

Electronic Supplementary Information
Cationic Iridium Complexes with an Alkyl-linked Bulky
Group at the Cyclometalating Ligand: Synthesis,
Characterizations, and Suppression of Phosphorescence
Concentration-quenching

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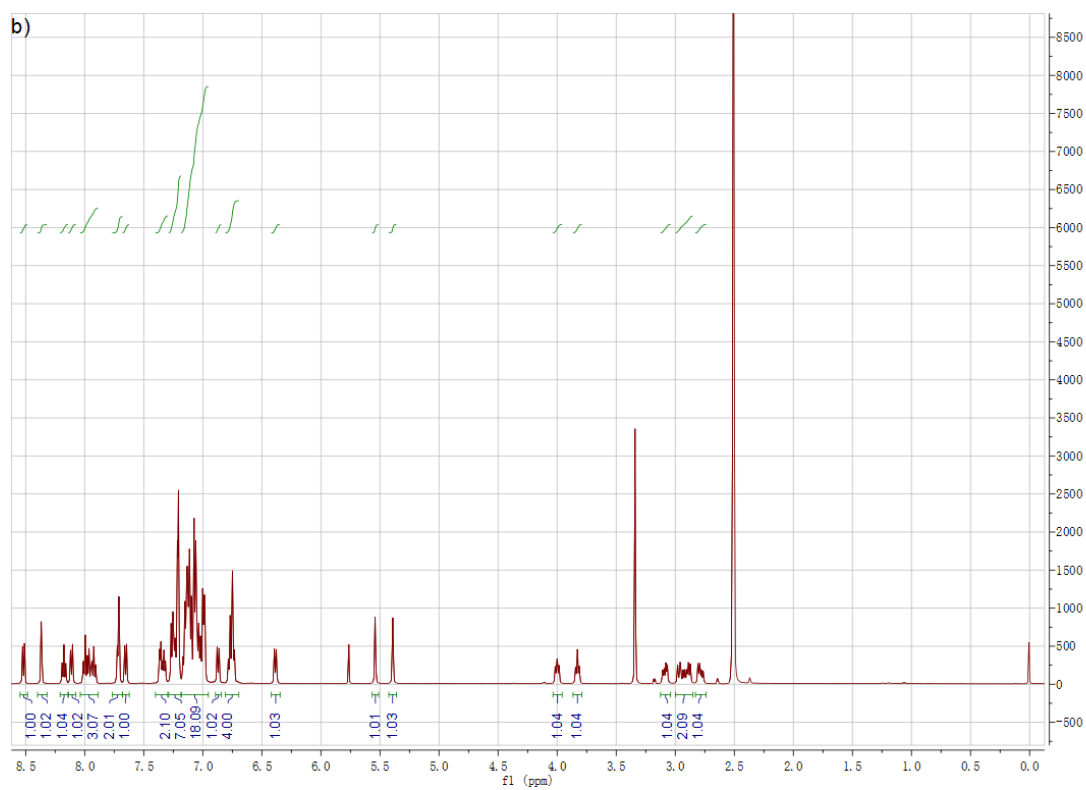
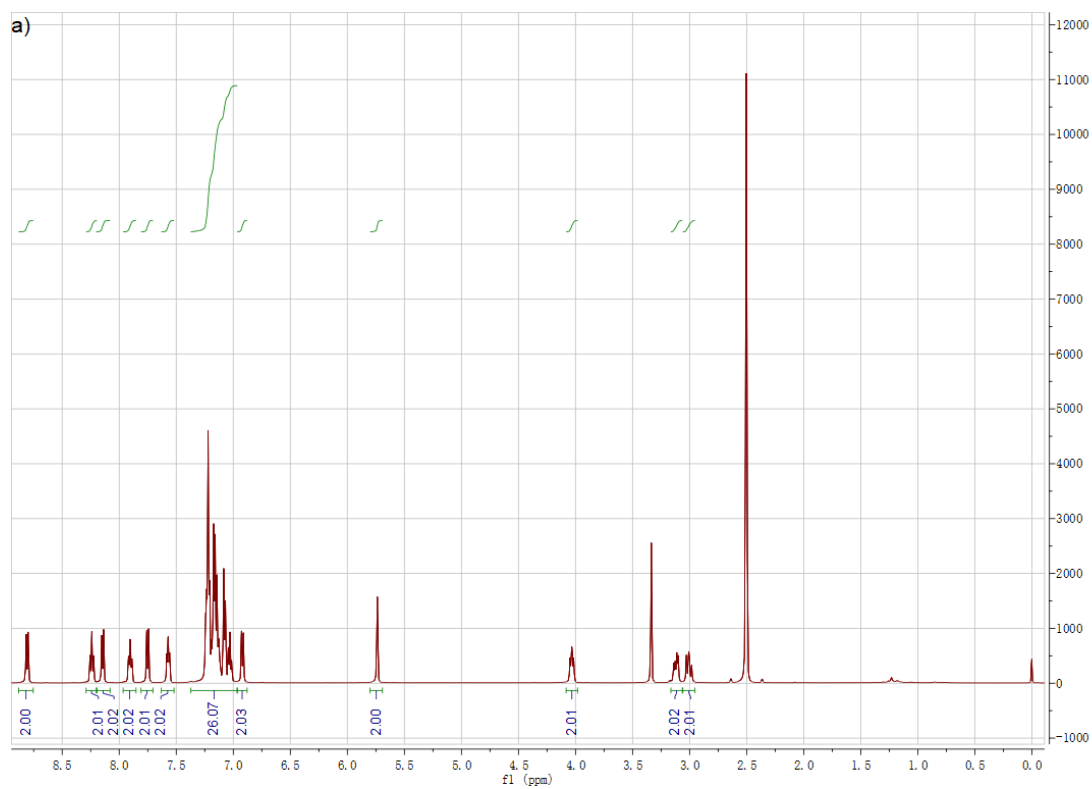
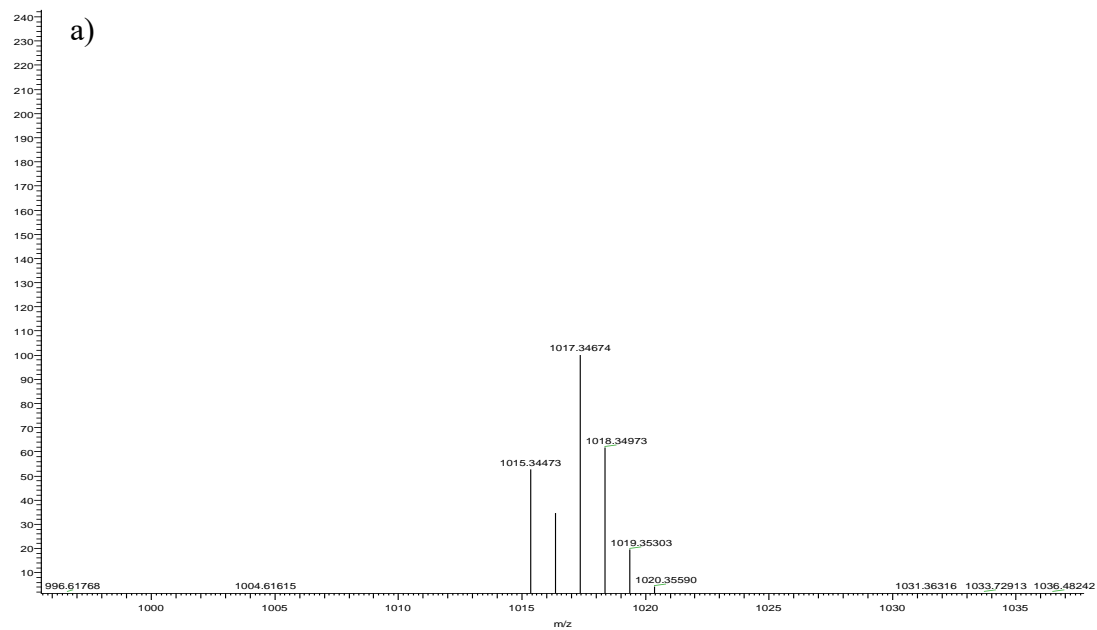


