

Electronic Supplementary Information
Green to Blue-green-emitting Cationic Iridium Complexes
with a CF₃ Substituted Phenyl-triazole Type
Cyclometalating Ligand: Synthesis, Characterization and
Their Use for Efficient Light-emitting Electrochemical Cells

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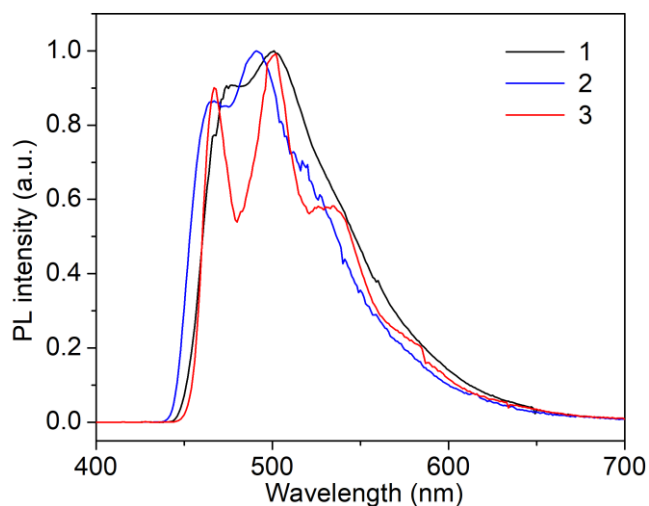


Figure S1. PL spectra of complexes 1-3 at 77 K in CH₃CN glass.[^]

Table S1. Selected bond lengths and dihedral angles on the ground and triplet states for complexes 1-3.

	State	Bond length (Å)			Angles (°)	
		Ir-C ^{^N} ^a	Ir-N ^{^C} ^b	Ir-N ^{^N} ^c	Φ ₁ ^d	Φ ₂ ^e
1	Crystal	2.021/2.032	2.014/2.017	2.120/2.088	79.3/79.2	77.0
	S ₀	2.043/2.043	2.049/2.049	2.189/2.189	79.0/79.0	75.6
	T ₁	2.016/2.016	2.051/2.051	2.179/2.179	79.9/79.9	76.0
2	S ₀	2.043/2.043	2.049/2.049	2.187/2.187	79.0/79.0	75.4
	T ₁	2.018/2.018	2.050/2.050	2.175/2.175	79.8/79.8	76.0
3	S ₀	2.042/2.038	2.050/2.049	2.223/2.169	79.0/79.1	75.0
	T ₁	2.047/2.043	2.051/2.046	2.197/2.132	79.0/79.1	76.4

^a The Ir-C bond length between iridium and the C^{^N} ligand. ^b The Ir-N bond length between iridium and the C^{^N} ligand. ^c The Ir-N bond length between iridium and the N^{^N} ligand. ^d The ligand bite angles of C^{^N} ligands. ^e The ligand bite angles of N^{^N} ligands.

Table S2. Distributions of HOMO-1, HOMO-2, HOMO-3, and LUMO+1, LUMO+2, LUMO+3 on complexes 1-3.

	HOMO-3	HOMO-2	HOMO-1	LUMO+1	LUMO+2	LUMO+3
1						
2						
3						

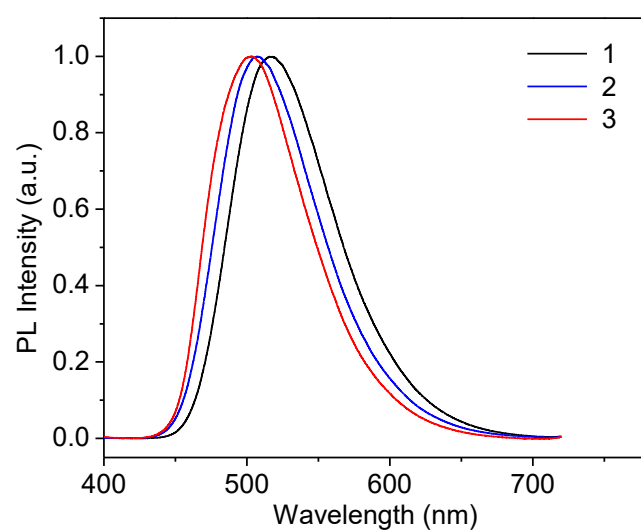


Figure S2. PL spectra of the emissive layers of LECs based on complexes 1-3.

