600
H	-4.90407600	-0.63075000	-2.23024600
H	-6.10261000	-0.44664600	-0.05702600

Table S124. Cartesien coordinates of pyridyl-4-ylidene 16

C	0.13642800	-1.17552000	-0.01241400
C	-1.24208600	-1.17562700	0.00596300
C	-2.05786000	-0.00003000	0.01279100
C	-1.24211700	1.17560300	0.00597300
C	0.13639000	1.17555000	-0.01242000
H	0.75160000	-2.07281900	-0.02194600
H	-1.71111100	-2.16241500	0.00796500
N	0.82737200	0.00001500	-0.02508400
C	2.29205000	0.00000100	0.02069300
H	2.67169500	-0.88796800	-0.48887600
H	2.67162600	0.88869400	-0.48764200
H	2.64741300	-0.00070500	1.05656000
H	0.75153600	2.07287200	-0.02198100
H	-1.71119300	2.16237200	0.00799300

Table S125. Cartesien coordinates of pyridyl-4-ylidene 16, IM-1

C	2.87078400	0.79630900	0.59650400
C	1.64393600	1.26676700	0.20143500
C	0.74746900	0.43033900	-0.48921500
C	1.16292700	-0.88364800	-0.76283400
C	2.40977000	-1.31380700	-0.36510600
H	3.59502900	1.39038700	1.14423700
H	1.28204700	2.28243100	0.36357200
N	3.25644100	-0.48088400	0.30915900
C	4.60526600	-0.94564000	0.66119900
H	4.98081200	-0.35538400	1.49825900
H	4.56266600	-1.99521100	0.95874300
H	5.28233400	-0.83622600	-0.19166500
H	2.78291800	-2.31515000	-0.54932400
H	0.50785600	-1.57989100	-1.27719500
C	-0.56562100	1.14278000	-0.95388600
H	-0.55360600	0.87838200	-2.05967900
O	-0.55774000	2.41988800	-0.66986100
C	-1.75069600	0.31681900	-0.36323800
C	-2.25638300	-0.84607100	-0.95392700
C	-2.34908000	0.79503100	0.80653100
C	-3.32195000	-1.53810300	-0.37095900
H	-1.83831300	-1.19972000	-1.89645400
C	-3.40870600	0.10574800	1.39474500
H	-1.97472900	1.73233200	1.20793300
C	-3.89632100	-1.06791500	0.81138500
H	-3.71278000	-2.43449900	-0.84799200
H	-3.86623300	0.48841000	2.30477500
H	-4.72954000	-1.60043000	1.26375600

Table S126. Cartesien coordinates of pyridyl-4-ylidene 16, TS-2

C	3.15840700	1.65257600	0.65442500
C	1.87240500	1.24865200	0.88610500
C	1.35191300	0.08269700	0.26712600
C	2.23802900	-0.62766700	-0.57857300
C	3.52364300	-0.18988100	-0.77377600
H	3.58721700	2.54105300	1.10362200
H	1.22519400	1.81152800	1.54667900
N	3.99137200	0.94063900	-0.16812400
C	5.34357000	1.43400000	-0.44987200
H	5.75583500	1.89708000	0.44891500
H	5.98155600	0.59701200	-0.73863900
H	5.32424600	2.17046000	-1.26004500
H	4.23205300	-0.71642600	-1.40299700
H	1.91580600	-1.53923800	-1.06861700
C	-0.08055000	-0.23931900	0.47548900
H	-0.63405500	0.47832300	-0.24994500
O	-0.53140300	0.23717400	1.72124400
C	-0.48049200	-1.67647100	0.19670100
C	-0.66328800	-2.13914100	-1.11338700
C	-0.68890900	-2.56313300	1.26071300
C	-1.01725800	-3.46860000	-1.35837600
H	-0.55059000	-1.44853700	-1.94701900
C	-1.04468200	-3.88928200	1.01779600
H	-0.58881900	-2.18741700	2.27375100
C	-1.20423300	-4.34910500	-0.29235900
H	-1.16318700	-3.80928400	-2.38049500
H	-1.20470100	-4.56608500	1.85365100
H	-1.48682400	-5.38188800	-0.47950000
H	-1.13887600	0.99623500	1.39260800
O	-1.50429700	1.91634800	0.14687800
C	-2.80603800	2.14164900	-0.28464200
C	-3.71535200	0.92034900	-0.01221500
H	-3.71415100	0.68169600	1.05830300
H	-4.75471100	1.09279000	-0.32344100
H	-3.34113600	0.04071000	-0.55067500
C	-2.80133000	2.45068800	-1.79990900
H	-3.80153700	2.68413600	-2.18984900

H	-2.14207200	3.30358100	-2.00020100
H	-2.41170100	1.58831500	-2.35601300
C	-3.36407900	3.36722200	0.48164500
H	-4.38438500	3.62874800	0.16893300
H	-3.37524300	3.15927400	1.55818500
H	-2.71445100	4.23387800	0.31333300

Table S127. Cartesien coordinates of pyridyl-4-ylidene 16, IM-2

C	3.21035200	0.88047200	-0.13697900
C	1.94681700	1.35350800	-0.21881700
C	0.78606500	0.48684400	-0.04017100
C	1.13628200	-0.88348100	0.31302200
C	2.42320600	-1.29248200	0.39344100
H	4.07698900	1.51491800	-0.29155900
H	1.78950300	2.40386000	-0.42725100
N	3.49593300	-0.44248700	0.17009800
C	4.84261500	-0.96578200	0.02905600
H	5.56738400	-0.19469500	0.30661200
H	4.97790700	-1.81803500	0.70186700
H	5.06017900	-1.29496400	-0.99787800
H	2.68872400	-2.30744900	0.67047900
H	0.36088300	-1.59539200	0.56739100
C	-0.49042000	0.97917600	-0.13046900
O	-0.61088400	2.36898400	-0.22090700
C	-1.75426300	0.24120900	-0.05527300
C	-1.92124900	-1.05079500	-0.60055300
C	-2.88992600	0.85828400	0.51603000
C	-3.14970700	-1.70335000	-0.54042700
H	-1.08836600	-1.52674300	-1.10807300
C	-4.11833000	0.20404000	0.56733200
H	-2.78685800	1.84959800	0.94790900
C	-4.25721100	-1.08383800	0.04541600
H	-3.24883900	-2.69577700	-0.97371500
H	-4.97055700	0.70052000	1.02524800
H	-5.21564300	-1.59416400	0.08553400
H	-1.38115100	2.56102700	-0.77963600