Figure S1. ^1H NMR spectra of a) complex 1 and b) complex 2 in $\text{DMSO-}d_6$. The single peak at 5.76 in the spectrum of complex 2 arises from the H^1 NMR signal of residual CH_2Cl_2 solvent because complex 2 was recrystallized from $\text{CH}_2\text{Cl}_2/\text{hexane}$ solution.

15 #19 RT: 0.16 AV: 1 NL: 4.40E5
T: FTMS + c ESI Full ms [150.00-1500.00]



16 #14 RT: 0.12 AV: 1 NL: 6.21E5
T: FTMS + c ESI Full ms [150.00-1500.00]

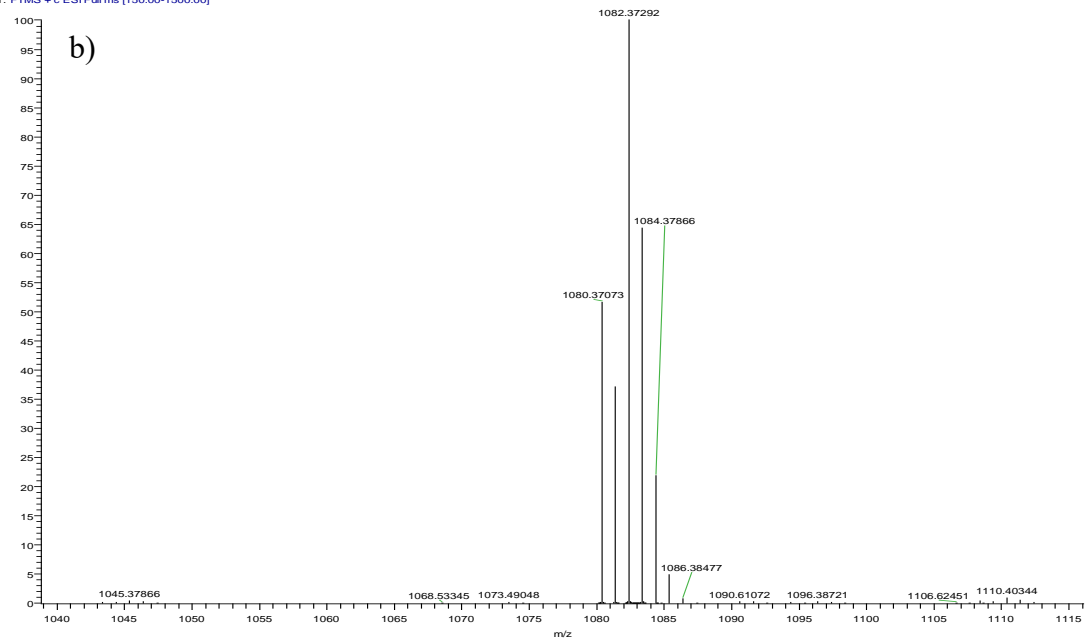
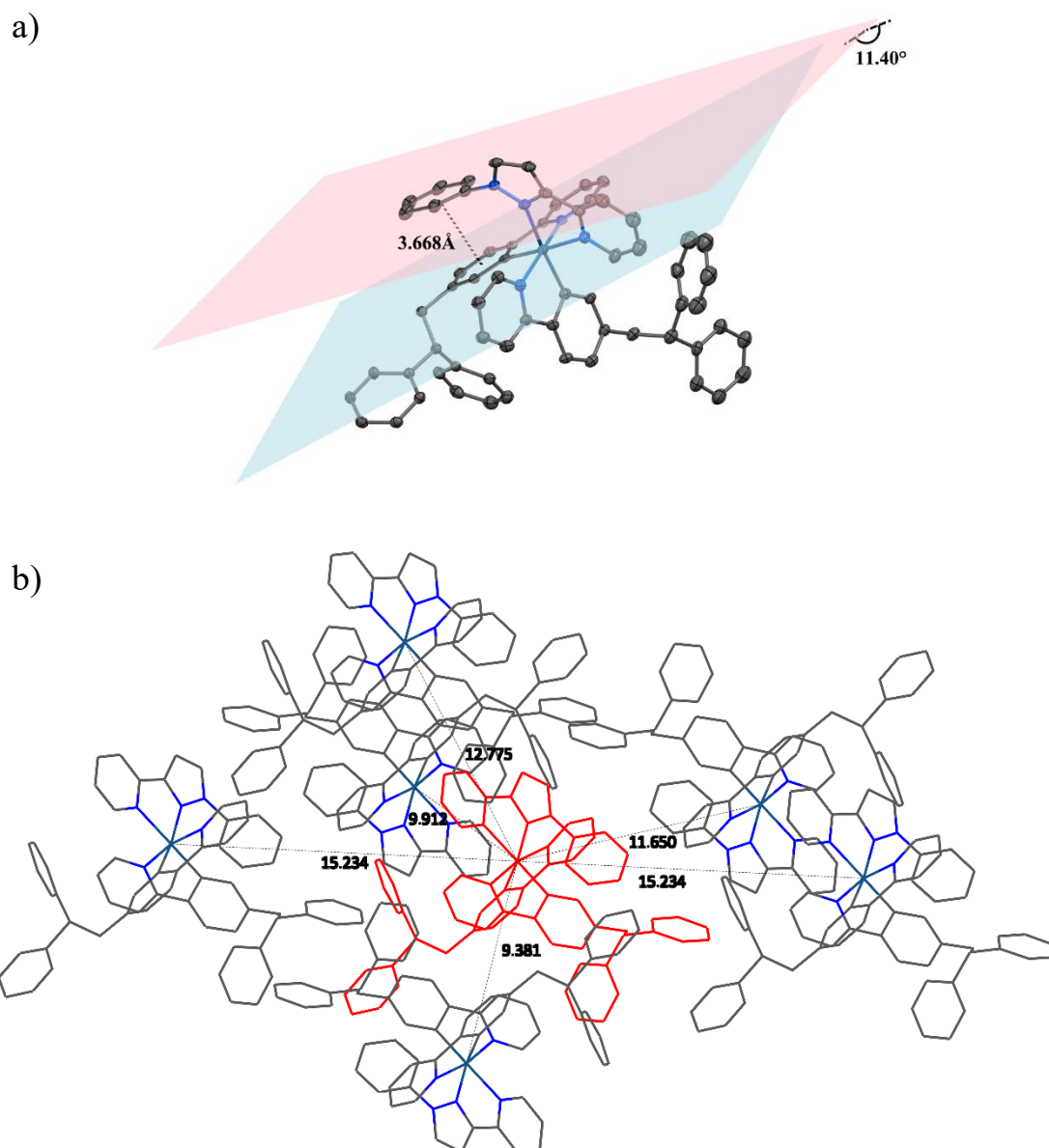


