Supporting Information

Tuning alkynyl-extended 9,10-dihydroanthracene-based systems into aggregation-induced emission (AIE) luminophores

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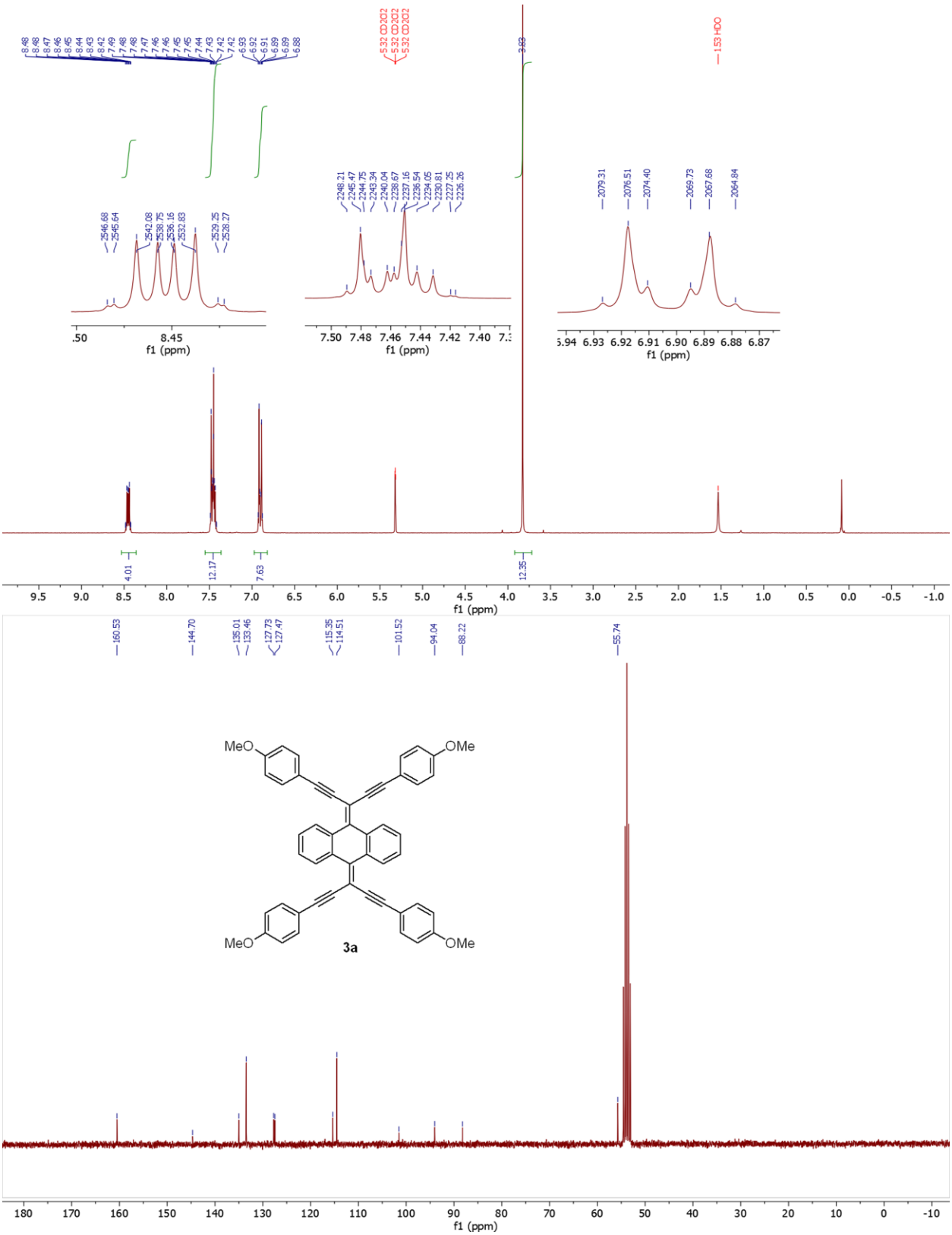

Fig. S-1. ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra of **3a** measured in CD_2Cl_2.

