Electronic Supplementary Material (ESI) for Dalton Transactions.

Non-palindromic (C^C^D) Gold(III) Pincer Complexes are Not Accessible by Intramolecular Oxidative Addition of Biphenylenes – An Experimental and Quantum Chemical Study

Wolfram Feuerstein [ID][a] and Frank Breher *[ID][a]

[a] Dr. W. Feuerstein, Prof. Dr. F. Breher
Institute of Inorganic Chemistry
Division Molecular Chemistry
Karlsruhe Institute of Technology (KIT)
Engesserstr. 15
76131 Karlsruhe, Germany
E-mail: breher@kit.edu

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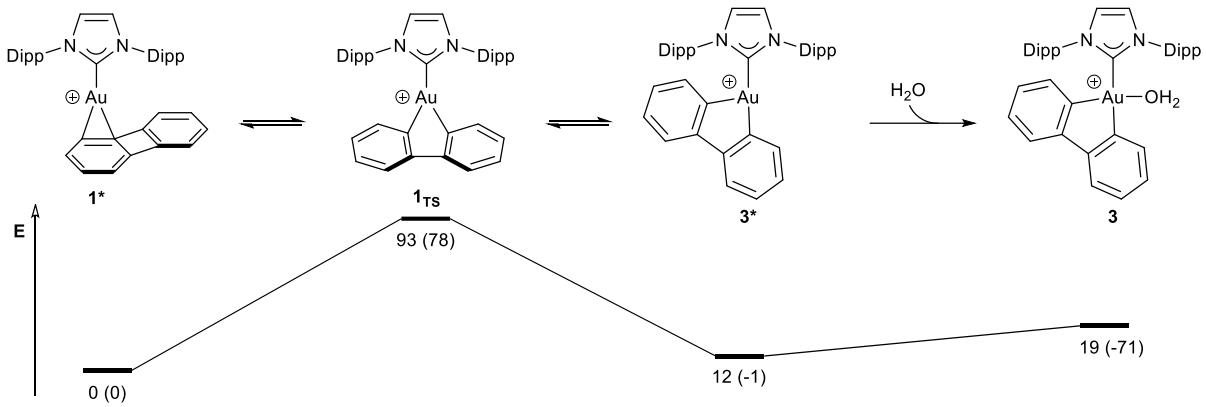
S 1. Oxidative Addition of Biphenylene to [(IPr)Au(I)]+



Oxidative addition of biphenylene (**2**) to $[(IPr)Au(I)]^+$ (**1***) calculated on the RI-TPSSh-D3(BJ)/def2-TZVPP level of theory neglecting the $[SbF_6]^-$ anion. Gibbs free energies (electronic energies in parentheses) are given in kJ mol^{-1} relative to the reactant complex **1***. Solvent effects of CH_2Cl_2 were only considered by single point calculations of gas phase optimized structures by means of the SMD model. Obviously, the incorporation of anion and solvent effects for structure optimizations and not only by means of single point calculations has a large impact on the theoretically predicted reaction outcome. The huge discrepancy between Gibbs free energy and electronic energy upon water coordination underlines the need to include the anion as well as solvent effects for the structure optimizations.

Gibbs free energies (electronic energies) obtained using other functionals are listed in the following table. Again, solvent effects were included by single point calculations of gas phase optimized structures only by means of the SMD model.

Species	Main text[a]	TPSSh	B97D3	BP86	PBE	TPSS	TPSSh/ B2PLYP[b]	B97D3/ B2PLYP[b]	BP86/ B2PLYP[b]	PBE/ B2PLYP[b]	TPSS/ B2PLYP[b]
1_{TS}	88 (82)	93 (78)	73 (74)	79 (70)	70 (72)	78 (72)	93 (79)	78 (78)	87 (78)	76 (79)	85 (79)
3*	10 (-2)	12 (−1)	−12 (−10)	3 (−11)	−1 (−6)	−5 (−10)	11 (−2)	−5 (−2)	11 (−3)	3 (−2)	3 (−2)
3	-37 (-79)	19 (−71)	8 (−67)	11 (−80)	11 (−74)	4 (−79)	22 (−68)	8 (−68)	22 (−69)	17 (−68)	15 (−68)

[a] Energies reported in the main text, i.e. calculations on the RIJCOSX-TPSSh-D3(BJ)/def2-TZVPP level of theory including $[SbF_6]^-$ anion and solvent effects (C-PCM) for structure optimizations as well. [b] Electronic energies obtained on the RI-B2PLYP-D3(BJ)/def2-TZVPP level of theory by single point calculations using the structures obtained applying the indicated functional.

S 2. Additional Solid State Structure

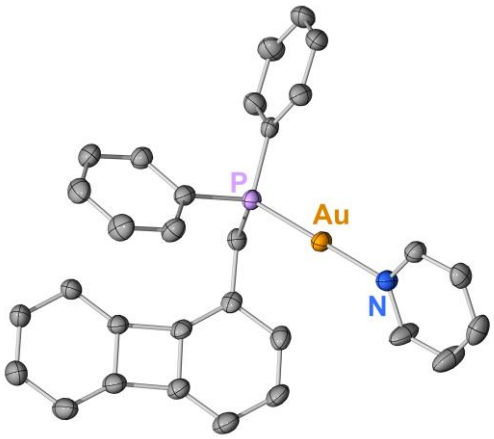


Figure S 1. Molecular structure of **S1** in the solid state. **S1** forms upon chloride abstraction of **19** using $Ag[SbF_6]$ in CH_2Cl_2 in the presence of pyridine. Crystals were grown by layering a solution of **S1** in CH_2Cl_2 with *n*-hexane. Thermal ellipsoids are drawn at the 30 % probability level. Hydrogen atoms and the SbF_6 anion are omitted for clarity. Selected bond lengths (pm) and angles (°): P–Au 224.0(1), Au–N 206.9(5).

S 3. **Crystallographic Details**

Compound	**11**	**19**	**S1**
Empirical Formula	$C_{12}H_7Br$	$C_{25}H_{19}AuClP$	$C_{30}H_{24}AuF_6NPSb$
M	231.09	582.822	862.19
Temperature / K	200	200	200
Crystal system	monoclinic	triclinic	orthorhombic
Space group	$P2_1/n$	P-1	Pbca
a / Å	11.984(2)	8.4150(17)	16.301(3)
b / Å	11.811(2)	11.176(2)	17.737(4)
c / Å	14.110(3)	12.451(3)	20.159(4)
α / °	90	109.57(3)	90
β / °	110.81(3)	106.82(3)	90
γ / °	90	93.89(3)	90
V / Å³	1866.9(7)	1038.4(5)	5829(2)
Z	8	2	8
ρ_{calc} g/cm³	1.644	1.864	1.965
μ /mm^{-1}	4.346	7.298	6.069
Crystal size / mm³	0.4 × 0.35 × 0.35	0.4 × 0.3 × 0.3	0.2 x 0.2 x 0.2
Radiation	Mo K_α (λ = 0.71073)	Mo K_α (λ = 0.71073)	Mo K_α (λ = 0.71073)
$2\theta_{min}$ / °	3.844	3.68	3.95
$2\theta_{max}$ / °	56.558	54	50.694
Reflections collected	17619	12924	75062
Independent Reflections	4641 (R_{int} = 0.0522)	4525 (R_{int} = 0.0309)	5334 (R_{int} = 0.1100)
Data/restraints/parameters	4641/0/235	4525/0/253	5334/0/361
GooF on F²	1.036	1.045	1.111
R_1 [$I \geq 2\sigma(I)$]	0.0355	0.0201	0.0389
wR_2 [$I \geq 2\sigma(I)$]	0.0823	0.0486	0.1010
R_1 (all data)	0.0534	0.0221	0.0446
wR_2 (all data)	0.0938	0.0499	0.1053
Largest diff. peak/holes /e · Å³	0.53 / −0.99	0.75 / −0.97	1.66 / −3.11
Diffractometer	Stoe IPDS II	Stoe IPDS II	Stoe IPDS II
CCDC number	2018371	2018369	2018372

Compound	**20**	**23**
Empirical Formula	$C_{17}H_{14}AuClN_2$	$C_{35}H_{28}AuF_3N_4O_3S$
M	478.733	838.64
Temperature / K	200	200
Crystal system	triclinic	orthorhombic
Space group	P-1	$P2_12_12_1$
a / Å	8.5300(17)	8.0660(16)
b / Å	9.0320(18)	19.896(4)
c / Å	10.772(2)	20.237(4)
α / °	83.91(3)	90
β / °	67.45(3)	90
γ / °	88.61(3)	90
V / Å³	762.0(3)	3247.7(11)
Z	2	4
ρ_{calc} g/cm³	2.086	1.715
μ /mm^{-1}	9.822	4.653
Crystal size / mm³	0.4 × 0.3 × 0.3	0.25 × 0.1 × 0.1
Radiation	Mo K_α (λ = 0.71073)	Mo K_α (λ = 0.71073)
$2\theta_{min}$ / °	4.12	2.87
$2\theta_{max}$ / °	50.7	56.562
Reflections collected	10302	59026
Independent Reflections	2783 (R_{int} = 0.0517)	8060 (R_{int} = 0.0948)
Data/restraints/parameters	2783/0/191	8060/0/427
GooF on F²	1.045	1.194
R_1 [$I \geq 2\sigma(I)$]	0.0239	0.0436
wR_2 [$I \geq 2\sigma(I)$]	0.0595	0.0983
R_1 (all data)	0.0243	0.0523
wR_2 (all data)	0.0597	0.1105
Largest diff. peak/holes /e · Å³	0.71 / −1.66	1.65 / −1.48
Diffractometer	Stoe IPDS II	Stoe IPDS II
CCDC number	2018370	2018373