Figure S2. HRMS spectra of a) complex 1 and b) complex 2.

Table S1. Selected bond lengths and dihedral angles for complexes 1 and 2

State	Bond length (Å)			Bite angles (°)		
	Ir-C [^] N [^] ^a	Ir-N [^] C [^] N [^] ^b	Ir-N [^] N [^] N [^] ^c	Φ ₁ ^d	Φ ₂ ^e	
1	S ₀	2.023/2.023	2.083/2.083	2.211/2.211	80.1/80.1	74.9
	T ₁	1.997/1.997	2.082/2.082	2.199/2.199	80.9/80.9	75.4
2	crystal	2.000/2.013	2.065/2.058	2.187/2.145	80.5/80.5	74.9
	S ₀	2.025/2.014	2.080/2.084	2.277/2.241	80.3/80.0	73.8
	T ₁	1.986/2.010	2.056/2.097	2.264/2.314	81.8/80.3	72.9
	T ₃	2.005/1.988	2.083/2.082	2.234/2.239	80.9/81.0	74.0

^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 angle of N[^]N ligand. ^f The dihedral angle between the phenyl and pyridine rings of C[^]N ligand. ^g The dihedral angle between the pyridine rings or between the pyridine and pyrazole rings of N[^]N ligand.



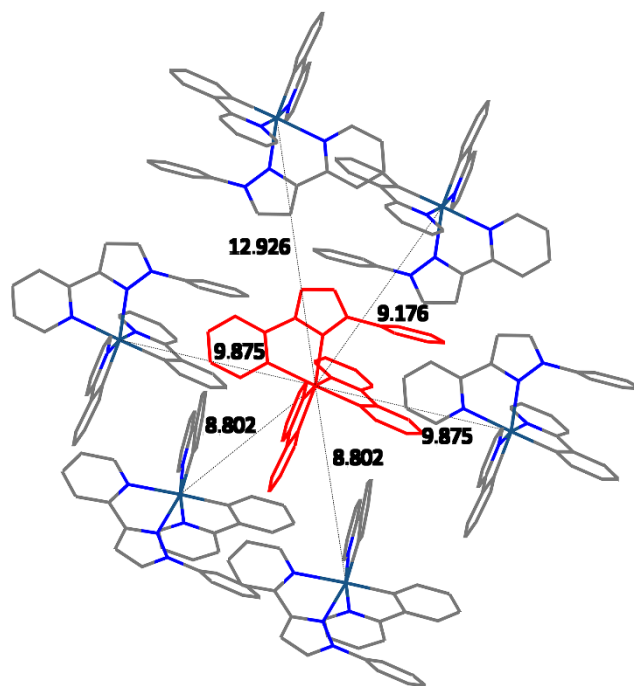


Figure S4. Ir-to-Ir distances (in Å) in the single crystal structure of [Ir(ppy)₂(phzpy)]PF₆; the central iridium complex was marked in red.

