Supporting Information for

Activation of metal-involved halogen bonds and classical halogen bonds in gold(I) catalysis

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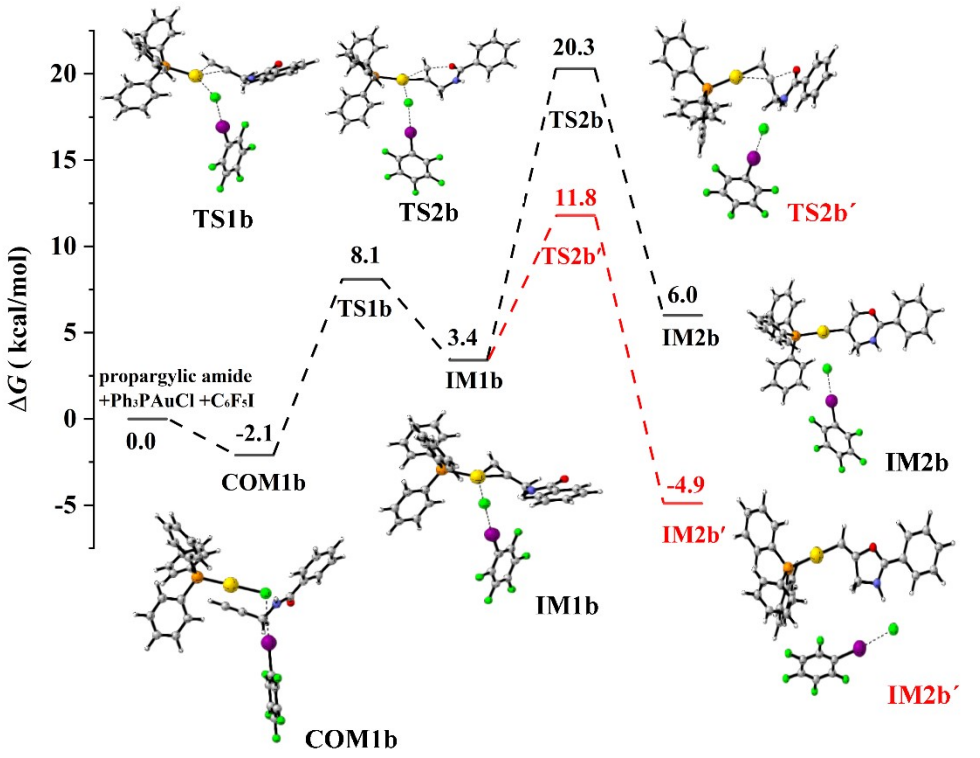

Figure S1. Gibbs energy curves of the cyclization via C_6F_5I activating the Cl atom of Ph_3PAuCl.

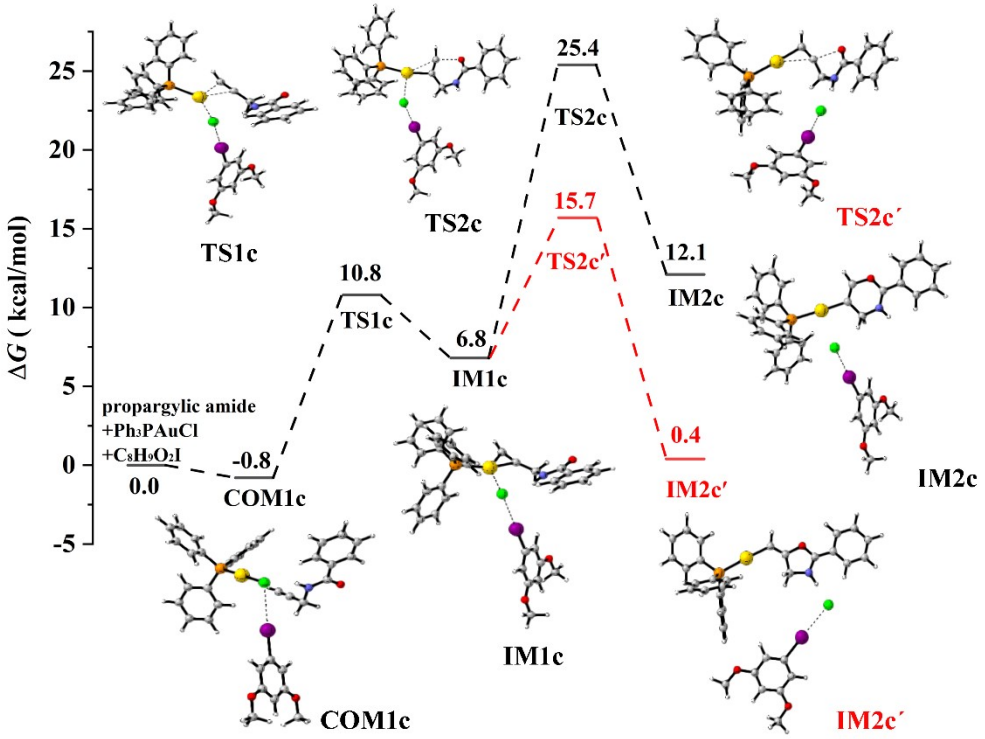

Figure S2. Gibbs energy curves of the cyclization via $C_8H_9O_2I$ activating the Cl atom of Ph_3PAuCl.

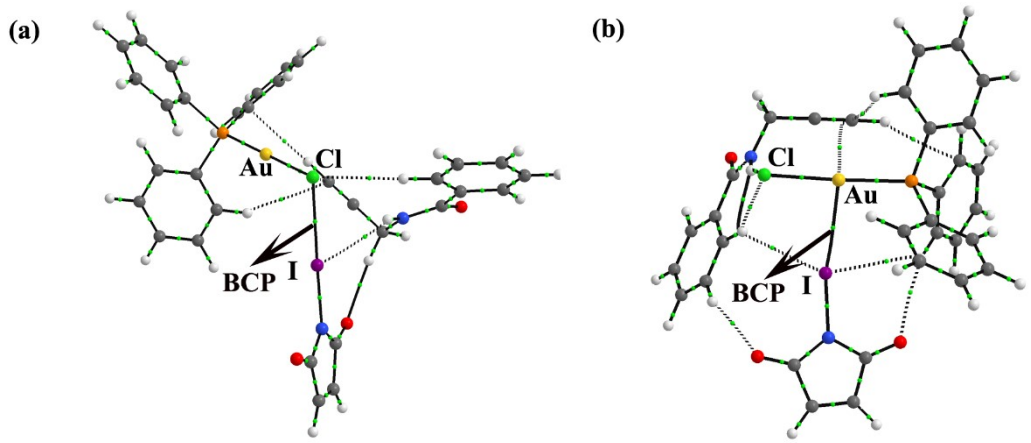

Figure S3. AIM molecular graphs of the complexes: (a) N–I···Cl; (b) N-I···Au.

Table S1. The angles (in °) of Cl–I–N from COM1 to IM2 (IM2′) via $C_4H_2INO_2$ activating the Cl atom.

	COM1	TS1	IM1	TS2	IM2	TS2′	IM2′
Cl–I–N	178.5	176.1	175.0	179.5	179.2	179.4	174.0

Table S2. The angles (in °) of Au–I–N from COM1a to IM2a (IM2a′) via $C_4H_2INO_2$ activating the Au atom.

	COM1a	TS1a	IM1a	TS2a	IM2a	TS2a′	IM2a′
Cl–I–N	169.5	171.7	169.5	169.3	173.1	171.8	164.6

Table S3. Topological and energetic properties at the BCPs of the N–I···Cl halogen bond in COM1 (all values in a.u.).

N–I···Cl	ρ	$\nabla^2\rho_b$	G_b	V_b	$-G_b/V_b$
I···Cl	0.0320	0.0687	0.0189	-0.0206	0.9164

Table S4. Topological and energetic properties at the BCPs of the N–I···Au halogen bond in COM1a (all values in a.u.).

N–I···Au	ρ	$\nabla^2\rho_b$	G_b	V_b	$-G_b/V_b$
I···Au	0.0307	0.0566	0.0168	-0.0194	0.8641

Table S5. Topological and energetic properties at the BCPs of the Au–Cl bond in COM1 (all values in a.u.).

Au–Cl	ρ	$\nabla^2\rho_b$	G_b	V_b	$-G_b/V_b$
	0.0848	0.2018	0.0751	-0.0998	0.7525

Table S6 Topological and energetic properties at the BCPs of the Au–Cl bond in COM1a (all values in a.u.).

Au–Cl	ρ	$\nabla^2\rho_b$	G_b	V_b	$-G_b/V_b$
	0.0899	0.1990	0.0776	-0.1055	0.7355

Table S7. Calculated Gibbs energy and XYZ coordinates for all atoms in **COM1** activated by $C_4H_2INO_2$.

G= -2803.3342Hartree

P	-3.20641600	-0.08417100	0.04614300
C	-3.34071100	1.48565900	0.99205600
Au	-1.19860600	-0.27690300	-1.00471000
C	-4.55831200	2.19076000	1.09101800
H	-5.45959100	1.82042300	0.57920800
C	-4.62002100	3.37598000	1.84215900
H	-5.57146600	3.92535100	1.91309000
C	-3.47471500	3.85997400	2.49532900
H	-3.52643200	4.79153200	3.07998000
C	-2.26024400	3.15949600	2.39593100
H	-1.35836600	3.53856200	2.90070900
C	-2.18827400	1.97804900	1.64310000
H	-1.23224600	1.43649000	1.55615000
C	-3.50189000	-1.44738800	1.24235100
C	-3.11288900	-2.75451500	0.87507800
H	-2.62866600	-2.93135400	-0.09897500
C	-3.33027600	-3.82387800	1.75607200
H	-3.02276700	-4.84022300	1.46573700
C	-3.92531100	-3.59581300	3.00926500
H	-4.08582500	-4.43521900	3.70339000
C	-4.30687200	-2.29584600	3.37922700
H	-4.76918100	-2.11305500	4.36155700
C	-4.09870500	-1.21980100	2.49977700
H	-4.39793000	-0.20360800	2.79831500
C	-4.61969000	-0.10881200	-1.12768100
C	-5.83831800	-0.74355300	-0.80951300
H	-5.96007700	-1.26400200	0.15263500
C	-6.90084600	-0.71488900	-1.72789500
H	-7.84905200	-1.21527800	-1.47757000
C	-6.75409900	-0.05563900	-2.95925300
H	-7.58849100	-0.03886500	-3.67748600
C	-5.53944000	0.57600800	-3.27816500
H	-5.41811400	1.08788000	-4.24521700
C	-4.47159100	0.54713300	-2.36923800
H	-3.51445100	1.03049400	-2.62434800
Cl	0.89058400	-0.48223000	-2.13295500

C	1.16374000	-1.13086700	2.74689200
C	-0.05097500	-1.25523700	2.84392600
H	-1.12369800	-1.37951500	2.94113400
C	2.61816100	-0.97036500	2.62248400
H	2.87357200	0.11238500	2.60874900
H	3.11970000	-1.42723900	3.50209700
N	3.17424900	-1.61547800	1.44363100
H	3.02159700	-1.15851100	0.54061800
C	3.93953300	-2.74619500	1.53061200
O	4.22760100	-3.27224100	2.61445900
C	4.43979100	-3.31457700	0.22427100
C	5.51573900	-4.22512600	0.28936300
C	3.87297000	-3.01224800	-1.03282500
C	6.03228000	-4.80447300	-0.87744400
H	5.93387400	-4.46487300	1.27860500
C	4.38619800	-3.59899900	-2.20028800
H	3.01003400	-2.33332100	-1.11863100
C	5.46870500	-4.49148700	-2.12698200
H	6.87802200	-5.50690200	-0.81347500
H	3.93013200	-3.35928000	-3.17344200
H	5.87048700	-4.94843200	-3.04490000
C	4.04844800	3.07930200	1.44739700
C	4.90598000	4.30461000	1.64027500
C	5.03339100	4.93025200	0.45301600
C	4.26562500	4.15027800	-0.58370400
N	3.70670600	3.05402900	0.09208300
H	5.32212600	4.57311700	2.62074100
H	5.58160200	5.84851000	0.20219500
O	3.71620200	2.26961200	2.30241800
O	4.14240900	4.40414200	-1.77113800
I	2.49001400	1.57626500	-0.83898700

Table S8. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS1** activated by $C_4H_2INO_2$.

G= -2803.3199 Hartree Frequency = -50.45

P	3.12593900	-0.13636900	-0.03012200
C	3.39826300	-1.92381300	-0.36246300
Au	0.87622800	0.33720600	0.17232100
C	4.51889200	-2.38031900	-1.08835300
H	5.25001800	-1.66326500	-1.49208300
C	4.69940400	-3.75619900	-1.30254400
H	5.57291100	-4.10741300	-1.87337700

C	3.76947100	-4.67961300	-0.79596700
H	3.91303300	-5.75727200	-0.97040200
C	2.65103300	-4.22716100	-0.07561500
H	1.91490100	-4.94641700	0.31505700
C	2.46084200	-2.85336700	0.13741500
H	1.57415000	-2.49344800	0.68519400
C	4.08692600	0.25985500	1.48804700
C	3.93340800	1.54783400	2.05020900
H	3.25815700	2.27983900	1.57779000
C	4.63862800	1.89708800	3.21123600
H	4.51730100	2.90369600	3.64037300
C	5.48957600	0.96279600	3.82797800
H	6.03664200	1.23614100	4.74353400
C	5.63544800	-0.32063900	3.27809300
H	6.29757600	-1.05693300	3.75944500
C	4.93915600	-0.67531300	2.10999800
H	5.06241300	-1.68308000	1.68572100
C	3.96352300	0.77146700	-1.39337300
C	5.28833700	1.24125800	-1.26973200
H	5.84503200	1.09409800	-0.33186700
C	5.89937500	1.90294800	-2.34768700
H	6.93219100	2.27035900	-2.24492100
C	5.19754900	2.09643400	-3.54869200
H	5.67923300	2.61815200	-4.39016300
C	3.87737300	1.63013900	-3.67326400
H	3.32119800	1.78537200	-4.61058500
C	3.25768700	0.97449500	-2.59913300
Cl	-1.11658300	0.56446000	-1.42650300
C	-0.87507700	0.91855000	2.29978300
C	0.34174800	0.71333600	2.44122400
H	1.29713100	0.63118800	2.95998500
C	-2.31462000	1.14042300	2.14404600
H	-2.82120800	0.16189700	1.98001200
H	-2.71873700	1.56559000	3.09004300
N	-2.64982800	2.08302000	1.09293800
H	-2.38128600	1.82097000	0.13581000
C	-3.27189800	3.26854900	1.37538200
O	-3.59812100	3.58275700	2.52912900
C	-3.55876700	4.18054900	0.20572200
C	-4.29465700	5.35279200	0.48163600
C	-3.13209100	3.93744500	-1.11841200
C	-4.60495900	6.26070500	-0.53955100
H	-4.61458000	5.52861800	1.51953400
C	-3.44226300	4.84822000	-2.14036000

H	-2.54910600	3.03894300	-1.37640100
C	-4.17900600	6.01013500	-1.85543800
H	-5.18200400	7.16983500	-0.30889700
H	-3.10318400	4.64705300	-3.16839500
H	-4.42055300	6.72143600	-2.66071700
H	2.21770300	0.62275700	-2.69358000
C	-4.66044500	-3.22813000	1.25729400
C	-5.51344600	-4.47147500	1.30362300
C	-5.44844800	-5.07861300	0.10160400
C	-4.54883300	-4.26631000	-0.79781300
N	-4.11895400	-3.17630400	-0.03112100
H	-6.06670500	-4.76490100	2.20619600
H	-5.93464500	-6.00182000	-0.24201300
O	-4.47247300	-2.42213900	2.15839700
O	-4.24792400	-4.50002600	-1.95852300
I	-2.81716800	-1.61824600	-0.69698800

Table S9. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM1** activated by $C_4H_2INO_2$.