Table S128. Cartesien coordinates of pyridyl-4-ylidene 16, TS-3

C	-3.97955400	-0.61570200	0.69688300
C	-2.69470600	-0.46721200	1.14404800
C	-1.70215300	0.14109300	0.33209800
C	-2.13687500	0.61548500	-0.92902200
C	-3.43925000	0.45440200	-1.33135000
H	-4.76129500	-1.07840700	1.28916800
H	-2.39815700	-0.78365900	2.13595500
N	-4.35890400	-0.16592500	-0.53591000
C	-5.72271600	-0.39963500	-1.02427000
H	-6.41178100	-0.41564100	-0.17800200
H	-6.01045200	0.40930400	-1.69846600
H	-5.78210800	-1.35411200	-1.55716600
H	-3.80853500	0.81937300	-2.28310700
H	-1.45676000	1.14149400	-1.58709200
C	-0.30386200	0.13405800	0.87819300
O	-0.24480400	-0.11508000	2.17499900
C	0.58117000	1.27502600	0.38247700
C	0.94232800	1.49938300	-0.95485200
C	1.04543000	2.17558900	1.35130300
C	1.71909100	2.60288100	-1.31483200
H	0.66190800	0.78740200	-1.72521000
C	1.82231100	3.27735800	0.99504400
H	0.78477200	1.97592700	2.38482600
C	2.15764400	3.50128600	-0.34190100
H	1.99579500	2.74790500	-2.35648600
H	2.16929300	3.96297500	1.76475700
H	2.76556400	4.35818300	-0.62141600
H	-0.19433800	-1.63979300	1.95247400
C	0.17490100	-1.52890700	0.13178900
O	-0.19759600	-2.32858800	1.18046000
H	-0.42607300	-1.72333700	-0.76526400
C	1.63770800	-1.53801400	-0.18259500
C	2.08869000	-1.65763800	-1.50400800
C	2.58783900	-1.45451300	0.84840000
C	3.45298600	-1.69178700	-1.79636300
H	1.36133900	-1.74444000	-2.30989500
C	3.94893600	-1.48174200	0.55737400
H	2.24174000	-1.35299800	1.87170500
C	4.38853400	-1.60184300	-0.76500900
H	3.78402500	-1.79661600	-2.82692600
H	4.67361100	-1.41064900	1.36489100
H	5.45226500	-1.62950000	-0.98748900

Table S129. Cartesien coordinates of pyridyl-4-ylidene 16, IM-3

C	3.94138400	-0.62297900	-0.89196800
C	2.60514100	-0.51351700	-1.18975700
C	1.66830200	-0.20895800	-0.18749600
C	2.16421900	-0.01096200	1.11404200
C	3.51047700	-0.14101300	1.37438600
H	4.70141800	-0.85522400	-1.63004000
H	2.19073900	-0.65138000	-2.18628800
N	4.39030400	-0.44626500	0.38241500
C	5.81313900	-0.64507900	0.70046900
H	6.41214000	-0.43177100	-0.18583200
H	6.10536100	0.03821500	1.49951400
H	5.98809700	-1.67698600	1.01872100
H	3.93852200	-0.00727900	2.36153000
H	1.50360100	0.25775300	1.93029900

C	0.17493600	-0.17510900	-0.64624600
O	0.10288600	-0.45598100	-1.95407900
C	-0.35607600	1.22787300	-0.26005400
C	-0.72955200	1.60556800	1.03738000
C	-0.43516700	2.18043100	-1.28251800
C	-1.16055200	2.90650300	1.30680500
H	-0.72825500	0.87600800	1.84346600
C	-0.86250300	3.48108200	-1.01626500
H	-0.17297300	1.85477800	-2.28386300
C	-1.22251600	3.85170300	0.28153300
H	-1.46199700	3.17642000	2.31635200
H	-0.92200000	4.20667900	-1.82451000
H	-1.56178100	4.86338800	0.49021600
H	-0.00342200	-2.14465100	-1.44956100
C	-0.52973500	-1.38917200	0.16485100
O	-0.10697100	-2.53940800	-0.53635600
H	-0.15311200	-1.46223700	1.19544000
C	-2.04374300	-1.27894900	0.21718100
C	-2.72197100	-1.42773300	1.43184400
C	-2.79410800	-1.07891900	-0.95246000
C	-4.11694800	-1.37838200	1.48936000
H	-2.15223600	-1.59637200	2.34469700
C	-4.18520900	-1.02495800	-0.89666300
H	-2.26215500	-0.94350400	-1.88895800
C	-4.85332100	-1.17651400	0.32247700
H	-4.62534800	-1.50179600	2.44290900
H	-4.75387400	-0.86274300	-1.80945200
H	-5.93936000	-1.13782800	0.36053200

Table S130. Cartesien coordinates of pyridyl-4-ylidene 16, TS-4

C	4.28916800	-0.26650200	-0.92287300
C	2.94648300	-0.02745000	-0.72259100
C	2.32385100	0.02077700	0.56140300
C	3.26780600	-0.21297200	1.60474800
C	4.61076900	-0.45184400	1.39799700
H	4.76385800	-0.30366100	-1.90022200
H	2.34947400	0.13064500	-1.62150600
N	5.12137400	-0.47612900	0.13605600
C	6.53502700	-0.79664200	-0.08782300
H	6.89245500	-0.26549100	-0.97219000
H	7.12022500	-0.47839900	0.77692400
H	6.66667700	-1.87333100	-0.23589100
H	5.32983900	-0.62992300	2.19379300
H	2.94649400	-0.20741800	2.64797500
C	-0.57575600	0.06425400	-0.96178200
O	-0.21886900	-0.11751900	-2.12273400
C	-0.95554400	1.42034600	-0.47723200
C	-0.66659500	1.85468900	0.82458900
C	-1.60211000	2.28783900	-1.36980500
C	-1.03910800	3.13602500	1.22806300
H	-0.08218000	1.21383600	1.47590200
C	-1.98756000	3.56132400	-0.95693200
H	-1.80378700	1.94554500	-2.38014400
C	-1.70865600	3.98610800	0.34440100
H	-0.79812400	3.47638900	2.23175500
H	-2.50139700	4.22326600	-1.64894300
H	-2.00356700	4.98177600	0.66608600
H	0.08541300	-1.93646600	-1.59973200
C	-0.73939000	-1.17970700	-0.05838700
O	-0.15128000	-2.28020700	-0.71379500
H	-0.20708100	-0.98466000	0.87829900
C	-2.22420200	-1.41595000	0.21606300
C	-2.82138100	-0.97407900	1.40122800
C	-3.01227000	-2.07708400	-0.73362800
C	-4.18252300	-1.18072100	1.63214500
H	-2.21797200	-0.46802700	2.15090500
C	-4.37203000	-2.28455300	-0.50563800
H	-2.54316100	-2.44575800	-1.64059300
C	-4.96284800	-1.83484300	0.67774200
H	-4.63073500	-0.83645300	2.56085800
H	-4.97140500	-2.80188700	-1.25080000
H	-6.02224700	-1.99937700	0.85722600

Table S131. Cartesien coordinates of pyridyl-3-ylidene 17

C	-0.12611200	1.16292400	-0.05217000
C	1.25464800	1.11962400	-0.04953400
C	1.89002300	-0.12747800	0.08934100
C	1.20929200	-1.36282500	0.01889500
C	-0.16634300	-1.20346600	-0.09443100
H	2.96757700	-0.11261000	0.27584800
H	-0.69996700	2.08269700	-0.03951900
H	1.80510000	2.05745400	-0.08706400
N	-0.83207800	0.00456900	-0.03588300
C	-2.29512900	0.04764300	0.08788000
H	-2.68408600	0.93539900	-0.41542700
H	-2.71576900	-0.84402400	-0.38189900
H	-2.59159500	0.06919600	1.14145300
H	-0.85498400	-2.03862100	-0.24209800

Table S132. Cartesien coordinates of pyridyl-3-ylidene 17, IM-1

C	3.45613000	0.21034600	-0.54932100
C	3.21345000	-1.13720300	-0.68857700
C	1.94483700	-1.66267400	-0.40054700
C	0.93794900	-0.82193200	0.08969100
C	1.24114900	0.53632100	0.22524800
H	1.74600100	-2.72141900	-0.53549800