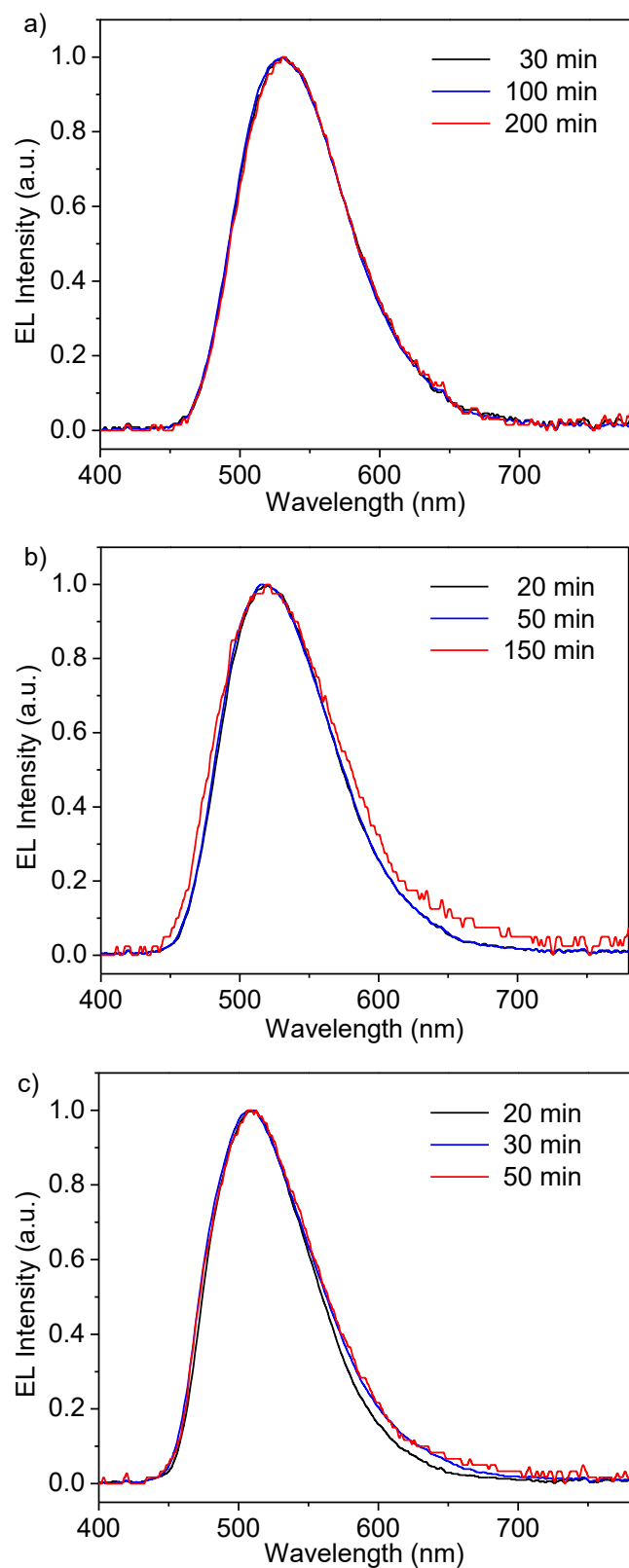


Figure S3. Time-dependent EL spectra of the LECs based on a) complex 1, b) complex 2 and c) complex 3 driven under a constant-voltage at 4.0 V.

Table S3. Cartesian coordinates of optimized geometries for complexes 1-3.**Complex1**

