

Supporting information for

Iridium-phosphine ligand complexes as an alternative to rhodium-based catalyst for the efficient hydroformylation of propene

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† C. Yao and W. Xiong contributed equally to this work and should be considered as co-first authors.

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1.¹H, ¹³C, ³¹P NMR spectra and MS data

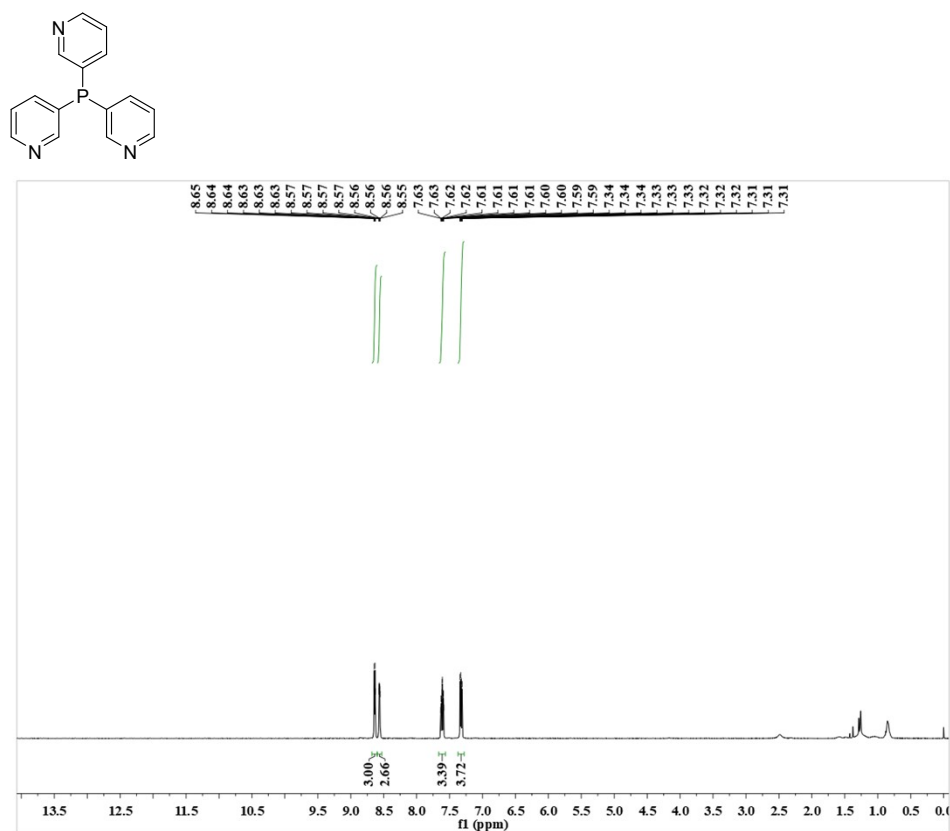


Figure S1 ¹H NMR of tri(3-pyridyl)phosphine (L5)

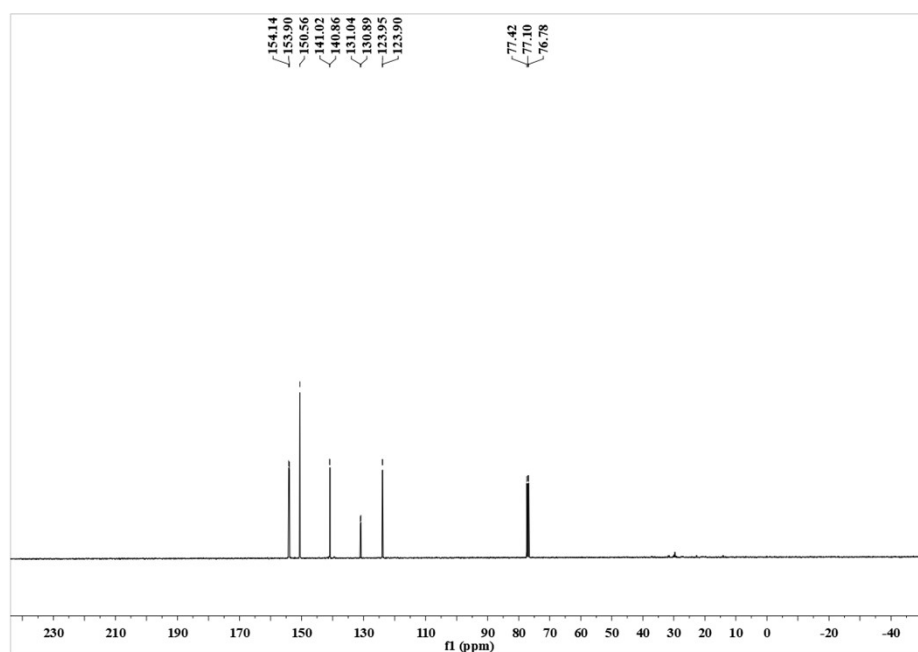


Figure S2 ¹³C NMR of tri(3-pyridyl)phosphine (L5)

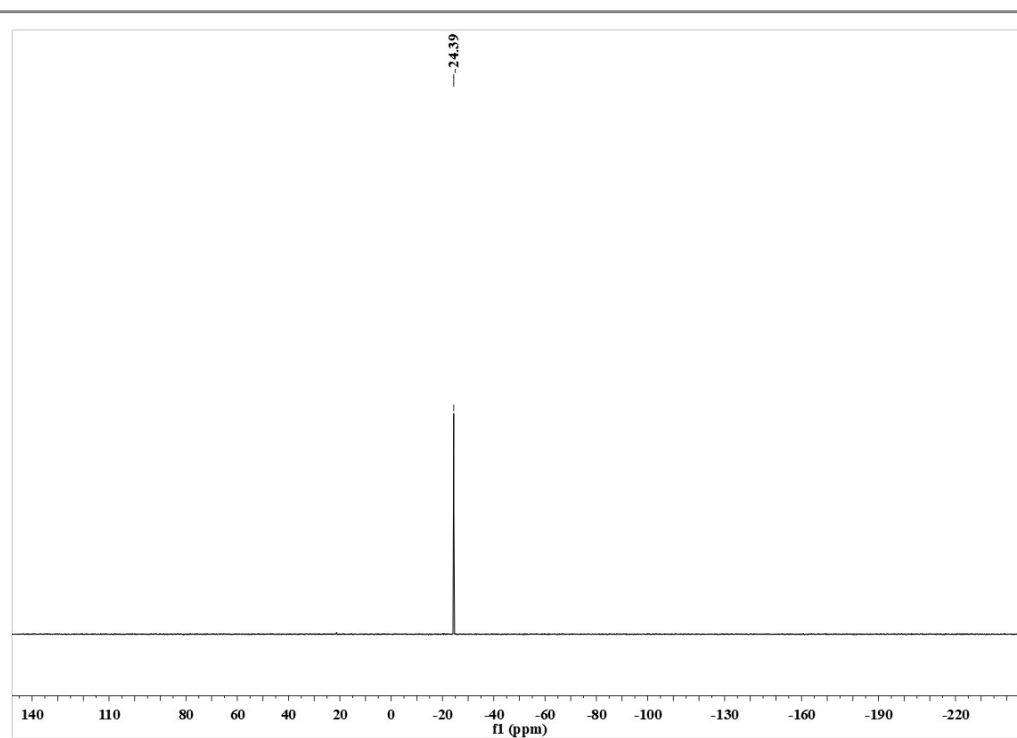


Figure S3 ^{31}P NMR of tri(3-pyridyl)phosphine (L5)

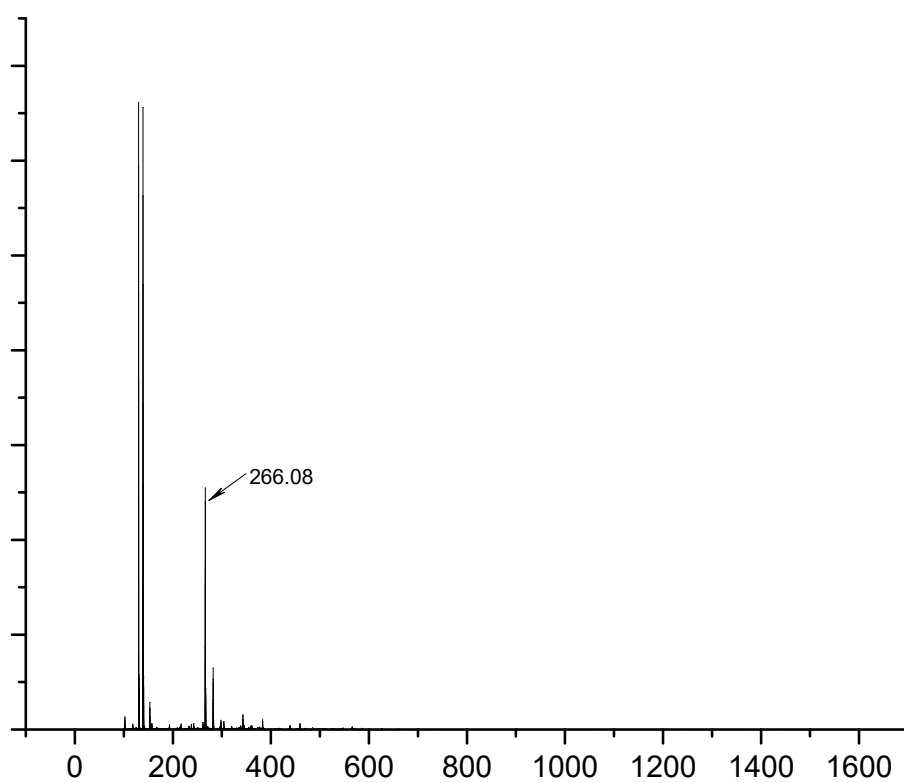


Figure S4 Electrospray mass spectrometry of tri(3-pyridyl)phosphine (L5)

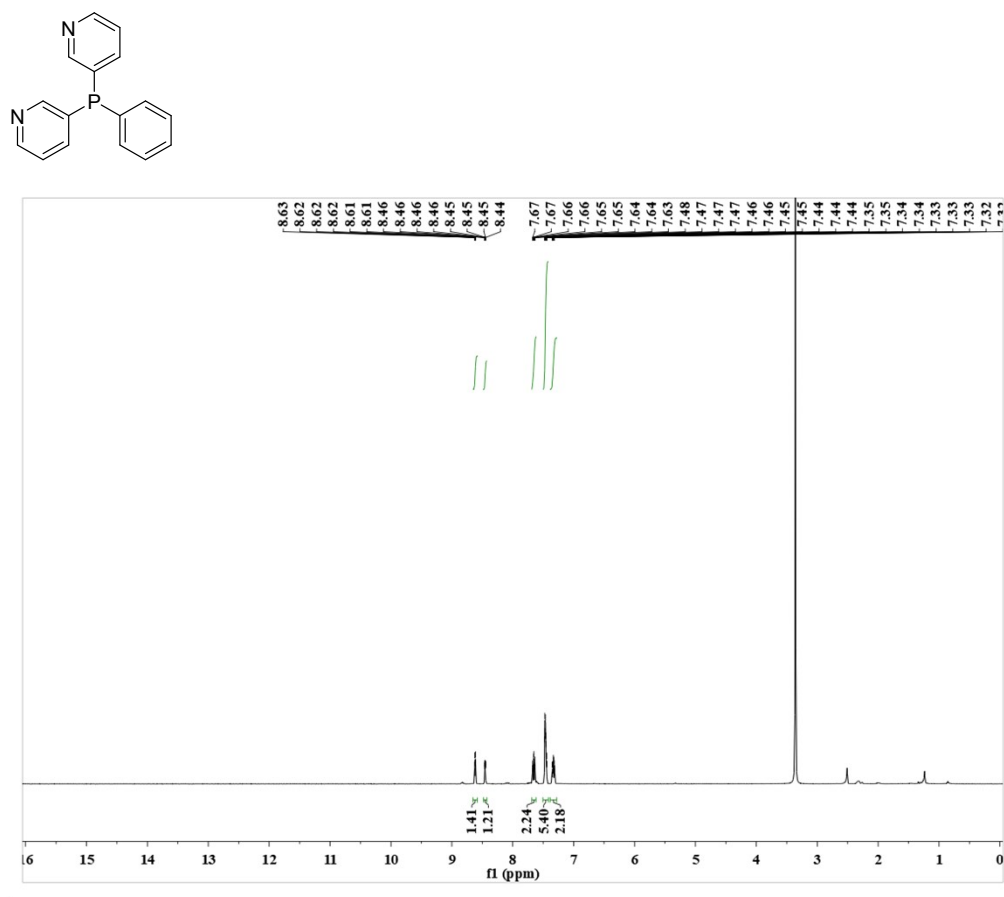


Figure S5 ¹H NMR of di(3-pyridyl)phenylphosphine (L6)

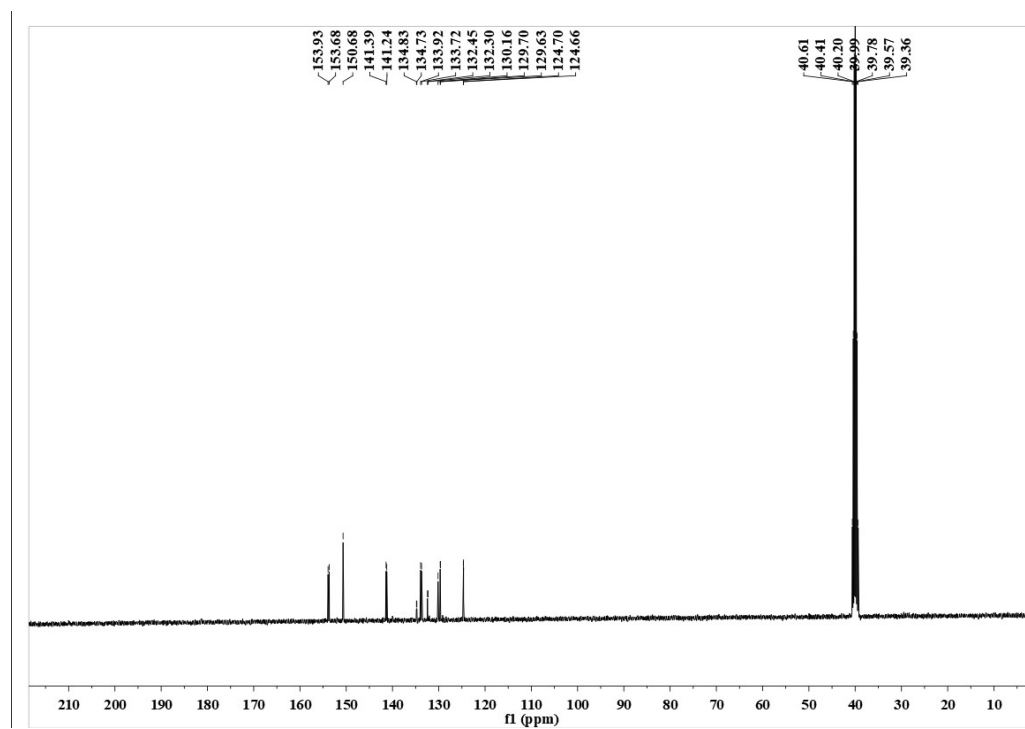


Figure S6 ¹³C NMR of di(3-pyridyl)phenylphosphine (L6)

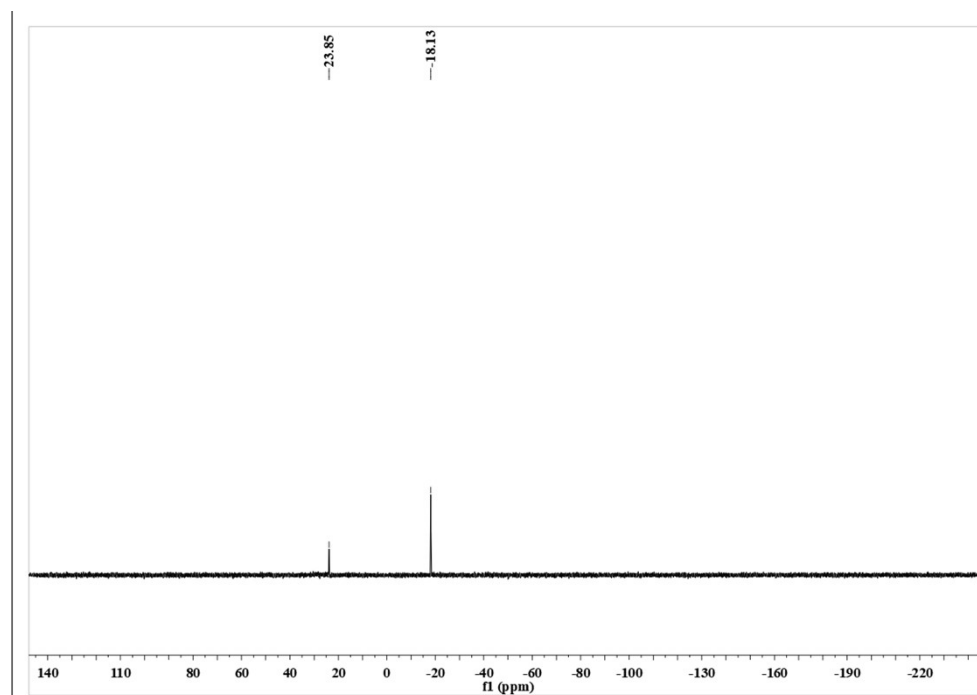


Figure S7 ^{31}P NMR of di(3-pyridyl)phenylphosphine (L6)

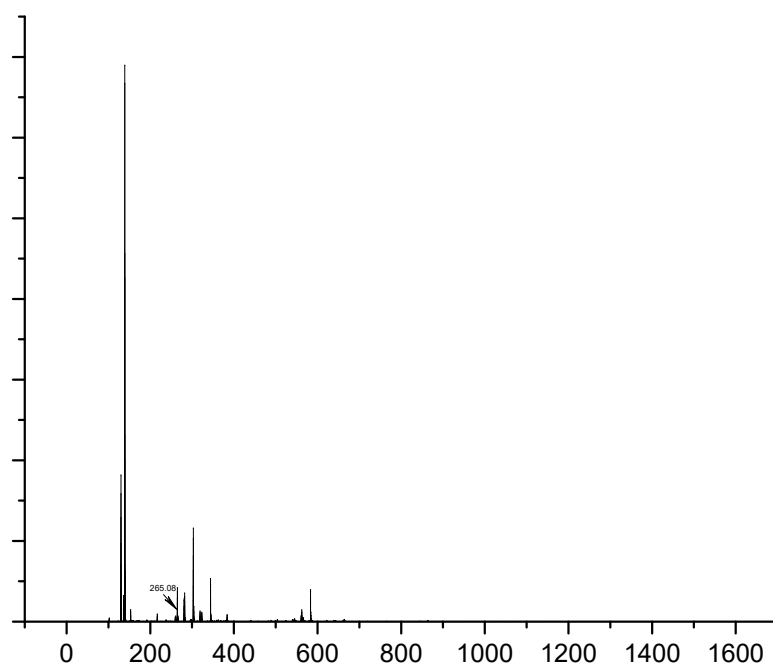


Figure S8 Electrospray mass spectrometry of di(3-pyridyl)phenylphosphine (L6)

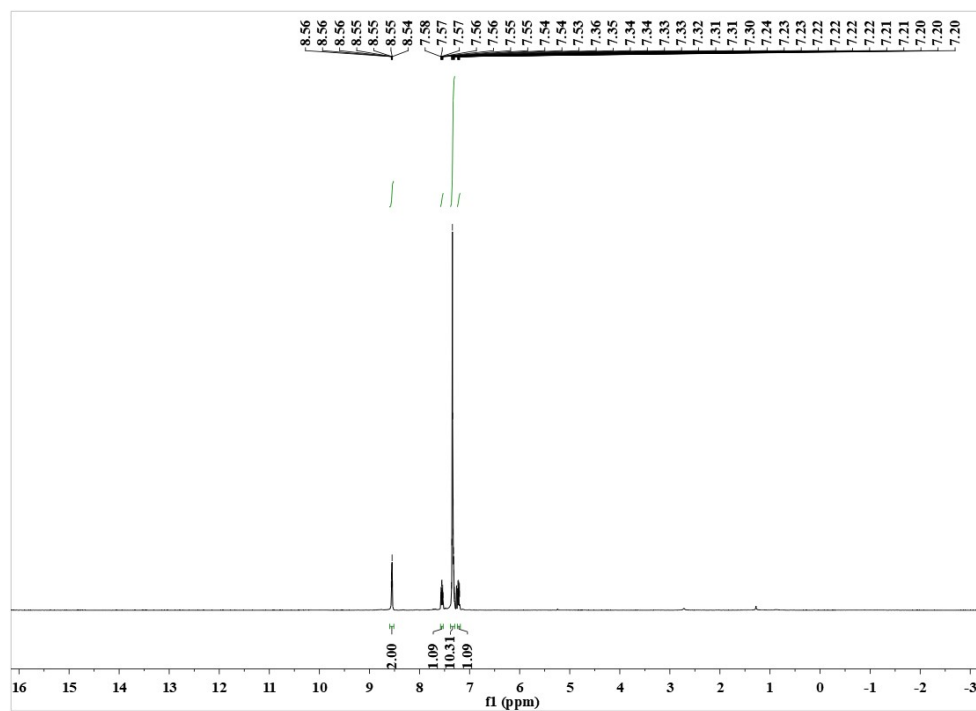
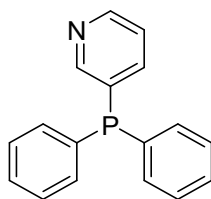


Figure S9 ¹H NMR of diphenyl(3-pyridyl)phosphine (L7)

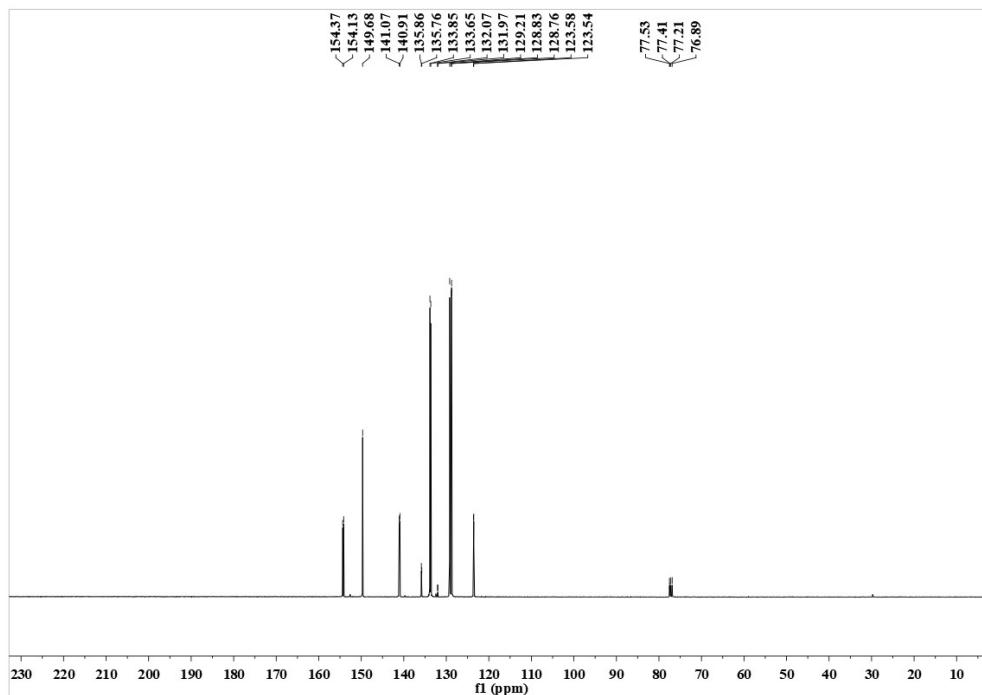


Figure S10 ¹³C NMR of diphenyl(3-pyridyl)phosphine (L7)