H	4.40255600	0.68816300	-0.76578200
H	4.01715200	-1.77733300	-1.03904700
N	2.44365800	1.03346500	-0.10809000
C	2.71037000	2.47571000	-0.00314900
H	2.93101900	2.88552900	-0.99280500
H	1.83269300	2.97374400	0.40793600
H	3.56354500	2.64206000	0.65952500
H	0.50694300	1.22794700	0.61862500
C	-0.35456100	-1.25287700	0.78260900
H	-0.49561800	-2.34349000	0.57251400
O	-0.01588700	-0.93456600	2.04452800
C	-1.59679600	-0.53613400	0.21605500
C	-2.04619700	-0.73052200	-1.09641400
C	-2.30387900	0.32845700	1.05382800
C	-3.17759500	-0.06353700	-1.56615600
H	-1.50785600	-1.41195500	-1.75493400
C	-3.44067400	0.99584300	0.58910800
H	-1.93733200	0.44024100	2.07059100
C	-3.87887600	0.80431000	-0.72226500
H	-3.51745800	-0.22170300	-2.58738900
H	-3.98834900	1.66247700	1.25200300
H	-4.76365500	1.32137100	-1.08598800

Table S133. Cartesien coordinates of pyridyl-3-ylidene 17, TS-2

C	-3.63788800	-2.07494800	-0.02839800
C	-2.66484800	-2.60016400	-0.87178200
C	-1.49956500	-1.89324700	-1.11785100
C	-1.26862700	-0.63216900	-0.50362000
C	-2.29348100	-0.15647600	0.32385900
H	-0.73533800	-2.27225600	-1.78508100
H	-4.57027300	-2.56992400	0.20910900
H	-2.84084700	-3.56543900	-1.33477600
N	-3.42711000	-0.86034900	0.54207700
C	-4.45042100	-0.31609800	1.45342400
H	-4.34571700	-0.77174000	2.44188500
H	-4.32232000	0.76331500	1.53284600
H	-5.44234400	-0.53192300	1.05246700
H	-2.22856900	0.80544500	0.81642700
C	0.02241000	0.04875700	-0.69976700
H	0.83260200	-0.60475100	-0.03165300
O	0.56054300	-0.26295200	-1.97666900
C	0.08274100	1.51699900	-0.36357200
C	0.04482400	1.95952100	0.96961300
C	0.21200500	2.47672200	-1.37861800
C	0.09442300	3.32129100	1.27757100
H	0.00957100	1.22824300	1.77542800
C	0.26775300	3.83571400	-1.07166300
H	0.28369500	2.13288800	-2.40505200
C	0.20087200	4.26622600	0.25629100
H	0.07229100	3.64061800	2.31688700
H	0.36726200	4.56406900	-1.87307000
H	0.24873700	5.32598500	0.49298100
H	1.35882900	-0.79928900	-1.70459300
O	1.88501300	-1.59923000	-0.21386200
C	3.08816100	-1.40570600	0.46808800
C	3.75090100	-0.06423700	0.08048800
H	3.09428700	0.77603800	0.33675700
H	4.71288300	0.09009200	0.58821300
H	3.92815100	-0.03311700	-1.00150900
C	2.84135400	-1.43573400	1.99425100
H	2.33559300	-2.36927600	2.26763800
H	3.77140300	-1.36090600	2.57381300
H	2.19246900	-0.60042000	2.28927000
C	4.03121200	-2.56886400	0.08401400
H	5.00499800	-2.50124100	0.58798900
H	3.56657600	-3.52562400	0.34883700
H	4.20041400	-2.56640200	-0.99906500

Table S134. Cartesien coordinates of pyridyl-3-ylidene 17, IM-2

C	3.68185400	-0.15863300	0.03624300
C	3.36211300	1.20208000	0.19902500
C	2.06420200	1.63848200	0.19368700
C	0.95061500	0.70421300	0.06737300
C	1.36138000	-0.64837700	-0.17912400
H	1.83284100	2.69190900	0.28551100
H	4.67973300	-0.57195000	0.03918900
H	4.17682500	1.91010000	0.31959700
N	2.64807100	-1.02333800	-0.17507600
C	2.97791700	-2.44028600	-0.39249300
H	3.32936500	-2.88399600	0.54324600
H	2.09315400	-2.97315300	-0.74014600
H	3.76540900	-2.51356000	-1.14613800
H	0.64864800	-1.42347000	-0.42261000
C	-0.37071100	1.11933400	0.08044000
O	-0.54898100	2.51099500	0.01986800
C	-1.58098900	0.31601300	0.04528100
C	-1.68066400	-0.97830500	0.61579700
C	-2.76644300	0.85834200	-0.51298400
C	-2.87356000	-1.69391200	0.58808300
H	-0.82699400	-1.40188400	1.13636900
C	-3.95731100	0.13898200	-0.53028000
H	-2.72539000	1.84510700	-0.96414100
C	-4.02406400	-1.14759500	0.01120200
H	-2.91205300	-2.68071600	1.04453400
H	-4.84163300	0.58483300	-0.98034900
H	-4.95462800	-1.70802600	-0.00458100
H	-1.27597200	2.73818200	0.62259900

Table S135. Cartesien coordinates of pyridyl-3-ylidene 17, TS-3

C	4.10439200	-0.29561300	-0.35731100
C	3.91254800	0.15566500	0.94262600
C	2.68280800	0.66379600	1.32932700
C	1.58512100	0.68937900	0.42281400
C	1.85556600	0.25253200	-0.87791600
H	2.50652100	1.07776500	2.31574600
H	5.03693700	-0.69462400	-0.73415700
H	4.74783000	0.12314500	1.63478000
N	3.07038500	-0.21951900	-1.23971200
C	3.28265000	-0.69481500	-2.61840200
H	3.27049900	-1.78799500	-2.63892600
H	2.48801100	-0.31024100	-3.25726200
H	4.24563500	-0.33126700	-2.98272300
H	1.11625300	0.29546300	-1.66514300
C	0.28198100	1.17310800	0.92221700
O	0.33243400	1.86935300	2.02586700
C	-0.77918600	1.58042400	-0.08077400
C	-1.23515400	0.80375800	-1.16130400
C	-1.36016200	2.84649000	0.10719000
C	-2.20522500	1.29342500	-2.03992900
H	-0.87933300	-0.21195500	-1.29784400
C	-2.32707500	3.33451500	-0.76832800
H	-1.02650400	3.42718600	0.95998200
C	-2.75116600	2.56289000	-1.85348400
H	-2.54778300	0.66692300	-2.86021500
H	-2.75358000	4.32126300	-0.60305100
H	-3.50806900	2.94086300	-2.53622700
H	-0.58460000	0.91058600	2.83283100
C	-0.30178200	-0.62473500	1.81928100
H	0.71550700	-0.93149300	2.10904800
O	-1.01729500	-0.02709300	2.79248900
C	-1.00050200	-1.59721700	0.97826200
C	-0.27782200	-2.57986100	0.27166300
C	-2.40094500	-1.56548700	0.83221400
C	-0.92806800	-3.48582000	-0.56318900
H	0.80173300	-2.63840500	0.40018200
C	-3.04794900	-2.47625600	0.00133900
H	-2.95972800	-0.82044300	1.38793300
C	-2.31858800	-3.43751300	-0.70545700
H	-0.35345500	-4.24288800	-1.09246100
H	-4.13026000	-2.43849900	-0.09611900
H	-2.82807600	-4.14883100	-1.35026300