S₀				T₁			
Ir	0.00000000	0.37154900	0.00000000	Ir	0.00000000	0.24082800	0.00000000
C	-0.53427200	-1.08682600	-1.32742600	C	0.61176300	-1.11562300	1.36023700
N	-2.01143800	0.22949200	0.36643600	N	1.99585500	0.14306200	-0.46025900
N	2.01143800	0.22949200	-0.36643600	N	-1.99585500	0.14306100	0.46026000
C	0.53427100	-1.08682600	1.32742600	C	-0.61176200	-1.11562300	-1.36023700
N	-2.85039100	0.87359700	1.21673600	N	2.78026500	0.78809800	-1.35350400
N	2.85039100	0.87359700	-1.21673600	N	-2.78026500	0.78809800	1.35350400
C	0.28017500	-1.75097600	-2.25696500	C	-0.16729800	-1.76025400	2.34126800
C	-0.23933100	-2.71324500	-3.12892700	C	0.39842100	-2.68575700	3.21639300
C	-1.59723900	-3.04858200	-3.10168500	C	1.76413700	-2.98975800	3.14378800
C	-2.44391500	-2.41210300	-2.19899400	C	2.57908300	-2.36378800	2.19617100
C	-1.91755300	-1.44609500	-1.32701300	C	2.01378300	-1.43302900	1.32370500
C	-2.67379300	-0.67880100	-0.35679800	C	2.71662000	-0.68793400	0.29569000
C	-4.02958900	0.34399900	1.00491200	C	3.99066400	0.33327000	-1.13463800
C	-0.28017500	-1.75097600	2.25696400	C	0.16729800	-1.76025400	-2.34126800
C	0.23933100	-2.71324600	3.12892700	C	-0.39842100	-2.68575700	-3.21639200
C	1.59723900	-3.04858300	3.10168400	C	-1.76413600	-2.98975900	-3.14378700
C	2.44391500	-2.41210300	2.19899400	C	-2.57908300	-2.36378800	-2.19617000
C	1.91755300	-1.44609600	1.32701300	C	-2.01378300	-1.43303000	-1.32370400
C	2.67379300	-0.67880100	0.35679800	C	-2.71662000	-0.68793400	-0.29568900
C	4.02958900	0.34399900	-1.00491200	C	-3.99066400	0.33327000	1.13463800
N	-0.33125300	2.10140500	-1.29950600	N	0.44039500	1.95802000	1.26685000
C	-0.16993500	3.31944900	-0.72117700	C	0.23256000	3.20092300	0.67205900
C	-0.31753700	4.49024100	-1.47187700	C	0.49732300	4.37637600	1.43299800
C	-0.63377800	4.40495500	-2.82483500	C	0.94992500	4.29063300	2.72616700
C	-0.79421600	3.14857700	-3.40532800	C	1.15227400	3.01118200	3.31004500
C	-0.63245200	2.02180000	-2.60611300	C	0.88512900	1.89673500	2.54422900
H	1.33849600	-1.51472100	-2.31306000	H	-1.22445800	-1.53217800	2.42415000
H	-1.99252900	-3.79743600	-3.78058400	H	2.19775700	-3.71079600	3.82877800
H	-3.49837000	-2.66218400	-2.17777000	H	3.63393200	-2.60554900	2.14916800
H	-1.33849600	-1.51472100	2.31306000	H	1.22445800	-1.53217900	-2.42415000
H	1.99252800	-3.79743700	3.78058400	H	-2.19775600	-3.71079600	-3.82877700
H	3.49837000	-2.66218400	2.17777000	H	-3.63393200	-2.60554900	-2.14916800
H	-0.18371300	5.46064100	-1.01202600	H	0.33956500	5.34812700	0.98030700
H	-1.03782700	3.03394000	-4.45509700	H	1.50077100	2.89652900	4.32952300
H	-0.73954300	1.02090700	-3.00684000	H	1.01550200	0.90094600	2.95102000
C	0.16993500	3.31944900	0.72117700	C	-0.23256000	3.20092300	-0.67206000
C	0.31753800	4.49024000	1.47187700	C	-0.49732300	4.37637500	-1.43299900
C	0.63377800	4.40495500	2.82483500	C	-0.94992500	4.29063200	-2.72616800
H	0.18371400	5.46064100	1.01202600	H	-0.33956600	5.34812700	-0.98030800