G= -2803.3290 Hartree

P	2.87185400	-0.12931800	-0.07639700
C	2.79920600	-1.57117800	-1.21265900
Au	0.75863100	0.37512100	0.91159700
C	3.61425600	-1.65929000	-2.36059400
H	4.30794100	-0.84275500	-2.61290000
C	3.53683300	-2.79118000	-3.18821400
H	4.17211400	-2.85318400	-4.08533500
C	2.65132300	-3.83629900	-2.87658200
H	2.58984500	-4.71945600	-3.53126800
C	1.83728300	-3.75022900	-1.73432300
H	1.13469700	-4.56227000	-1.49180300
C	1.90630300	-2.62061100	-0.90523300
H	1.25708100	-2.54768300	-0.01772500
C	4.13832000	-0.55006500	1.19321900
C	4.24392300	0.28134800	2.33072600
H	3.57518800	1.15025600	2.44142900
C	5.19955400	0.00466900	3.31940100
H	5.27827000	0.66048700	4.20027100
C	6.04593500	-1.11054600	3.18983100
H	6.78933000	-1.33179200	3.97126300
C	5.93784000	-1.94381300	2.06508700
H	6.59647400	-2.81988900	1.96040800

C	4.99016700	-1.66621000	1.06533400
H	4.91558500	-2.32389700	0.18623700
C	3.59666600	1.25216100	-1.05525300
C	4.94790800	1.63460100	-0.92242000
H	5.60729900	1.11013500	-0.21460800
C	5.45713800	2.69170000	-1.69511200
H	6.51254800	2.98541000	-1.58471600
C	4.62677100	3.36907400	-2.60239600
H	5.02881500	4.19824900	-3.20505200
C	3.28029100	2.98881500	-2.73738300
H	2.62386500	3.51741200	-3.44585300
C	2.76187300	1.93799700	-1.96618000
Cl	-0.63404900	0.52823100	-1.35787300
C	-0.77884300	0.78368200	2.43449300
C	0.33185600	0.53245100	2.99263000
H	1.04759100	0.39126100	3.80555800
C	-2.21903500	1.07276200	2.25253300
H	-2.75706300	0.10479600	2.12524000
H	-2.61224000	1.56092200	3.16989100
N	-2.49697200	1.96927300	1.14812600
H	-2.19229600	1.66905600	0.21388400
C	-3.12255500	3.17043400	1.34821000
O	-3.50119900	3.53663400	2.47014700
C	-3.34804200	4.03242100	0.12824100
C	-4.12951900	5.19351800	0.31042200
C	-2.82175600	3.75661200	-1.15302000
C	-4.38993500	6.05733300	-0.76160100
H	-4.52504400	5.39626300	1.31687400
C	-3.08169300	4.62414800	-2.22564000
H	-2.19437100	2.86977900	-1.33762200
C	-3.86629400	5.77387900	-2.03489900
H	-5.00442500	6.95751900	-0.60429100
H	-2.66410600	4.39867300	-3.21920000
H	-4.06846800	6.45057800	-2.87988700
H	1.70447200	1.64631200	-2.07433300
C	-4.44164800	-3.07062200	1.16338400
C	-5.32842700	-4.29053200	1.20609800
C	-5.21587200	-4.93993100	0.02999900
C	-4.24922100	-4.17966000	-0.84577500
N	-3.83388800	-3.07363000	-0.09476600
H	-5.93494000	-4.53976900	2.08747200
H	-5.70667400	-5.86262900	-0.30842800
O	-4.27984500	-2.24132700	2.04946500
O	-3.89158800	-4.46159800	-1.97955200

I	-2.44299700	-1.57249700	-0.73320400

Table S10. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS2** activated by $C_4H_2INO_2$.

G= -2803.3059 Hartree Frequency = -260.32

P	2.29634300	-1.68481000	-0.04930000
C	3.42239900	-0.24007500	-0.18110700
Au	0.02553100	-1.10177700	-0.12569400
C	4.73640000	-0.27457900	0.33469900
H	5.11098800	-1.17660300	0.84292700
C	5.56555400	0.85089800	0.20733400
H	6.58948300	0.82070800	0.61118800
C	5.08764900	2.01503200	-0.41946200
H	5.73743600	2.90032200	-0.50188800
C	3.77761600	2.05684600	-0.92507500
H	3.37768800	2.97477200	-1.38320400
C	2.94858000	0.92979900	-0.81025000
H	1.91537500	0.96595700	-1.19180100
C	2.75706000	-2.83860400	-1.41017900
C	1.87323300	-3.89973300	-1.70830800
H	0.93433900	-4.00743800	-1.14103200
C	2.18521200	-4.81208100	-2.72683300
H	1.49259800	-5.63829300	-2.95019400
C	3.37155200	-4.66434100	-3.46678200
H	3.61043300	-5.37500000	-4.27312800
C	4.24663700	-3.60429200	-3.18111900
H	5.17388900	-3.48016400	-3.76167200
C	3.94555600	-2.69330800	-2.15439700
H	4.63858800	-1.86601900	-1.93991500
C	2.77905000	-2.53649500	1.51214800
C	3.49716000	-3.74957200	1.51937500
H	3.78861500	-4.22941800	0.57291400
C	3.84245700	-4.35228600	2.74111300
H	4.40258100	-5.30026700	2.73979600
C	3.47774000	-3.74931200	3.95533700
H	3.74927700	-4.22481700	4.91066800
C	2.76213500	-2.53900700	3.94927000
H	2.47192700	-2.06277100	4.89870700
C	2.40764100	-1.93284900	2.73503700
Cl	-0.07349300	0.88803600	2.08865600
C	-2.03649000	-0.77811500	-0.41794800
C	-2.19975500	-1.65720600	-1.32341900

H	-2.10016100	-2.45112200	-2.06039100
C	-2.98316500	0.19302600	0.22442400
H	-2.61446900	0.50479900	1.21913900
H	-3.00258100	1.10565800	-0.41368900
N	-4.31473000	-0.37541900	0.35953300
H	-4.74016900	-0.31938700	1.28827000
C	-4.92981600	-1.14688800	-0.57475600
O	-4.39184200	-1.45114700	-1.66642100
C	-6.30570200	-1.64907900	-0.24432300
C	-6.76932500	-2.79531200	-0.92489600
C	-7.15420800	-1.00343200	0.68161700
C	-8.04809800	-3.30459500	-0.66346200
H	-6.10643600	-3.27799900	-1.65824700
C	-8.43648300	-1.51225900	0.93624500
H	-6.82968600	-0.08259400	1.19148400
C	-8.88365900	-2.66520100	0.26905800
H	-8.39749600	-4.20529700	-1.19148000
H	-9.09413600	-0.99872900	1.65432800
H	-9.89047800	-3.06255700	0.47123600
H	1.83948800	-0.98708100	2.73580100
C	0.92541900	5.52788400	-1.32645000
C	0.53908500	6.90795100	-1.80848000
C	-0.55564300	7.30021800	-1.12785800
C	-0.93565400	6.19413700	-0.17038400
N	0.00101700	5.17333300	-0.34691900
H	1.10682300	7.43523300	-2.58743600
H	-1.12687900	8.23602400	-1.19845500
O	1.86980800	4.85590500	-1.72699200
O	-1.88014400	6.18713800	0.60829200
I	-0.02447500	3.26857400	0.74471600

Table S11. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM2** activated by $C_4H_2INO_2$.

G= -2803.3322 Hartree

P	3.03625300	-0.50023200	-0.09809500
C	3.12017600	1.33446500	-0.14862100
Au	0.85669000	-1.36136800	-0.26394000
C	4.22781600	2.03970100	0.37174200
H	5.06789100	1.49531100	0.83042300
C	4.25257400	3.44178600	0.31518200
H	5.11782800	3.98793000	0.72222100
C	3.17240800	4.14589100	-0.24530500

H	3.19029900	5.24670600	-0.27397100
C	2.06252200	3.45015400	-0.75299100
H	1.19654600	3.99558400	-1.16104700
C	2.03826900	2.04674200	-0.70706700
H	1.16276200	1.49714200	-1.08928400
C	4.13783400	-1.12763300	-1.43516400
C	4.01707300	-2.48815400	-1.79782100
H	3.27607500	-3.12699000	-1.28987900
C	4.83307200	-3.02548500	-2.80451600
H	4.73434800	-4.08740700	-3.07813300
C	5.76396400	-2.20771100	-3.46835100
H	6.39801700	-2.62795700	-4.26447400
C	5.87788700	-0.85213500	-3.12009900
H	6.60055700	-0.20576100	-3.64194200
C	5.07054400	-0.31033200	-2.10577300
H	5.16739500	0.75370700	-1.84280200
C	3.86023000	-0.96076000	1.48705600
C	5.11642500	-1.59751200	1.53779400
H	5.65620900	-1.83649300	0.60892900
C	5.68497400	-1.93062300	2.77951100
H	6.66673900	-2.42827000	2.81132100
C	5.00744900	-1.62950700	3.97149900
H	5.45564200	-1.89186400	4.94245800
C	3.75400900	-0.99377900	3.92314400
H	3.21732800	-0.75575900	4.85465700
C	3.17673900	-0.66380100	2.68833100
Cl	-0.95734600	1.02501400	2.53317000
C	-1.05524400	-2.11494600	-0.38590700
C	-1.31266500	-3.38722500	-0.72871600
H	-0.61142100	-4.18271700	-1.00912300
C	-2.21725700	-1.21188600	-0.05547200
H	-2.04029300	-0.65202700	0.88953400
H	-2.36821300	-0.44451100	-0.84799300
N	-3.46719600	-1.98471900	0.09899900
H	-4.25670700	-1.51176500	0.55478600
C	-3.64473500	-3.22914900	-0.29528100
O	-2.64410100	-3.93117100	-0.78241200
C	-4.93813600	-3.92467100	-0.20681100
C	-4.95696600	-5.33945100	-0.22043400
C	-6.15460700	-3.20712000	-0.12052300
C	-6.17540300	-6.02207200	-0.13042500
H	-4.01144600	-5.89569500	-0.28872700
C	-7.36771100	-3.89965100	-0.03263800
H	-6.16489000	-2.10659600	-0.15037400

C	-7.38059600	-5.30536900	-0.03444300
H	-6.18464100	-7.12244700	-0.13264300
H	-8.31138800	-3.33708100	0.02690800
H	-8.33743700	-5.84539800	0.03431200
H	2.19302400	-0.16696200	2.65967700
C	-2.02015100	5.17031300	-1.43313600
C	-2.98762100	6.12168600	-2.10429500
C	-4.19560200	5.96006900	-1.53045400
C	-4.06544600	4.89637800	-0.46189400
N	-2.73594100	4.47742700	-0.46495800
H	-2.67936500	6.79654700	-2.91481500
H	-5.14690900	6.46735800	-1.74290800
O	-0.82939500	5.04423900	-1.70681500
O	-4.95956900	4.47949000	0.26553200
I	-1.91056400	2.91232100	0.90404300

Table S12. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS2′** activated by $C_4H_2INO_2$.

G= -2803.3180 Hartree Frequency = -129.08

P	3.00006700	-0.50156100	0.18645700
C	3.49792100	0.94580100	-0.83056400
Au	1.42828800	-1.81853300	-0.90500400
C	2.86366300	2.19224700	-0.64691500
H	2.10914800	2.33432300	0.14113100
C	3.17823600	3.26960000	-1.49107200
H	2.66226600	4.22886100	-1.33498800
C	4.12307100	3.11256900	-2.51742000
H	4.37097500	3.96024200	-3.17501000
C	4.74679700	1.86730500	-2.71035500
H	5.48303900	1.73596000	-3.51846000
C	4.43197000	0.78238200	-1.87840300
H	4.91872800	-0.19106500	-2.04572600
C	4.52629800	-1.42525400	0.62164600
C	4.41603000	-2.81358900	0.85356600
H	3.44177100	-3.31319700	0.72461500
C	5.54235200	-3.55403100	1.24333900
H	5.44853300	-4.63629200	1.42161700
C	6.78480800	-2.91664600	1.39756200
H	7.66947600	-3.49933500	1.69778700
C	6.89983400	-1.53634400	1.16244600
H	7.87273200	-1.03450100	1.27925500
C	5.77661700	-0.78782000	0.77611400
H	5.87957100	0.29193000	0.58980300

C	2.31514600	0.17224000	1.75564900
C	3.14916500	0.79545100	2.71003300
H	4.23312600	0.87932100	2.53820200
C	2.59379500	1.31146900	3.89031100
H	3.24843400	1.79406100	4.63244700
C	1.21057700	1.21511400	4.12601200
H	0.78108600	1.62408000	5.05372100
C	0.37811500	0.59930800	3.17856400
H	-0.70845800	0.52209800	3.34002500
C	0.92955100	0.07483600	1.99853600
Cl	-3.29429700	0.15842200	1.80652900
C	-1.02965700	-2.39146300	-1.76252600
C	0.02197600	-3.09716800	-1.85000300
H	0.32162000	-4.10049200	-2.17593500
C	-1.94866900	-1.26427600	-1.55636200
H	-1.42156200	-0.44640800	-1.02436500
H	-2.24585600	-0.86203100	-2.55304000
N	-3.10450900	-1.67412600	-0.78577500
H	-3.35396200	-1.11932000	0.06192100
C	-3.57745500	-2.90783200	-1.08063000
O	-2.97079600	-3.58946200	-1.94519000
C	-4.79635300	-3.41830500	-0.38542900
C	-5.17652000	-4.75699400	-0.62388800
C	-5.57739800	-2.61621500	0.47664100
C	-6.31594900	-5.28947800	-0.00711800
H	-4.55951400	-5.36708000	-1.30013700
C	-6.71566100	-3.15528200	1.09332800
H	-5.30318700	-1.56898200	0.67961600
C	-7.08774400	-4.48916200	0.85314700
H	-6.60459800	-6.33478800	-0.19711200
H	-7.31880900	-2.52556600	1.76525800
H	-7.98394100	-4.90632400	1.33836700
H	0.27467000	-0.41365600	1.25919800
C	-2.95747400	5.34892700	-0.81939800
C	-2.14530200	6.50674800	-1.35399800
C	-0.84156400	6.23121700	-1.15404900
C	-0.74365100	4.88162700	-0.47984100
N	-2.04534100	4.41910900	-0.31552800
H	-2.61286800	7.38836100	-1.81355000
H	0.04641300	6.82781800	-1.40495400
O	-4.17680700	5.24166300	-0.82489300
O	0.28731700	4.30592300	-0.14419300
I	-2.61104600	2.50989800	0.62448200

Table S13. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM2′** activated by $C_4H_2INO_2$.