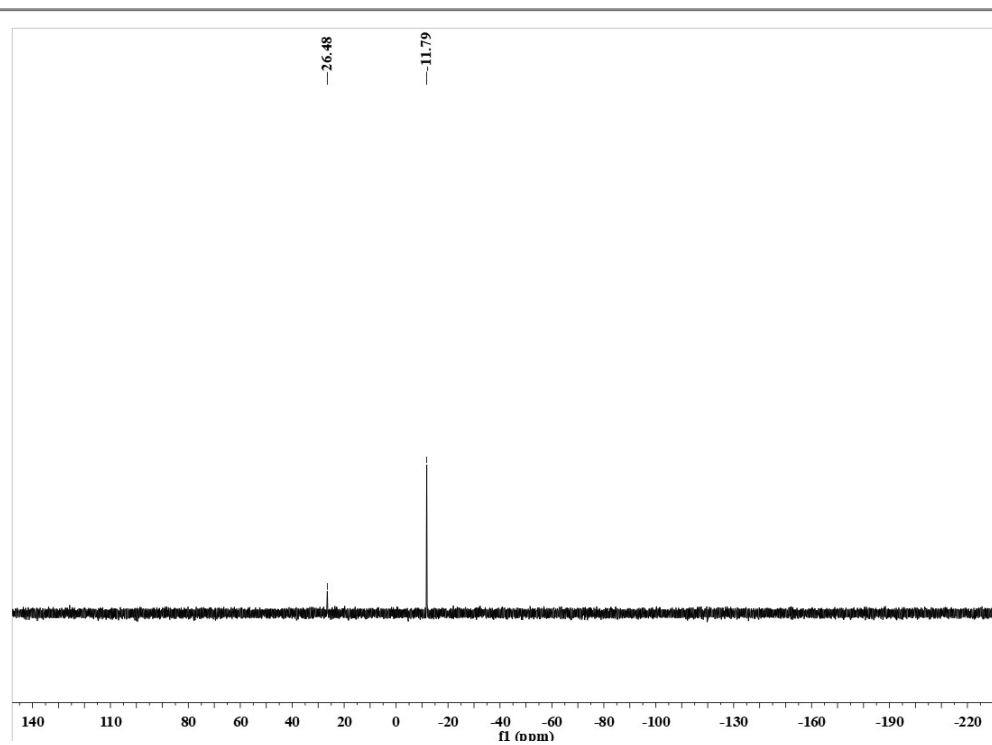


Figure S11 ^{31}P NMR of diphenyl(3-pyridyl)phosphine (L7)

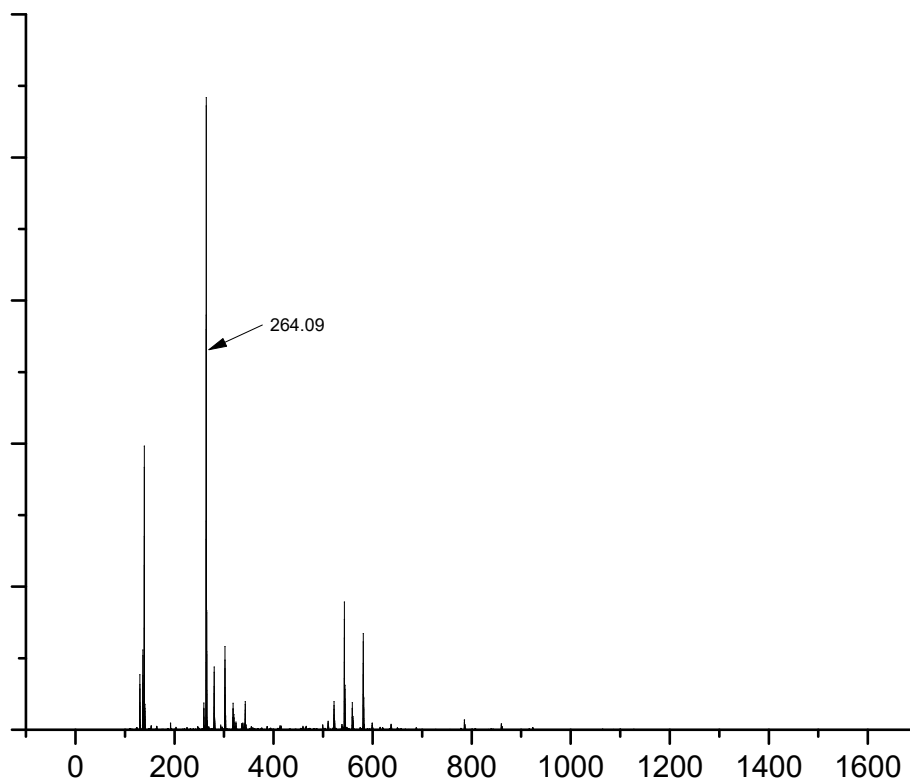


Figure S12 Electrospray mass spectrometry of diphenyl(3-pyridyl)phosphine (L7)

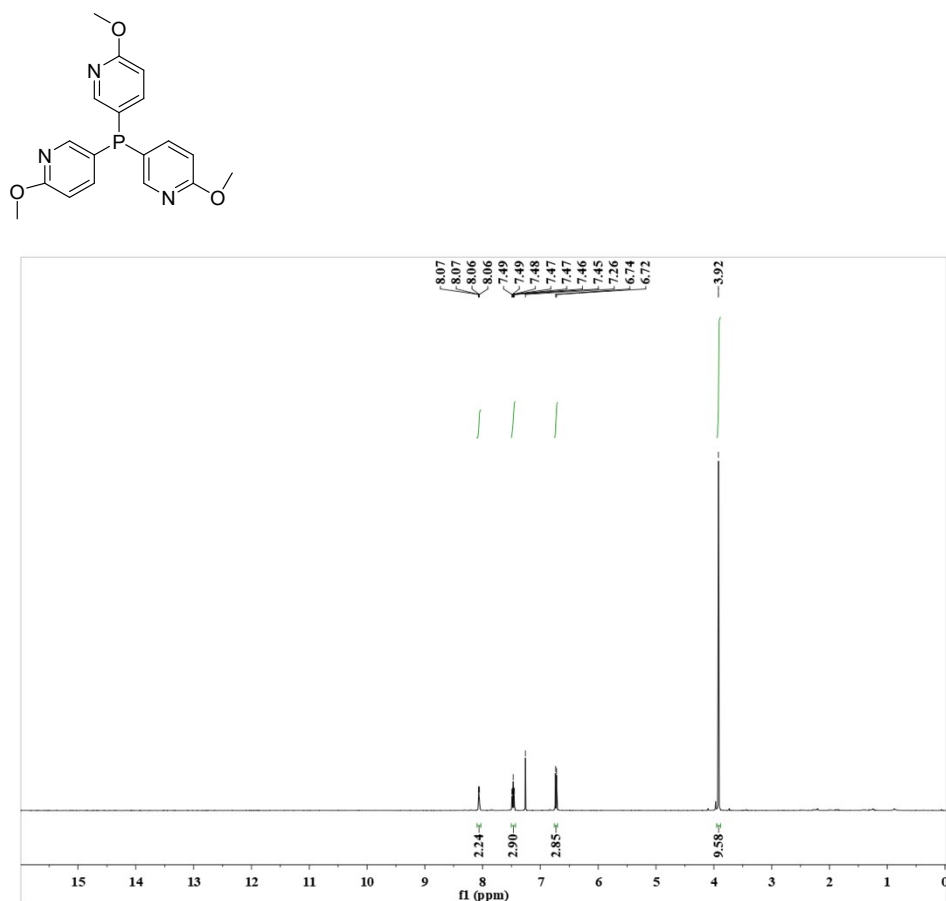


Figure S13 ¹H NMR of tri(4-methoxypyridyl)phosphine (L8)

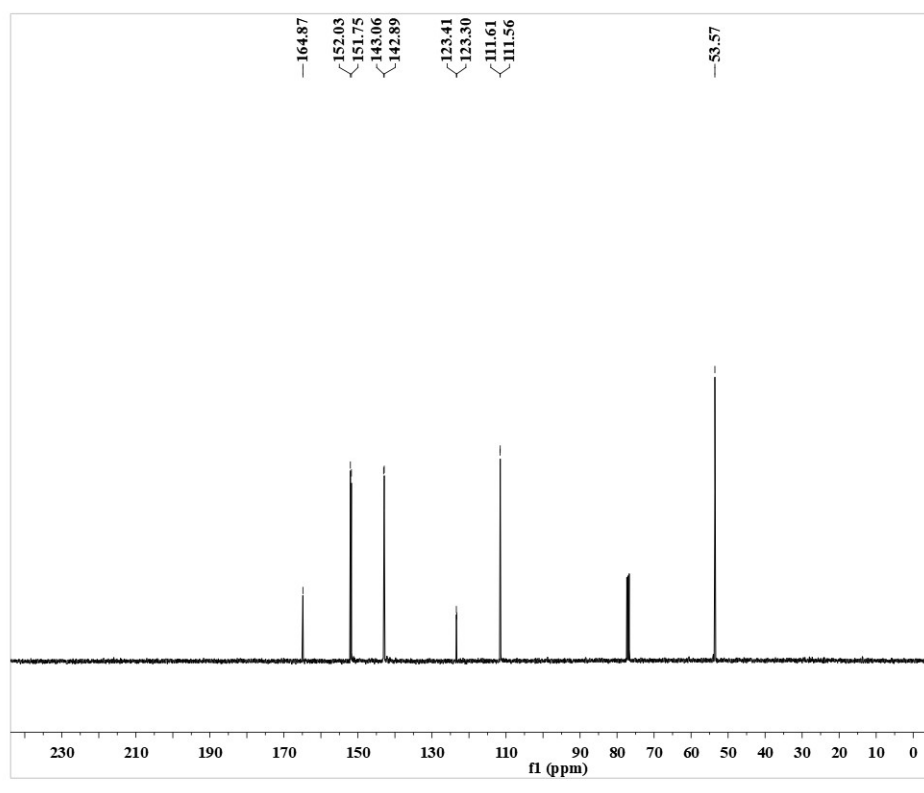


Figure S14 ^{13}C NMR of tri(4-methoxypyridyl)phosphine (L8)

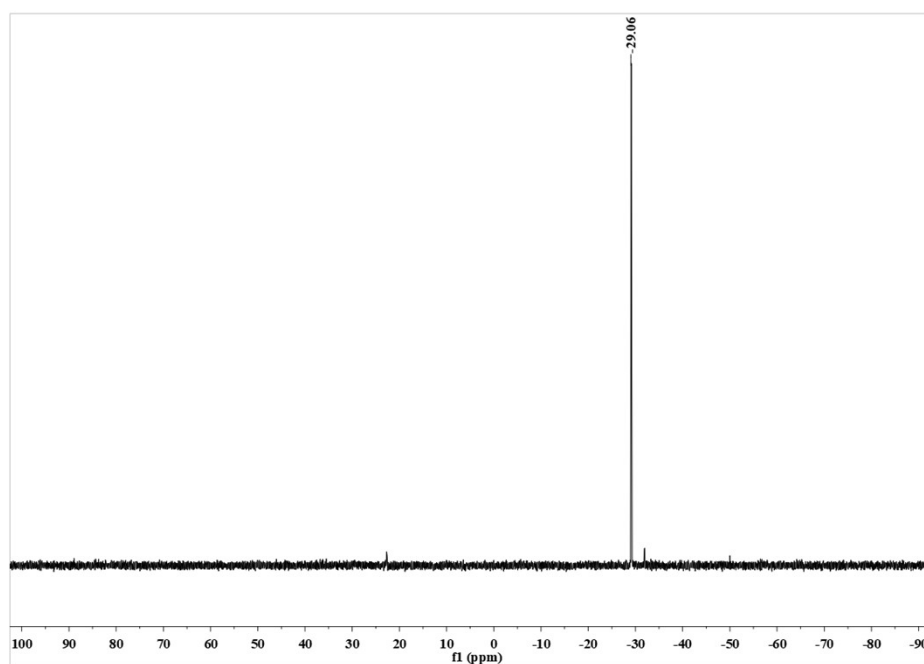


Figure S15 ^{31}P NMR of tri(4-methoxypyridyl)phosphine (L8)

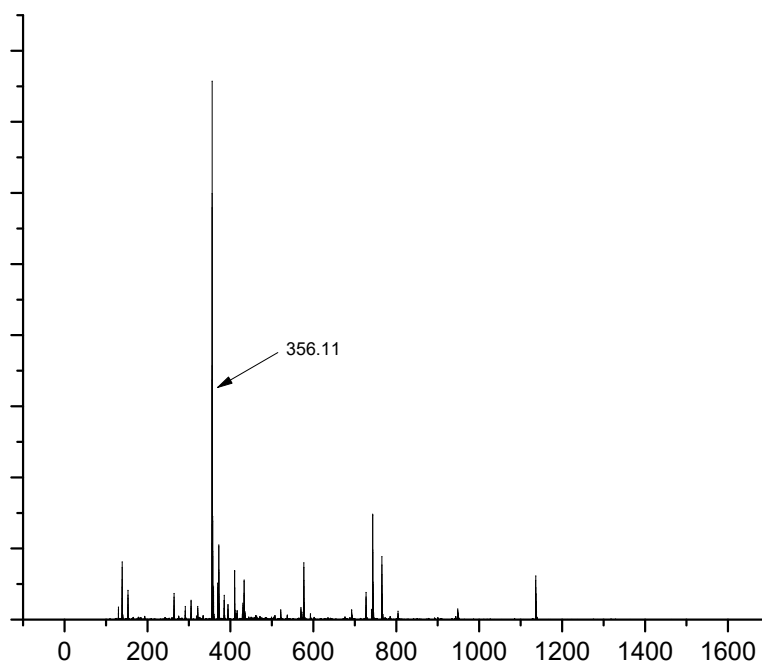


Figure S16 Electrospray mass spectrometry of tri(4-methoxypyridyl)phosphine (L8)

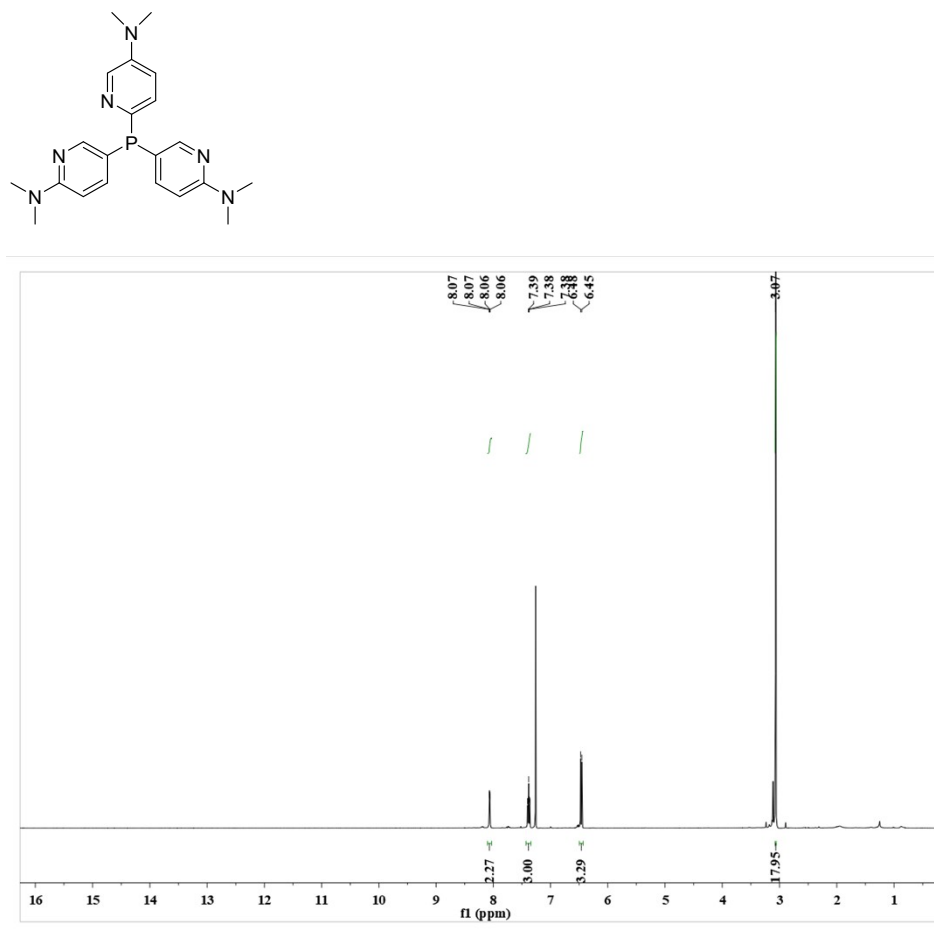


Figure S17 ¹H NMR of tri(4-N,N-dimethyl-pyridyl)phosphine (L9)

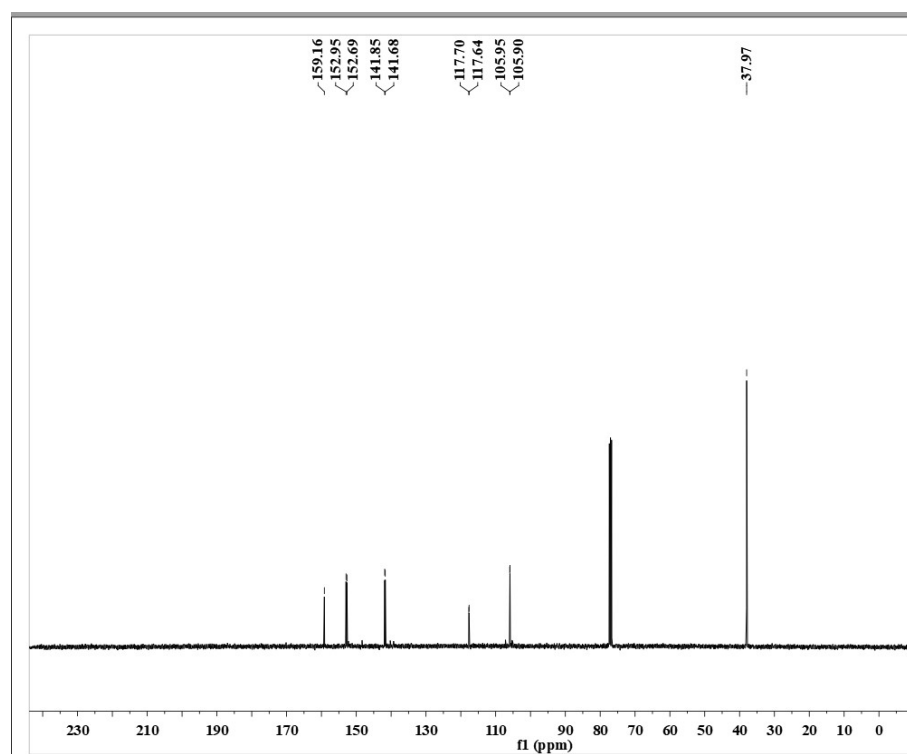


Figure S18 ¹³C NMR of tri(4-N,N-dimethyl-pyridyl)phosphine (L9)

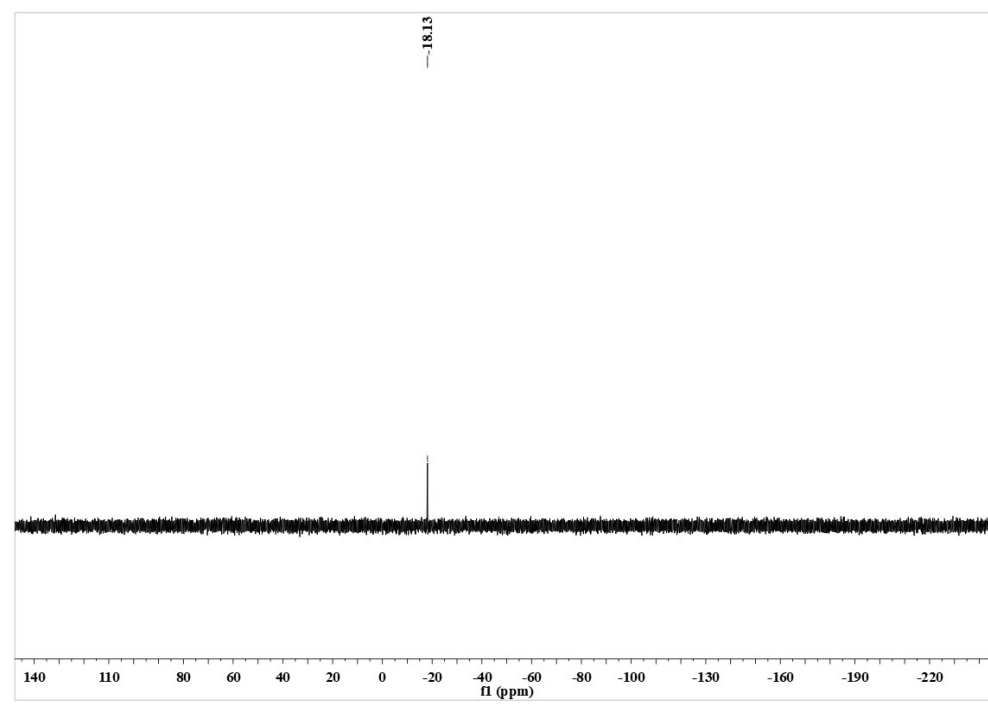


Figure S19 ^{31}P NMR of tri(4-N,N-dimethyl-pyridyl)phosphine (L9)