C	0.63245200	2.02180000	2.60611300	C	-0.88512900	1.89673400	-2.54422900
C	0.79421600	3.14857700	3.40532900	C	-1.15227400	3.01118100	-3.31004500
H	0.73954300	1.02090700	3.00684000	H	-1.01550200	0.90094600	-2.95102000
H	1.03782700	3.03394000	4.45509700	H	-1.50077100	2.89652800	-4.32952400
N	0.33125300	2.10140500	1.29950600	N	-0.44039500	1.95802000	-1.26685000
N	3.98370100	-0.63154800	-0.03167700	N	-4.01314100	-0.59254900	0.11498800
C	5.08668200	-1.43783600	0.43927100	C	-5.16838200	-1.29952300	-0.39555100
C	5.90536600	-0.94463300	1.45610800	C	-5.93701000	-0.70487100	-1.39688900
C	5.31071900	-2.68612600	-0.14379500	C	-5.48527900	-2.55087700	0.13479400
C	6.96955300	-1.72920700	1.90272000	C	-7.04935100	-1.39210400	-1.88395400
H	5.70860000	0.03126500	1.88639600	H	-5.66598000	0.27115100	-1.78442600
C	6.37719900	-3.46062900	0.31333100	C	-6.59965400	-3.22637600	-0.36371500
C	7.20384800	-2.98377100	1.33420200	C	-7.37855300	-2.64897600	-1.37002100
H	8.03271400	-3.59006500	1.68571600	H	-8.24479300	-3.17888400	-1.75312700
N	-3.98370100	-0.63154700	0.03167600	N	4.01314100	-0.59254900	-0.11498800
C	-5.08668200	-1.43783600	-0.43927100	C	5.16838200	-1.29952300	0.39555100
C	-5.31071900	-2.68612600	0.14379500	C	5.48527900	-2.55087700	-0.13479300
C	-5.90536600	-0.94463300	-1.45610800	C	5.93701100	-0.70487100	1.39688900
C	-6.37719900	-3.46062900	-0.31333200	C	6.59965400	-3.22637500	0.36371500
C	-6.96955300	-1.72920700	-1.90272100	C	7.04935100	-1.39210300	1.88395400
H	-5.70860100	0.03126600	-1.88639600	H	5.66598000	0.27115100	1.78442600
C	-7.20384900	-2.98377100	-1.33420200	C	7.37855300	-2.64897600	1.37002000
H	-8.03271400	-3.59006500	-1.68571600	H	8.24479300	-3.17888400	1.75312700
H	-0.42161300	-3.20674900	3.83673500	H	0.22191600	-3.17509700	-3.96084500
H	0.42161300	-3.20674900	-3.83673500	H	-0.22191600	-3.17509600	3.96084500
H	-6.56154000	-4.43352500	0.13032400	H	6.85828000	-4.20085100	-0.03706100
H	-7.61321600	-1.35850500	-2.69366800	H	7.65618800	-0.94376500	2.66358500
H	6.56154000	-4.43352500	-0.13032500	H	-6.85828000	-4.20085100	0.03706100
C	-5.28002400	0.75396900	1.72727900	C	5.20680900	0.76621300	-1.90642300
H	7.61321600	-1.35850600	2.69366800	H	-7.65618800	-0.94376600	-2.66358500
C	5.28002400	0.75396900	-1.72727800	C	-5.20680900	0.76621300	1.90642300
F	5.00527100	1.69326300	-2.63952000	F	-4.86803800	1.65614300	2.84387800
F	6.19640800	1.24947100	-0.86989600	F	-6.11888900	1.32848500	1.08994300
F	5.84510600	-0.29750400	-2.35411100	F	-5.79387400	-0.28766200	2.50575700
F	-6.19640800	1.24947000	0.86989600	F	6.11888900	1.32848500	-1.08994300
F	-5.00527100	1.69326300	2.63952000	F	4.86803800	1.65614300	-2.84387800
F	-5.84510500	-0.29750400	2.35411200	F	5.79387400	-0.28766200	-2.50575700
H	-4.66095900	-3.03911500	0.93744500	H	4.87130300	-2.98242700	-0.91803300
H	4.66095900	-3.03911500	-0.93744500	H	-4.87130300	-2.98242700	0.91803400
H	-0.74983300	5.30826700	-3.41396600	H	1.14881400	5.19303400	3.29575900
H	0.74983300	5.30826700	3.41396600	H	-1.14881400	5.19303400	-3.29576000