Table S136. Cartesien coordinates of pyridyl-3-ylidene 17, IM-3

C	4.04458700	0.68636600	0.29260700
C	3.92374100	0.09097600	-0.94901300
C	2.68432200	-0.40308900	-1.35718700
C	1.55451800	-0.27122600	-0.53238800
C	1.73784800	0.33977400	0.69886800
H	2.50787400	-0.92520000	-2.29440900
H	4.97605000	1.07449000	0.68608100
H	4.80328100	0.00890700	-1.57930800
N	2.95591900	0.79734400	1.09621800
C	3.09885100	1.36868400	2.44847200
H	2.18693900	1.90895900	2.70582000
H	3.26804500	0.56865000	3.17449200
H	3.94182000	2.06068000	2.46117700
H	0.93849100	0.46439100	1.41611800
C	0.23407000	-0.85095200	-1.09251300
O	0.51156400	-1.64589100	-2.13322200
C	-0.53092300	-1.59911800	0.04177600
C	-1.10790800	-1.01505200	1.18159400
C	-0.61841000	-2.99129200	-0.09527000
C	-1.73869200	-1.79960600	2.15248600
H	-1.11501400	0.06200200	1.31098900
C	-1.24413100	-3.77644000	0.87192800
H	-0.18325000	-3.42065600	-0.99112300
C	-1.80657200	-3.18443900	2.00510200
H	-2.18889700	-1.31956100	3.01865900
H	-1.29724800	-4.85486300	0.73910300
H	-2.30019900	-3.79335600	2.75875000
H	-0.92765100	-1.03015900	-2.87802300
C	-0.61035500	0.41057800	-1.76278800
H	0.18258500	0.96808600	-2.29714400
O	-1.47252700	-0.21685800	-2.66425600
C	-1.35897000	1.38013300	-0.88761300
C	-0.71416700	2.50232500	-0.34451900
C	-2.72062300	1.19489000	-0.60496600
C	-1.39373900	3.39114800	0.49082600
H	0.32649500	2.69469100	-0.60134800
C	-3.40362900	2.08518300	0.22284700
H	-3.22676700	0.34721200	-1.05296900
C	-2.74331500	3.18198100	0.78330400
H	-0.87669700	4.25922700	0.89436900
H	-4.45927300	1.92517200	0.42900100
H	-3.27932300	3.87698500	1.42474300

Table S137. Cartesien coordinates of pyridyl-3-ylidene 17, TS-4

C	5.00446500	-1.40916500	-0.10878600
C	3.99146000	-2.34424400	-0.01198900
C	2.65876500	-1.92446900	-0.14203400
C	2.27989300	-0.58941900	-0.43194600
C	3.37942000	0.25959400	-0.52917800
H	1.87726800	-2.67259100	0.00097400
H	6.05659600	-1.64239400	0.01053600
H	4.25667200	-3.38101600	0.18180600

N	4.69269000	-0.11371700	-0.35405800
C	5.76744800	0.89031300	-0.37906900
H	5.42185300	1.76488100	-0.93217500
H	6.03024200	1.19031900	0.63989400
H	6.64881100	0.47778400	-0.87509800
H	3.28453500	1.32354100	-0.75357200
C	-0.57392900	-0.06587400	1.01257300
O	-0.35755000	-0.35111200	2.18553200
C	-0.63609200	1.35350700	0.56190400
C	-0.27539200	1.74673700	-0.73526700
C	-1.06233800	2.32121200	1.48309000
C	-0.35876600	3.08827000	-1.10527900
H	0.13446900	1.00906800	-1.41639200
C	-1.15643900	3.65924300	1.10619400
H	-1.32366900	2.00524600	2.48815600
C	-0.80750300	4.04453100	-0.19037500
H	-0.06813800	3.39010400	-2.10829900
H	-1.50048800	4.40117200	1.82196900
H	-0.87785000	5.08859000	-0.48512400
H	-0.35841200	-2.17398600	1.60045200
C	-0.93167100	-1.22301200	0.05083000
H	-0.33894400	-1.10733700	-0.86037300
O	-0.58086200	-2.43837900	0.68277500
C	-2.42347100	-1.16832700	-0.27429100
C	-2.88035300	-0.62926800	-1.48114700
C	-3.35858600	-1.65114100	0.64922500
C	-4.24663800	-0.56768200	-1.76108000
H	-2.16272000	-0.25883400	-2.20917100
C	-4.72356800	-1.59121200	0.37229600
H	-3.00458500	-2.09086600	1.57668900
C	-5.17265100	-1.04712000	-0.83371800
H	-4.58601600	-0.15132600	-2.70624900
H	-5.43867900	-1.97224700	1.09719100
H	-6.23679700	-1.00301900	-1.05099000

Table S138. Cartesien coordinates of pyridyl-2-ylidene 18

C	0.21775100	1.13825900	0.00017500
C	-1.15200300	1.20599300	0.00016300
C	-1.87169800	-0.00524700	-0.00003100
C	-1.17822400	-1.20169400	-0.00020000
C	0.24717500	-1.31573200	-0.00019400
H	-2.96026000	0.01676000	-0.00004600
H	0.84832100	2.02286100	0.00032000
H	-1.64791400	2.17078800	0.00030100
H	-1.74444200	-2.13195800	-0.00034900
N	0.84905000	-0.07646900	0.00000100
C	2.32319100	-0.05135700	0.00003000
H	2.69706100	0.46229000	0.89236800
H	2.64964300	-1.08936900	-0.00013600
H	2.69709100	0.46258600	-0.89212400

Table S139. Cartesien coordinates of pyridyl-2-ylidene 18, TS-1

C	3.18488200	-0.58146600	-0.88374800
C	3.90040800	0.56343500	-0.62287800
C	3.27012300	1.59265400	0.09545000
C	1.96463000	1.41221100	0.52446300
C	1.22242200	0.24653900	0.24527600
H	3.80992600	2.51150400	0.31316700
H	3.60083800	-1.42272100	-1.42765200
H	4.92524100	0.64784100	-0.96693700
H	1.47768800	2.19418000	1.10376700
N	1.89359000	-0.70545300	-0.46263900
C	1.15335800	-1.94203200	-0.79791000
H	1.85719400	-2.71514600	-1.11254700
H	0.59966600	-2.25040000	0.09393700
H	0.45150800	-1.72730500	-1.60734500
C	-0.44461700	-0.35376300	1.48160800
H	-0.15135800	0.48284900	2.15295000
O	-0.23498200	-1.53213700	1.82775000
C	-1.60536700	0.00852300	0.58216600
C	-1.93468900	1.34293600	0.31631500
C	-2.41002900	-1.00715800	0.05656800
C	-3.03227600	1.65829100	-0.48243500
H	-1.32259400	2.13807200	0.73893900
C	-3.50913400	-0.69615800	-0.74544800
H	-2.16509800	-2.03518500	0.30709200
C	-3.82152200	0.63690900	-1.02049500
H	-3.27766500	2.69848100	-0.68316200
H	-4.12961400	-1.49338200	-1.14826400
H	-4.68013200	0.88095700	-1.64106300

