Picosecond time-resolved infrared spectroscopy of rhodium and iridium azides
Supplementary Information

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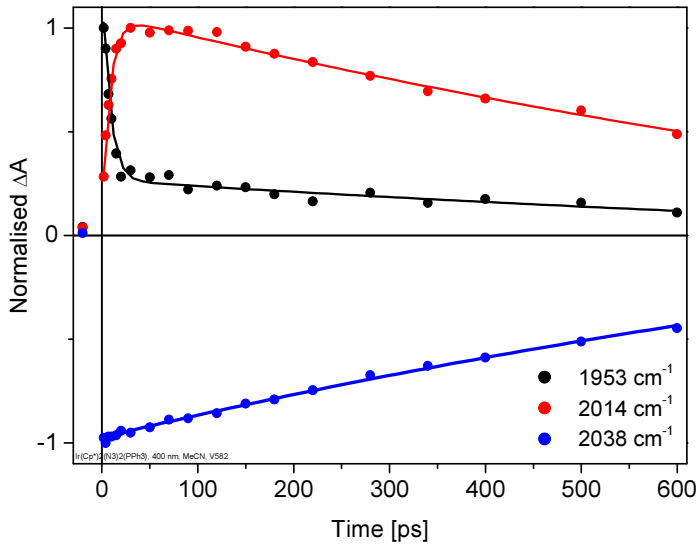


Figure S1a. Normalised kinetic traces at 1953 cm^{-1} (black), 1985 and 2014 cm^{-1} (green and red) and 2038 cm^{-1} (blue) of a solution of $Ir(Cp^*)(N_3)_2(PPh_3)$ (2) in MeCN, λ_{exc} = 400 nm.

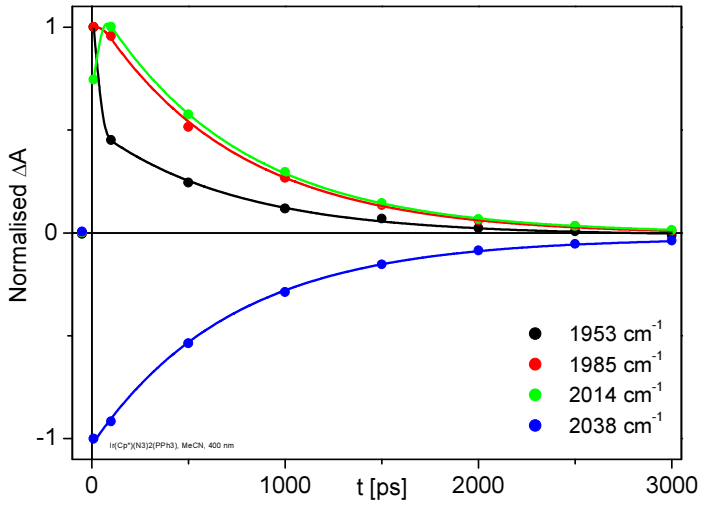


Figure S1b. Normalised kinetic traces at 1953 cm^{-1} (black), 1985 and 2014 cm^{-1} (green and red) and 2038 cm^{-1} (blue) of a solution of $Ir(Cp^*)(N_3)_2(PPh_3)$ (2) in MeCN, λ_{exc} = 400 nm.

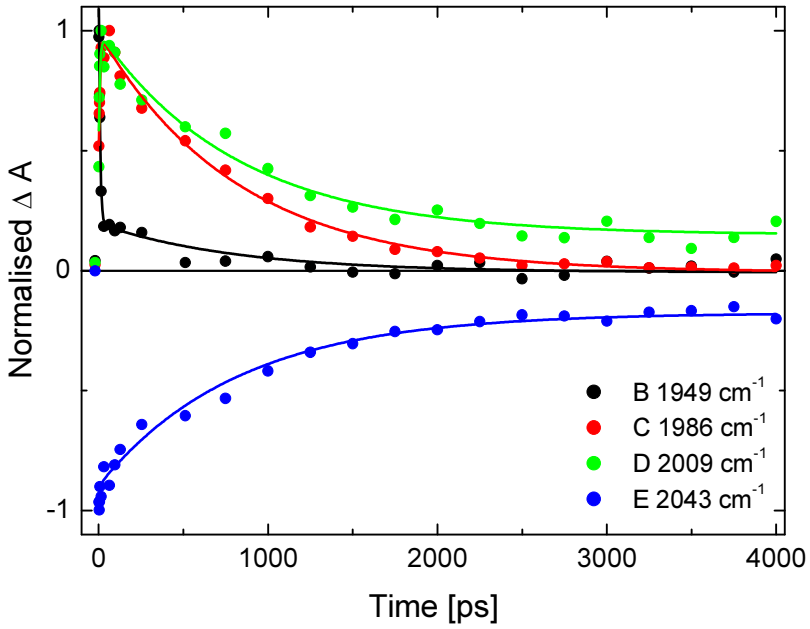


Figure S2. Normalised kinetic traces at 1946 cm^{-1} (black), 1983 and 2006 cm^{-1} (green and red) and 2040 cm^{-1} (blue) of a solution of $Ir(Cp^*)(N_3)_2(PPh_3)$ (**2**) in MeCN, λ_{exc} = 266 nm.

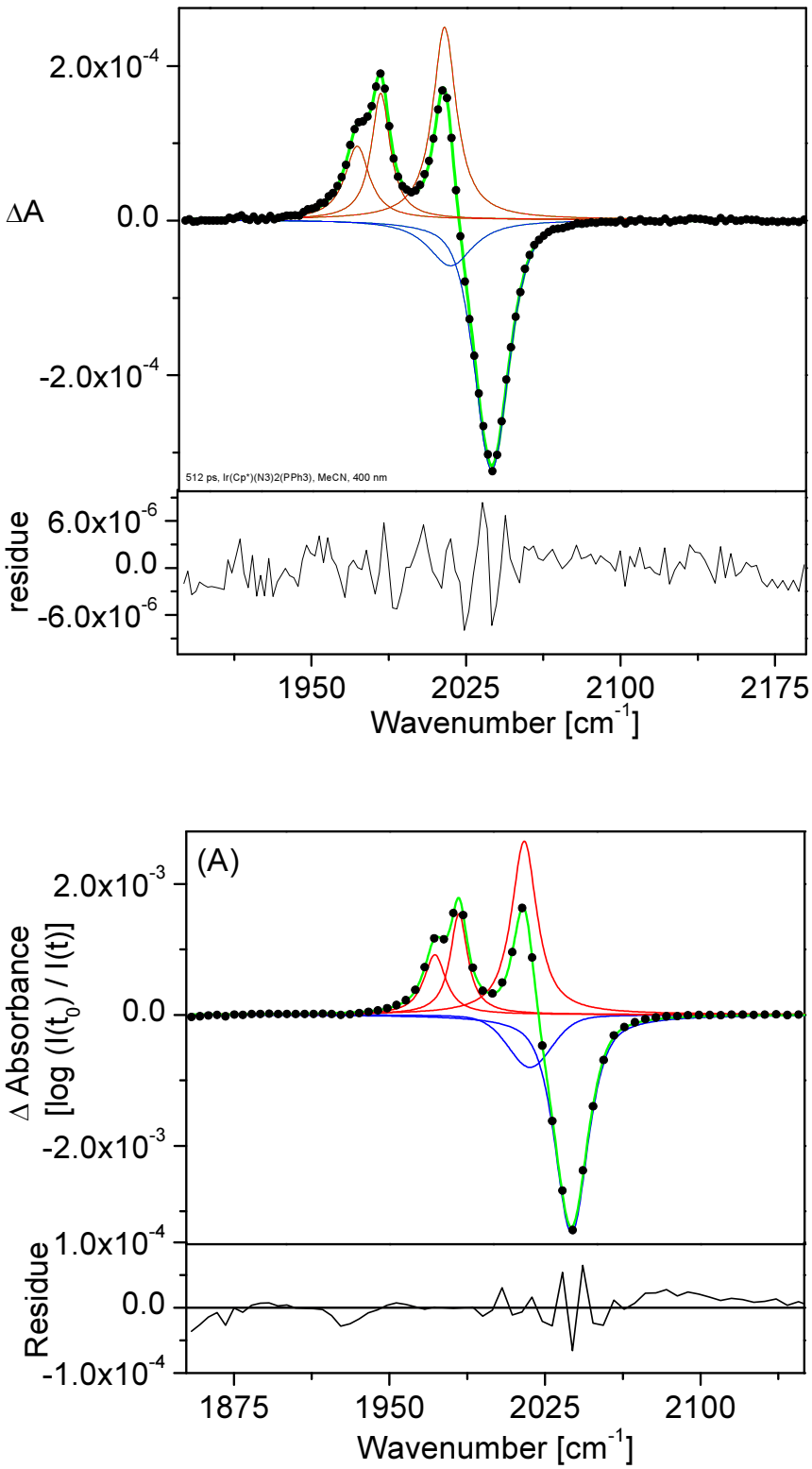


Figure S3. Time resolved infrared difference spectrum (black dots) obtained ca. 256 ps after laser flash (λ_{exc}= 400 nm) of a solution of Ir**(**Cp***)**(N_3)$_2$(PPh_3) (**2**) in MeCN, high digital resolution (top) and low digital resolution (bottom). The overlap of *pseudo* Voigt profiles for parent bleach (blue) and transient bands (red) results in a fit curve (green) and a residual (black).

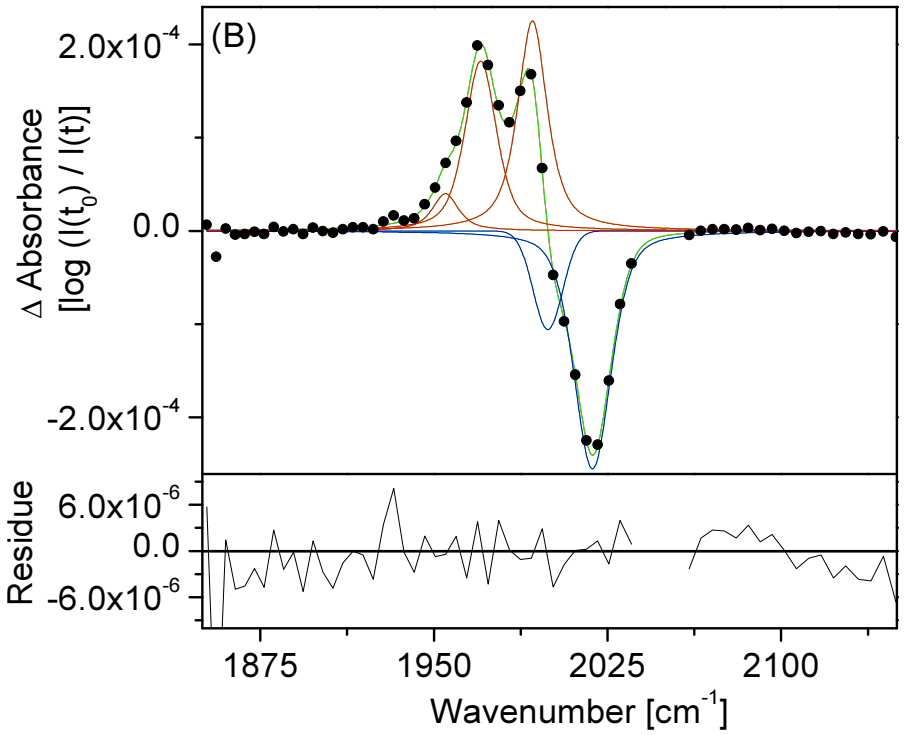


Figure S4. Time resolved infrared difference spectrum (black dots) obtained ca. 55 ps after laser flash (λ_{exc} = 400 nm) of a solution of Rh(Cp*)$(N_3)_2(PPh_3)$ (1) in toluene. The overlap of *pseudo* Voigt profiles for parent bleach (blue) and transient bands (red) results in a fit curve (green) and a residual (black).