G= -2803.3439Hartree

P	3.41091500	-0.37299100	0.08249200
C	3.75039100	0.84473300	-1.25709600
Au	1.43432700	-1.60014000	-0.25607300
C	4.35271500	2.09530200	-1.00542700
H	4.62519600	2.38298100	0.02161900
C	4.60098100	2.98086900	-2.06749300
H	5.07011300	3.95618900	-1.86455300
C	4.25242400	2.62506600	-3.38135700
H	4.44594000	3.32289400	-4.21085200
C	3.65079200	1.38030300	-3.63503200
H	3.36940500	1.10039600	-4.66198700
C	3.39538600	0.49371300	-2.57785300
H	2.90792200	-0.47526500	-2.77375500
C	4.91437000	-1.43172200	0.18653500
C	4.78453100	-2.70805800	0.77714100
H	3.79933900	-3.04532100	1.13884500
C	5.90324400	-3.54683500	0.89623300
H	5.79352000	-4.54037700	1.35780100
C	7.15496200	-3.12371000	0.41753900
H	8.03041700	-3.78604400	0.50327900
C	7.28653600	-1.85818100	-0.17802300
H	8.26461900	-1.52530300	-0.55869300
C	6.17217300	-1.01103800	-0.29368400
H	6.28490200	-0.02197700	-0.76348900
C	3.38140400	0.61144100	1.63978200
C	4.43266000	0.58102000	2.57822300
H	5.32491100	-0.03591100	2.39253200
C	4.34209900	1.33918800	3.75818500
H	5.16619200	1.30898800	4.48792300
C	3.20857400	2.12975400	4.00586900
H	3.14021700	2.72088600	4.93234400
C	2.15905900	2.16206000	3.07061800
H	1.26648400	2.77823500	3.26092600
C	2.23795500	1.40322300	1.89332800
Cl	-5.42300700	0.77916200	1.84316700
C	-1.50064100	-2.30416100	-0.14539800
C	-0.28665100	-2.65561400	-0.59057500
H	-0.26477000	-3.56776400	-1.21715300
C	-2.01186000	-1.16641900	0.71524500

H	-1.66168000	-1.23007500	1.76864700
H	-1.73059400	-0.16332500	0.32607600
N	-3.45991500	-1.37297800	0.65158000
H	-4.15932300	-0.73091800	1.11442000
C	-3.75107500	-2.45343000	-0.04365800
O	-2.67532500	-3.07020600	-0.51078900
C	-5.07228200	-3.00040000	-0.33838100
C	-5.16907600	-4.27131900	-0.95413400
C	-6.24395600	-2.27093400	-0.02509300
C	-6.42849700	-4.80843000	-1.24219900
H	-4.25519100	-4.83165200	-1.19787900
C	-7.49689700	-2.81914200	-0.32174400
H	-6.17576900	-1.27247600	0.43860000
C	-7.59202100	-4.08505500	-0.92646600
H	-6.50412200	-5.79827000	-1.71684700
H	-8.40808700	-2.25077900	-0.08171200
H	-8.58131500	-4.51032900	-1.15603500
H	1.41004900	1.43318200	1.16518100
C	-2.17932900	4.79339100	-1.04568700
C	-0.82594500	5.11022100	-1.64311500
C	-0.02661200	4.03920800	-1.46686500
C	-0.82477800	2.97485100	-0.75200400
N	-2.09376900	3.49467300	-0.53708900
H	-0.60869600	6.07428600	-2.12320400
H	1.02024700	3.88790700	-1.76439000
O	-3.15933200	5.52438800	-1.00954700
O	-0.42849300	1.85818800	-0.41894200
I	-3.66598500	2.37603500	0.51451300

Table S14. Calculated Gibbs energy and XYZ coordinates for all atoms in **COM1a** activated by $C_4H_2INO_2$.

G= -2803.3360 Hartree

P	2.60480100	-0.10790400	0.10293000
C	3.98764300	-1.27819800	-0.21541800
Au	0.73392400	-0.85370500	-1.01314100
C	5.33378900	-0.85915700	-0.15712800
H	5.58243700	0.19072900	0.06045400
C	6.36337500	-1.78513200	-0.38587900
H	7.41205200	-1.45281000	-0.34349600
C	6.05899000	-3.12706500	-0.67154400
H	6.87048800	-3.84867000	-0.85324800
C	4.71972500	-3.54624800	-0.73202500
H	4.47616100	-4.59514200	-0.96069500

C	3.68411400	-2.62521300	-0.50916700
H	2.63188200	-2.95032900	-0.56516600
C	2.41013500	-0.01229400	1.92753300
C	1.58681900	0.99406200	2.48175100
H	1.09595700	1.74179400	1.83936600
C	1.39084600	1.04884000	3.86957600
H	0.74986400	1.83847900	4.29115400
C	2.00324500	0.10486300	4.71174700
H	1.84343900	0.15079600	5.80011700
C	2.81998100	-0.89625500	4.16213000
H	3.30581900	-1.63656100	4.81637800
C	3.02621600	-0.95838800	2.77370900
H	3.67128000	-1.74466500	2.35347800
C	3.17213500	1.54257400	-0.46116700
C	3.89134600	2.40955600	0.38932900
H	4.08799300	2.12906500	1.43516400
C	4.35290200	3.64220000	-0.09997700
H	4.90990400	4.31730700	0.56782500
C	4.10283100	4.01362000	-1.43130500
H	4.46334900	4.98294300	-1.80905000
C	3.38583100	3.15206400	-2.27882300
H	3.18125100	3.44269900	-3.32065700
C	2.91718000	1.92092300	-1.79688500
Cl	-1.08759800	-1.69336500	-2.25816900
C	-0.76788700	-3.96857000	1.14056200
C	0.20061500	-3.55559300	1.76617700
H	1.04607600	-3.18797500	2.33712800
C	-1.92435500	-4.44889400	0.37359700
H	-1.56775400	-4.94317200	-0.55699400
H	-2.47711200	-5.21120000	0.96336600
N	-2.87878600	-3.40180100	0.05111100
H	-2.57729200	-2.69492700	-0.63185500
C	-4.12506900	-3.37660400	0.61599900
O	-4.51809500	-4.26247200	1.38900900
C	-5.01510100	-2.21365400	0.24616200
C	-6.37168100	-2.30190300	0.62582600
C	-4.56367300	-1.04728000	-0.40850100
C	-7.26153600	-1.25595800	0.34689700
H	-6.70470200	-3.21119300	1.14828900
C	-5.45219200	0.00582300	-0.67823400
H	-3.51088200	-0.93375400	-0.70989200
C	-6.80267500	-0.09733900	-0.30432500
H	-8.31867000	-1.34115300	0.64375200
H	-5.07830000	0.91777100	-1.16965500

H	-7.49799600	0.72996200	-0.51683700
H	2.34269400	1.25033100	-2.45607800
I	-1.07883000	1.53014100	-0.45226400
N	-2.07417100	3.29495500	0.19841100
C	-3.28784300	3.77768300	-0.30910800
C	-1.58299400	4.12876600	1.21063900
C	-3.57641200	5.04573300	0.45483200
C	-2.58236300	5.24941700	1.34311100
H	-4.47562500	5.64646200	0.26217000
H	-2.45143200	6.06152700	2.07104100
O	-0.55311300	3.96751400	1.84896000
O	-3.96487100	3.26450200	-1.18674800

Table S15. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS1a** activated by $C_4H_2INO_2$.

G= -2803.3180 Hartree Frequency = -49.47

P	2.68261600	0.13993900	-0.09533400
C	4.08567100	-0.77143400	-0.85896000
Au	0.84173700	-1.29932100	0.07863000
C	5.02971500	-0.12467600	-1.68422400
H	4.93315500	0.94999600	-1.90189900
C	6.09505200	-0.85617000	-2.23376900
H	6.82697300	-0.34781000	-2.88042800
C	6.22553300	-2.22864100	-1.96356500
H	7.06018800	-2.79865500	-2.40030700
C	5.28572400	-2.87555100	-1.14292600
H	5.37983200	-3.95249500	-0.93489000
C	4.21547400	-2.15240800	-0.59505700
H	3.46709100	-2.66095900	0.03549200
C	3.30808700	0.75524900	1.52298100
C	2.38896900	1.36513500	2.40689700
H	1.33150800	1.47289300	2.11439300
C	2.82070700	1.83994100	3.65425500
H	2.09872200	2.31828900	4.33403300
C	4.16624900	1.69803300	4.03668400
H	4.50164700	2.06370200	5.01957000
C	5.07992300	1.08492800	3.16467400
H	6.13446400	0.96975000	3.45961800
C	4.65720400	0.61521200	1.90964500
H	5.38287900	0.13975500	1.23300300
C	2.42607100	1.63008700	-1.14041100
C	2.92224800	2.89776900	-0.77198800

H	3.47685600	3.02607000	0.16968500
C	2.70209400	4.00539800	-1.60764000
H	3.08643600	4.99378700	-1.31154800
C	1.99374400	3.85452100	-2.81039000
H	1.81733600	4.72631100	-3.45931100
C	1.50233700	2.59077500	-3.18126500
H	0.94094000	2.46850300	-4.12028700
C	1.71081000	1.48150200	-2.34928700
Cl	-0.36067100	-2.54005000	-1.75496200
C	-0.53408400	-2.52135300	1.91184100
C	0.38012700	-1.76005200	2.28382900
H	1.02849300	-1.20576900	2.96289600
C	-1.62467100	-3.44333900	1.56587900
H	-1.18642400	-4.40931200	1.22954100
H	-2.22572600	-3.64721600	2.47959600
N	-2.53215000	-2.91728900	0.56697200
H	-2.11764900	-2.75665800	-0.36580300
C	-3.81970500	-2.58082700	0.87960500
O	-4.29716200	-2.76648200	2.00861700
C	-4.64804600	-1.98289400	-0.23379800
C	-6.00470200	-1.72281300	0.05386500
C	-4.14563600	-1.66138400	-1.51419800
C	-6.84792200	-1.16373800	-0.91567800
H	-6.37470900	-1.97104700	1.05984300
C	-4.99140300	-1.10017700	-2.48397500
H	-3.08862200	-1.83447100	-1.77424700
C	-6.34261100	-0.85130100	-2.18967200
H	-7.90530200	-0.96884800	-0.67734700
H	-4.58775700	-0.85243300	-3.47806500
H	-7.00208800	-0.41122000	-2.95415500
H	1.30837800	0.49681200	-2.63599500
I	-1.23960100	1.12870100	0.31592700
N	-2.81597000	2.52055700	0.38332100
C	-2.84301100	3.72742200	-0.33433300
C	-4.00986700	2.32475700	1.09848600
C	-4.17612800	4.35505100	-0.01875400
C	-4.85467800	3.53927600	0.81361500
H	-4.47308800	5.32474100	-0.44086600
H	-5.85375100	3.66435700	1.25272000
O	-4.28520000	1.36595500	1.79974400
O	-1.96123800	4.16005400	-1.05748200

Table S16. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM1a** activated by $C_4H_2INO_2$.