S 4. **NMR spectra**

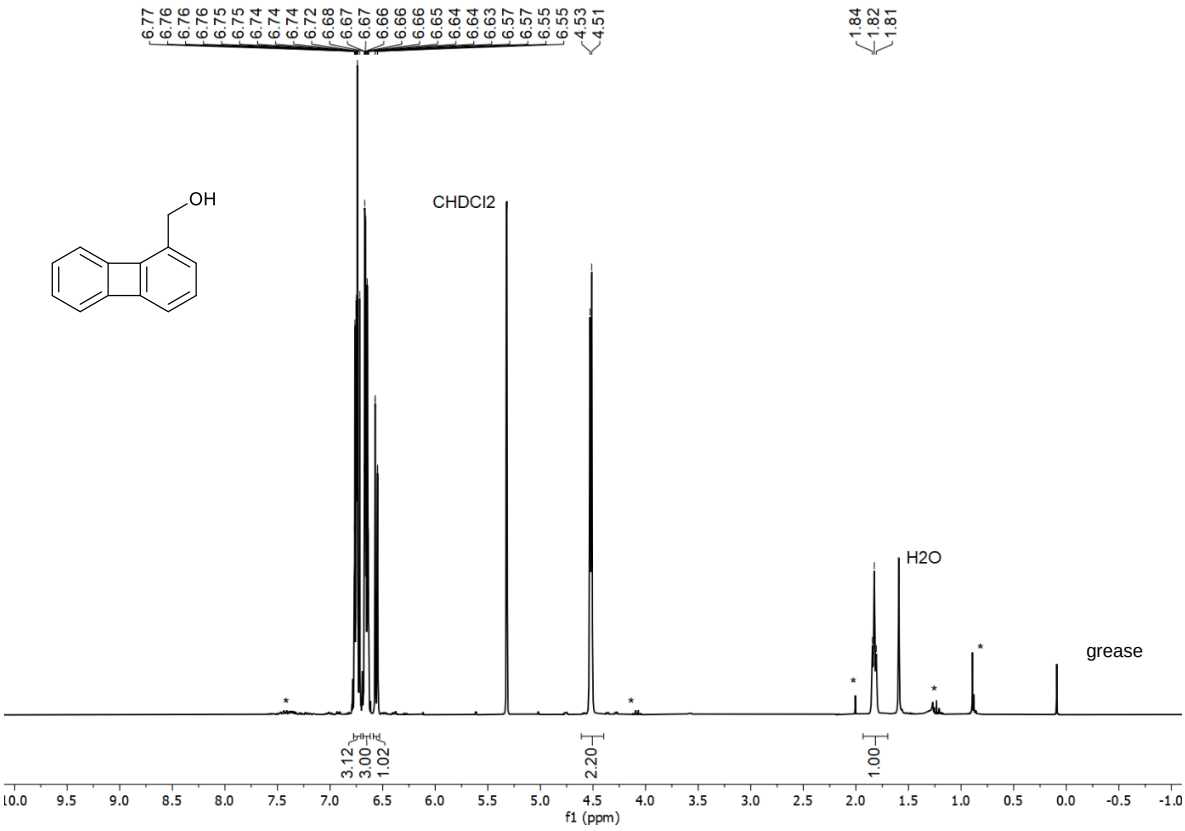


Figure S 2. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of **13**. Impurities are marked with an asterisk.

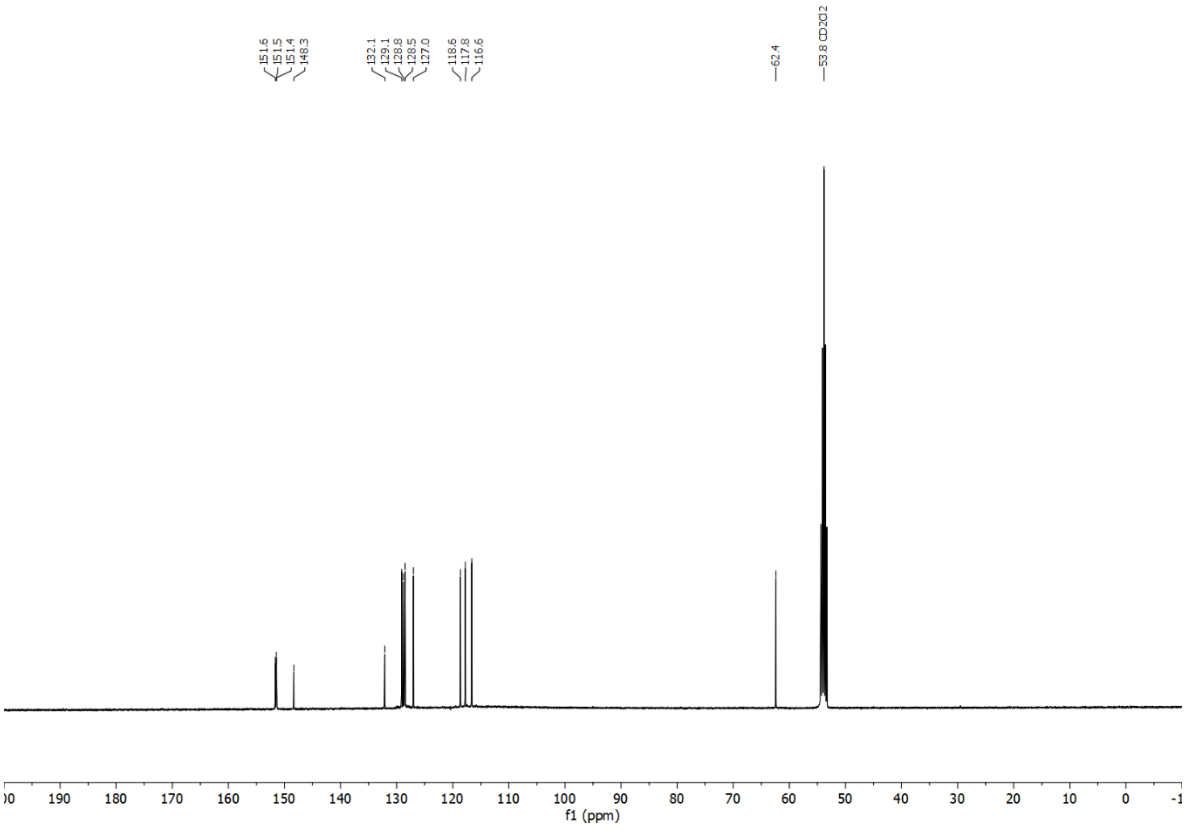


Figure S 3. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of **13**.

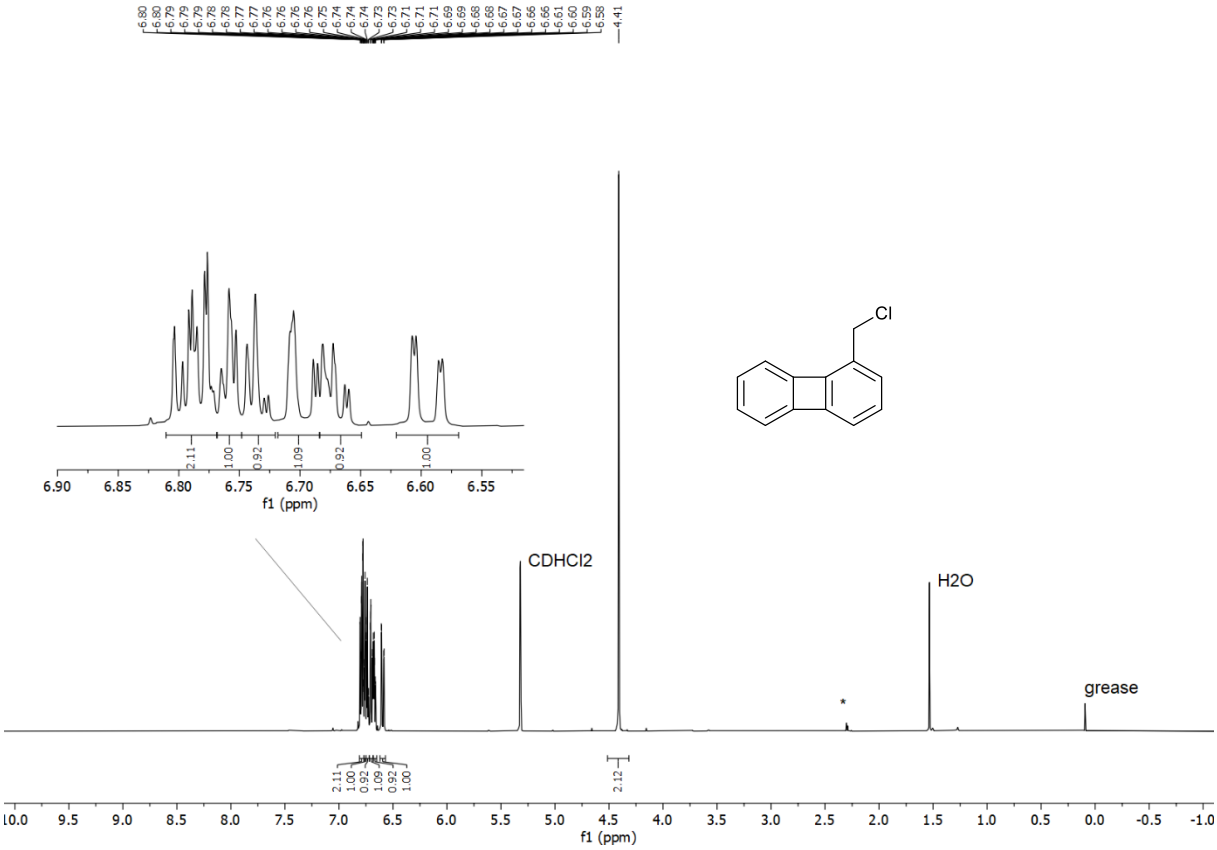


Figure S 4. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of **14**. Impurities are marked with an asterisk.