Complex2

S ₀				T ₁			
Ir	0.00008400	0.16841800	0.00011200	Ir	0.00000000	0.05168600	0.00000000
C	0.55132600	-1.28756800	1.32341500	C	-0.63031900	-1.31150600	-1.34722700
N	2.00706600	0.02731400	-0.38982400	N	-1.98841200	-0.04642200	0.48819200
N	-2.00688100	0.02691700	0.39011500	N	1.98841100	-0.04642200	-0.48819200
C	-0.55065500	-1.28860300	-1.32224700	C	0.63031900	-1.31150600	1.34722600
N	2.83528100	0.66963800	-1.25184600	N	-2.76118500	0.60403200	1.38768900
N	-2.83537200	0.66960000	1.25160600	N	2.76118500	0.60403000	-1.38769100
C	-0.25106400	-1.95225500	2.26340400	C	0.13448600	-1.96054700	-2.33629700
C	0.27981700	-2.91225400	3.13082300	C	-0.44349200	-2.88972200	-3.19948800
C	1.63802000	-3.24532800	3.08881700	C	-1.80766400	-3.19501000	-3.10544200
C	2.47313400	-2.60872900	2.17559900	C	-2.60851800	-2.56627300	-2.14823700
C	1.93518600	-1.64485100	1.30818500	C	-2.03092100	-1.63086500	-1.28824200
C	2.67903900	-0.87847500	0.32781700	C	-2.71895400	-0.88268400	-0.25289500
C	4.01773900	0.14244800	-1.05213000	C	-3.97393000	0.14629500	1.18896400
C	0.25201200	-1.95361400	-2.26176700	C	-0.13448600	-1.96054700	2.33629600
C	-0.27859400	-2.91400400	-3.12892300	C	0.44349100	-2.88972200	3.19948700
C	-1.63678500	-3.24714300	-3.08710300	C	1.80766300	-3.19501100	3.10544100
C	-2.47216000	-2.61022800	-2.17434200	C	2.60851700	-2.56627400	2.14823600
C	-1.93448600	-1.64596700	-1.30718400	C	2.03092100	-1.63086600	1.28824100
C	-2.67860700	-0.87925100	-0.32727600	C	2.71895400	-0.88268500	0.25289500
C	-4.01759800	0.14171000	1.05234700	C	3.97393000	0.14629400	-1.18896400
N	0.34651900	1.89911600	1.29166400	N	-0.46665600	1.76613300	-1.25486900
C	0.17821900	3.11712500	0.71834200	C	-0.24614600	3.00903900	-0.66694300
C	0.33098700	4.28740300	1.46692400	C	-0.52918100	4.18542300	-1.42163800
C	0.66404400	4.23000600	2.82286900	C	-1.02248300	4.12313000	-2.70456000
C	0.82794900	2.95827200	3.38725000	C	-1.24317500	2.82949500	-3.26789200
C	0.66099800	1.83053800	2.59678100	C	-0.95532200	1.71310100	-2.51540600
H	-1.30919700	-1.71795600	2.33114900	H	1.19041700	-1.73305100	-2.43548100
H	2.04227400	-3.99252700	3.76428600	H	-2.25056200	-3.91953000	-3.78077100
H	3.52770200	-2.85721300	2.14273900	H	-3.66222400	-2.80910700	-2.08397900
H	1.31013200	-1.71922200	-2.32938100	H	-1.19041700	-1.73305100	2.43548000
H	-2.04083600	-3.99462700	-3.76237900	H	2.25056100	-3.91953200	3.78076900
H	-3.52672100	-2.85875900	-2.14165000	H	3.66222300	-2.80910800	2.08397800
H	0.18607200	5.25415400	1.00111500	H	-0.35285400	5.15474500	-0.96888600
H	1.08068200	2.84091000	4.43568400	H	-1.62260300	2.71413300	-4.27724200
H	0.77340200	0.83292200	3.00445400	H	-1.10202400	0.71997800	-2.92394100
C	-0.17857600	3.11668900	-0.72100200	C	0.24614600	3.00903800	0.66694300
C	-0.33015100	4.28569200	-1.47056300	C	0.52918100	4.18542300	1.42163900
C	-0.66376100	4.22692700	-2.82714900	C	1.02248300	4.12312900	2.70456000
H	-0.18346200	5.25283200	-1.00588100	H	0.35285400	5.15474500	0.96888600
C	-0.66070700	1.82770800	-2.59787400	C	0.95532200	1.71310000	2.51540500
C	-0.82677700	2.95523900	-3.39000000	C	1.24317500	2.82949400	3.26789200

