Electronic Supplementary Information

Luminescent Monocyclometalated Cationic Gold(III) Complexes: Synthesis, Photophysical Characterization and Catalytic Investigations

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Table S1. Selected singlet and triplet excited states of **3** at the optimized ground-state geometry computed by TD-DFT (CPCM, dichloromethane solvent).

S_n	Excitation	Coefficient	Vertical excitation energy (nm)	*f*
S_1	H → L	0.67	307.7 (4.03 eV)	0.224
S_2	H → L+2	0.52	295.3 (4.20)	0.011
	H → L+1	0.39		
S_3	H-1 → L+1	0.54	286.9 (4.32)	0.885
	H-1 → L	0.36		
S_4	H-3 → L	0.59	282.2 (4.39)	0.014
S_5	H-2 → L+1	0.62	276.6 (4.48)	0.015
S_6	H → L+1	0.54	275.9 (4.49)	0.003
S_7	H-1 → L	0.60	272.0 (4.56)	0.022
S_8	H-3 → L+2	0.50	270.1 (4.59)	0.002
	H-3 → L+1	0.32		
S_9	H → L+3	0.55	255.1 (4.86)	0.177
S_{10}	H-1 → L+2	0.65	254.8 (4.87)	0.007
T_1	H → L	0.59	439.5 (2.82)	0.000
T_2	H-1 → L+1	0.55	403.6 (3.07)	0.000

Table S2. Selected singlet and triplet excited states of **4** at the optimized ground-state geometry computed by TD-DFT (CPCM, dichloromethane solvent).

S_n	Excitation	Coefficient	Vertical excitation energy (nm)	*f*
S_1	H → L+1	0.59	309.1 (4.01 eV)	0.179
	H → L	0.33		
S_2	H → L	0.43	303.9 (4.08)	0.078
	H-1 → L	0.35		
S_3	H-1 → L	0.52	299.1 (4.15)	0.126
	H → L+2	0.40		
S_4	H → L	0.43	291.9 (4.25)	0.002
	H → L+2	0.39		
S_5	H-2 → L+1	0.56	282.5 (4.39)	0.064
S_6	H-1 → L+1	0.65	279.9 (4.43)	0.008
S_7	H-2 → L+2	0.56	274.9 (4.51)	0.004
S_8	H-3 → L	0.57	274.5 (4.52)	0.070
	H-1 → L+6	0.31		
S_9	H-1 → L+2	0.65	268.4 (4.62)	0.004
S_{10}	H-2 → L	0.57	264.2 (4.69)	0.002
	H-2 → L+2	0.30		
T_1	H-1 → L	0.60	462.8 (2.68)	0.000
T_2	H → L+1	0.56	438.5 (2.83)	0.000

Table S3. Selected singlet and triplet excited states of **7** at the optimized ground-state geometry computed by TD-DFT (CPCM, dichloromethane solvent).

S_n	Excitation	Coefficient	Vertical excitation energy (nm)	*f*
S_1	H → L	0.63	318.4 (3.89 eV)	0.142
S_2	H → L+1	0.65	310.5 (3.99)	0.023
S_3	H-1 → L	0.61	291.6 (4.25)	0.021
S_4	H-2 → L	0.47	289.9 (4.28)	0.152
S_5	H-2 → L+1	0.48	288.9 (4.29)	0.041
S_6	H-1 → L+1	0.63	284.3 (4.36)	0.258
S_7	H-3 → L	0.40	280.2 (4.42)	0.005
	H-2 → L	0.34		
	H-4 → L	0.31		
S_8	H-2 → L	0.59	277.7 (4.46)	0.006
S_9	H-3 → L+1	0.45	267.6 (4.63)	0.010
	H-2 → L+1	0.36		
S_{10}	H-6 → L	0.57	265.7 (4.67)	0.033
T_1	H → L	0.68	443.6 (2.80)	0.000
T_2	H-8 → L+2	0.45	361.3 (3.43)	0.000

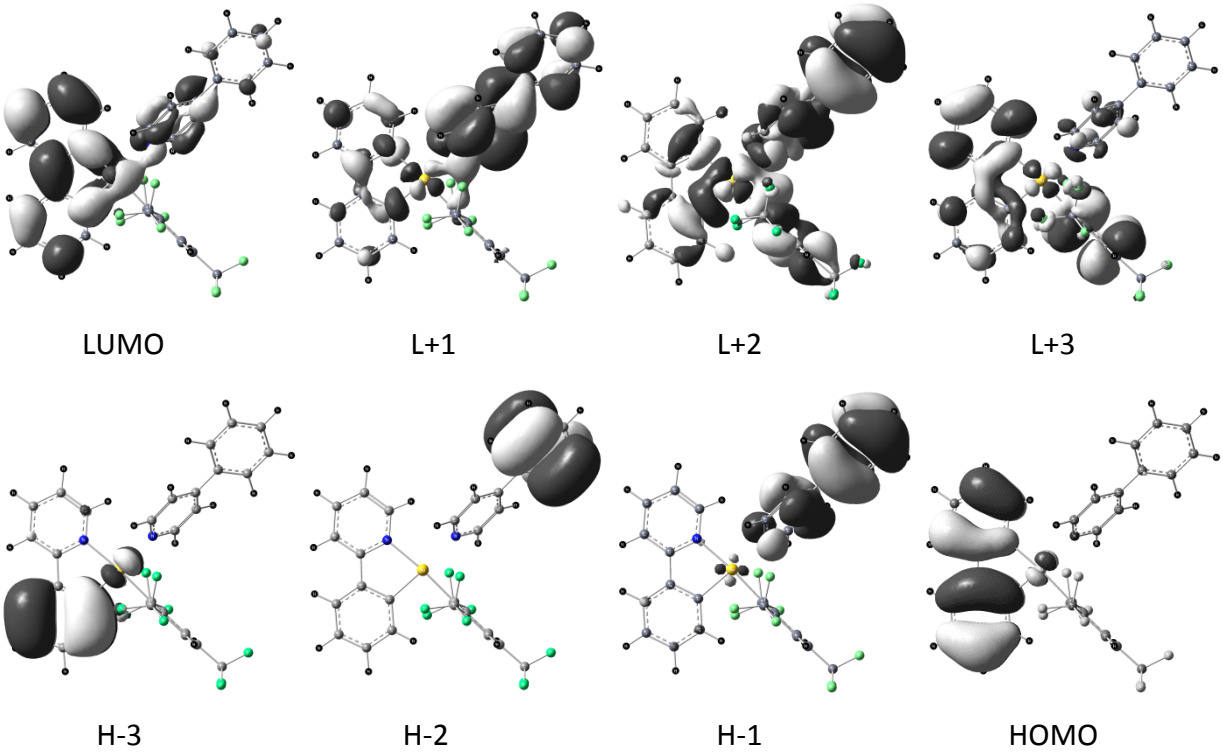

Figure S1. Spatial plots of selected frontier orbitals of the optimized ground state of **3**.