G= -2803.3233 Hartree

P	-2.62278000	0.08532800	0.23660200
C	-3.92287300	-1.00251400	0.94906000
Au	-0.84984600	-1.21548300	-0.73470000
C	-4.62703000	-0.66426400	2.12332400
H	-4.39447700	0.26817200	2.66009900
C	-5.62599900	-1.52216500	2.61230400
H	-6.17054000	-1.25480800	3.53117200
C	-5.92821600	-2.71520000	1.93520500
H	-6.70991800	-3.38632900	2.32370200
C	-5.22634400	-3.05621200	0.76620400
H	-5.45436000	-3.99406100	0.23652000
C	-4.22287000	-2.20725000	0.27611100
H	-3.66203700	-2.48195700	-0.63236400
C	-3.49250300	1.15141600	-0.98937000
C	-2.71398100	1.86808800	-1.92500500
H	-1.61590500	1.77302800	-1.91572300
C	-3.33431100	2.70420800	-2.86547500
H	-2.71878400	3.26263000	-3.58765500
C	-4.73492100	2.82077600	-2.89048500
H	-5.22098400	3.47032500	-3.63492600
C	-5.51297700	2.10306000	-1.96777000
H	-6.61059000	2.18855300	-1.98496400
C	-4.89761800	1.27226300	-1.01643600
H	-5.51660300	0.71633800	-0.29613600
C	-2.10654400	1.21614400	1.59353000
C	-2.52189900	2.56297900	1.64386800
H	-3.17999900	2.97194200	0.86257700
C	-2.08982100	3.39104100	2.69319000
H	-2.41361800	4.44294000	2.72327100
C	-1.24918100	2.88178000	3.69577000
H	-0.91069400	3.53435100	4.51559200
C	-0.83482300	1.53946100	3.64697800
H	-0.16956400	1.13710600	4.42677500
C	-1.25364800	0.70646500	2.59890700
Cl	-0.08521100	-2.51071900	1.32162600
C	0.43973300	-2.02510800	-2.29291200
C	-0.38762700	-1.21307100	-2.81914000
H	-0.84914200	-0.64264500	-3.62886600
C	1.53308900	-3.01528500	-2.14880000
H	1.08569500	-4.03452600	-2.18180600

H	2.23239200	-2.92652700	-3.00759600
N	2.31506800	-2.83128700	-0.94296800
H	1.79472400	-2.85050700	-0.05126600
C	3.64686400	-2.51956700	-1.00481700
O	4.26348500	-2.46998100	-2.07915000
C	4.34550900	-2.26214900	0.30951100
C	5.74968500	-2.12880300	0.26676500
C	3.68204100	-2.12833100	1.54908100
C	6.48143000	-1.88386700	1.43637300
H	6.24773100	-2.22146500	-0.70984700
C	4.41677900	-1.87988900	2.71930400
H	2.58399100	-2.19974400	1.62090600
C	5.81573400	-1.76035400	2.66832800
H	7.57729900	-1.78603600	1.38800400
H	3.88795600	-1.77418400	3.67942300
H	6.38734300	-1.56639300	3.58958300
H	-0.90576600	-0.33926900	2.54943100
I	1.47351600	1.23655700	-0.68554400
N	2.90240500	2.70379000	-0.27492800
C	2.61059700	3.97204200	0.25630400
C	4.28821900	2.52204800	-0.43770600
C	3.94376900	4.65182800	0.42609000
C	4.91764300	3.81011700	0.02350300
H	4.02497700	5.67326600	0.82177400
H	6.00537000	3.96149400	0.00339900
O	4.84084200	1.52294800	-0.86381300
O	1.50286500	4.40960800	0.51694800

Table S17. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS2a** activated by $C_4H_2INO_2$.

G= -2803.2985Hartree Frequency = -229.85

P	-2.44270600	-0.65532900	-0.03366100
C	-3.49182300	-2.16171000	-0.21035000
Au	-0.12583700	-1.19506700	-0.10374600
C	-4.72190900	-2.29981900	0.46498700
H	-5.05459800	-1.53518300	1.18293500
C	-5.52984300	-3.42395600	0.22577200
H	-6.48643300	-3.52841200	0.76093200
C	-5.12165100	-4.40757700	-0.68952600
H	-5.75727700	-5.28761900	-0.87369900
C	-3.89900800	-4.26807500	-1.36834800
H	-3.57218900	-5.03739800	-2.08489600

C	-3.08364600	-3.15237200	-1.12828000
H	-2.12324000	-3.04869500	-1.65726800
C	-3.11039100	0.43134800	-1.36398100
C	-2.35033600	0.65122500	-2.53020100
H	-1.33008700	0.24237300	-2.60108400
C	-2.88954900	1.39238200	-3.59398800
H	-2.28849400	1.56024600	-4.50091900
C	-4.18620300	1.92195200	-3.49713200
H	-4.60602000	2.50864400	-4.32897600
C	-4.94957300	1.70072500	-2.33778400
H	-5.96835500	2.11070700	-2.25912300
C	-4.42061900	0.95155400	-1.27597700
H	-5.03360200	0.77188100	-0.37941100
C	-2.85076600	0.09803000	1.58755700
C	-3.05873000	1.48645500	1.72837000
H	-3.02695400	2.15504200	0.85587500
C	-3.27542400	2.03393500	3.00387300
H	-3.43183200	3.11914300	3.10358500
C	-3.28059200	1.20867500	4.13961100
H	-3.45341500	1.64267600	5.13679600
C	-3.04839300	-0.17103600	4.00279100
H	-3.03226600	-0.82095200	4.89146700
C	-2.82529300	-0.72846100	2.73498900
Cl	-0.41372400	-3.29269700	1.36346000
C	1.93582400	-1.62909100	-0.35935900
C	2.20351900	-0.85920500	-1.33641300
H	2.24891000	-0.12987500	-2.14129800
C	2.75099500	-2.66767400	0.35910300
H	2.32380900	-2.89420000	1.35211400
H	2.68053000	-3.60412600	-0.23911200
N	4.13450900	-2.25101600	0.50233000
H	4.51197500	-2.22548800	1.45297300
C	4.86141600	-1.68046800	-0.49563000
O	4.38213200	-1.46383200	-1.63266300
C	6.27957600	-1.30274000	-0.17998600
C	6.89343800	-0.32034700	-0.98616800
C	7.02294200	-1.91279100	0.85422200
C	8.21872700	0.06533800	-0.74571800
H	6.30936500	0.13549500	-1.79931000
C	8.35176100	-1.52890300	1.08819500
H	6.57706900	-2.71133000	1.46778400
C	8.95017400	-0.53701200	0.29287600
H	8.68594100	0.84036400	-1.37274600
H	8.92618400	-2.01456100	1.89197500

H	9.99315200	-0.23705400	0.47919500
H	-2.60281900	-1.80277000	2.63542800
C	1.70594500	4.66314900	0.10271800
C	1.34354700	6.10496700	0.38069300
C	0.00839300	6.17852700	0.55036300
C	-0.56652600	4.78860900	0.39083900
N	0.50921300	3.94573500	0.12245200
H	2.09989600	6.90106500	0.42136600
H	-0.62327500	7.05095800	0.76760100
O	2.82465500	4.21063100	-0.10094800
O	-1.74755600	4.47216700	0.47987400
I	0.34477900	1.74880400	-0.18551700

Table S18. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM2a** activated by $C_4H_2INO_2$.

G= -2803.3269Hartree

P	-2.33023500	-0.99192500	-0.04741300
C	-3.20401900	-2.59771900	-0.31075900
Au	0.08907900	-1.00894000	-0.02281500
C	-4.47318400	-2.84733400	0.25487200
H	-4.93063200	-2.11976400	0.94210400
C	-5.16166100	-4.03070500	-0.05677300
H	-6.14912200	-4.21889000	0.39269800
C	-4.59587400	-4.96645400	-0.93874700
H	-5.13843100	-5.89334500	-1.18202200
C	-3.33594600	-4.71773200	-1.50746600
H	-2.88522900	-5.44968900	-2.19558600
C	-2.63758800	-3.54100800	-1.19371300
H	-1.64038600	-3.36356100	-1.62145200
C	-3.08009900	0.05401100	-1.36594800
C	-2.33501100	0.30148000	-2.53736300
H	-1.29613800	-0.05750700	-2.60918800
C	-2.91325200	1.00601400	-3.60504000
H	-2.32394200	1.19640700	-4.51525400
C	-4.23381400	1.47347400	-3.50687300
H	-4.68429900	2.03333300	-4.34118800
C	-4.98080300	1.22555500	-2.34256800
H	-6.01726900	1.58831900	-2.26247800
C	-4.41243200	0.51104900	-1.27669300
H	-5.01207900	0.31249800	-0.37534200
C	-2.88964600	-0.36097700	1.58477400
C	-3.17158700	1.00693100	1.79150100

H	-3.13298000	1.72952900	0.96271100
C	-3.47599000	1.47058400	3.08231500
H	-3.69061400	2.54033500	3.22981500
C	-3.49424100	0.58528300	4.17177800
H	-3.73467400	0.95475500	5.18087800
C	-3.19337900	-0.77304100	3.97193500
H	-3.19326900	-1.47217400	4.82260200
C	-2.88568700	-1.24645900	2.68741100
Cl	0.31263700	-3.50969600	0.44272700
C	2.15114700	-0.87642300	0.01454200
C	2.87633900	-0.54925400	-1.06346300
H	2.53082500	-0.22057500	-2.05060600
C	2.84117200	-1.29428800	1.28228800
H	2.53121500	-0.65729000	2.13819500
H	2.56623800	-2.34275700	1.53522300
N	4.30610300	-1.18718600	1.14350700
H	4.86708600	-1.34569800	1.98878800
C	4.95434700	-0.89698500	0.03239400
O	4.30758700	-0.60151000	-1.07367200
C	6.42203600	-0.87004000	-0.05317600
C	7.03520600	-0.17158800	-1.12007000
C	7.22382100	-1.53684800	0.90299100
C	8.43092700	-0.12904000	-1.21401500
H	6.41199500	0.34596000	-1.86291200
C	8.61848300	-1.48996000	0.79830600
H	6.76502000	-2.11805400	1.71777700
C	9.22381700	-0.78485200	-0.25667300
H	8.90409800	0.42253900	-2.04018900
H	9.23760100	-2.01584700	1.54040500
H	10.32132200	-0.75067600	-0.33516600
H	-2.63654900	-2.30976500	2.54536600
C	0.79621900	5.12283200	-0.12891400
C	0.14780600	6.48804300	0.03586900
C	-1.15129900	6.28785700	0.33025500
C	-1.38675800	4.78678800	0.36495400
N	-0.18375500	4.16819700	0.08390400
H	0.70562900	7.42819300	-0.08070200
H	-1.95043600	7.01832800	0.52085700
O	1.97820300	4.92017900	-0.40225900
O	-2.46772500	4.24360000	0.60241800
I	0.08530500	1.77009400	-0.03074500

Table S19. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS2a′** activated by $C_4H_2INO_2$.

G= -2803.3044 Hartree Frequency = -104.82

P	-0.83505100	1.94404900	-0.18179900
C	-1.70683000	2.25820600	1.40469500
Au	0.19519200	-0.15459300	-0.39205600
C	-1.15048500	3.11008200	2.38231700
H	-0.19786200	3.62761800	2.19501000
C	-1.81666800	3.30261300	3.60361200
H	-1.37707400	3.97092800	4.35995900
C	-3.03378100	2.65022500	3.85747400
H	-3.55241900	2.80391000	4.81648800
C	-3.58828700	1.80079600	2.88469400
H	-4.54075300	1.28165100	3.07231500
C	-2.93084500	1.59981600	1.66232000
H	-3.38130000	0.92591300	0.91815800
C	-2.03385600	2.25251000	-1.53119600
C	-1.85752400	1.57423500	-2.75644400
H	-1.04083600	0.84113800	-2.86240000
C	-2.72437700	1.82802200	-3.82971700
H	-2.58381900	1.29472600	-4.78234800
C	-3.77265000	2.75234500	-3.68389300
H	-4.45654500	2.94578600	-4.52477900
C	-3.95346100	3.42492800	-2.46378600
H	-4.77627600	4.14685400	-2.34662800
C	-3.08788500	3.18013800	-1.38581800
H	-3.23715900	3.70944900	-0.43249300
C	0.49251000	3.20625400	-0.32280000
C	0.29318700	4.42666000	-1.00283900
H	-0.67251700	4.64972500	-1.48092500
C	1.33883700	5.36108600	-1.07597500
H	1.17979800	6.31020000	-1.61101000
C	2.58034500	5.08818400	-0.47529700
H	3.39631600	5.82484600	-0.54115500
C	2.78012400	3.87411300	0.20209200
H	3.73835200	3.61891800	0.68327900
C	1.74238900	2.93299000	0.27473100
Cl	4.44201100	1.30950000	2.24016900
C	2.05012100	-2.00402200	0.13005500
C	1.24949600	-1.95311700	-0.85096000
H	1.05427000	-2.45115800	-1.80789900
C	2.75244300	-1.79728800	1.39696800
H	2.28912000	-0.94938100	1.94668300
H	2.61759900	-2.70815000	2.02643400
N	4.14741300	-1.48499900	1.17852300
H	4.46881600	-0.54456300	1.57763900

C	4.74516600	-2.19344900	0.19372600
O	4.08527200	-3.06799500	-0.42369900
C	6.18180000	-1.92077400	-0.12402600
C	6.85506300	-2.82755600	-0.97066600
C	6.86700600	-0.78950100	0.37402600
C	8.20035400	-2.61968700	-1.30309300
H	6.30198700	-3.69574300	-1.35926100
C	8.21118800	-0.58266600	0.02893100
H	6.34718100	-0.05206500	1.01264200
C	8.88170800	-1.49632700	-0.80262800
H	8.72082900	-3.33572300	-1.95798700
H	8.73952600	0.30385900	0.41308100
H	9.93841500	-1.33024200	-1.06489500
H	1.93411600	1.98872600	0.81163200
C	-5.34363700	-2.10740700	0.69954600
C	-6.44535400	-3.13460900	0.75249700
C	-5.94808200	-4.32169800	0.34946000
C	-4.48959000	-4.14483600	0.01015100
N	-4.20711800	-2.79051300	0.24906200
H	-7.46303200	-2.87755200	1.07631500
H	-6.45083000	-5.29389300	0.25632200
O	-5.41430400	-0.92083100	0.98476300
O	-3.70434300	-4.98790300	-0.39008700
I	-2.31604000	-1.86517700	-0.03599100

Table S20. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM2a′** activated by $C_4H_2INO_2$.