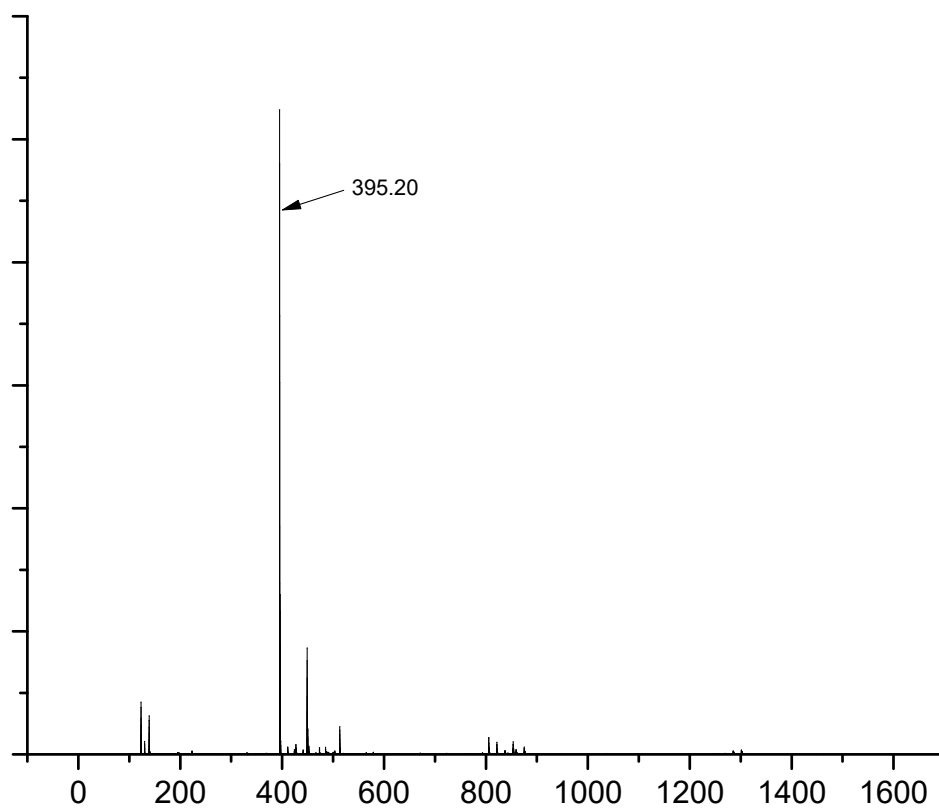


Figure S20 Electrospray mass spectrometry of tri(4-N,N-dimethyl-pyridyl)phosphine

(L9)

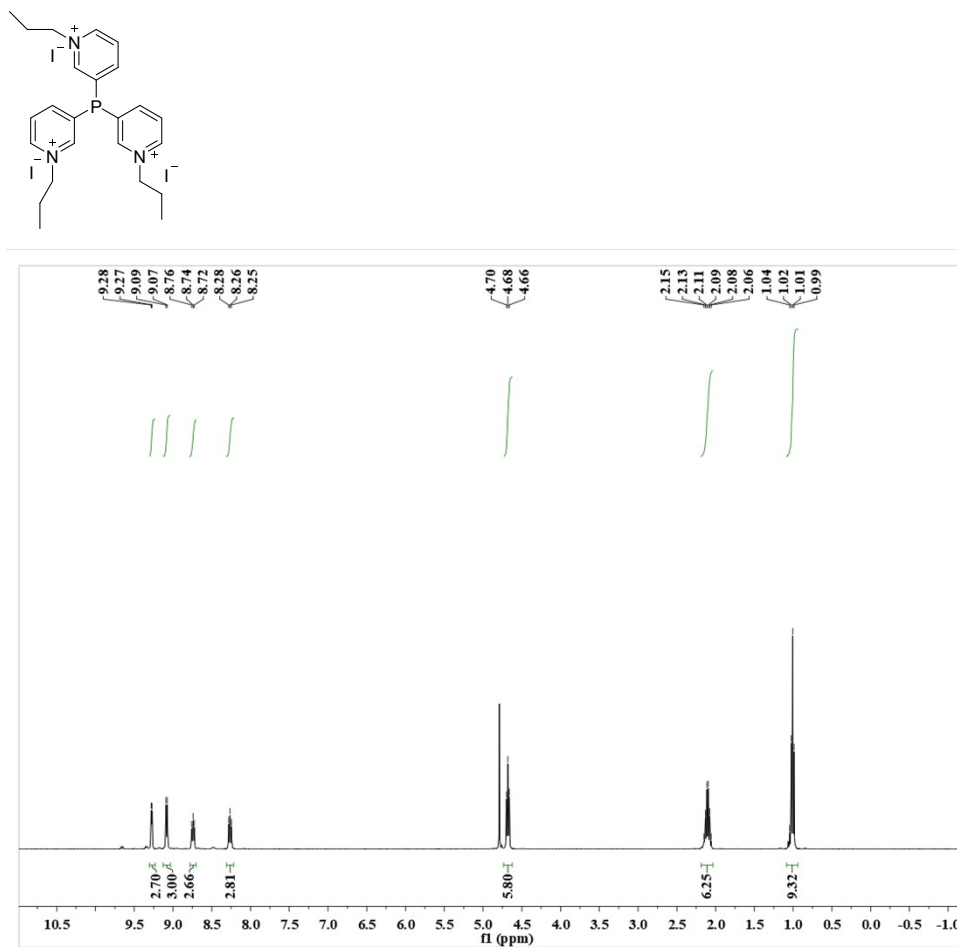


Figure S21 ¹H NMR of tri(1-propylpyridinium iodide)phosphine (L5-1)

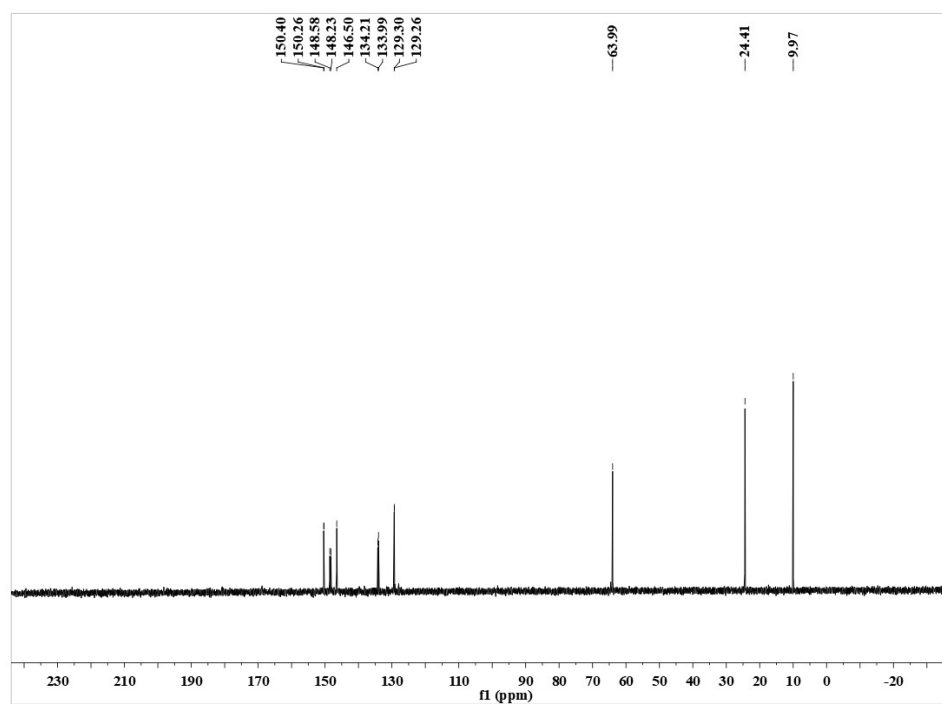


Figure S22 ^{13}C NMR of tri(1-propylpyridinium iodide)phosphine (L5-1)

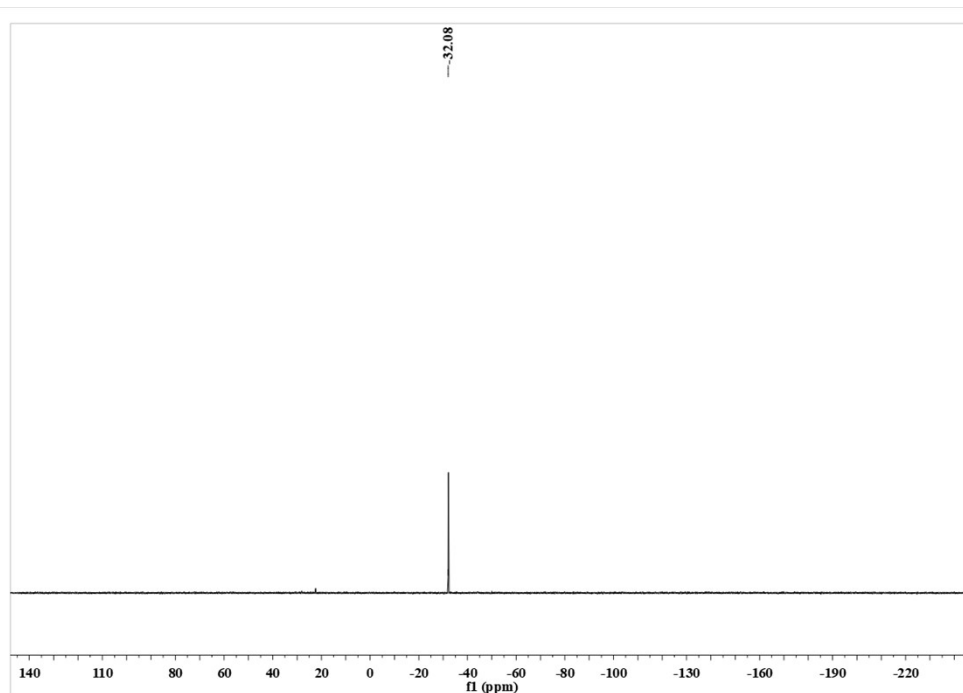


Figure S23 ^{31}P NMR of tri(1-propylpyridinium iodide)phosphine (L5-1)

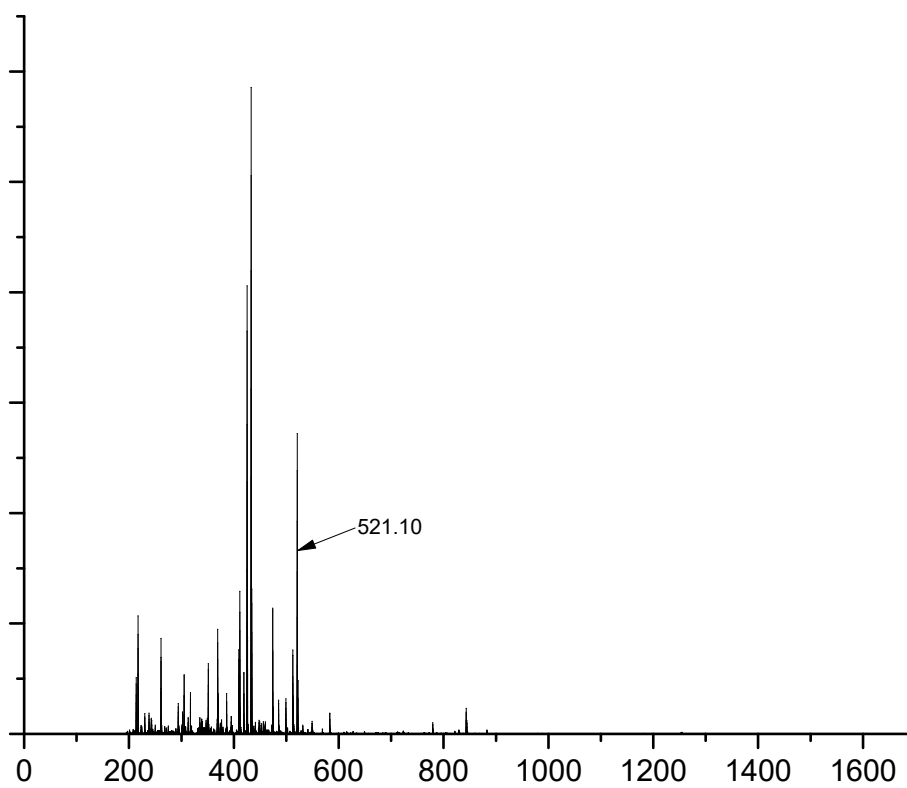


Figure S24 Electrospray mass spectrometry of tri(1-propylpyridinium iodide)phosphine (L5-1)- $\text{C}_{24}\text{H}_{32}\text{IN}_3\text{P}^+$

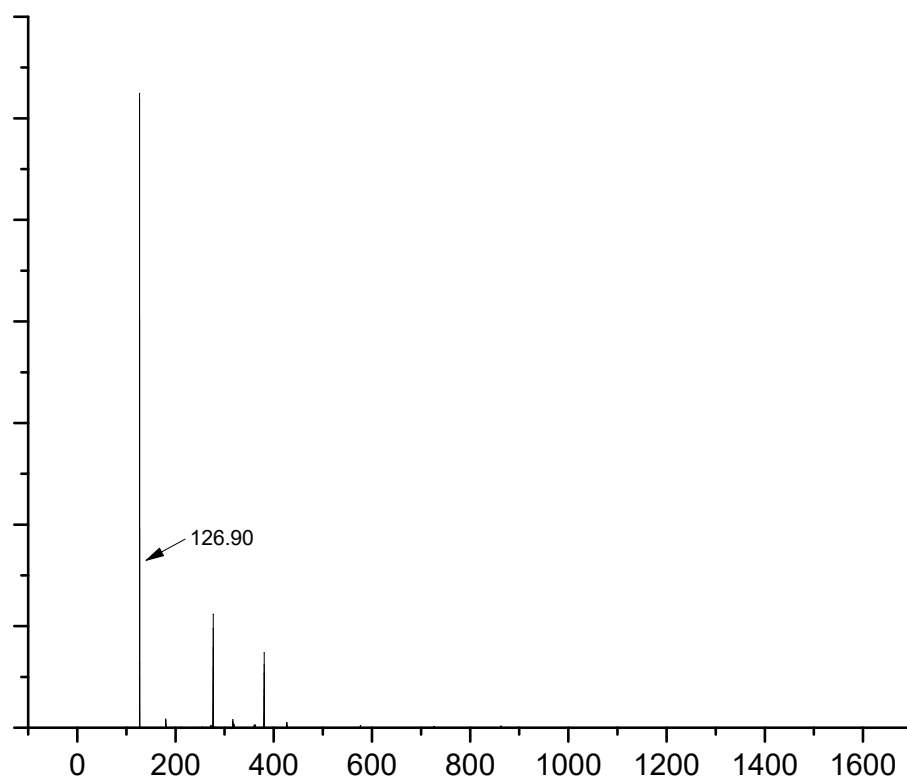


Figure S25 Electrospray mass spectrometry of tri(1-propylpyridinium iodide)phosphine (L5-1)-I⁻.

2.The results of the optimized structures based on Ir-L5 and Ir-L5-1.

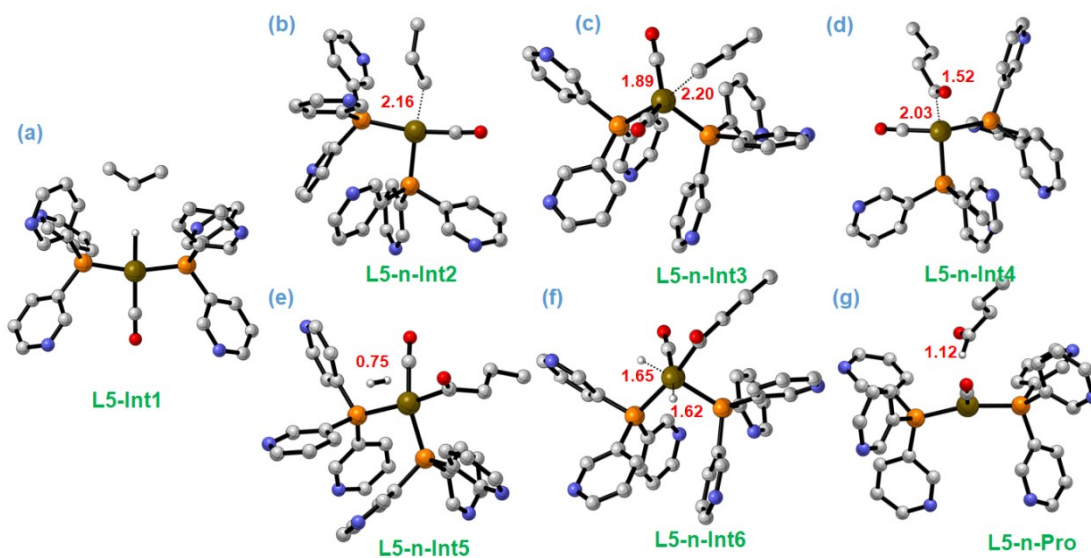


Figure S26 The results of the optimized structures based on Ir-L5.

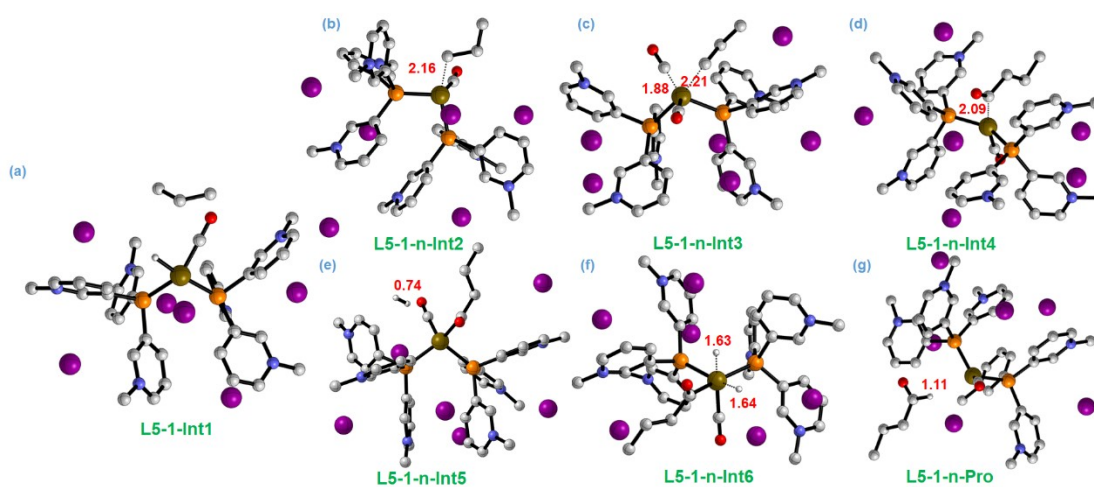


Figure S27 The results of the optimized structures based on Ir-L5-1.

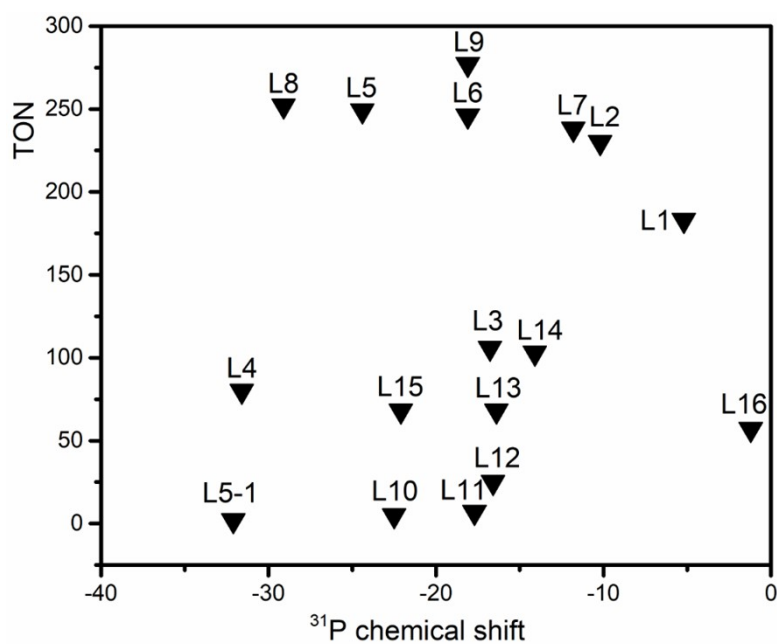


Figure S28. The ³¹P Chemical shift of different ligands VS TON of the reactions

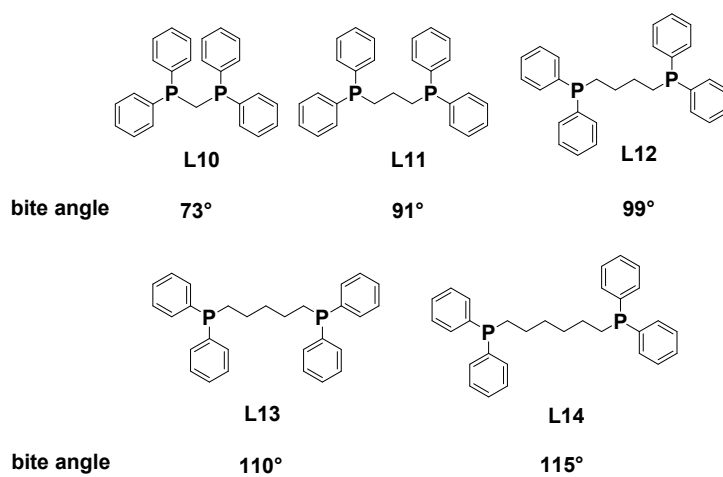


Table S1. L10-L14 Bite angle of L10-L14 cited from the literature¹⁻¹⁶

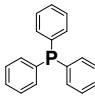
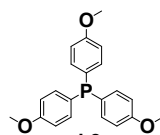
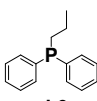
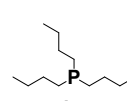
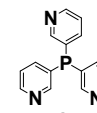
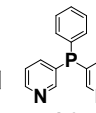
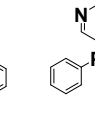
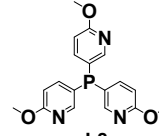
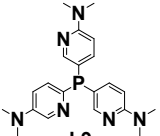
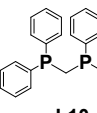
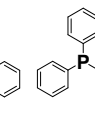
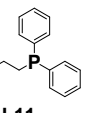
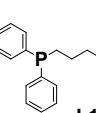
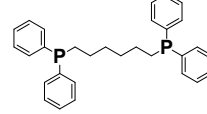
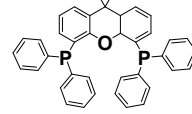
							
TON	118	66	53	54	145	84	61
n/i	2.1	2.2	2.1	2.8	1.6	1.8	1.8
Selectivity	>99%	>99%	>99%	>99%	>99%	>99%	>99%
							
TON	61	160	trace	6	9	20	
n/i	1.9	2.2	-	2.2	1.8	2.0	
Selectivity	>99%	>99%		>99%	>99%	>99%	
							
TON	33	72					
n/i	2.2	1.5					
Selectivity	>99%	>99%					

Table S2. Reactivity of monodentate ligands and bidentate ligands in two hours.