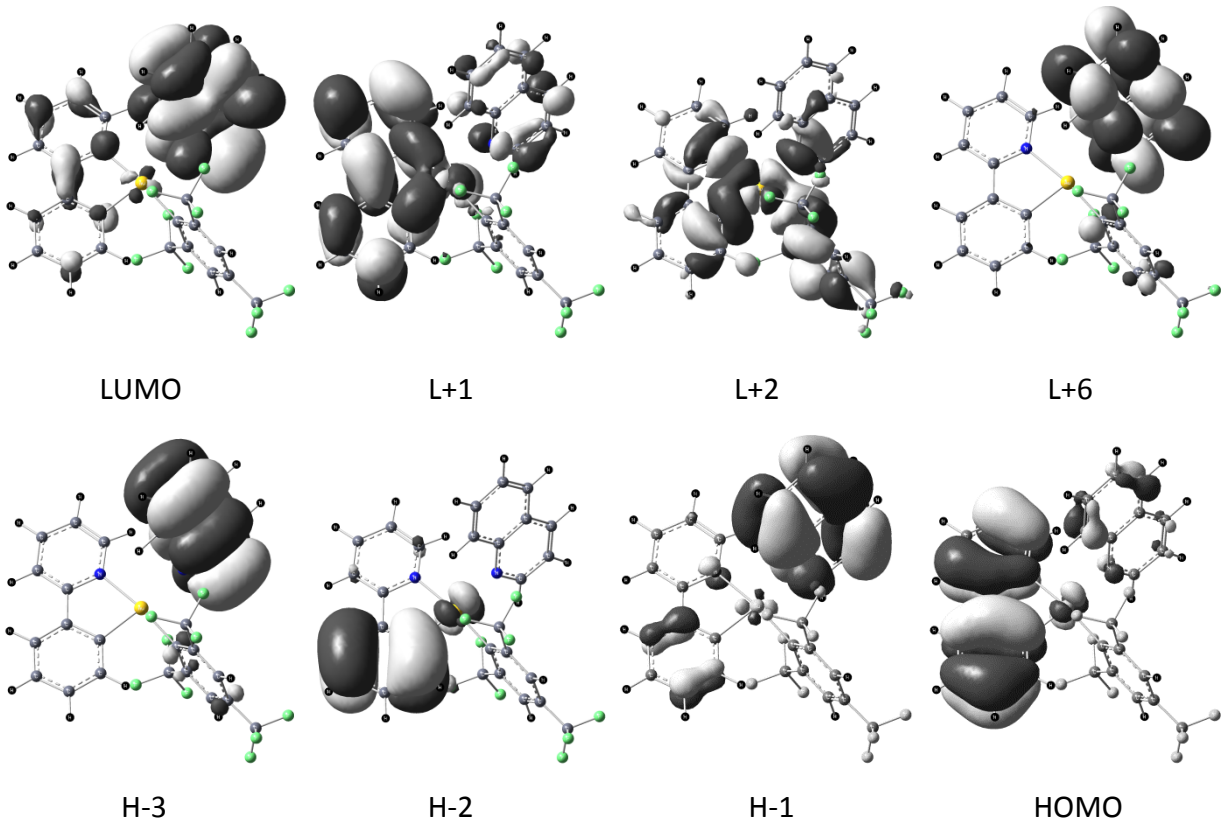

Figure S2. Spatial plots of selected frontier orbitals of the optimized ground state of **4**.

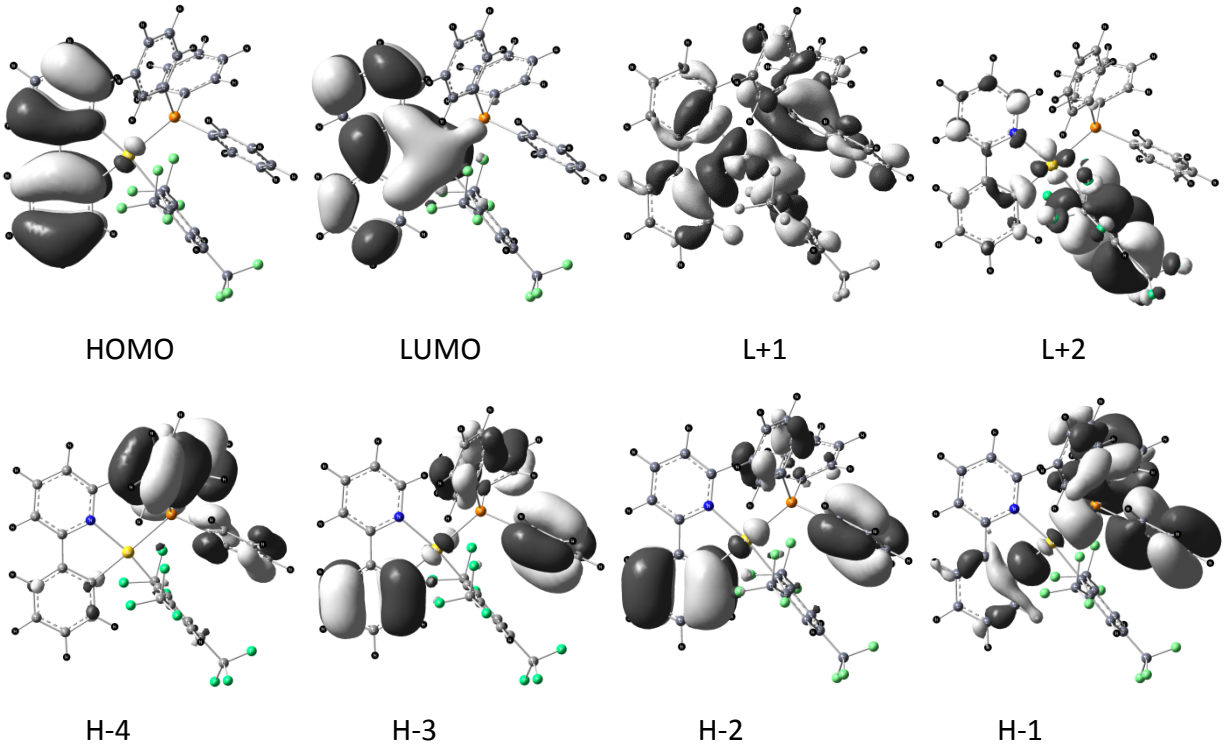

Figure S3. Spatial plots of selected frontier orbitals of the optimized ground state of **7**.