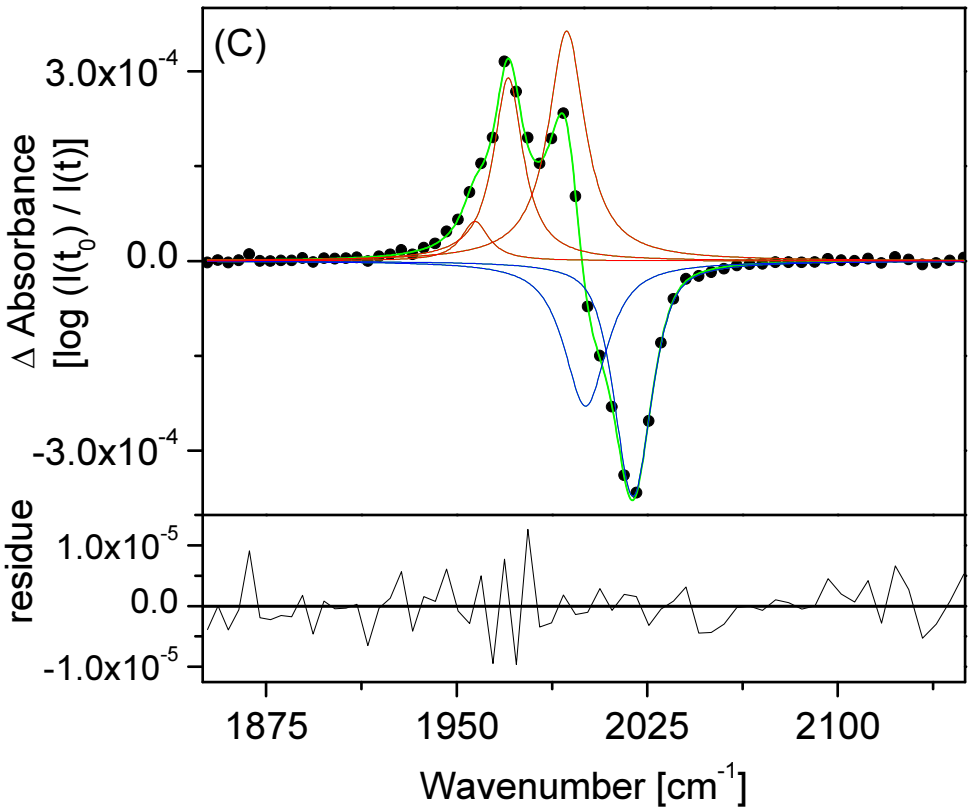


Figure S5. Time resolved infrared difference spectrum (black dots) obtained ca. 256 ps after laser flash (□exc = 400 nm) of

a solution of Rh(Cp*)(N3)2(PPh3) in THF (ca. 180 ps, C). The overlap of pseudo Voigt profiles for parent bleach (blue) and transient bands (red) results in a fit curve (green) and a residual (black).

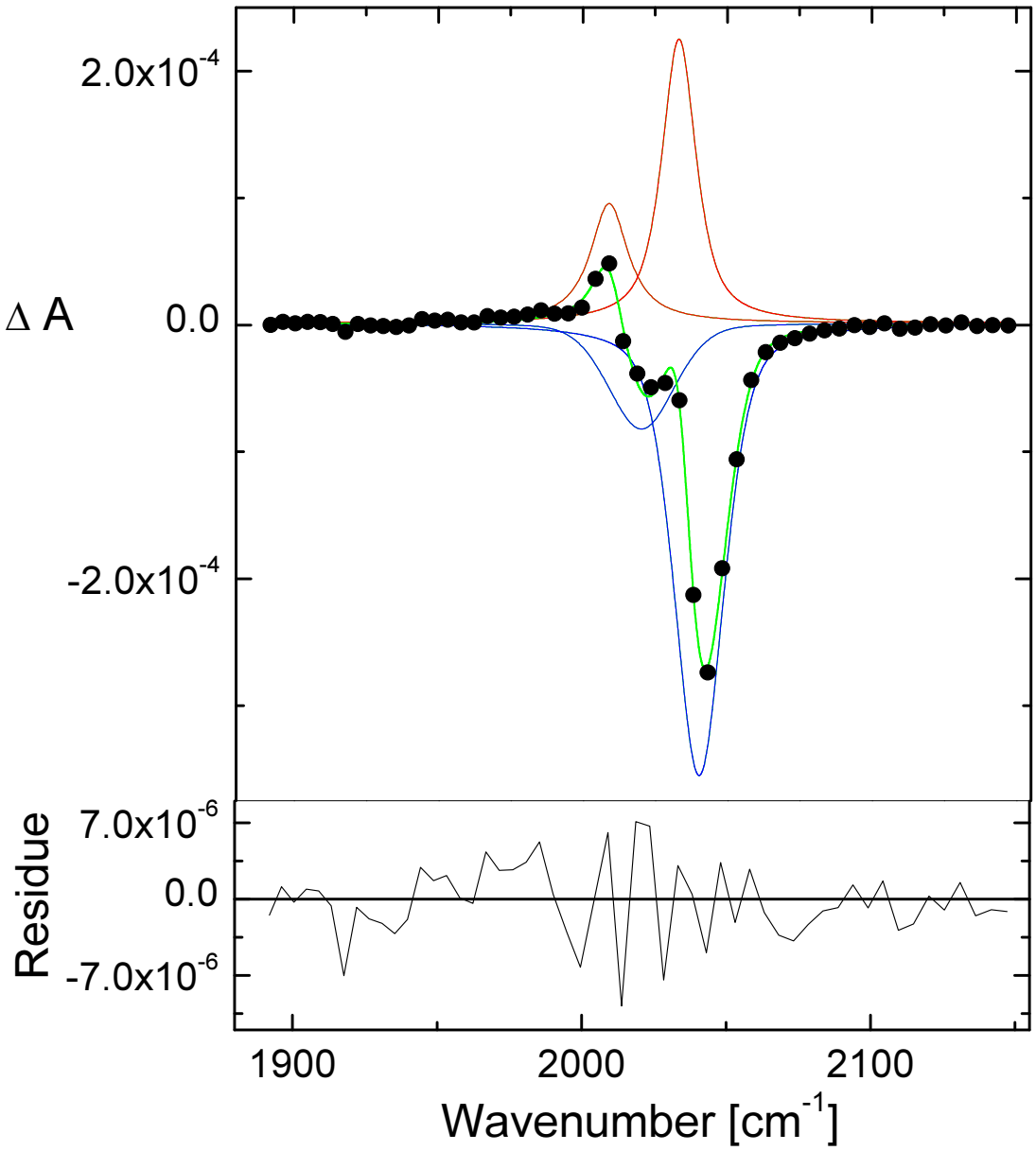


Figure S6. Time resolved infrared difference spectrum (black dots) obtained ca. 3500 ps after laser flash (λ_{exc} = 266 nm) of a solution of Ir(Cp*)$(N_3)_2(PPh_3)$ in MeCN. The overlap of *pseudo* Voigt profiles for parent bleach (blue) and transient bands (red) results in a fit curve (green) and a residual (black).

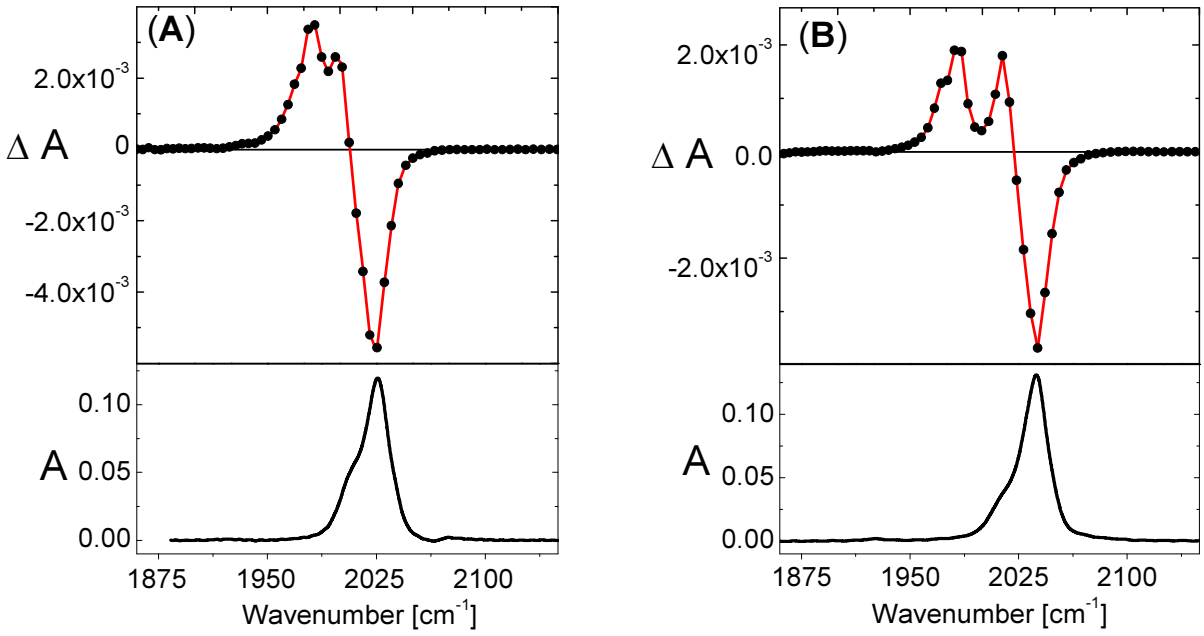


Figure S7. Time resolved spectra (top) in MeCN solution (λ_{exc} = 400 nm, top row) at *t* = 30 ps of $Rh(Cp^*)(N_3)_2(PPh_3)$ (**1**, A) and $Ir(Cp^*)(N_3)_2(PPh_3)$ (**2**, B) and respective FTIR spectra of the ground state (bottom).

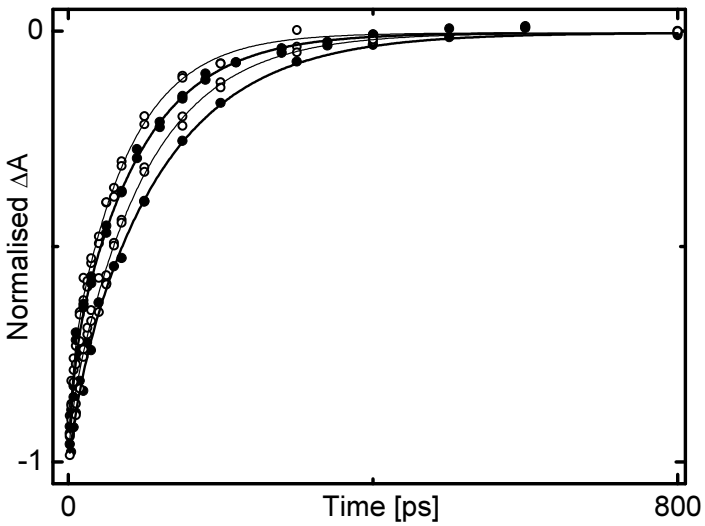


Figure S8. Normalised kinetic traces of $Rh(Cp^*)(N_3)_2(PPh_3)$ (**1**) solutions in MeCN, CH_2Cl_2, THF and toluene under 400 nm femtosecond excitation.

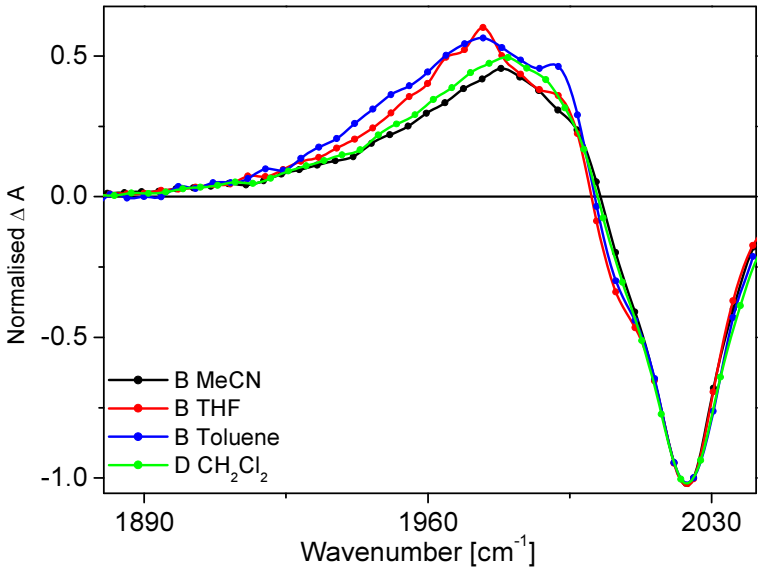


Figure S9. Normalised (parent bleach cross section at minimum) TRIR spectra of $Rh(Cp^*)(N_3)_2(PPh_3)$ (**1**) solutions in MeCN, CH_2Cl_2, THF and toluene 2 ps after 400 nm femtosecond excitation. For better comparability, the wavenumber scales of individual spectra were offset so that the bleach minima coincide with the one observed in MeCN.