3.The coordinates of the optimized structures

H ₂			
H	0.00000000	0.00000000	0.37142000
H	0.00000000	0.00000000	-0.37142000

CO			
C	0.00000000	0.00000000	-0.65024200
O	0.00000000	0.00000000	0.48768100

C-C=C			
C	-0.13360400	0.45673500	0.00025900
H	-0.16363200	1.54724400	-0.00041300
C	-1.28152100	-0.22068800	0.00005600
H	-2.24459500	0.28238900	-0.00059700
H	-1.30049100	-1.30886200	-0.00011400
C	1.23351200	-0.16309400	-0.00004900
H	1.81034600	0.14840500	-0.88125600
H	1.81129800	0.14979100	0.87994700
H	1.17675400	-1.25668800	0.00083500

Ir-L5			
P	-2.27255400	-0.00236700	-0.03103900
C	-2.77983400	-1.16820800	1.28864300
C	-3.53984200	-2.89303500	3.27002400

C	-3.84817800	-2.06485000	1.15982700
C	-3.03278900	-0.69175600	-1.55350500
C	-4.04790100	-1.83517800	-3.82440600
C	-4.83396100	-0.91127200	-3.13523100
C	-4.31735900	-0.33054000	-1.97954400
C	-3.31411100	1.47282700	0.29116100
C	-4.75291200	3.78101400	0.59100700
C	-5.08333400	2.68149200	1.38263300
C	-4.35464800	1.50327000	1.22502700
H	-3.86904300	-3.59229300	4.03648700
H	-4.41935800	-2.10980400	0.23592400
H	-4.41967900	-2.30815500	-4.73138600
H	-5.82414000	-0.65169800	-3.49644500
H	-4.90128300	0.39334100	-1.42073000
H	-5.30476700	4.71431100	0.68415100
H	-5.89314000	2.74519200	2.10277900
H	-4.59029000	0.62607900	1.81884000
P	2.28210100	-0.03817100	-0.04598900
C	2.81223800	-1.51911000	0.89585800
C	4.10691800	-2.05007000	0.80284600
C	3.64734800	-3.70503400	2.31096300
C	3.32547200	1.30287500	0.64558800
C	4.72673600	3.47083100	1.55748900
C	4.78743000	2.28289900	2.28398900
C	4.07688300	1.17728000	1.81736400
C	3.00474600	-0.27724300	-1.71436700
C	3.91103400	-0.72543100	-4.25554900
C	4.80193000	-0.21072200	-3.31204000
C	4.33905900	0.02039900	-2.01961000

H	4.83910100	-1.59955900	0.13675600
H	4.01326200	-4.57182200	2.85810600
H	5.27392200	4.35087700	1.88950600
H	5.37986400	2.22207600	3.19159300
H	4.10895400	0.23596400	2.35566400
H	4.23936300	-0.91688600	-5.27544800
H	5.82894800	0.00889500	-3.58648600
H	4.99939300	0.43789500	-1.26554700
C	0.03770600	2.08467900	0.52366800
O	0.06372600	3.18179200	0.90068500
H	-0.00226300	-1.34764500	-0.45705400
N	-2.81735800	-2.19312100	-3.43719800
N	-3.76264400	3.77189400	-0.31191800
N	4.01154800	3.61330800	0.43257000
N	2.62874200	-1.00221300	-3.98954400
C	2.19348000	-0.77660600	-2.74594900
C	-2.32739800	-1.62564300	-2.33065700
C	-3.06089300	2.64398600	-0.44253800
C	-2.06857200	-1.16722500	2.49697300
C	1.90741900	-2.15416300	1.75421400
C	3.32397400	2.55361300	0.00372200
H	2.73991400	2.69924400	-0.90329100
H	0.89023400	-1.78063300	1.82581800
H	1.14632400	-0.99019900	-2.54802300
H	-1.32300400	-1.91848700	-2.03949900
H	-2.24947500	2.66480400	-1.16757200
H	-1.22363600	-0.49393800	2.61808200
C	-2.45625200	-2.04300500	3.50607500
C	2.33293200	-3.26689300	2.47566300

H	-1.93103300	-2.07275000	4.45580500
H	1.65854500	-3.79020700	3.14636200
N	-4.22917200	-2.91312000	2.12352500
N	4.52820500	-3.11586400	1.49072100
Ir	0.00728700	0.28205000	-0.03230600

Ir-L5-Int1			
P	-2.26527400	-0.30457700	0.01744100
C	-2.92241300	0.90587200	-1.18930700
C	-2.21359200	1.14277500	-2.37339000
C	-2.71030400	2.07407000	-3.28068400
C	-3.90276700	2.73197000	-2.97198300
C	-2.86607900	0.35216700	1.62322100
C	-2.43245800	1.61657000	2.05000000
C	-2.88261500	2.09926000	3.27295200
C	-3.73735600	1.29880700	4.03650100
C	-3.29002000	-1.80240500	-0.23779600
C	-4.67404200	-4.15076600	-0.46549300
C	-5.21417700	-2.99935900	-1.03954500
C	-4.51247500	-1.80215300	-0.91791300
H	-1.28257100	0.61145600	-2.55095300
H	-2.18250200	2.29441800	-4.20299500
H	-4.32054400	3.46656100	-3.65765300
H	-1.76972600	2.20952800	1.42777400
H	-2.57750600	3.07758900	3.63164200
H	-4.10009200	1.64413100	5.00310100
H	-5.19901000	-5.10130100	-0.53747200
H	-6.16197700	-3.04026600	-1.56703600

H	-4.90578700	-0.88757300	-1.34918800
P	2.28489500	-0.22173400	0.03378700
C	2.85269500	1.22165900	-0.94680100
C	3.95798000	2.01132000	-0.61499700
C	4.28509200	3.08884600	-1.43589500
C	3.49407300	3.33677100	-2.55928700
C	3.39035400	-1.57562500	-0.52061400
C	4.89592600	-3.75238700	-1.21100200
C	5.19388800	-2.52252200	-1.79638700
C	4.42936900	-1.41178300	-1.44105400
C	2.90485600	0.12268900	1.72615600
C	2.04361000	0.62087400	2.71284900
C	2.56030400	0.90132000	3.97500200
C	3.91710400	0.67273700	4.20907300
H	4.54335300	1.79927200	0.27398800
H	5.13106600	3.72947000	-1.20729200
H	3.71869500	4.17346600	-3.21793000
H	5.47596800	-4.63829500	-1.46162100
H	6.00583200	-2.43588100	-2.51165200
H	4.63716300	-0.43812800	-1.87255800
H	0.99367100	0.77017000	2.48346400
H	1.92285300	1.28399600	4.76593200
H	4.35347200	0.88587000	5.18306200
C	0.06368200	-2.18335400	-1.04802400
O	0.09887900	-3.16582100	-1.66443600
C	-0.31505500	3.64706200	-0.40885100
H	-0.24459200	2.79142100	-1.07622900
C	-1.46838100	4.31374200	-0.32903600
H	-2.33412400	4.03334500	-0.92110100

H	-1.58684000	5.17097800	0.33172100
C	0.92413400	3.96583600	0.37367100
H	0.77268800	4.82382900	1.03774100
H	1.23178100	3.10492900	0.98051600
H	1.76388000	4.19097900	-0.29538600
H	-0.01013600	0.97315900	0.60153600
N	-3.50759200	-4.17278700	0.19213300
N	-4.16067900	0.09228700	3.64805500
N	-4.59519800	2.52307500	-1.84403900
N	4.75446800	0.18214400	3.28631400
N	3.90365300	-3.93068900	-0.32773900
N	2.43231700	2.59210600	-2.89587800
C	4.24673200	-0.09049100	2.07974700
C	3.16953600	-2.86428800	-0.00552400
C	2.12835300	1.56305800	-2.09954700
C	-4.10378400	1.63029400	-0.97712600
C	-2.83552000	-3.02247000	0.28932200
C	-3.73280900	-0.35964800	2.46098700
H	-1.88270300	-3.06398800	0.81320800
H	-4.67307300	1.49376100	-0.06022100
H	-4.10187300	-1.33885100	2.16979500
H	4.94394400	-0.50932400	1.35724900
H	2.35693800	-3.03547900	0.69836500
H	1.25277300	0.97406400	-2.36654500
Ir	0.01937400	-0.53867200	-0.12212300

Ir-L5-n-Int2			
P	1.63507800	0.38681600	-0.02770000

C	1.14441600	2.12849600	-0.39940800
C	0.40384800	2.87847400	0.52335600
C	-0.07521600	4.13158500	0.15202300
C	0.20368000	4.60207300	-1.13066600
C	1.39199200	2.71810800	-1.64901200
C	3.22022800	0.24294900	-0.94731100
C	3.17575100	-0.02646600	-2.32550600
C	5.45238300	-0.06324800	-2.50737400
C	5.61636600	0.17304200	-1.14273100
C	4.48082000	0.33312600	-0.35069900
C	2.13391500	0.50764300	1.73136400
C	1.86347500	-0.55878800	2.60357000
C	2.76826100	0.54180900	4.39165100
C	3.09514100	1.65541200	3.61483000
C	2.77322200	1.63649400	2.26061400
H	0.20800000	2.49456400	1.51633600
H	-0.65900800	4.72687000	0.84641800
H	-0.16737300	5.57068900	-1.45945600
H	1.98834400	2.20030800	-2.39435800
H	2.21571800	-0.15099000	-2.82432100
H	6.31740500	-0.18683200	-3.15568100
H	6.61003700	0.22808900	-0.70946800
H	4.57718300	0.50956200	0.71502300
H	1.36391000	-1.44498300	2.21852200
H	2.99618900	0.52715500	5.45566900
H	3.58279500	2.51556900	4.06271900
H	3.00028300	2.48937300	1.62806400
P	-1.85698300	-0.14664400	-0.06293400
C	-1.98092800	0.93722000	1.42302400

C	-2.61405300	2.18360400	1.47436800
C	-2.55558400	2.92384300	2.65335300
C	-1.85986600	2.39455200	3.74155400
C	-1.32919000	0.49410200	2.58621100
C	-3.41004100	-1.12518400	0.03378600
C	-3.71459800	-2.00475600	-1.01509400
C	-4.88257900	-2.75410400	-0.94945800
C	-5.70775000	-2.60496900	0.16879800
C	-4.30807000	-1.05640100	1.10500700
C	-2.25690500	0.95968700	-1.47525200
C	-1.30247500	1.17380100	-2.47376800
C	-1.60074800	2.03537200	-3.52643900
C	-2.85795100	2.63832500	-3.55207300
C	-3.50662400	1.58104700	-1.63177300
H	-3.11714700	2.58816200	0.60414000
H	-3.03169100	3.89705100	2.72532000
H	-1.78008200	2.95397600	4.67175500
H	-0.82502700	-0.46832300	2.58011600
H	-3.04150100	-2.09930000	-1.86285200
H	-5.14971200	-3.44494100	-1.74283400
H	-6.62886900	-3.17838700	0.25419900
H	-4.11445600	-0.39204000	1.94247700
H	-0.35217000	0.65374500	-2.41837600
H	-0.87391200	2.24163300	-4.30495400
H	-3.12309800	3.32719600	-4.35166900
H	-4.30662100	1.38546900	-0.92008800
C	-0.79809300	-3.02110800	-0.05238600
O	-1.30679400	-4.03696800	0.17955200
C	4.06085800	-3.68522600	-0.28655600

H	4.55637800	-3.10051400	-1.07193200
H	3.75759900	-4.64225300	-0.72812800
C	1.78549400	-2.65970900	-0.80665600
H	4.80066300	-3.89422600	0.49659700
H	2.25587800	-2.18571300	-1.67634200
H	1.42606000	-3.63154900	-1.16572000
C	2.84928200	-2.92394500	0.26491700
H	3.20835700	-1.98669800	0.70659600
H	2.40302900	-3.48899400	1.09439400
N	0.93660900	3.91933300	-2.01824700
N	-3.80906100	2.40999600	-2.63489700
N	-5.43505200	-1.77685700	1.18176200
N	-1.25632100	1.19862800	3.72068500
N	2.17077900	-0.55126500	3.90390900
N	4.25481700	-0.16156600	-3.09929000
Ir	0.10003400	-1.41441000	-0.30161200

Ir-L5-n-Int3			
P	1.66449000	0.44808300	0.01193800
C	1.17129900	2.14330900	-0.52456600
C	0.39790800	2.96848000	0.30293900
C	-0.11687600	4.15799000	-0.20412800
C	0.16060900	4.49342200	-1.52892300
C	1.41364300	2.60071600	-1.83060700
C	3.27853900	0.23261400	-0.84599400
C	3.29274400	-0.15566400	-2.19390100
C	4.51305600	-0.33078500	-2.83883600
C	5.68586500	-0.13741100	-2.10686800

C	4.51844900	0.39490600	-0.21178900
C	2.15031500	0.73923700	1.76597400
C	1.96000100	-0.26848100	2.71733000
C	2.31064200	-0.02884800	4.04367300
C	2.83234700	1.22142300	4.37760200
C	2.70537500	1.94979500	2.21290300
H	0.20506200	2.69082800	1.33112100
H	-0.73348000	4.79810100	0.41843600
H	-0.23849800	5.40641100	-1.96569100
H	2.03033000	2.02092100	-2.51086900
H	2.36187600	-0.33006700	-2.72393700
H	4.55507100	-0.62714800	-3.88204600
H	6.65863200	-0.27552000	-2.57475600
H	4.56745700	0.67260100	0.83669600
H	1.53172700	-1.21768700	2.41667300
H	2.17704600	-0.79274600	4.80334000
H	3.10590000	1.45080900	5.40575900
H	2.88577400	2.76102700	1.51189200
P	-1.93129000	-0.14746700	-0.01689400
C	-1.92944500	1.02757300	1.39404700
C	-2.50587800	2.30399000	1.33600200
C	-1.73016300	2.86375700	3.41660700
C	-1.14231600	1.60840000	3.59426400
C	-1.24659300	0.67712600	2.56669400
C	-3.31485100	-1.27406700	0.41140200
C	-3.40974600	-2.51704700	-0.23615700
C	-5.32859100	-3.06434800	0.88163500
C	-5.32612800	-1.86311000	1.59132400
C	-4.30197500	-0.95019300	1.34925300

C	-2.61257200	0.84587400	-1.39608800
C	-1.74047400	1.45438100	-2.30429300
C	-2.26144700	2.26769400	-3.30517300
C	-3.64578900	2.42989300	-3.37209700
C	-3.98822100	1.06788500	-1.56523200
H	-3.04157400	2.62466900	0.44776600
H	-1.65039500	3.62525400	4.18968900
H	-0.59422100	1.37715600	4.50166200
H	-0.78156800	-0.29752100	2.65763700
H	-2.64385400	-2.81486000	-0.94756800
H	-6.11471000	-3.79907200	1.04435100
H	-6.10609900	-1.64921600	2.31526100
H	-4.26923600	-0.00551800	1.88301000
H	-0.67454600	1.29202400	-2.22322200
H	-1.60427000	2.76547000	-4.01051300
H	-4.09210000	3.05879500	-4.13987400
H	-4.70706200	0.60009400	-0.89732700
C	-0.28477100	-2.46101300	1.06839000
O	-0.53635500	-3.17611800	1.95250900
C	3.96966900	-3.77202500	-0.03893000
H	4.52758600	-3.27306800	-0.84055700
H	3.64748800	-4.75071300	-0.41432900
H	4.66031500	-3.94049900	0.79608900
C	2.76756800	-2.92024600	0.38824800
H	2.25894200	-3.39831400	1.23578400
H	3.14403100	-1.96087300	0.76102400
C	1.78285900	-2.70836300	-0.75913700
H	1.33230600	-3.66681800	-1.03460400
H	2.32636800	-2.35176200	-1.63663900

C	-0.16122200	-1.45470200	-2.28345600
O	-0.28730700	-1.57805300	-3.43165000
N	-4.39312600	-3.39454300	-0.01799300
N	-4.50275400	1.83991700	-2.52755500
N	0.92238900	3.73909600	-2.33224700
N	-2.40913400	3.21147500	2.31631900
N	5.69832800	0.21349900	-0.81613000
N	3.03255900	2.19977700	3.48479300
Ir	0.10709300	-1.32969000	-0.40038700

Ir-L5-n-Int4			
P	1.50960000	0.73752900	0.02251100
C	0.97670500	2.36516200	-0.66647700
C	-0.12588600	3.03171300	-0.10916100
C	-0.20426900	4.57280100	-1.79414700
C	0.90575000	4.00989200	-2.42331000
C	1.50455400	2.89079100	-1.85166100
C	3.31103100	0.71266600	-0.34450900
C	3.76945400	0.45537000	-1.64657500
C	5.14000700	0.39081900	-1.87845700
C	6.01097600	0.56990800	-0.80289600
C	4.27784200	0.88033400	0.65858000
C	1.46347100	1.00801200	1.83871500
C	1.32161700	-0.10321900	2.68457700
C	1.42377200	1.18537300	4.57026300
C	1.57786500	2.35667600	3.82769300
C	1.60970100	2.26448900	2.43822200
H	-0.55727600	2.68189500	0.82170500

H	-0.70885700	5.43442800	-2.22594600
H	1.28587900	4.43134500	-3.34813600
H	2.36355600	2.43392100	-2.32920100
H	3.07039600	0.26152400	-2.45052700
H	5.52492100	0.18747700	-2.87276600
H	7.08833300	0.51451300	-0.94737600
H	3.97913100	1.06799200	1.68506900
H	1.20261100	-1.08980300	2.24330500
H	1.39557600	1.22243500	5.65768800
H	1.67409300	3.31625100	4.32555900
H	1.73971500	3.15512700	1.83247600
P	-1.91096500	-0.24574000	-0.06132800
C	-2.21923200	0.60751300	1.53342400
C	-2.70782800	1.91329900	1.68436900
C	-2.52174600	1.83231800	3.96568600
C	-2.02571800	0.52716300	3.93445200
C	-1.86674100	-0.08988200	2.69955700
C	-3.29328400	-1.45552500	-0.11577400
C	-3.26528700	-2.45497600	-1.10259600
C	-5.27036600	-3.32092400	-0.42794500
C	-5.39939900	-2.37584900	0.58940500
C	-4.39488600	-1.42175800	0.74467300
C	-2.41112400	0.92155700	-1.38112800
C	-1.51871400	1.19161900	-2.42906500
C	-2.98063700	2.63114500	-3.43577700
C	-3.96018500	2.40623600	-2.46618500
C	-3.67379200	1.52538400	-1.42817100
H	-2.96453000	2.51473100	0.81730000
H	-2.65025700	2.35147600	4.91364200

H	-1.74464600	0.01721300	4.84951200
H	-1.45885400	-1.09430300	2.63421000
H	-2.41845300	-2.51879100	-1.78326400
H	-6.03652200	-4.07917800	-0.57757900
H	-6.26520800	-2.38663200	1.24428500
H	-4.46404600	-0.67124000	1.52554500
H	-0.54823200	0.70009300	-2.45414200
H	-3.16981400	3.31756700	-4.25900600
H	-4.92261100	2.90379300	-2.53029700
H	-4.41932900	1.30708900	-0.66918900
C	-0.25989100	-2.85764300	0.22857200
O	-0.52023400	-3.83535000	0.80612000
C	4.24516600	-4.06632400	0.59927600
H	4.95279600	-4.41966800	-0.16040200
H	3.56425100	-4.89442200	0.83032900
H	4.81522900	-3.83575700	1.50613000
C	3.47040900	-2.84141000	0.10992200
H	2.77775300	-2.50231300	0.88959700
H	4.16348300	-2.01231200	-0.07135400
C	2.67397900	-3.12739400	-1.17133000
H	2.04344100	-4.01352700	-1.00736000
H	3.34360300	-3.34119900	-2.01350200
C	1.73744400	-1.99670600	-1.56330800
O	1.75908300	-1.52029100	-2.69485200
N	-1.78602000	2.02826000	-3.43687500
N	-2.85648100	2.52084200	2.86929900
N	-4.22717200	-3.36590900	-1.26772600
N	-0.71195100	4.10475100	-0.64749000
N	1.30455400	-0.02910200	4.01926200

N	5.59696200	0.80920500	0.44674900
Ir	0.23752900	-1.20518900	-0.45039300

Ir-L5-n-Int5			
P	-1.50801400	-0.68916700	-0.00910100
C	-0.82906000	-2.40232600	-0.05212100
C	-0.09140000	-2.93173900	1.01354500
C	0.53831200	-4.16391200	0.85945900
C	0.40340900	-4.83420100	-0.35596900
C	-0.92366500	-3.18184800	-1.21609800
C	-3.03848600	-0.87597300	-1.00614100
C	-2.96635600	-0.70166600	-2.39587500
C	-4.12161900	-0.86100600	-3.15450700
C	-5.31253000	-1.17290900	-2.49735400
C	-4.28881500	-1.18336200	-0.45206900
C	-2.09355500	-0.51574500	1.72193800
C	-2.04621200	0.73843600	2.34253900
C	-2.48827700	0.86051700	3.65688600
C	-2.95373400	-0.28206700	4.31035000
C	-2.59295900	-1.59317500	2.47012200
H	-0.01381600	-2.39795100	1.95214700
H	1.13148900	-4.58143100	1.66640100
H	0.89383800	-5.79167500	-0.51809300
H	-1.51079200	-2.83597900	-2.06260500
H	-2.03375500	-0.41593200	-2.86920600
H	-4.10275600	-0.72695700	-4.23103700
H	-6.23645000	-1.29720400	-3.05871900
H	-4.40194300	-1.30579900	0.62129900

H	-1.64247500	1.58234900	1.79196500
H	-2.46775700	1.81870800	4.16671300
H	-3.29903200	-0.22803000	5.34102800
H	-2.65014800	-2.58711200	2.03288800
P	1.92898700	0.16712300	-0.00118600
C	1.98970100	-0.59764700	1.66592600
C	2.65369500	-1.79016200	1.98465500
C	1.81858400	-1.80769000	4.11765800
C	1.13502500	-0.60566500	3.91944600
C	1.22385700	0.00618300	2.67294300
C	3.35917500	1.32172300	0.02026300
C	3.63824300	2.05699200	-1.13869600
C	4.71422500	2.94111200	-1.12853900
C	5.22636900	2.43955000	1.03778000
C	4.17671700	1.52190100	1.13451100
C	2.53633600	-1.11364800	-1.16115400
C	1.68945900	-1.58848600	-2.16671800
C	2.15263000	-2.57718300	-3.03107400
C	3.45727500	-3.04111200	-2.86766900
C	3.84531800	-1.62162900	-1.11819700
H	3.24622500	-2.30863700	1.23795100
H	1.75663300	-2.32783600	5.07138900
H	0.52766400	-0.17736800	4.71019600
H	0.67984400	0.91894700	2.45387200
H	3.02424100	1.94987900	-2.02808000
H	4.95135400	3.52179600	-2.01764600
H	5.87606900	2.61325100	1.89382800
H	4.01124000	0.98105100	2.05968500
H	0.69330400	-1.17342100	-2.26948000

H	1.51448300	-2.98481800	-3.80766600
H	3.85073500	-3.82066300	-3.51683500
H	4.55956700	-1.23521200	-0.39350600
C	0.57195000	2.89976800	-0.44182100
O	0.99073900	3.96499300	-0.25596000
C	-2.63479000	3.77802500	0.23262200
H	-1.75861000	3.52462300	0.84126000
H	-2.33169500	4.62416800	-0.39661200
C	-1.81664200	2.03703400	-1.45651300
O	-1.83515900	2.07535600	-2.67874300
N	-5.40669700	-1.32846700	-1.17110100
N	-3.00905700	-1.49102900	3.73677600
N	-0.32581800	-4.36555500	-1.37703700
N	4.30314500	-2.56824200	-1.94049200
N	2.57087000	-2.39367500	3.17664400
N	5.50448100	3.14128100	-0.06470600
H	0.36507400	0.51835700	-4.36416300
H	-0.07911900	0.94847000	-3.94569300
Ir	-0.14253700	1.17724200	-0.57162500
C	-3.79151200	4.18717200	1.14715600
H	-3.52114800	5.04715400	1.77021700
H	-4.68104800	4.45895900	0.56725400
H	-4.07171200	3.36129500	1.81354700
C	-2.99865000	2.58653400	-0.66421200
H	-3.38271800	1.77177400	-0.03445200
H	-3.79128500	2.86448400	-1.36980400
Ir-L5-n-Int6			