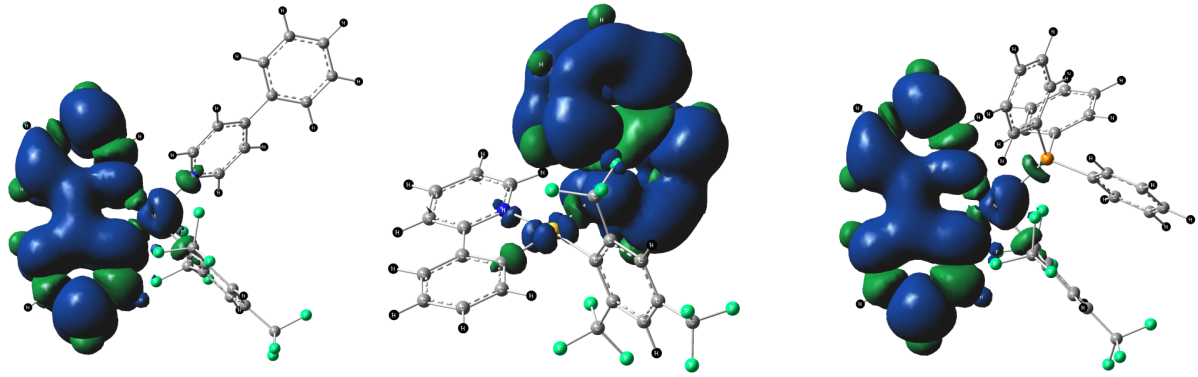

Figure S4. Spin density surfaces for the optimized triplet states of **3**, **4** and **7**, showing the ^{3}ILCT character of the emission processes.

Table S4. Frontier orbitals of the DFT optimized ground state S_0 and triplet state T_1 structures of **3**: energy levels and compositions.

	MO	Energy (eV)	Composition (%)			
			ppy	*FMes*	*4-ppy*	*Au*
Ground-state	L+3	-1.97	19	**74**	5	2
	L+2	-2.21	27	**31**	15	27
	L+1	-2.52	12	2	**82**	4
	LUMO	-2.65	**86**	0	8	6
	HOMO	-7.49	**97**	0	2	1
	H-1	-7.58	3	0	**96**	1
	H-2	-7.82	0	0	**100**	0
	H-3	-7.93	**95**	0	1	4
Triplet-state	α-HOMO	-4.77	**98**	0	0	2
	α-H-1	-7.57	0	0	**99**	1
	α-H-2	-7.82	0	0	**100**	0
	α-H-3	-7.89	**98**	0	0	2

[a] *Sum of Mulliken spin densities per fragment (given in %).*

Table S5. Frontier orbitals of the DFT optimized ground state S_0 and triplet state T_1 structures of **4**: energy levels and compositions.

	MO	Energy (eV)	Composition (%)			
			ppy	*FMes*	*quin*	*Au*
Ground-state	L+6 …	-1.46	1	1	**95**	3
	L+2	-2.33	**32**	31	6	31
	L+1	-2.63	**87**	0	10	7
	LUMO	-2.76	10	0	**89**	1
	HOMO	-7.50	**93**	0	6	1
	H-1	-7.70	6	0	**93**	1
	H-2	-7.95	**94**	0	1	5
	H-3	-8.24	0	2	**98**	0
Triplet-state	α-HOMO	-5.05	0	0	**100**	0
	α-H-1	-7.50	**98**	0	0	2
	α-H-2	-7.94	**95**	0	0	5
	α-H-3	-8.40	2	1	**96**	1

[a] *Sum of Mulliken spin densities per fragment (given in %).*

Table S6. Frontier orbitals of the DFT optimized ground state S_0 and triplet state T_1 structures of **7**: energy levels and compositions.

	MO	Energy (eV)	Composition (%)			
			ppy	*FMes*	*PPh_3*	*Au*
Ground-state	L+2	-2.00	9	**87**	2	2
	L+1	-2.43	**32**	23	27	18
	LUMO	-2.67	**91**	0	1	8
	HOMO	-7.45	**98**	0	1	1
	H-1	-7.67	14	0	**79**	7
	H-2	-7.87	**57**	1	40	2
	H-3	-7.88	37	0	**61**	2
	H-4	-7.96	2	0	**98**	0
	H-5	-8.09	2	2	**96**	0
	H-6	-8.10	1	3	**95**	1
	H-7	-8.31	2	0	**98**	0
	H-8	-8.50	6	**68**	22	4
Triplet-state	α-HOMO	-4.76	**98**	0	0	2
	α-H-1	-7.69	12	0	**81**	7
	α-H-2	-7.84	**59**	0	40	1
	α-H-3	-7.88	32	0	**67**	1