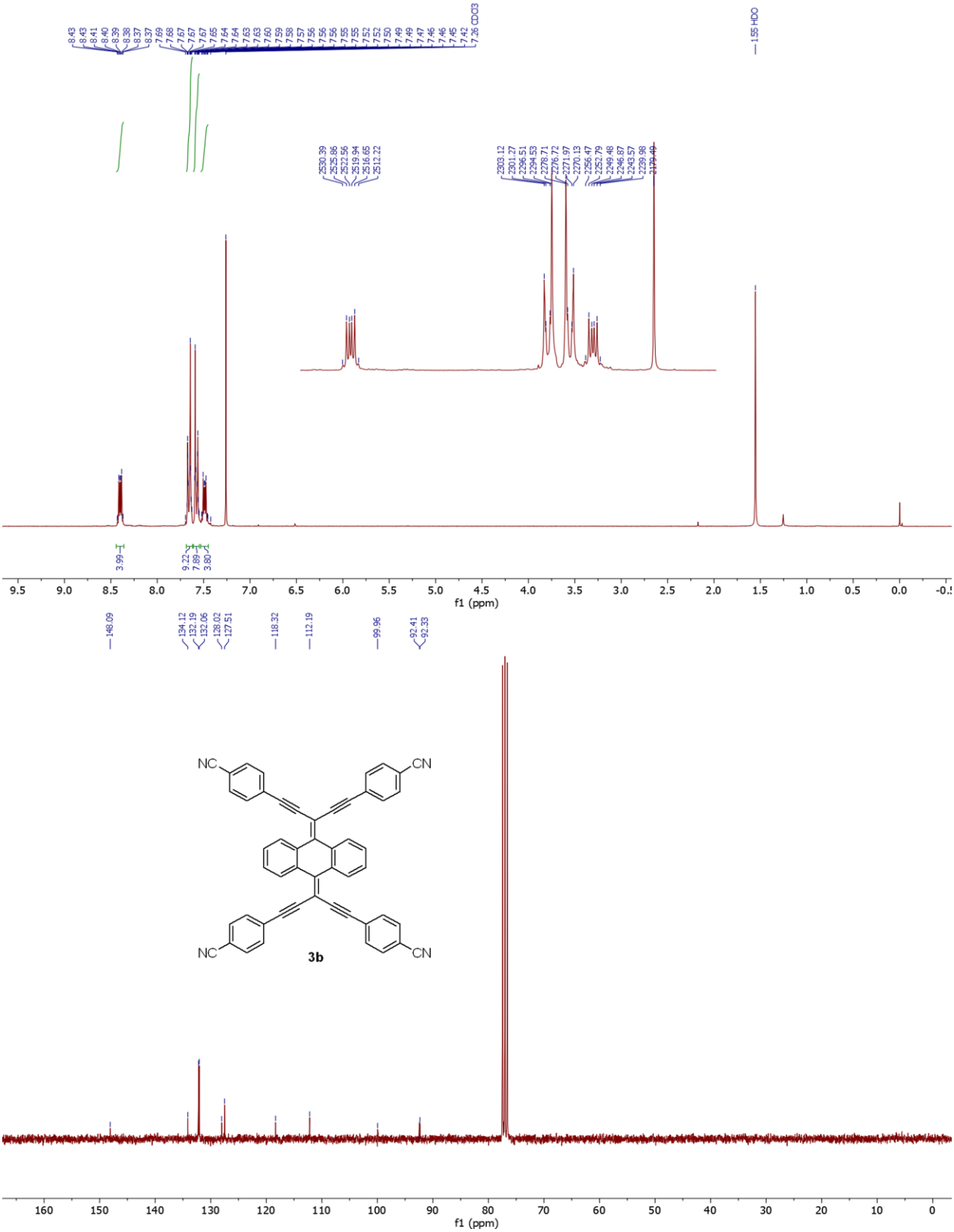

Fig. S-2. ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra of **3b** in measured $CDCl_3$.