H	-0.77213500	0.82982300	-3.00521500	H	1.10202500	0.71997700	2.92394000
H	-1.07727400	2.83668800	-4.43873500	H	1.62260300	2.71413200	4.27724200
N	-0.34728000	1.89749400	-1.29326700	N	0.46665600	1.76613200	1.25486900
N	-3.98397600	-0.83156700	0.07640400	N	4.00969600	-0.78612400	-0.17571700
C	-5.09321000	-1.63500700	-0.38448300	C	5.16889400	-1.50590800	0.30670500
C	-5.91734500	-1.14145000	-1.39674400	C	5.96067400	-0.92789500	1.29963800
C	-5.31752700	-2.88109900	0.20312600	C	5.46565700	-2.75422100	-0.24222800
C	-6.98729100	-1.92339000	-1.83408900	C	7.07632300	-1.62919200	1.75854100
H	-5.72032700	-0.16718700	-1.83064500	H	5.70472800	0.04602500	1.70239000
C	-6.38989400	-3.65299700	-0.24463800	C	6.58349900	-3.44386200	0.22811500
C	-7.22194200	-3.17577500	-1.26091000	C	7.38566600	-2.88318200	1.22560800
H	-8.05531900	-3.78004500	-1.60518800	H	8.25453300	-3.42390700	1.58704800
N	3.98435400	-0.83069500	-0.07604300	N	-4.00969600	-0.78612300	0.17571700
C	5.09374400	-1.63399400	0.38471300	C	-5.16889400	-1.50590900	-0.30670400
C	5.31828600	-2.87994500	-0.20311700	C	-5.46565000	-2.75422500	0.24222500
C	5.91783600	-1.14043300	1.39700400	C	-5.96068000	-0.92789400	-1.29963100
C	6.39085100	-3.65168900	0.24443600	C	-6.58349200	-3.44386800	-0.22811600
C	6.98796700	-1.92222900	1.83415400	C	-7.07632900	-1.62919200	-1.75853200
H	5.72064600	-0.16628000	1.83107000	H	-5.70473900	0.04602900	-1.70237900
C	7.22285700	-3.17446200	1.26073800	C	-7.38566500	-2.88318600	-1.22560400
H	8.05639300	-3.77860700	1.60485100	H	-8.25453200	-3.42391200	-1.58704200
H	0.37363100	-3.40790900	-3.84455100	H	-0.16623900	-3.38145300	3.95115200
H	-0.37220800	-3.40592600	3.84679400	H	0.16623800	-3.38145200	-3.95115300
H	6.57563300	-4.62276600	-0.20302500	H	-6.82656100	-4.41614500	0.18743900
H	7.63586400	-1.55117500	2.62148400	H	-7.70128600	-1.19405100	-2.53129200
H	-6.57449200	-4.62419500	0.20263600	H	6.82657300	-4.41613700	-0.18744400
C	5.25875800	0.55081500	-1.79111800	C	-5.17983300	0.58396500	1.97393000
H	-7.63521600	-1.55233700	-2.62139800	H	7.70127600	-1.19405200	2.53130500
C	-5.25872200	0.54986900	1.79126900	C	5.17983300	0.58396300	-1.97393000
F	-4.97377700	1.49068600	2.69872100	F	4.82911100	1.48015300	-2.90100500
F	-6.18820000	1.04221900	0.94614100	F	6.10274100	1.14074400	-1.16577000
F	-5.81298900	-0.50216700	2.42708800	F	5.75895900	-0.46587300	-2.58789200
F	6.18818900	1.04341000	-0.94608000	F	-6.10273900	1.14074900	1.16576900
F	4.97358300	1.49148600	-2.69864900	F	-4.82911000	1.48015200	2.90100700
F	5.81319300	-0.50116300	-2.42688300	F	-5.75896200	-0.46587200	2.58788900
H	4.66420200	-3.23327700	-0.99305100	H	-4.83359000	-3.17233900	1.01837000
H	-4.66341300	-3.23443000	0.99303500	H	4.83360100	-3.17233400	-1.01837700
C	0.84906800	5.47902700	3.64129100	C	-1.32455100	5.36118700	-3.50594500
H	1.90641400	5.61374100	3.89592700	H	-2.38001800	5.38845500	-3.80259300
H	0.51454400	6.36684700	3.10063300	H	-1.10495200	6.27084600	-2.94132000
H	0.29634300	5.41349400	4.58331700	H	-0.73674800	5.38240100	-4.43156400
C	-0.85793900	5.47783800	-3.64059800	C	1.32455100	5.36118700	3.50594500
H	-1.92427700	5.72491500	-3.70397000	H	2.38001700	5.38845400	3.80259300
H	-0.34473500	6.33108200	-3.19123600	H	1.10495200	6.27084500	2.94132100

H	-0.49302900	5.34451700	-4.66245700	H	0.73674800	5.38239900	4.43156500
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Complex3