[a] *Sum of Mulliken spin densities per fragment (given in %).*

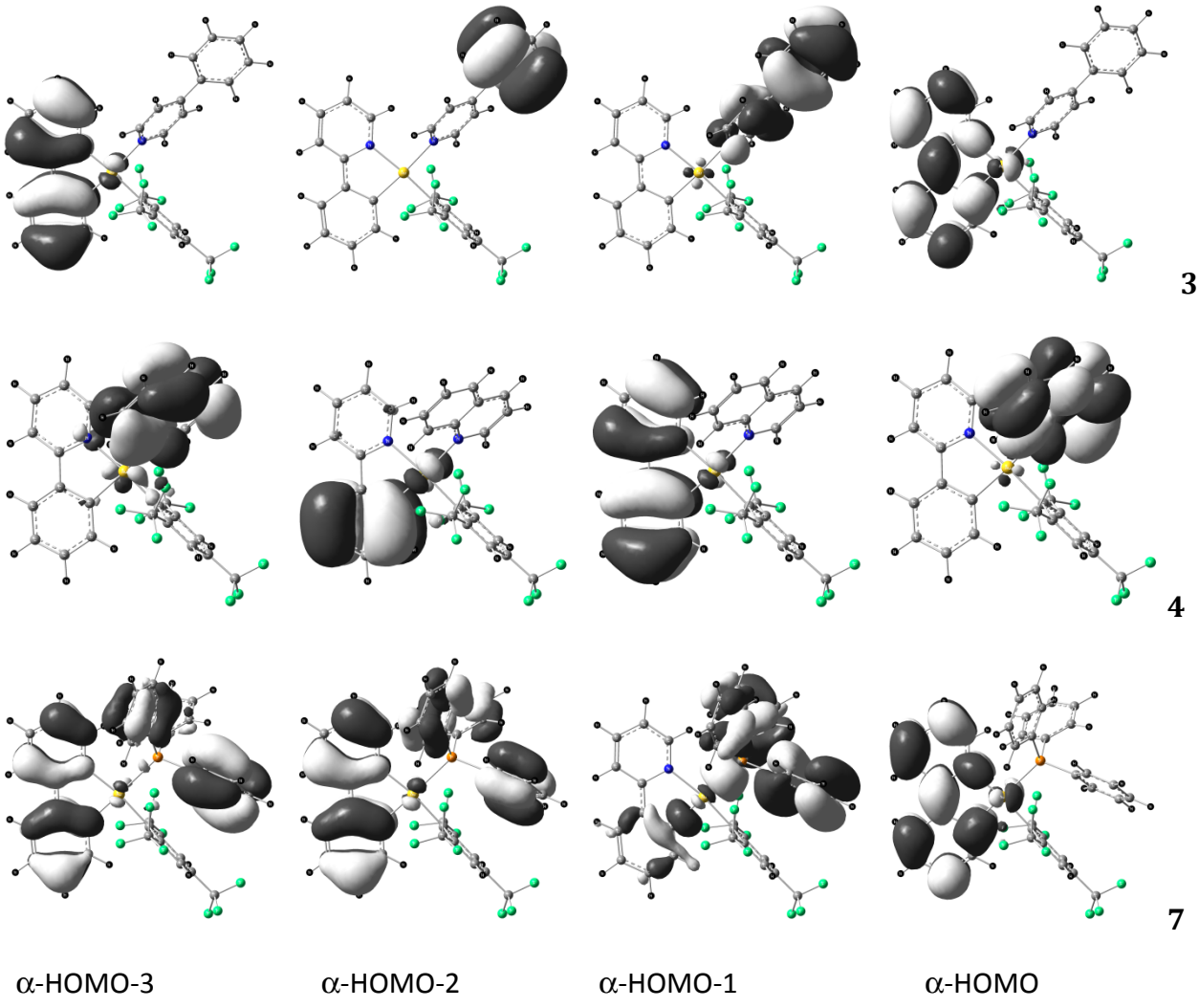

Figure S5. Spatial plots of selected frontier orbitals of the optimized triplet states of **3**, **4** and **7**.

Cartesian coordinates of the optimized ground-state structure of 3

Au	0.68297100	-0.95833900	-0.01725200
F	0.60556500	0.08634400	-2.74281300
F	1.52634600	1.87684600	-3.51883900
N	-1.45797500	-0.65806200	-0.11758400
N	0.57111800	-3.06016700	-0.15093100
F	0.68295000	2.00146200	3.55026000
C	1.36560100	3.84398400	0.01488200
C	0.90931100	1.79608500	1.20313500
F	-0.59473200	0.56618200	2.56426300
F	2.72937800	0.40085400	-2.49951600
C	1.30545500	1.74181700	-1.16714200
F	1.98318300	5.80451600	1.16823900
F	1.51313000	0.15306300	2.80478000
C	2.90505500	-2.76835500	0.20586600
C	-6.25267300	1.12822500	-0.63229300
H	-5.60360800	1.89268700	-1.05186900
C	1.48196200	3.12683200	-1.16701800
H	1.72126900	3.64126300	-2.09165700
C	1.00092100	1.04651500	0.01723100

C	2.64086000	-1.38217400	0.21477400
F	2.32238100	5.75806800	-0.97371700
C	-4.24633600	-0.25451200	-0.09385400
C	-2.07053700	-0.00041200	-1.11869800
H	-1.43944000	0.35131800	-1.92558500
C	1.77680700	-3.67035200	-0.01935700
C	1.08543700	3.17922200	1.20153300
H	1.01389800	3.73470500	2.13052700
C	-3.58752800	-0.93721700	0.94199800
H	-4.13371400	-1.29984900	1.80684200
C	3.67855000	-0.48251700	0.42121000
H	3.49780000	0.58623800	0.43570000
C	1.85781400	-5.06143200	-0.12295200
H	2.81615900	-5.55653100	-0.01697600
C	1.54557000	1.03143400	-2.48259900
F	0.30915900	5.93427000	-0.19799500
C	-2.21792800	-1.11448800	0.89688200
H	-1.69706700	-1.62002200	1.70435700
C	-3.43730900	0.21152000	-1.14154300
H	-3.87075500	0.72292000	-1.99505800
C	-7.62683000	1.33859500	-0.60799300
H	-8.03951200	2.25214200	-1.02659300
C	-0.53449000	-3.77420700	-0.40810900
H	-1.45489400	-3.21310500	-0.52495900
C	0.63391500	1.13421400	2.53486300
C	-0.50920800	-5.15310800	-0.52499100
H	-1.42459800	-5.69620300	-0.73374500
C	5.24888400	-2.31636900	0.60499300
H	6.26182800	-2.67673500	0.75742600
C	1.50280600	5.34522300	0.00390000
C	-6.55928100	-0.98651700	0.49660100
H	-6.15595600	-1.90945700	0.90602100
C	-5.70084100	-0.03642200	-0.07737700
C	4.98011100	-0.95025700	0.61361100
H	5.78452100	-0.23727800	0.77275600
C	-8.47072400	0.38463500	-0.04036300
H	-9.54464300	0.54829300	-0.02543400
C	4.21516700	-3.22192600	0.40261700
H	4.43610200	-4.28537500	0.40305200
C	0.71388000	-5.80493100	-0.37235700
H	0.77595700	-6.88625100	-0.45550900
C	-7.93403100	-0.77930500	0.50887600
H	-8.58862400	-1.52961100	0.94329000

Cartesian coordinates of the optimized ground-state structure of 4

C	3.70190100	-0.17163800	0.95512300
H	3.40607500	0.82088300	1.27533100
C	4.98602300	-0.64519900	1.16099600
H	5.72161300	-0.01854700	1.65360500
C	5.29243400	-1.93304900	0.72318200
H	6.28870500	-2.34131400	0.86751800
C	4.31149700	-2.69734000	0.10844600
H	4.53323000	-3.70570700	-0.22161600
C	3.02979100	-2.17106700	-0.07153400
C	1.90072400	-2.87323700	-0.67957300
C	0.65150100	-2.21711300	-0.68874300
C	-0.44743600	-2.83066700	-1.27610900
H	-1.41507500	-2.34242700	-1.29996200