P	1.42836300	0.77952600	0.01072600
C	0.63444200	2.30208200	-0.64340400
C	-0.26309800	3.07019900	0.10688100
C	-0.94677200	4.11031000	-0.51699700
C	-0.70898600	4.35682500	-1.86794600
C	0.81562700	2.65636100	-1.98936200
C	3.11036700	0.85250700	-0.72529100
C	3.33137900	0.37165700	-2.02385300
C	4.61670800	0.43780100	-2.55423200
C	5.63890800	0.96750900	-1.76631300
C	4.20960100	1.37621300	-0.02778100
C	1.76057800	1.16152400	1.79233500
C	1.99683900	0.11010400	2.68491300
C	2.24260200	0.41113100	4.02281600
C	2.23675800	1.74542400	4.42282200
C	2.00499900	2.72409500	3.45626900
H	-0.41654400	2.87227000	1.15691700
H	-1.65370100	4.71760100	0.03945800
H	-1.23585700	5.15453500	-2.38793300
H	1.51429800	2.10677400	-2.61301700
H	2.52401100	-0.07247700	-2.59279100
H	4.82287400	0.06780600	-3.55328300
H	6.65758000	1.02128400	-2.14565500
H	4.08775300	1.77032700	0.97662900
H	1.98137800	-0.91664100	2.34308200
H	2.42521900	-0.38466100	4.73856700
H	2.40746800	2.02577900	5.45705500
H	2.00081700	3.77864300	3.72380400
P	-2.02405500	-0.38009100	-0.10135100

C	-2.23399000	0.80040300	1.29520200
C	-3.09491700	1.90373000	1.26711100
C	-3.11190400	2.77604800	2.35344400
C	-2.26946600	2.51553300	3.43511000
C	-1.44707400	0.62568800	2.44561400
C	-3.16840400	-1.73948700	0.35670500
C	-3.35882800	-2.79460300	-0.55364500
C	-4.77021200	-3.89988700	0.86697600
C	-4.64794900	-2.91460900	1.84469900
C	-3.83632200	-1.81134100	1.58222200
C	-2.90737700	0.44595400	-1.47327100
C	-2.19306800	1.12938700	-2.46159500
C	-2.89406600	1.82363200	-3.44352400
C	-4.28831700	1.79757300	-3.40868800
C	-4.30993800	0.47436400	-1.54322600
H	-3.72222600	2.09291900	0.40323800
H	-3.76041500	3.64671000	2.35914900
H	-2.24643800	3.18492500	4.29268900
H	-0.76744500	-0.21702100	2.51567300
H	-2.84811300	-2.78382100	-1.51356600
H	-5.39701500	-4.77307000	1.03651000
H	-5.17727000	-3.00516500	2.78806100
H	-3.72800600	-1.02316900	2.31965600
H	-1.11190100	1.10928700	-2.46144400
H	-2.36413700	2.37323200	-4.21451000
H	-4.87033800	2.33010600	-4.15844000
H	-4.90602300	-0.06209100	-0.80802200
C	0.17077100	-2.23435300	1.12895200
O	0.10047100	-2.88605200	2.08269200

C	5.38260600	-3.27522100	0.40496500
H	5.04272000	-4.03881200	1.11600300
H	5.58271200	-2.35793200	0.97322400
H	6.33376100	-3.61602100	-0.01966100
C	4.34127400	-3.02716900	-0.68830300
H	4.70948700	-2.26910600	-1.38854900
H	4.18012200	-3.93426100	-1.28066100
C	3.00544900	-2.55854200	-0.11369400
H	3.15542400	-1.68479400	0.53265900
H	2.56601600	-3.33332000	0.53242100
O	2.15247000	-2.50173000	-2.33047500
H	0.17664900	-0.59146600	-2.02114900
C	1.94817000	-2.20537500	-1.17206700
H	-0.52500200	-2.45607500	-1.26946200
N	-4.14361500	-3.84713900	-0.31713200
N	1.78193500	2.44801600	2.16734000
N	5.45006700	1.43056600	-0.52434500
N	-1.45326000	1.45418900	3.49472400
N	0.16335200	3.65205200	-2.59960700
N	-4.99478900	1.13326400	-2.48281200
Ir	0.20610200	-1.22637700	-0.50214600

Ir-L5-n-Pro			
P	2.40909700	0.10415900	0.00778300
C	3.05725600	1.60551600	-0.81628300
C	2.24239700	2.73898800	-0.95031200
C	3.89412100	3.91902300	-2.00375700
C	4.78822600	2.84845800	-1.92853300

C	4.36032500	1.66986200	-1.32504100
C	3.11566800	-1.26171300	-0.99119400
C	2.38255100	-1.77567900	-2.06820200
C	2.92454900	-2.81401600	-2.81879200
C	4.18870400	-3.29482400	-2.47457300
C	4.37459900	-1.82530700	-0.73135700
C	3.36584700	0.00710300	1.56707800
C	3.23009600	-1.13081300	2.37604100
C	3.91890500	-1.18884200	3.58096900
C	4.71231900	-0.09787800	3.94712200
C	4.18514300	1.04218300	2.03453500
H	1.21936600	2.71103000	-0.58419800
H	4.19549400	4.85486200	-2.47089000
H	5.79007400	2.93746600	-2.33666800
H	5.02446300	0.81369500	-1.25469500
H	1.40088100	-1.38285300	-2.30271200
H	2.36270600	-3.24943200	-3.63772900
H	4.64415200	-4.10610700	-3.03948800
H	4.97495800	-1.46958400	0.10263800
H	2.59489000	-1.95437900	2.06218100
H	3.83956200	-2.05501300	4.23003200
H	5.26179300	-0.10710500	4.88653000
H	4.31502600	1.94789600	1.44911200
P	-2.11744300	0.61135800	-0.02181300
C	-2.32991600	2.39061900	-0.39403900
C	-3.26047800	2.88126300	-1.31487900
C	-3.33734600	4.25770600	-1.52049300
C	-2.48550900	5.08957000	-0.79291100
C	-1.51901900	3.31842500	0.28091300

C	-3.22463400	0.33518000	1.41266100
C	-3.13212300	-0.87242000	2.11654800
C	-3.98540900	-1.09784800	3.19032100
C	-4.89976300	-0.09829200	3.53240900
C	-4.17794700	1.26752600	1.84390500
C	-3.01530200	-0.23733900	-1.38095200
C	-2.35857700	-0.52162900	-2.58642200
C	-3.04696600	-1.20204700	-3.58541200
C	-4.37037300	-1.57694800	-3.34795500
C	-4.35084800	-0.65143500	-1.25568700
H	-3.90712500	2.20269300	-1.86229100
H	-4.04197900	4.67828300	-2.23101400
H	-2.51854900	6.16845900	-0.93062700
H	-0.77654600	2.96394800	0.99365700
H	-2.39874700	-1.61602900	1.82619400
H	-3.93881600	-2.02231700	3.75695700
H	-5.58059000	-0.23705100	4.36998600
H	-4.28405100	2.22121800	1.33388800
H	-1.32132700	-0.23352200	-2.71712500
H	-2.55964000	-1.45807200	-4.52027300
H	-4.93428500	-2.12146800	-4.10281800
H	-4.90439500	-0.45375200	-0.34195800
C	0.07344500	-0.33841600	2.06061100
O	0.05173400	-0.63118700	3.18492300
C	-2.49287400	-4.56919500	1.58896200
H	-2.90843900	-5.48501600	1.15331400
H	-3.31024600	-3.84161500	1.66247300
H	-2.15517400	-4.80334100	2.60450600
C	-1.34560800	-4.02433500	0.73537100

H	-0.91266000	-3.13247600	1.20895900
H	-0.53630200	-4.76423700	0.68628100
C	-1.79274600	-3.66237500	-0.69009400
H	-2.63466900	-2.95595900	-0.63269400
H	-2.13309800	-4.53794700	-1.25278900
O	-0.36323700	-3.22703700	-2.59468000
H	0.17699000	0.50000300	-1.40702800
C	-0.69705600	-2.96542900	-1.45609500
H	-0.20114000	-2.13840200	-0.88811100
N	-5.02151500	-1.30824800	-2.20949700
N	-5.00055300	1.06540200	2.88069200
N	4.91068300	-2.81582000	-1.45286200
N	2.64383700	3.87604800	-1.52908300
N	4.84720000	1.00087100	3.19835800
N	-1.59121600	4.63867900	0.09702900
Ir	0.11435900	0.10484100	0.23085300

Ir-L5-n-TS1			
P	-1.82494900	0.08948400	-0.05155300
C	-2.50299100	0.46428400	1.62181100
C	-1.68046700	0.30338700	2.74094300
C	-2.16604700	0.64173800	4.00199200
C	-3.46941500	1.12695800	4.10181800
C	-3.32242500	-0.49605200	-0.94080700
C	-5.43042000	-1.67090300	-2.25001500
C	-4.60587700	-0.79316600	-2.95676900
C	-3.53457000	-0.20277300	-2.29401300
C	-1.59068700	1.78424500	-0.74549000

C	-0.94349500	4.20738200	-1.86248200
C	-1.73473200	4.18885200	-0.71280000
C	-2.06834500	2.95822300	-0.15023100
H	-0.67253200	-0.07505700	2.61774200
H	-1.54145500	0.53547800	4.88324900
H	-3.88493800	1.40391600	5.06893200
H	-6.27307200	-2.15506900	-2.73964400
H	-4.79893300	-0.57965200	-4.00353100
H	-2.87397900	0.47746200	-2.82195100
H	-0.65573300	5.15096900	-2.32231800
H	-2.07952800	5.11723900	-0.26734200
H	-2.66837000	2.91785200	0.75176600
P	1.81644800	0.06032800	0.00535500
C	1.54241300	1.16550300	1.45038800
C	0.85884900	2.55810500	3.71409000
C	0.55935300	3.11330700	2.47040600
C	0.90613700	2.40659000	1.32213600
C	2.40953200	1.23247500	-1.28751800
C	3.26387100	2.83261200	-3.34403400
C	3.46655800	3.26525000	-2.03312700
C	3.04129400	2.44749500	-0.99074400
C	3.39094600	-0.77895300	0.46429800
C	5.64952700	-2.19463000	1.07721000
C	5.65462700	-0.81062200	1.27552300
C	4.50665500	-0.09189900	0.96041900
H	0.59337700	3.07875500	4.63191400
H	0.05734500	4.07302200	2.39905900
H	0.68156600	2.81482200	0.34485200
H	3.57753600	3.44927700	-4.18412100

H	3.94585200	4.21907400	-1.83496100
H	3.18459500	2.76242500	0.03748400
H	6.53122900	-2.78664700	1.31626800
H	6.53724800	-0.31507900	1.66787800
H	4.47619100	0.98378500	1.10550200
C	0.39385700	-1.86678900	-2.11333100
O	0.58746100	-2.23125300	-3.20519400
C	-1.17890200	-3.17635400	-0.06286700
C	-0.45710500	-3.14042900	1.17909600
H	-2.25215000	-3.00848200	-0.05148600
H	-0.85864600	-3.92334800	-0.78511500
C	0.68853900	-4.08181700	1.46562000
H	-1.05069500	-2.88157200	2.05637400
H	0.09203500	-1.62012900	1.34363700
H	0.30322700	-4.97591100	1.97601200
H	1.17638600	-4.39918300	0.54044200
H	1.44582900	-3.62959000	2.11245500
N	1.47318700	1.37668700	3.86299500
N	-4.28284500	1.28463400	3.04743200
N	-0.49276300	3.09833900	-2.46285300
N	2.69368400	1.66356200	-3.65280400
N	4.60013500	-2.87001600	0.59726500
N	-5.24733000	-1.96989800	-0.95884600
C	3.50029900	-2.16457800	0.29981300
C	1.80288700	0.70866300	2.75184900
C	2.27705700	0.89384800	-2.64252400
C	-0.81134800	1.92494400	-1.90614500
C	-4.21714100	-1.39228100	-0.33177400
C	-3.80083000	0.95686600	1.84452700

H	-4.48355400	1.09077400	1.00828200
H	-4.10475000	-1.64729700	0.72007400
H	2.29141400	-0.25109400	2.90376000
H	2.64755600	-2.71361100	-0.09069800
H	-0.40853100	1.03865400	-2.38696100
H	1.81010800	-0.04175400	-2.92925700
Ir	0.01414400	-1.35723700	-0.34376200

Ir-L5-n-TS2			
P	-1.81116200	0.38440300	0.01642800
C	-1.34561800	2.11220300	0.43533300
C	-0.41844100	4.65531200	0.87340200
C	-0.95522200	3.94569500	1.94537700
C	-1.44157300	2.65725700	1.71949300
C	-2.74651900	-0.15054500	1.50602500
C	-3.96087300	-0.93775400	3.83415600
C	-4.75723900	-0.45385400	2.79594100
C	-4.13882400	-0.04375000	1.61739700
C	-3.14454700	0.64247000	-1.22310500
C	-3.40323500	-0.35447100	-2.17149500
C	-4.42659600	-0.16189800	-3.09505400
C	-5.15336800	1.02897300	-3.04325800
H	-0.02415100	5.65879800	1.01379000
H	-0.99913900	4.39254700	2.93369800
H	-1.88278700	2.08528500	2.52964900
H	-4.40959700	-1.25392700	4.77396300
H	-5.83501800	-0.39227300	2.91073700
H	-4.73037400	0.35005100	0.79821200

H	-2.79997800	-1.25698200	-2.18427700
H	-4.65234800	-0.91239400	-3.84602000
H	-5.95712800	1.21623400	-3.75267500
P	2.02950900	-0.05697600	-0.03596200
C	2.36224300	1.71355800	-0.38827200
C	2.83336300	4.35583400	-0.93625800
C	2.56919800	3.48977000	-2.00051700
C	2.32737900	2.15178100	-1.72164100
C	3.54941100	-0.84159600	-0.70176300
C	5.71487000	-2.16224100	-1.71715200
C	5.91848100	-0.92555200	-1.09825000
C	4.81559500	-0.25317100	-0.58175300
C	2.22572000	-0.21143800	1.77555000
C	1.31845000	0.44573600	2.61903100
C	1.39871000	0.24053600	3.99070900
C	2.37917500	-0.62959000	4.47603100
H	3.00873900	5.41410900	-1.11802600
H	2.53991700	3.86269400	-3.01918900
H	2.10675500	1.45684000	-2.52493400
H	6.55688500	-2.71347600	-2.13187800
H	6.91656200	-0.50472800	-1.02677100
H	4.93048900	0.71106900	-0.09501300
H	0.56668800	1.10583700	2.19991200
H	0.70786700	0.72835600	4.67100900
H	2.46467100	-0.82290400	5.54350700
C	0.07479400	-0.26778100	-2.50777600
O	0.10130000	0.04683800	-3.62702700
C	-2.90129300	-4.69120000	-1.14253600
H	-2.29369500	-5.60184800	-1.19919900

H	-3.06957900	-4.34070300	-2.16868800
H	-3.87430700	-4.96227300	-0.71599200
C	-2.20854200	-3.61672200	-0.29602500
H	-2.84406200	-2.72386300	-0.24486100
H	-2.09447200	-3.97231100	0.73390900
C	-0.84054000	-3.23917900	-0.85510600
H	-0.91921700	-2.92622000	-1.90065700
H	-0.12146200	-4.05986400	-0.82237300
C	-0.02770100	-2.29636500	0.59647400
O	0.10805700	-2.92302000	1.58957000
N	-4.92171400	1.99909200	-2.14969500
N	-2.62908200	-1.04795700	3.75176200
N	-0.34785800	4.16329800	-0.37239800
N	3.25087100	-1.26901300	3.69070700
N	4.51488900	-2.73944400	-1.84638100
N	2.88883100	3.96039200	0.33804600
C	-3.93813100	1.79917400	-1.26554800
C	-0.78433000	2.92022500	-0.57044800
C	2.66174200	2.66482400	0.59503900
C	3.16726900	-1.05972000	2.37059500
C	3.46113100	-2.08151800	-1.34706500
C	-2.04745600	-0.67859800	2.60570900
H	-0.97288900	-0.81511600	2.55985800
H	3.88292700	-1.60202200	1.75959100
H	2.72179200	2.37697900	1.63995900
H	2.48592400	-2.54987100	-1.46559700
H	-0.68484200	2.53576500	-1.58320900
H	-3.76608700	2.60528700	-0.55608200
Ir	-0.00032000	-0.89680600	-0.69562900

Ir-L5-n-TS3			
P	1.91786200	0.24504000	0.16920600
C	2.07428300	-0.87436400	1.61752500
C	1.79186300	-2.24556500	1.51039400
C	2.11302000	-2.60676700	3.74359900
C	3.26732200	1.45513100	0.51458400
C	3.01929700	2.83093300	0.48801300
C	4.06588800	3.71410400	0.75125400
C	5.32424200	3.18843700	1.03705200
C	2.61308300	-0.77606600	-1.19635100
C	2.14403700	-0.60240100	-2.50288400
C	2.69532700	-1.36435400	-3.53010800
C	3.69878800	-2.27812700	-3.21671900
H	1.55232400	-2.67406700	0.54243200
H	2.12144300	-3.32123800	4.56409200
H	2.02315600	3.19536800	0.26077800
H	3.90762800	4.78783000	0.73342300
H	6.16512900	3.84663800	1.24657200
H	1.35234600	0.10361800	-2.71252000
H	2.33319800	-1.26044900	-4.54710600
H	4.15107500	-2.89299000	-3.99245200
P	-1.50930500	-0.65908600	-0.05978500
C	-0.97163500	-1.82635500	-1.36936700
C	-0.46809400	-3.10930200	-1.14022800
C	-0.00212700	-3.85612100	-2.22293700
C	-0.08291900	-3.30377300	-3.49865700
C	-3.33478800	-0.53772100	-0.28798700

C	-6.04197000	-0.27388200	-0.60810800
C	-3.99922300	-0.81202700	-1.48947500
C	-1.52738800	-1.64238000	1.49621500
C	-0.98761400	-1.11515100	2.67060700
C	-1.11122700	-1.83169500	3.85879600
C	-1.76488300	-3.06221000	3.82540300
H	-0.42907100	-3.52423400	-0.13941300
H	0.41118500	-4.84881200	-2.07611200
H	-7.11370600	-0.17862900	-0.77234400
H	-3.45134900	-1.15080600	-2.36151800
H	-0.47563700	-0.16037400	2.64685000
H	-0.70006200	-1.44966700	4.78709700
H	-1.86761300	-3.65876400	4.72968100
C	0.51868200	2.24080500	-1.75449800
O	0.94510700	2.74301700	-2.71509200
C	-3.27498200	3.23240900	1.08820200
H	-2.80527300	2.48040100	1.73594700
H	-4.17690100	2.76681400	0.67606200
O	-2.66812200	1.96119700	-1.78674200
H	-0.52356000	1.81259500	1.82812500
C	-1.95353300	2.30880700	-0.86493900
H	-0.09743900	2.31149700	1.39241600
N	-2.30845900	-3.58131200	2.71562100
N	-0.56944000	-2.07802300	-3.74288000
N	4.16315800	-2.46658700	-1.97360000
N	5.58472600	1.87345200	1.07609500
C	3.62780700	-1.72907800	-0.99860500
C	-0.98305500	-1.35842000	-2.69798300
C	-2.19843600	-2.87401300	1.58914400

C	-4.11220900	-0.11556100	0.79742200
C	2.38711800	-0.38159200	2.89074400
C	4.57536800	1.03992200	0.81737800
H	-2.68179100	-3.30000000	0.71231800
H	-3.64977900	0.09999600	1.75571500
H	2.62165500	0.66915100	3.03237800
H	4.81965200	-0.01826500	0.85926400
H	4.01708300	-1.92277900	-0.00255800
H	-1.33329800	-0.34998100	-2.91045200
H	0.26383200	-3.86187500	-4.36582300
Ir	-0.20390700	1.29765800	-0.32420600
N	-5.32112900	-0.69057000	-1.65360000
N	1.81078400	-3.09969800	2.53652400
C	2.40787400	-1.26101500	3.97029400
C	-5.48656300	0.02176600	0.63793400
H	2.65686500	-0.91316500	4.96811700
H	-6.11549400	0.34700100	1.46085100
C	-3.64436500	4.46335700	1.91811400
H	-4.13553200	5.22278200	1.29860900
H	-4.32787500	4.20324100	2.73466200
H	-2.75194700	4.92300100	2.36052600
C	-2.32487600	3.56847500	-0.07170500
H	-2.82376800	4.26045700	-0.76200700
H	-1.42199600	4.05494100	0.31372400

Ir-L5-n-TS4			
P	1.63722400	0.67108900	-0.01512600
C	0.94176800	2.27971000	-0.58563200

C	0.06191400	3.00346000	0.23083200
C	-0.57157300	4.12965000	-0.28466000
C	-0.31447200	4.49619900	-1.60600700
C	3.23127500	0.55137200	-0.91605900
C	3.22606600	0.10782800	-2.24697800
C	4.43836200	-0.03411200	-2.91424100
C	5.61785200	0.24838000	-2.22347400
C	2.15486900	1.07478800	1.70121500
C	2.16866900	0.09848200	2.70233700
C	2.56948700	0.44706100	3.98924400
C	2.94720700	1.76679300	4.23383900
H	-0.12515500	2.69440600	1.25197200
H	-1.25905700	4.70461400	0.32676200
H	-0.80446200	5.36227100	-2.04647000
H	2.29543200	-0.15778100	-2.73339000
H	4.46775200	-0.38141800	-3.94186900
H	6.58459000	0.13562600	-2.71073600
H	1.86649500	-0.91751500	2.48506900
H	2.58079000	-0.28779400	4.78759300
H	3.25540600	2.07887600	5.22958300
P	-2.06715100	-0.32081600	-0.08559900
C	-2.25718800	0.90921700	1.27795400
C	-3.07885800	2.03780900	1.18254300
C	-3.09031100	2.95944300	2.22893600
C	-2.28130300	2.72040500	3.33930300
C	-3.27567600	-1.62106500	0.38447400
C	-3.17394100	-2.88850200	-0.20382500
C	-4.09934100	-3.86824900	0.13986000
C	-5.08883400	-3.55139600	1.07375800