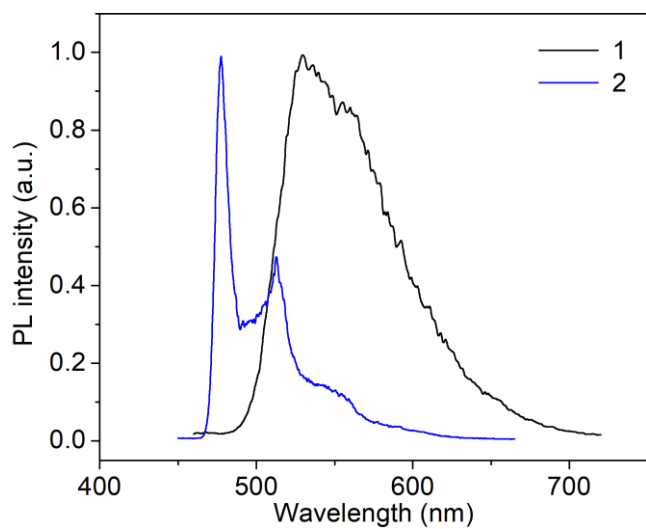


Figure S5. PL spectra of complexes 1 and 2 at 77 K in CH₃CN glass.

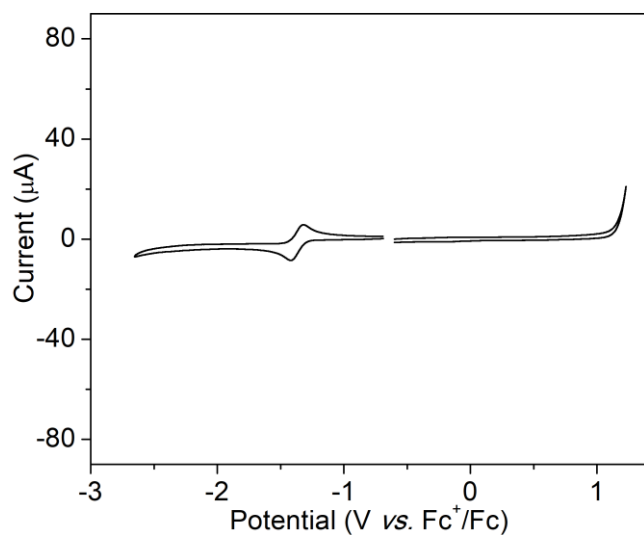


Figure S6. The blank test for cyclic voltammetry measurement in DMF solution. The only difference between the blank test and the sample test is that in the former, no sample was added in the solution.

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

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

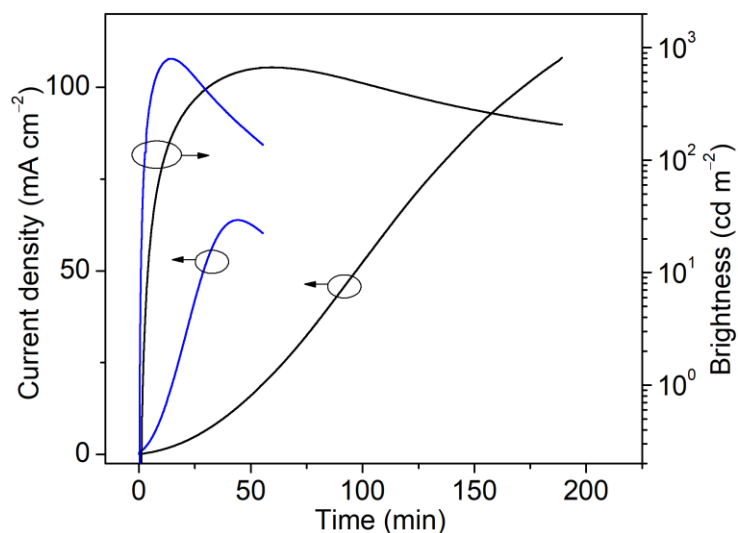


Figure S7. Time-dependent current-density and brightness curves of the LECs based on $[\text{Ir}(\text{ppy})_2(\text{phzpy})]\text{PF}_6$ at 5.0 V. a) device C and b) device D.

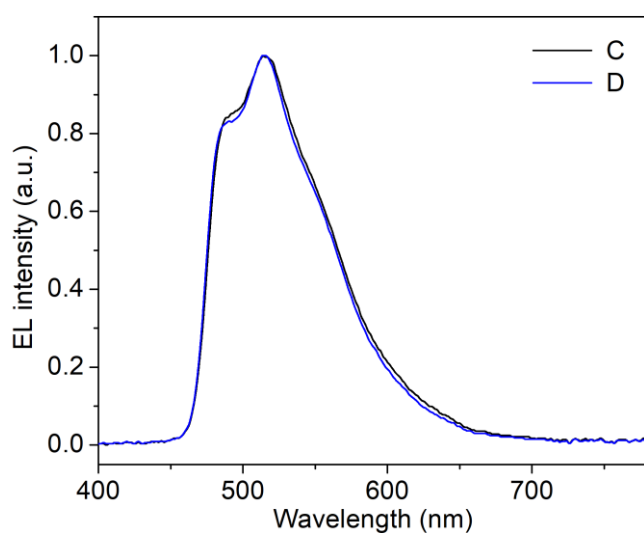


Figure S8. EL spectra of devices C and D.

Table S3. Cartesian coordinates of optimized geometries for complexes 1 and 2.

Complex 1

S_0				T_1			
Ir	0.00020824	-2.22128583	-0.00000254	Ir	-0.00004092	-2.12046307	-0.00000460
N	-0.85933579	-2.10847568	1.89379256	N	-0.84413476	-2.05550017	1.90172428
C	-1.92613324	-2.82708151	2.29803458	C	-1.91284469	-2.77282645	2.29197027
H	-2.35082804	-3.50309951	1.56691995	H	-2.36198503	-3.40677098	1.53824109
C	-2.46208342	-2.71220331	3.57203258	C	-2.41340448	-2.70019621	3.58605603
H	-3.32205241	-3.31042153	3.84914732	H	-3.27818623	-3.29298447	3.85919969
C	-1.86881165	-1.81721166	4.46649808	C	-1.78207729	-1.85859825	4.50298181