C	-0.31684700	-4.09959700	-1.84468900
H	-1.18355500	-4.57104900	-2.30000600
C	0.91002200	-4.75763700	-1.83099200
H	1.00799500	-5.74395800	-2.27456700
C	2.01492600	-4.14579000	-1.25252800
H	2.97004900	-4.66301400	-1.25890400
C	0.39001200	2.05368900	1.94156500
H	-0.19215800	1.29780400	2.45494100
C	0.48853500	3.34929800	2.47084000
H	-0.02803000	3.58543400	3.39508600
C	1.23872500	4.28262800	1.79781200
H	1.33802200	5.29745500	2.17562900
C	1.88993000	3.92401900	0.59707300
C	1.74233800	2.58896300	0.11379000
C	2.38168100	2.22334900	-1.09155300
H	2.25494500	1.21979100	-1.48687300
C	3.13876900	3.14247200	-1.78094200
H	3.61713500	2.84963900	-2.71133700
C	3.29235100	4.46322000	-1.30414200
H	3.89183900	5.17324700	-1.86592600
C	2.67635100	4.84573800	-0.13816000
H	2.77899100	5.86022800	0.23857500
C	-1.28255600	-0.12683600	0.00300700
C	-1.92258500	0.53482200	-1.05827700
C	-3.30764000	0.70318600	-1.08039400
H	-3.77624200	1.21410800	-1.91492400
C	-4.08689500	0.20738600	-0.04508800
C	-3.48382300	-0.46114400	1.01081600
H	-4.09165100	-0.86293800	1.81436800
C	-2.09869000	-0.63101500	1.03525700
C	-1.15438500	1.13756000	-2.21218500
C	-5.57740500	0.43394600	-0.04431000
C	-1.54442500	-1.44050100	2.19026500
Au	0.73467000	-0.36472700	0.10662400
F	-0.15748500	0.34235800	-2.64691700
F	-0.58969800	2.31206600	-1.85912700
F	-1.94228800	1.38370800	-3.26449600
F	-5.88477200	1.59492700	0.56324900
F	-6.06676400	0.49288800	-1.29108700
F	-6.22378100	-0.54250200	0.60873100
F	-2.43635500	-1.57707500	3.17719400
F	-1.17379100	-2.67205800	1.81149400
F	-0.44664900	-0.86377000	2.74689600
N	2.76035500	-0.90883500	0.34840400
N	0.98885300	1.67716300	0.81853900

Cartesian coordinates of the optimized ground-state structure of 7

C	-3.73699300	0.69110400	0.12321500
H	-3.57249100	-0.37871000	0.13402100
C	-5.02279200	1.20053300	0.16839200
H	-5.86714400	0.52199200	0.22491600
C	-5.18706500	2.58323900	0.13647900
H	-6.17906400	3.02493500	0.16770200
C	-4.06566500	3.39443200	0.06644000
H	-4.17666300	4.47204200	0.04488200

C	-2.78777700	2.82853800	0.02830300
C	-1.54455800	3.59427400	-0.02950200
C	-0.33327700	2.87512300	-0.03815300
C	0.87099100	3.56849600	-0.08125300
H	1.81946700	3.04329800	-0.08795500
C	0.88112600	4.96367700	-0.11874800
H	1.83124100	5.49026500	-0.15239300
C	-0.31413100	5.67785400	-0.11380700
H	-0.30580300	6.76337300	-0.14403100
C	-1.52222500	4.99533100	-0.06909700
H	-2.44703800	5.56463400	-0.06517500
C	1.40289600	0.55654100	0.00221800
C	2.13342200	0.43947200	-1.19246700
C	3.51540000	0.24355300	-1.18243900
H	4.05409900	0.15067200	-2.11869800
C	4.20116700	0.17951400	0.02032600
C	3.51017100	0.33058000	1.21540600
H	4.04632900	0.30667500	2.15849800
C	2.12947000	0.51855500	1.20784700
C	1.47744500	0.57765500	-2.54735100
C	5.68417200	-0.08078100	0.05208000
C	1.45259600	0.68158400	2.55047200
Au	-0.61378100	0.84036900	0.00805500
F	0.99726600	1.81733700	-2.74862200
F	0.42949100	-0.26497400	-2.69616000
F	2.32420800	0.31332400	-3.54850500
F	5.94044600	-1.35052500	0.42629600
F	6.25195100	0.10639100	-1.14676200
F	6.30353600	0.72091500	0.93266000
F	2.32142100	0.61201600	3.56573100
F	0.80478700	1.85310000	2.66330300
F	0.53209600	-0.28887400	2.75799200
N	-2.64821800	1.47527000	0.05353300
P	-1.00796600	-1.60851900	-0.00176100
C	0.43057100	-2.63708000	-0.44270500
C	0.53675000	-3.21562400	-1.71169900
C	1.45636600	-2.82506900	0.49449700
C	1.66024900	-3.97197600	-2.04033000
H	-0.25270100	-3.08143600	-2.44536000
C	2.57507000	-3.58122800	0.15938700
H	1.37587700	-2.39710000	1.48982700
C	2.68010500	-4.15319100	-1.10903800
H	1.73374800	-4.42176600	-3.02667300
H	3.36515200	-3.72687400	0.89118400
H	3.55451300	-4.74445400	-1.36706500
C	-1.58068900	-2.24258000	1.60902500
C	-1.42479500	-3.59801800	1.93289800
C	-2.21600300	-1.38883100	2.51868600
C	-1.91425400	-4.08897200	3.14036600
H	-0.91051200	-4.26899000	1.24958500
C	-2.70559100	-1.88445700	3.72408500
H	-2.30715700	-0.32698100	2.30591100
C	-2.55838200	-3.23497700	4.03465600
H	-1.78618800	-5.14010200	3.38402100
H	-3.18783400	-1.21108400	4.42730000
H	-2.93419100	-3.61973200	4.97875300

C	-2.31406400	-2.04154600	-1.21093500
C	-2.48373900	-1.27053400	-2.36953900
C	-3.14366200	-3.15120000	-0.99865700
C	-3.45490400	-1.61533100	-3.30661200
H	-1.86177800	-0.39899100	-2.54892400
C	-4.11582300	-3.48886600	-1.93744200
H	-3.04021500	-3.75185900	-0.09967600
C	-4.27116400	-2.72478000	-3.09305400
H	-3.57313300	-1.01310100	-4.20331200
H	-4.75256500	-4.35191000	-1.76302700
H	-5.02953300	-2.99150200	-3.82409600

Cartesian coordinates of the optimized triplet-state structure of 3

Au	0.68624700	-0.94958500	-0.02571700
F	0.59808000	0.12522300	-2.75477600
F	1.49907800	1.93233900	-3.51335400
N	-1.44693200	-0.66038500	-0.12049000
N	0.57361100	-3.02616900	-0.15361400
F	0.64753200	1.99769500	3.55491800
C	1.33027500	3.86499000	0.03529000
C	0.89912200	1.80328900	1.20878000
F	-0.55726400	0.50584900	2.56247800
F	2.71962200	0.45839900	-2.51278800
C	1.28562600	1.77109300	-1.16223100
F	1.93310200	5.82264000	1.20132000
F	1.56614500	0.18965500	2.81482900
C	2.90226400	-2.81212600	0.18605800
C	-6.25639300	1.09251500	-0.61171800
H	-5.61324100	1.87144900	-1.01339900
C	1.44899700	3.15790800	-1.15228500
H	1.67932300	3.68191600	-2.07379500
C	0.99192300	1.06154600	0.01713900
C	2.63462200	-1.35954800	0.19355900
F	2.26312700	5.79655000	-0.94240300
C	-4.23853700	-0.28186000	-0.09564600
C	-2.06292000	0.01130600	-1.11022600
H	-1.43308200	0.38301900	-1.90888600
C	1.82538300	-3.66453500	0.01038000
C	1.06197200	3.18807100	1.21777200
H	0.98868300	3.73577600	2.15118300
C	-3.57597500	-0.97853000	0.92835900
H	-4.12087700	-1.36297700	1.78454300
C	3.67058400	-0.48187200	0.38136400
H	3.49766300	0.58850600	0.39840000
C	1.88051800	-5.09786600	-0.04924600
H	2.83225200	-5.59343800	0.10759600
C	1.52786000	1.07610400	-2.48579000
F	0.25172300	5.94614100	-0.15641700
C	-2.20482500	-1.14305300	0.88353600
H	-1.68061000	-1.65996700	1.68132100
C	-3.43132400	0.21198600	-1.13186300
H	-3.86731600	0.73596700	-1.97640900
C	-7.63259300	1.28915000	-0.58761800
H	-8.05281100	2.20712600	-0.98867900
C	-0.49908600	-3.75848400	-0.42747500