G= -2803.3381Hartree

P	2.68046100	-1.15509900	0.00206500
C	3.00455400	-0.65322600	1.74409900
Au	0.43146300	-0.84017700	-0.71465600
C	3.38317800	-1.58496200	2.73254500
H	3.52683600	-2.64449000	2.47250000
C	3.57971000	-1.16149200	4.05809600
H	3.87580300	-1.89555100	4.82347600
C	3.40199700	0.18734500	4.40488400
H	3.55707500	0.51500200	5.44460700
C	3.02258700	1.11745400	3.42147300
H	2.87627800	2.17772300	3.67912000
C	2.81905600	0.70301600	2.09725300
H	2.51321500	1.44812600	1.34615600
C	3.91402000	-0.25305300	-1.02015300
C	3.62440900	-0.05531800	-2.38773300

H	2.66567800	-0.40860000	-2.80099900
C	4.55067100	0.59575600	-3.21648600
H	4.31730300	0.74799800	-4.28155900
C	5.76557500	1.06096000	-2.68513600
H	6.48867900	1.57824100	-3.33469500
C	6.05380100	0.87306400	-1.32313800
H	7.00254700	1.24107100	-0.90280400
C	5.13356400	0.21765400	-0.48886800
H	5.36500700	0.07941000	0.57829300
C	3.13353400	-2.93582300	-0.10522300
C	4.46011700	-3.36598600	-0.31805100
H	5.26997400	-2.63092000	-0.44305200
C	4.74965300	-4.73849300	-0.37676300
H	5.78610100	-5.06892600	-0.54663100
C	3.72352800	-5.68630500	-0.22216600
H	3.95541800	-6.76157400	-0.27135500
C	2.40092200	-5.26165700	-0.01200400
H	1.59302800	-6.00054200	0.10368600
C	2.10398700	-3.89078900	0.04137600
Cl	-5.46742200	-1.38704400	3.59827800
C	-2.58640100	-0.81881100	-0.60911800
C	-1.49445600	-0.71136500	-1.38613100
H	-1.67761900	-0.61093300	-2.47175900
C	-2.79249700	-0.92683300	0.88713500
H	-2.29198400	-1.81208600	1.33448600
H	-2.42952500	-0.02886000	1.43451300
N	-4.24269400	-1.04307900	0.99780800
H	-4.76036900	-1.17247900	2.01277600
C	-4.78725900	-0.98596000	-0.19087500
O	-3.89421700	-0.84414200	-1.18254500
C	-6.20575500	-1.06187800	-0.53321100
C	-6.60030100	-0.97576800	-1.88956800
C	-7.17780700	-1.22300500	0.48367800
C	-7.95750600	-1.05009500	-2.22357800
H	-5.83996300	-0.85041200	-2.67366200
C	-8.53122400	-1.29608400	0.13332300
H	-6.86673700	-1.29127600	1.54346700
C	-8.92342000	-1.21018100	-1.21449200
H	-8.26472300	-0.98243200	-3.27814400
H	-9.28905600	-1.42143700	0.92170900
H	-9.99030200	-1.26833400	-1.48082000
H	1.06501300	-3.55278300	0.19309700
C	1.01399400	4.71840500	0.94206500
C	0.73190000	6.19886800	1.01810900

C	-0.33969500	6.46956100	0.24576800
C	-0.81909800	5.18067600	-0.37724600
N	0.04639200	4.18292700	0.08876800
H	1.34593400	6.87824500	1.62491000
H	-0.83726700	7.42967400	0.05195500
O	1.90837000	4.10381900	1.50855100
O	-1.76561100	5.02494600	-1.13318900
I	-0.09526300	2.08446000	-0.39152600

Table S21. Calculated Gibbs energy and XYZ coordinates for all atoms in **COM1b** activated by C_6F_5I.

G= -3172.1518 Hartree

P	3.40820500	-1.11693200	0.07450400
C	2.87033400	-2.76362500	0.69110500
Au	1.66650500	0.08484300	-0.75791300
C	3.66164000	-3.91905800	0.52535400
H	4.62498500	-3.86324400	-0.00381600
C	3.21511600	-5.15046600	1.03300900
H	3.83430500	-6.05066900	0.89746600
C	1.98537100	-5.23450100	1.70598100
H	1.63789400	-6.20233300	2.09944100
C	1.19400300	-4.08429700	1.86945200
H	0.22588500	-4.14705800	2.38975500
C	1.62945400	-2.85209700	1.35997200
H	1.00173800	-1.95334700	1.47552500
C	4.23446200	-0.27964800	1.48681500
C	4.41546800	1.11948000	1.42087900
H	4.04305200	1.68152800	0.54914800
C	5.05797800	1.79333900	2.46984100
H	5.19500000	2.88416700	2.41380800
C	5.51270400	1.07999800	3.59268100
H	6.00886600	1.61219900	4.41898200
C	5.32681700	-0.31031900	3.66395700
H	5.67748400	-0.87106800	4.54414100
C	4.69034700	-0.99404100	2.61422200
H	4.54627400	-2.08335000	2.67825500
C	4.71703000	-1.43007200	-1.17734300
C	6.08451400	-1.45754100	-0.83268000
H	6.40137000	-1.26680400	0.20392400
C	7.04840800	-1.72424800	-1.81901600
H	8.11493600	-1.74057600	-1.54639400
C	6.65528900	-1.96532200	-3.14560700
H	7.41444400	-2.16996500	-3.91635200

C	5.29312100	-1.93648500	-3.49114000
H	4.98143600	-2.11769100	-4.53132300
C	4.32479400	-1.66529700	-2.51325300
Cl	-0.15869600	1.30784000	-1.66547000
C	-0.17820500	1.54037000	2.63029700
C	0.83225600	0.95734200	3.00327400
H	1.72785100	0.45409300	3.34944300
C	-1.39315800	2.22597300	2.17401000
H	-2.14293000	1.46944100	1.85162900
H	-1.83914600	2.79628200	3.01658800
N	-1.15758700	3.18719500	1.10861900
H	-0.86822300	2.81637600	0.19500400
C	-1.30645000	4.53048900	1.32680500
O	-1.67351100	4.98211200	2.42146500
C	-1.01973500	5.45346600	0.16466400
C	-1.31979100	6.81977500	0.35410100
C	-0.46699000	5.04139500	-1.06740900
C	-1.08392800	7.75356400	-0.66361500
H	-1.74261300	7.12513000	1.32280100
C	-0.22903300	5.97791600	-2.08582000
H	-0.21071700	3.98696900	-1.25578000
C	-0.53720000	7.33430200	-1.88891700
H	-1.32692600	8.81534000	-0.50129000
H	0.20270400	5.64178200	-3.04137400
H	-0.35003300	8.06534700	-2.69103200
H	3.25768300	-1.62797400	-2.78654500
C	-4.64811600	-1.27246900	-0.29996700
C	-5.13081200	-1.10465500	1.00777700
C	-6.31737600	-1.72883400	1.42640200
C	-7.03273100	-2.53592500	0.52720300
C	-6.56182800	-2.71342100	-0.78361000
C	-5.37389800	-2.08218000	-1.18791800
I	-2.85806100	-0.32049100	-0.91300700
F	-4.95354000	-2.27391400	-2.44466700
F	-7.24564400	-3.48255600	-1.63856800
F	-8.16158600	-3.13328300	0.91847500
F	-6.76801700	-1.56091600	2.67483400
F	-4.47401700	-0.34435000	1.89512600

Table S22. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS1b** activated by C_6F_5I.

G= -3172.1356 Hartree Frequency = -49.90

P	3.37238700	-1.11209500	0.01234600
C	2.91326500	-2.82673000	-0.47173800

Au	1.49763800	0.22601300	0.22917500
C	3.77891400	-3.64557000	-1.22750200
H	4.75369500	-3.26220000	-1.56559000
C	3.39366400	-4.95518400	-1.55638800
H	4.07106700	-5.58817600	-2.15027900
C	2.15008400	-5.45468400	-1.13443400
H	1.85095700	-6.48110800	-1.39777800
C	1.28437300	-4.64041100	-0.38485400
H	0.30493800	-5.02386600	-0.05987900
C	1.66021400	-3.32849700	-0.05811400
H	0.97484200	-2.68087700	0.51326600
C	4.35493000	-1.26804200	1.56171100
C	4.76533700	-0.07854200	2.20652000
H	4.50912900	0.90161300	1.77220300
C	5.49920200	-0.14189700	3.40005700
H	5.81924900	0.78907000	3.89314700
C	5.81699800	-1.38847800	3.96814600
H	6.38685700	-1.43595200	4.90900300
C	5.40163700	-2.57113600	3.33614100
H	5.64503600	-3.54958700	3.77855700
C	4.67373000	-2.51596100	2.13505200
H	4.35516200	-3.44916500	1.64664000
C	4.56116800	-0.52143200	-1.26276400
C	5.95452200	-0.69912000	-1.12374100
H	6.36727500	-1.17773500	-0.22267600
C	6.82111800	-0.25990400	-2.13805400
H	7.90729300	-0.39873500	-2.02269800
C	6.30633200	0.35400900	-3.29176700
H	6.98927200	0.70002800	-4.08312800
C	4.91949000	0.53383700	-3.43144300
H	4.51168700	1.02121700	-4.33044700
C	4.04770100	0.10358800	-2.41985700
Cl	-0.13524300	1.24863900	-1.42956200
C	0.09830000	1.38327800	2.28241600
C	1.11832900	0.70067600	2.48300600
H	1.92518600	0.23582600	3.05021100
C	-1.12604600	2.16146700	2.07265900
H	-1.96512400	1.46251600	1.85195700
H	-1.38281800	2.69819000	3.01331600
N	-1.00770600	3.17022800	1.03731000
H	-0.81497000	2.82350400	0.08516800
C	-1.14638800	4.49992300	1.32485100
O	-1.40298600	4.90574300	2.46810700
C	-0.98641600	5.46206800	0.17118100

C	-1.29513000	6.81562500	0.42486800
C	-0.53771800	5.09215300	-1.11591200
C	-1.16944200	7.77990400	-0.58408000
H	-1.63552400	7.08702200	1.43536400
C	-0.40974300	6.05977300	-2.12481800
H	-0.27754100	4.04773100	-1.35240800
C	-0.72575100	7.40365500	-1.86376100
H	-1.41777900	8.83167800	-0.37237100
H	-0.05764000	5.75897400	-3.12382000
H	-0.62458300	8.15890000	-2.65891300
H	2.96179200	0.26052900	-2.52315000
C	-4.62056800	-1.25003200	-0.26976900
C	-5.16221000	-1.06956300	1.01244900
C	-6.35547400	-1.70601700	1.39173600
C	-7.02029400	-2.53735000	0.47596600
C	-6.49111100	-2.72794000	-0.81057100
C	-5.29669200	-2.08380500	-1.17346300
I	-2.80875700	-0.27796400	-0.81781000
F	-4.81999700	-2.28945500	-2.40873900
F	-7.12673800	-3.52141100	-1.68117200
F	-8.15595400	-3.14671700	0.82879300
F	-6.86166200	-1.52623800	2.61765100
F	-4.55493800	-0.28431400	1.91484900

Table S23. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM1b** activated by C_6F_5I.
G= -3172.1430Hartree

P	3.19867500	-1.04200300	-0.05642000
C	2.57322000	-2.35152500	-1.18502400
Au	1.43947900	0.27079500	0.89587100
C	3.28037200	-2.74880400	-2.33888600
H	4.23144200	-2.26123500	-2.60215300
C	2.76727900	-3.76717200	-3.15875200
H	3.32160400	-4.07030700	-4.06050900
C	1.55260700	-4.39319900	-2.83329900
H	1.15172500	-5.18814600	-3.48119000
C	0.84472700	-3.99796300	-1.68536300
H	-0.11222800	-4.47929800	-1.43126700
C	1.34874200	-2.97753600	-0.86513100
H	0.78515700	-2.65793500	0.02642700
C	4.19202400	-1.92025300	1.22314700
C	4.62419900	-1.18457700	2.34954100

H	4.36273900	-0.11799300	2.44377500
C	5.38659100	-1.80749900	3.34851700
H	5.72292200	-1.22546000	4.22054600
C	5.71114300	-3.17138200	3.24094200
H	6.30160100	-3.66155500	4.03048000
C	5.27646100	-3.90767000	2.12743200
H	5.52569300	-4.97655400	2.03942300
C	4.52194900	-3.28693700	1.11727200
H	4.18951800	-3.87241800	0.24680200
C	4.41671700	-0.06917400	-1.03750300
C	5.80675100	-0.28665400	-0.93371200
H	6.20059600	-1.04991800	-0.24574300
C	6.69598000	0.47520500	-1.70989700
H	7.77968600	0.30099100	-1.62223100
C	6.20666100	1.45218400	-2.59194500
H	6.90662500	2.04880700	-3.19739200
C	4.82204100	1.66969800	-2.69752200
H	4.43310200	2.43632100	-3.38556200
C	3.92649600	0.91759000	-1.92235400
Cl	0.26604100	0.99946700	-1.29905700
C	0.22699400	1.23420300	2.43410500
C	1.15419000	0.56050800	2.98445200
H	1.74745800	0.15766300	3.80881200
C	-0.99017800	2.06205700	2.27842300
H	-1.86314000	1.37521700	2.18477800
H	-1.14692300	2.67789600	3.18978300
N	-0.92672000	2.97603100	1.15492900
H	-0.71727300	2.56618500	0.23276800
C	-1.12052700	4.31985600	1.32510200
O	-1.39137800	4.81245000	2.43041800
C	-1.00501600	5.18579900	0.09282400
C	-1.40006500	6.53423400	0.22582000
C	-0.51636300	4.73507300	-1.15316300
C	-1.32182900	7.41366300	-0.86229400
H	-1.76888700	6.87012900	1.20650700
C	-0.43542600	5.61852100	-2.24123000
H	-0.18509800	3.69321500	-1.29463300
C	-0.83887800	6.95699500	-2.10098700
H	-1.63829100	8.46191200	-0.74487300
H	-0.05078900	5.25577200	-3.20713400
H	-0.77511200	7.64564400	-2.95808000
H	2.84116500	1.09493400	-2.00411200
C	-4.38613100	-1.21196600	-0.27055100
C	-4.90317200	-1.08329900	1.02788000

C	-6.14873300	-1.63465900	1.37085200
C	-6.89161100	-2.32724200	0.40113100
C	-6.38754300	-2.46611300	-0.90204900
C	-5.14036100	-1.90777900	-1.22770700
I	-2.49950400	-0.36089300	-0.77032900
F	-4.69050600	-2.05828000	-2.48096300
F	-7.09746400	-3.12845800	-1.82338400
F	-8.07741300	-2.85493800	0.71881000
F	-6.63097800	-1.50547400	2.61270200
F	-4.22242300	-0.42920500	1.98177400

Table S24. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS2b** activated by C_6F_5I.