H	-2.26042197	-1.69955836	5.47166058	H	-2.14817071	-1.77753802	5.52090761
C	-0.77000221	-1.07555997	4.05386958	C	-0.67348513	-1.12236229	4.09930142
H	-0.29939013	-0.37483148	4.73271031	H	-0.16961669	-0.46599956	4.79794946
C	-0.26521275	-1.22578798	2.75414262	C	-0.20697197	-1.23092272	2.78478236
C	0.87785834	-0.50885818	2.18955618	C	0.94976474	-0.53126168	2.22283565
C	1.66384794	0.39929876	2.91604624	C	1.75858811	0.34888306	2.94653198
H	1.43716302	0.62158243	3.95483595	H	1.54974492	0.57233192	3.98762833
C	2.75499168	1.02191764	2.31899232	C	2.86175223	0.94729856	2.33888843
H	3.35063624	1.71485360	2.90370409	H	3.48029416	1.61483424	2.92898351
C	3.07835619	0.75723173	0.97808184	C	3.18226598	0.69471293	0.98973741
C	2.27292879	-0.14036973	0.25802889	C	2.35522323	-0.17097625	0.26807407
H	2.53059449	-0.33505112	-0.77996734	H	2.59648267	-0.36800177	-0.77207854
C	1.17730239	-0.80139338	0.83100510	C	1.23605650	-0.79998832	0.84715155
N	0.85972938	-2.10827428	-1.89380018	N	0.84405356	-2.05550787	-1.90173343
C	-1.17708269	-0.80151986	-0.83094268	C	-1.23611650	-0.79996466	-0.84715617
C	1.92662133	-2.82671713	-2.29808240	C	1.91275190	-2.77285014	-2.29198188
C	0.26547908	-1.22562944	-2.75410732	C	0.20690327	-1.23091812	-2.78478910
C	-0.87768960	-0.50888394	-2.18948336	C	-0.94982170	-0.53123961	-2.22283980
C	-2.27279984	-0.14067924	-0.25793114	C	-2.35527046	-0.17093306	-0.26807534
H	2.35140998	-3.50271509	-1.56700365	H	2.36188251	-3.40680378	-1.53825460
C	2.46254782	-2.71170767	-3.57207862	C	2.41331207	-2.70022459	-3.58606773
C	0.77023990	-1.07527372	-4.05383061	C	0.67341755	-1.12236164	-4.09930810
C	-1.66381638	0.39918989	-2.91592852	C	-1.75863088	0.34892081	-2.94653310
C	-3.07836611	0.75683225	-0.97794081	C	-3.18229938	0.69477194	-0.98973551
H	-2.53043155	-0.33544101	0.78005860	H	-2.59653058	-0.36795503	0.77207778
H	3.32259561	-3.30979716	-3.84922664	H	3.27808420	-3.29302595	-3.85921342
C	1.86914855	-1.81675598	-4.46649936	C	1.78199774	-1.85861423	-4.50299100
H	0.29952764	-0.37457934	-4.73263700	H	0.16955930	-0.46598895	-4.79795413
H	-1.43717038	0.62155295	-3.95470980	H	-1.54978498	0.57236851	-3.98762915
C	-2.75504923	1.02162352	-2.31884136	C	-2.86178339	0.94735469	-2.33888661
H	2.26073674	-1.69900344	-5.47165889	H	2.14809187	-1.77755721	-5.52091682
H	-3.35079659	1.71449922	-2.90351918	H	-3.48031387	1.61490302	-2.92897938
C	-4.30491397	1.34553499	-0.30074979	C	-4.41953853	1.27276996	-0.32762330
H	-5.13590076	0.63652718	-0.41775539	H	-5.25434503	0.58071814	-0.50133571
H	-4.12774706	1.39795893	0.77959445	H	-4.27341958	1.27912012	0.75773102
C	-4.81450912	2.71543391	-0.81177029	C	-4.88787499	2.67102792	-0.80304634
H	-5.06684056	2.59626435	-1.87173194	H	-5.13584230	2.58906657	-1.86735165
C	-6.12713450	3.06408727	-0.10330423	C	-6.19745671	3.03197800	-0.09455788
C	-7.35217904	2.83515783	-0.74495941	C	-7.42196487	2.83140762	-0.74659594
C	-6.14445029	3.57518400	1.20284282	C	-6.21342008	3.52468955	1.21837118
C	-8.56293764	3.10666874	-0.10261259	C	-8.63171550	3.11324882	-0.10716460
H	-7.35816625	2.44145152	-1.75870990	H	-7.42838554	2.45192213	-1.76570056
C	-7.35196133	3.84645994	1.84875979	C	-7.42030849	3.80644874	1.86111051
H	-5.20697610	3.77378540	1.71467840	H	-5.27632956	3.70090955	1.73868927