H	-1.42838900	-3.21878300	-0.58155400
C	0.64369300	1.12921400	2.53881200
C	-0.47043700	-5.15067800	-0.51922900
H	-1.38523900	-5.68598000	-0.74840900
C	5.27160600	-2.35047900	0.54025800
H	6.29524000	-2.68861700	0.67280000
C	1.45200800	5.36746900	0.03548500
C	-6.54606200	-1.04805000	0.47207100
H	-6.13500100	-1.97539300	0.86344600
C	-5.69511700	-0.07799300	-0.07913700
C	4.99129700	-0.94970900	0.55697000
H	5.79771600	-0.23838600	0.70540700
C	-8.46900500	0.31551100	-0.04277000
H	-9.54451000	0.46844600	-0.02814200
C	4.27406500	-3.25680600	0.36069700
H	4.49970000	-4.31784900	0.34837000
C	0.75543000	-5.83141300	-0.30726500
H	0.79837400	-6.91465800	-0.35591200
C	-7.92280800	-0.85440500	0.48394500
H	-8.57145300	-1.61993700	0.90034400

Cartesian coordinates of the optimized triplet-state structure of 4

C	3.72459400	-0.05967800	0.94163900
H	3.38755600	0.91219700	1.28466600
C	5.02993400	-0.48204300	1.12446900
H	5.74584500	0.16739100	1.61661800
C	5.38207300	-1.75193000	0.66793900
H	6.39596400	-2.12078000	0.79463200
C	4.42463900	-2.54995000	0.05915000
H	4.68289400	-3.54512800	-0.28411000
C	3.11959900	-2.07517900	-0.09817900
C	2.00994800	-2.81662400	-0.69551400
C	0.73693000	-2.20575400	-0.68719800
C	-0.34541600	-2.86203600	-1.25965400
H	-1.33105600	-2.41055100	-1.26925200
C	-0.17566300	-4.12583600	-1.82948200
H	-1.03045600	-4.63038400	-2.27168500
C	1.07509600	-4.73738700	-1.83297100
H	1.20365700	-5.72001100	-2.27697600
C	2.16427700	-4.08425900	-1.26978300
H	3.13736400	-4.56666200	-1.28790100
C	0.36865500	1.97460600	2.07787200
H	-0.11886600	1.15544400	2.58770800
C	0.40837600	3.23109100	2.60361400
H	-0.06742600	3.42299100	3.56009400
C	1.06666400	4.27471100	1.90002600
H	1.10007900	5.28259300	2.30140000
C	1.67151500	3.97968800	0.67135400
C	1.59873900	2.63497700	0.16809200
C	2.21875800	2.34364200	-1.07756600
H	2.14976900	1.33561500	-1.47553800
C	2.90220200	3.34721400	-1.84702200
H	3.34603900	3.06947100	-2.79740100
C	2.96664000	4.61881000	-1.37585800
H	3.46858200	5.40247900	-1.93493400

C	2.35245500	4.94511300	-0.10952300
H	2.40605400	5.96590400	0.25886500
C	-1.25838800	-0.16534800	0.00094500
C	-1.90395700	0.49060000	-1.06165000
C	-3.29093700	0.63957800	-1.09006100
H	-3.76302500	1.14712600	-1.92472000
C	-4.06868900	0.12852100	-0.06106500
C	-3.46126600	-0.54120300	0.99074100
H	-4.06738000	-0.95887300	1.78766200
C	-2.07352400	-0.69186200	1.02184700
C	-1.14733800	1.10704300	-2.21531000
C	-5.56159100	0.33745100	-0.06752300
C	-1.53228900	-1.53001100	2.16266900
Au	0.76322200	-0.35461900	0.11687600
F	-0.10639300	0.35459200	-2.62427000
F	-0.64137600	2.31562800	-1.87973100
F	-1.92966900	1.29801200	-3.28274500
F	-5.88463500	1.50470900	0.51915700
F	-6.04754500	0.37041100	-1.31707800
F	-6.19914200	-0.63556700	0.59892700
F	-2.38286700	-1.56707000	3.19580100
F	-1.30883500	-2.79750700	1.78339100
F	-0.35831900	-1.06281700	2.65408000
N	2.80656800	-0.82877400	0.33823200
N	0.96152600	1.66290200	0.86146300

Cartesian coordinates of the optimized triplet-state structure of 7

C	-3.72939800	0.62425400	0.11825900
H	-3.56693900	-0.44697300	0.13973400
C	-5.03641900	1.11262000	0.14974800
H	-5.85788800	0.40661900	0.20309800
C	-5.25758000	2.51193700	0.10753500
H	-6.26482000	2.91525600	0.12733700
C	-4.17051600	3.33746600	0.04184800
H	-4.30331100	4.41309900	0.00874600
C	-2.83569700	2.80737100	0.01803600
C	-1.67833500	3.56599500	-0.02895400
C	-0.38984000	2.85169800	-0.03792800
C	0.77447100	3.57764300	-0.07178600
H	1.73947600	3.08241900	-0.07611900
C	0.75513700	4.98800100	-0.10642600
H	1.69040000	5.53843200	-0.13770000
C	-0.48553400	5.69401900	-0.10341400
H	-0.48080400	6.77993900	-0.13017400
C	-1.66518600	5.01901800	-0.06645500
H	-2.60152300	5.56687800	-0.06248400
C	1.39669100	0.57646900	0.00088000
C	2.12842500	0.47042100	-1.19488100
C	3.51307600	0.29304100	-1.18891200
H	4.05070100	0.20701100	-2.12638400
C	4.20301700	0.23905900	0.01184300
C	3.51301900	0.38271900	1.20827100
H	4.05233000	0.36764200	2.14968800
C	2.12955800	0.55101200	1.20397500
C	1.47029600	0.60334500	-2.54977800