C	-2.89098800	0.54443900	-1.47651000
C	-2.15281500	1.43445300	-2.26631800
C	-2.79936100	2.14689800	-3.26956800
C	-4.16636000	1.93330300	-3.46055700
H	-3.68480700	2.20566800	0.29889000
H	-3.71136400	3.84873300	2.18161700
H	-2.25406600	3.42479500	4.16808400
H	-2.37186000	-3.09265800	-0.90810700
H	-4.05298100	-4.86082800	-0.29705700
H	-5.82440400	-4.29603100	1.37186200
H	-1.09170400	1.55649800	-2.09798200
H	-2.24971700	2.84674200	-3.89089500
H	-4.70626900	2.46896600	-4.23919500
C	0.13177200	-2.04778900	1.25268900
O	0.09885700	-2.70972300	2.20597800
C	4.20931100	-3.84834700	0.92511100
H	4.57416900	-4.73713100	0.39700900
H	3.57896300	-4.18945700	1.75546700
H	5.07634800	-3.33142600	1.35073700
C	3.43133400	-2.92466700	-0.01243600
H	3.09653200	-2.03646700	0.53405400
H	4.07745000	-2.56460000	-0.82103300
C	2.20629900	-3.62083600	-0.63282400
H	1.53943900	-3.98713800	0.15340600
H	2.54387300	-4.48115500	-1.22565000
O	1.83763300	-2.47323500	-2.70320000
H	0.06198800	-0.30497500	-1.84670000
C	1.46088800	-2.68795100	-1.57030200
H	0.20002900	-2.55309600	-1.36129300

N	-4.89038500	1.07930700	-2.72698900
N	-5.19912500	-2.35180300	1.65590100
N	-1.49930600	1.63770200	3.46075300
N	0.52971000	3.82839100	-2.40163800
N	5.64729800	0.65609400	-0.94883500
N	2.96199100	2.71611800	3.28935500
C	-4.25828100	0.40739300	-1.75639800
C	-4.30947400	-1.41428900	1.30878100
C	-1.49761900	0.76321100	2.45108200
C	2.57801800	2.36690100	2.05863700
C	1.14376200	2.75349200	-1.89032900
C	4.47565600	0.80592400	-0.32050500
H	-4.42359300	-0.45015600	1.79726700
H	-0.83762200	-0.08920000	2.57115600
H	-4.87404800	-0.27484000	-1.17642100
H	2.60521100	3.15859000	1.31448000
H	1.82644500	2.24148900	-2.56162400
H	4.53701200	1.13116200	0.71374500
Ir	0.12311900	-1.04535500	-0.37279700

Ir-L5-1			
P	1.93288100	-0.00806500	-0.71079400
C	2.02949000	-0.79502700	0.96725100
C	3.07947300	-1.65638200	1.30694600
C	2.17861000	-2.00681800	3.45774900
C	1.10935100	-1.18455700	3.17745200
C	1.03579900	-0.57476200	1.92051800
C	2.51542400	1.70393500	-0.28752700

C	3.22998000	2.08156100	0.87253700
C	3.54348700	3.41554200	1.07641200
C	3.13895800	4.37672800	0.15140400
C	2.15881700	2.69258300	-1.18826900
C	3.45161000	-0.72300700	-1.49856600
C	3.34463700	-1.96532600	-2.13982900
C	4.47856500	-2.53910900	-2.72831000
C	5.66654100	-1.84405000	-2.72246800
C	4.68382400	-0.08183000	-1.49415200
H	3.89915900	-1.88241200	0.64821600
H	2.30396200	-2.51193200	4.40664300
H	0.31860800	-1.03203500	3.90441100
H	0.18704500	0.06533700	1.71140700
H	3.56423000	1.33685400	1.58454700
H	4.08547100	3.73416300	1.95834300
H	3.39630000	5.42096700	0.23002000
H	1.57270100	2.47742600	-2.07544200
H	2.38502900	-2.46024000	-2.19527200
H	4.42524300	-3.52133200	-3.18105000
H	6.57532800	-2.21806200	-3.17608600
H	4.85302200	0.87674800	-1.02789400
P	-1.68977200	-0.50331600	-0.65377900
C	-1.91121600	-2.02320400	0.36709200
C	-3.10522200	-2.31575300	1.03181600
C	-2.21794800	-4.35321100	1.81594100
C	-1.01039300	-4.10367600	1.20104000
C	-0.85817800	-2.92989300	0.45015700
C	-3.20599500	-0.61279500	-1.69371000
C	-4.00042700	0.50122700	-1.93717000

C	-5.32222300	-0.69515900	-3.47240500
C	-4.57244600	-1.83532200	-3.26489700
C	-3.49362900	-1.79291000	-2.38053600
C	-2.07152600	0.90165300	0.48401100
C	-1.14407800	1.94045100	0.58676300
C	-1.38126100	3.01607500	1.44695300
C	-2.56978200	3.05643300	2.14489600
C	-3.23818100	0.98065700	1.24579300
H	-4.00680900	-1.71506400	0.95050000
H	-2.41197400	-5.23927800	2.40739600
H	-0.18529200	-4.80621700	1.26516400
H	0.07414900	-2.74929600	-0.07821100
H	-3.84269000	1.45085200	-1.44993900
H	-6.17513900	-0.65869200	-4.13687400
H	-4.82972900	-2.74450900	-3.79444500
H	-2.87994700	-2.67490200	-2.23525100
H	-0.24167400	1.90594000	-0.01085000
H	-0.67100800	3.83684900	1.54782100
H	-2.82685100	3.86929700	2.81293100
H	-4.06097700	0.28039700	1.17329300
C	-0.27496500	-1.87718400	-3.06464300
O	-0.46819800	-2.87739100	-3.63051400
Ir	0.14957900	-0.35050300	-2.06328400
N	3.14300200	-2.22385400	2.53347000
N	-3.49015200	2.07160100	2.00857900
N	-3.25533500	-3.48560700	1.68941800
N	5.75067100	-0.61903900	-2.13994400
N	2.49568200	3.98946400	-0.98470700
N	-5.00882900	0.45506600	-2.83392700

C	-5.88408600	1.63245500	-2.94725100
H	-5.26335800	2.52848600	-2.99549400
H	-6.48174800	1.55064500	-3.85457800
H	-6.53098100	1.64636100	-2.06301900
C	-4.72130200	2.07658700	2.82352900
H	-5.53418700	1.64240700	2.23669400
H	-4.53435500	1.45347300	3.70408300
H	-4.95154200	3.10360100	3.10660800
C	-4.50258400	-3.69214800	2.45081600
H	-4.39632700	-3.14676100	3.39543600
H	-5.33786300	-3.27728200	1.88285000
H	-4.64360600	-4.75963700	2.62094200
C	4.27089500	-3.12980600	2.81320000
H	4.18354800	-3.98289000	2.13194700
H	5.19845700	-2.57774100	2.63393700
H	4.21283300	-3.45420900	3.85161000
C	2.00446300	5.03383900	-1.90038800
H	1.40042600	4.56710000	-2.67817500
H	1.39337800	5.72204000	-1.30399500
H	2.85282100	5.56400000	-2.33943700
C	7.03073100	0.10807900	-2.09307400
H	6.90689000	1.08831900	-2.55861600
H	7.31172100	0.22073300	-1.03862200
H	7.78467900	-0.46265700	-2.63413100
I	-1.09060600	2.15321400	-3.01439300
I	2.47636700	-4.63461500	-0.18270900
I	6.17857700	-0.02599200	1.57241000
I	-2.53486400	-0.80067100	3.93500000
I	-6.47158200	-0.59487900	0.27755200

I	0.87659600	6.03944600	1.61024700
H	1.23797700	-0.05165900	-3.23628100

Ir-L5-1-Int1			
P	1.89127900	-0.34794500	-0.40385900
C	1.67521000	-1.72479500	0.81493900
C	2.42223400	-2.89683200	0.68497200
C	1.23536500	-3.92232400	2.44708400
C	0.48489700	-2.78400800	2.64186400
C	0.68664800	-1.68433700	1.79596700
C	1.94433700	1.05500900	0.78815900
C	2.39364200	0.91284500	2.11111200
C	2.45667700	2.02761600	2.94081500
C	2.05857900	3.26036600	2.45155900
C	1.62517800	2.32727300	0.32687300
C	3.67463600	-0.51828100	-0.86152900
C	4.04497100	-1.29749100	-1.95357300
C	5.39978400	-1.41832300	-2.29457900
C	6.34444800	-0.74135300	-1.55580500
C	4.67613000	0.14412400	-0.14848400
H	3.18804700	-3.02186100	-0.06392800
H	1.13091900	-4.81208400	3.05441500
H	-0.28725000	-2.75901200	3.40503800
H	0.07035700	-0.79985300	1.92825800
H	2.73405700	-0.05037300	2.48108800
H	2.78789700	1.94641200	3.96855200
H	2.08254000	4.16548600	3.03869000
H	1.30425200	2.50714300	-0.68962800

H	3.28558300	-1.81030300	-2.53474200
H	5.71101900	-2.02391000	-3.13713400
H	7.40484500	-0.77813700	-1.76891800
H	4.48476300	0.77234700	0.70327600
P	-1.58010400	-0.53620400	-1.13144000
C	-2.33836200	-2.02171000	-0.34208400
C	-3.70242800	-2.04949100	-0.09202400
C	-3.50687200	-4.10854400	1.02535700
C	-2.16476700	-4.19177900	0.68286300
C	-1.56436100	-3.14118100	0.00283600
C	-2.85974000	-0.26231500	-2.44204500
C	-3.58859700	0.91460100	-2.56788100
C	-4.50229500	0.19263700	-4.62101500
C	-3.82577000	-1.00736500	-4.52875900
C	-2.97800400	-1.23312400	-3.44046800
C	-1.98667500	0.79790500	0.07277200
C	-1.60748100	2.10955700	-0.29076700
C	-2.02315600	3.18593100	0.47016900
C	-2.76241800	2.95985400	1.63141500
C	-2.70907000	0.62672800	1.24323600
H	-4.37562300	-1.23318500	-0.35293600
H	-4.02178200	-4.86718900	1.59802300
H	-1.59040300	-5.04810100	1.01376100
H	-0.51882400	-3.17502900	-0.27368200
H	-3.53876200	1.72265100	-1.85620700
H	-5.15689900	0.44239700	-5.44586200
H	-3.93769300	-1.74302900	-5.31617500
H	-2.37870900	-2.13870200	-3.38865000
H	-1.00478400	2.25249800	-1.18092800

H	-1.76522300	4.20367900	0.20419600
H	-3.18178700	3.75251000	2.22923300
H	-2.99433400	-0.33794000	1.65165000
C	-0.24282800	0.45002900	-3.70045000
O	-0.67093400	1.01515400	-4.62686200
Ir	0.46766500	-0.42868800	-2.21077300
N	2.15545300	-3.97928700	1.44849300
N	-3.07661300	1.69411200	1.99325000
N	-4.27241100	-3.09361500	0.54657600
N	5.97436000	0.02389600	-0.50445200
N	1.66085400	3.38949800	1.16376500
N	-4.35577800	1.13878400	-3.66466700
C	-5.11275500	2.40161700	-3.72055500
H	-4.41145900	3.23814700	-3.69735800
H	-5.69373500	2.43121300	-4.64152100
H	-5.77109400	2.42844000	-2.84369300
C	-3.88082200	1.49659400	3.21657300
H	-4.92274900	1.72665300	2.97943500
H	-3.79035800	0.45781400	3.53800700
H	-3.48443900	2.16466000	3.98497300
C	-5.68386300	-3.00980100	0.96933100
H	-5.68585300	-2.88561600	2.05789500
H	-6.14574100	-2.14151500	0.49779900
H	-6.20076100	-3.92733800	0.68215300
C	3.03508700	-5.14811100	1.29785700
H	3.06021200	-5.43863300	0.24564000
H	4.03356900	-4.85398400	1.64206000
H	2.64870700	-5.96960800	1.90033500
C	1.36767900	4.73921300	0.65739100

H	0.79279000	4.65566300	-0.26352600
H	0.79852100	5.27006200	1.42388400
H	2.31880400	5.22859800	0.42997600
C	6.96337400	0.75641900	0.30003000
H	6.69416900	1.81737500	0.26308400
H	6.92135000	0.36441500	1.32056100
H	7.95479300	0.60171200	-0.12428500
I	4.43869800	3.32109600	-1.12507600
I	0.82056400	-3.32700800	-2.68682800
I	5.02543100	-2.00728800	2.41972300
I	-3.11319200	-2.40996700	3.75492900
I	-5.98091700	0.92197100	-0.29826900
I	-0.81768500	3.98823400	3.90876400
H	1.83695500	-0.22542400	-3.06009800
C	0.91928400	4.88490100	-2.82406300
H	1.95946400	4.68764300	-2.57395700
H	0.61756800	5.92783400	-2.91472400
C	0.05542000	3.88875300	-3.03758700
H	0.41429900	2.86289000	-2.96075000
C	-1.38352800	4.06678500	-3.43698400
H	-1.64365500	5.12584200	-3.53790500
H	-1.57916300	3.56299800	-4.39146700
H	-2.06817400	3.62142500	-2.69977700

Ir-L5-1-n-Int2			
P	-1.71334600	-0.14535400	0.26052600
C	-1.00429300	1.47440000	0.78900100
C	-0.62706900	1.68759200	2.12278300

C	-0.14994900	2.93652900	2.51042500
C	-0.00906500	3.94446600	1.56955100
C	-3.03152300	-0.35635300	1.53446900
C	-3.54579800	-1.64239400	1.78918700
C	-4.53160400	-1.78881200	2.78204600
C	-5.02800400	-0.68059300	3.41964000
C	-2.70816600	0.37648400	-1.20492300
C	-4.18234100	1.15418400	-3.41600900
C	-2.85463500	0.83285600	-3.57576900
C	-2.11500500	0.41870500	-2.45893300
H	-0.72481400	0.88208000	2.84510300
H	0.12569000	3.14221100	3.53817200
H	0.38692600	4.92631900	1.79749500
H	-3.10087900	-2.50193300	1.30518200
H	-4.92968800	-2.76735900	3.01798600
H	-5.80312200	-0.72550700	4.17432300
H	-4.82112900	1.47238600	-4.22955300
H	-2.38803400	0.91654100	-4.54938300
H	-1.06387300	0.18886900	-2.57479300
P	1.71999700	-1.51751500	-0.24088600
C	2.42985800	0.09312800	0.30638600
C	2.26071100	0.48263600	1.64420500
C	2.89278300	1.63002600	2.11384800
C	3.62938600	2.41618600	1.24303100
C	2.28738900	-1.58746700	-2.00961800
C	2.90223800	-1.69132200	-4.70829700
C	3.92167000	-1.74155700	-3.78140600
C	3.61776800	-1.71325500	-2.41212100
C	2.98700300	-2.67077400	0.45676800

C	3.12256000	-3.95856200	-0.06714600
C	3.99674400	-4.87514400	0.52900800
C	4.70298700	-4.50584300	1.65235000
H	1.65721200	-0.13336200	2.30679600
H	2.80707100	1.94089700	3.14807500
H	4.11578600	3.33709300	1.53590100
H	3.06694700	-1.71800300	-5.77798500
H	4.94980700	-1.80499900	-4.11852800
H	4.42415500	-1.73864600	-1.67839100
H	2.55697300	-4.25126100	-0.94317000
H	4.11925300	-5.87427600	0.12823300
H	5.39493500	-5.16032000	2.16542800
C	-1.50213600	-2.62192100	-1.49623200
O	-1.92796700	-2.89261600	-2.55315400
C	3.75179200	-2.34771700	1.57889700
C	1.30559700	-1.50544300	-2.99155300
C	3.16336200	0.92901900	-0.52706800
C	-0.83956100	2.51893100	-0.11307800
C	-4.06018400	0.71549300	-1.10097500
C	-3.58032900	0.72774600	2.19317600
H	-4.60524600	0.71029300	-0.17507100
H	-1.08808100	2.44490000	-1.16048400
H	-3.30456900	1.75609500	1.98309100
H	3.71075700	-1.38367100	2.05964000
H	0.25995600	-1.45668000	-2.72881600
H	3.31036500	0.74012600	-1.57784400
Ir	-0.49963700	-2.12034200	-0.03378500
N	4.54700500	-3.26340500	2.17608500
N	-0.32076400	3.70260100	0.27551400

N	-4.57331200	0.56721900	3.10283300
N	3.70850100	2.07317700	-0.06366000
N	1.60966700	-1.61689400	-4.30217700
N	-4.76214900	1.09206900	-2.19280100
C	4.49088900	2.91929400	-0.98572900
H	4.44508700	3.94818700	-0.62086900
H	5.51699800	2.54154600	-1.00228000
H	4.03389100	2.85564000	-1.97477000
C	0.51815400	-1.45334100	-5.27844000
H	0.30741500	-0.38070800	-5.35561400
H	0.82984500	-1.85932900	-6.24067200
H	-0.36051000	-1.98802900	-4.91326800
C	5.40365100	-2.80475800	3.28180100
H	5.90035800	-3.66345300	3.73219800
H	6.13571600	-2.10610200	2.85854100
H	4.78569500	-2.30359000	4.02862700
C	-5.13334600	1.76322300	3.75903400
H	-4.56786000	1.98821500	4.66775700
H	-5.07099100	2.60252200	3.06030900
H	-6.17709600	1.57219400	4.01157200
C	-6.18453900	1.40875900	-1.99811800
H	-6.24886900	2.23805300	-1.28676000
H	-6.62266900	1.69330600	-2.95415600
H	-6.66702000	0.50726100	-1.60482300
C	-0.20920700	4.79507100	-0.71339400
H	-1.16904900	5.31848800	-0.74039600
H	0.60445400	5.45312500	-0.39826000
H	0.02150700	4.35399000	-1.68459600
I	-4.07493700	3.81244100	0.34588100

I	-0.16712600	-2.16588400	2.95496800
I	-5.55592700	-2.18025100	-0.62561300
I	6.19457100	-0.70261900	0.15681300
I	1.14668000	1.82198000	-3.32582100
I	2.98442600	5.83284100	1.33581500
C	-0.02209600	-4.22033800	0.08169000
C	-1.20822900	-5.05977300	0.55857800
H	0.33107900	-4.60720600	-0.88513200
H	0.79536900	-4.31873300	0.80264700
C	-0.81619300	-6.52435400	0.79732300
H	-2.02495100	-5.01245600	-0.17195400
H	-1.59795400	-4.63493800	1.49102600
H	-0.43342400	-6.98674500	-0.12192900
H	-0.03179400	-6.59915200	1.56107400
H	-1.67331300	-7.11790500	1.13729100

Ir-L5-1-n-Int3			
P	-1.40636000	-0.52934200	-0.17277300
C	-1.32592200	0.08587700	1.57354800
C	-0.75407400	1.33267000	1.81387900
C	-0.71757700	1.85482300	3.11248900
C	-1.26770000	1.12470200	4.14161900
C	-1.88825200	-0.60396200	2.65598500
C	-2.69594800	-1.84029500	-0.00394000
C	-2.29479100	-3.08106200	0.49633800
C	-3.24459000	-4.08974700	0.69097000
C	-4.55110900	-3.85985900	0.31982200
C	-4.03748400	-1.65371100	-0.34353200

C	-2.31642200	0.89526800	-0.90427900
C	-2.00116200	1.37227400	-2.18362200
C	-2.78356200	2.36225800	-2.75529300
C	-3.88094600	2.84465900	-2.05710500
C	-3.34594700	1.50959800	-0.20231900
H	-0.39658400	1.94204600	0.99488100
H	-0.32663600	2.84722000	3.29747100
H	-1.29678000	1.47111900	5.16635700
H	-2.41596600	-1.53569700	2.56325200
H	-1.26382500	-3.26393100	0.78021600
H	-2.95683000	-5.03890500	1.12657400
H	-5.33768200	-4.59520700	0.42978800
H	-4.42861000	-0.76107800	-0.82122000
H	-1.18267200	0.92279900	-2.72993500
H	-2.60924200	2.71009000	-3.76576600
H	-4.56065900	3.58162900	-2.46036400
H	-3.64106300	1.21671200	0.80109600
P	2.20489600	0.11396400	-0.65197700
C	1.85196500	1.91221600	-0.55973500
C	2.13048900	2.67863300	0.55871600
C	1.21842800	4.60725300	-0.46019700
C	0.99327200	3.89721700	-1.64047300
C	1.29809300	2.55081300	-1.69116900
C	3.62641400	0.14251400	-1.83031000
C	3.91675000	-1.03667600	-2.53295700
C	5.67288800	0.04033100	-3.68701100
C	5.47938400	1.19504700	-2.96762600
C	4.41907200	1.26366200	-2.04564300
C	3.00628700	-0.29291000	0.94698000

C	2.27442000	-0.92194800	1.95056400
C	2.91089100	-1.30500500	3.13809800
C	4.25680400	-1.05532200	3.28631000
C	4.37838900	-0.09592600	1.13705600
H	2.57901200	2.27525800	1.45303000
H	1.03768300	5.66693900	-0.36604300
H	0.53753300	4.40960300	-2.47832600
H	1.10887300	1.98384100	-2.59533800
H	3.28449900	-1.90995900	-2.46514300
H	6.45130800	-0.07143500	-4.43098400
H	6.13416900	2.04449700	-3.11899700
H	4.26810000	2.17959400	-1.48314000
H	1.22718800	-1.17563900	1.82115600
H	2.34746500	-1.83512000	3.89857900
H	4.81804800	-1.33836700	4.16758100
H	5.02228800	0.37413800	0.41292100
C	0.72841400	-0.58494300	-3.18642500
O	0.93804200	-0.17974200	-4.26100100
C	-3.07867700	-3.07235900	-3.72307200
H	-3.49654700	-3.61088100	-2.86242300
H	-2.62930000	-3.81653900	-4.39149200
H	-3.90696600	-2.58145600	-4.24419900
C	-2.04600000	-2.03904800	-3.25967500
H	-1.65634400	-1.49410700	-4.12894800
H	-2.57364000	-1.28702500	-2.66395900
C	-0.89471700	-2.67728600	-2.48574300
H	-0.27566900	-3.27590900	-3.16010300
H	-1.28395000	-3.36147300	-1.72904000
C	1.12113200	-2.89557700	-0.59457000

O	1.47654200	-3.91142100	-0.18587600
Ir	0.48061500	-1.29121200	-1.45729700
N	1.83049600	4.00302900	0.58545600
N	-1.84757700	-0.07571100	3.90236700
N	4.96427000	-0.44559500	2.30216200
N	4.86378200	-1.03684600	-3.50380800
N	-4.92035800	-2.67238800	-0.21985300
N	-4.09891800	2.46545600	-0.77805900
C	5.13777300	-2.30865000	-4.18997000
H	4.20245200	-2.71522300	-4.57863300
H	5.83322600	-2.13330400	-5.01020400
H	5.56828500	-2.99325600	-3.44907300
C	6.42172600	-0.26009000	2.41111000
H	6.89175400	-0.94783600	1.70021600
H	6.65038300	0.77989500	2.15861500
H	6.73342500	-0.48655100	3.43012700
C	-2.50199900	-0.83152800	4.98326400
H	-2.03910400	-1.82320300	5.01971100
H	-2.35819700	-0.30078700	5.92378800
H	-3.56681200	-0.90160900	4.73741800
C	-5.25079700	3.03412500	-0.05404300
H	-5.04482500	4.08642000	0.15191900
H	-6.13221500	2.90492400	-0.68746300
H	-5.38857200	2.48269100	0.87634100
C	-6.34238000	-2.40639500	-0.51672400
H	-6.40508100	-1.79820000	-1.42402400
H	-6.85589000	-3.35865900	-0.64834100
H	-6.75132600	-1.84808900	0.33195900
C	2.06461100	4.78982500	1.80562700