Table S140. Cartesien coordinates of pyridyl-2-ylidene 18, IM-1

C	-2.76956200	0.29807600	-1.28007000
C	-3.72846900	-0.48529100	-0.68376800
C	-3.42020300	-1.08593800	0.54993900
C	-2.18256600	-0.86098900	1.11819700
C	-1.20489600	-0.06678000	0.48608500
H	-4.14718100	-1.72230700	1.04661500
H	-2.93568100	0.80282000	-2.22446800
H	-4.69047400	-0.61738800	-1.16473400
H	-1.92238600	-1.29483800	2.07788400
N	-1.54342800	0.48356700	-0.72554200
C	-0.59126400	1.40116800	-1.38560400
H	-1.11918600	1.95306000	-2.16422000
H	-0.22220400	2.05232800	-0.58190200
H	0.23431800	0.83162400	-1.81491800

C	0.07422000	0.36775900	1.22892800
H	0.05436800	-0.25961900	2.15965800
O	-0.12033700	1.67502600	1.43836100
C	1.38314800	-0.04161900	0.51414900
C	1.60712000	-1.32826100	0.00942200
C	2.40507100	0.90637500	0.43363700
C	2.82903300	-1.65713700	-0.58110000
H	0.82258900	-2.08174200	0.07766700
C	3.63195800	0.57937000	-0.14700900
H	2.19989500	1.89441700	0.83680600
C	3.84651600	-0.70217500	-0.65997300
H	2.98953100	-2.65780800	-0.97615300
H	4.42268300	1.32444400	-0.20105000
H	4.79977700	-0.95751900	-1.11627400

Table S141. Cartesien coordinates of pyridyl-2-ylidene 18, TS-2

C	3.25177800	2.05248300	0.41598500
C	3.38070600	2.40005000	-0.90210200
C	2.52163100	1.79364000	-1.84246700
C	1.55876600	0.91415200	-1.40012200
C	1.41808100	0.58340800	-0.03390000
H	2.59390700	2.04569400	-2.89586600
H	3.88254200	2.46992500	1.19145200
H	4.12897500	3.12751900	-1.19408600
H	0.83489600	0.48781400	-2.08515700
N	2.32554300	1.13940800	0.83866900
C	2.36944500	0.72979200	2.25989500
H	3.34187200	1.02025100	2.66089500
H	1.55260500	1.19119100	2.81141100
H	2.24882800	-0.35077900	2.32366200
C	0.24267300	-0.20060600	0.41089900
H	-0.67360100	0.39152800	-0.15562100
O	-0.16975200	0.09251500	1.73474300
C	0.23159300	-1.67656700	0.09227600
C	1.11703700	-2.29629800	-0.80448400
C	-0.74536700	-2.47383900	0.71307200
C	1.01469700	-3.65879200	-1.08928400
H	1.90761000	-1.72157400	-1.27931800
C	-0.84150200	-3.83539600	0.43297000
H	-1.41524600	-2.00975200	1.42765000
C	0.03383600	-4.43694200	-0.47417700
H	1.71499500	-4.11364600	-1.78581300
H	-1.60581800	-4.42998400	0.92735400
H	-0.04267600	-5.49878200	-0.69237500
H	-0.91097600	0.74407100	1.52639800
O	-1.62340500	1.47292600	0.14550000
C	-2.97536200	1.41742500	-0.20133300
C	-3.11678800	1.47513900	-1.73910800
H	-4.16475300	1.49891900	-2.06684000
H	-2.61284600	2.37049600	-2.12148100
H	-2.63981400	0.59756000	-2.19446900
C	-3.67213400	2.64796100	0.42276500
H	-4.74258000	2.68971000	0.18061400
H	-3.56540500	2.62258800	1.51377000
H	-3.19657400	3.56653100	0.06052800
C	-3.64643600	0.13040800	0.32808200
H	-4.71630100	0.08654000	0.08409600
H	-3.16447800	-0.75598900	-0.10243000
H	-3.54462700	0.07467900	1.41920800

Table S142. Cartesien coordinates of pyridyl-2-ylidene 18, IM-2

C	3.47972100	0.02408500	-0.24667100
C	3.52662800	-1.29227000	-0.54350300
C	2.31456700	-2.07383400	-0.43490800
C	1.13443600	-1.46633500	-0.15907000
C	1.04827600	-0.02533800	-0.01042100
H	2.35132300	-3.14703000	-0.59721500
H	4.36362100	0.65660100	-0.24558000
H	4.46124000	-1.74833600	-0.85035400
H	0.21590200	-2.03892700	-0.12927000
N	2.29983800	0.68258900	0.10143700
C	2.43357700	1.64630400	1.20851800
H	3.35982100	2.21320800	1.07155600
H	1.59176900	2.33887000	1.21527600
H	2.47751100	1.13272300	2.17852200
C	-0.10215400	0.71675500	-0.12777100
O	-0.01059300	2.07968000	-0.36510800
C	-1.48553000	0.24107600	-0.03323800
C	-1.86786700	-0.79559900	0.84050000
C	-2.49035300	0.86326000	-0.80097100
C	-3.19095500	-1.22715500	0.90399300
H	-1.12638000	-1.24209700	1.49605500
C	-3.81276800	0.43479400	-0.72799400
H	-2.21660100	1.68334200	-1.45598500
C	-4.17132700	-0.61833000	0.11754500
H	-3.46043400	-2.02848900	1.58743400
H	-4.56880800	0.92510200	-1.33624000
H	-5.20436800	-0.95073100	0.17332600
H	0.84377100	2.22572400	-0.81277400

Table S143. Cartesien coordinates of pyridyl-2-ylidene 18, TS-3

C	4.29511100	-0.38202300	0.19326200
C	4.27671500	-0.52369000	1.55317100
C	3.05027300	-0.32867900	2.22115100
C	1.91961700	-0.06981100	1.48170900
C	1.93828200	0.04010200	0.06845100

H	2.99287700	-0.40583900	3.30262300
H	5.20074300	-0.48764000	-0.39212400
H	5.18838700	-0.77417100	2.08286500
H	0.95821500	0.02444700	1.96949400
N	3.17399000	-0.06587100	-0.52735500
C	3.40290400	0.28900100	-1.95183800
H	4.19834300	-0.34925800	-2.34141100
H	2.45993400	0.14419700	-2.48361800
H	3.71261600	1.33727100	-1.99977800
C	0.65392200	0.10822200	-0.72281600
O	0.71878000	-0.15332300	-2.01216700
C	-0.28357400	1.25342300	-0.35635200
C	-0.08436500	2.18866500	0.67031300
C	-1.40279300	1.42714200	-1.18817300
C	-0.99071400	3.23077600	0.88542700
H	0.79833100	2.14313300	1.30023000
C	-2.30941000	2.46040600	-0.97224000
H	-1.53271800	0.74382100	-2.01827400
C	-2.11350600	3.36754200	0.07225200
H	-0.80422600	3.94353700	1.68535700
H	-3.17064900	2.56289500	-1.62781200
H	-2.81882300	4.17753600	0.23925100
H	0.49356900	-1.62493400	-1.87124700
C	-0.07793400	-1.64478200	-0.09253200
O	0.26376900	-2.37137700	-1.18534700
H	0.49416800	-1.91697600	0.80105100
C	-1.53190900	-1.51893500	0.19457400
C	-2.47992000	-1.77202900	-0.80920300
C	-1.99004600	-1.15623500	1.47145000
C	-3.84315000	-1.65374100	-0.54524700
H	-2.12503400	-2.08393700	-1.78584800
C	-3.35206300	-1.03443600	1.73591400
H	-1.27170800	-0.97923700	2.27020300
C	-4.28597600	-1.27978200	0.72577400
H	-4.56451500	-1.85978600	-1.33245400
H	-3.68715600	-0.75429300	2.73157300
H	-5.34946200	-1.18888600	0.93123400