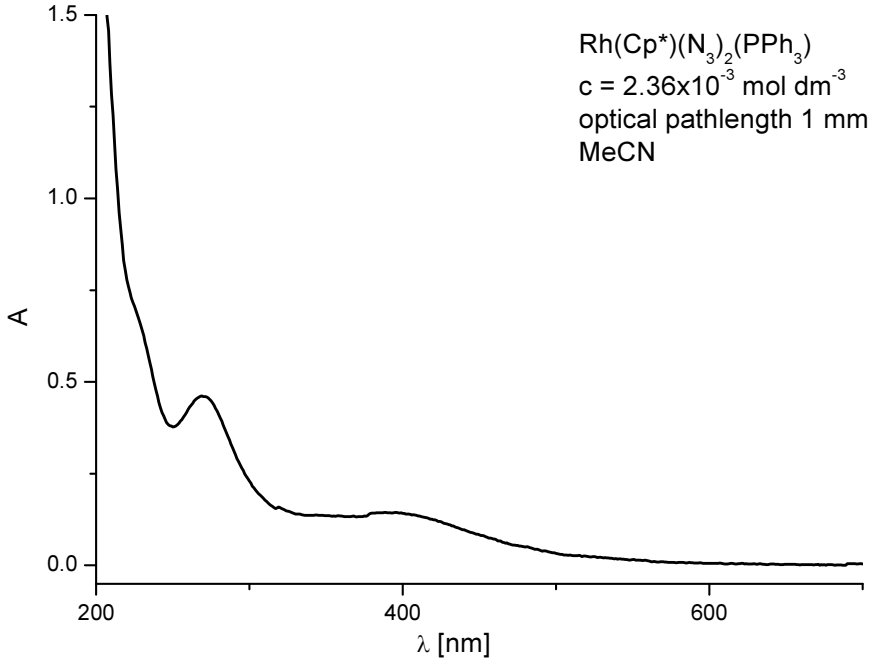


Figure S10. UV/vis absorption spectrum of $Rh(Cp^*)(N_3)_2(PPh_3)$ in MeCN solution, λ_{max} = 393 nm (ε = 6100) and 269 nm (ε = 20000); optical density [dm^3 mol^{-1} cm^{-1}] = 19000 (266 nm), 6000 (400 nm)**.**

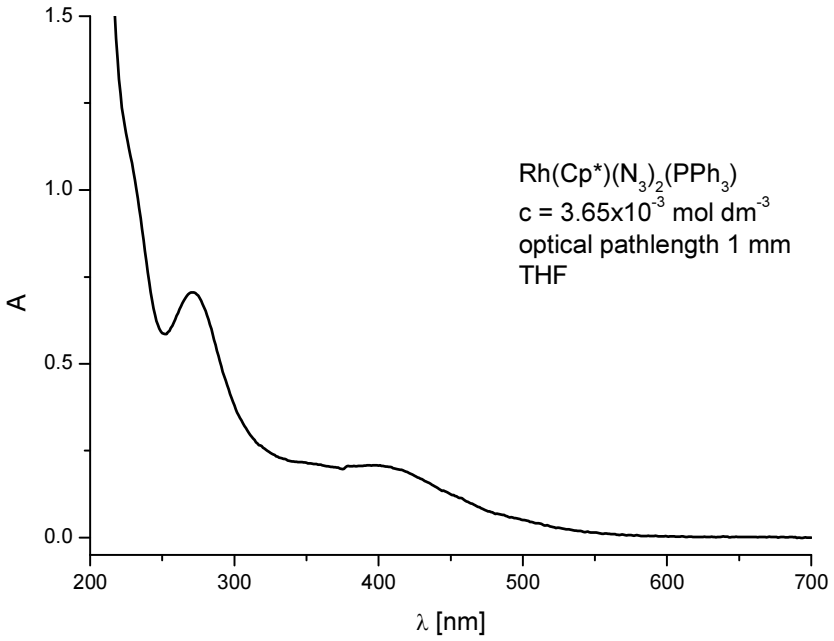


Figure S11. UV/vis absorption spectrum of $Rh(Cp^*)(N_3)_2(PPh_3)$ in THF solution, λ_{max} = 398 nm (ε = 5700) and 272 nm (ε = 19000).

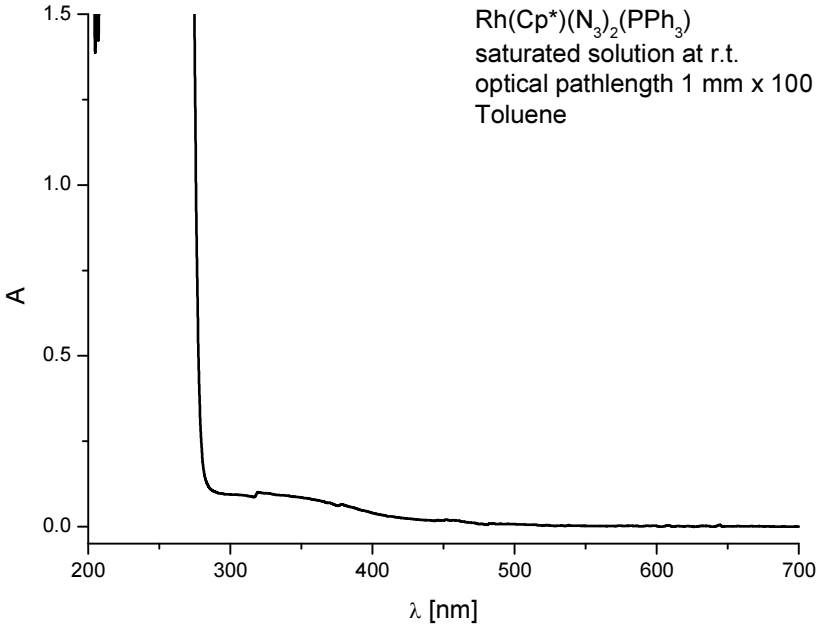


Figure S12. UV/vis absorption spectrum of $Rh(Cp^*)(N_3)_2(PPh_3)$ in toluene solution, λ_{max} = 326 nm.

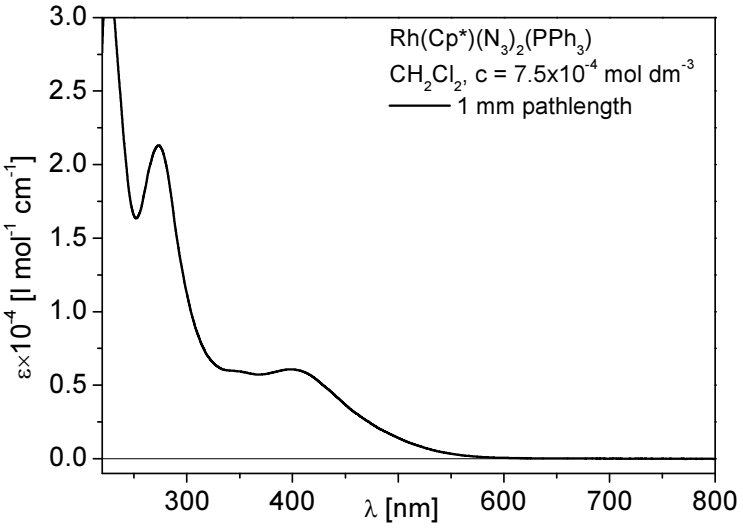


Figure S13. UV/vis absorption spectrum of $Rh(Cp^*)(N_3)_2(PPh_3)$ in CH_2Cl_2 solution, λ_{max} = 398 nm.

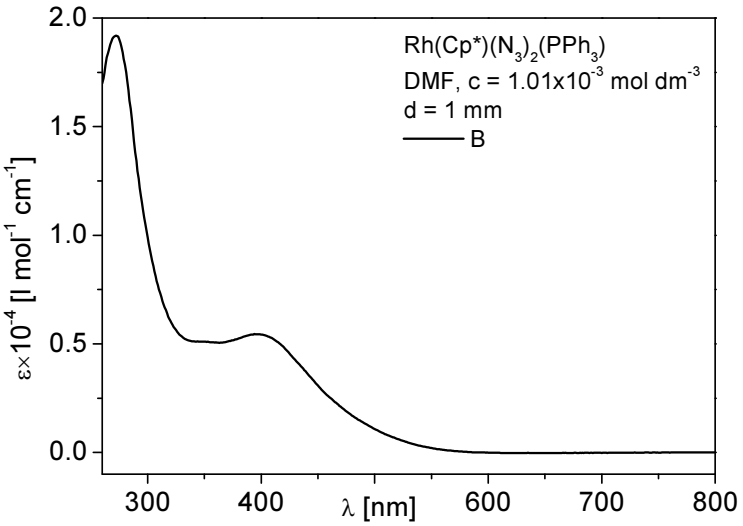


Figure S14. UV/vis absorption spectrum of $Rh(Cp^*)(N_3)_2(PPh_3)$ in DMF solution, λ_{max} = 397 nm.

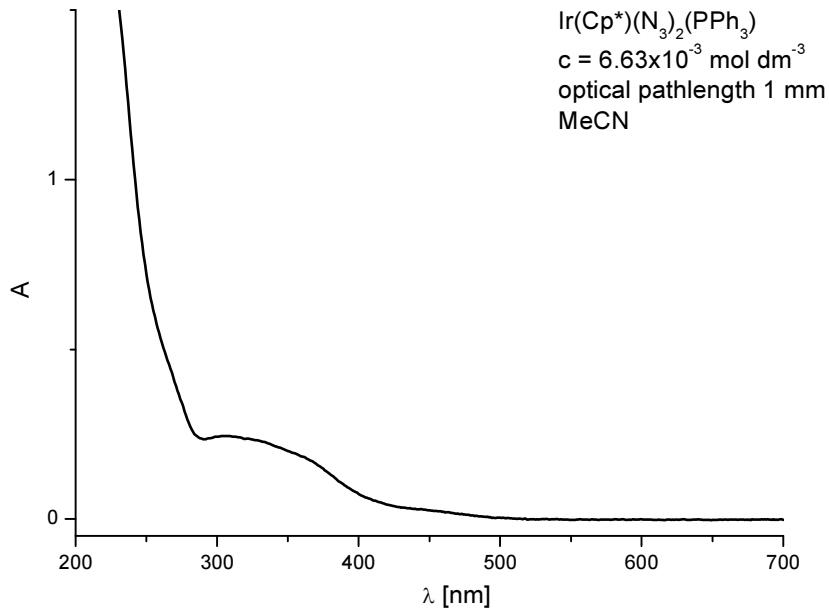


Figure S15. UV/vis absorption spectrum of $Ir(Cp^*)(N_3)_2(PPh_3)$ in MeCN solution, λ_{max} = 305 nm (ε = 3700); optical density [$dm^3\ mol^{-1}\ cm^{-1}$] = 6900 (266 nm), 1100 (400 nm).

Table S1. Residual parent bleach 800 ns ($Rh(Cp^*)(N_3)_2(PPh_3)$ and 3-4 ns ($Ir(Cp^*)(N_3)_2(PPh_3)$ after femtosecond excitation.