H	1.08537900	5.02498300	2.23729800
H	2.69325600	4.21395600	2.48220800
H	2.59589100	5.70439900	1.53967800
I	-1.67475400	4.70716400	0.71144100
I	-0.15020300	-3.35407800	3.41309600
I	5.43260100	3.24745800	0.92459400
I	5.57510000	-2.70326600	-0.48821200
I	-5.29505600	-0.21030900	2.44384600
I	-5.74157400	0.36332500	-3.12835700

Ir-L5-1-n-Int4			
P	-1.95137800	0.06846200	-0.21767000
C	-1.87164000	1.77566000	0.46598100
C	-0.78050400	2.62074500	0.24090900
C	-0.78007400	3.88679200	0.82268100
C	-1.84791500	4.27618600	1.60805700
C	-2.96933800	2.25935300	1.16808600
C	-2.80965300	-0.78099600	1.16604000
C	-2.47085400	-0.45545400	2.48671300
C	-3.09269400	-1.13515000	3.53586600
C	-4.00943200	-2.12765500	3.25728900
C	-3.69581700	-1.82478000	0.94305000
C	-3.15291700	0.42336800	-1.57146300
C	-2.71637800	1.29497500	-2.56878000
C	-3.56240700	1.60296800	-3.64152400
C	-4.82401700	1.05162900	-3.68302700
C	-4.43931100	-0.10567000	-1.65908500
H	0.04574500	2.28803400	-0.37580300

H	0.05421700	4.56117700	0.68073800
H	-1.88435000	5.21931300	2.13542100
H	-3.88839200	1.69037700	1.31250400
H	-1.75887000	0.32841000	2.73274500
H	-2.86417000	-0.86648800	4.56066000
H	-4.55262500	-2.67094400	4.02003800
H	-3.92375800	-2.21533800	-0.04892300
H	-1.73878100	1.77305000	-2.53130300
H	-3.23074400	2.27967500	-4.41991900
H	-5.53292200	1.24208700	-4.47858300
H	-4.91216100	-0.67736300	-0.88115700
P	2.35298900	-0.37779000	-0.64298100
C	2.84425700	0.99999900	-1.74890400
C	3.21093900	2.23539600	-1.23610700
C	3.29862800	3.16434700	-3.39603000
C	3.03205800	1.92955600	-3.96656200
C	2.80255400	0.83786500	-3.13998700
C	3.60079800	-1.64931600	-1.12529800
C	3.24788800	-2.99626800	-0.96405000
C	5.30158300	-3.68684200	-1.89516500
C	5.72872900	-2.38325400	-1.99666100
C	4.85441100	-1.33950200	-1.64287300
C	2.88879700	0.16360000	1.01789900
C	2.01321900	0.88979300	1.83009900
C	2.41483600	1.27022000	3.11758200
C	3.65592600	0.88308000	3.56737200
C	4.13172700	-0.20128500	1.52924200
H	3.29820700	2.43064800	-0.17876700
H	3.44230300	4.06376700	-3.97750900

H	2.95047500	1.85129100	-5.04330700
H	2.55500000	-0.12420200	-3.57410000
H	2.26755000	-3.29870100	-0.62826100
H	5.91272700	-4.53431600	-2.17862200
H	6.72665500	-2.17054700	-2.36086600
H	5.18618200	-0.30666500	-1.72651700
H	1.02961500	1.16756600	1.47811300
H	1.72832400	1.81760600	3.75946500
H	4.02546400	1.12156600	4.55650400
H	4.85198400	-0.78814800	0.98604400
C	-0.04522900	-0.43676800	-2.67556100
O	-0.16867700	-0.41764000	-3.82444500
C	-0.56693900	-5.30627200	-0.14817900
H	-1.25975100	-5.63077700	0.63758300
H	0.41581800	-5.73416300	0.09081800
H	-0.91720400	-5.73065600	-1.09448700
C	-0.50909900	-3.77928400	-0.22351800
H	0.17383200	-3.48204100	-1.03531900
H	-1.48940300	-3.40129100	-0.52998500
C	-0.06471300	-3.14535000	1.09694800
H	0.88654000	-3.57917700	1.44298300
H	-0.78774800	-3.36403900	1.89519300
C	0.17658500	-1.62777100	1.11388400
O	0.35070000	-1.09275400	2.19894800
Ir	0.12446900	-0.75315500	-0.78492900
N	3.44401700	3.28282300	-2.05948800
N	-2.95606000	3.49509300	1.69977900
N	4.49066300	0.15660700	2.77911700
N	4.05318300	-3.97804100	-1.44372800

N	-4.26745100	-2.47877900	1.97360900
N	-5.24996600	0.23710500	-2.68681200
C	3.64444500	-5.37294400	-1.21836900
H	2.60435400	-5.49716000	-1.52439900
H	4.28361600	-6.03496100	-1.80199700
H	3.74453600	-5.57051100	-0.14397400
C	5.82078700	-0.26442900	3.24928700
H	5.85902200	-1.35725000	3.21531700
H	6.56803600	0.17618000	2.58237400
H	5.96505700	0.08856900	4.26969500
C	-4.04468500	3.88989900	2.61263400
H	-3.68077500	3.70803000	3.63128200
H	-4.27204100	4.94624900	2.46312800
H	-4.92287200	3.27703400	2.40183000
C	-6.58279200	-0.38833400	-2.71673500
H	-7.15657700	0.03045700	-3.54291100
H	-6.43390900	-1.46539700	-2.84945100
H	-7.07558400	-0.18467200	-1.76093700
C	-5.33766500	-3.44685700	1.66315800
H	-5.12045700	-3.90994500	0.69836700
H	-5.37830700	-4.20183900	2.44877400
H	-6.27868900	-2.89038100	1.60672400
C	3.71189500	4.59887000	-1.46245800
H	2.74775900	5.07062300	-1.24619100
H	4.31578900	4.44997900	-0.56586800
H	4.27036500	5.20528900	-2.17488300
I	0.05900800	4.00831000	-2.88342200
I	-0.96963200	2.49817800	4.41498300
I	6.32411800	1.78778100	-0.15396200

I	3.93456600	-3.56772500	2.03675500
I	-6.37179600	0.49393200	1.24707900
I	-3.87721100	-3.23912500	-2.42163900

Ir-L5-1-n-Int5			
P	-1.39300300	0.23633000	-0.19590800
C	-1.04368000	1.63377100	0.99288600
C	-0.07516500	2.58871900	0.69081300
C	0.13348600	3.67837900	1.54381000
C	-0.62557900	3.79397200	2.68625800
C	-1.79250400	1.81825800	2.15531800
C	-3.13829400	-0.10553200	0.22529400
C	-3.40220500	-0.83262300	1.41551800
C	-4.70491400	-1.10866400	1.76965700
C	-5.75465000	-0.70303300	0.93744000
C	-4.20976100	0.32079700	-0.52953400
C	-1.38269100	1.30679200	-1.70494500
C	-0.50581900	1.05268300	-2.77196100
C	-0.30235900	2.03281100	-3.73825800
C	-0.98566300	3.23581000	-3.64188000
C	-2.08176600	2.50862600	-1.68900900
H	0.48796300	2.56040100	-0.23343400
H	0.83306900	4.45462500	1.25613500
H	-0.53594200	4.61731500	3.38248300
H	-2.59176400	1.16228000	2.45688000
H	-2.58169000	-1.17059700	2.03953100
H	-4.93938100	-1.67936300	2.65932800
H	-6.79224700	-0.79562000	1.21373200

H	-4.10138100	0.88339600	-1.44450000
H	0.06363800	0.12976100	-2.81213000
H	0.44067400	1.88441700	-4.51413900
H	-0.84866200	4.05451200	-4.33435100
H	-2.76893600	2.79418100	-0.88896000
P	2.00485000	-1.28857600	0.16677000
C	2.59119900	0.40670700	0.53783000
C	2.80816700	0.84213500	1.84078700
C	3.41689800	2.98309100	1.06489400
C	3.25042100	2.59226000	-0.24946500
C	2.78313000	1.30269800	-0.51920600
C	3.37854100	-1.93736600	-0.87468600
C	3.19030100	-3.18065300	-1.51653700
C	3.98855100	-3.53456200	-2.57498800
C	5.20049200	-1.52894900	-2.38654000
C	4.46087300	-1.15926200	-1.26941500
C	2.22089800	-2.24389600	1.72679000
C	1.11349300	-2.72952200	2.44150300
C	1.33651400	-3.48801600	3.60261400
C	2.61967300	-3.68833500	4.04906200
C	3.49770800	-2.49515800	2.21095500
H	2.62743700	0.22905100	2.71158000
H	3.73299300	3.97980100	1.34399600
H	3.41608000	3.30374100	-1.04870000
H	2.60625000	1.00510400	-1.55419200
H	2.37810200	-3.83723200	-1.23083500
H	3.85009600	-4.45005500	-3.13501100
H	5.99455000	-0.91017600	-2.78084100
H	4.72028200	-0.23386700	-0.77404400

H	0.10616600	-2.60692000	2.05931000
H	0.50197600	-3.87838200	4.17101700
H	2.85512800	-4.23599200	4.95286500
H	4.39916000	-2.11158700	1.74092600
C	0.25711500	-2.59523000	-2.22053900
O	0.46921100	-3.06649300	-3.26036100
C	-2.77929400	-4.92161000	-1.48604700
H	-1.75539300	-5.27157700	-1.67817500
H	-3.07598100	-5.30903600	-0.50610300
C	-1.81499000	-2.85990000	-0.40468500
O	-1.83719400	-3.19077800	0.77585900
H	0.95407500	-5.49198400	0.28163400
H	0.53089400	-4.89241200	0.15709800
Ir	-0.16676800	-1.71584200	-0.63779200
N	3.68294200	-3.18472600	3.36080400
N	4.98056500	-2.70724900	-3.00831800
N	3.14622600	2.12782400	2.08048600
N	-1.91854800	3.41880700	-2.67144500
N	-5.48315400	0.04750000	-0.16106400
N	-1.56853700	2.86680600	2.97323900
C	5.58470800	-2.91968500	-4.33091100
H	5.51128400	-3.97357200	-4.59907900
H	5.02584900	-2.29549800	-5.04011300
H	6.63228400	-2.61675900	-4.30547200
C	5.06171400	-3.39609300	3.84873700
H	5.65733800	-2.51566600	3.58573200
H	5.03529800	-3.52054200	4.93150100
H	5.48302800	-4.28951600	3.38059800
C	3.38532200	2.51646800	3.48018000

H	3.41202600	3.60378300	3.54861800
H	2.57393100	2.11529100	4.09260100
H	4.34724700	2.08775500	3.78088900
C	-2.41880900	2.98771200	4.16715200
H	-2.27934700	2.08916400	4.77367800
H	-2.11746200	3.86906000	4.73202100
H	-3.45443500	3.09443500	3.82908300
C	-6.61344700	0.54066900	-0.95589100
H	-6.24181800	0.92323400	-1.90575500
H	-7.28677600	-0.30433800	-1.13097100
H	-7.10012800	1.35123900	-0.40823100
C	-2.57783800	4.73573200	-2.55351500
H	-1.79359500	5.46015300	-2.30503200
H	-3.04845200	4.98496300	-3.50620200
H	-3.32246100	4.68867900	-1.75707900
I	3.00804200	0.04611000	-4.23494900
I	6.06034400	-0.02172500	2.05641400
I	-6.62918700	-3.28486200	-0.40273200
I	-4.58655700	3.45512800	0.94126300
I	1.11656400	5.07411800	-1.79083000
I	0.09021900	-0.13689900	4.11724000
C	-2.79172200	-3.38192200	-1.41951600
H	-2.57140600	-2.94390700	-2.39716400
H	-3.79880200	-3.05927900	-1.11314500
C	-3.72639300	-5.43922700	-2.56939100
H	-3.71603700	-6.53451700	-2.60328500
H	-4.75161300	-5.11134800	-2.37056800
H	-3.43177900	-5.06987600	-3.55959400

Ir-L5-1-n-Int6			
P	1.13729000	-0.47844800	0.32267000
C	1.71125900	-1.11045500	-1.32963700
C	1.52920300	-0.32513100	-2.46234900
C	2.04565300	-0.73321700	-3.69926500
C	2.75231600	-1.91023400	-3.77383800
C	2.45900900	-2.28865400	-1.46522800
C	2.28136200	-1.42363400	1.41211600
C	1.99166000	-2.77578600	1.62097900
C	2.87255900	-3.55382100	2.38017700
C	3.97362700	-2.95803200	2.95668300
C	3.42332500	-0.87667200	1.99417600
C	1.77459600	1.24283900	0.16608200
C	1.40582400	3.62852800	0.15038600
C	2.73879000	3.80542300	-0.16005700
H	1.06573600	0.65018500	-2.39799200
H	1.96247500	-0.08451900	-4.56173500
H	3.20718100	-2.27433800	-4.68554600
H	2.72786300	-2.92108800	-0.63936000
H	1.11377000	-3.23946900	1.18165100
H	2.68209400	-4.60936500	2.52983100
H	4.68697100	-3.49540600	3.56840800
H	3.67760700	0.17971900	1.96627300
H	0.74463700	4.47755800	0.28556100
H	3.19590500	4.77818000	-0.28161800
P	-2.43205200	-0.16686700	-0.78720000
C	-1.80597200	0.69443900	-2.30091400
C	-1.44991500	0.06420200	-3.50702500

C	-0.90366800	0.81662400	-4.54011400
C	-0.71781500	2.18706100	-4.38246100
C	-1.61942700	2.07134300	-2.20276800
C	-3.91037300	0.89652900	-0.48569900
C	-4.30126800	1.12970800	0.83505100
C	-5.90376200	2.70283100	0.14206100
C	-5.66325400	2.40513300	-1.18384800
C	-4.63637300	1.51072700	-1.50315700
C	-3.18354700	-1.70888700	-1.46030700
C	-2.36521700	-2.81370800	-1.71627400
C	-2.93630000	-4.03931800	-2.07018200
C	-4.30850800	-4.14623200	-2.13674400
C	-4.56432400	-1.86990300	-1.55321200
H	-1.59566000	-1.00319100	-3.63508900
H	-0.60011200	0.35296800	-5.47116300
H	-0.32510300	2.83111900	-5.15449700
H	-1.88755900	2.65434300	-1.31444600
H	-3.79966200	0.67338100	1.67163000
H	-6.62440500	3.44494400	0.45818200
H	-6.22861300	2.91537600	-1.95378100
H	-4.38581200	1.33041400	-2.54318200
H	-1.28504400	-2.77677800	-1.59994500
H	-2.29058200	-4.89761500	-2.22818600
H	-4.82181300	-5.07096100	-2.36766400
H	-5.27636800	-1.08655700	-1.33940600
C	-1.39969600	0.95108500	2.14702200
O	-1.66339400	1.80516800	2.86986800
C	1.79059000	-0.35528400	5.97455000
H	1.03558100	0.22559200	6.51797600

H	2.43346400	0.35814000	5.44600500
H	2.39938700	-0.88409200	6.71743700
C	1.13224400	-1.33890800	5.00468600
H	1.89863400	-1.94162300	4.50426600
H	0.49467300	-2.05113700	5.53909000
C	0.29905500	-0.61794900	3.94444100
H	0.90358500	0.13388600	3.42146400
H	-0.51089400	-0.05293700	4.42750400
O	-0.47602400	-2.73424800	3.16840500
H	-1.00852500	-2.21608000	0.57074400
C	-0.37253500	-1.55471700	2.93410400
H	-2.50663000	-1.26354300	1.73055000
Ir	-1.10705600	-0.68130200	1.13433100
N	-5.23180500	2.06551400	1.12258900
N	-1.14046100	2.79077400	-3.23990700
N	4.21192600	-1.63549100	2.78932300
N	2.95388400	-2.66099600	-2.66585700
N	-5.09812800	-3.06825200	-1.89564100
C	-6.56750800	-3.19912400	-1.88287900
H	-6.91659900	-2.92203400	-0.88041700
H	-6.99786600	-2.52682500	-2.62812900
H	-6.83448600	-4.22903500	-2.11588200
C	-5.43055900	2.41336000	2.53831500
H	-4.55582200	2.98223100	2.86755000
H	-6.33050300	3.01923900	2.63476500
H	-5.54689200	1.48335000	3.10000200
C	5.44273500	-1.02126500	3.32505500
H	5.79191900	-1.61348600	4.17088300
H	6.18014700	-1.01208500	2.51581800

H	5.21107600	0.00311500	3.63340500
C	3.79077500	-3.87127100	-2.71323200
H	3.20146500	-4.69990900	-2.30880600
H	4.06835200	-4.06838900	-3.74809400
H	4.68298000	-3.67814100	-2.10870400
C	-0.92660300	4.24476100	-3.09015700
H	0.15865300	4.39989900	-3.05600200
H	-1.34490600	4.75103800	-3.96193900
H	-1.41250500	4.58444100	-2.17306600
I	5.61548900	-1.28133500	-0.55845900
C	3.10197500	1.48537600	-0.17934000
H	3.82994700	0.69184800	-0.34560600
N	3.54994500	2.73962500	-0.34898100
C	0.91421500	2.33326900	0.30371100
H	-0.13371900	2.20137000	0.53933500
C	4.98664900	2.96001500	-0.59671400
H	5.43301800	2.02468500	-0.93491500
H	5.09399700	3.72696400	-1.36422300
H	5.43359900	3.26418200	0.35506700
I	0.51033100	-4.97901500	-1.20706800
I	-6.16663200	-1.35502800	1.41726800
I	3.72695200	2.49208800	3.23911500
I	2.44704600	2.90023900	-3.88428800
I	-2.54331600	4.41415500	0.46189300

Ir-L5-1-n-Pro			
P	2.09479100	0.42351600	0.07442400
C	1.90368600	-0.18794200	1.80118500

C	1.65077500	-1.51663100	2.15652200
C	1.21472500	-1.82231100	3.44481600
C	0.99773300	-0.80582700	4.35471000
C	1.70249000	0.79547400	2.76899900
C	3.64070300	1.42698200	0.21951100
C	3.66046900	2.58036800	-0.54546200
C	5.67103200	3.30109100	0.45317000
C	5.71656600	2.17156400	1.22747300
C	4.72273100	1.18174700	1.08566700
C	2.63667800	-1.04889700	-0.89633900
C	2.15016400	-1.15754900	-2.20096000
C	2.53403100	-2.23254200	-3.00695400
C	3.38423600	-3.18525700	-2.48474900
C	3.51068800	-2.03557000	-0.43100000
H	1.76207500	-2.34448500	1.46186600
H	1.02876000	-2.85778500	3.70912200
H	0.60876900	-0.96090200	5.35076100
H	1.80298900	1.85382200	2.54991000
H	2.85551800	2.82149100	-1.22671900
H	6.41442600	4.08575400	0.50344700
H	6.54777100	2.02207900	1.90509400
H	4.72202700	0.32473100	1.74475200
H	1.44783400	-0.42588100	-2.59033800
H	2.12882100	-2.32693400	-4.00857400
H	3.71426300	-4.05294000	-3.04104000
H	3.92208000	-2.05563700	0.56598700
P	-1.76089800	0.49556700	-0.58567600
C	-1.49942200	-1.28525900	-0.17465000
C	-1.82737000	-1.86132900	1.04132300

C	-1.05446500	-3.97542000	0.31919400
C	-0.66859500	-3.43690200	-0.89918400
C	-0.85774900	-2.08569900	-1.13812000
C	-2.87591400	0.38865100	-2.05669800
C	-3.39045100	1.57604100	-2.57485100
C	-4.56790000	0.31512600	-4.24380800
C	-3.22893500	-0.81441700	-2.66972400
C	-3.00855700	1.04839100	0.66990800
C	-2.83634000	2.28595800	1.29642000
C	-3.73644700	2.68077800	2.28531000
C	-4.75049800	1.82105400	2.65906400
C	-4.09331000	0.26028500	1.02473600
H	-2.24189000	-1.31635900	1.88344600
H	-0.94506600	-5.01984300	0.56800500
H	-0.21226400	-4.07851200	-1.64275400
H	-0.56590100	-1.66845300	-2.10025000
H	-3.15599200	2.52674900	-2.09976700
H	-5.21659300	0.20863700	-5.10352900
H	-2.92989200	-1.78299800	-2.30643500
H	-1.98860900	2.90636000	1.02551400
H	-3.62110300	3.62513600	2.80306500
H	-5.43695600	2.02746400	3.46986900
H	-4.31813200	-0.70252700	0.55962100
C	0.43369100	2.18026900	-2.30769800
O	0.54476200	2.66028700	-3.35802700
H	-0.18853400	1.23699100	1.05426000
Ir	0.19577700	1.55410700	-0.51998500
C	-4.23599800	1.53373900	-3.68979400
H	-4.64038000	2.44223600	-4.12010400

N	-4.09017500	-0.83170000	-3.71196200
N	-4.93021100	0.64579900	2.01152300
N	-1.58724200	-3.17676800	1.26817100
N	3.84638200	-3.08577800	-1.21618000
N	1.27013800	0.48113000	4.00569800
N	4.66342000	3.48178800	-0.45259100
C	-4.39023000	-2.14098900	-4.31536800
H	-3.46767800	-2.49890400	-4.78605800
H	-4.71490400	-2.81467400	-3.51633500
H	-5.17961000	-2.01907800	-5.05660200
C	-5.93113100	-0.31774000	2.51685100
H	-6.08089800	-1.09705000	1.76664800
H	-5.52530900	-0.75410800	3.43475400
H	-6.86535600	0.20860500	2.71837500
C	-2.00419000	-3.78618700	2.54542300
H	-1.23833000	-4.50871900	2.83718800
H	-2.10146600	-3.00131800	3.29798100
H	-2.97011300	-4.27367900	2.38729900
C	4.76769300	-4.09834200	-0.66659700
H	4.26544600	-4.59302900	0.17150400
H	4.99765200	-4.82170800	-1.44767200
H	5.67596800	-3.57555400	-0.35128000
C	0.92247200	1.55144900	4.95979300
H	1.18763300	2.51405900	4.52406300
H	-0.15890400	1.49161800	5.13043600
H	1.46707500	1.39464900	5.89290300
C	4.56393500	4.71684800	-1.24708500
H	4.54790900	4.46591700	-2.30988200
H	3.64065400	5.23467400	-0.97120900

H	5.42686900	5.34793000	-1.03621600
I	6.61913700	-0.78467600	-0.40580800
I	1.86683500	-5.09963700	1.60667600
I	-2.42691100	-0.25021200	4.50319400
I	0.84263400	4.13223200	0.71669300
I	-4.95322300	-3.02832200	-0.44605500
I	-0.66191200	-1.26290600	-4.78101800
O	-2.92837800	4.27919100	-0.99913000
C	-1.98681800	4.89039300	-1.47738800
H	-1.33962300	4.40665300	-2.23412100
C	-2.34227900	6.83664600	0.11980200
H	-3.42681700	6.72274100	0.01018900
H	-2.04508600	6.19849000	0.96071900
C	-1.65112500	6.31637600	-1.13920900
H	-1.92663600	6.91985700	-2.02149000
H	-0.55987800	6.38945300	-1.05783800
C	-1.98581300	8.29372800	0.41895600
H	-2.28632900	8.95544600	-0.40289600
H	-2.48486500	8.64496900	1.32875400
H	-0.90540200	8.41268200	0.56355400

