Electronic Supplementary Information

Synthesis and Reactivity at the Ir-^{Me}Tpm Platform: From κ^1-*N* Coordination to κ^3 –N-based Organometallic Chemistry.

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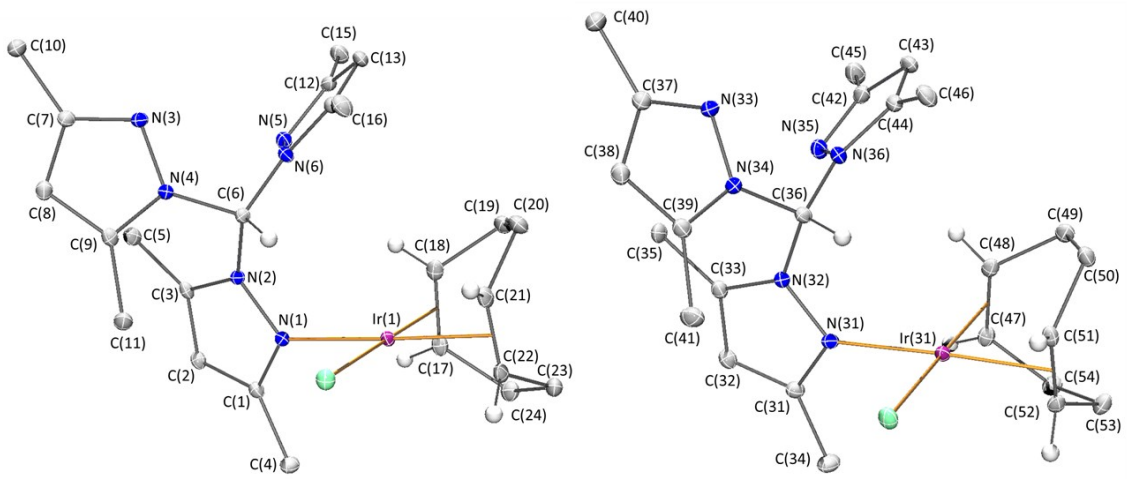


Figure S1. Molecular structure of both independent molecules of complex **1**. For clarity most of hydrogen atoms have been excluded.

Table S1. Dihedral angles (°) between pyrazole rings for complex **1**.

		Molecule 1					Molecule 2		
		PL(1)	PL(2)	PL(3)			PL(31)	PL(32)	PL(33)
Molec 1	PL(1)	-	71.90(10)	66.22(1)	Molec 2	PL(31)	-	74.72(11)	73.66(11)
	PL(2)		-	87.16(10)		PL(32)		-	88.19(11)
	PL(3)			-		PL(33)			-

Plane's definition: PL(1): N(1)-N(2)-C(1)-C(2)-C(3), PL(2): N(3)-N(4)-C(7)-C(8)-C(9), PL(3): N(5)-N(6)-C(12)-C(13)-C(14), PL(31): N(31)-N(32)-C(31)-C(32)-C(33), PL(32): N(33)-N(34)-C(37)-C(38)-C(39), PL(33): N(35)-N(36)-C(42)-C(43)-C(44).

Table S2. Ring puckering parameters (Å, °) for complexes **2·OTf**, **3·OTf**, and **4·OTf**.

	2·OTf	**3·OTf**	**4·OTf**
Ir-N(1)-N(2)-C(6)-N(4)-N(3)			
q_T	0.920(7)	0.9111(19)	0.9748(19)
φ	-179.25(11)	-8.00(13)	-2.30(12)
θ	99.93(14)	81.70(12)	79.58(11)
conf	$B_{4,1}$	$^{1,4}B$	$^{1,4}B$
Ir-N(5)-N(6)-C(6)-N(4)-N(3)			
q_T		0.828(6)	0.756(3)
φ		-179.30(13)	177.70(16)
θ		91.87(13)	89.25(14)
conf		$B_{4,1}$	$B_{4,1}$
Ir-N(1)-N(2)-C(6)-N(6)-N(5)			
q_T		0.978(9)	0.977(2)
φ		179.53(11)	176.17(11)
θ		101.90(15)	100.73(12)
conf		$B_{4,1}$	$B_{4,1}$