G= -3172.1162 Hartree Frequency = -269.47

P	-2.12654600	-2.41320900	-0.08493600
C	-0.60499100	-3.42988200	-0.27916100
Au	-1.68056900	-0.10944800	-0.06296800
C	-0.49845000	-4.72632200	0.26774600
H	-1.33201900	-5.15569300	0.84450200
C	0.67833700	-5.46996000	0.08328300
H	0.75732600	-6.47993200	0.51469900
C	1.75270100	-4.92587500	-0.64049100
H	2.67760400	-5.50814500	-0.77470900
C	1.65218600	-3.63308000	-1.18138800
H	2.49892400	-3.19387100	-1.72994200
C	0.47849800	-2.88533200	-1.00106400
H	0.40541700	-1.86424400	-1.40932800
C	-3.25035100	-2.91722700	-1.45759400
C	-4.36867400	-2.09848400	-1.73043000
H	-4.53410700	-1.18313100	-1.13888100
C	-5.26299400	-2.44329800	-2.75432800
H	-6.13376300	-1.80092600	-2.95799200
C	-5.04077500	-3.59785700	-3.52548500
H	-5.73714600	-3.86185000	-4.33648400
C	-3.92486200	-4.40888900	-3.26438300
H	-3.74297400	-5.31127100	-3.86855200
C	-3.03181400	-4.07507900	-2.23175700
H	-2.16136200	-4.71879500	-2.03456200
C	-2.93251400	-3.03185100	1.45331800
C	-4.02815900	-3.91933000	1.42426400
H	-4.44153800	-4.26119700	0.46332000
C	-4.59809300	-4.36964400	2.62715700
H	-5.45436600	-5.06138800	2.59755800

C	-4.07952600	-3.94005000	3.85936100
H	-4.52932100	-4.29376000	4.80019900
C	-2.98833700	-3.05413200	3.88930100
H	-2.58100400	-2.71104000	4.85315600
C	-2.41536800	-2.59424000	2.69385700
Cl	0.05366800	0.12850100	2.14441700
C	-1.54800500	1.96108600	-0.41260500
C	-2.39502200	2.07794700	-1.36037000
H	-3.14497000	1.88571100	-2.12425600
C	-0.68694700	2.98987000	0.25890200
H	-0.41001800	2.66098800	1.27850700
H	0.26080200	3.06592300	-0.32191300
N	-1.35496300	4.28155900	0.33020100
H	-1.34121900	4.75072900	1.23954800
C	-2.14448700	4.80786800	-0.63889700
O	-2.38675900	4.21535500	-1.72075500
C	-2.75269500	6.15304700	-0.37004000
C	-3.91658900	6.50654800	-1.08604200
C	-2.18861500	7.07898100	0.53464200
C	-4.52239100	7.75298900	-0.88027900
H	-4.33627400	5.78433400	-1.80183000
C	-2.79426200	8.32856100	0.73346500
H	-1.25611000	6.84258700	1.07088700
C	-3.96360200	8.66593100	0.03123200
H	-5.43598200	8.01613300	-1.43546800
H	-2.34389100	9.04719200	1.43528800
H	-4.43719500	9.64729300	0.18968100
H	-1.56515800	-1.88958200	2.72123200
I	2.80842300	0.21064300	1.00191600
C	4.79824700	0.28601500	0.17626000
C	5.32802400	-0.80223600	-0.53152600
C	5.59604700	1.42916600	0.32814700
C	6.61942900	-0.75835000	-1.08247100
C	6.89038600	1.49559600	-0.21370500
C	7.40269500	0.39555100	-0.91996900
F	5.14209700	2.50141600	0.99671700
F	7.63951100	2.59597300	-0.06056500
F	8.63444900	0.44700000	-1.43867500
F	7.11062500	-1.80646000	-1.75762200
F	4.61191500	-1.92594000	-0.70895200

Table S25. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM2b** activated by C_6F_5I.

G= -3172.1389 Hartree

P	-2.42941400	-2.23820300	-0.09385000
C	-0.84000600	-3.09603300	-0.44475300
Au	-2.28273600	0.09065800	-0.35608200
C	-0.45099400	-4.26561300	0.24162500
H	-1.09753100	-4.68989800	1.02499200
C	0.77216900	-4.88388500	-0.06495000
H	1.07407500	-5.79225300	0.47937700
C	1.61153900	-4.34096300	-1.05164100
H	2.57801500	-4.81760200	-1.27718100
C	1.22694800	-3.17595800	-1.73676000
H	1.89043800	-2.73778000	-2.49767900
C	0.00741100	-2.55221200	-1.43415700
H	-0.28607700	-1.62630300	-1.95526200
C	-3.68577700	-3.02766600	-1.18531700
C	-4.86634200	-2.30499300	-1.46576400
H	-4.99910500	-1.29323100	-1.04880500
C	-5.86278600	-2.86896900	-2.27702000
H	-6.78057100	-2.29929700	-2.49020000
C	-5.68383000	-4.15135800	-2.82360300
H	-6.46245700	-4.59003200	-3.46683900
C	-4.50701900	-4.86980700	-2.55470700
H	-4.36074000	-5.87248500	-2.98557800
C	-3.50937400	-4.31362200	-1.73719100
H	-2.58974900	-4.88340200	-1.53407200
C	-2.87899300	-2.72869600	1.62534500
C	-3.91169900	-3.64709400	1.90430400
H	-4.48048800	-4.11030200	1.08376200
C	-4.21984800	-3.97364800	3.23612700
H	-5.02882700	-4.69051000	3.44677500
C	-3.50106000	-3.38942200	4.29136600
H	-3.74552100	-3.64597100	5.33402100
C	-2.47163400	-2.47305400	4.01349600
H	-1.90571000	-2.00722500	4.83541700
C	-2.15959200	-2.13475400	2.68797600
Cl	0.41760700	0.61552800	2.39428500
C	-2.08939100	2.13176800	-0.53350900
C	-3.10717400	2.94281100	-0.86251200
H	-4.14295300	2.68525400	-1.11570900
C	-0.74492300	2.74795400	-0.23637000
H	-0.31205400	2.33200400	0.70373500
H	-0.01301600	2.52311000	-1.04507800
N	-0.85207500	4.21451100	-0.09211800

H	-0.05531400	4.70345800	0.33338100
C	-1.88451600	4.94250500	-0.46557100
O	-2.97758500	4.37535500	-0.92910100
C	-1.90348600	6.41106600	-0.38058300
C	-3.14495500	7.08796100	-0.43220000
C	-0.70545600	7.15274300	-0.25586500
C	-3.18276000	8.48438000	-0.34601000
H	-4.07546900	6.51158200	-0.52862900
C	-0.75372400	8.54872200	-0.17052700
H	0.27330300	6.64868300	-0.25297100
C	-1.99016600	9.21633400	-0.21313100
H	-4.15110000	9.00569900	-0.37989000
H	0.18205000	9.12047200	-0.08007800
H	-2.02331600	10.31466400	-0.14689500
H	-1.35335300	-1.40432200	2.48936000
I	2.95538200	0.12712400	1.13678400
C	4.89471600	-0.21533400	0.18325100
C	5.15568200	-1.39699200	-0.52188400
C	5.91561600	0.74068300	0.26135900
C	6.39729700	-1.63115100	-1.13568300
C	7.16700500	0.53317300	-0.34246900
C	7.40656700	-0.65953800	-1.04351700
F	5.72779200	1.89764400	0.92198100
F	8.13318500	1.46016300	-0.25833900
F	8.59458900	-0.86926100	-1.62409100
F	6.62838200	-2.76906900	-1.80769400
F	4.21570200	-2.35450700	-0.63601900

Table S26. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS2b′** activated by C_6F_5I.

G= -3172.1298 Hartree Frequency = -126.83

P	0.50837000	3.05998500	0.14486100
C	-1.14822700	3.18417600	-0.64309400
Au	1.93869400	1.70785000	-1.08269600
C	-2.27743100	2.55370000	-0.08276300
H	-2.19761600	2.01116700	0.87062300
C	-3.51270700	2.60666100	-0.75108100
H	-4.38621200	2.10221900	-0.31121100
C	-3.62731400	3.28827300	-1.97266500
H	-4.59703900	3.32919000	-2.49241400
C	-2.50009100	3.91208000	-2.53670400
H	-2.58383800	4.44282800	-3.49765800

C	-1.26141900	3.85470200	-1.88226900
H	-0.38039700	4.33564500	-2.33636400
C	1.12878000	4.77485700	0.35783800
C	2.52223000	4.96782300	0.47877000
H	3.20393100	4.10510400	0.40176300
C	3.03682300	6.25519000	0.69285300
H	4.12425400	6.39957500	0.78526100
C	2.16737400	7.35583000	0.78050400
H	2.57320400	8.36651800	0.94194200
C	0.78105500	7.16744800	0.65567300
H	0.09753900	8.02807200	0.72071400
C	0.25745300	5.88131900	0.44579700
H	-0.82994000	5.74378500	0.34596500
C	0.24639000	2.37486700	1.83038100
C	-0.24925800	3.17499700	2.88307200
H	-0.47002700	4.24128800	2.72073900
C	-0.45694700	2.60778800	4.14991000
H	-0.84004000	3.23568500	4.96923100
C	-0.17677100	1.24806500	4.37498600
H	-0.34163600	0.81092400	5.37211500
C	0.31638400	0.44959300	3.33061400
H	0.54158900	-0.61855300	3.47996300
C	0.53213500	1.01333100	2.06344700
Cl	1.10861200	-3.09768800	1.91104400
C	2.84263800	-0.64005300	-1.95521300
C	3.32663200	0.51573100	-2.16093500
H	4.21691300	0.97403200	-2.60798000
C	1.93408600	-1.73460800	-1.59073100
H	1.07452400	-1.33023300	-1.01787300
H	1.51872800	-2.17513300	-2.52751200
N	2.61706000	-2.73035500	-0.79216600
H	2.18048700	-3.00459400	0.12591900
C	3.88793500	-2.98692300	-1.17764300
O	4.36332200	-2.34174500	-2.14785600
C	4.68485000	-4.02488300	-0.45683600
C	6.01690400	-4.23750800	-0.87376100
C	4.15652800	-4.79258500	0.60540400
C	6.81118500	-5.20271100	-0.24125200
H	6.41236000	-3.63042600	-1.70158500
C	4.95831600	-5.75419400	1.23762700
H	3.12302500	-4.63698300	0.95710800
C	6.28279000	-5.96344800	0.81629400
H	7.84870400	-5.36282800	-0.57313300
H	4.54257300	-6.34657400	2.06729900

H	6.90584800	-6.72240700	1.31486700
H	0.93133800	0.38590700	1.25055400
C	-3.62830300	-2.32551700	0.17319400
C	-4.29088700	-1.12969100	0.48091200
C	-5.58738600	-0.86741100	0.01036400
C	-6.24084500	-1.81861600	-0.78904400
C	-5.59704800	-3.02652300	-1.10256600
C	-4.29794500	-3.26490000	-0.62287200
I	-1.62120800	-2.69711500	0.90223200
F	-3.70095400	-0.18819700	1.24029100
F	-6.19963100	0.29193600	0.30232400
F	-6.22389200	-3.93584700	-1.86150100
F	-3.71492600	-4.42911800	-0.95171400
F	-7.47465100	-1.57777800	-1.24557600

Table S27. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM2b′** activated by C_6F_5I.

G= -3172.1563 Hartree

P	3.02952200	-1.34179400	-0.00444300
C	3.24754800	0.00364300	-1.24699600
Au	0.92033700	-2.37049400	-0.16797000
C	3.58189700	1.32448600	-0.88724100
H	3.74576400	1.58936200	0.16749000
C	3.68913100	2.31730600	-1.87695300
H	3.92872600	3.35077300	-1.58241500
C	3.47574500	1.99655500	-3.22684300
H	3.55962300	2.77657700	-3.99943900
C	3.14523500	0.67857600	-3.58955300
H	2.97155500	0.42259400	-4.64625300
C	3.02091300	-0.31302800	-2.60562500
H	2.74409200	-1.34005200	-2.89419200
C	4.44374000	-2.48799600	-0.26875000
C	4.29282700	-3.83659300	0.12082700
H	3.33500600	-4.17891300	0.54557800
C	5.35612000	-4.73867600	-0.03880200
H	5.23097000	-5.78923800	0.26581000
C	6.57127800	-4.30376100	-0.59444000
H	7.40224700	-5.01416400	-0.72586400
C	6.72349100	-2.96361000	-0.98840800
H	7.67345500	-2.62072800	-1.42696000
C	5.66541300	-2.05467000	-0.82661400

H	5.79169800	-1.00675600	-1.13935300
C	3.31393200	-0.55264600	1.63448800
C	4.53673700	-0.65710000	2.32868200
H	5.37201700	-1.23156600	1.90042800
C	4.69058600	-0.02726000	3.57500500
H	5.64608900	-0.11732300	4.11470200
C	3.63509100	0.71581400	4.12875000
H	3.76217600	1.21129300	5.10383200
C	2.41603400	0.82434300	3.43799000
H	1.58650700	1.41186400	3.85968200
C	2.24982100	0.18258400	2.20168900
Cl	-5.48516900	1.29163200	0.75024500
C	-2.08698100	-2.61744400	-0.16113700
C	-0.91935800	-3.25415300	-0.32828300
H	-1.00057400	-4.32963000	-0.57653200
C	-2.45264200	-1.18477800	0.17340400
H	-2.07715600	-0.85928800	1.16723900
H	-2.08213700	-0.45476700	-0.57757400
N	-3.91317400	-1.23232200	0.16757700
H	-4.52184500	-0.36693600	0.38259200
C	-4.33624900	-2.44590300	-0.10977200
O	-3.34682900	-3.31097000	-0.30879800
C	-5.71782200	-2.90841100	-0.21579100
C	-5.96960900	-4.28219800	-0.44499200
C	-6.79574000	-1.99863600	-0.09414700
C	-7.28834000	-4.73909200	-0.54653500
H	-5.12825900	-4.98349900	-0.53900800
C	-8.10948700	-2.46977100	-0.19849800
H	-6.60596700	-0.92510900	0.07844300
C	-8.35831900	-3.83545200	-0.42314400
H	-7.48373900	-5.80755800	-0.72292500
H	-8.94779300	-1.76300400	-0.10499600
H	-9.39473000	-4.19827200	-0.50387300
H	1.28955000	0.26386200	1.66831800
C	-1.07877400	3.80452800	0.11230000
C	0.03224900	3.40747200	0.86882600
C	1.29626600	3.98595700	0.67384600
C	1.45492100	4.98678400	-0.29748100
C	0.35353200	5.40520600	-1.06068700
C	-0.90214800	4.81168400	-0.84622100
I	-2.98549100	2.82143200	0.37527400
F	-0.08197500	2.44140400	1.80000900
F	2.35688900	3.58337200	1.39135800
F	0.50922900	6.36090100	-1.98634100

F	-1.93034900	5.23249400	-1.59927200
F	2.66140100	5.53007800	-0.50555200

Table S28. Calculated Gibbs energy and XYZ coordinates for all atoms in **COM1c** activated by $C_8H_9O_2I$.