Complex	λ_{exc} [nm]	Solvent	Residual parent bleach [%]
$Rh(N_3)_2(Cp^*)(PPh_3)$	400	CH_3CN	0
$Rh(N_3)_2(Cp^*)(PPh_3)$	400	CH_2Cl_2	0
$Rh(N_3)_2(Cp^*)(PPh_3)$	400	THF	0
$Rh(N_3)_2(Cp^*)(PPh_3)$	400	Toluene	0
$Rh(N_3)_2(Cp^*)(PPh_3)$	266	CH_3CN	3.3(±1.8)
$Rh(N_3)_2(Cp^*)(PPh_3)$	266	THF	0.6(±0.5)
$Ir(N_3)_2(Cp^*)(PPh_3)$	400	CH_3CN	2.1(±0.6)
$Ir(N_3)_2(Cp^*)(PPh_3)$	266	CH_3CN	17(±2)

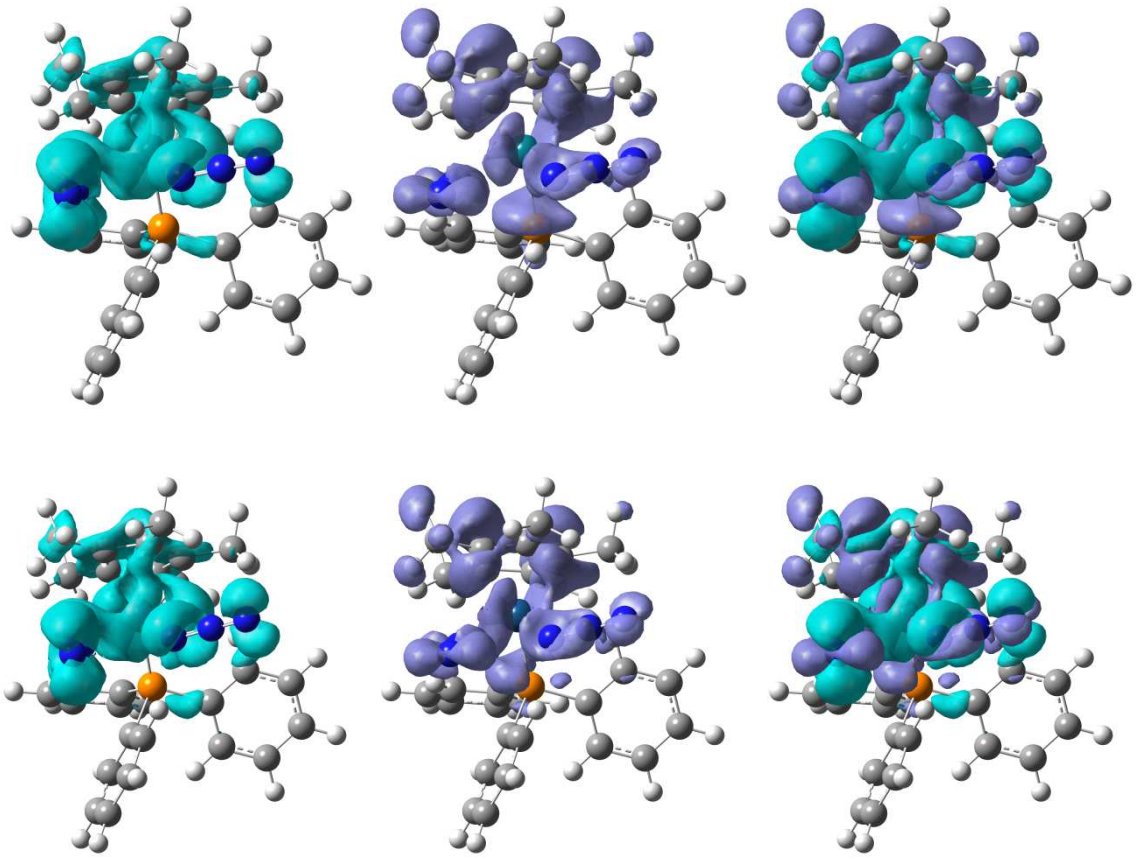
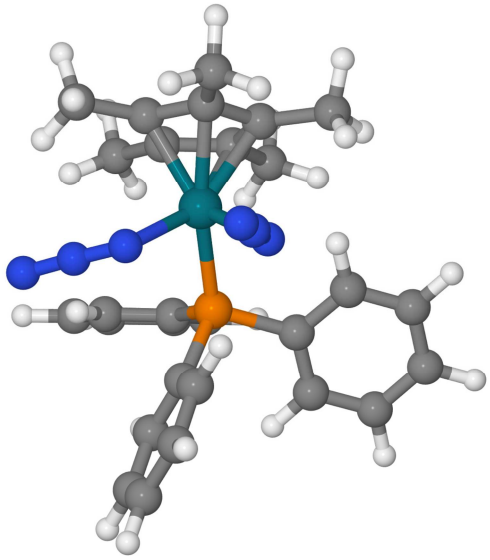


Figure S16. Isosurface diagrams of electron density change (teal, reduction; pale blue, increase) between singlet and triplet of rotamers **1c** (top row) and **2c** (bottom row); reductions are shown on the left, increases in the middle and the superposition of both on the right.

Table S2: Calculated (unscaled) vibrational frequencies and infrared intensities and relative total free energies of the local minima on the singlet ground state and triplet excited state surface at the B3LYP/6-311g(d,p) level of theory.

Isomer	$\nu_{as}(N_3)/cm^1$	G (a.u.)	ΔG/kJ mol^{-1}
1a	2106(2373), 2116(1997)	-1860.724257	0.0
1b	2096(3774), 2109(450)	-1860.721466	+7.3
1c	2110(2051), 2119(2346)	-1860.723791	+1.2
1a*	2066(2786), 2092(1642)	-1860.676987	+2.8
1b*	2069(2162), 2101(2224)	-1860.675219	+7.4
1c*	2061(1219), 2097(2834)	-1860.678056	0.0
2a	2115(2246), 2125(2015)	-1854.531450	+0.9
2b	2108(3912), 2121(332)	-1854.530049	4.6
2c	2121(2010), 2129(2413)	-1854.531785	0.0
2a*	2066(2384), 2104(1982)	-1854.473656	+5.1
2b*	2066(1820), 2114(2496)	-1854.472499	+8.1
2c*	2059(1297), 2109(2797)	-1854.475598	0.0

S17. **1a** (S_0)



S17.1. General Information

SMILES	: CC12C3([Rh]145(C2(C4(C53C)C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c6ccccc6)(c7ccccc7)c8ccccc8)C
Formula	: $C_{28}H_{30}N_6PRh$
Charge	: 0
Multiplicity	: 1
Dipole	: 15.2659 Debye
Energy	: -1861.15332955 a.u.
Number of imaginary frequencies	: 0

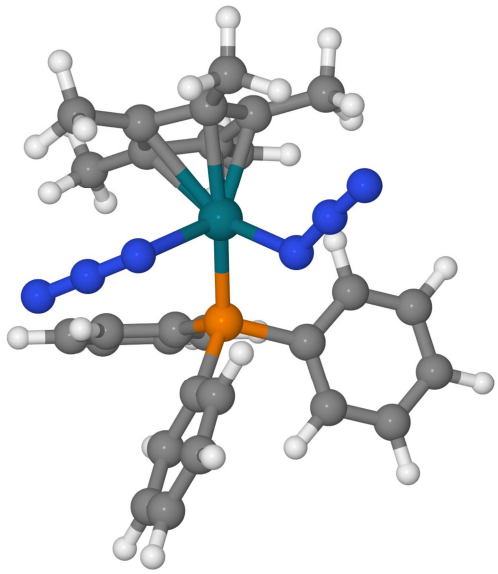
S17.2. Cartesian Co-ordinates (XYZ format)

66

P	1.07255554	-0.07152909	0.06439155
N	-1.19321573	-0.30518797	-2.22791457
N	-0.85260278	0.61773705	-2.91072917
N	-0.52708983	1.46966779	-3.62578678
N	-1.22267926	-2.30308270	-0.04971046
N	-1.84949803	-2.91046667	-0.87466818
N	-2.42791224	-3.55191326	-1.64324391
C	3.25262189	-0.17178285	-1.88949192
H	3.62693715	0.78083414	-1.44887590
C	1.78950071	-1.03631508	1.50340414
C	3.23164701	-1.16304052	1.67551017
H	3.92570543	-0.67646658	0.94915944
C	3.77106619	-1.91303062	2.78539658
H	4.87863970	-1.99580455	2.90776086
C	2.88113332	-2.55799460	3.72817779
H	3.30139732	-3.14169383	4.58347940
C	1.45075357	-2.45364165	3.55444169
H	0.75755113	-2.95976448	4.26966524
C	3.99340105	-0.79788828	-2.96358013
H	4.93291473	-0.31793204	-3.33238983

C	3.52414608	-2.03168869	-3.55134678
H	4.09868813	-2.51177073	-4.38116789
C	2.30726337	-2.64164519	-3.06086826
H	1.93411732	-3.59404922	-3.51115155
C	1.55806601	-2.02066708	-1.99328923
H	0.62032998	-2.48597717	-1.61608148
C	-3.52690768	-0.01747103	0.34498543
C	-3.12234211	1.25456119	-0.30137563
C	-2.06783891	1.89842772	0.53290242
C	-1.88517249	1.04963565	1.76252711
C	-2.77523112	-0.12670438	1.64426899
C	-4.62775326	-1.00279737	-0.14621632
H	-5.62484646	-0.68754655	0.27126563
H	-4.41112041	-2.04577565	0.20297320
H	-4.69562149	-1.00460446	-1.26532626
C	-3.67935300	1.82052064	-1.63941073
H	-4.11624336	1.00509846	-2.27124691
H	-2.87960124	2.34931564	-2.21992683
H	-4.49112511	2.56217217	-1.39688027
C	-1.49019730	3.32670951	0.31040293
H	-2.22052574	4.07969379	0.72191107
H	-1.34269404	3.53573799	-0.78109038
H	-0.51071161	3.45477366	0.83560610
C	-1.01994383	1.43795216	2.99842238
H	-1.63119245	2.11437869	3.65925884
H	-0.09742371	1.99031532	2.68479252
H	-0.72017241	0.53528106	3.58992314
C	-2.97058296	-1.27267265	2.67953491
H	-2.25005889	-1.17212260	3.53192592
H	-2.82846689	-2.27240372	2.19065952
H	-4.01672316	-1.21554577	3.08977437
C	1.78201735	1.65245163	0.24741165
C	1.65869570	2.57910752	-0.87200707
H	1.19534636	2.24045658	-1.82924700
C	2.14875627	3.93286419	-0.75872111
H	2.05868316	4.62404823	-1.63191879
C	2.73800564	4.39466095	0.48022857
H	3.10799193	5.44522095	0.56871510
C	2.84820652	3.48955727	1.60093296
H	3.30315185	3.83343244	2.56172132
C	2.38058972	2.12379551	1.48700893
H	2.48890328	1.43133318	2.35331941
C	2.02310324	-0.77641445	-1.39662373
C	0.90618461	-1.69898117	2.44606638
H	-0.19351415	-1.64129102	2.29270196
Rh	-1.33804452	-0.13273621	-0.09852234

S18. **1a*** (T_1)



S18.1. General Information

SMILES	:	C12C3([Rh]145(C2(C4(C53C)C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c6ccccc6)(c7ccccc7)c8ccccc8)C
Formula	:	$C_{28}H_{30}N_6PRh^3$
Charge	:	0
Multiplicity	:	3
Dipole	:	15.2659 Debye
Energy	:	-1861.10203875 a.u.
Number of imaginary frequencies	:	0

S18.2. Cartesian Co-ordinates (XYZ format)

66

P	1.28966010	-0.02718679	-0.00858025
N	-0.99314600	1.17922366	-2.16788840
N	-0.49200955	2.26015043	-2.15010881
N	-0.00610116	3.31975269	-2.15287876
N	-0.86203641	-1.89691794	-1.34806347
N	-1.75396824	-2.65591860	-1.61358452
N	-2.56743169	-3.42929077	-1.89016783
C	3.51086593	0.93316585	-1.64230037
H	3.90752363	1.41855693	-0.72084498
C	1.95697546	-1.64750659	0.66692621
C	3.27540493	-2.13354230	0.28621396
H	3.89582324	-1.54978633	-0.43304169
C	3.78264594	-3.37361026	0.82949233
H	4.79422140	-3.73426580	0.52068889
C	2.98634672	-4.14319897	1.75919569
H	3.38003445	-5.10307646	2.17425466
C	1.67764199	-3.66688466	2.14830709
H	1.05195022	-4.25349188	2.86411166
C	4.25066471	1.03786492	-2.88125014
H	5.21373034	1.60436094	-2.89864302