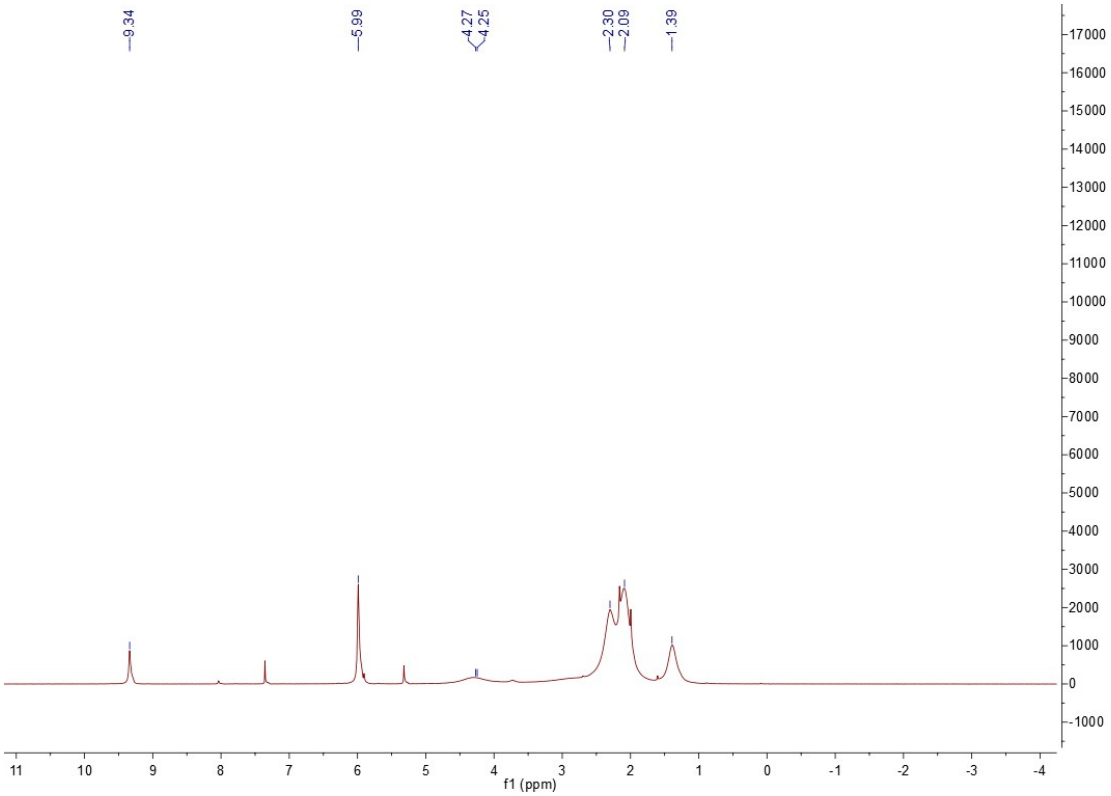


Figure S2. ^{1}H NMR spectrum of complex **1** in CD_2Cl_2 at 298 K

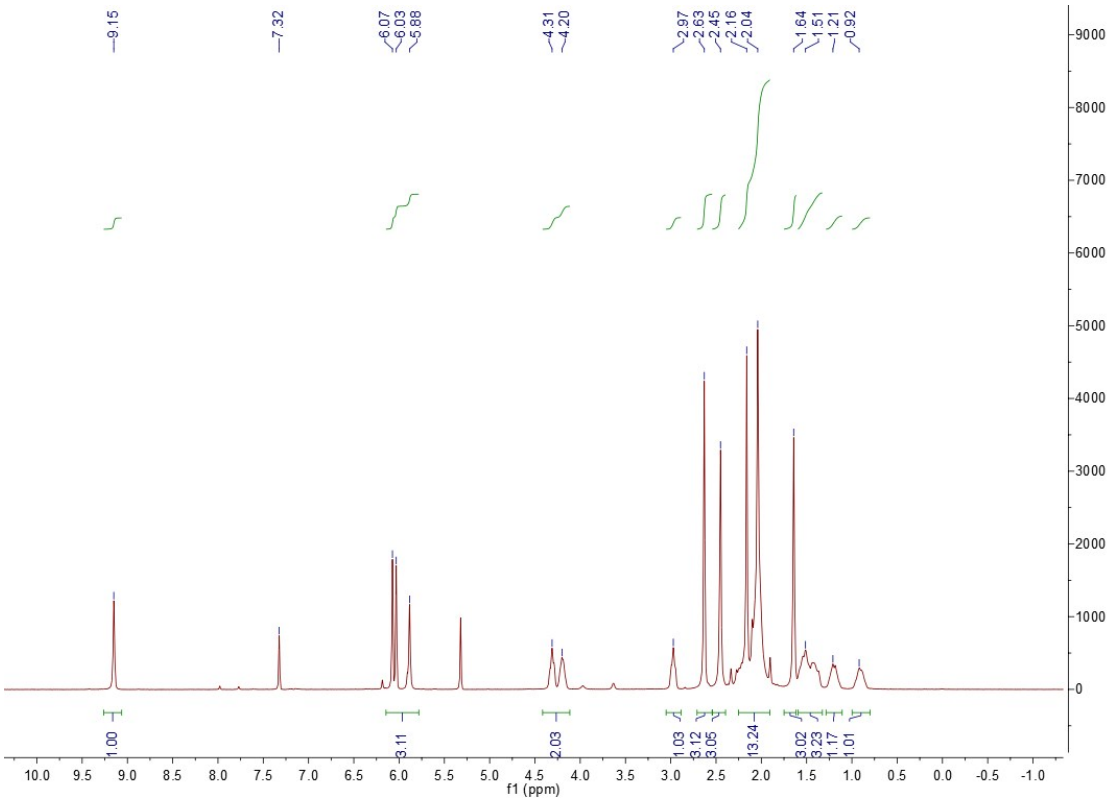


Figure S3. ^{1}H NMR spectrum of complex **1** in CD_2Cl_2 at 193 K

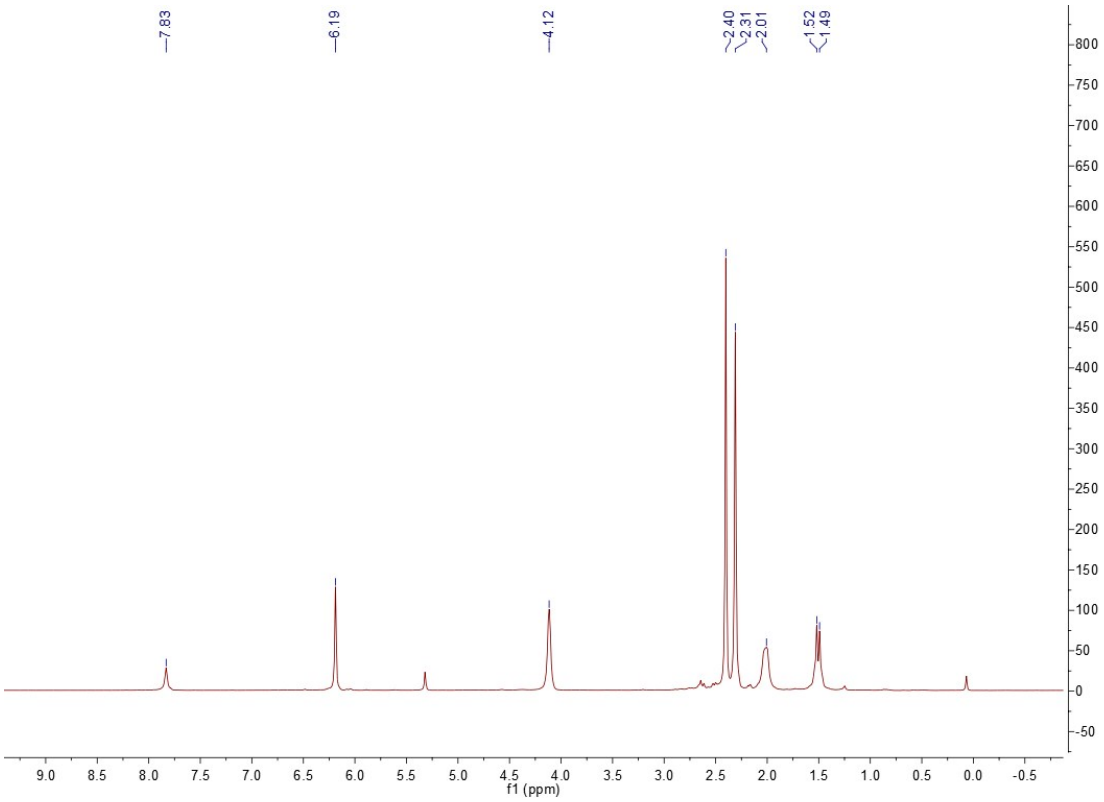


Figure S4. ^{1}H NMR Spectrum of complex **2.OTf** in CD_2Cl_2 at 298 K

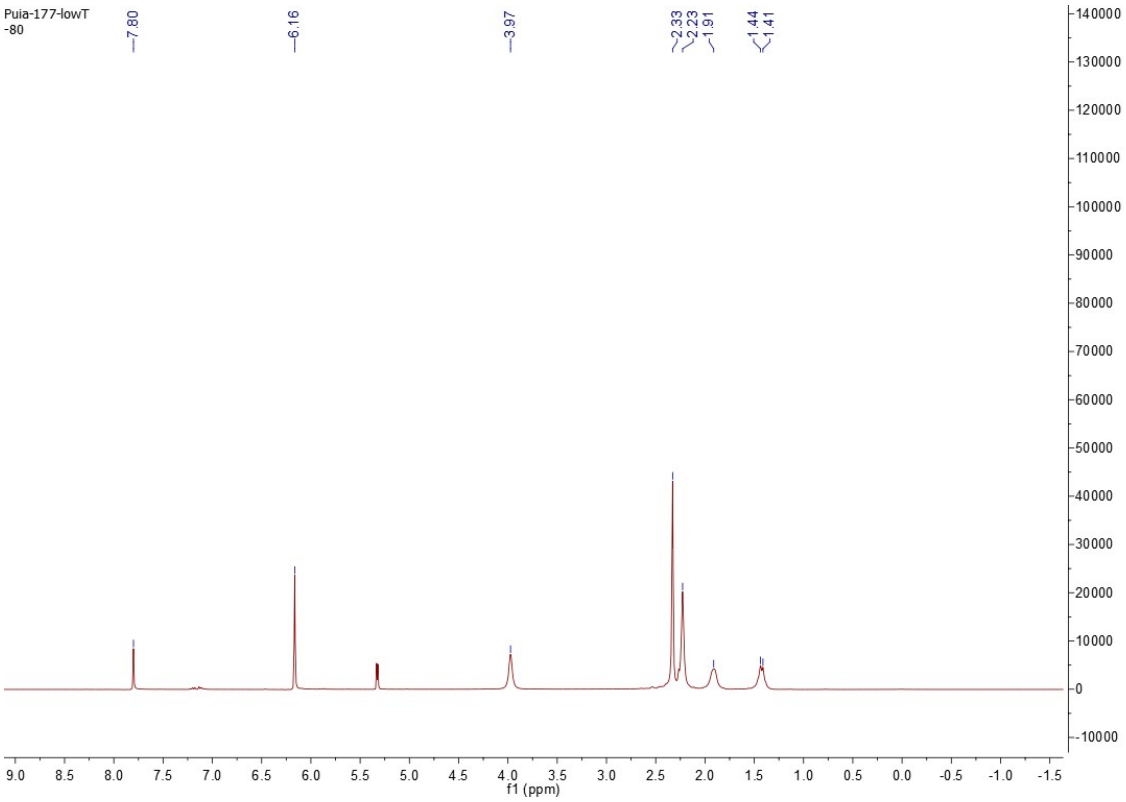


Figure S5. ^{1}H NMR spectrum of complex **2.OTf** in CD_2Cl_2 at 193 K

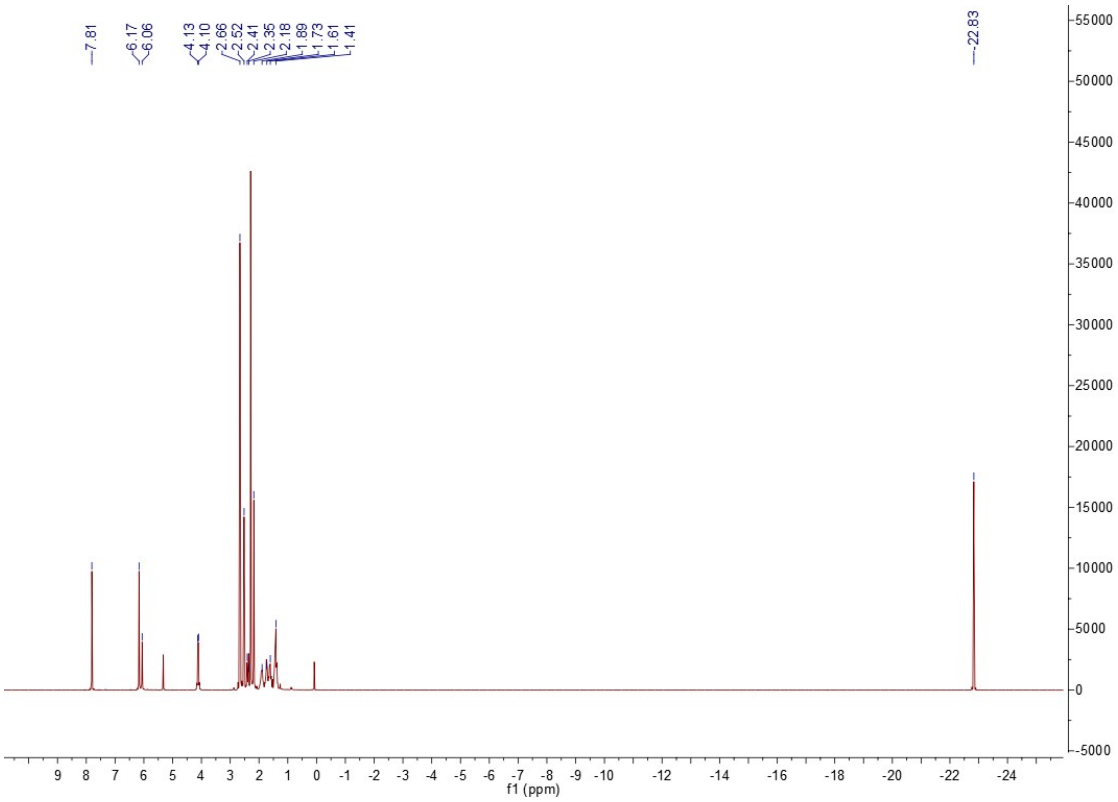


Figure S6. ^{1}H NMR spectrum of complex **3.OTf** in CD_2Cl_2 at 298

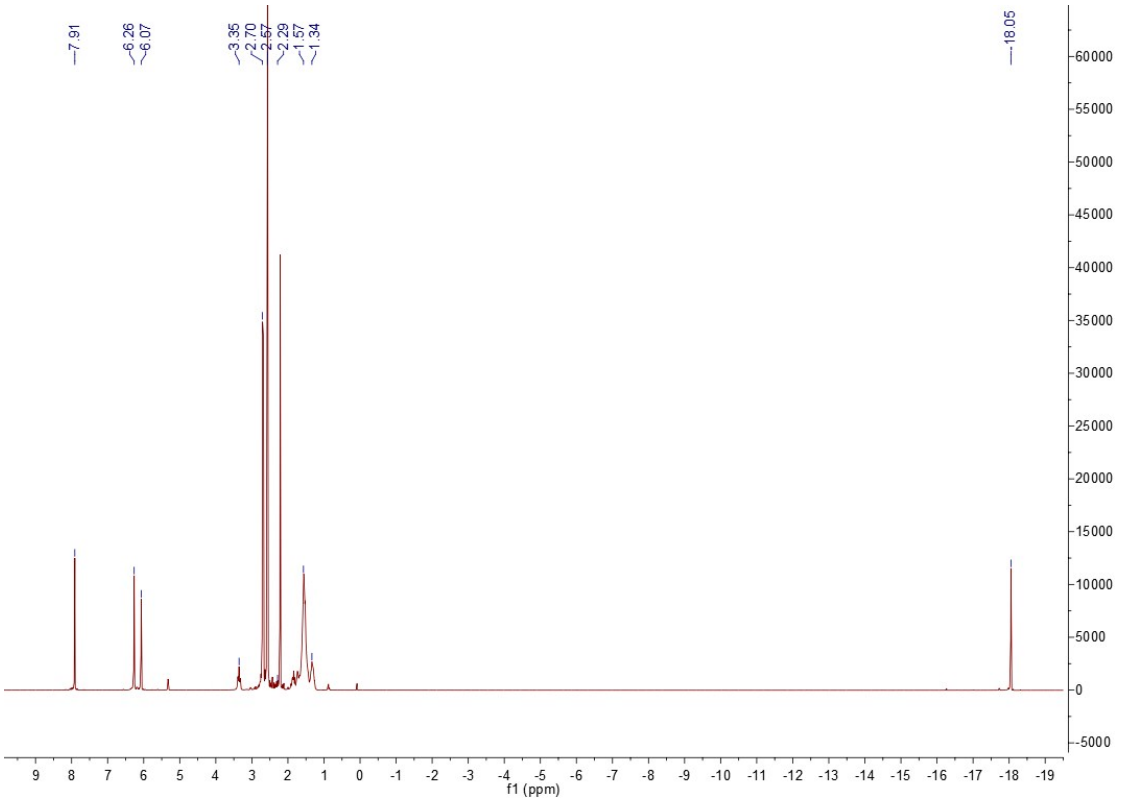


Figure S7. ^{1}H NMR spectrum of complex **4.OTf** in CD_2Cl_2 at 298

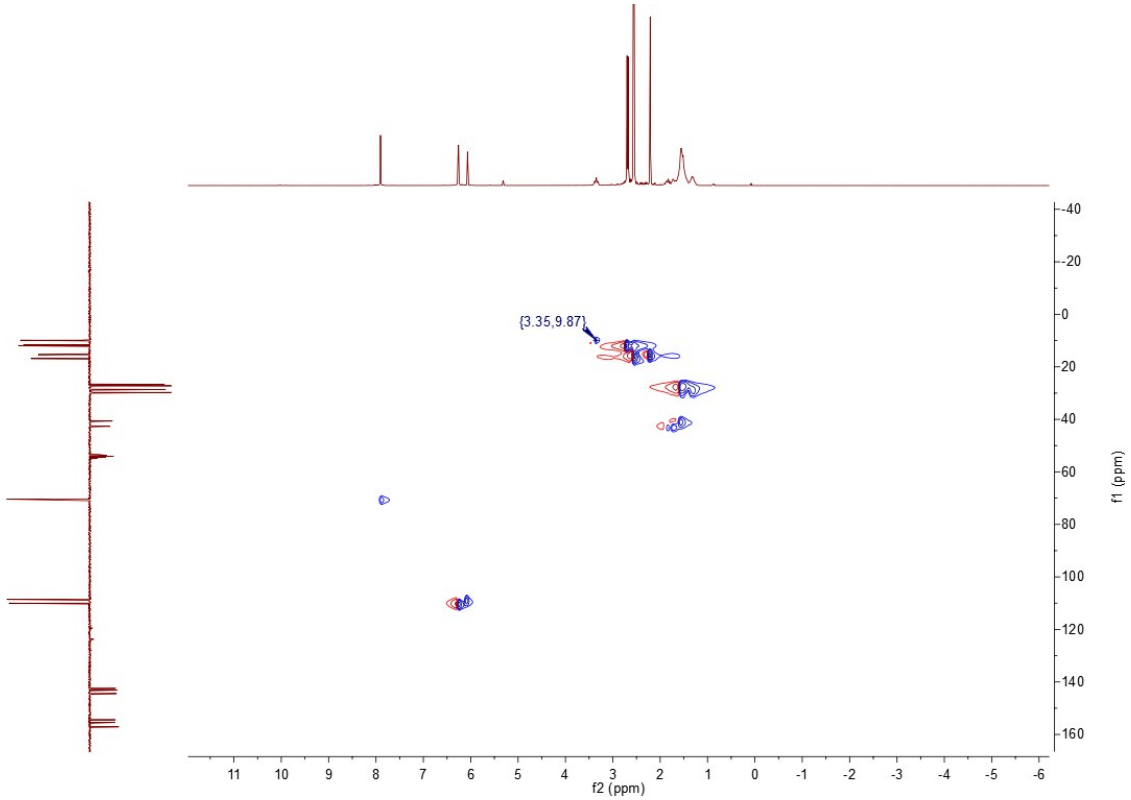