S ₀				T ₁			
Ir	0.00392500	-0.21064000	0.04242300	Ir	-0.05780700	-0.21666800	0.04778000
C	-0.53205000	-1.50204900	-1.44053000	C	-0.68979500	-1.42263200	-1.47548600
N	-2.00094400	-0.41609800	0.41329900	N	-2.06502400	-0.30894600	0.43328300
N	2.01356900	-0.27929200	-0.35658100	N	1.94459900	-0.39256400	-0.36174200
C	0.57741700	-1.78614800	1.20735700	C	0.42047100	-1.87764300	1.14410100
N	-2.83609300	0.11288300	1.34276200	N	-2.85564400	0.24835400	1.38461000
N	2.83295300	0.46224800	-1.14433900	N	2.80866700	0.33900900	-1.10918200
C	0.28260400	-2.05245200	-2.44167000	C	0.08081000	-1.99277300	-2.49930300
C	-0.23658900	-2.90940800	-3.41673400	C	-0.50047800	-2.78416500	-3.49426000
C	-1.59381800	-3.25017900	-3.42559900	C	-1.87714600	-3.03711000	-3.49872700
C	-2.43995300	-2.72414800	-2.45441400	C	-2.68063500	-2.48924300	-2.50384200
C	-1.91425000	-1.86230700	-1.47867200	C	-2.09230800	-1.69235000	-1.50865600
C	-2.66735900	-1.22195800	-0.41928800	C	-2.79086000	-1.04068700	-0.41983200
C	-4.01767700	-0.38105200	1.06665400	C	-4.06933800	-0.15559500	1.10351600
C	-0.21827400	-2.56521300	2.06188500	C	-0.42214500	-2.64982100	1.95800400
C	0.32624000	-3.59989700	2.82900700	C	0.05882300	-3.75317300	2.66961400
C	1.69265500	-3.89501100	2.76978200	C	1.40447500	-4.12779600	2.58980100
C	2.52132800	-3.14731900	1.93856500	C	2.27738300	-3.39045000	1.79557700
C	1.96900500	-2.11049000	1.16998600	C	1.78970200	-2.28201500	1.08562800
C	2.70184200	-1.23474100	0.27665700	C	2.57407800	-1.41185400	0.23178200
C	4.02593400	-0.05524900	-0.98610300	C	3.96994800	-0.25026300	-0.96854200
H	1.34021000	-1.80881400	-2.47141600	H	1.15147200	-1.81531000	-2.53125900
H	-1.98799700	-3.91836100	-4.18467500	H	-2.31926100	-3.65532900	-4.27349900
H	-3.49325700	-2.97999500	-2.45789500	H	-3.74787900	-2.67856100	-2.50396400
H	-1.28251900	-2.36332500	2.13931300	H	-1.47198800	-2.38838100	2.04949200
H	2.10802500	-4.69961600	3.36820800	H	1.76961600	-4.98680100	3.14362200
H	3.58167700	-3.36741800	1.89291300	H	3.32160900	-3.67394200	1.73224800
C	0.17772000	2.67967800	1.09024300	C	0.32443800	2.62823300	1.15582100
C	0.34523300	3.76952900	1.95048600	C	0.53197300	3.69344400	2.11030000
C	0.68819700	3.53945600	3.28060700	C	0.89241500	3.39559600	3.39711100
H	0.20767000	4.77863300	1.58915100	H	0.38438800	4.71856500	1.80051800
C	0.67108600	1.19123000	2.81842000	C	0.78877800	1.03478000	2.83613000
C	0.85320900	2.23017700	3.72654100	C	1.05060100	2.03956100	3.78187100
H	0.78255700	0.15462700	3.11404400	H	0.86149800	-0.01214000	3.11241700
H	1.11640900	2.00773600	4.75401300	H	1.33999100	1.76395600	4.78847900
N	0.34562200	1.40130700	1.53398500	N	0.42568800	1.27723600	1.58459400
N	4.00857100	-1.11847200	-0.10836400	N	3.88743400	-1.35057300	-0.14171400
C	5.13434100	-1.93222700	0.28966600	C	4.96721600	-2.23553900	0.23246400
C	5.95596700	-1.49407500	1.32906800	C	5.75480200	-1.91434800	1.33876600
C	5.37718100	-3.13099300	-0.38310700	C	5.20165500	-3.38157100	-0.52894800