C	-8.56686467	3.61355361	1.19827498	C	-8.63478758	3.60208159	1.20065069
H	-9.50056088	2.92531551	-0.62070421	H	-9.56908970	2.95421273	-0.63283825
H	-7.34367987	4.24395294	2.85994086	H	-7.41146171	4.18977427	2.87767771
H	-9.50611835	3.82871418	1.69958455	H	-9.57331804	3.82532123	1.69970061
C	-3.80127339	3.85486255	-0.72436427	C	-3.84043384	3.77498340	-0.67852325
C	-3.92688221	4.93903575	-1.60780191	C	-3.89852418	4.86240043	-1.56474140
C	-2.76877027	3.88963759	0.22255896	C	-2.84024318	3.77381831	0.30384230
C	-3.05551529	6.02609398	-1.54642002	C	-2.99310155	5.91896596	-1.47178442
H	-4.72072937	4.92840302	-2.35108456	H	-4.66620346	4.87867935	-2.33476948
C	-1.89340564	4.97824089	0.28941725	C	-1.93067114	4.83142721	0.40143741
H	-2.63255222	3.06145413	0.91068209	H	-2.75748431	2.94397980	0.99875748
C	-2.03353404	6.05062637	-0.59288362	C	-2.00429086	5.90786673	-0.48393454
H	-3.17223471	6.85177797	-2.24287052	H	-3.05753084	6.74833678	-2.17050092
H	-1.09601297	4.98210880	1.02673995	H	-1.16025916	4.80919837	1.16665569
H	-1.35312180	6.89577604	-0.54112261	H	-1.29848553	6.72978610	-0.40765891
C	4.30482399	1.34615483	0.30093980	C	4.41951987	1.27268597	0.32763087
H	5.13597180	0.63735996	0.41809219	H	5.25430722	0.58061098	0.50134318
H	4.12774342	1.39843204	-0.77942497	H	4.27340671	1.27904659	-0.75772437
C	4.81403797	2.71623023	0.81187591	C	4.88789412	2.67092757	0.80306569
H	5.06632572	2.59721771	1.87186509	H	5.13577314	2.58897110	1.86739210
C	6.12662697	3.06515242	0.10347424	C	6.19755312	3.03179104	0.09467654
C	7.35168235	2.83649040	0.74520462	C	7.42199636	2.83117462	0.74682218
C	6.14391191	3.57622426	-1.20268257	C	6.21365106	3.52446582	-1.21826473
C	8.56242154	3.10823945	0.10292276	C	8.63181493	3.11293522	0.10748391
H	7.35769216	2.44280518	1.75896318	H	7.42831203	2.45171682	1.76593780
C	7.35140432	3.84773869	-1.84853487	C	7.42060774	3.80614415	-1.86091127
H	5.20642611	3.77461731	-1.71457699	H	5.27661284	3.70071983	-1.73866547
C	8.56631824	3.61509887	-1.19797507	C	8.63502116	3.60173176	-1.20034460
H	9.50005245	2.92709268	0.62107268	H	9.56913712	2.95386472	0.63323989
H	7.34309857	4.24520952	-2.85972446	H	7.41186568	4.18944206	-2.87748979
H	9.50555610	3.83044578	-1.69923430	H	9.57360480	3.82490872	-1.69932259
C	3.80051426	3.85538972	0.72430589	C	3.84052636	3.77494120	0.67843757
C	3.92574043	4.93963346	1.60771106	C	3.89860474	4.86236856	1.56464381
C	2.76811180	3.88985708	-0.22273931	C	2.84042082	3.77382040	-0.30401453
C	3.05410117	6.02646525	1.54618054	C	2.99325141	5.91898522	1.47159365
H	4.71950429	4.92923488	2.35108572	H	4.66621949	4.87861466	2.33473694
C	1.89247409	4.97823149	-0.28974533	C	1.93091845	4.83148066	-0.40170324
H	2.63219102	3.06161132	-0.91084618	H	2.75767441	2.94397634	-0.99892456
C	2.03222440	6.05069231	0.59252460	C	2.00452420	5.90792843	0.48365977
H	3.17052687	6.85220936	2.24260887	H	3.05766911	6.74836277	2.17030326
H	1.09516676	4.98186411	-1.02716163	H	1.16057078	4.80928538	-1.16698722
H	1.35160105	6.89566476	0.54064701	H	1.29877257	6.72988718	0.40731216
C	-0.62334145	-5.19422568	-0.40094315	C	-0.61483272	-5.10302922	-0.35905942
C	-1.24369650	-6.36736372	-0.84418945	C	-1.30292424	-6.28123652	-0.77231493

C	-2.41610780	-6.28707668	-1.59005481	C	-2.48311113	-6.20019975	-1.46892609
H	-0.81791821	-7.33595907	-0.61717147	H	-0.88430658	-7.25185629	-0.53408349
C	-2.28222426	-3.90393399	-1.41697506	C	-2.32913164	-3.80613847	-1.36226627
C	-2.94839716	-5.03280667	-1.88198184	C	-3.02134906	-4.92263163	-1.78006654
H	-2.90272280	-7.19207530	-1.93746253	H	-2.99726720	-7.10466516	-1.77864259
H	-2.65113509	-2.90461320	-1.61573746	H	-2.70532496	-2.81133344	-1.57063113
H	-3.85893895	-4.92164964	-2.45920537	H	-3.94964247	-4.81101078	-2.32765147
C	0.62419157	-5.19415721	0.40076091	C	0.61470007	-5.10304078	0.35904131
C	1.24473098	-6.36723063	0.84392044	C	1.30277103	-6.28126103	0.77229412
C	2.28286533	-3.90368022	1.41689874	C	2.32902131	-3.80618224	1.36225160
C	2.41712614	-6.28681469	1.58979717	C	2.48295920	-6.20024648	1.46890569
H	0.81910785	-7.33587630	0.61682618	H	0.88413649	-7.25187296	0.53406041
C	2.94921377	-5.03248246	1.88182478	C	3.02121930	-4.92268841	1.78004926
H	2.65161784	-2.90431606	1.61573669	H	2.70523181	-2.81138423	1.57061894
H	2.90388385	-7.19176266	1.93713673	H	2.99709947	-7.10472152	1.77862019
H	3.85973441	-4.92122490	2.45906233	H	3.94951460	-4.81108501	2.32763454
N	-1.15054082	-3.97711466	-0.69506594	N	-1.16667020	-3.86105092	-0.66811752
N	1.15119909	-3.97698516	0.69497530	N	1.16655903	-3.86107285	0.66810258