C	3.74804497	0.41341630	-4.08402586
H	4.32134533	0.49750328	-5.03981829
C	2.50206470	-0.32098621	-4.04611826
H	2.10720301	-0.80449611	-4.97313833
C	1.75166082	-0.42631522	-2.81593275
H	0.79093337	-0.98869449	-2.78340220
C	-3.47476435	0.07364015	-0.05429710
C	-3.06969595	1.50456452	-0.04833088
C	-2.07204556	1.67094958	1.02530539
C	-2.00374532	0.38517389	1.81583226
C	-2.90664506	-0.58902639	1.16239119
C	-4.51538467	-0.56486428	-1.02091944
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H	-2.44056296	-2.42329359	2.33149934
H	-3.31013680	-2.74078059	0.75891346
H	-4.21524382	-2.04577231	2.17448449
C	2.00456834	1.26366484	1.14579475
C	1.94166446	2.67161202	0.77199012
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C	2.46971273	3.68366838	1.65769255
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C	3.03939199	3.31299829	2.93556905
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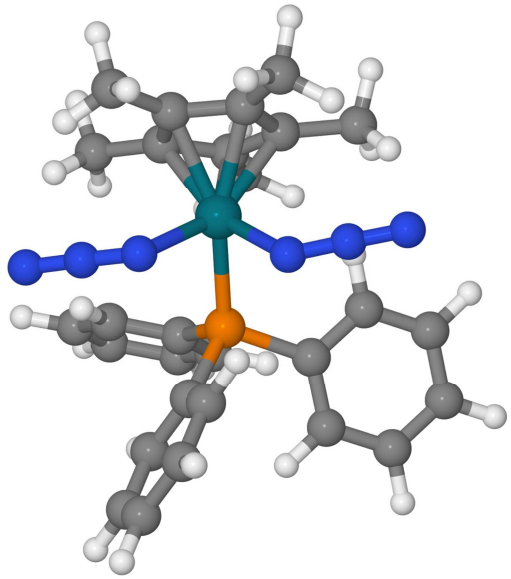
H	3.52860141	1.62238109	4.30359554
C	2.58062768	0.89867187	2.43162227
H	2.63743806	-0.17281106	2.73292089
C	2.25142550	0.20340128	-1.60114872
C	1.16401458	-2.43121219	1.60148001
H	0.15130655	-2.07859707	1.90298378
Rh	-1.10569322	-0.11670736	-0.24422419

S19. **1b** (S_0)



S19.1. General Information

SMILES	:	CC12C3([Rh]145(C2(C4(C53C)C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c6ccccc6)(c7ccccc7)c8ccccc8)C
Formula	:	$C_{28}H_{30}N_6PRh$
Charge	:	0
Multiplicity	:	1
Dipole	:	12.1730 Debye
Energy	:	-1861.15379480 a.u.
Number of imaginary frequencies	:	0

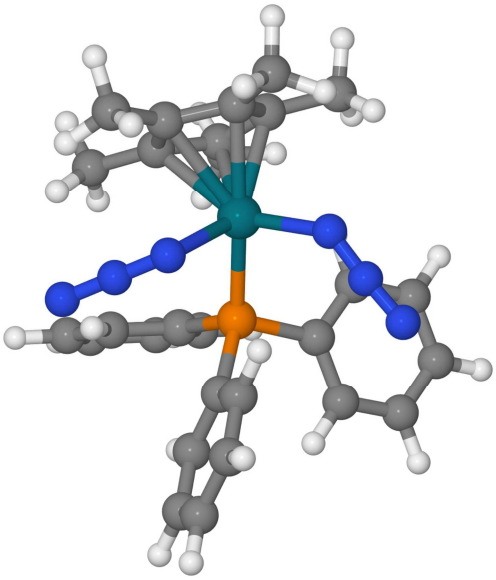
S19.2. Cartesian Co-ordinates (XYZ format)

66

P	-1.00567234	-0.07527797	0.09052285
N	0.98926526	-1.34169841	-2.07431698
N	0.86001295	-2.51423955	-1.87349367
N	0.72808319	-3.65974689	-1.73990309
N	0.83672625	1.53684711	-1.89812493
N	1.01797104	2.70403838	-1.70569384
N	1.17937791	3.84597230	-1.58166254
C	-3.23313379	-1.55617905	-1.07487297
H	-3.42273307	-1.96342802	-0.05503510
C	-1.77701426	1.56580794	0.56215841
C	-3.20695090	1.80068588	0.40805259
H	-3.85821915	1.00794256	-0.02936626
C	-3.78514171	3.06045818	0.81576341
H	-4.88279009	3.22713661	0.68902254
C	-2.95013523	4.09991646	1.37891901
H	-3.40161848	5.07400227	1.68870580
C	-1.53067183	3.87689972	1.53217578
H	-0.87449056	4.67535353	1.95598865
C	-4.10756397	-1.93024611	-2.16642141

H	-4.96244621	-2.62287354	-1.97055018
C	-3.87825847	-1.40869915	-3.49395251
H	-4.55543470	-1.69895315	-4.33456278
C	-2.76860976	-0.50981605	-3.73037934
H	-2.58305287	-0.10609531	-4.75607777
C	-1.88496804	-0.13569467	-2.65079379
H	-1.02231407	0.54691505	-2.82792163
C	3.51741242	0.64328730	-0.28629392
C	3.44804835	-0.82719731	-0.25447920
C	2.60659862	-1.23674023	0.92380852
C	2.24053192	0.00832128	1.66585588
C	2.76275826	1.17388105	0.90632349
C	4.27853346	1.51796353	-1.32599711
H	5.31835699	1.71784317	-0.94318259
H	3.76198316	2.50164747	-1.47520614
H	4.35723543	0.99084198	-2.31205535
C	4.11953688	-1.80374956	-1.26287806
H	4.24560785	-1.32389486	-2.26743937
H	3.52081370	-2.74399018	-1.37472034
H	5.13685226	-2.07593918	-0.86408675
C	2.40509391	-2.70314527	1.40751684
H	3.35269547	-3.06005049	1.90065110
H	2.17582870	-3.38165212	0.54400331
H	1.56753707	-2.76763177	2.14708567
C	1.53707516	0.05745487	3.05405927
H	2.33058739	-0.04712846	3.84619236
H	0.80323976	-0.77907717	3.17047334
H	1.00465345	1.03090918	3.21083784
C	2.76475072	2.66731071	1.35071182
H	2.12149072	2.82016420	2.25584459
H	2.41495800	3.34553599	0.52761865
H	3.81954002	2.95543337	1.61913371
C	-1.46270037	-1.21519494	1.50472009
C	-1.11272395	-2.62685227	1.40432751
H	-0.61298126	-3.01381874	0.48434040
C	-1.43046212	-3.53734446	2.47963715
H	-1.16419041	-4.61791611	2.38172102
C	-2.08110118	-3.05062652	3.67814898
H	-2.31952596	-3.75503111	4.51209879
C	-2.42354488	-1.65160847	3.78977132
H	-2.92741919	-1.26568258	4.70932770
C	-2.12193465	-0.73639160	2.70906591
H	-2.39699674	0.33937272	2.80360675
C	-2.11234498	-0.65780747	-1.30966449
C	-0.94914007	2.61816382	1.12211764
H	0.14563033	2.45238137	1.22267485
Rh	1.35310209	0.01609872	-0.42983311

S20. **1b*** (T_1)



S20.1. General Information

SMILES	:	CC12C3([Rh]145(C2(C4(C53C)C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c6ccccc6)(c7ccccc7)c8ccccc8)C
Formula	:	$C_{28}H_{30}N_6PRh^3$
Charge	:	0
Multiplicity	:	3
Dipole	:	12.1730 Debye
Energy	:	-1861.09990284 a.u.
Number of imaginary frequencies	:	0

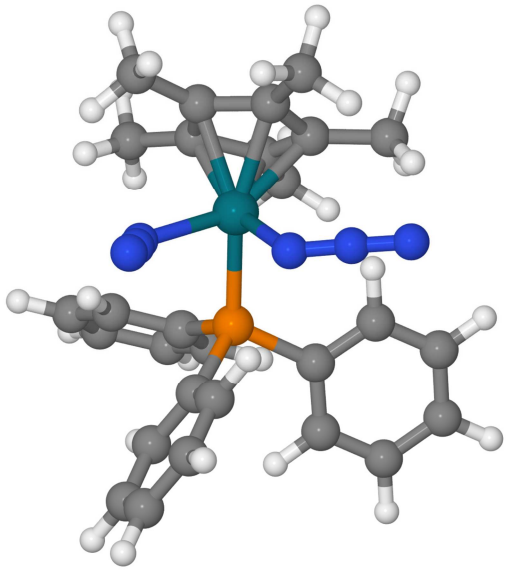
S20.2. Cartesian Co-ordinates (XYZ format)

66

P	-1.02399600	-0.03400095	0.09356219
N	1.22462344	-1.24294269	-2.08917403
N	0.87997949	-2.37085485	-1.91819906
N	0.54941964	-3.47879243	-1.77131569
N	1.04794490	2.04922748	-1.53674293
N	0.08716141	2.62138653	-1.97715628
N	-0.78803545	3.22532582	-2.42466545
C	-3.32030225	-1.36747169	-1.09797275
H	-3.61099315	-1.65308452	-0.06026866
C	-1.84215450	1.56388521	0.64320588
C	-3.22551775	1.87342155	0.31181687
H	-3.82154632	1.16491747	-0.30877230
C	-3.82991195	3.10234928	0.77509767
H	-4.89085865	3.32655239	0.50534707
C	-3.06809592	4.03597832	1.57407963
H	-3.53823280	4.98606110	1.92747378
C	-1.69391739	3.73733687	1.91121566
H	-1.09440649	4.45118952	2.52677298

C	-4.16382599	-1.75168216	-2.20743775
H	-5.10000610	-2.32912016	-2.01094127
C	-3.79569983	-1.39292967	-3.55910230
H	-4.44755507	-1.69421649	-4.41544437
C	-2.57957101	-0.64883810	-3.79945850
H	-2.28327703	-0.37567243	-4.84153843
C	-1.72969794	-0.26366866	-2.69566369
H	-0.77968627	0.28023306	-2.89186573
C	3.64369702	0.58126485	-0.29836932
C	3.49857545	-0.89549083	-0.18728779
C	2.61683631	-1.16093314	0.96299398
C	2.37007952	0.14885357	1.68284595
C	3.05688429	1.21285856	0.92509264
C	4.45607519	1.34228444	-1.38650954
H	5.50431585	1.52837479	-1.01822650
H	3.97839689	2.33143210	-1.61338687
H	4.51533604	0.74188966	-2.33203602
C	4.11287212	-1.94089222	-1.15774643
H	4.06100655	-1.58505726	-2.22012639
H	3.57889485	-2.92364478	-1.08143258
H	5.19571209	-2.10548186	-0.89157540
C	2.26873875	-2.56676960	1.53699279
H	3.13075089	-2.92664218	2.16795754
H	2.09775400	-3.30946851	0.71481425
H	1.35401571	-2.52797937	2.18033624
C	1.72035003	0.26694584	3.09452367
H	2.44635701	-0.11704889	3.86566901
H	0.78114486	-0.34058112	3.16380906
H	1.47934222	1.33358991	3.34330320
C	3.13289928	2.73041129	1.26649678
H	2.41332626	2.99886942	2.08372259
H	2.90312171	3.35463738	0.36257783
H	4.17316580	2.98387074	1.61581600
C	-1.45153165	-1.24240303	1.46203101
C	-1.20919788	-2.66477060	1.25158095
H	-0.79689252	-3.02496672	0.27834740
C	-1.52052248	-3.61725640	2.29216695
H	-1.33914077	-4.70497179	2.11201763
C	-2.05397940	-3.16727042	3.56035972
H	-2.28816080	-3.90667605	4.36473560
C	-2.28592181	-1.75827634	3.78025889
H	-2.70152402	-1.39931262	4.75332975
C	-1.99261510	-0.79792935	2.73741102
H	-2.18682194	0.28514197	2.91390300
C	-2.09196782	-0.61826873	-1.33167756
C	-1.08397162	2.51294518	1.44456661
H	-0.02360929	2.29286861	1.70544183
Rh	1.28908849	0.31594172	-0.38284963

S21. **1c** (S_0)



S21.1. General Information

SMILES	:	CC12C3([Rh]145(C2(C4(C53C)C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c6ccccc6)(c7ccccc7)c8ccccc8)C
Formula	:	$C_{28}H_{30}N_6PRh$
Charge	:	0
Multiplicity	:	1
Dipole	:	15.4190 Debye
Energy	:	-1861.15401109 a.u.
Number of imaginary frequencies	:	0

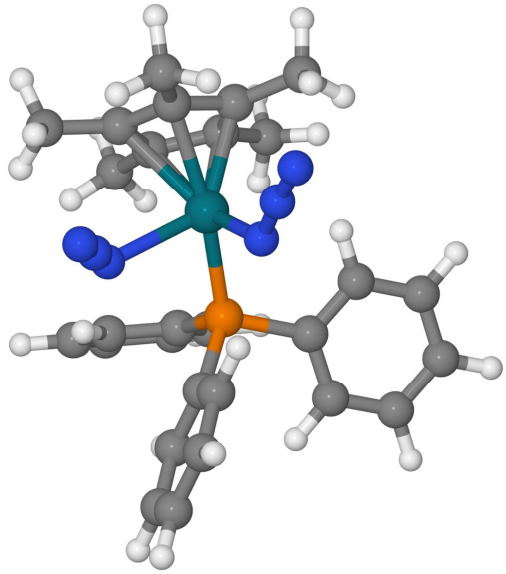
S21.2. Cartesian Co-ordinates (XYZ format)