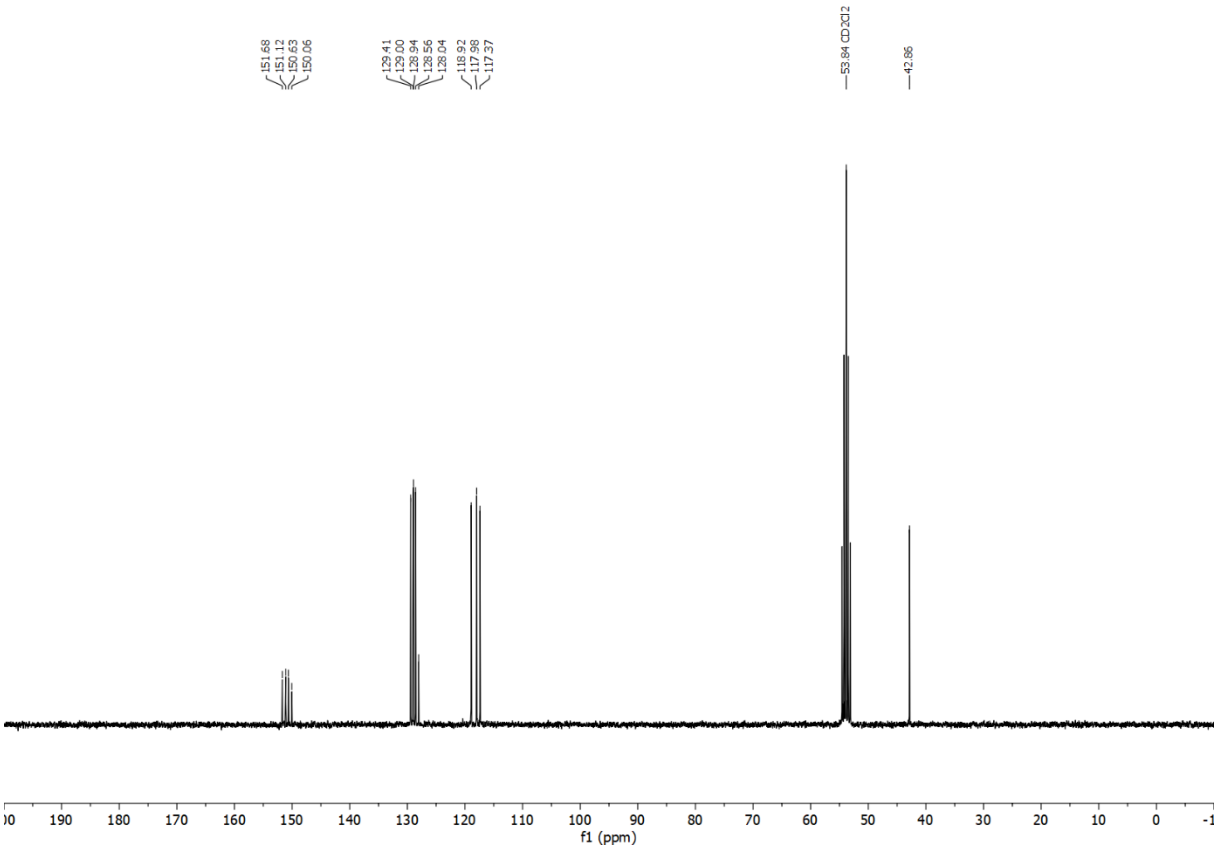


Figure S 5. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of **14**.

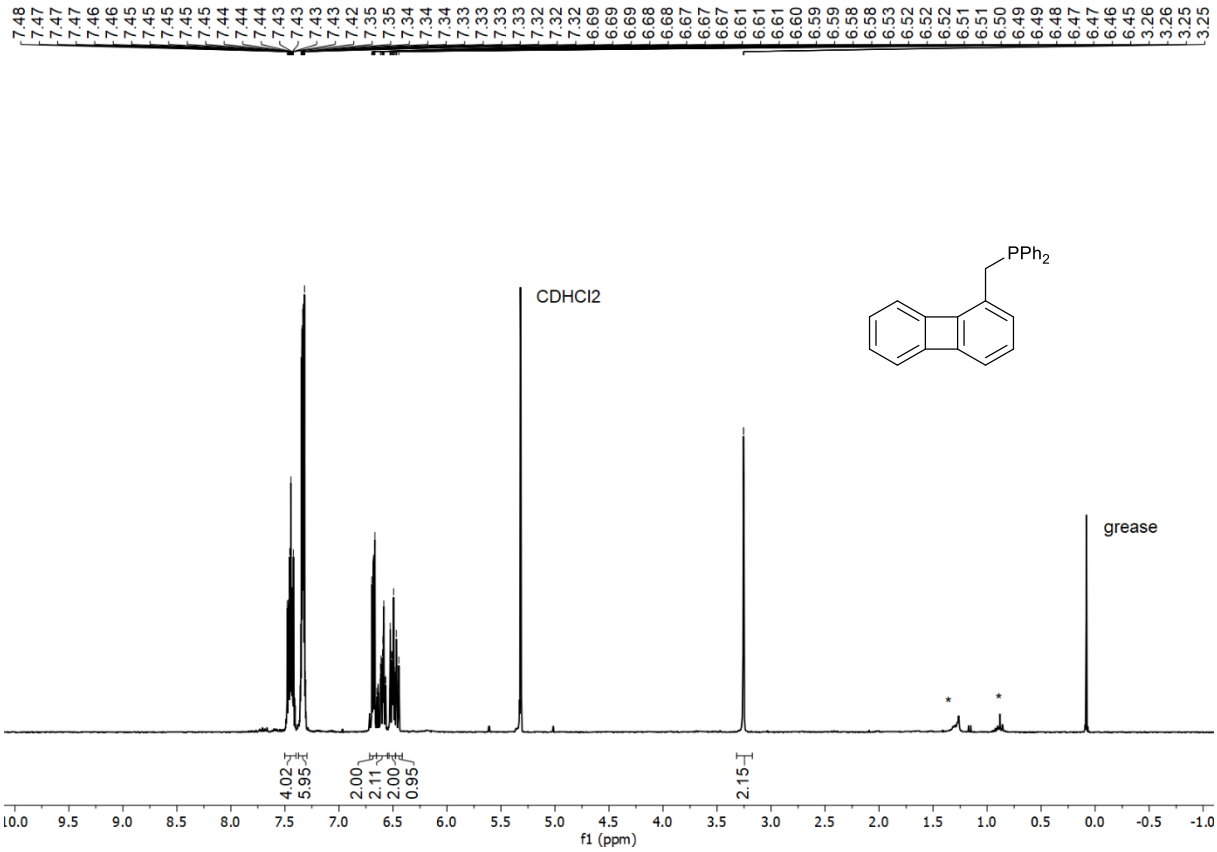


Figure S 6. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of **15**. Impurities are marked with an asterisk.