Complex 2

S ₀			T ₁				
Ir	-1.37274450	-1.53927057	0.17645206	Ir	-1.11062156	-1.69397933	0.18048550
N	-1.87502506	-0.65741176	1.99639272	N	-1.72867932	-0.90692674	2.02294067
C	-3.12603936	-0.33833357	2.38337687	C	-3.00808524	-0.76557496	2.42037112
H	-3.91401291	-0.56297742	1.67702768	H	-3.76447285	-1.08221239	1.71403097
C	-3.39996812	0.24688899	3.61098107	C	-3.34829938	-0.23781560	3.65769177
H	-4.42314950	0.48634112	3.87559343	H	-4.39201115	-0.14086966	3.93218993
C	-2.33508055	0.51215503	4.47569149	C	-2.32157089	0.16023077	4.51752081
H	-2.51022324	0.96929219	5.44415014	H	-2.54901573	0.58027132	5.49184933
C	-1.04455703	0.18536048	4.08041152	C	-1.00138492	0.01476878	4.11108638
H	-0.20593850	0.38696233	4.73528466	H	-0.19305681	0.32115625	4.76344315
C	-0.81948677	-0.40368534	2.82841073	C	-0.71018368	-0.52701460	2.85184790
C	0.48183290	-0.79298836	2.28620100	C	0.62854472	-0.74638860	2.30238340
C	1.68861356	-0.67613902	2.99580390	C	1.81469892	-0.47948198	3.00526234
H	1.70090218	-0.27419057	4.00444931	H	1.78211382	-0.08076894	4.01459018
C	2.88352517	-1.08995867	2.42045687	C	3.04918873	-0.73621195	2.42139936
H	3.80574565	-1.01040106	2.98925193	H	3.95601957	-0.53894297	2.98617916
C	2.90180935	-1.62206298	1.11953241	C	3.13196517	-1.25901465	1.11887058
C	1.69068136	-1.73285434	0.42065100	C	1.94264028	-1.52598867	0.42641586
H	1.71435823	-2.15611907	-0.57923103	H	2.00847088	-1.94007890	-0.57477934
C	0.46429374	-1.33785122	0.97602851	C	0.68228162	-1.28548724	0.99108476
N	-0.69577455	-2.27181697	-1.64912252	N	-0.36817157	-2.34431651	-1.62332404
C	-1.07409794	0.20335683	-0.81134435	C	-1.10639301	0.04908955	-0.77061699

C	-0.58711824	-3.57933477	-1.95968199	C	-0.10198233	-3.61253858	-1.97256444
C	-0.31996938	-1.31998892	-2.55872956	C	-0.10123656	-1.30298496	-2.55253097
C	-0.51782126	0.05603336	-2.10912166	C	-0.49445317	-0.02758105	-2.12079471
C	-1.32626922	1.50842587	-0.36097873	C	-1.54817193	1.29590580	-0.31407898
H	-0.90105312	-4.27738800	-1.19457801	H	-0.33593157	-4.36895660	-1.23243884
C	-0.09566186	-4.01761015	-3.18032422	C	0.45318856	-3.96481913	-3.19546181
C	0.18608218	-1.71462305	-3.80631495	C	0.49397180	-1.63566054	-3.80898315
C	-0.23146724	1.18026695	-2.90197221	C	-0.35625796	1.17984672	-2.88313548
C	-1.06070683	2.63714806	-1.14823876	C	-1.45355641	2.45774892	-1.08554496
H	-1.75003282	1.66292262	0.62739618	H	-1.99296334	1.37119924	0.67416429
H	-0.02686834	-5.08003163	-3.38214004	H	0.64215668	-5.00930025	-3.41278205
C	0.30159306	-3.06224716	-4.11991189	C	0.77052405	-2.93831195	-4.13453863
H	0.48536315	-0.96125373	-4.52482359	H	0.71971305	-0.83666947	-4.50658888
H	0.18838992	1.06545524	-3.89718763	H	0.09783213	1.15756149	-3.86841129
C	-0.50251893	2.45637284	-2.42657465	C	-0.82933774	2.36255976	-2.38139025
H	0.69428158	-3.36613172	-5.08487107	H	1.22077723	-3.18779006	-5.08927489
H	-0.29400930	3.32036090	-3.05235822	H	-0.74241583	3.26487025	-2.98254355
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H	-1.90099880	4.58011948	-1.44720277	H	-2.59514740	4.23368161	-1.41104537
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C	-0.12074133	4.86100860	-0.25477788	C	-0.87957601	4.81818010	-0.23390030
H	0.60072770	4.75439364	-1.07334689	H	-0.15498683	4.82404709	-1.05674586
C	-0.40379901	6.35752171	-0.11598192	C	-1.41055049	6.24669914	-0.11474457
C	0.64965404	7.26578074	-0.30984782	C	-0.54482367	7.31739405	-0.38988896
C	-1.66493980	6.87070786	0.21766765	C	-2.72446321	6.54327076	0.27461153
C	0.45361885	8.63964802	-0.17315126	C	-0.97291304	8.64013661	-0.27759113
H	1.63528728	6.88727222	-0.57032204	H	0.47736125	7.10782446	-0.69619071
C	-1.86562658	8.24798129	0.35735864	C	-3.15750331	7.86802118	0.38972982
H	-2.50556049	6.20046524	0.36732938	H	-3.42579332	5.74234824	0.48625974
C	-0.80879112	9.13770960	0.16316912	C	-2.28480584	8.92139914	0.11482800
H	1.28427722	9.32159890	-0.33267187	H	-0.28447432	9.45062459	-0.50035488
H	-2.85239644	8.62220671	0.61574673	H	-4.18089287	8.07295904	0.69166679
H	-0.96580768	10.20727101	0.26870075	H	-2.62267108	9.95007774	0.20084048
C	0.55149418	4.30385939	1.00063512	C	-0.11664176	4.39120779	1.01987709
C	1.77429735	3.62623223	0.91148692	C	1.19877104	3.91864049	0.92195364
C	-0.03952745	4.44907312	2.26535115	C	-0.70994164	4.45145537	2.29031321
C	2.39213336	3.10475706	2.05168819	C	1.90542773	3.51602418	2.05878212
H	2.25034646	3.50233622	-0.05778630	H	1.67847394	3.86391963	-0.05190184
C	0.57301431	3.92877992	3.40603150	C	-0.00850402	4.05006067	3.42793073
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C	1.79370477	3.25455998	3.30382682	C	1.30417577	3.58125083	3.31685559
H	3.33850744	2.58072196	1.95450640	H	2.92380728	3.15243887	1.95497172
H	0.10042685	4.05521007	4.37625704	H	-0.48484537	4.10898119	4.40274052
H	2.27344848	2.85385895	4.19217780	H	1.85220929	3.27410878	4.20302418