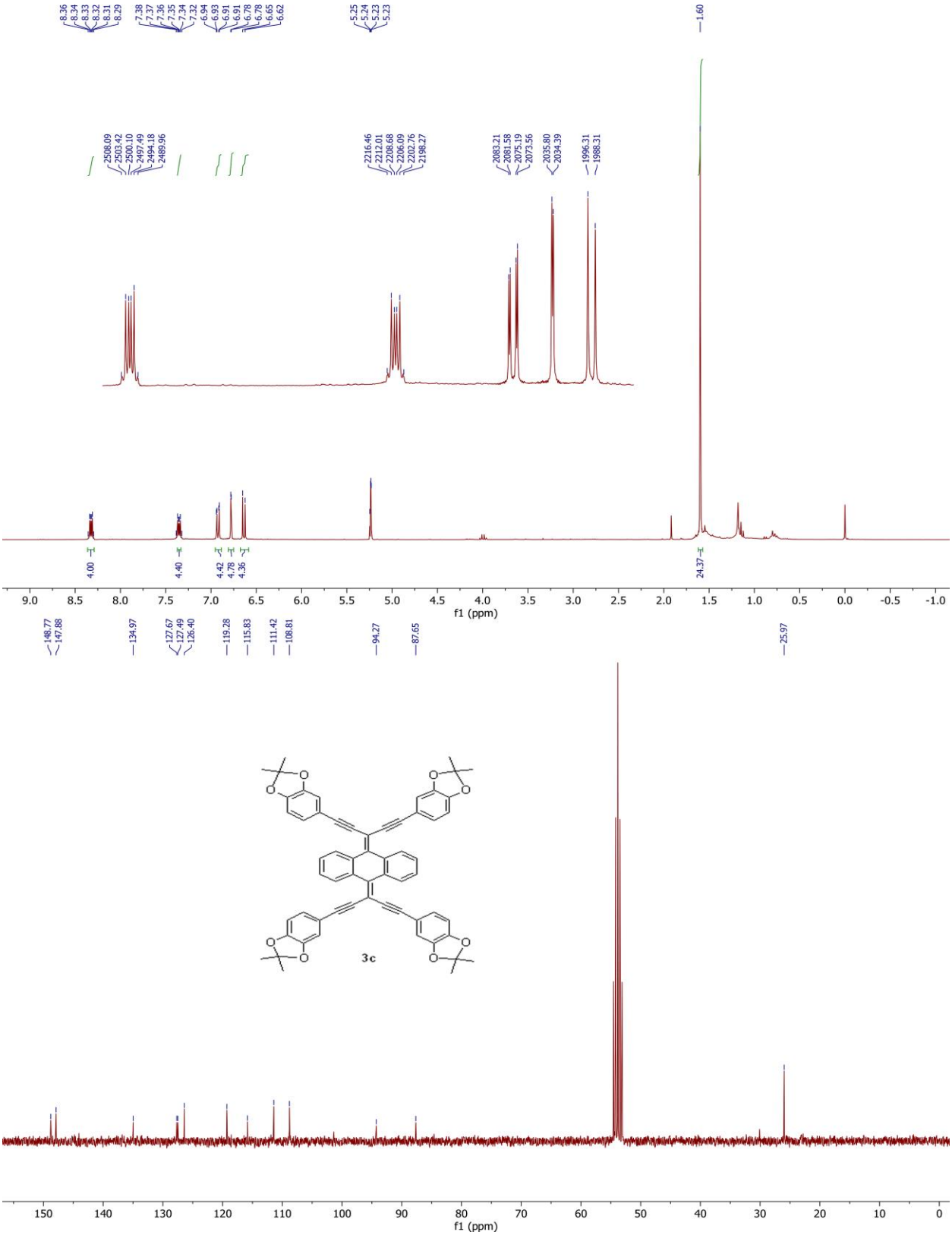

Fig. S-3. ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra of **3c** measured in $CDCl_3$.

Table S-1: Crystallographic data and refinement conditions for **3a** and **3c**

Compound 3a	
formula	$C_{53}H_{37}Cl_3O_4$
formula weight	844.17
crystal dimensions (mm)	0.44 × 0.30 × 0.05
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters	
a (Å)	11.149(2)
b (Å)	13.306(3)
c (Å)	15.211(3)
α (deg)	81.578(3)
β (deg)	87.381(3)
γ (deg)	71.177(3)
V (Å^3)	2112.8(8)
Z	2
ρ_{calcd} (g cm^{-3})	1.327
μ (mm^{-1})	0.265
diffractometer	Bruker PLATFORM/APEX II CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	50.50
total data collected	14465 ($-13 \le h \le 13$, $-15 \le k \le 15$, $-18 \le l \le 18$)
independent reflections	7640 (R_{int} = 0.0596)
number of observed reflections (*NO*)	3820 [$F_o^2 \ge 2\sigma(F_o^2)$]

Compound 3c

formula	$C_{60}H_{44}O_8$
formula weight	892.95
crystal dimensions (mm)	0.32 × 0.12 × 0.11
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	8.58110(10)
b (Å)	16.8286(3)
c (Å)	17.0367(3)
α (deg)	81.6064(9)
β (deg)	75.5209(8)
γ (deg)	77.4936(11)
V (Å^3)	2314.57(7)
Z	2
ρ_{calcd} (g cm^{-3})	1.281
μ (mm^{-1})	0.679