66

P	-1.07376730	0.03904792	-0.02211326
N	0.93413460	0.76534921	-2.24137425
N	1.27481973	1.88296676	-2.51404405
N	1.57903910	2.94964123	-2.83931780
N	1.40956306	2.02837443	0.46360177
N	1.68570876	2.28898859	1.59890759
N	1.95544338	2.60422993	2.68158412
C	-3.22949243	1.21405756	-1.59659314
H	-3.64435577	0.18390395	-1.68673539
C	-1.75033009	0.16521835	1.72034907
C	-3.16892028	0.39741573	1.96696377
H	-3.87358427	0.51170874	1.10923755
C	-3.66898179	0.48578098	3.31876898
H	-4.75914717	0.65997237	3.49123240
C	-2.76358700	0.35840300	4.44178534
H	-3.15434265	0.43337032	5.48597574
C	-1.35420179	0.14626905	4.20809793
H	-0.64476353	0.06092517	5.06667948
C	-3.94640779	2.32346773	-2.18746114

H	-4.90859032	2.13020802	-2.72238660
C	-3.42433596	3.66703272	-2.08505893
H	-3.98016286	4.52140570	-2.54373670
C	-2.17756581	3.89826012	-1.38898373
H	-1.76114535	4.93262577	-1.31125820
C	-1.45243776	2.79753208	-0.79625231
H	-0.48351017	2.97085857	-0.27336308
C	3.50100207	-0.40488431	0.22926621
C	3.18909001	-1.00558805	-1.07775831
C	2.08683228	-2.01013613	-0.88499260
C	1.78620708	-2.07378387	0.57633752
C	2.62168169	-1.05626214	1.26703525
C	4.57485914	0.68358529	0.52521294
H	5.54104996	0.17761332	0.80460864
H	4.25792217	1.33480179	1.38083017
H	4.75514221	1.32542419	-0.37566841
C	3.85602808	-0.67099130	-2.44241810
H	4.43017578	0.28985760	-2.38416433
H	3.08091736	-0.58911276	-3.24752021
H	4.56991482	-1.50072837	-2.70570374
C	1.57151151	-2.97478580	-1.99164248
H	2.32471180	-3.79964161	-2.13801885
H	1.45049965	-2.42984486	-2.96455669
H	0.58910936	-3.43027663	-1.71006811
C	0.83374655	-3.09731030	1.26248646
H	1.43170607	-4.01841879	1.51139879
H	-0.00537850	-3.38952541	0.58173126
H	0.40325987	-2.68515158	2.21138883
C	2.76971364	-0.83990741	2.80325723
H	2.00068808	-1.42740369	3.36875725
H	2.68347263	0.24486420	3.07986045
H	3.78817320	-1.20176232	3.11835003
C	-1.88010395	-1.48717177	-0.74622273
C	-1.69250250	-1.75005031	-2.16803145
H	-1.09965706	-1.03345966	-2.78464246
C	-2.27751660	-2.92163086	-2.77656627
H	-2.13517928	-3.10363531	-3.86966681
C	-3.03424978	-3.85915852	-1.97319472
H	-3.48148108	-4.76807356	-2.44487572
C	-3.21066880	-3.61457348	-0.56020522
H	-3.79218721	-4.33240843	0.06824712
C	-2.64229941	-2.43245006	0.05352068
H	-2.79313445	-2.24774671	1.14216101
C	-1.97261357	1.44110620	-0.89681411
C	-0.85168755	0.05257198	2.85439467
H	0.23580804	-0.09154428	2.67385602
Rh	1.32972360	-0.00487141	-0.25794432

S22. **1c*** (T_1)



S22.1. General Information

SMILES	:	CC12C3([Rh]145(C2(C4(C53C)C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c6ccccc6)(c7ccccc7)c8ccccc8)C
Formula	:	$C_{28}H_{30}N_6PRh^3$
Charge	:	0
Multiplicity	:	3
Dipole	:	15.4190 Debye
Energy	:	-1861.10172072 a.u.
Number of imaginary frequencies	:	0

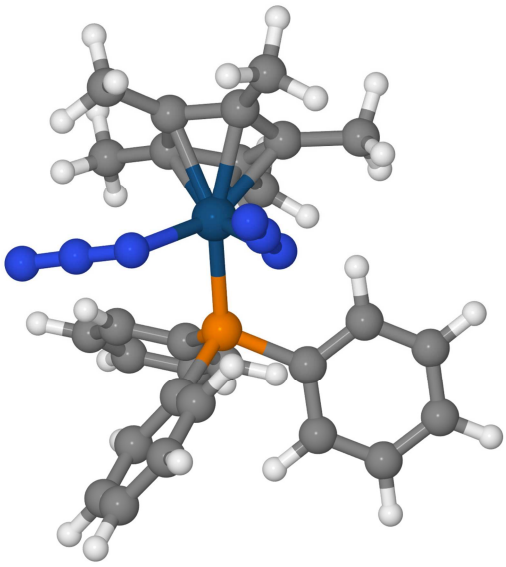
S22.2. Cartesian Co-ordinates (XYZ format)

66

P	1.17836094	-0.19756401	0.01291448
N	-0.86103708	1.33591831	-1.78789628
N	-1.46985221	1.13213265	-2.79492760
N	-2.05670857	0.95560312	-3.78479218
N	-1.10749876	-1.92351103	-1.47997391
N	-2.04511476	-2.56438160	-1.87251592
N	-2.90117359	-3.22270656	-2.28248620
C	3.33815813	0.70095617	-1.73202229
H	3.69915819	1.31532979	-0.87530267
C	1.96236920	-1.67656076	0.86114895
C	3.39242506	-1.93474984	0.74151736
H	4.03053427	-1.25633097	0.12726042
C	3.99086118	-3.06920934	1.40523601
H	5.08848238	-3.25067997	1.30071974
C	3.17355633	-3.96789885	2.19192696
H	3.63830924	-4.84823084	2.69957280
C	1.75447774	-3.72596550	2.31364131
H	1.11275184	-4.41678143	2.91271710
C	4.08044147	0.70729405	-2.97420406

H	5.00845146	1.32498145	-3.05406284
C	3.62637496	-0.07804529	-4.09901810
H	4.20130253	-0.06945751	-5.05746984
C	2.42381191	-0.87298453	-3.97771621
H	2.06225634	-1.47951818	-4.84419346
C	1.67256153	-0.88351977	-2.74318933
H	0.74156088	-1.48919857	-2.65170670
C	-3.56701946	0.07317436	0.01026388
C	-3.03812790	1.43678081	0.26852316
C	-2.08256555	1.32766461	1.39090776
C	-2.16625476	-0.06418436	1.95886052
C	-3.10779667	-0.83345443	1.11485839
C	-4.61421156	-0.30361417	-1.08040452
H	-5.65158129	-0.18682626	-0.65671468
H	-4.49130583	-1.36764884	-1.41227245
H	-4.51696682	0.36659622	-1.97381043
C	-3.37028265	2.72379065	-0.53379053
H	-3.62027454	2.48578310	-1.60097313
H	-2.50723433	3.43859220	-0.51672596
H	-4.26367044	3.23303390	-0.07123458
C	-1.36601734	2.52412701	2.08028078
H	-2.08332086	2.99835992	2.80924225
H	-1.05989921	3.29883575	1.33158350
H	-0.45819578	2.19023657	2.64394617
C	-1.53385425	-0.51326567	3.31133986
H	-2.15473223	-0.11022764	4.16096163
H	-0.48966256	-0.11998930	3.42490101
H	-1.51015592	-1.63097358	3.39817405
C	-3.57833338	-2.30338740	1.33183324
H	-2.84055352	-2.87580132	1.95284641
H	-3.71748829	-2.83427525	0.35334560
H	-4.56780529	-2.30284119	1.87033093
C	1.79590511	1.28173041	0.97387654
C	1.62125170	2.61217427	0.40366128
H	1.14916670	2.72125745	-0.60105115
C	2.05995750	3.77929711	1.13226712
H	1.93366742	4.79175711	0.67676556
C	2.64832997	3.63989305	2.44772196
H	2.98218989	4.54513407	3.01144147
C	2.80228853	2.32600975	3.02970552
H	3.25486803	2.20820618	4.04451132
C	2.38431859	1.14907610	2.29729199
H	2.52440286	0.13846178	2.74695897
C	2.12418413	-0.09383346	-1.60611773
C	1.15183043	-2.58887982	1.65211737
H	0.05503434	-2.42100978	1.75011647
Rh	-1.23021221	-0.31328174	-0.14352173

S23. **2a** (S_0)



S23.1. General Information

SMILES	: CC12C3([Ir]145(C2(C4(C53C)C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c6ccccc6)(c7ccccc7)c8ccccc8)C
Formula	: $C_{28}H_{30}IrN_6P$
Charge	: 0
Multiplicity	: 1
Dipole	: 14.8498 Debye
Energy	: -1854.96145398 a.u.
Number of imaginary frequencies	: 0

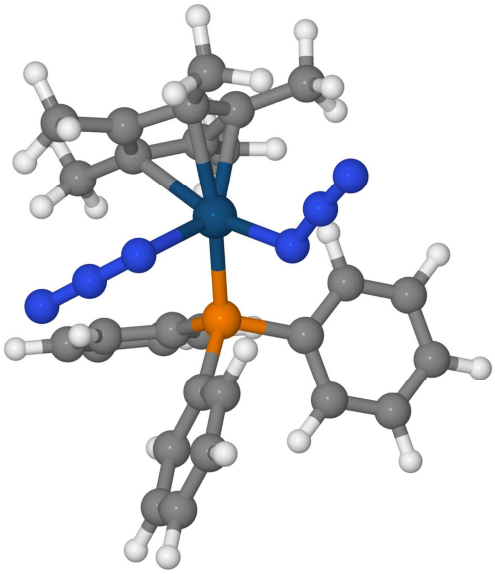
S23.2. Cartesian Co-ordinates (XYZ format)

66

Ir	5.67918110	0.93609816	2.87660146
P	4.77517176	0.07525454	4.91693211
N	7.65725183	0.60657555	3.67623734
N	8.13129807	1.38856602	4.45193863
N	8.64289856	2.10581136	5.20290089
N	5.83233452	-1.13619494	2.20963073
N	6.86878443	-1.49525213	1.71617544
N	7.83286238	-1.90703607	1.23237109
C	6.14530468	-0.65259880	7.40755320
H	5.59898138	0.18401630	7.90003300
C	3.36109257	-1.13927674	4.72626829
C	2.92436624	-1.95455825	5.85294771
H	3.44303060	-1.87035549	6.83755064
C	1.82085097	-2.87393713	5.70124817
H	1.49475813	-3.49120641	6.57371473
C	1.14791179	-2.99970603	4.42533970
H	0.29861602	-3.71685505	4.31011534
C	1.58328855	-2.20394659	3.30064273
H	1.07848167	-2.30466008	2.30904508

C	7.03588200	-1.48237741	8.19320679
H	7.16162920	-1.26940179	9.28311825
C	7.74806261	-2.57630920	7.57641649
H	8.43323231	-3.21489143	8.18628979
C	7.56784439	-2.84382701	6.16462946
H	8.11441898	-3.68821144	5.67742872
C	6.68849659	-2.01729369	5.37337589
H	6.54825687	-2.21971130	4.28695536
C	5.74668026	1.75178397	0.75353491
C	6.44266701	2.70239043	1.63979399
C	5.48120546	3.16109061	2.70557976
C	4.14964437	2.53968525	2.39524412
C	4.31588459	1.63396478	1.22454810
C	6.34582138	1.02457356	-0.48663080
H	6.18195152	1.66065753	-1.40073490
H	5.84108257	0.03642473	-0.64567566
H	7.44632626	0.85347819	-0.36132741
C	7.93215227	3.14324832	1.52832878
H	8.54191780	2.37414932	0.98792428
H	8.37755299	3.32263255	2.54090261
H	7.97214842	4.10722589	0.94807684
C	5.76880550	4.29989052	3.72919679
H	5.69334221	5.29461813	3.20623970
H	6.80189562	4.19990587	4.15536547
H	5.03168392	4.27910089	4.57093191
C	2.80394816	2.87114811	3.10601377
H	2.32156539	3.72407031	2.55134392
H	2.97095633	3.18135405	4.16763258
H	2.10570240	1.99458873	3.08957767
C	3.20107698	0.86261070	0.45619431
H	2.25613475	0.80851889	1.05636311
H	3.53548384	-0.17764837	0.20150861
H	2.97736597	1.40805209	-0.50305235
C	4.11009073	1.37860847	6.08728504
C	5.01623487	2.41192460	6.57314491
H	6.08888674	2.40360403	6.26502132
C	4.54243565	3.44088840	7.46963453
H	5.25496817	4.21737909	7.84020185
C	3.15290499	3.47015357	7.87490034
H	2.78568935	4.27207422	8.56085491
C	2.24465394	2.45749354	7.38926506
H	1.16982186	2.47065067	7.69410133
C	2.71837306	1.41153991	6.50743675
H	2.00808001	0.63289768	6.14614153
C	5.96854067	-0.90917695	5.98761988
C	2.68637347	-1.27979696	3.45023584
H	3.04436445	-0.68186945	2.58484507