G= -2904.9886 Hartree

P	3.37070200	-1.37890400	0.05130400
C	2.78171700	-2.94908800	0.80566200
Au	1.66437500	-0.10527200	-0.74659600
C	3.51142200	-4.15044300	0.68931100
H	4.45102600	-4.17773100	0.11673400
C	3.03336700	-5.32065600	1.30189000
H	3.60395600	-6.25721400	1.20462900
C	1.83313600	-5.29782800	2.03090500
H	1.46004700	-6.21808900	2.50655700
C	1.10370900	-4.10183900	2.14624100
H	0.15868800	-4.08130900	2.71051400
C	1.57108900	-2.93014900	1.53260900
H	0.99172200	-1.99565500	1.61113000
C	4.34041200	-0.51280900	1.35168500
C	4.59452900	0.86660800	1.18649200
H	4.19575800	1.39727200	0.30669700
C	5.34235100	1.56229600	2.14780000
H	5.53509000	2.63789700	2.01439400
C	5.83061400	0.89145400	3.28258600
H	6.40917700	1.44150100	4.04088300
C	5.57284300	-0.47863700	3.45311100
H	5.94965700	-1.00612700	4.34303200
C	4.83044600	-1.18430200	2.49113900
H	4.63042500	-2.25717100	2.63397400
C	4.57309600	-1.85569200	-1.25522200
C	5.96113000	-1.90091400	-1.01043800
H	6.36102900	-1.62693100	-0.02232400
C	6.83917600	-2.29186900	-2.03502300
H	7.92240900	-2.32160400	-1.84035800
C	6.33941000	-2.63952700	-3.30053800
H	7.03113700	-2.94232300	-4.10185900
C	4.95614300	-2.59303700	-3.54675300
H	4.56097500	-2.85795200	-4.53956200
C	4.07342400	-2.19782700	-2.53095900
Cl	-0.10675000	1.21983000	-1.59570200
C	0.21826600	1.60439800	2.67402400

C	1.17702300	0.96733000	3.09225800
H	2.02864600	0.41605900	3.47440400
C	-0.93539200	2.35678000	2.16345600
H	-1.71728000	1.64278600	1.82212900
H	-1.37059300	2.96613600	2.98365500
N	-0.60720800	3.27575500	1.08598700
H	-0.40397900	2.86015500	0.16738400
C	-0.56130000	4.62605500	1.29985600
O	-0.81177900	5.12528900	2.40682800
C	-0.20213800	5.49898200	0.11859300
C	-0.21593000	6.89332100	0.33788000
C	0.14489200	5.01366600	-1.16122800
C	0.10534500	7.78516400	-0.69398800
H	-0.48628200	7.25338500	1.34177300
C	0.46701000	5.90782900	-2.19445000
H	0.17026100	3.93357400	-1.37692800
C	0.44830600	7.29380800	-1.96555500
H	0.08860800	8.87025000	-0.50658400
H	0.73518300	5.51503700	-3.18756300
H	0.70138500	7.99130900	-2.77937700
H	2.99025900	-2.14715500	-2.72864900
C	-5.13820400	-0.86151100	-0.31431100
C	-5.62755400	-0.69227400	0.98714700
C	-6.91071200	-1.19937500	1.29524800
C	-7.68076900	-1.86124400	0.31411000
C	-7.15461300	-2.01357800	-0.98728400
C	-5.87337000	-1.51273400	-1.31310600
H	-5.49139700	-1.64570600	-2.33435300
H	-5.05293800	-0.18102800	1.77138400
H	-8.67506700	-2.25112700	0.55924700
O	-7.32704600	-1.00251900	2.57343000
O	-7.81640500	-2.63395800	-1.99879300
C	-8.60896300	-1.47966600	2.96264900
H	-8.72926400	-1.20899300	4.02862100
H	-9.42489400	-1.00184100	2.37671800
H	-8.68889100	-2.58461900	2.86127900
C	-9.11248200	-3.16431400	-1.75079800
H	-9.83455300	-2.37255200	-1.45242700
H	-9.44993300	-3.61498900	-2.70318600
H	-9.09487900	-3.95317300	-0.96654900
I	-3.20111600	-0.09943700	-0.79397400

Table S29. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS1c**

activated by $C_8H_9O_2I$.

G= -2904.9701 Hartree Frequency = -59.48

P	-3.44899200	-1.27892500	0.04118700
C	-2.90402100	-3.03582600	0.09626200
Au	-1.66488200	0.14472200	-0.32062700
C	-3.53016000	-3.98962000	0.92596700
H	-4.36278400	-3.69420800	1.58234500
C	-3.08692900	-5.32233500	0.91935100
H	-3.57651800	-6.06122200	1.57254400
C	-2.02326700	-5.71066800	0.08802400
H	-1.67639200	-6.75563600	0.08897000
C	-1.39553600	-4.76218800	-0.73743400
H	-0.55518600	-5.05926500	-1.38359400
C	-1.82879600	-3.42776700	-0.73090000
H	-1.32445700	-2.67872800	-1.36317900
C	-4.75930700	-1.20093600	-1.25123100
C	-5.21176800	0.07532900	-1.65616900
H	-4.77949800	0.98246500	-1.20295300
C	-6.20884500	0.19120300	-2.63601200
H	-6.55806600	1.18925700	-2.94297000
C	-6.75254700	-0.96192700	-3.22917400
H	-7.52952200	-0.86913100	-4.00381400
C	-6.29833800	-2.23111000	-2.83651900
H	-6.71859400	-3.13684800	-3.30064100
C	-5.30587600	-2.35516900	-1.84921600
H	-4.95860100	-3.35475200	-1.54697900
C	-4.32089100	-0.96559600	1.63273300
C	-5.71008700	-1.16944000	1.77596500
H	-6.31418300	-1.50176100	0.91793400
C	-6.32707300	-0.94388300	3.01741700
H	-7.41171700	-1.10181600	3.12233900
C	-5.56595700	-0.51779500	4.11842900
H	-6.05385400	-0.33923200	5.08928000
C	-4.18306200	-0.31065900	3.97725800
H	-3.58372900	0.03167500	4.83502100
C	-3.56058000	-0.52700800	2.73854000
Cl	0.14757000	1.06886500	1.17657400
C	-0.60727500	1.53779400	-2.39521700
C	-1.64314500	0.86685100	-2.54641000
H	-2.51805200	0.45156900	-3.04638400
C	0.62391700	2.32174500	-2.24492000
H	1.48710700	1.62644700	-2.14133600
H	0.78760700	2.92075000	-3.16807500

N	0.58432200	3.25459100	-1.13585000
H	0.53782800	2.82876600	-0.19658800
C	0.57929300	4.60603900	-1.33927500
O	0.65608800	5.10713700	-2.47095400
C	0.49028400	5.47157100	-0.10415600
C	0.68012000	6.85834800	-0.28342000
C	0.21092600	4.98007800	1.19018200
C	0.60548900	7.73757500	0.80519700
H	0.88669700	7.22385000	-1.30051900
C	0.13328900	5.86260900	2.27911500
H	0.04508000	3.90539000	1.36969700
C	0.33166000	7.24085800	2.09143500
H	0.76063000	8.81689500	0.65093900
H	-0.08664600	5.46784400	3.28323100
H	0.27100800	7.92903400	2.94913000
H	-2.47974700	-0.34345600	2.62393700
C	5.13952500	-0.97089800	0.22360200
C	5.69603500	-0.88060800	-1.05900100
C	6.99160200	-1.40461300	-1.27198400
C	7.71019600	-2.00653400	-0.21578300
C	7.11843200	-2.08004200	1.06423700
C	5.82382500	-1.56133200	1.29409500
H	5.39117100	-1.63370600	2.30129200
H	5.16332500	-0.41738000	-1.90073500
H	8.71479800	-2.41041100	-0.38537800
O	7.47195600	-1.28422500	-2.53769900
O	7.72719300	-2.63764200	2.14383700
C	8.77055000	-1.78292700	-2.83241900
H	8.94508700	-1.57739400	-3.90543900
H	9.55715400	-1.27005100	-2.23590200
H	8.84310000	-2.87967400	-2.66027100
C	9.03132700	-3.18355200	1.99336800
H	9.77025500	-2.41370300	1.67925900
H	9.32141000	-3.57163100	2.98805000
H	9.04862500	-4.02186300	1.26212400
I	3.17921400	-0.18210600	0.56370700

Table S30. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM1c** activated by $C_8H_9O_2I$.

G= -2904.9765Hartree

P	-3.38541000	-1.09275200	0.11476200

C	-2.64665200	-2.54663500	0.96495600
Au	-1.74814500	0.27856000	-0.96049700
C	-3.16057300	-3.04811800	2.17891800
H	-4.02165500	-2.56026600	2.66063900
C	-2.56881800	-4.17130400	2.77972000
H	-2.97183200	-4.55543700	3.72963600
C	-1.46712500	-4.79906300	2.17539500
H	-1.00303200	-5.67645400	2.65204900
C	-0.95149200	-4.30064600	0.96678400
H	-0.08241900	-4.78337000	0.49388900
C	-1.53440100	-3.17579100	0.36427900
H	-1.11903200	-2.77745400	-0.57558900
C	-4.62502900	-1.78372200	-1.06090400
C	-5.20020100	-0.90929600	-2.01020500
H	-4.89998100	0.15097300	-2.03469600
C	-6.15354800	-1.38647000	-2.92166900
H	-6.59997700	-0.69690900	-3.65483200
C	-6.52956400	-2.74126600	-2.90499600
H	-7.27098800	-3.11682400	-3.62718500
C	-5.95378700	-3.61506800	-1.96904900
H	-6.24268000	-4.67744100	-1.95324200
C	-5.00653000	-3.14095000	-1.04553600
H	-4.56414100	-3.83326800	-0.31344200
C	-4.37254400	-0.21036700	1.39522300
C	-5.76590700	-0.39114800	1.52286300
H	-6.30344400	-1.06833400	0.84197600
C	-6.47380700	0.29723000	2.52213100
H	-7.56143100	0.15261200	2.61509500
C	-5.79926700	1.16412200	3.39721800
H	-6.35761600	1.70354600	4.17810800
C	-4.41102200	1.34487500	3.27187600
H	-3.87796800	2.02576800	3.95355600
C	-3.69606500	0.66566500	2.27369200
Cl	-0.19205900	0.70758200	1.05231200
C	-0.75200200	1.38635100	-2.54791100
C	-1.78283900	0.81211900	-3.02239700
H	-2.50961300	0.53279300	-3.78883900
C	0.50516700	2.16637500	-2.47704900
H	1.35872600	1.45694000	-2.57430000
H	0.55813400	2.87431900	-3.33162900
N	0.62421400	2.95243000	-1.26513300
H	0.55148700	2.43761800	-0.37376400
C	0.77661400	4.31085900	-1.31302500
O	0.87159600	4.92812400	-2.38455600

C	0.84046200	5.03408700	0.01185500
C	1.19362300	6.40002000	-0.02656500
C	0.55109000	4.43595000	1.25814900
C	1.26864200	7.15339300	1.15256500
H	1.40585600	6.85127100	-1.00739300
C	0.62377000	5.19334900	2.43799800
H	0.25675900	3.37574800	1.32883700
C	0.98391700	6.55057900	2.39021200
H	1.54976400	8.21721500	1.10743400
H	0.39393600	4.71639900	3.40354200
H	1.04048500	7.13984800	3.31890500
H	-2.60734900	0.81315000	2.17421900
C	4.90312500	-1.05184600	0.19577800
C	5.46158200	-0.95536500	-1.08557600
C	6.79082800	-1.39588000	-1.27880100
C	7.54092000	-1.92223800	-0.20436700
C	6.94655200	-2.00443600	1.07394200
C	5.61822600	-1.56915700	1.28392700
H	5.18488800	-1.64524100	2.29059200
H	4.90521200	-0.54875300	-1.94120400
H	8.57126200	-2.26188900	-0.35924700
O	7.27084800	-1.27374400	-2.54450600
O	7.58435600	-2.49270400	2.17028300
C	8.60209800	-1.69014300	-2.82037200
H	8.77060100	-1.49573400	-3.89643000
H	9.34832400	-1.11358200	-2.23014400
H	8.74664900	-2.77577700	-2.62477100
C	8.92869100	-2.93778900	2.04296700
H	9.60712300	-2.11921600	1.71554300
H	9.23904800	-3.27810800	3.04896000
H	9.01890500	-3.78900600	1.33240600
I	2.89333800	-0.38281200	0.50573300

Table S31. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS2c** activated by $C_8H_9O_2I$.

G= -2904.9469 Hartree Frequency = -266.29

P	-2.69472500	-2.07063200	-0.15971300
C	-1.41577200	-3.32680800	-0.58121800
Au	-1.81133600	0.10202000	-0.08172000
C	-1.42527100	-4.62585700	-0.03190500
H	-2.20459100	-4.91780100	0.68857400
C	-0.43319200	-5.54990000	-0.39956300
H	-0.44357500	-6.56126500	0.03571000

C	0.56961300	-5.18535500	-1.31308000
H	1.34903100	-5.91051200	-1.59428000
C	0.58442000	-3.89031300	-1.85876200
H	1.37558100	-3.59569600	-2.56534200
C	-0.40105100	-2.96148500	-1.49232500
H	-0.37914400	-1.93966200	-1.90499200
C	-4.03264300	-2.29459800	-1.41024100
C	-4.96858400	-1.25027100	-1.57592400
H	-4.86692400	-0.32700800	-0.98213200
C	-6.01835500	-1.38217300	-2.49704400
H	-6.74505100	-0.56374100	-2.61751100
C	-6.13412900	-2.54981600	-3.27147000
H	-6.95206300	-2.64827000	-4.00208500
C	-5.20007400	-3.58697900	-3.11702700
H	-5.28305300	-4.50133900	-3.72491300
C	-4.15331700	-3.46521200	-2.18745700
H	-3.42785800	-4.28494200	-2.07319000
C	-3.43008300	-2.63556000	1.43464700
C	-4.65620800	-3.33051700	1.49224000
H	-5.21585600	-3.54780500	0.56982800
C	-5.16922800	-3.74791200	2.73194400
H	-6.12769800	-4.28878000	2.76933100
C	-4.46427400	-3.47687600	3.91583200
H	-4.86930700	-3.80425800	4.88612200
C	-3.24332600	-2.78237400	3.85972700
H	-2.68935900	-2.56262100	4.78585400
C	-2.72489900	-2.35572700	2.62733500
Cl	0.07162200	-0.10034500	1.93267400
C	-1.32995700	2.12954500	-0.37384800
C	-2.23088500	2.49611000	-1.20244200
H	-3.08794500	2.50219600	-1.87224100
C	-0.20473300	2.91117400	0.23660600
H	0.09273300	2.46494800	1.20526400
H	0.67671800	2.82210100	-0.43929600
N	-0.56553400	4.30837600	0.43383500
H	-0.33657100	4.71098000	1.34607100
C	-1.32936700	5.04965300	-0.40479100
O	-1.83222800	4.59086400	-1.46270500
C	-1.57926400	6.47804200	-0.01857000
C	-2.72179200	7.11648800	-0.54697300
C	-0.70104300	7.20698300	0.81336400
C	-2.99765200	8.45200000	-0.22550000
H	-3.38817800	6.54458400	-1.20955600
C	-0.97702300	8.54597000	1.12753100

H	0.21988000	6.74179900	1.19942300
C	-2.12693000	9.16898200	0.61380600
H	-3.89687200	8.93891700	-0.63344400
H	-0.28329800	9.10908300	1.77058900
H	-2.34113600	10.22006500	0.86236200
H	-1.77207300	-1.79673300	2.58923400
C	5.09829900	-0.39278500	0.20769100
C	5.45093200	0.25029600	-0.98712600
C	6.79331400	0.18582800	-1.42438500
C	7.76512100	-0.51173200	-0.67371900
C	7.37823400	-1.14904600	0.52572100
C	6.03930000	-1.09373000	0.97466600
H	5.77137400	-1.60108100	1.91205300
H	4.71966700	0.80165200	-1.59474900
H	8.80501100	-0.55668500	-1.01678400
O	7.06437000	0.83091000	-2.59087400
O	8.23683600	-1.84421700	1.31905100
C	8.39119300	0.80435900	-3.09966400
H	8.37358900	1.38340000	-4.04237700
H	9.11460100	1.27970200	-2.40073400
H	8.73071700	-0.23167400	-3.32151800
C	9.60100600	-1.94560900	0.93352400
H	10.09262400	-0.94905600	0.87712200
H	10.10109500	-2.54598700	1.71696200
H	9.71956400	-2.46245600	-0.04455300
I	3.05773300	-0.29856900	0.88398200

Table S32. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM2c** activated by $C_8H_9O_2I$.