C	7.04263700	-2.28435300	1.70630000	C	6.79655400	-2.77181500	1.69434000
H	5.74464000	-0.55573600	1.83031100	H	5.55155800	-1.01332800	1.90738400
C	6.46564700	-3.91214900	0.00580400	C	6.24620100	-4.23057600	-0.16158400
C	7.29562200	-3.49031200	1.04803900	C	7.04049100	-3.92712800	0.94740100
H	8.14168300	-4.10152100	1.34600900	H	7.85198200	-4.59091900	1.22850600
N	-3.97635500	-1.22287300	-0.02439700	N	-4.09336200	-0.96360300	-0.01364000
C	-5.08751200	-1.93558100	-0.61201100	C	-5.25468400	-1.58277300	-0.61108400
C	-5.41098900	-3.20526200	-0.13160700	C	-5.64783300	-2.84915300	-0.17625800
C	-5.81438600	-1.33157400	-1.63904600	C	-5.95769700	-0.89383400	-1.60047100
C	-6.48515100	-3.88748100	-0.70460300	C	-6.76927400	-3.44147700	-0.75815900
C	-6.88551900	-2.02500500	-2.20327300	C	-7.07684300	-1.49818400	-2.17406100
H	-5.54246900	-0.34039300	-1.98593400	H	-5.63091200	0.09244500	-1.91197800
C	-7.21916900	-3.29977300	-1.73801400	C	-7.48060800	-2.76862000	-1.75496800
H	-8.05357400	-3.83498300	-2.18015700	H	-8.35209500	-3.23405400	-2.20446100
H	-0.32097700	-4.18208300	3.47992200	H	-0.62218300	-4.32718900	3.29252200
H	0.42403300	-3.31710300	-4.17758900	H	0.12556100	-3.20951200	-4.27429700
H	-6.74664500	-4.87613600	-0.34185800	H	-7.08525200	-4.42658500	-0.43094700
H	-7.45794800	-1.56772300	-3.00365200	H	-7.63172200	-0.97497900	-2.94588500
H	6.66471600	-4.84708500	-0.50766800	H	6.43851600	-5.12597200	-0.74350200
C	-5.26239600	-0.07523600	1.84742100	C	-5.28672100	0.21444800	1.90072400
H	7.68874400	-1.95608800	2.51385000	H	7.41557800	-2.53513800	2.55349200
C	5.26380200	0.46052400	-1.66053000	C	5.23748000	0.21849700	-1.62280100
F	4.95525200	1.44622500	-2.51105000	F	4.99806800	1.28903000	-2.38835300
F	6.14530700	0.94022400	-0.75800400	F	6.16423200	0.55315000	-0.70156600
F	5.88723300	-0.51747800	-2.34765600	F	5.77123400	-0.74879500	-2.39569000
F	-6.21973900	0.44512200	1.05247900	F	-6.19271700	0.85333300	1.13287700
F	-4.99789200	0.80325100	2.82133800	F	-4.95190600	1.01733800	2.91677200
F	-5.77123000	-1.19144100	2.40883200	F	-5.88914800	-0.88196500	2.40434000
H	-4.83025300	-3.64596300	0.67153500	H	-5.08369500	-3.35626200	0.59900500
H	4.72454300	-3.44139800	-1.19205400	H	4.57631900	-3.59969000	-1.38803600
H	0.82090600	4.37708500	3.95699900	H	1.04415000	4.19061000	4.11928700
C	-0.71348300	1.99523600	-2.30456000	C	-0.79613500	2.08615600	-2.13001500
C	-0.74836900	3.36425100	-2.38020000	C	-0.72301700	3.47795300	-2.18037700
H	-0.90647300	1.26155100	-3.07127300	H	-1.14891100	1.41750100	-2.90146600
H	-0.97009500	4.03589300	-3.19397600	H	-0.95939600	4.16302000	-2.97916400
C	-0.19406500	2.75785700	-0.32273200	C	0.00719300	2.77404500	-0.18281500
N	-0.41911000	3.84294600	-1.12782200	N	-0.19195000	3.91790100	-0.98086700
N	-0.37034600	1.63734900	-1.03013000	N	-0.32920000	1.64243800	-0.95928200
C	-0.33775700	5.24739500	-0.80893000	C	0.23092600	5.26275600	-0.74501300
C	0.88623100	5.90782300	-0.93631100	C	1.56333800	5.53238600	-0.40817500
C	-1.49267500	5.92593700	-0.41406900	C	-0.68948500	6.30385100	-0.90746900
C	0.95326300	7.27181100	-0.64806200	C	1.96520200	6.85394800	-0.21633500
H	1.76646100	5.35840300	-1.25331800	H	2.27269400	4.71764600	-0.30669100
C	-1.41333400	7.29022300	-0.12974900	C	-0.27021000	7.62272100	-0.72968900

H	-2.43213600	5.38984400	-0.32907100	H	-1.72092300	6.07887900	-1.15914000
C	-0.19317500	7.96122100	-0.24447700	C	1.05317600	7.90051900	-0.37895800
H	1.90011900	7.79368500	-0.74194200	H	2.99698100	7.06480200	0.04681100
H	-2.30475700	7.82613400	0.17985600	H	-0.98356800	8.43116400	-0.85499500
H	-0.13616600	9.02208400	-0.02174400	H	1.37321000	8.92750600	-0.23410400