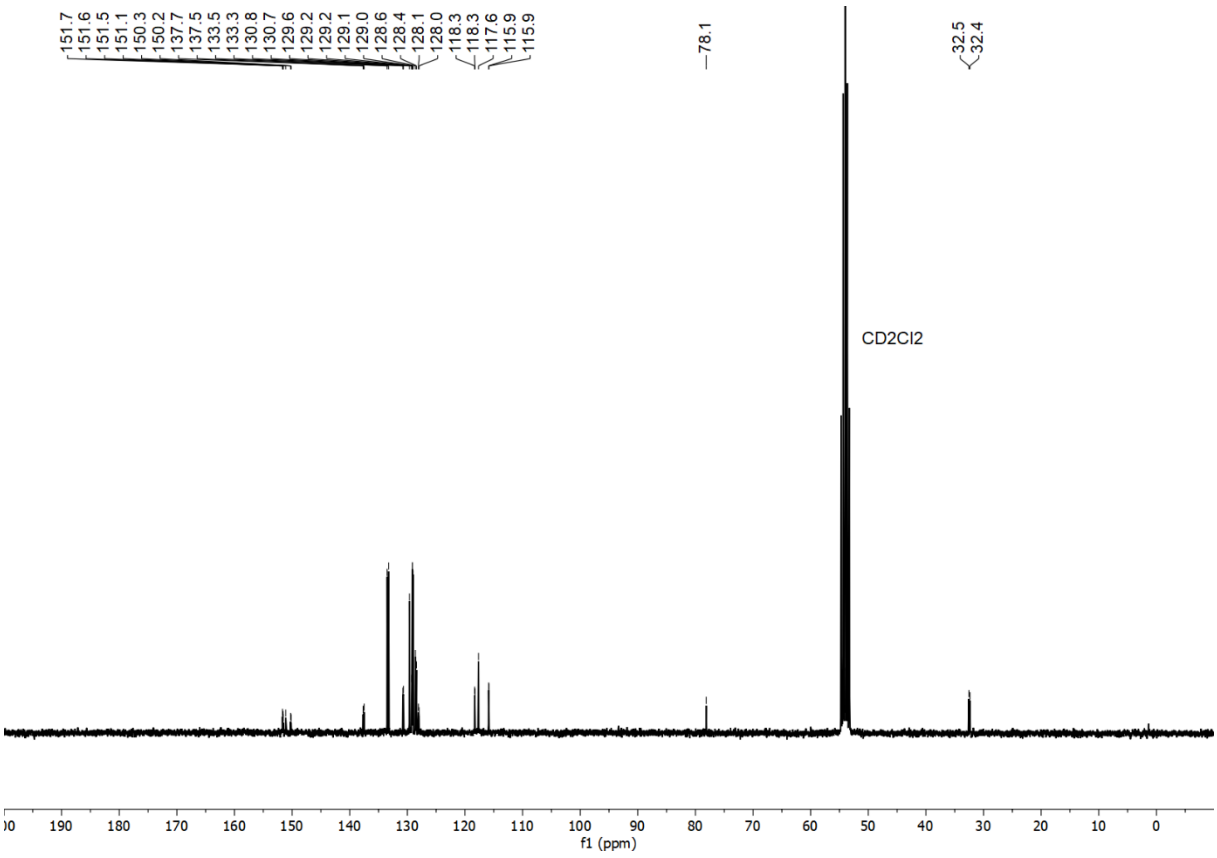


Figure S 7. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of **15**.

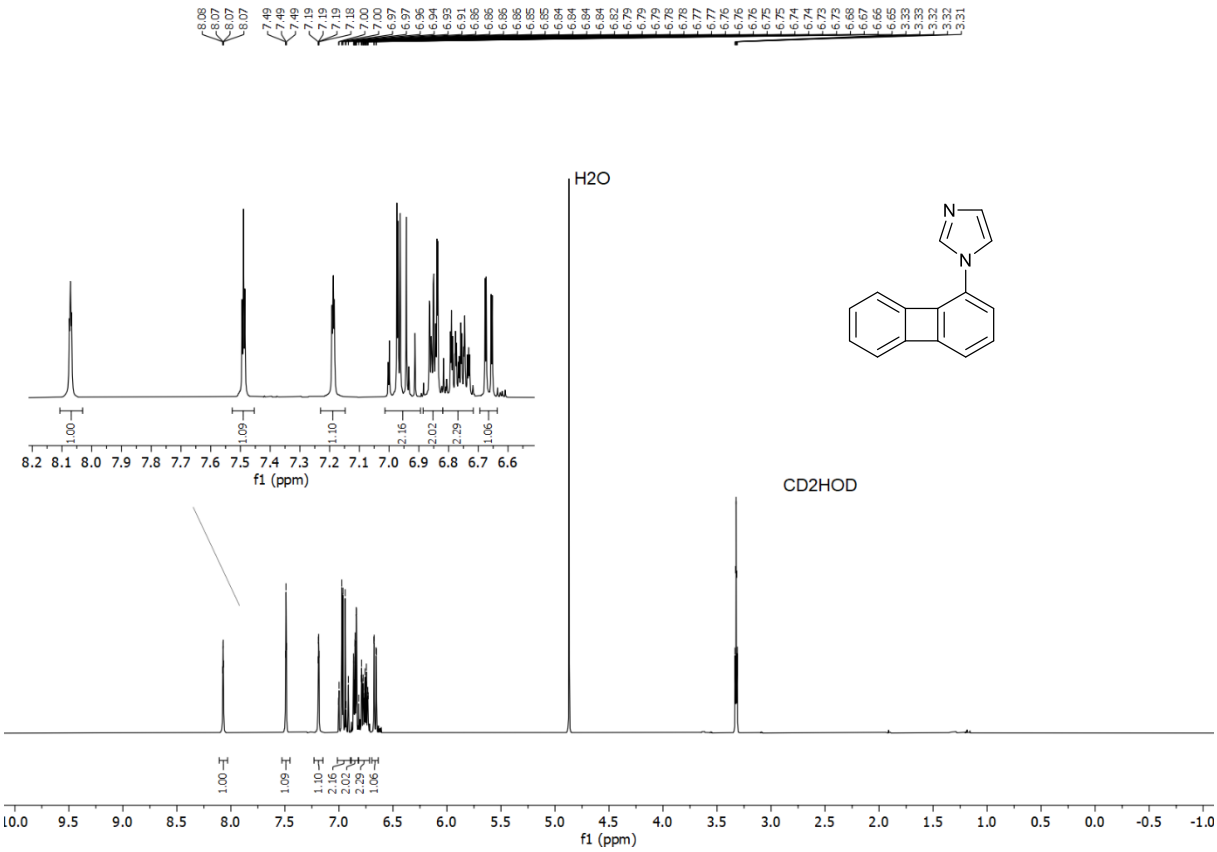


Figure S 8. ^{1}H NMR spectrum (300 MHz, MeOH-*d4*) of **16**.

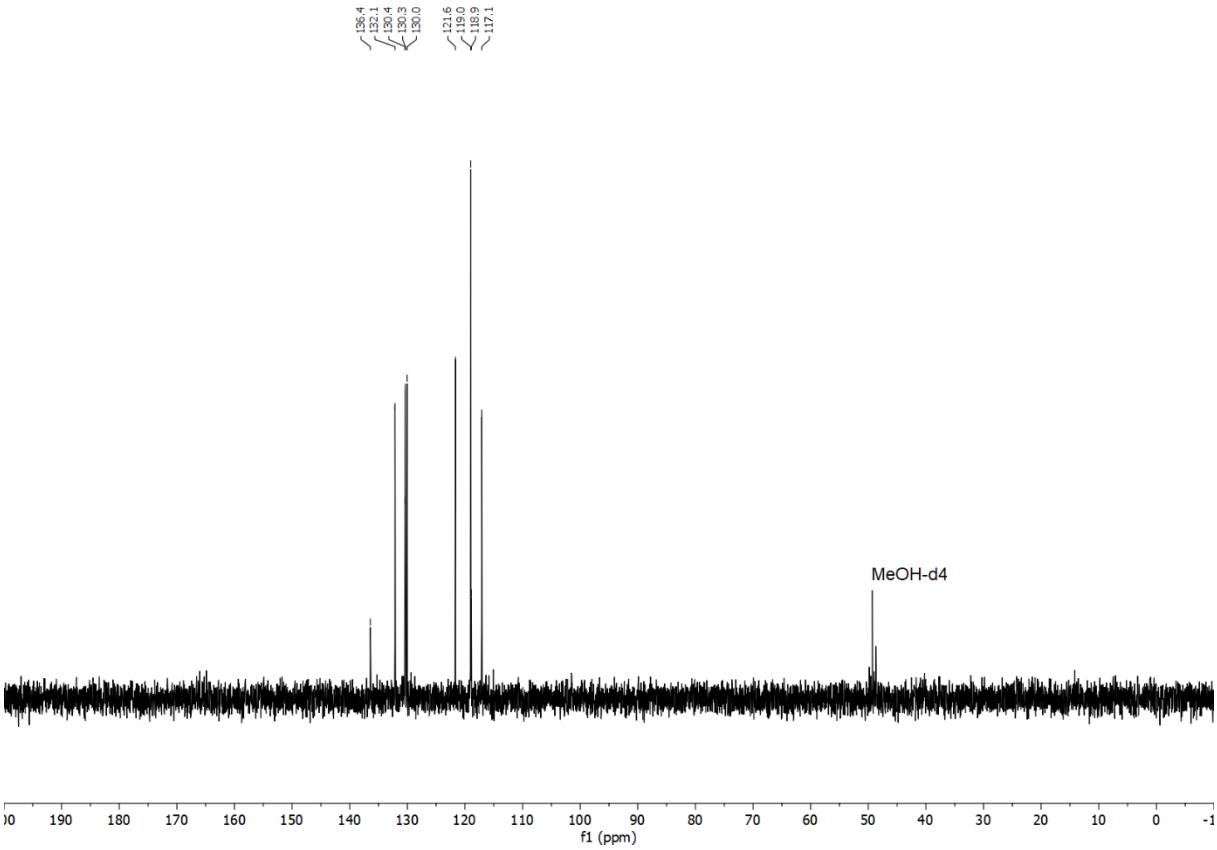


Figure S 9. ^{13}C NMR spectrum (75 MHz, MeOH-*d4*) of **16**.