Figure S8. ^{1}H-^{13}C(APT) HSQC NMR spectrum of complex **4.OTf** in CD_2Cl_2 at 298 K

Computational Details

All DFT theoretical calculations were carried out using the Gaussian program package.[1] The B3LYP method,[2] including the D3 dispersion correction scheme developed by Grimme[3] with Becke Johnson damping, has been used for both energies and gradient calculations. All atoms were treated with the def2-SVP basis set[4] together with the corresponding core potential for Ir for geometry optimizations. Energies were further refined by single point calculations using the def2-TZVP basis set. The "ultrafine" grid was employed in all calculations. All reported energies are Gibbs free energies referred to a 1 atm standard state at 298.15 K removing the contribution to the translational entropy, as indicated by Morokuma et al.[5] The nature of the stationary points was confirmed by analytical frequency analysis, and transition states were characterized by a single imaginary frequency corresponding to the expected motion of the atoms.

[1] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[2] a) C. Lee, W. Yang, R. G. Parr, Phys. Rev. B 1988, 37, 785–789; b) A. D. Becke, J. Chem. Phys. 1993, 98, 1372–1377; c) A. D. Becke, J. Chem. Phys. 1993, 98, 5648–5652.

[3] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, J. Chem. Phys. 2010, 132, 154104.

[4] F. Weigend, R. Ahlrichs, Phys. Chem. Chem. Phys. 2005, 7, 3297–3305.

[5] R. Tanaka, M. Yamashita, L. W. Chung, K. Morokuma, K. Nozaki, Organometallics, 2011, 30, 6742–6750.