Table S144. Cartesien coordinates of pyridyl-2-ylidene 18, IM-3

C	4.21883100	0.19771000	-0.29646300
C	4.70573400	-0.75881100	0.56148300
C	3.78319500	-1.61583300	1.17571200
C	2.43223000	-1.46125600	0.92165700
C	1.94491500	-0.45208300	0.06640500
H	4.12294200	-2.39788100	1.84853800
H	4.86664500	0.88323100	-0.82879000
H	5.77340200	-0.83936600	0.72916000
H	1.71977900	-2.14873100	1.35206300
N	2.88866600	0.34601900	-0.53464500
C	2.48804800	1.35388800	-1.54635700
H	3.37220600	1.62934100	-2.12225400
H	1.72763900	0.86653200	-2.16492600
H	2.06913900	2.22977300	-1.05039800
C	0.45145900	-0.32737300	-0.37212900
O	0.48095800	-0.66980900	-1.68381900
C	-0.09691100	1.07143800	-0.03609400
C	0.12727400	1.68737800	1.20181000
C	-0.87961400	1.73189500	-0.98790800
C	-0.41750400	2.94287000	1.48218000
H	0.73294500	1.18718700	1.95620900
C	-1.42972200	2.98266100	-0.70899800
H	-1.03598200	1.24034700	-1.94291200
C	-1.19910300	3.59431400	0.52624400
H	-0.23210700	3.41026600	2.44644700
H	-2.04053400	3.48307300	-1.45660900
H	-1.62490100	4.57084500	0.74247500
H	0.27191800	-2.36951500	-1.06625400
C	-0.41383700	-1.43204100	0.39526700
O	0.00680600	-2.66807900	-0.15366200
H	-0.18196000	-1.42110300	1.46967800
C	-1.91170200	-1.22996700	0.24392900
C	-2.54758100	-1.49277300	-0.97749900
C	-2.68755800	-0.79917900	1.32505500
C	-3.92451500	-1.31966700	-1.11028500
H	-1.95113400	-1.82274000	-1.82079800
C	-4.06706000	-0.62650600	1.19598700
H	-2.20768800	-0.59676600	2.28046900
C	-4.69047300	-0.88712100	-0.02441200
H	-4.40347600	-1.52657300	-2.06445300
H	-4.65311200	-0.29495300	2.04976900
H	-5.76514400	-0.75925600	-0.12856800

Table S145. Cartesien coordinates of pyridyl-2-ylidene 18, TS-4

C	4.48250300	-0.22856700	-0.33082900
C	4.85681800	-1.22465500	0.53868500
C	3.85056900	-1.88076300	1.26460800
C	2.52970100	-1.50152700	1.08477500
C	2.13857000	-0.46246600	0.21164500
H	4.11131600	-2.68232500	1.95185000
H	5.19638300	0.31861600	-0.93665200
H	5.90402200	-1.48804500	0.63826900
H	1.74947100	-2.03274200	1.62113000
N	3.16982700	0.11935800	-0.46983800
C	2.83938000	1.20352400	-1.42219400
H	3.70871500	1.41564100	-2.04760600
H	1.99559200	0.87542600	-2.03132900
H	2.55636200	2.09895300	-0.86510000
C	0.03807500	-0.14271300	-0.60876500
O	0.19400500	-0.35912900	-1.83240100

C	-0.22488200	1.26109500	-0.11515400
C	-0.08807000	1.64049500	1.22740700
C	-0.67862700	2.20718900	-1.04208200
C	-0.39176100	2.93909100	1.63148700
H	0.28572000	0.92333500	1.95267400
C	-0.98418300	3.50828500	-0.63927500
H	-0.79016800	1.90079800	-2.07735600
C	-0.84154200	3.87844100	0.69848400
H	-0.27403800	3.22172100	2.67465800
H	-1.33825300	4.23123600	-1.36999900
H	-1.07834400	4.89105700	1.01489100
H	0.16484300	-2.23565600	-1.28012300
C	-0.58363300	-1.31866400	0.19533500
O	-0.10238300	-2.51789800	-0.37821900
H	-0.26857000	-1.27592800	1.24314000
C	-2.10712700	-1.23416000	0.15183400
C	-2.79718400	-1.48343200	-1.04196100
C	-2.83944300	-0.90674300	1.29707000
C	-4.18787400	-1.40555300	-1.08556100
H	-2.23542500	-1.73630600	-1.93573200
C	-4.23315800	-0.82728300	1.25707100
H	-2.31546200	-0.71548100	2.23125800
C	-4.91157300	-1.07692500	0.06419000
H	-4.71001400	-1.60214100	-2.01877600
H	-4.78672600	-0.57616300	2.15847000
H	-5.99654900	-1.01930800	0.02954200

Table S146. Cartesien coordinates of isoquinoline-6-ylidene 19

C	3.09227700	0.41019600	0.12353900
C	1.96845500	1.26053000	0.03041400
C	0.63976400	0.81989900	-0.03876700
C	0.37225200	-0.60666800	-0.01727100
C	1.47869000	-1.50233300	-0.03000800
C	2.75660200	-0.98604800	-0.04174300
H	-0.36015400	2.75439900	-0.07344600
H	2.10756100	2.34614900	0.08384900
C	-0.50190600	1.67773000	-0.05056900
C	-0.94344200	-1.04276900	0.00404300
H	1.28554000	-2.57611400	-0.03612500
H	3.57589500	-1.70490800	-0.13304900
C	-1.76980800	1.17920800	-0.03082900
H	-1.19262900	-2.09857500	0.02995800
H	-2.66043400	1.79651100	-0.03553200
N	-1.99146100	-0.18494800	-0.00990700
C	-3.36951100	-0.67765400	0.05581600
H	-3.37726000	-1.75467000	-0.11625100
H	-3.80546800	-0.46845700	1.03823800
H	-3.97307200	-0.19224300	-0.71604400

Table S147. Cartesien coordinates of isoquinoline-6-ylidene 19, TS-1

C	0.03799100	-0.75995900	-0.79883300
C	-0.74083500	0.38773800	-0.53724100
C	-2.10102800	0.36689600	-0.19877900
C	-2.78477700	-0.90812100	-0.10592600
C	-2.04303200	-2.09581100	-0.35820200
C	-0.70749500	-1.99526000	-0.67976400
H	-2.41982300	2.50903800	0.00963400
H	-0.27292900	1.37511600	-0.59738400
C	-2.88493600	1.52921500	0.06484000
C	-4.13198200	-0.92436100	0.22422300
H	-2.55074000	-3.05876100	-0.28914900
H	-0.17904300	-2.93543900	-0.85923100
C	-4.20617300	1.43929300	0.38490200
H	-4.68659200	-1.85373300	0.30473800
H	-4.83746200	2.29503400	0.59215700
N	-4.82941800	0.20620000	0.46391400
C	-6.25350700	0.15940100	0.81045500
H	-6.58637200	-0.87866600	0.83337300
H	-6.41411200	0.60799900	1.79520600
H	-6.83835500	0.70622400	0.06498600
C	2.51917200	1.15984500	-1.10610400
H	2.03406500	0.54819000	-1.88371800
O	2.20555900	2.32780900	-0.92291900
C	3.56197200	0.45780700	-0.31309900
C	3.70813400	-0.93067700	-0.43112800
C	4.41407200	1.18067900	0.53307200
C	4.70554000	-1.59002100	0.28543500
H	3.00016200	-1.47496100	-1.05014800
C	5.41318300	0.52141400	1.24474200
H	4.27726600	2.25543400	0.60976300
C	5.56052800	-0.86415200	1.11999500
H	4.81479200	-2.66833400	0.20122400
H	6.07961900	1.08179600	1.89579300
H	6.34000800	-1.37834800	1.67718500