S24. **2a*** (T_1)



S24.1. General Information

SMILES	:	C[C]1C2(C3([Ir]24(C1(C43C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c5ccccc5)(c6ccccc6)c7ccccc7)C)C
Formula	:	$C_{28}H_{30}IrN_6P^3$
Charge	:	0
Multiplicity	:	3
Dipole	:	14.8498 Debye
Energy	:	-1854.90009756 a.u.
Number of imaginary frequencies	:	0

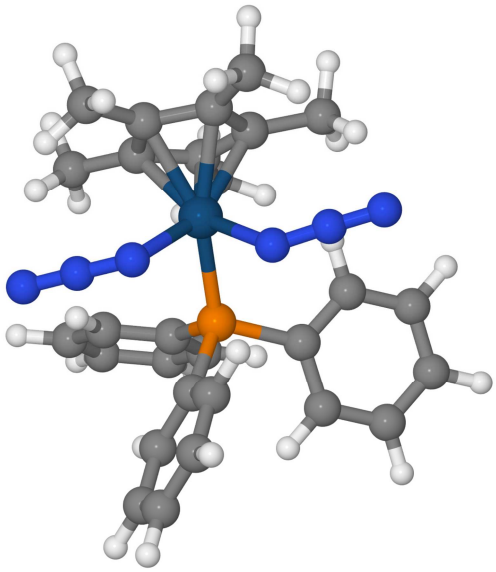
S24.2. Cartesian Co-ordinates (XYZ format)

66

Ir	-1.04955685	-0.35815609	0.21934532
P	1.29538345	-0.05202483	0.05632901
N	-1.27483630	-0.46288937	-2.12698221
N	-0.85658759	0.44389144	-2.78096128
N	-0.45369533	1.32092237	-3.43286705
N	-0.70236832	-2.43929148	0.21991237
N	-1.56319344	-3.25650883	0.42539045
N	-2.33218575	-4.09295130	0.62374848
C	3.29004073	-0.04841663	-2.07789397
H	3.68303370	0.89590174	-1.63573837
C	2.18228984	-0.96938109	1.43566215
C	3.52929473	-1.48684752	1.24353075
H	4.03700638	-1.36193585	0.25877753
C	4.21057272	-2.17191648	2.31909895
H	5.24135399	-2.56899214	2.15023136
C	3.56181216	-2.34719086	3.59926367
H	4.08943605	-2.88069224	4.42730045
C	2.22629237	-1.83145082	3.80303812
H	1.71364450	-1.96278930	4.78692245

C	3.93720603	-0.61517578	-3.24113345
H	4.82518625	-0.09824698	-3.68049240
C	3.43888927	-1.83845055	-3.82781196
H	3.93968964	-2.27230644	-4.72793913
C	2.29140592	-2.49918771	-3.24497318
H	1.90033555	-3.44502139	-3.69397545
C	1.63402164	-1.93889976	-2.08668351
H	0.74978381	-2.44444299	-1.63621402
C	-3.47106576	-0.16752617	0.40242839
C	-3.19078946	1.05244219	-0.40024939
C	-2.10927677	1.79065561	0.30102280
C	-1.89938581	1.16290224	1.65592980
C	-2.77253342	-0.04946769	1.71894240
C	-4.50004339	-1.27528644	0.02485762
H	-5.52484751	-0.97243959	0.38074711
H	-4.23782301	-2.25553870	0.50145084
H	-4.54083776	-1.41411483	-1.08762324
C	-3.82087278	1.40939677	-1.77243090
H	-4.06824112	0.48381060	-2.35594225
H	-3.12873030	2.04674196	-2.38262248
H	-4.77575493	1.98727739	-1.61057532
C	-1.56976318	3.18943524	-0.12591110
H	-2.33468151	3.96979666	0.15015970
H	-1.39839375	3.23736334	-1.23292708
H	-0.61109442	3.43284130	0.39588419
C	-1.12332606	1.81859076	2.83996272
H	-1.76668859	2.61526680	3.30984664
H	-0.17189774	2.29359841	2.48529196
H	-0.87507558	1.06114292	3.62919426
C	-2.95765018	-1.00246310	2.93930745
H	-2.05002356	-0.99535280	3.59848499
H	-3.15053296	-2.05546999	2.60442829
H	-3.84039187	-0.66097480	3.55018878
C	1.93428922	1.70218372	0.20698045
C	1.70946836	2.64284873	-0.88323641
H	1.17761278	2.30915117	-1.80631149
C	2.18523288	4.00310898	-0.78048980
H	2.01644397	4.70917702	-1.62987125
C	2.86361313	4.45178175	0.41675314
H	3.22379231	5.50662136	0.49560520
C	3.07490754	3.52961254	1.50892198
H	3.59989882	3.86392736	2.43686390
C	2.62194157	2.15889311	1.40512824
H	2.80531478	1.45185375	2.24689054
C	2.12774086	-0.70349741	-1.49401009
C	1.53900051	-1.15148282	2.72817039
H	0.50685352	-0.76653159	2.89446354

S25. **2b** (S_0)



S25.1. General Information

SMILES	:	CC12C3([Ir]145(C2(C4(C53C)C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c6ccccc6)(c7ccccc7)c8ccccc8)C
Formula	:	$C_{28}H_{30}IrN_6P$
Charge	:	0
Multiplicity	:	1
Dipole	:	11.9615 Debye
Energy	:	-1854.96218258 a.u.
Number of imaginary frequencies	:	0

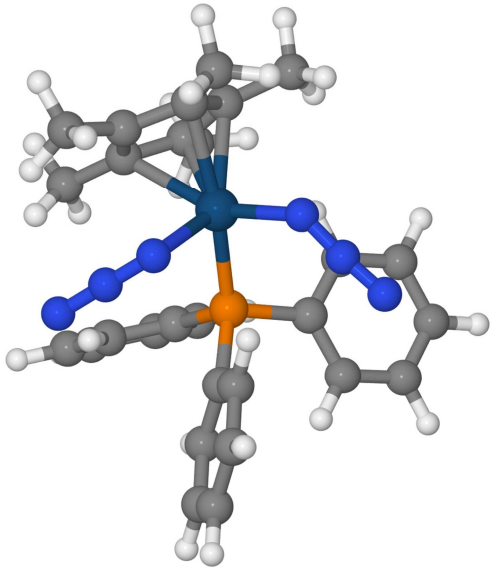
S25.2. Cartesian Co-ordinates (XYZ format)

66

Ir	1.23668015	-0.04474850	-0.37832028
P	-1.11044085	-0.12360939	0.09101138
N	0.87556702	-1.33275795	-2.08739233
N	0.72009391	-2.51151800	-1.93410444
N	0.56387478	-3.65656638	-1.85352337
N	0.75317067	1.49271178	-1.85264254
N	0.93677074	2.65890288	-1.64395976
N	1.09789169	3.79774308	-1.51147497
C	-3.32551861	-1.58482146	-1.12650824
H	-3.51634955	-2.02383995	-0.12026209
C	-1.88446331	1.51250970	0.57856405
C	-3.31537628	1.74273658	0.42642605
H	-3.96299076	0.95352918	-0.02260274
C	-3.90022993	2.99403167	0.85041350
H	-4.99847507	3.15715885	0.72429293
C	-3.07075763	4.02973413	1.42837143
H	-3.52709174	4.99752760	1.75059533
C	-1.65045583	3.81104279	1.57988846
H	-0.99843842	4.60692644	2.01495385
C	-4.19480562	-1.93197882	-2.23135471

H	-5.04554892	-2.63571453	-2.05839300
C	-3.96569180	-1.36997843	-3.54196954
H	-4.63866949	-1.63929284	-4.39286709
C	-2.86142874	-0.45691860	-3.74805093
H	-2.67576075	-0.02101865	-4.76051140
C	-1.98335290	-0.10995816	-2.65515685
H	-1.12517297	0.58361149	-2.81024742
C	3.42476535	0.55462927	-0.19962500
C	3.33928657	-0.91665727	-0.18931121
C	2.46578884	-1.33968759	0.96523458
C	2.09568691	-0.09592794	1.71790183
C	2.64421082	1.08037376	0.98422956
C	4.20977831	1.43511689	-1.21805084
H	5.24782753	1.61590087	-0.82181257
H	3.70705676	2.42727733	-1.35805988
H	4.29064322	0.92265582	-2.21166182
C	4.00766706	-1.88613498	-1.20802486
H	4.18532801	-1.38043821	-2.19187808
H	3.37788248	-2.79845500	-1.37020648
H	4.99950743	-2.20998454	-0.78511786
C	2.26199937	-2.81112409	1.43563247
H	3.19164443	-3.15966010	1.96733975
H	2.07610893	-3.48853779	0.56096762
H	1.39465272	-2.88798237	2.13859057
C	1.36730671	-0.05651541	3.09439278
H	2.14919066	-0.15158111	3.89905500
H	0.64202332	-0.90201932	3.19703054
H	0.82051504	0.91036230	3.24216628
C	2.66149569	2.56574512	1.45874369
H	1.96556199	2.72122717	2.32370400
H	2.38320446	3.26847148	0.62976116
H	3.70432281	2.81629467	1.80159104
C	-1.59388161	-1.28474212	1.47887087
C	-1.24305916	-2.69448256	1.36237693
H	-0.71551389	-3.06301475	0.45059353
C	-1.59230983	-3.62448311	2.41075635
H	-1.32414246	-4.70340538	2.30069518
C	-2.27617502	-3.15855622	3.59907389
H	-2.53835154	-3.87776303	4.41303349
C	-2.62091112	-1.76159275	3.72624350
H	-3.14990163	-1.39183831	4.63829660
C	-2.28975129	-0.82754421	2.67042327
H	-2.56772470	0.24630219	2.77669168
C	-2.20917964	-0.67416000	-1.33074963
C	-1.06230164	2.56040692	1.15452409
H	0.03256336	2.39567780	1.25359547

S26. **2b*** (T_1)



S26.1. General Information

SMILES	:	C[C]1C2(C3([Ir]24(C1(C43C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c5ccccc5)(c6ccccc6)c7ccccc7)C)C
Formula	:	$C_{28}H_{30}IrN_6P^3$
Charge	:	0
Multiplicity	:	3
Dipole	:	11.9615 Debye
Energy	:	-1854.89703287 a.u.
Number of imaginary frequencies	:	0

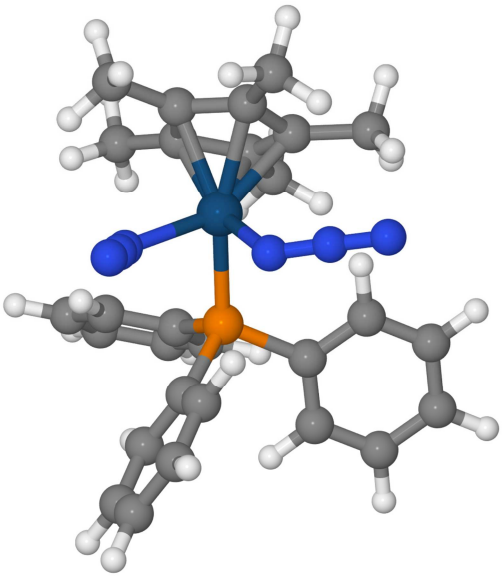
S26.2. Cartesian Co-ordinates (XYZ format)