Table S3. Energetic values for DFT (B3LYP-D3) calculated structures. Geometrical optimizations using the def2-SVP, E(DZ), basis set and single point energies with def2-TZVP basis set, E(TZ). Corrections to the Gibbs free energy at 298.15 K and 1 atm. All absolute energies in a.u. Gibbs free energies relative to **A** and isolated molecules in kcal mol^{-1} considering triple-Z corrections.

	E(DZ)	E(TZ)	Gcorr	ΔG(TZ)
A	-2141.58967	-2143.45840	0.70292	0
B	-1828.49073	-1830.02218	0.50981	4.2
TSBC	-1828.47641	-1830.00867	0.50949	12.5
C	-1828.49943	-1830.03207	0.50812	-3.0
TSCD	-1828.45881	-1829.99719	0.50404	16.3
D	-1828.48093	-1830.01781	0.50690	5.2
E	-1827.31430	-1828.84595	0.48971	-11.5
F	-1829.69232	-1831.22934	0.52508	-2.5
TSFG	-1829.69222	-1831.22951	0.52648	-1.7
G	-1829.69265	-1831.23046	0.52535	-3.0
TSGH	-1829.67950	-1831.21622	0.52512	5.8
H	-1829.68001	-1831.21630	0.52649	6.6
TSHI	-1829.66379	-1831.19724	0.52900	20.1
I	-314.30122	-314.64105	0.19487	-18.0
H_2	-1.17393	-1.17961	-0.00159	
COE	-313.06728	-313.40708	0.17074	

Figure S9. DFT calculated Gibbs free energy profile (in kcal mol^{-1}, respect to **A**), for the alternative allylic C-H bond oxidative addition.

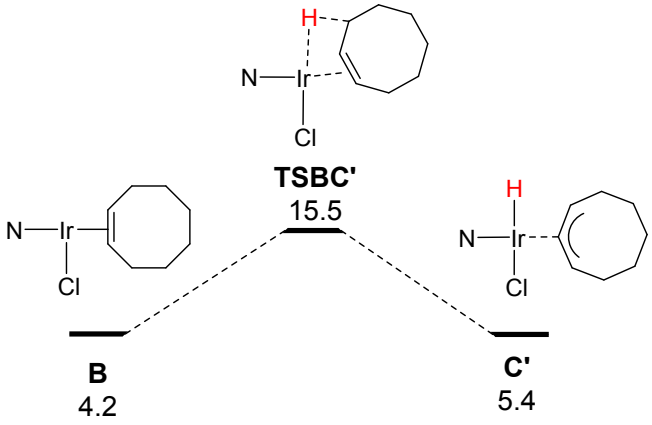


Figure S10. DFT optimized structure of **3·OTf** complex.

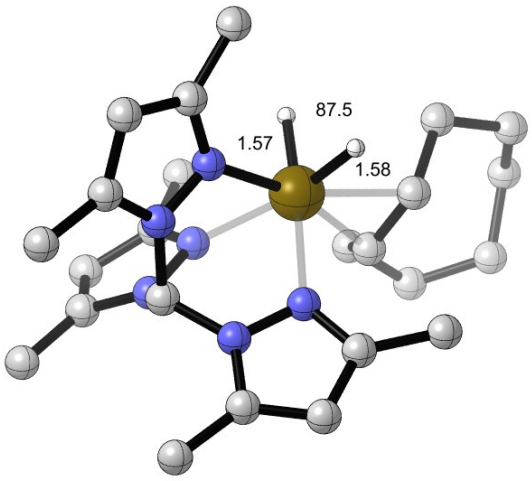


Figure S11. IR spectrum obtained from DFT calculated frequencies for **3.OTf** complex:

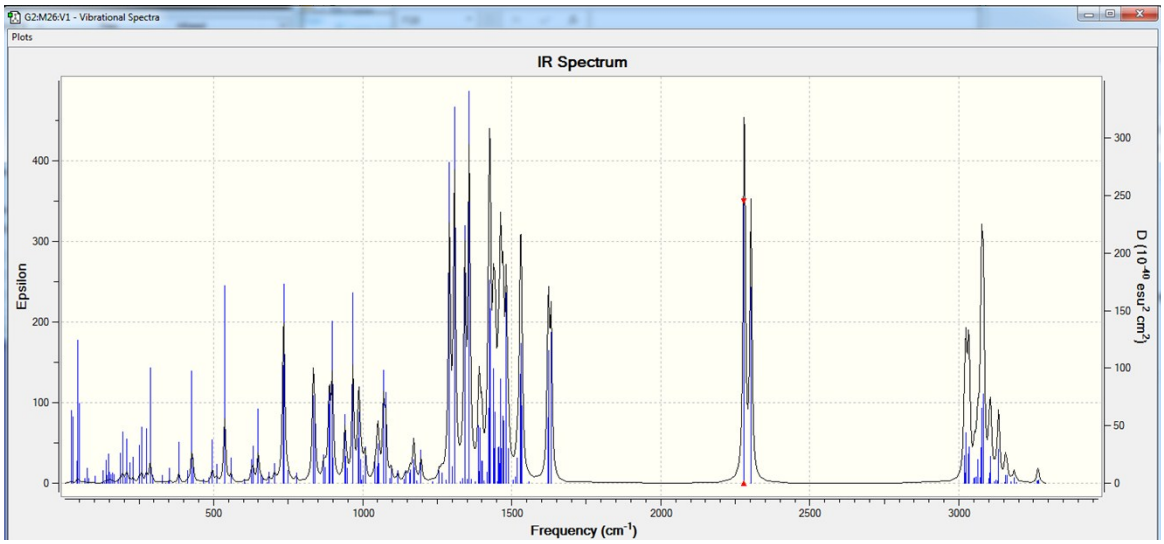


Figure S12. IR spectrum obtained for **3.OTf** complex:

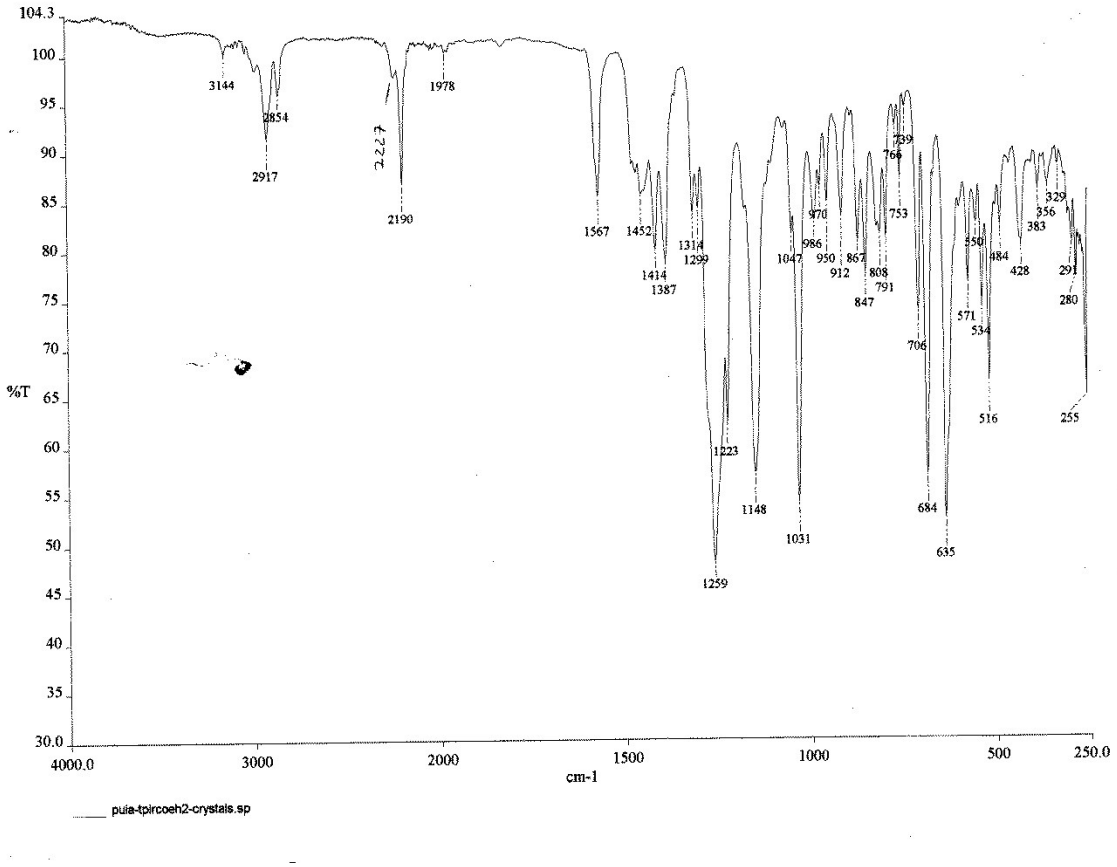
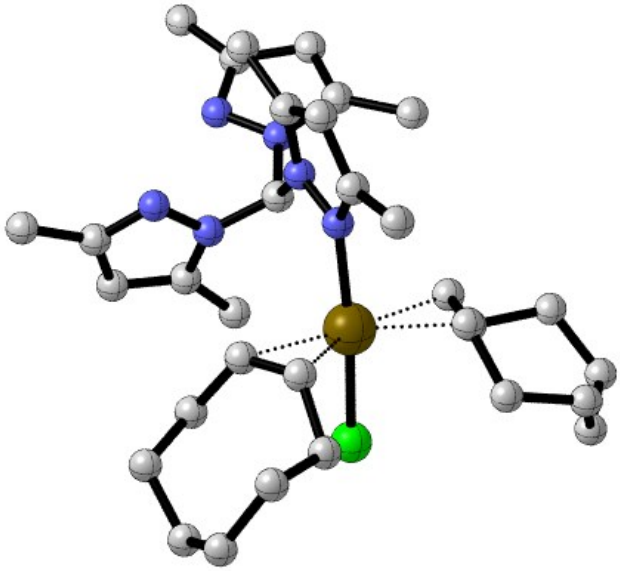


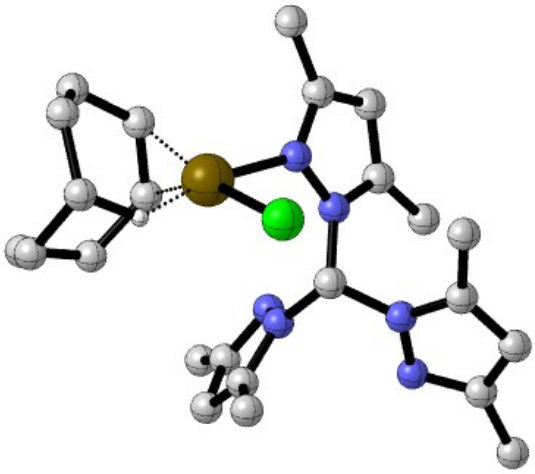
Table S4. Infrared bands (cm^{-1}) associated to Iridium hydride vibrational modes obtained from DFT calculations of **3.OTf** (scaling factor of 0.964).

Vibrational mode	frequency	scaled frequency	Experimental values	description
1	2280.0	2197.9	2190	Ir-H1, Ir-H2 asymmetric stretching
2	2302.4	2219.5	2227	Ir-H1, Ir-H2 symmetric stretching

Figure S13. Geometrical representation for the DFT optimized structures. Only most relevant hydrogen atoms are shown for clarity.



A



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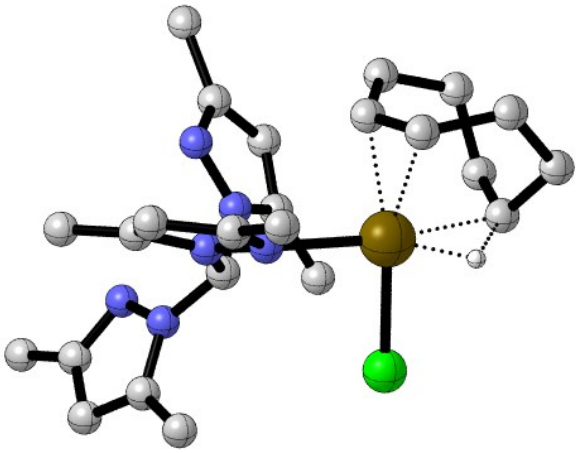
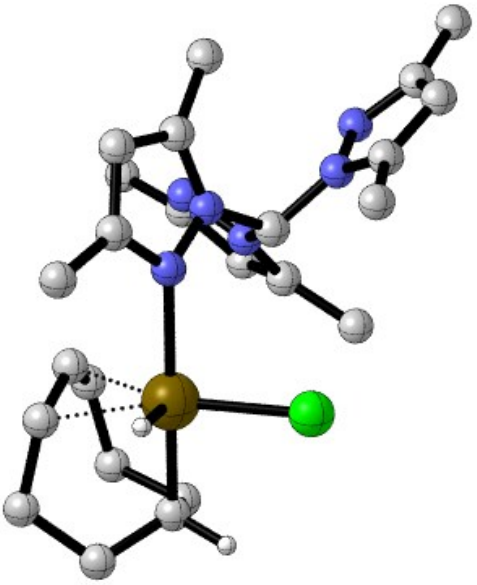
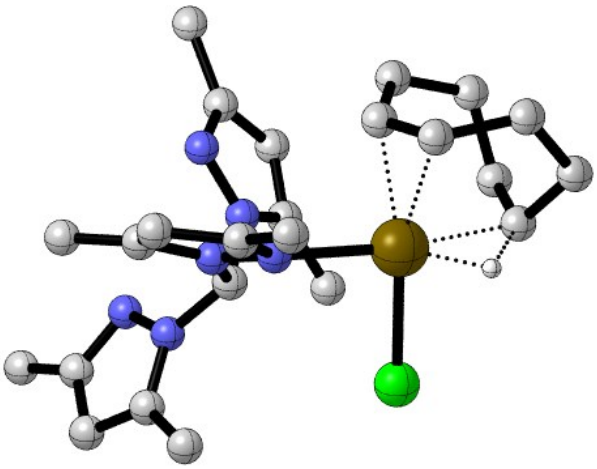