Table S148. Cartesien coordinates of isoquinoline-6-ylidene 19, IM-1

C	0.43491900	0.36554500	-0.72088900
C	-0.60114000	1.20510600	-0.31378000
C	-1.88446500	0.70641500	-0.08649500
C	-2.14557400	-0.70409800	-0.28778800
C	-1.08075600	-1.54714900	-0.71710600
C	0.17022300	-1.01409500	-0.92998400
H	-2.84008700	2.57182600	0.50726800
H	-0.33222100	2.25384800	-0.19759900
C	-2.98353100	1.50826500	0.34816400
C	-3.42582300	-1.18998700	-0.04167400

H	-1.26926300	-2.60848800	-0.86108000
H	0.98157000	-1.66282700	-1.24810300
C	-4.21286900	0.96189500	0.56609700
H	-3.67174100	-2.23892100	-0.16460100
H	-5.07075700	1.53453000	0.89687100
N	-4.43475100	-0.38490900	0.36985200
C	-5.75832600	-0.93952600	0.67543700
H	-5.84415400	-1.93376600	0.23547800
H	-5.90212200	-1.01033400	1.75842200
H	-6.53209900	-0.29660100	0.24904400
C	1.79038000	1.06707400	-1.00303900
H	1.92086200	0.77641500	-2.09715800
O	1.77973500	2.36014700	-0.78192400
C	2.91710600	0.28385800	-0.26435200
C	3.57234100	-0.82558300	-0.80785100
C	3.31471300	0.75034200	0.99383300
C	4.58378700	-1.47936700	-0.09657900
H	3.31268900	-1.16811400	-1.80895600
C	4.31678100	0.09811500	1.70961500
H	2.83620900	1.65049000	1.36820800
C	4.95354600	-1.02426200	1.16918600
H	5.09139900	-2.33418800	-0.53873100
H	4.61377700	0.47062200	2.68792400
H	5.74343900	-1.52659500	1.72266200

Table S149. Cartesien coordinates of isoquinoline-6-ylidene 19, TS-2

C	-0.41765000	-0.41455800	0.20952000
C	-1.36803300	0.39190000	0.86176400
C	-2.71549100	0.33957500	0.52835400
C	-3.17035100	-0.56716800	-0.50525600
C	-2.20305200	-1.39177100	-1.15545400
C	-0.88184800	-1.31050000	-0.80761400
H	-3.43990400	1.84596600	1.93447100
H	-1.01419200	1.05812500	1.64010700
C	-3.72196200	1.14421200	1.15652500
C	-4.51719900	-0.61000800	-0.82546200
H	-2.53031600	-2.08917200	-1.92274300
H	-0.16033900	-1.95043300	-1.30407300
C	-5.02733700	1.05160900	0.78937300
H	-4.90139400	-1.27511900	-1.59104700
H	-5.81497600	1.64467200	1.23814900
N	-5.43239300	0.17815200	-0.20417200
C	-6.85764600	0.07797300	-0.52783500
H	-6.97796100	-0.47132600	-1.46248900
H	-7.39796500	-0.44549400	0.26822600
H	-7.27909600	1.07912600	-0.65115100
C	1.01474100	-0.23132900	0.52307100
H	1.38087200	0.66613400	-0.16159800
O	1.20267500	0.35199500	1.79772600
C	1.91956800	-1.42823700	0.28752500
C	2.39299300	-1.74625700	-0.99287900
C	2.31791300	-2.22777500	1.36752200
C	3.21704900	-2.85631600	-1.19712300
H	2.13100100	-1.10795100	-1.83431800
C	3.14237200	-3.33384300	1.16615400
H	1.98655800	-1.95479300	2.36417000
C	3.59054300	-3.65708200	-0.11768400
H	3.57890200	-3.08318400	-2.19704000
H	3.44131800	-3.94452500	2.01493500
H	4.23705700	-4.51729200	-0.27184900
H	1.62861900	1.22040300	1.52976300
O	1.85751400	2.17152500	0.11335500
C	3.07244000	2.62947000	-0.38429800
C	3.24457600	4.09366200	0.09401800
H	4.18033800	4.54009000	-0.26919400
H	2.40465900	4.70072600	-0.26215200
H	3.24526100	4.12808500	1.18958100
C	4.26053700	1.78617200	0.13290300
H	4.15858500	0.74412600	-0.19255600
H	5.22789800	2.16235700	-0.22700900
H	4.27723400	1.79413400	1.22947900
C	3.05337800	2.60266000	-1.93047700
H	2.19156300	3.17146300	-2.29824500
H	3.96606000	3.02505600	-2.37217900
H	2.95220700	1.56924700	-2.28655900

Table S150. Cartesien coordinates of isoquinoline-6-ylidene 19, IM-2

C	0.39825400	0.39704100	-0.00082000
C	-0.77221900	1.23558100	-0.16025600
C	-2.04340600	0.73165400	-0.10890100
C	-2.27570500	-0.69013800	0.13916600
C	-1.11215200	-1.51940100	0.34899500
C	0.14144000	-1.00517000	0.28821600
H	-3.15475100	2.58819100	-0.49352000
H	-0.62094500	2.29339100	-0.34495900
C	-3.24282700	1.52400700	-0.29813100
C	-3.55061500	-1.18355500	0.17931200
H	-1.25833800	-2.57170900	0.58353800
H	0.98413600	-1.65534800	0.49656800
C	-4.47565400	0.96654800	-0.24778900
H	-3.75546900	-2.23300200	0.36420800
H	-5.38396500	1.54274400	-0.38638700
N	-4.66308600	-0.38785800	-0.02674000
C	-5.99589300	-0.92480500	0.19657200
H	-6.04301500	-1.95649900	-0.16448700
H	-6.27343700	-0.91255500	1.26013400
H	-6.72612900	-0.33353400	-0.36211400
C	1.67131700	0.92797300	-0.04782500
O	1.75842400	2.31531300	-0.05360600
C	2.95280700	0.21898800	-0.02720900

C	3.16242700	-1.00320300	-0.70395100
C	4.06441100	0.80438500	0.62136800
C	4.40839700	-1.62369100	-0.69604100
H	2.34775500	-1.44344800	-1.26971000
C	5.31072800	0.18322500	0.61902900
H	3.92862000	1.73812600	1.16018800
C	5.49164400	-1.03780200	-0.03439200
H	4.54108000	-2.56130700	-1.23032800
H	6.14320500	0.65107500	1.13901400
H	6.46435300	-1.52189600	-0.03669300
H	2.58338800	2.55845100	-0.50349500