B. Data Collection and Refinement Conditions

diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	Cu Kα (1.54178) (microfocus source)
temperature (°C)	–100
scan type	ω and ϕ scans (1.0°) (5 s exposures)
data collection 2θ limit (deg)	148.67
total data collected	64886 (-10 ≤ *h* ≤ 10, -20 ≤ *k* ≤ 20, -21 ≤ *l* ≤ 21)
independent reflections	9038 (R_{int} = 0.0475)
number of observed reflections (*NO*)	7757 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT-2014*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2017*[d])

absorption correction method	multi-scan (*SADABS*)
range of transmission factors	1.0000 – 0.7956
data/restraints/parameters	9038 / 0 / 621
goodness-of-fit (*S*)[e] [all data]	1.039
final *R* indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0409
wR_2 [all data]	0.1146
largest difference peak and hole	0.439 and –0.457 e Å^{-3}

Table S-2. Calculated UV-Vis absorption properties for compound **3a** and **3b** in the gas phase at the TD-CAM-B3LYP/6-31G(d) level of theory

Entry	λ_{max}	***f***	**MO Composition**
3a	448 nm	1.2097	H → L (68.4 %) H – 1 → L + 1 (13.1 %)
3b	451 nm	1.2057	H → L (68.1 %) H – 1 → L + 1 (13.6 %)

Table S-3. Geometries of **3a** and **3b** optimized at the B3LYP/6-31G(d) level of theory

3a				**3b**			
0 1				0 1			
C	-0.69917700	3.51252300	3.13767700	C	0.69806900	-3.50805600	3.06409600
C	-1.39299000	2.38305300	2.71569400	C	1.39341200	-2.38107600	2.63670900
C	-0.71074400	1.23443900	2.27975400	C	0.71022400	-1.23455300	2.19897500
C	0.71046700	1.23460400	2.27974700	C	-0.71073000	-1.23435400	2.19897200
C	1.39245000	2.38337800	2.71567800	C	-1.39425800	-2.38069200	2.63667900
C	0.69837900	3.51268600	3.13766800	C	-0.69923400	-3.50786600	3.06408000
C	-1.40788100	-0.00015800	1.87498700	C	1.40440500	-0.00011900	1.79087200
C	1.40788700	0.00016800	1.87497900	C	-1.40456200	0.00025500	1.79085900
C	0.71075200	-1.23442400	2.27976400	C	-0.71039100	1.23467700	2.19902300
C	-0.71045900	-1.23459000	2.27976500	C	0.71056300	1.23448800	2.19900500
C	-1.39244000	-2.38335900	2.71571300	C	1.39408600	2.38084200	2.63668000
H	-2.47491600	-2.37465600	2.75167000	H	2.47643400	2.37146400	2.67646600
C	-0.69836600	-3.51266200	3.13771100	C	0.69904100	3.50801000	3.06406700
C	0.69919000	-3.51249900	3.13771200	C	-0.69826000	3.50817600	3.06411700
C	1.39300100	-2.38303400	2.71571300	C	-1.39359600	2.38117400	2.63675300
H	-1.24809000	4.38138200	3.49120200	H	1.24578300	-4.37465500	3.42383600
H	-2.47546400	2.37409900	2.75165500	H	2.47576000	-2.37202600	2.67650200
H	2.47492700	2.37467700	2.75162800	H	-2.47661000	-2.37132800	2.67643400
H	1.24709300	4.38167300	3.49118700	H	-1.24718300	-4.37431000	3.42383000
H	-1.24707900	-4.38164600	3.49124300	H	1.24697800	4.37448100	3.42377100