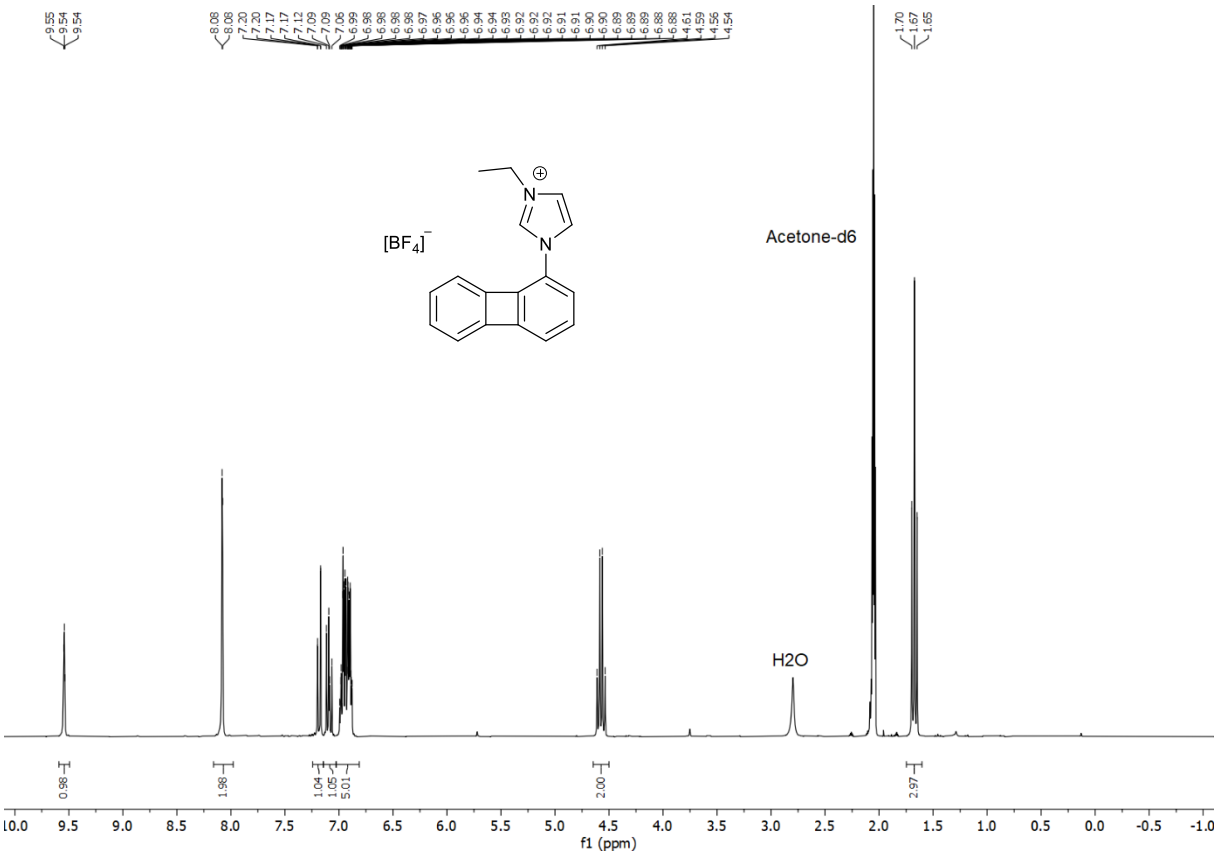


Figure S 10. ^{1}H NMR spectrum (300 MHz, Acetone-*d6*) of **17a**.

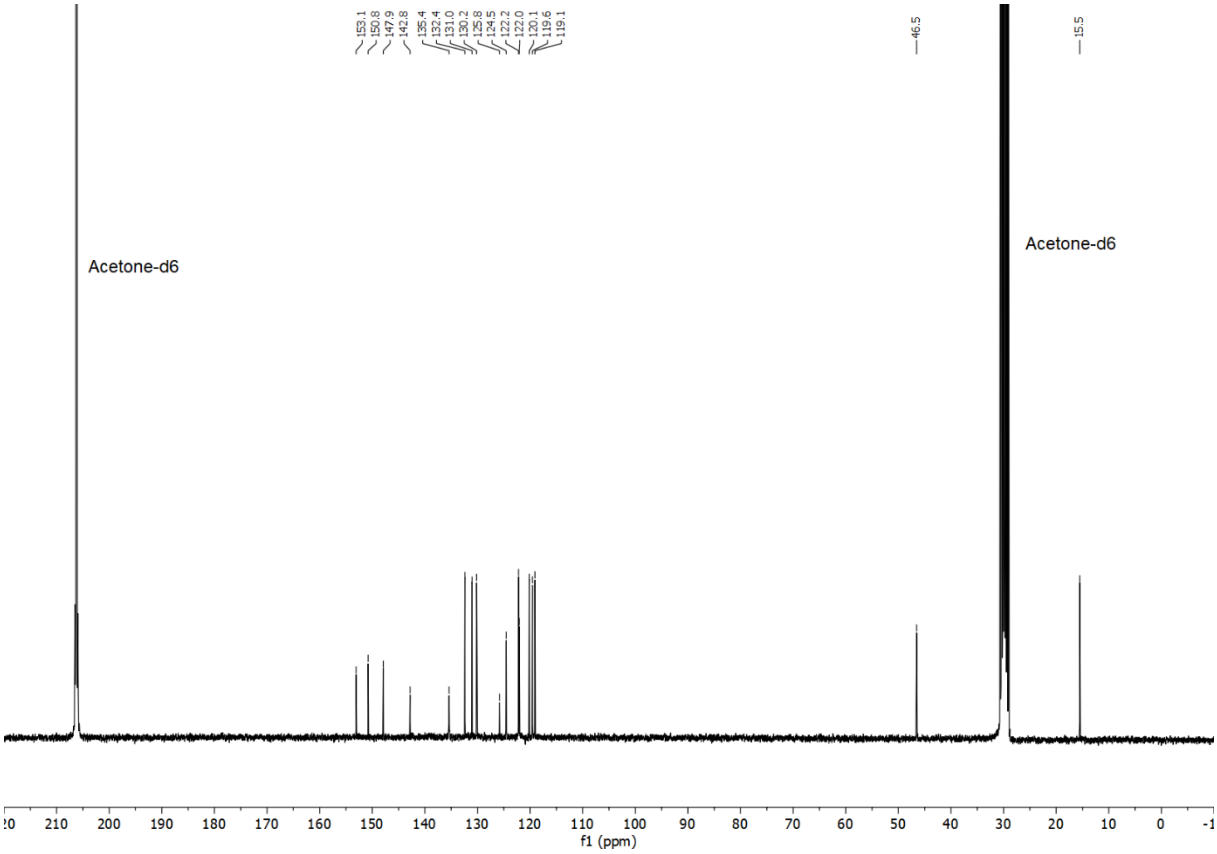


Figure S 11. ^{13}C NMR spectrum (75 MHz, Acetone-*d6*) of **17a**.

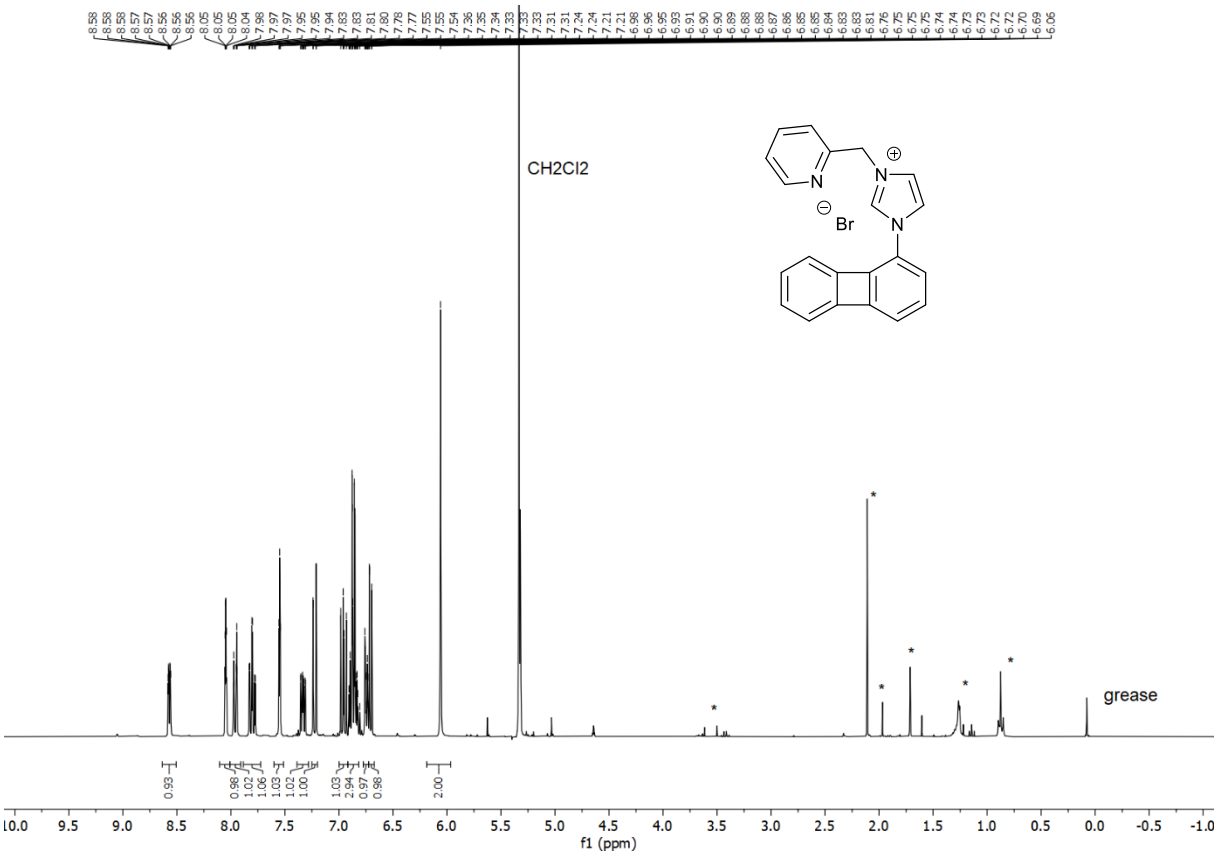


Figure S 12. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of **18**. Impurities are marked with an asterisk.