C	5.68935200	-0.00082700	0.04011600
C	1.45804500	0.71099500	2.55013200
Au	-0.62922700	0.82510700	0.00852000
F	0.99282500	1.84442100	-2.75549400
F	0.42153500	-0.23690500	-2.69685200
F	2.31632700	0.33588200	-3.55148900
F	5.96472600	-1.26569900	0.41706100
F	6.25147100	0.19111900	-1.16077400
F	6.30032800	0.81189900	0.91684800
F	2.32990900	0.62578100	3.56253000
F	0.82498200	1.89018500	2.67413600
F	0.52824400	-0.24939100	2.75613100
N	-2.65121300	1.40001600	0.05356800
P	-0.97418200	-1.61851700	0.00243600
C	0.48302100	-2.62201300	-0.43520100
C	0.60270300	-3.19476800	-1.70564600
C	1.50808300	-2.79761200	0.50514000
C	1.73917300	-3.93213600	-2.03275200
H	-0.18623300	-3.07079500	-2.44162100
C	2.63972600	-3.53499900	0.17169600
H	1.41683800	-2.37493600	1.50177400
C	2.75836800	-4.10063600	-1.09834300
H	1.82327400	-4.37735000	-3.02032900
H	3.42913800	-3.67106300	0.90603600
H	3.64280000	-4.67737000	-1.35512500
C	-1.53539800	-2.25788000	1.61574300
C	-1.35550100	-3.60934300	1.94379000
C	-2.18794600	-1.41307700	2.52154800
C	-1.83859600	-4.10582700	3.15160500
H	-0.82787100	-4.27306100	1.26356700
C	-2.67138500	-1.91453400	3.72701400
H	-2.29629000	-0.35349900	2.30528700
C	-2.50046800	-3.26128500	4.04181400
H	-1.69176200	-5.15373200	3.39856500
H	-3.16785100	-1.24818900	4.42701900
H	-2.87159000	-3.65021700	4.98606600
C	-2.27058800	-2.08411500	-1.20564000
C	-2.46765100	-1.31540100	-2.36119000
C	-3.06251400	-3.22124800	-0.99538300
C	-3.42996000	-1.68840700	-3.29667700
H	-1.87536500	-0.42274500	-2.53717400
C	-4.02537300	-3.58761500	-1.93281600
H	-2.93733900	-3.82103100	-0.09868300
C	-4.20893700	-2.82472400	-3.08503900
H	-3.57061500	-1.08696500	-4.19066000
H	-4.63328800	-4.47144500	-1.75969100
H	-4.96048400	-3.11314500	-3.81489500

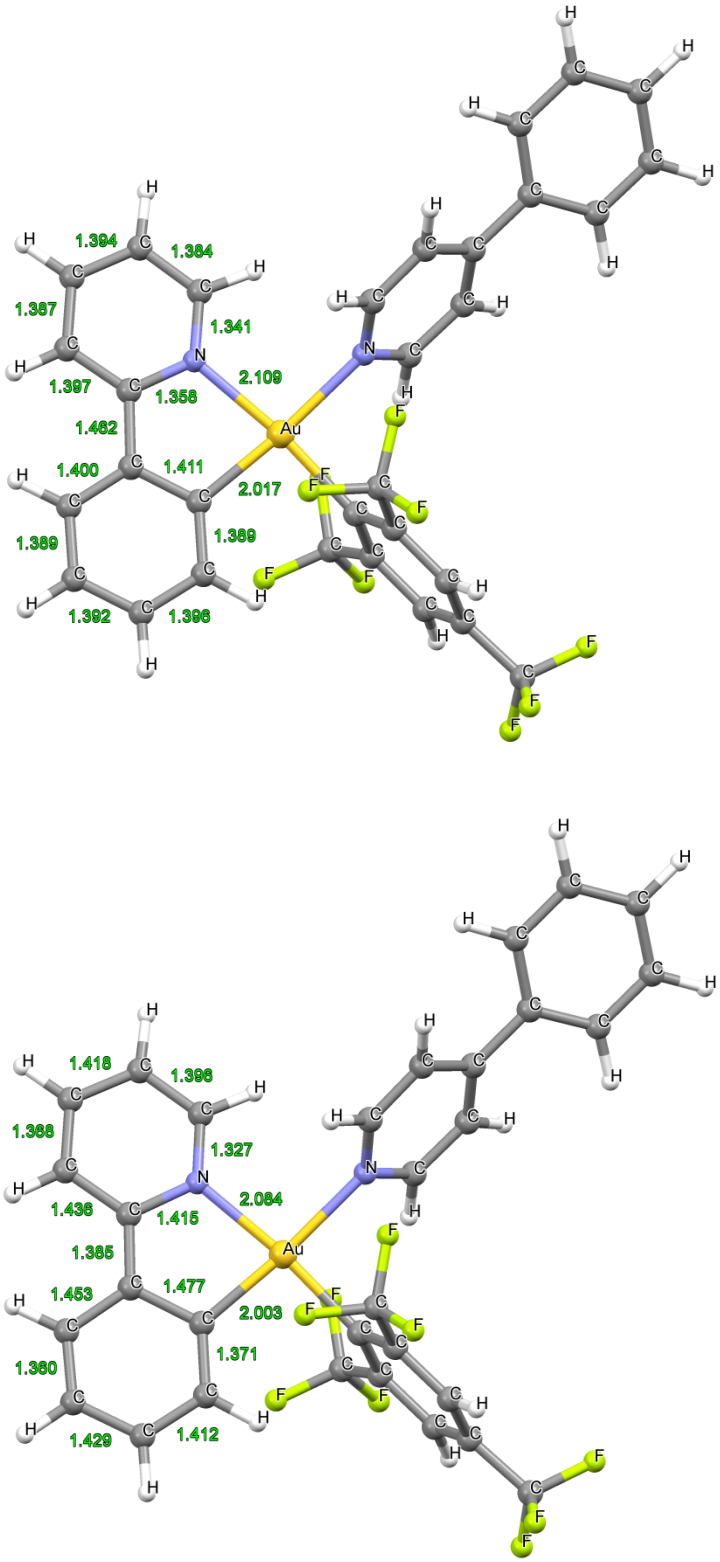

Figure S6. DFT optimized ground state and triplet state of **3** with selected bond distances.