G= -2904.9680Hartree

P	-2.75841500	-1.96939300	-0.16152400
C	-1.36778600	-3.08503500	-0.62193900
Au	-2.18648300	0.30503600	-0.26612900
C	-1.18642800	-4.35192900	-0.03197300
H	-1.87908200	-4.70170900	0.74869600
C	-0.11526400	-5.16772600	-0.43209800
H	0.02331700	-6.15351800	0.03855500
C	0.77871700	-4.72245200	-1.42172300
H	1.62155300	-5.36169100	-1.72745400
C	0.60391600	-3.45918800	-2.00897600
H	1.30949000	-3.10390300	-2.77578800
C	-0.46169000	-2.63904700	-1.61081900

H	-0.59007800	-1.63998300	-2.05859500
C	-4.13775400	-2.40571100	-1.30804800
C	-5.16579400	-1.45781200	-1.50044700
H	-5.11147100	-0.48238700	-0.98991800
C	-6.24874800	-1.75203600	-2.34386600
H	-7.04722300	-1.00424900	-2.48660800
C	-6.30698500	-2.98452200	-3.01113700
H	-7.15263600	-3.21150800	-3.68208400
C	-5.28090100	-3.92980100	-2.83055900
H	-5.31945000	-4.89366800	-3.35892000
C	-4.19875400	-3.64399000	-1.98046800
H	-3.39933300	-4.38858300	-1.84607500
C	-3.31329900	-2.53807000	1.50227700
C	-4.47799900	-3.31484600	1.68371800
H	-5.09666600	-3.60416600	0.82069000
C	-4.85495200	-3.71977000	2.97582400
H	-5.76668200	-4.32199100	3.11302700
C	-4.07691500	-3.35727000	4.08493000
H	-4.37586300	-3.67829700	5.09676300
C	-2.91774100	-2.58508900	3.90444700
H	-2.30334500	-2.29385900	4.77099900
C	-2.53361600	-2.16691900	2.61949200
Cl	0.18007400	0.18257000	2.16147400
C	-1.71670400	2.30689300	-0.41862600
C	-2.61571600	3.26034900	-0.71310000
H	-3.67837100	3.15870900	-0.96247900
C	-0.30179700	2.73177100	-0.11515600
H	0.07565200	2.19130700	0.78615900
H	0.38528400	2.47676400	-0.95489700
N	-0.22618500	4.18462900	0.13869100
H	0.60785800	4.53698000	0.62210900
C	-1.14761400	5.06092500	-0.20703500
O	-2.29030800	4.66500600	-0.72490100
C	-0.98430100	6.51209000	-0.02056000
C	-2.12782700	7.34356100	-0.07256100
C	0.29038900	7.08634400	0.19783200
C	-1.99532100	8.72567800	0.10737500
H	-3.11753600	6.89650000	-0.24170900
C	0.41213700	8.46927300	0.37778900
H	1.19769200	6.46275100	0.21009500
C	-0.72826200	9.29026800	0.33283200
H	-2.88859500	9.36735000	0.07253600
H	1.40633700	8.91091700	0.54255200
H	-0.62714400	10.37775000	0.47112300

H	-1.62514200	-1.54714300	2.49197800
C	4.97019700	-0.65078100	0.24109700
C	5.30340700	-0.15565600	-1.03030800
C	6.61204600	-0.35394600	-1.52367100
C	7.57898700	-1.03974200	-0.75201800
C	7.21583700	-1.52761400	0.52584900
C	5.90921900	-1.33495400	1.02568500
H	5.66164600	-1.72428400	2.02458600
H	4.57479200	0.38018000	-1.65712300
H	8.59148400	-1.18895800	-1.13711200
O	6.86237800	0.15463000	-2.76069100
O	8.06873100	-2.19571000	1.34558000
C	8.15935100	0.00094200	-3.31691400
H	8.13287100	0.48497200	-4.31173300
H	8.94009800	0.49571700	-2.70016500
H	8.43194000	-1.07293800	-3.44685200
C	9.40416800	-2.42488700	0.90913600
H	9.95063900	-1.47245600	0.72829100
H	9.90541400	-2.97469800	1.72790100
H	9.44146900	-3.04425600	-0.01433900
I	2.96920500	-0.33841400	1.01206300

Table S33. Calculated Gibbs energy and XYZ coordinates for all atoms in **TS2c′** activated by $C_8H_9O_2I$.

G= -2904.9624 Hartree Frequency = -127.44

P	0.63919800	2.95552500	0.15223100
C	-1.02449900	3.10366100	-0.61565900
Au	2.03823800	1.59201600	-1.09566100
C	-2.18750900	2.63578400	0.02797500
H	-2.12674300	2.20257300	1.03776200
C	-3.42951500	2.71223200	-0.62618700
H	-4.33133500	2.32328000	-0.12761700
C	-3.51546900	3.26163000	-1.91506700
H	-4.48924700	3.31830500	-2.42582900
C	-2.35623100	3.73049100	-2.55882800
H	-2.41930000	4.15709400	-3.57184100
C	-1.11203200	3.64434600	-1.91871000
H	-0.20475200	3.99856900	-2.43427300
C	1.27628900	4.66545400	0.35928000
C	2.67023200	4.84774000	0.49029500
H	3.34555600	3.97882800	0.42852800
C	3.19371400	6.13307100	0.69462100
H	4.28150800	6.26942200	0.79488400
C	2.33287700	7.24203100	0.76232400

H	2.74596900	8.25101200	0.91589600
C	0.94619300	7.06397500	0.62739700
H	0.26958300	7.93111600	0.67656200
C	0.41369100	5.77985000	0.42708300
H	-0.67384300	5.64948900	0.31859900
C	0.39723400	2.27434900	1.84128800
C	-0.00426400	3.09447800	2.91819500
H	-0.16157600	4.17396700	2.76970600
C	-0.19870300	2.52955900	4.18847300
H	-0.50841900	3.17266000	5.02685300
C	0.00335900	1.15284600	4.39254500
H	-0.14889500	0.71775700	5.39261600
C	0.40515900	0.33480400	3.32406100
H	0.57438400	-0.74635100	3.45437300
C	0.60625700	0.89525300	2.05330500
Cl	1.11662400	-3.13256200	1.82266000
C	2.90614900	-0.76321500	-1.99422300
C	3.40814200	0.38811600	-2.18321500
H	4.31101900	0.83456300	-2.61684600
C	1.98140700	-1.84893400	-1.64592300
H	1.11645300	-1.43788500	-1.08560600
H	1.57710500	-2.28431500	-2.58996000
N	2.64105300	-2.85050300	-0.83581500
H	2.18314400	-3.10426700	0.08547200
C	3.91587400	-3.11447000	-1.19911400
O	4.41140200	-2.47955200	-2.16728100
C	4.69669300	-4.15098000	-0.45791700
C	6.01185600	-4.42098500	-0.89461900
C	4.16994200	-4.85822000	0.64633900
C	6.79018600	-5.38653000	-0.24288400
H	6.40691900	-3.85819600	-1.75338600
C	4.95666700	-5.81952400	1.29802600
H	3.15155600	-4.65062900	1.01753400
C	6.26329800	-6.08850200	0.85529100
H	7.81412100	-5.59267000	-0.59129300
H	4.54323100	-6.36391400	2.16115800
H	6.87394100	-6.84724000	1.36941100
H	0.93745800	0.24920700	1.22460200
C	-3.84235000	-2.27871200	0.25443300
C	-4.37938400	-1.01119200	0.52245000
C	-5.70002700	-0.72800900	0.11050500
C	-6.47420900	-1.70321100	-0.55483600
C	-5.90825500	-2.97287200	-0.80657100
C	-4.58543900	-3.26752600	-0.40490500

H	-4.17515900	-4.26463800	-0.61886800
H	-3.80351000	-0.23532000	1.04586200
H	-7.49902500	-1.47916500	-0.87164600
O	-6.15322500	0.52680600	0.39508800
O	-6.57094300	-3.97901000	-1.43805600
C	-7.48105300	0.87845400	0.02557100
H	-7.62939700	1.92304200	0.35843900
H	-7.63422500	0.82693200	-1.07510300
H	-8.23409600	0.23134400	0.52674900
C	-7.90724900	-3.75922100	-1.86947200
H	-7.97336700	-2.93619200	-2.61539500
H	-8.23799400	-4.70073800	-2.34746100
H	-8.58675600	-3.53094600	-1.01849700
I	-1.81707800	-2.69422400	0.87494100

Table S34. Calculated Gibbs energy and XYZ coordinates for all atoms in **IM2c′** activated by $C_8H_9O_2I$.

G= -2904.9867 Hartree

P	-3.59049100	-0.52355200	0.03256200
C	-2.73211400	-1.79808600	-0.98539700
Au	-2.55200000	1.56494000	-0.26304900
C	-1.87611400	-2.75518600	-0.40363600
H	-1.77293600	-2.81585000	0.69046900
C	-1.13802200	-3.62976600	-1.21979100
H	-0.45161100	-4.35438300	-0.75403300
C	-1.25952600	-3.56341400	-2.61681300
H	-0.67982100	-4.24893800	-3.25430600
C	-2.11452700	-2.61230900	-3.20122800
H	-2.21029300	-2.55251300	-4.29653500
C	-2.83944800	-1.72437800	-2.39306300
H	-3.49153500	-0.96936700	-2.86062700
C	-5.36600900	-0.58849100	-0.44669900
C	-6.14310200	0.57262500	-0.24150800
H	-5.66930600	1.48325100	0.15992200
C	-7.51139000	0.56967300	-0.55315700
H	-8.10979000	1.47940400	-0.39064100
C	-8.11132800	-0.58674100	-1.07961800
H	-9.18355900	-0.58616900	-1.33003400
C	-7.34052600	-1.74183600	-1.29280900
H	-7.80661200	-2.64830400	-1.70928500
C	-5.97191200	-1.74755200	-0.97767200
H	-5.37562500	-2.65612800	-1.15259200

C	-3.51283100	-1.13583500	1.76857900
C	-4.37418700	-2.14668900	2.24622400
H	-5.13887300	-2.58447300	1.58646500
C	-4.26249200	-2.59430400	3.57169300
H	-4.93987300	-3.38049300	3.93969700
C	-3.29343000	-2.04117100	4.42671400
H	-3.21059800	-2.39437800	5.46634000
C	-2.43510900	-1.03419200	3.95594300
H	-1.67748900	-0.59480300	4.62302200
C	-2.54601000	-0.57811600	2.63248700
Cl	4.54976700	2.42605400	1.35190900
C	-0.26440100	3.50580300	-0.29072200
C	-1.56796700	3.33595900	-0.55493800
H	-2.09005400	4.22117800	-0.96500600
C	0.81002900	2.59064000	0.26436300
H	0.58915600	2.23343900	1.29338300
H	0.98901300	1.69379000	-0.36724300
N	1.98369900	3.45858800	0.26708100
H	2.95414400	3.11872100	0.64830000
C	1.67564500	4.64985300	-0.19068000
O	0.39462200	4.76664900	-0.53598400
C	2.56276500	5.79982600	-0.35204800
C	2.03258500	7.02300100	-0.82691800
C	3.93973100	5.69388800	-0.04061500
C	2.87456500	8.12954000	-0.98586700
H	0.96251900	7.09836800	-1.06760500
C	4.76949400	6.80924500	-0.20451800
H	4.35712500	4.74010800	0.32955800
C	4.24178300	8.02472500	-0.67530200
H	2.46212700	9.08084500	-1.35448200
H	5.84018700	6.72836500	0.03699400
H	4.90150400	8.89721000	-0.80160800
H	-1.88255600	0.22061800	2.26185500
C	4.08000800	-2.70255400	0.11123900
C	2.87170700	-3.37864900	0.33556000
C	2.79883800	-4.75743600	0.03520400
C	3.91661600	-5.44626700	-0.48329900
C	5.11902400	-4.73758400	-0.69912300
C	5.20686200	-3.35874900	-0.40327600
H	6.15815700	-2.83732900	-0.58020000
H	1.98527300	-2.87199700	0.74252300
H	3.85309500	-6.51559400	-0.71420700
O	1.59729400	-5.35592300	0.27935200
O	6.25085400	-5.30821300	-1.19178000

C	1.46095600	-6.75093100	0.03452200
H	0.42436900	-7.01553000	0.31648700
H	1.61712200	-7.00261300	-1.03768300
H	2.16556600	-7.34841500	0.65375100
C	6.24321700	-6.69419700	-1.50683400
H	5.50298900	-6.93578600	-2.30153400
H	7.25720900	-6.93299800	-1.87975900
H	6.03242600	-7.32269500	-0.61322500
I	4.23150100	-0.60525900	0.58806800