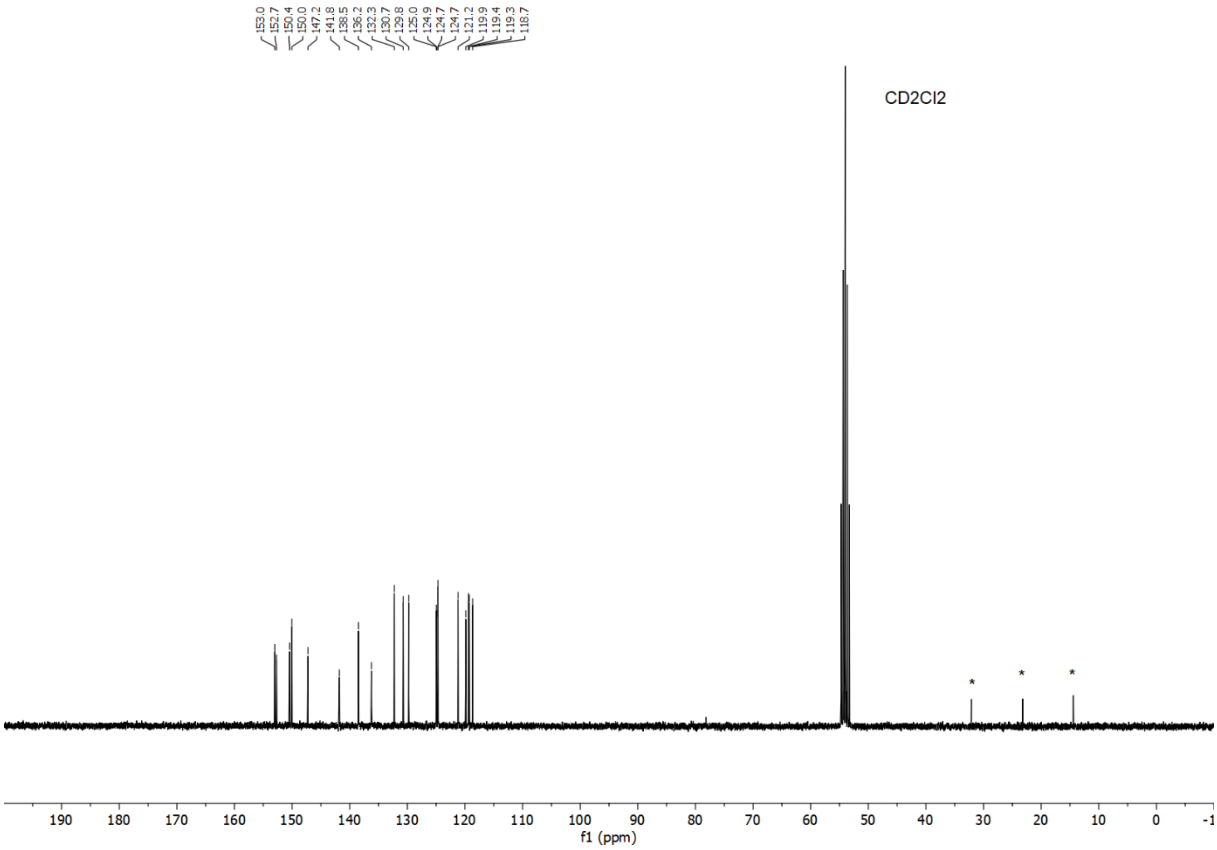


Figure S 13. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of **18**. Impurities are marked with an asterisk.

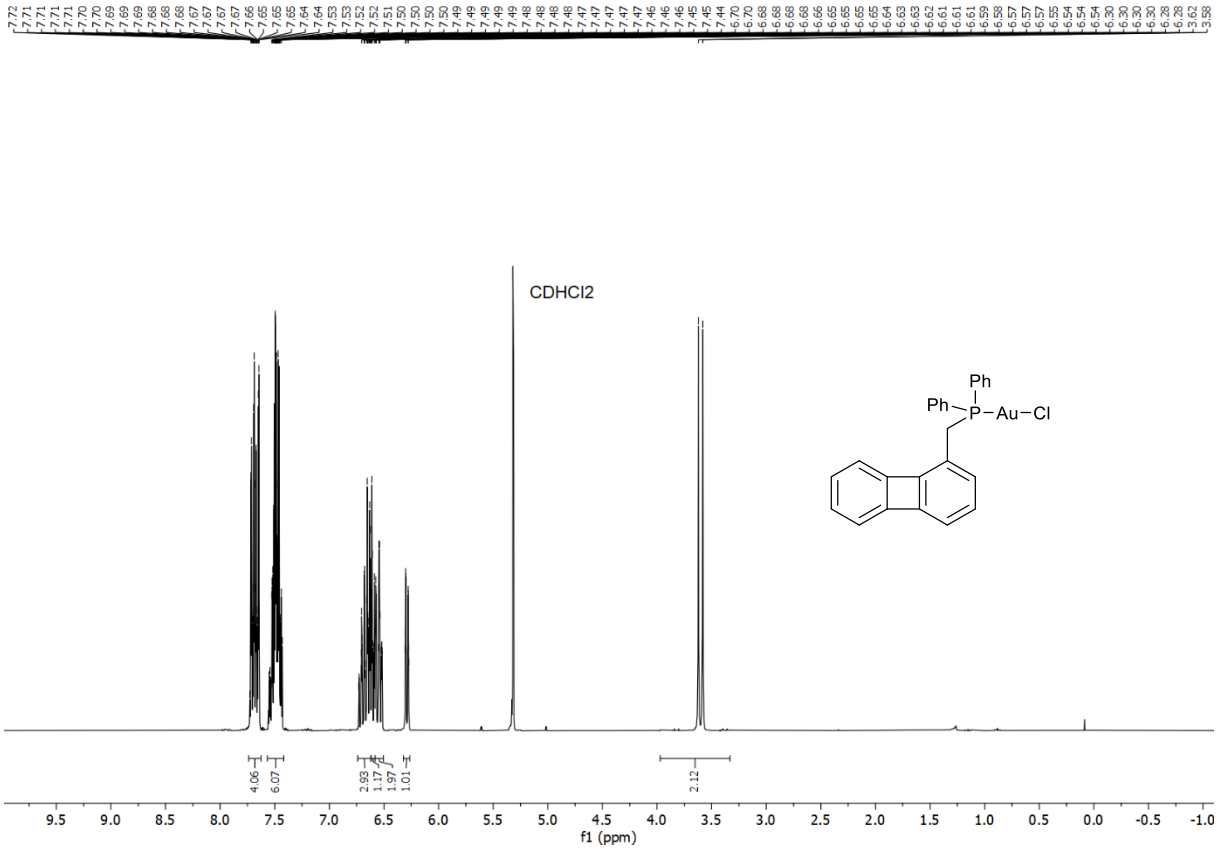


Figure S 14. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of **19**.