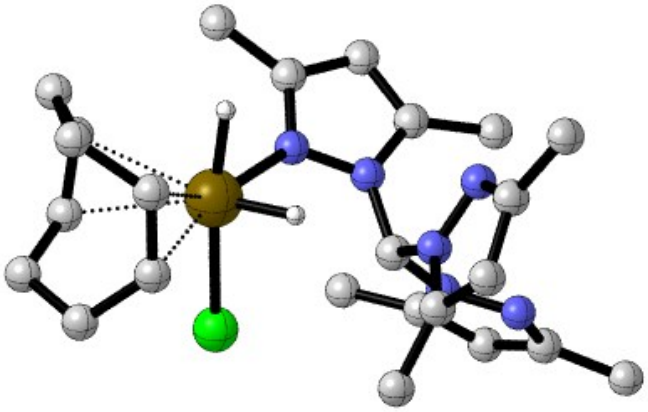
TSBC



C



TSCD



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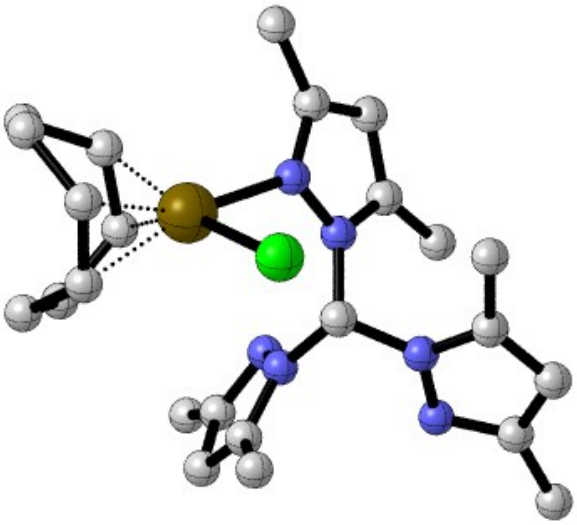

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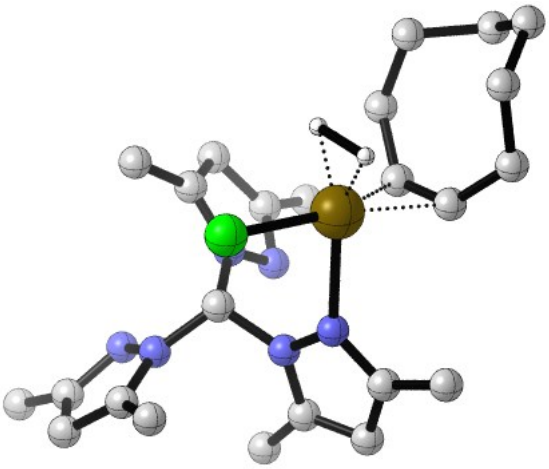

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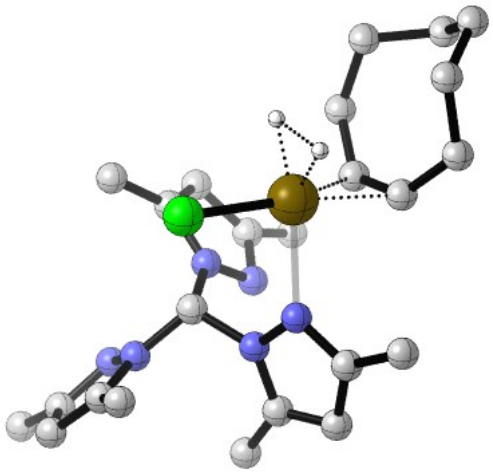
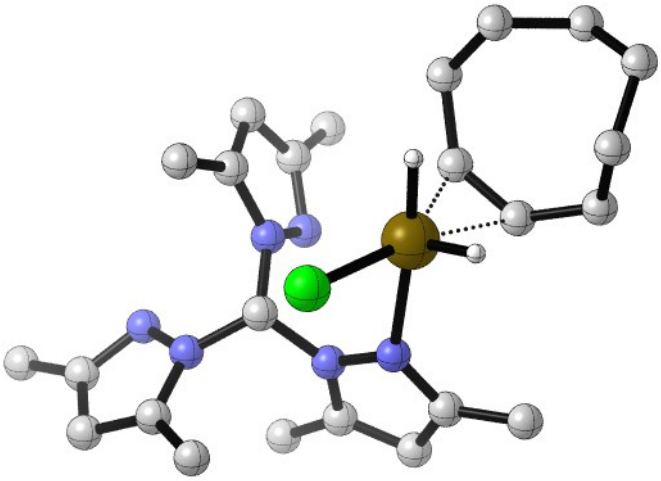


TSFG



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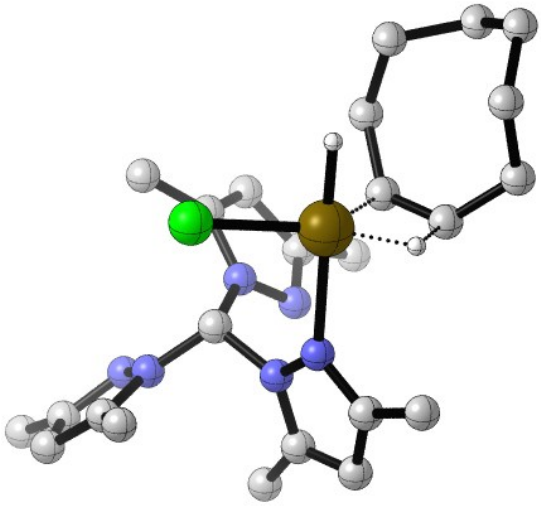