C	4.20000793	-2.10510927	0.50322685	C	4.47826860	-1.55844558	0.49029166
H	4.61816966	-2.90162142	1.13129619	H	5.00094368	-2.30444310	1.10184967
H	4.00047581	-2.56493149	-0.47012977	H	4.33345013	-2.02286474	-0.49040119
C	5.30824599	-1.02269969	0.36023635	C	5.43238415	-0.33615744	0.36341131
H	5.48441809	-0.61670022	1.36257627	H	5.57204143	0.06112698	1.37502949
C	6.62179865	-1.67749952	-0.07566554	C	6.81266802	-0.80098397	-0.10800411
C	7.64301152	-1.88960872	0.86080576	C	7.85173596	-0.95404148	0.82062791
C	6.82696485	-2.11221238	-1.39369455	C	7.06728948	-1.11915622	-1.45027485
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H	7.50305784	-1.55827888	1.88703083	H	7.67354674	-0.71076816	1.86546791
C	8.01623658	-2.74313008	-1.76249884	C	8.32318458	-1.57892946	-1.85063362
H	6.05692321	-1.94692950	-2.14181319	H	6.28289714	-0.99591592	-2.19147485
C	9.02665810	-2.94882346	-0.81900628	C	9.35077520	-1.72669519	-0.91507066
H	9.61525534	-2.66899454	1.23744568	H	9.90218646	-1.51861091	1.16031461
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H	9.95350157	-3.43642076	-1.10710329	H	10.32902120	-2.08029429	-1.22779045
C	4.93742691	0.16214101	-0.52915272	C	4.89074695	0.81471507	-0.48144190
C	5.46145640	1.42801757	-0.22215208	C	5.26017698	2.12761797	-0.14797368
C	4.12957454	0.04209868	-1.66892122	C	4.06915986	0.62505828	-1.60182930
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H	6.09204317	1.54275002	0.65640357	H	5.89743395	2.29579006	0.71706804
C	3.85936369	1.14951297	-2.47821444	C	3.63573701	1.71232020	-2.36652331
H	3.69812608	-0.91777284	-1.93411525	H	3.75226468	-0.37338017	-1.88555122
C	4.39107204	2.40102572	-2.16239623	C	4.01453481	3.01164311	-2.02466605
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C	-1.10363068	-5.44172391	2.43765184	C	-0.38129808	-5.56404450	2.43598050
H	0.15970278	-3.77170292	1.88981099	H	0.68947383	-3.78126083	1.84346620
H	-2.64396450	-6.91804520	2.78298208	H	-1.75202119	-7.18705743	2.83301949
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C	-5.31754718	-3.44164699	-0.00506779	C	-4.84295038	-4.04179482	0.09668306
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H	-3.24179562	-1.18541018	-3.21998157	H	-2.94081097	-1.75366968	-3.18367139
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C	-4.67661171	1.90614114	-3.32386958	C	-4.75247896	1.10886671	-3.57236940
H	-3.30937538	0.86554588	-4.62867278	H	-3.20788297	0.16465359	-4.74605982
H	-6.03756501	2.68691792	-1.84174584	H	-6.26354650	1.81040059	-2.20014484
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T₃							
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H	-1.80893100	-0.05898000	-4.09085000				
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C	-3.28891600	-0.99027000	-1.15947000				
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C	-0.85324600	-1.22267200	-1.00030300				
N	0.08688500	-2.29819800	1.67561200				
C	1.13170800	-0.02093800	0.83382900				
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C	-0.91226900	-3.83774900	3.20892200				
C	-0.54314400	-1.55386400	3.86283900				
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H	2.16188400	1.20073700	-0.62256400				

H	-1.25785600	-4.84555300	3.40615800			
C	-1.01187500	-2.82836900	4.16715800			
H	-0.60366000	-0.75992700	4.59693800			
H	0.19729400	1.13896400	3.94280900			
C	1.21200800	2.28579500	2.44611200			
H	-1.44559800	-3.03110900	5.14058200			
H	1.24774300	3.17351700	3.07157100			
C	2.42356000	3.59920500	0.65459400			
H	3.03027900	4.03136700	1.45858700			
H	3.10321700	3.36302100	-0.17000900			
C	1.39223200	4.67289700	0.19817500			
H	0.64942700	4.75875400	1.00018200			
C	2.01131300	6.06071600	0.02832800			
C	1.18776500	7.18883600	0.17331200			
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C	1.69411800	8.47777500	0.00988600			
H	0.13709700	7.05136400	0.41754200			
C	3.87390000	7.55505200	-0.45012300			
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C	3.04331900	8.66633600	-0.30446300			
H	1.03745600	9.33465200	0.13193300			
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H	3.44178400	9.66883800	-0.43040600			
C	0.63643100	4.23668600	-1.05732600			
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C	-1.40993600	3.45222500	-2.11916400			
H	-1.21811800	3.87438200	-0.01801000			
C	0.57313200	3.79737500	-3.45053400			
H	2.30724900	4.50681300	-2.39802500			
C	-0.77096500	3.42235600	-3.35980300			
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C	-6.85864100	-0.00809100	0.06298900			
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C	-4.68856500	1.18360200	0.64669300			
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H	-5.21002100	2.92866000	-0.50523600			
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H	-1.27471200	-3.76682800	-1.51739000			
H	0.96809000	-7.13799100	-3.01004500			
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C	5.05422900	-3.06352900	0.11361500			
H	4.96735800	-4.81046700	-1.19720200			
H	6.09338200	-2.87332600	0.33613700			
N	2.81714100	-2.76577400	0.33091600			
N	4.07015500	-2.25478700	0.66035000			
C	3.05669500	-3.83228900	-0.51417700			
C	4.27660500	-1.42950600	1.79453500			
C	3.49752600	-1.58232300	2.94806000			
C	5.31543700	-0.48735000	1.76302300			
C	3.76034900	-0.78983300	4.06507400			
H	2.71495500	-2.33121700	2.96434000			
C	5.57778400	0.28689100	2.89170200			
H	5.90361500	-0.36281300	0.85927900			
C	4.80003300	0.14344000	4.04519800			
H	3.15615900	-0.91361100	4.95888600			
H	6.38428500	1.01337500	2.86423000			

H	5.00274200	0.75424900	4.91936100			
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