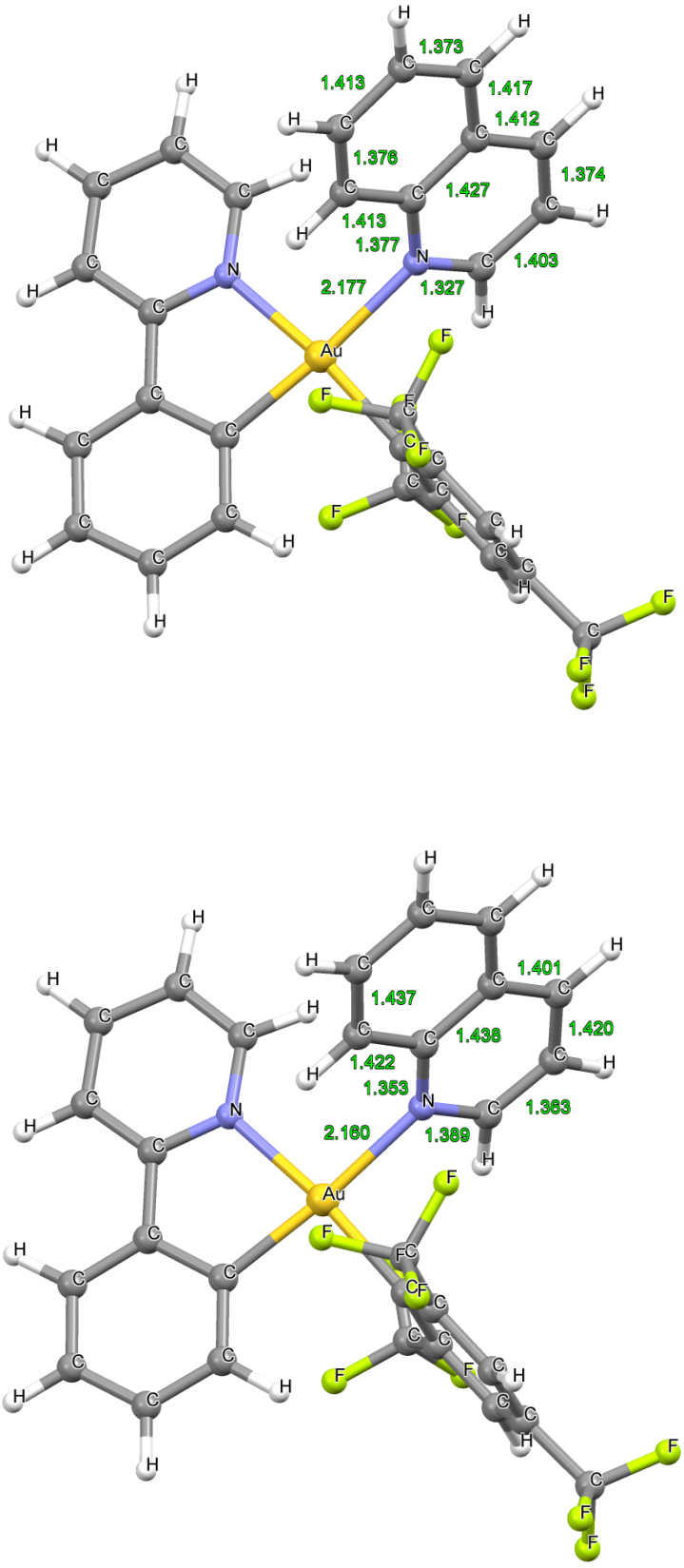

Figure S7. DFT optimized ground state and triplet state of **4** with selected bond distances.

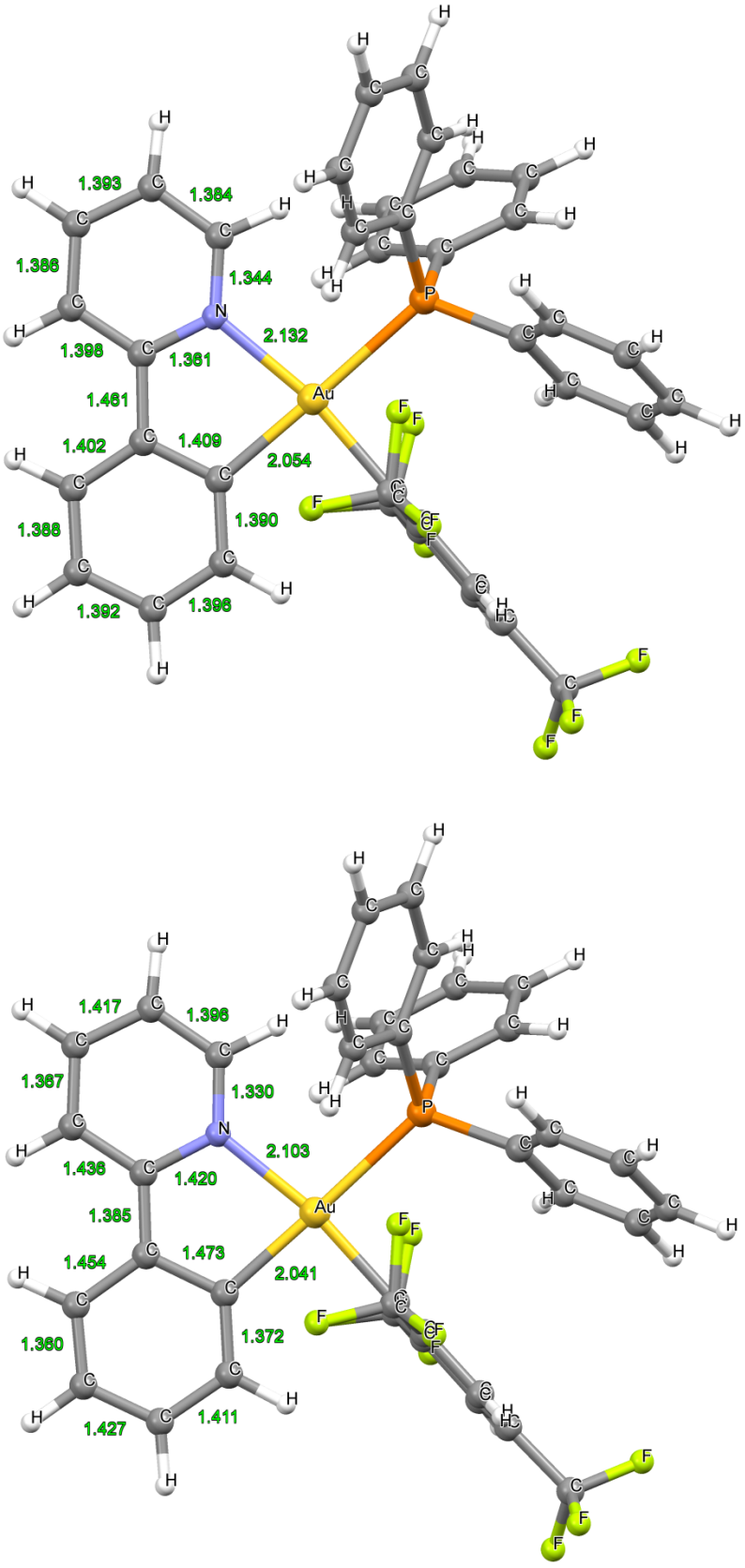

Figure S8. DFT optimized ground state and triplet state of **7** with selected bond distances.