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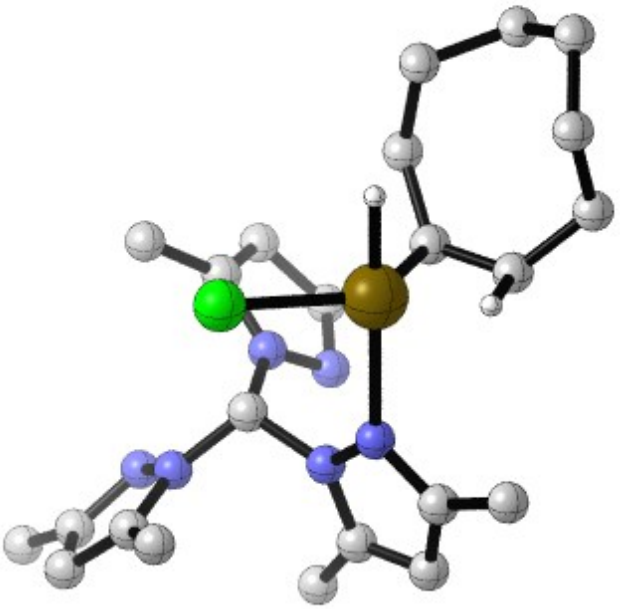

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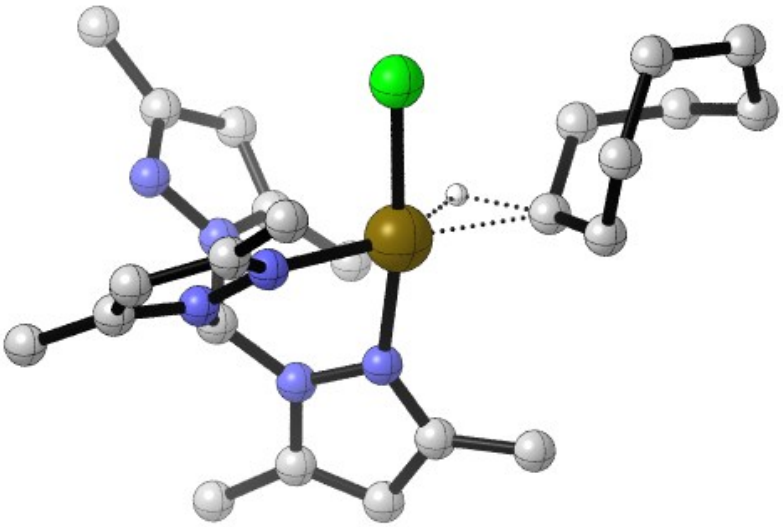

TSHI

Table S5. Cartesian coordinates (in Å) for all calculated structures.

A

77	1.001961	0.137068	0.091547
17	2.253384	0.018381	-1.941266
7	-0.356568	0.210359	1.648923
7	-1.694974	0.140928	1.345899
7	-2.129522	-1.115993	-0.637821
7	-2.600268	-2.165168	0.076679
7	-3.375155	0.865607	-0.212291
7	-4.455864	0.176838	-0.642533
6	-0.271154	0.163444	2.985164
6	-1.568020	0.029005	3.532777
6	-2.456100	-0.001818	2.472423
6	1.012264	0.252976	3.745704
1	1.156408	-0.644735	4.367283
1	0.991145	1.120483	4.424440
1	1.870126	0.354713	3.074102
6	-3.935520	-0.182573	2.478573
1	-4.467072	0.735385	2.183611
1	-4.255386	-0.454181	3.493448
1	-4.223295	-0.979770	1.779515
6	-2.095362	0.188884	-0.049000
6	-1.998221	-1.392670	-1.975674
6	-2.381034	-2.712340	-2.110751
6	-2.740089	-3.148976	-0.801831
6	-1.484686	-0.397638	-2.959645
1	-2.072714	0.534491	-2.940681
1	-1.548888	-0.813531	-3.973639
1	-0.426378	-0.149197	-2.765429
6	-3.193913	-4.507237	-0.372455
1	-3.454031	-4.496284	0.694874
1	-2.402933	-5.259158	-0.529249
1	-4.075690	-4.832670	-0.947369
6	-3.654383	2.188552	0.033488
6	-4.999919	2.337468	-0.250166
6	-5.449999	1.053793	-0.673602
6	-2.642388	3.180287	0.497070
1	-2.148400	2.863168	1.428605
1	-3.130491	4.146580	0.679127
1	-1.854135	3.338361	-0.255513
6	-6.819747	0.644989	-1.114370
1	-6.821515	-0.421850	-1.375994
1	-7.145914	1.222382	-1.994672
1	-7.563403	0.812694	-0.318395
1	-1.824125	-0.051341	4.585997
1	-1.309207	0.772491	-0.557335
1	-2.376262	-3.295026	-3.028825
1	-5.575882	3.257362	-0.176248
6	0.962239	-2.117735	0.266252
6	2.008938	-1.598208	1.048085
6	3.403371	-4.161531	-1.110496
6	3.483001	-1.755822	0.775146
6	4.330271	-4.126326	0.113399
6	3.955386	-3.156846	1.244280
1	1.788998	-1.497748	2.114238
1	3.695130	-1.597410	-0.289346
1	3.581126	-3.267083	-1.730197
1	5.344915	-3.880836	-0.247474
1	0.034888	-2.316199	0.816757
1	3.730935	-5.011477	-1.732803
1	4.027033	-0.966955	1.316542
1	4.404697	-5.140732	0.544547
1	4.822896	-3.058985	1.917802
1	3.159350	-3.609917	1.859404
6	1.099122	-2.949358	-0.995085
1	1.558018	-2.361160	-1.801175
1	0.079643	-3.180321	-1.330496
6	1.883965	-4.277550	-0.859447
1	1.681152	-4.749038	0.118705
1	1.469534	-4.970823	-1.610102
6	1.966870	1.947541	0.803766
6	0.887798	2.302238	-0.055829
6	3.901581	4.057206	-1.112602
6	1.017580	3.044008	-1.369061
6	2.744590	4.992128	-1.494391
6	1.322278	4.543449	-1.123336
1	-0.003237	2.615357	0.500710
1	1.782289	2.578807	-2.003310
1	3.910455	3.190522	-1.793749
1	2.797251	5.145296	-2.586898
1	1.741265	2.039565	1.872128
1	4.835073	4.603328	-1.329575
1	0.072094	2.938262	-1.927942
1	2.917916	5.987073	-1.046363
1	0.611407	5.175829	-1.681791

1 1.137209 4.768858 -0.059102
6 3.446390 2.078616 0.511965
1 3.709047 1.505811 -0.385823
1 3.985537 1.605032 1.348435
6 3.959478 3.529696 0.337900
1 3.431422 4.213212 1.026726
1 5.012373 3.540765 0.663400

B

77 -1.568898 -0.598236 -0.283662
17 -0.721573 -1.657678 -2.277852
7 -0.101207 -1.379380 0.863512
7 1.157038 -0.843921 0.910476
7 1.438279 1.378220 0.072280
7 1.611110 1.872838 1.317598
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3-OTF

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