Table S151. Cartesien coordinates of isoquinoline-6-ylidene 19, TS-3

C	-0.74581200	0.33153300	-0.26597600
C	-1.79073100	-0.18633300	-1.04759600
C	-3.10541000	-0.19620600	-0.59274600
C	-3.42018600	0.35366000	0.70859500
C	-2.35970400	0.89851600	1.48968500
C	-1.07352800	0.87766500	1.01481300
H	-4.02381300	-1.13366800	-2.33420700
H	-1.52613100	-0.56002000	-2.03029800
C	-4.20312600	-0.71049500	-1.35142000
C	-4.73776000	0.34838100	1.14264400
H	-2.58527400	1.34047400	2.45726900
H	-0.28562900	1.31223000	1.61815100
C	-5.47204800	-0.68470600	-0.86057500
H	-5.02193500	0.75269600	2.10810400
H	-6.32931900	-1.06787000	-1.40055600
N	-5.74189000	-0.15631500	0.38794900
C	-7.12678600	-0.15702400	0.87121800
H	-7.16639700	0.31535300	1.85303700
H	-7.76424700	0.40229600	0.18031200
H	-7.49527700	-1.18390100	0.95332100
C	0.64636200	0.17482400	-0.82284600
O	0.68230400	-0.16467000	-2.09643100
C	1.63300200	1.26932400	-0.41488900
C	2.07757400	1.52616400	0.89091300
C	2.11363000	2.09024900	-1.44556100
C	2.94949400	2.58338500	1.16096700
H	1.78386000	0.87426900	1.70768500
C	2.98410000	3.14651200	-1.17972100
H	1.79084200	1.86448900	-2.45591200
C	3.40219400	3.40370700	0.12757000
H	3.28777400	2.75262200	2.18066200
H	3.34016000	3.76964200	-1.99719600
H	4.08389200	4.22448600	0.33704900
H	0.57355600	-1.69065600	-1.76769200
C	1.01008100	-1.47867700	0.02856900
H	0.42801000	-1.56300200	0.95358500
O	0.53263200	-2.31292200	-0.94998900
C	2.47742600	-1.59046800	0.29282100
C	2.96649400	-1.68519000	1.60317800
C	3.39327800	-1.63430500	-0.77174100
C	4.33293800	-1.82243200	1.85164500
H	2.26475500	-1.67101500	2.43586000
C	4.75688300	-1.76467400	-0.52461600
H	3.01887700	-1.54466600	-1.78615000
C	5.23398800	-1.86187600	0.78686200
H	4.69190000	-1.90652400	2.87485000
H	5.45477300	-1.79150000	-1.35812400
H	6.29925700	-1.96999500	0.97520000

Table S152. Cartesien coordinates of isoquinoline-6-ylidene 19, IM-3

C	-0.74117000	0.00750800	-0.04207100
C	-1.74081000	-0.31704800	-0.95363300
C	-3.08908700	-0.29944500	-0.58659600
C	-3.45277900	0.06198000	0.76540900
C	-2.42529400	0.40271600	1.68764200
C	-1.11161100	0.37393800	1.28431900
H	-3.93159200	-0.90338700	-2.49986400
H	-1.39287600	-0.58285200	-1.94993800
C	-4.15443400	-0.62548700	-1.47504300
C	-4.79933200	0.06965000	1.11749800
H	-2.69238100	0.68619000	2.70287800
H	-0.33645100	0.64853100	1.99167300
C	-5.45213700	-0.59841300	-1.05878600
H	-5.12475600	0.33561600	2.11738300
H	-6.29272000	-0.84085800	-1.69697500
N	-5.76951100	-0.25058000	0.23986400
C	-7.18411100	-0.24568700	0.63935100
H	-7.26549300	0.07605600	1.67765300
H	-7.74493400	0.44493100	0.00399600
H	-7.60043700	-1.25195700	0.54067000
C	0.72290100	-0.11852000	-0.56611300
O	0.72710700	-0.48051900	-1.85735500
C	1.41078200	1.24315200	-0.29323400
C	1.91117400	1.65310600	0.95070100
C	1.51175400	2.12780400	-1.37423800
C	2.48387200	2.91719600	1.11204800
H	1.89741500	0.97316800	1.79846100
C	2.07887000	3.39176600	-1.21613900
H	1.15320000	1.77548000	-2.33582600
C	2.56354100	3.79536200	0.03055600
H	2.88048600	3.20874200	2.08208100
H	2.15101600	4.06256400	-2.06973700
H	3.01237000	4.77804400	0.15489500
H	0.70876300	-2.12714100	-1.27164300
C	1.35770600	-1.35544900	0.28600900
H	1.01409500	-1.35132700	1.33026100

O	0.82408700	-2.49717000	-0.34779500
C	2.87686100	-1.37154600	0.28204500
C	3.58800700	-1.51344100	1.47862700
C	3.59484400	-1.30252300	-0.92260800
C	4.98340900	-1.58522400	1.48441600
H	3.04208200	-1.58154100	2.41876000
C	4.98638200	-1.36918900	-0.91881400
H	3.03751500	-1.17086900	-1.84482000
C	5.68748900	-1.51327100	0.28286600
H	5.51684200	-1.70146200	2.42527600
H	5.53032800	-1.30715900	-1.85876900
H	6.77359100	-1.56881200	0.28045500

Table S153. Cartesien coordinates of isoquinoline-6-ylidene 19, TS-4

C	-1.24982700	0.18594300	0.94829300
C	-2.01240800	0.16422400	-0.23861000
C	-3.40361200	-0.00045100	-0.28900900
C	-4.14026800	-0.15586000	0.94945600
C	-3.41855900	-0.13396500	2.17495900
C	-2.05130100	0.02821900	2.14363600
H	-3.66528500	0.07899500	-2.44775900
H	-1.50632600	0.27239800	-1.20204000
C	-4.16910100	-0.03241400	-1.49216800
C	-5.51634200	-0.32409200	0.89523800
H	-3.96543700	-0.25053500	3.11121200
H	-1.54139300	0.03375400	3.11042400
C	-5.52083300	-0.20158700	-1.47150300
H	-6.11021100	-0.44639900	1.79526300
H	-6.13942500	-0.23312400	-2.36031400
N	-6.19415700	-0.34749200	-0.27153700
C	-7.64816200	-0.53750600	-0.30001300
H	-8.02413500	-0.60711500	0.72111300
H	-8.12563900	0.31040100	-0.79951900
H	-7.89542000	-1.45863900	-0.83602900
C	1.44508100	0.01487200	-0.86236900
O	0.95861500	-0.20378600	-1.96823300
C	1.93117500	1.37411800	-0.48979800
C	1.75522300	1.90279100	0.79710600
C	2.57204000	2.14107200	-1.47325000
C	2.23566800	3.17720200	1.09520400
H	1.16427700	1.34085700	1.51352500
C	3.06441400	3.40798400	-1.16585300
H	2.68693800	1.72725100	-2.47047500
C	2.89985100	3.92656000	0.12066100
H	2.08181500	3.59197000	2.08814000
H	3.57317600	3.99155600	-1.92875100
H	3.27835200	4.91728100	0.35998800
H	0.64506600	-1.98070400	-1.31950900
C	1.67500100	-1.19412300	0.07532900
H	1.24751400	-0.94019900	1.05077700
O	0.99985600	-2.30607400	-0.46674600
C	3.17449900	-1.46161000	0.20371700
C	3.91601500	-0.93771500	1.26814200
C	3.83042300	-2.23448300	-0.76178500
C	5.28846800	-1.17379400	1.36349600
H	3.41681400	-0.34256700	2.02875600
C	5.20140000	-2.47181400	-0.66887200
H	3.24827900	-2.66509300	-1.57033600
C	5.93637100	-1.94031900	0.39347700
H	5.84959500	-0.76380300	2.19963900
H	5.69689800	-3.07654800	-1.42466600
H	7.00456900	-2.12793600	0.46824900