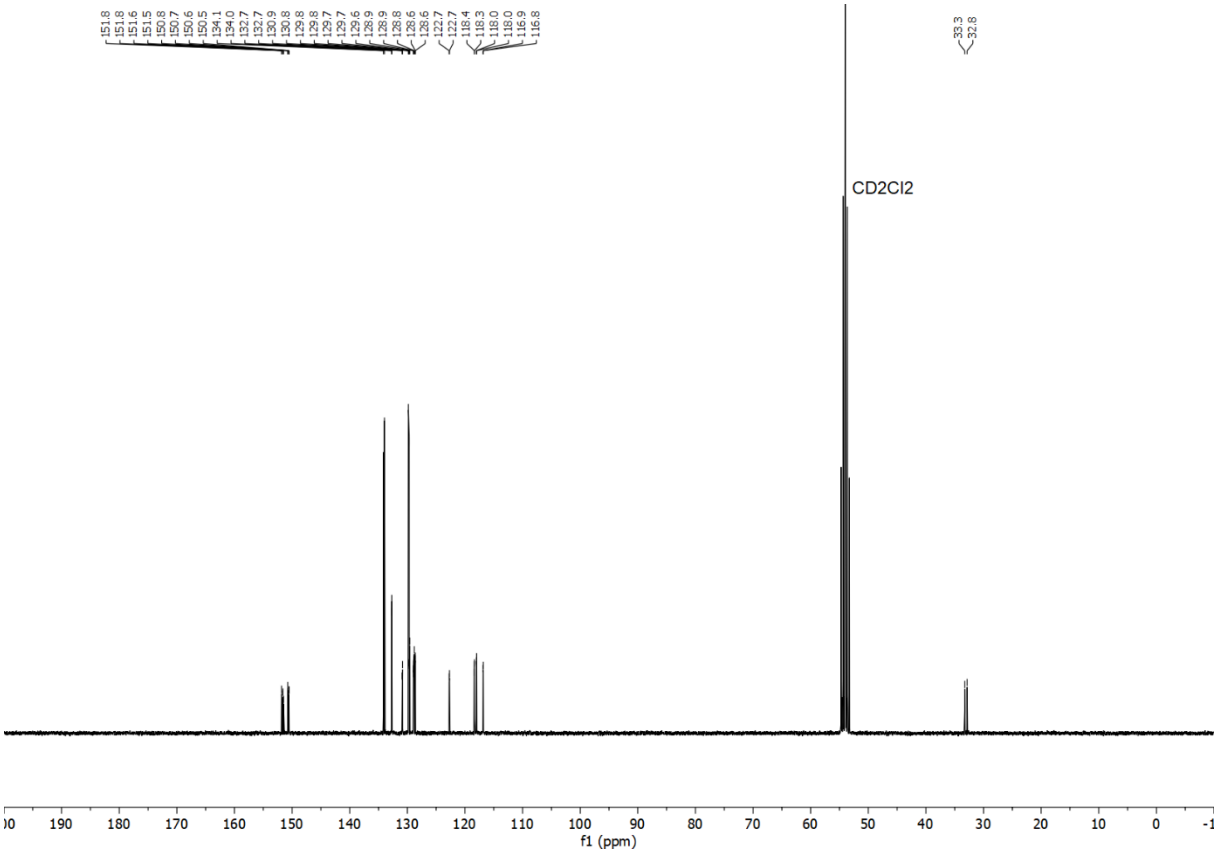


Figure S 15. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of **19**.

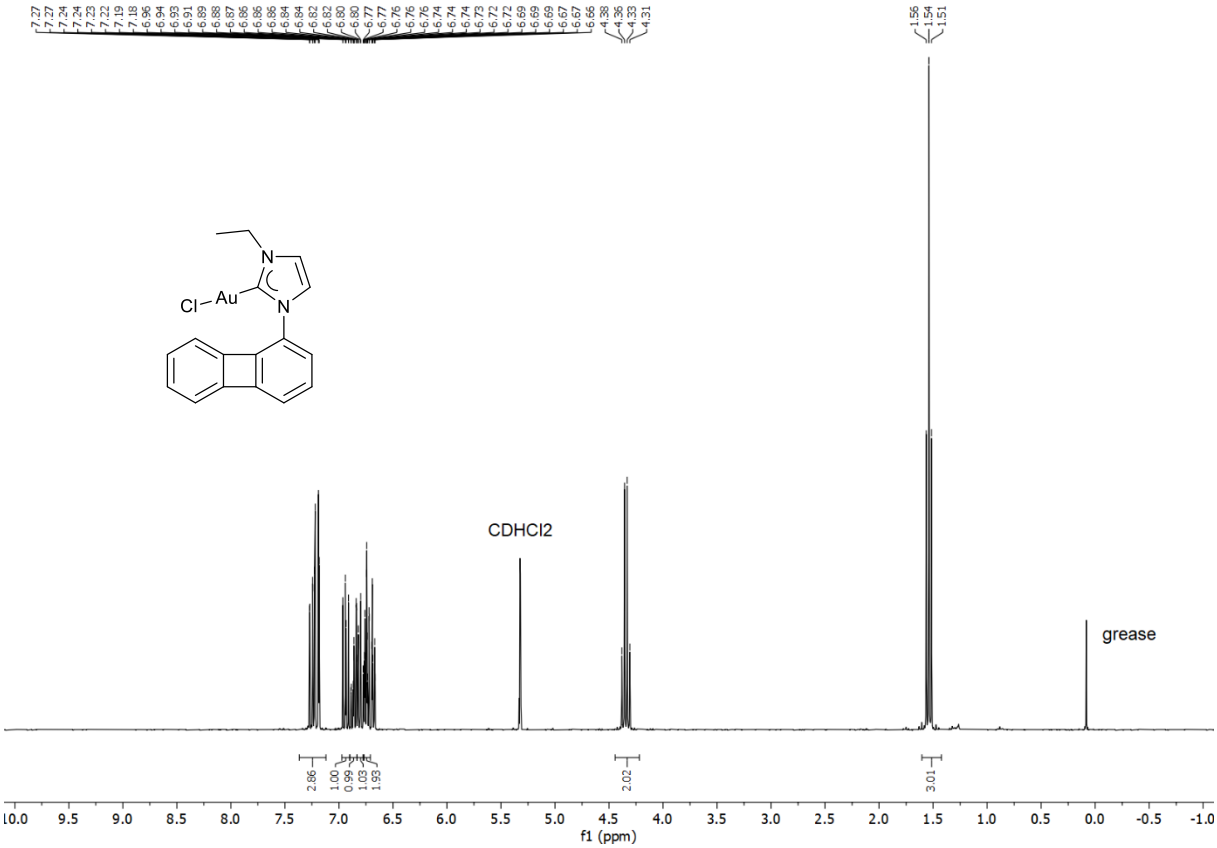


Figure S 16. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of **20**.

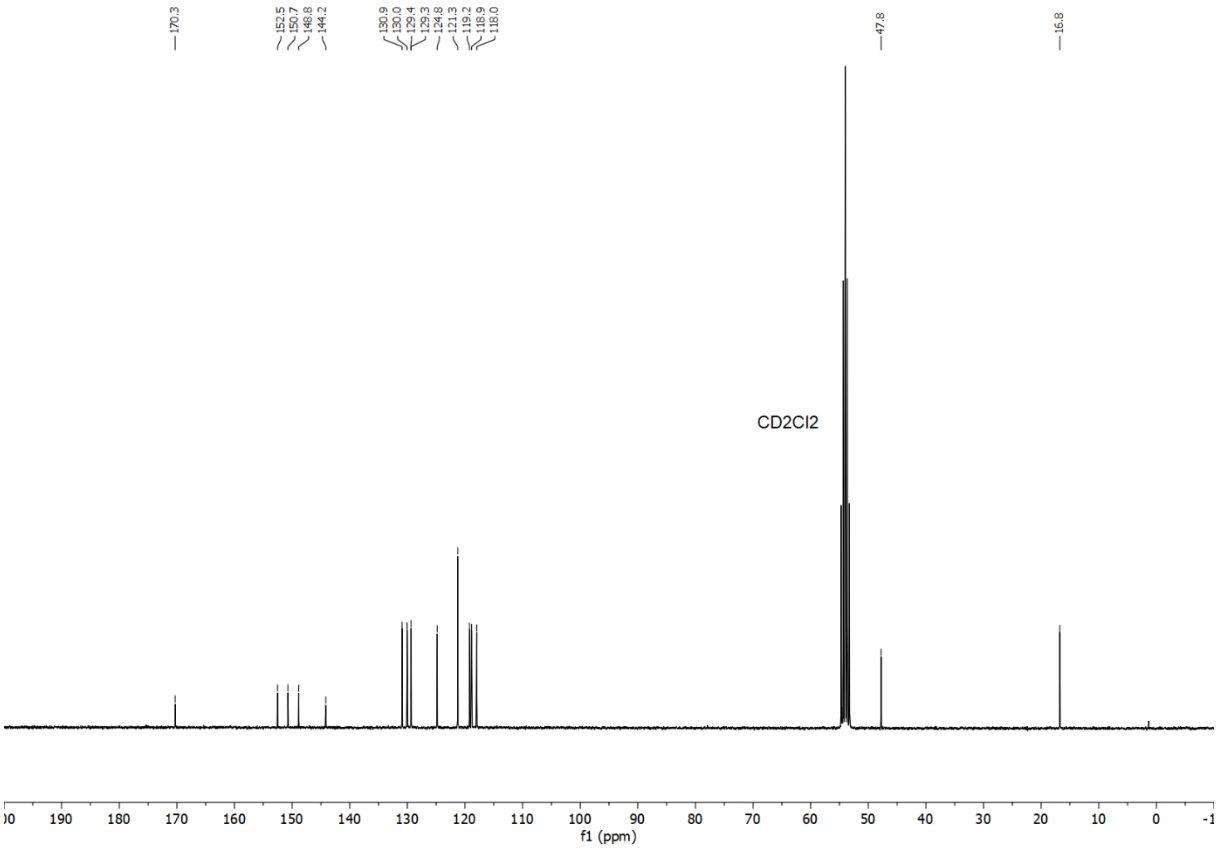


Figure S 17. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of **20**.