H	1.24810500	-4.38135400	3.49124400	H	-1.24596900	4.37477000	3.42387000
H	2.47547500	-2.37408000	2.75166800	H	-2.47594900	2.37210000	2.67654000
C	-2.57516200	-0.00029500	1.12680400	C	2.56729200	-0.00023900	1.03584100
C	2.57516400	0.00029600	1.12678900	C	-2.56736700	0.00044300	1.03571200
C	-3.20682900	1.18833600	0.65752400	C	3.19264600	-1.18960900	0.56161200
C	-3.20655400	-1.18907300	0.65753000	C	3.19305600	1.18893700	0.56163300
C	3.20682800	-1.18834000	0.65752000	C	-3.19272700	1.18985800	0.56157300
C	3.20655400	1.18906900	0.65749900	C	-3.19306900	-1.18874800	0.56146800
C	-3.79085300	2.15184600	0.19502600	C	3.77193600	-2.15174400	0.09154600
C	-3.79035700	-2.15271900	0.19503300	C	3.77279800	2.15078100	0.09153700
C	3.79085100	-2.15185600	0.19503100	C	-3.77196700	2.15199500	0.09147500
C	3.79035600	2.15270800	0.19498700	C	-3.77264400	-2.15067600	0.09134700
C	-5.68807900	5.63314000	-1.30878300	C	5.66396500	-5.61038300	-1.44290300
C	-6.28062900	4.37723200	-1.49572700	C	6.26502700	-4.34916800	-1.60343100
C	-5.65251000	3.23607400	-1.00094900	C	5.64451800	-3.21408300	-1.10184500
C	-4.42919400	3.31605200	-0.31231100	C	4.40927700	-3.31061200	-0.42716100
C	-3.84620300	4.59186600	-0.13521600	C	3.81252600	-4.58036500	-0.27253400
C	-4.46516200	5.72961900	-0.62441500	C	4.43165400	-5.71630500	-0.77340400
H	-7.22319200	4.27732300	-2.02160600	H	7.21531600	-4.27092200	-2.12136900
H	-6.11368500	2.26420100	-1.14738100	H	6.10712000	-2.24040500	-1.22473600
H	-2.89902100	4.66996200	0.38957700	H	2.86006100	-4.65767800	0.24165700
H	-4.02193600	6.71178300	-0.49324700	H	3.96975200	-6.69085900	-0.65333500
C	-5.65177600	-3.23736400	-1.00093500	C	5.64625500	3.21192700	-1.10148600
C	-6.27961300	-4.37866300	-1.49574200	C	6.26742800	4.34656800	-1.60325200
C	-5.68672500	-5.63442400	-1.30888000	C	5.66681200	5.60808900	-1.44344800
C	-4.46382400	-5.73064300	-0.62445500	C	4.43426900	5.71476200	-0.77450000
C	-3.84514400	-4.59274900	-0.13522700	C	3.81447600	4.57926100	-0.27344600
C	-4.42842900	-3.31706800	-0.31231700	C	4.41077600	3.30921200	-0.42733800
H	-6.11321000	-2.26560200	-1.14728800	H	6.10851400	2.23801600	-1.22381600
H	-7.22229400	-4.27902000	-2.02146100	H	7.21789900	4.26773900	-2.12077100
H	-4.02036500	-6.71270400	-0.49331000	H	3.97270600	6.68954700	-0.65499500
H	-2.89795100	-4.67062600	0.38958000	H	2.86183400	4.65716300	0.24031500
C	4.42918700	-3.31606800	-0.31229800	C	-4.40945000	3.31077100	-0.42723000
C	3.84618500	-4.59188000	-0.13519800	C	-3.81261900	4.58054000	-0.27312700
C	4.46513500	-5.72964100	-0.62438200	C	-4.43191600	5.71638100	-0.77402300
C	5.68804500	-5.63317000	-1.30876900	C	-5.66448600	5.61033400	-1.44301900
C	6.28062400	-4.37727200	-1.49569100	C	-6.26563700	4.34909300	-1.60302400
C	5.65251300	-3.23610600	-1.00091700	C	-5.64496200	3.21411400	-1.10141800
H	2.89900400	-4.66996400	0.38959900	H	-2.85995500	4.65795900	0.24066400
H	4.02190100	-6.71180000	-0.49321000	H	-3.96994100	6.69095300	-0.65435600
H	7.22322600	-4.27738800	-2.02150200	H	-7.21613000	4.27074800	-2.12057600
H	6.11371000	-2.26424000	-1.14732600	H	-6.10763400	2.24041700	-1.22390100
C	4.46385200	5.73062300	-0.62451100	C	-4.43360700	-5.71480500	-0.77441000
C	3.84515900	4.59273900	-0.13528300	C	-3.81399400	-4.57918100	-0.27341900
C	4.42842700	3.31705000	-0.31237800	C	-4.41045700	-3.30922500	-0.42744700
C	5.65175800	3.23733800	-1.00102000	C	-5.64592700	-3.21216400	-1.10164100
C	6.27960600	4.37862600	-1.49583900	C	-6.26692100	-4.34692900	-1.60334700
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H	4.02041500	6.71269100	-0.49334800	H	-3.97192000	-6.68951800	-0.65480400
H	2.89797900	4.67063100	0.38954500	H	-2.86136400	-4.65690300	0.24039300
H	6.11316900	2.26557000	-1.14740300	H	-6.10832100	-2.23832700	-1.22405300
H	7.22224400	4.27893700	-2.02162400	H	-7.21738200	-4.26827400	-2.12090600
O	6.21209900	-6.81172800	-1.74916200	C	6.30432000	-6.78324300	-1.95929400
O	6.21054100	6.81306600	-1.74938200	N	6.82467500	-7.73633400	-2.37742100
O	-6.21215800	6.81170500	-1.74916900	C	6.30786000	6.78049100	-1.96001700
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H	-7.36519900	-6.19137800	-3.37553500				
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H	-7.36810400	6.19057400	-3.37468200				
H	-8.25384700	6.37603500	-1.83048300				