Ir-L5-1-n-TS1			
P	1.86158100	-0.16800900	-0.04703400
C	1.15629100	1.52039800	0.16492000
C	0.23843600	1.98901300	-0.78246200
C	-0.30025700	3.26612300	-0.65491000
C	0.05941200	4.05277100	0.42321900
C	2.96111600	0.08755000	-1.50117900

C	3.67389300	-0.99143200	-2.02238600
C	4.48269600	-0.80512000	-3.15211200
C	4.52951000	0.43197300	-3.75525600
C	3.02950400	-0.24404300	1.36435000
C	4.79398800	-0.31489000	3.49500500
C	3.44061200	-0.35518600	3.74274400
C	2.54275900	-0.31205800	2.66401900
H	-0.00320500	1.38309200	-1.65012100
H	-1.01866200	3.67086300	-1.35714500
H	-0.38760400	5.02773700	0.58735000
H	3.64908700	-1.95905700	-1.52899500
H	5.06610100	-1.62513600	-3.55342600
H	5.11433400	0.64253300	-4.64107600
H	5.54310400	-0.32940000	4.27574100
H	3.08372700	-0.39584100	4.76468600
H	1.47388200	-0.26924800	2.85426900
P	-1.75971100	-1.65443300	0.07807500
C	-2.54389800	-0.03036200	-0.28039200
C	-2.42296900	0.52630200	-1.56414900
C	-3.06111900	1.72736800	-1.85691600
C	-3.76936400	2.39138200	-0.86434300
C	-2.37128200	-2.02466700	1.78681000
C	-3.10001200	-2.62474700	4.39563800
C	-4.03855000	-2.73124500	3.39350100
C	-3.66886600	-2.45595200	2.06832600
C	-2.91533800	-2.76917100	-0.85700000
C	-2.73973700	-4.14799800	-0.73205700
C	-3.55067500	-5.03030000	-1.45460600
C	-4.47681600	-4.51906100	-2.34212300

H	-1.81945700	0.04996200	-2.33528600
H	-2.97344400	2.17141700	-2.84204800
H	-4.24892000	3.35140600	-1.00823300
H	-3.30933700	-2.84317300	5.43504000
H	-5.05266600	-3.02874700	3.63268300
H	-4.41521500	-2.53453300	1.28313800
H	-1.95077600	-4.52392700	-0.08599900
H	-3.44778400	-6.10425400	-1.35384700
H	-5.11961200	-5.13921900	-2.95308800
C	0.99653000	-2.89289500	1.32076300
O	1.28022100	-3.41668400	2.32082300
C	-3.89337200	-2.30872900	-1.74241900
C	-1.47867400	-1.88745200	2.85010200
C	-3.25522000	0.67868700	0.67694300
C	1.51135000	2.36485300	1.20662200
C	4.41483900	-0.24410000	1.16798300
C	3.04952400	1.31709000	-2.15087000
H	4.87265800	-0.14506000	0.20025600
H	2.22835400	2.10451600	1.96728300
H	2.51574900	2.19583600	-1.83133000
H	-4.07454500	-1.26297800	-1.93022200
H	-0.45656900	-1.59006100	2.70412400
H	-3.37238900	0.34530400	1.69580800
Ir	0.47455800	-2.00838600	-0.24323400
N	-4.60479800	-3.17939000	-2.50291700
N	0.95677500	3.59334300	1.32328200
N	3.81738200	1.46806500	-3.24859200
N	-3.82556000	1.86628600	0.38412300
N	-1.82947800	-2.24351900	4.10742200

N	5.25748100	-0.23566100	2.22458000
C	-4.57234700	2.58502700	1.43523700
H	-4.48448400	3.65710400	1.23425500
H	-5.61221100	2.24948200	1.40656200
H	-4.11302300	2.35338000	2.39698600
C	-0.81850000	-2.09046400	5.16796500
H	-0.60686500	-1.01879300	5.26438900
H	-1.21086100	-2.49671500	6.09958400
H	0.08257100	-2.63157700	4.87217800
C	-5.63509000	-2.61677600	-3.39408900
H	-6.13001200	-3.42664600	-3.92870200
H	-6.34764600	-2.07029900	-2.76385300
H	-5.16214600	-1.93658800	-4.10511200
C	3.80598600	2.78642300	-3.90181700
H	2.80514500	2.94459900	-4.31555400
H	4.05181500	3.53924900	-3.14789500
H	4.54948700	2.79836700	-4.69804900
C	6.69534600	-0.18304000	1.92832000
H	6.88613100	0.72948900	1.35577700
H	7.25518700	-0.16741400	2.86289400
H	6.94409700	-1.07817900	1.34760400
C	1.34944500	4.41508400	2.48024800
H	2.44039900	4.48265500	2.49559400
H	0.91245000	5.40674100	2.37259600
H	0.96626400	3.93446700	3.38443500
I	4.75010600	3.03098600	0.21216600
I	0.32136900	0.73433200	-4.28556000
I	4.98544200	-3.33413000	0.41415300
I	-6.32354100	-1.04433000	0.01677400

I	-1.01375000	1.27509900	3.48450500
I	-3.05457100	5.75391000	-0.20541600
C	1.15207700	-3.65900300	-1.54487900
C	0.74849400	-2.70486800	-2.53864000
H	2.20870100	-3.80664800	-1.33549300
H	0.53254000	-4.54547300	-1.42640600
C	-0.43418900	-3.00200200	-3.43850100
H	1.53891800	-2.14006100	-3.03168100
H	0.25883100	-1.48135700	-1.90320800
H	-0.08135200	-3.62016600	-4.27259200
H	-1.20476300	-3.55973400	-2.90135500
H	-0.85050700	-2.08376000	-3.86156500

Ir-L5-1-n-TS2			
P	-1.47924400	-0.44252900	-0.10029900
C	-1.46640400	0.46236600	1.51256400
C	-0.70096800	1.62052700	1.59607100
C	-0.70850600	2.38438900	2.76996100
C	-1.52228000	2.00106300	3.81048900
C	-2.24341600	0.09533500	2.61914700
C	-2.71146900	-1.76960000	0.23373500
C	-2.34214100	-2.79150900	1.11529700
C	-3.25057700	-3.81411700	1.39969400
C	-4.47224500	-3.82764100	0.75855800
C	-3.97210300	-1.81515200	-0.36532400
C	-2.41119400	0.79987100	-1.08740400
C	-2.00175500	1.16923600	-2.37321400
C	-2.78001700	2.03933800	-3.11879300

C	-3.96439300	2.51301100	-2.57903000
C	-3.53395400	1.41581000	-0.54771200
H	-0.11911100	1.94853100	0.74593900
H	-0.13721200	3.30036300	2.84319200
H	-1.60599500	2.55860200	4.73396800
H	-2.92027600	-0.74244900	2.62262800
H	-1.38763100	-2.76801800	1.63590800
H	-3.00523800	-4.58480000	2.12072800
H	-5.22195400	-4.58978900	0.92759500
H	-4.33245900	-1.09513400	-1.09829700
H	-1.10475200	0.73693300	-2.79114500
H	-2.52748200	2.29377100	-4.14029100
H	-4.64762800	3.15181300	-3.12029800
H	-3.90498000	1.21607100	0.45296000
P	2.33558100	0.10828200	-0.70308200
C	1.99576000	1.90361800	-0.88840200
C	2.24373300	2.82041400	0.11662300
C	1.29220500	4.56966600	-1.16054400
C	1.09390800	3.69967600	-2.23371900
C	1.44460200	2.37071300	-2.10280200
C	3.74434600	-0.04757500	-1.88428000
C	3.90460600	-1.28059700	-2.53321000
C	5.76176600	-0.44397100	-3.72864000
C	5.68798700	0.75836000	-3.06714400
C	4.64017700	0.97984000	-2.15277800
C	3.10788000	-0.06472400	0.94545300
C	2.31109600	-0.30348200	2.06486300
C	2.90948000	-0.53576700	3.30892800
C	4.28307100	-0.56174900	3.39306800

C	4.49529900	-0.10323500	1.08999700
H	2.70543600	2.55771300	1.05670700
H	1.06697300	5.62405100	-1.20734900
H	0.62218300	4.08008000	-3.13093200
H	1.27872100	1.68147600	-2.92311200
H	3.17923700	-2.07393800	-2.42132300
H	6.52459000	-0.67009100	-4.46288600
H	6.42569300	1.52772700	-3.26053700
H	4.57755700	1.93143500	-1.63138500
H	1.23070500	-0.35163500	1.98981000
H	2.28753600	-0.76146600	4.16895900
H	4.81663400	-0.76631700	4.31226600
H	5.18427600	0.03360700	0.27457200
C	0.52102500	-0.90164200	-2.93130500
O	0.66505300	-0.84867000	-4.08582300
C	-1.17140500	-5.33545800	-2.14188600
H	-1.72142100	-5.67049400	-1.25401700
H	-0.32974900	-6.02152200	-2.29220200
H	-1.83912300	-5.42200800	-3.00635200
C	-0.68846400	-3.88896800	-1.96807700
H	-0.20165500	-3.55291600	-2.88904300
H	-1.55512400	-3.24027700	-1.81591600
C	0.28541900	-3.80682500	-0.77608200
H	1.21930700	-4.32751400	-0.99816800
H	-0.18486500	-4.29119200	0.08376900
C	1.00356400	-2.51654400	0.29282700
O	1.53321400	-2.92945800	1.26212400
Ir	0.53785700	-1.21191300	-1.03724100
N	1.92751600	4.13361300	-0.04778500

N	-2.30321000	0.89911600	3.70766500
N	5.05104900	-0.35200400	2.29353300
N	4.84316000	-1.42245400	-3.50420800
N	-4.79856400	-2.86118400	-0.13216800
N	-4.27943300	2.25639600	-1.28940400
C	4.98258100	-2.74435700	-4.13212700
H	4.01512800	-3.05800900	-4.52885300
H	5.71070200	-2.68502900	-4.94059500
H	5.31554800	-3.44188600	-3.35349400
C	6.52070000	-0.42129300	2.35830900
H	6.84430800	-1.24278800	1.71194300
H	6.91936200	0.53605800	2.00896300
H	6.82321700	-0.60641600	3.38827500
C	-3.14013100	0.46075500	4.83635900
H	-2.66757900	-0.43338900	5.25903600
H	-3.18893100	1.26306800	5.57201100
H	-4.13826900	0.23289000	4.45082200
C	-5.52513300	2.82221000	-0.73803900
H	-5.39484200	3.89953100	-0.61587500
H	-6.33186900	2.59118400	-1.43810300
H	-5.73501100	2.34578100	0.22023000
C	-6.16051800	-2.81972300	-0.70467800
H	-6.11305700	-2.38285000	-1.70612500
H	-6.55852000	-3.83422500	-0.73500600
H	-6.76329300	-2.17616600	-0.05559300
C	2.13757100	5.07227900	1.06447200
H	1.18141500	5.19788900	1.58382700
H	2.92291000	4.67765400	1.70970600
H	2.46328200	6.03123300	0.66030100

I	-1.65474900	4.65400900	-0.06826200
I	-0.43194400	-2.05737000	4.22027200
I	5.58906200	3.10100600	0.78049400
I	5.25946800	-3.05383200	-0.40031100
I	-5.76142000	-0.10911300	2.02264300
I	-5.49484500	-0.26362000	-3.53276300

Ir-L5-1-n-TS3			
P	-1.36938300	0.18874700	-0.20459700
C	-1.06499900	1.73711700	0.80132500
C	-0.13591100	2.68188900	0.36939000
C	0.00953800	3.89753900	1.04506300
C	-0.78873500	4.16095500	2.13518400
C	-1.85785200	2.07613800	1.89919600
C	-3.09602800	-0.15095100	0.29141000
C	-3.32831300	-0.67156300	1.58954700
C	-4.61645300	-0.93445100	2.00035700
C	-5.68131700	-0.74027200	1.11044100
C	-4.18050700	0.08073500	-0.52447100
C	-1.37585400	1.05875000	-1.83682800
C	-0.47418200	0.68521400	-2.84515200
C	-0.25219500	1.54124900	-3.91817000
C	-0.94895900	2.73873900	-3.98718700
C	-2.08987600	2.23865600	-1.98743200
H	0.44256100	2.54062400	-0.53357600
H	0.68734900	4.64735000	0.65257900
H	-0.75107500	5.08699900	2.69343500
H	-2.64130000	1.44652800	2.28493000

H	-2.49628000	-0.84423600	2.26724500
H	-4.82927600	-1.34436600	2.97953800
H	-6.71445800	-0.81813500	1.40739600
H	-4.08759500	0.45583700	-1.53175000
H	0.08503700	-0.23976100	-2.75416500
H	0.50011400	1.30397700	-4.66204100
H	-0.79531100	3.47287600	-4.76582100
H	-2.80984200	2.60427300	-1.25214700
P	1.87055100	-1.41654700	0.52917700
C	2.38798400	0.34042700	0.48734800
C	2.64482400	1.07365700	1.63678300
C	3.21549800	2.96723900	0.34796300
C	3.01417500	2.26785800	-0.82818400
C	2.54860400	0.95486200	-0.76125300
C	3.26869100	-2.19808400	-0.39514600
C	3.14417400	-3.54970400	-0.79742400
C	3.99374100	-4.06666800	-1.74065500
C	5.12766400	-2.00964100	-1.91502000
C	4.32898000	-1.46607400	-0.90976600
C	2.25618100	-1.95165000	2.25413400
C	1.23723000	-2.13026400	3.19720900
C	1.56688800	-2.54885700	4.49738000
C	2.88408700	-2.74686900	4.82949600
C	3.57445500	-2.17297100	2.64467600
H	2.50964800	0.68730600	2.63674500
H	3.52062900	4.00539900	0.36081700
H	3.16187000	2.76547000	-1.77800800
H	2.37042900	0.41011600	-1.68673400
H	2.34538400	-4.17480800	-0.41630500

H	3.91081600	-5.07826500	-2.11561500
H	5.93701300	-1.45639400	-2.36896800
H	4.54245400	-0.45375700	-0.59880700
H	0.20351200	-1.99655900	2.91606600
H	0.79645000	-2.67385800	5.24727500
H	3.20736700	-3.04903500	5.81721400
H	4.42040000	-2.02420000	1.98581800
C	0.47985200	-2.88054500	-1.91614400
O	0.83518100	-3.47364800	-2.84661000
H	-0.85902200	-3.09170000	0.98998500
H	-1.32028100	-2.63392400	1.41500000
Ir	-0.20439700	-1.86962200	-0.50470000
N	3.87136200	-2.55841500	3.90759500
N	4.97992300	-3.29967200	-2.29062200
N	2.98876900	2.38026800	1.54631200
N	-1.90191200	3.02880600	-3.06747600
N	-5.43995400	-0.18609700	-0.10666400
N	-1.70579300	3.25400000	2.53944000
C	5.68387000	-3.75113400	-3.49851100
H	5.59887400	-4.83414200	-3.58579200
H	5.21276800	-3.25297700	-4.35501100
H	6.73560600	-3.46731200	-3.43433100
C	5.29050300	-2.73745700	4.27239000
H	5.84768200	-1.87534300	3.88667700
H	5.37213100	-2.78939300	5.35770300
H	5.66917700	-3.66025800	3.82622900
C	3.26465900	3.09610500	2.80349000
H	3.30894900	4.16576500	2.60091200
H	2.46232100	2.87268300	3.51087500

H	4.22639700	2.73418900	3.18152200
C	-2.61080500	3.53572800	3.66381400
H	-2.47410600	2.75094200	4.41189000
H	-2.35586300	4.50480800	4.09076200
H	-3.63078000	3.55406500	3.26582900
C	-6.58792100	0.08285700	-0.97989800
H	-6.22774500	0.30581300	-1.98334800
H	-7.20992100	-0.81721700	-0.99834300
H	-7.13124400	0.94728000	-0.59047500
C	-2.57929400	4.34104300	-3.12651200
H	-1.81709000	5.10054800	-2.91906400
H	-3.00166300	4.47886200	-4.12323100
H	-3.36551800	4.36705300	-2.37034700
I	3.35190800	-0.61752200	-4.13375200
I	5.93905500	0.31479100	2.02339800
I	-6.32116800	-3.58116900	0.40070500
I	-4.71079100	3.39707900	0.41986200
I	1.11805700	4.92127000	-2.33189500
I	0.05424200	0.68692500	4.30235800
C	-3.42636800	-4.29402400	-2.38263600
H	-2.80843700	-4.28614500	-3.29006800
H	-4.28901500	-3.65036000	-2.57719600
O	-2.49645100	-1.61100300	-2.37543600
C	-2.00006100	-2.35199100	-1.54829400
C	-3.89534600	-5.71567800	-2.07124300
H	-4.46218900	-6.13128100	-2.91193500
H	-3.04316200	-6.38160200	-1.88066300
H	-4.54579700	-5.72214200	-1.19107100
C	-2.62395200	-3.69651200	-1.21967100

H	-3.29792700	-3.53323700	-0.36238800
H	-1.84468400	-4.38672000	-0.87755300

Ir-L5-1-n-TS4			
P	2.10059700	0.09512500	-0.35951600
C	1.50163400	0.26358900	1.38738300
C	1.09675800	-0.81519400	2.18134100
C	0.55808200	-0.58592800	3.44719900
C	0.42019800	0.70943900	3.90758900
C	1.36684000	1.54851400	1.91066100
C	3.59812900	1.17076800	-0.21711200
C	3.71406900	2.20297100	-1.13002900
C	5.56149900	3.11246000	0.01162700
C	5.50566800	2.11303300	0.94743900
C	4.54959000	1.08900400	0.82008400
C	2.67724700	-1.66274900	-0.38993900
C	2.21643700	-2.50010300	-1.40683100
C	2.56248800	-3.85318100	-1.42725000
C	3.39413500	-4.34168200	-0.44198800
C	3.51529800	-2.22258900	0.58086600
H	1.21065900	-1.84890100	1.87025300
H	0.27769200	-1.43362600	4.06353900
H	-0.00947900	0.96807100	4.86534500
H	1.64762200	2.45193700	1.36984000
H	3.00560300	2.31836300	-1.94056800
H	6.27804500	3.92218000	0.05109400
H	6.22525800	2.09546700	1.75600700
H	4.44470300	0.36820500	1.61752900

H	1.55322700	-2.12806600	-2.17571600
H	2.14828100	-4.50810600	-2.18473000
H	3.70356700	-5.37670400	-0.38697700
H	3.86802500	-1.69044000	1.44897200
P	-1.55579000	0.42153100	-0.95589400
C	-1.62460200	-0.93291300	0.29479900
C	-2.35400500	-0.89867100	1.47614300
C	-1.70071400	-3.11729300	1.99237100
C	-0.98552100	-3.21186600	0.81329200
C	-0.92614000	-2.10716400	-0.02819600
C	-2.80157900	-0.17026000	-2.18310900
C	-3.12037300	0.64399600	-3.27039300
C	-4.51285200	-1.09700500	-4.14870000
C	-3.35246900	-1.45463800	-2.12814000
C	-2.43217400	1.80909500	-0.11393900
C	-1.75205000	2.98460400	0.23635700
C	-2.40989400	3.96931600	0.96407000
C	-3.72333500	3.76084100	1.34885800
C	-3.77446700	1.69152200	0.22339700
H	-2.87806700	-0.03017300	1.85341400
H	-1.74749500	-3.92404300	2.71053800
H	-0.46363800	-4.12862900	0.57480200
H	-0.37504900	-2.17835000	-0.95538600
H	-2.67734300	1.62731800	-3.37125900
H	-5.18459100	-1.52727700	-4.87986900
H	-3.14775400	-2.16191400	-1.34370700
H	-0.71236000	3.13445200	-0.03640300
H	-1.88392700	4.86592700	1.27077900
H	-4.27971000	4.45343400	1.96607800

H	-4.37529800	0.80793500	0.00010700
C	0.43475100	-0.41068800	-3.35907700
O	0.42732600	-0.95763300	-4.36739400
H	0.63264400	2.08313600	-0.81835700
Ir	0.50108100	0.82734400	-1.85387600
C	-3.99319500	0.17650700	-4.25789200
H	-4.25104800	0.78888000	-5.11327000
N	-4.18871900	-1.88618500	-3.10093900
N	-4.39646500	2.66200800	0.92826900
N	-2.35971300	-1.97602600	2.30529700
N	3.85627200	-3.53013700	0.53589100
N	0.85174900	1.74666900	3.14304300
N	4.69580700	3.12729400	-1.04196000
C	-4.74149500	-3.24643900	-2.96963700
H	-3.89711000	-3.94469300	-2.95444100
H	-5.30500600	-3.28468400	-2.03212300
H	-5.39194600	-3.44715300	-3.82005800
C	-5.75481500	2.41682300	1.45932000
H	-6.16980000	1.52796000	0.98294400
H	-5.64637800	2.23934700	2.53458100
H	-6.37748500	3.29228000	1.26803700
C	-3.21613500	-1.93368000	3.50827500
H	-2.88383900	-2.70885100	4.19841500
H	-3.13425900	-0.94622700	3.96811200
H	-4.24829500	-2.10627600	3.18846600
C	4.76325800	-4.04614500	1.57886000
H	4.24224300	-3.98884000	2.53876400
H	4.99712200	-5.08574800	1.35557000
H	5.67061200	-3.43482800	1.55208400

C	0.70384200	3.11989000	3.67518200
H	1.03520800	3.83256200	2.91838300
H	-0.35515100	3.26258300	3.91309200
H	1.30992000	3.21189700	4.57887100
C	4.69306500	4.26615100	-1.97510800
H	4.40539500	3.91172700	-2.96569600
H	3.97031700	5.00492000	-1.61153700
H	5.69650300	4.68985700	-2.02100800
I	6.54857000	-1.10040300	-0.08051300
I	1.41770500	-4.24092800	3.28421500
I	-2.90673200	1.92009400	4.08904300
I	1.68390400	4.94019400	0.32887400
I	-5.64292300	-1.46897400	0.38048300
I	-1.00711500	-4.00397200	-2.95040200
O	-0.49295500	2.11813400	-4.57984500
C	-0.00123300	2.52146700	-3.54808900
H	1.09248500	1.97684000	-3.12609100
C	-1.63011800	4.35228100	-2.93516800
H	-2.08644500	4.30567400	-3.93079200
H	-2.16597600	3.62754500	-2.30940800
C	-0.15685600	3.92977900	-3.02831100
H	0.36216400	4.58926200	-3.74098500
H	0.34674400	4.04132400	-2.06657800
C	-1.77645900	5.75072000	-2.33262800
H	-1.30531600	6.50466200	-2.97332300
H	-2.83171600	6.02249200	-2.21498800
H	-1.28807700	5.80649900	-1.35365400

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