66

Ir	-1.08893692	-0.20191386	-0.14807233
P	1.25610840	-0.07373987	0.00048327
N	-1.13218963	1.04176688	-2.15176749
N	-0.63022816	2.12488651	-2.17501736
N	-0.14717829	3.18366003	-2.21600771
N	-1.19460368	-2.01510000	-1.19684565
N	-0.33610052	-2.74397922	-1.62445712
N	0.41840491	-3.50147414	-2.05292940
C	3.56742024	0.77426243	-1.54846036
H	4.00289202	1.11974418	-0.58211392
C	1.95204902	-1.67891788	0.68652821
C	3.23966575	-2.20659304	0.25994536
H	3.83364415	-1.66907907	-0.51484185
C	3.74954033	-3.43539810	0.82633424
H	4.73640442	-3.82937336	0.48056281
C	2.98841381	-4.15193844	1.82490170
H	3.38500905	-5.10279989	2.25752020
C	1.70953739	-3.63489676	2.25909853
H	1.11109161	-4.17929077	3.02948523
C	4.33517218	0.91302484	-2.76528406

H	5.35698652	1.36295497	-2.72116494
C	3.78172898	0.47619584	-4.02794886
H	4.37518358	0.58828336	-4.96830225
C	2.45675492	-0.10013775	-4.06969023
H	2.01780343	-0.43226594	-5.04206371
C	1.68278182	-0.24199893	-2.85694265
H	0.65159726	-0.65509987	-2.90427923
C	-3.48753476	0.01565878	0.06112597
C	-3.12509680	1.46000540	0.00748099
C	-2.06724834	1.67646992	1.02347398
C	-1.95350611	0.43038103	1.86795068
C	-2.87806606	-0.58614063	1.28391469
C	-4.50175238	-0.70292252	-0.87820649
H	-5.54441786	-0.60315228	-0.46430621
H	-4.25658798	-1.79378033	-0.96391231
H	-4.48375320	-0.24736649	-1.90318918
C	-3.66643858	2.49724388	-1.01153731
H	-3.86036921	2.01981950	-2.00803113
H	-2.94342804	3.34286070	-1.15086544
H	-4.63813162	2.92590094	-0.63226116
C	-1.44935405	3.05972576	1.39140034
H	-2.18831015	3.62922835	2.02383113
H	-1.22956598	3.66312551	0.47250259
H	-0.50280368	2.93970394	1.97498500
C	-1.23385108	0.34921902	3.24940634
H	-1.88279247	0.83465010	4.03217363
H	-0.24841677	0.88183266	3.22600675
H	-1.05990350	-0.71634412	3.55402660
C	-3.15980506	-2.01914167	1.82910287
H	-2.33018064	-2.36700225	2.49924326
H	-3.27522540	-2.75237417	0.98852015
H	-4.11464071	-2.00906539	2.42659187
C	1.96230626	1.23821068	1.13974202
C	1.90290594	2.63662839	0.73331267
H	1.45225728	2.91381860	-0.24995372
C	2.43831658	3.66746569	1.59206986
H	2.39442348	4.73413324	1.26221430
C	3.01922297	3.32349062	2.87255454
H	3.42789388	4.12403965	3.53644729
C	3.07189775	1.94037068	3.28692985
H	3.52256894	1.66225195	4.27082539
C	2.55387855	0.89926422	2.42448187
H	2.61412287	-0.16560522	2.74787235
C	2.22961736	0.19491187	-1.58157337
C	1.19322813	-2.41030645	1.69082129
H	0.20602901	-2.01965880	2.02876067

S27. **2c** (S_0)



S27.1. General Information

SMILES	:	CC12C3([Ir]145(C2(C4(C53C)C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c6ccccc6)(c7ccccc7)c8ccccc8)C
Formula	:	$C_{28}H_{30}IrN_6P$
Charge	:	0
Multiplicity	:	1
Dipole	:	15.2574 Debye
Energy	:	-1854.96193790 a.u.
Number of imaginary frequencies	:	0

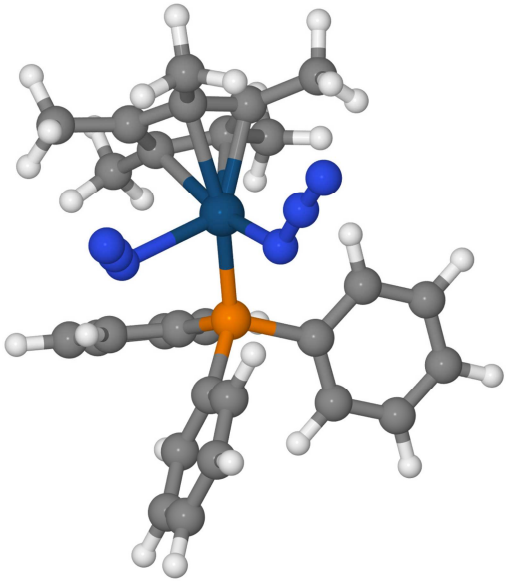
S27.2. Cartesian Co-ordinates (XYZ format)

66

Ir	-1.20930731	0.01133765	-0.28335929
P	1.17517972	-0.02649329	-0.04930371
N	-0.82636440	-0.87955725	-2.22698307
N	-1.22720706	-1.98524332	-2.47092223
N	-1.58375025	-3.04002666	-2.77637219
N	-1.27611244	-2.02345324	0.46544117
N	-1.60235143	-2.28178954	1.58951890
N	-1.91421974	-2.59995961	2.65800571
C	3.33721805	-1.20986140	-1.61585522
H	3.73920560	-0.17779870	-1.73711050
C	1.84820044	-0.13496466	1.69596577
C	3.27675486	-0.29691881	1.94059265
H	3.98760796	-0.35525289	1.08229125
C	3.78034425	-0.38387129	3.29101729
H	4.87821054	-0.50190324	3.46199226
C	2.86810160	-0.32760313	4.41429567
H	3.26124310	-0.40179914	5.45765018
C	1.44969416	-0.18652472	4.18169880
H	0.73604655	-0.15622745	5.04055166
C	4.06481314	-2.32421446	-2.18492532

H	5.02025938	-2.13074732	-2.73175192
C	3.56224513	-3.67147088	-2.04645801
H	4.12635899	-4.52943659	-2.48799038
C	2.32310271	-3.90168524	-1.33620262
H	1.92071521	-4.93915796	-1.23017275
C	1.58751452	-2.79644942	-0.76582634
H	0.62513047	-2.97194934	-0.23159483
C	-3.40076137	0.43333620	0.16219056
C	-3.06328154	1.02530861	-1.14517450
C	-1.94543505	2.01688099	-0.94901919
C	-1.66332734	2.08334684	0.52198553
C	-2.52037597	1.07674265	1.21089494
C	-4.49088669	-0.64277238	0.44985539
H	-5.44799423	-0.12668382	0.74111223
H	-4.17861652	-1.30999053	1.29491401
H	-4.68529367	-1.27138865	-0.45741400
C	-3.70530224	0.67729938	-2.51964831
H	-4.26287127	-0.29359463	-2.46932030
H	-2.91799212	0.60815203	-3.31390548
H	-4.42919779	1.49475741	-2.79286289
C	-1.41942167	2.98768830	-2.04725003
H	-2.15774345	3.82853603	-2.17741609
H	-1.31182861	2.45489359	-3.02861118
H	-0.42669782	3.42040920	-1.76529288
C	-0.70541000	3.09702921	1.21612823
H	-1.28906643	4.03463268	1.43498921
H	0.15722252	3.35763431	0.55241936
H	-0.30935979	2.68945718	2.18198800
C	-2.69929600	0.88376844	2.74768019
H	-1.87624037	1.38794208	3.31760049
H	-2.72809458	-0.20224185	3.02777624
H	-3.67522097	1.35426462	3.05442500
C	1.98154104	1.49182117	-0.78994203
C	1.80244672	1.72751009	-2.21745348
H	1.20865428	1.00293601	-2.82401037
C	2.39518380	2.88358116	-2.84736586
H	2.25800657	3.04388380	-3.94450998
C	3.15063763	3.83499861	-2.05922484
H	3.60214329	4.73342419	-2.54661059
C	3.31909704	3.61788058	-0.64101583
H	3.89893126	4.34665871	-0.02377022
C	2.74601650	2.44859457	-0.00691647
H	2.89249015	2.28610873	1.08582437
C	2.08761072	-1.43506634	-0.90273207
C	0.94304228	-0.09223219	2.82939267
H	-0.14975163	0.00055949	2.64655590

S28. **2c*** (T_1)



S28.1. General Information

SMILES	:	C[C]1C2(C3([Ir]24(C1(C43C)C)(N=[N+]=[N-])(N=[N+]=[N-])[P](c5ccccc5)(c6ccccc6)c7ccccc7)C)C
Formula	:	$C_{28}H_{30}IrN_6P^3$
Charge	:	0
Multiplicity	:	3
Dipole	:	15.2574 Debye
Energy	:	-1854.89977369 a.u.
Number of imaginary frequencies	:	0

S28.2. Cartesian Co-ordinates (XYZ format)

66

Ir	-1.09916377	-0.33473596	-0.05769635
P	1.27356517	-0.17635517	0.01218292
N	-0.81412739	1.27950585	-1.81238174
N	-1.44490290	1.01431489	-2.79273891
N	-2.05427742	0.77564639	-3.75517488
N	-0.97593307	-1.94038606	-1.40225291
N	-1.91859150	-2.59847689	-1.76312029
N	-2.76695132	-3.27720690	-2.14860368
C	3.41785145	0.68337095	-1.77003264
H	3.79297304	1.30420518	-0.92429334
C	2.08835196	-1.62769997	0.88264018
C	3.51725793	-1.87516606	0.73261088
H	4.13149118	-1.21214676	0.07880023
C	4.14684248	-2.98072767	1.41610742
H	5.24305391	-3.15397382	1.28600943
C	3.36246729	-3.86079955	2.25506282
H	3.85082173	-4.71900368	2.77822900
C	1.94493341	-3.62820148	2.40924764
H	1.32789207	-4.30437517	3.04964304

C	4.14826727	0.67192423	-3.01918769
H	5.08002853	1.28183973	-3.11358047
C	3.67689061	-0.11982881	-4.13211775
H	4.24207163	-0.12485405	-5.09637213
C	2.46917582	-0.90331596	-3.99083376
H	2.09390950	-1.51544213	-4.84753036
C	1.73012054	-0.89635438	-2.74889398
H	0.79668897	-1.49526095	-2.64280748
C	-3.47647524	0.08847374	0.07910634
C	-2.96240807	1.46982765	0.27516520
C	-1.94783843	1.40236807	1.35860932
C	-2.00840926	0.03878336	1.99144638
C	-2.98054671	-0.77353537	1.19930792
C	-4.54170752	-0.33929938	-0.97699547
H	-5.57251835	-0.17556119	-0.55347162
H	-4.44000196	-1.42432940	-1.23941541
H	-4.43978548	0.26831988	-1.91366327
C	-3.31804371	2.71996832	-0.57205206
H	-3.61405039	2.43480706	-1.61600757
H	-2.44933915	3.42658472	-0.62391818
H	-4.18759871	3.26100373	-0.09942330
C	-1.22387409	2.63666749	1.97280967
H	-1.94493699	3.17035103	2.65517426
H	-0.89541811	3.35227990	1.17618823
H	-0.32858375	2.33105850	2.57103610
C	-1.36864996	-0.34556982	3.36114383
H	-2.01722121	0.04705162	4.19479895
H	-0.34578478	0.10056210	3.47006750
H	-1.29079640	-1.45847690	3.47560930
C	-3.44233656	-2.23222160	1.50179791
H	-2.66274929	-2.78708816	2.08692932
H	-3.65052271	-2.79559755	0.55441296
H	-4.38984585	-2.20702338	2.11064053
C	1.90005600	1.32915652	0.92696148
C	1.74825537	2.64271951	0.31407106
H	1.28726387	2.72754097	-0.69805908
C	2.19685769	3.82659817	1.00891471
H	2.08724475	4.82566309	0.52073449
C	2.77347517	3.72089410	2.33257151
H	3.11471033	4.63907623	2.87032509
C	2.90716004	2.42389441	2.95596242
H	3.35185122	2.33197546	3.97688937
C	2.48009920	1.23024094	2.25664449
H	2.60507989	0.23236865	2.73805785
C	2.19764066	-0.09898324	-1.62374616
C	1.31074655	-2.51980495	1.72869146
H	0.21589904	-2.35788465	1.85494339