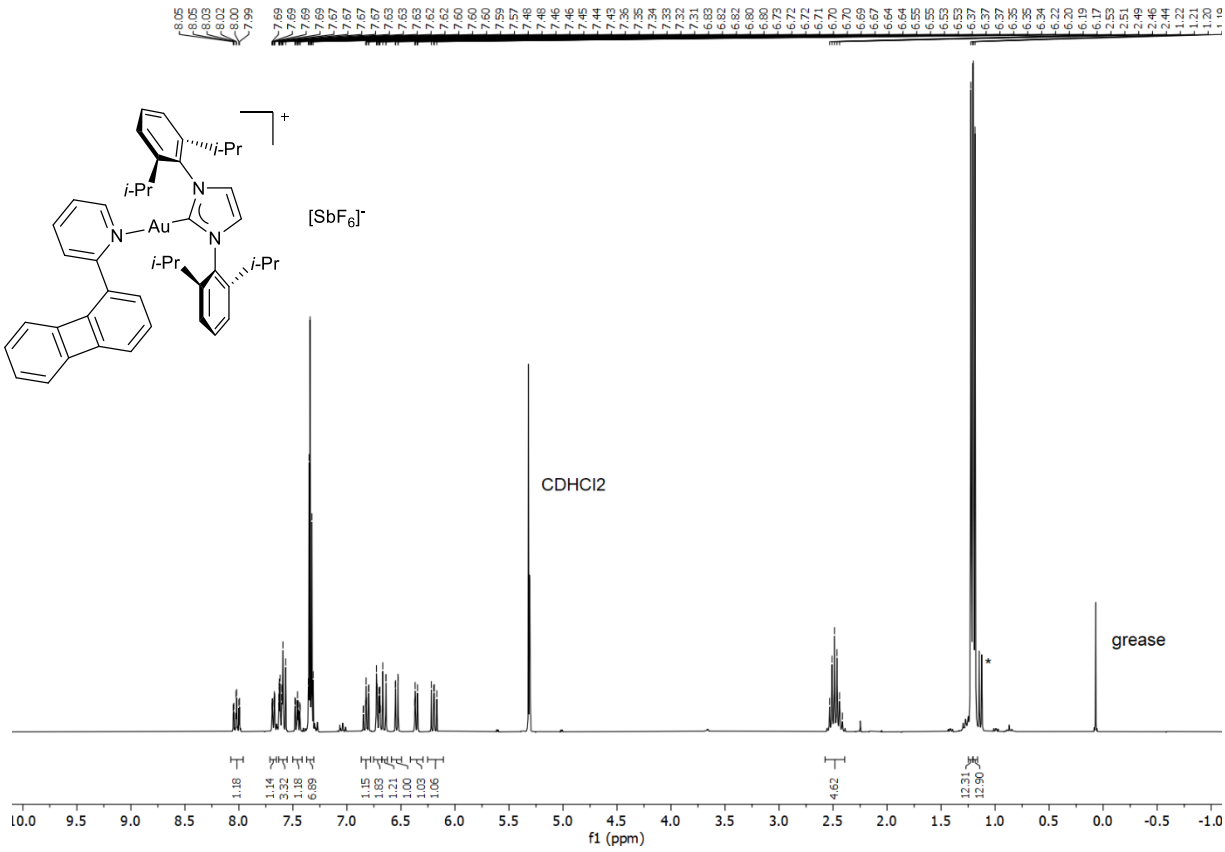


Figure S 18. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of **21**.

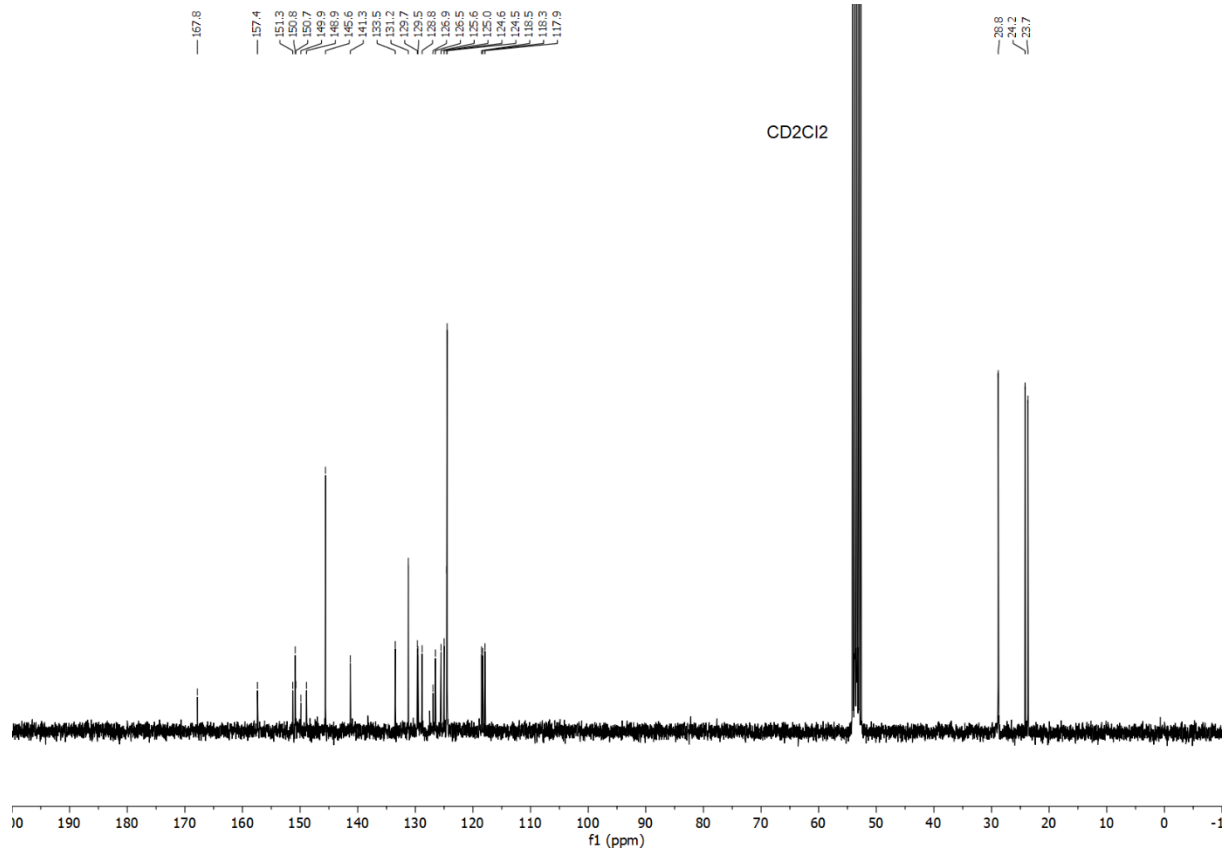


Figure S 19. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of **21**.

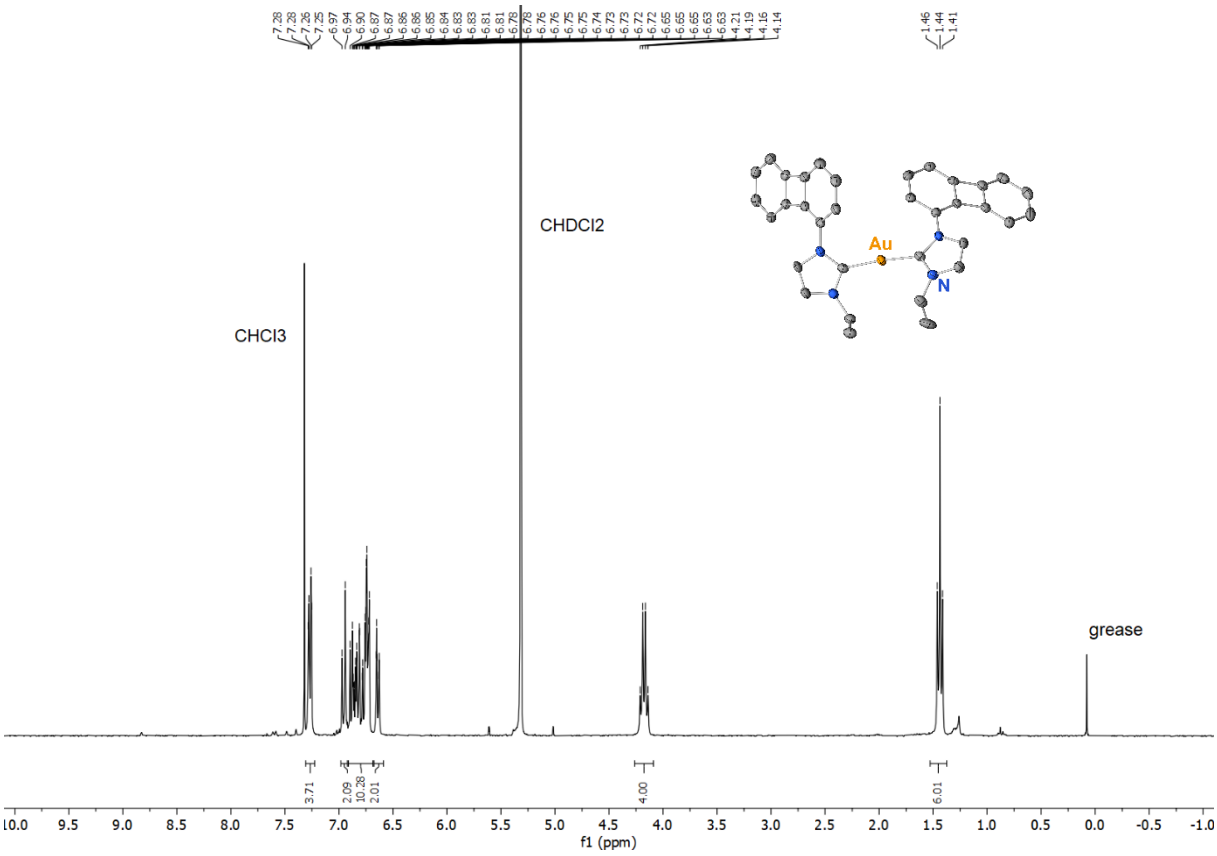


Figure S 20. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of **23**.

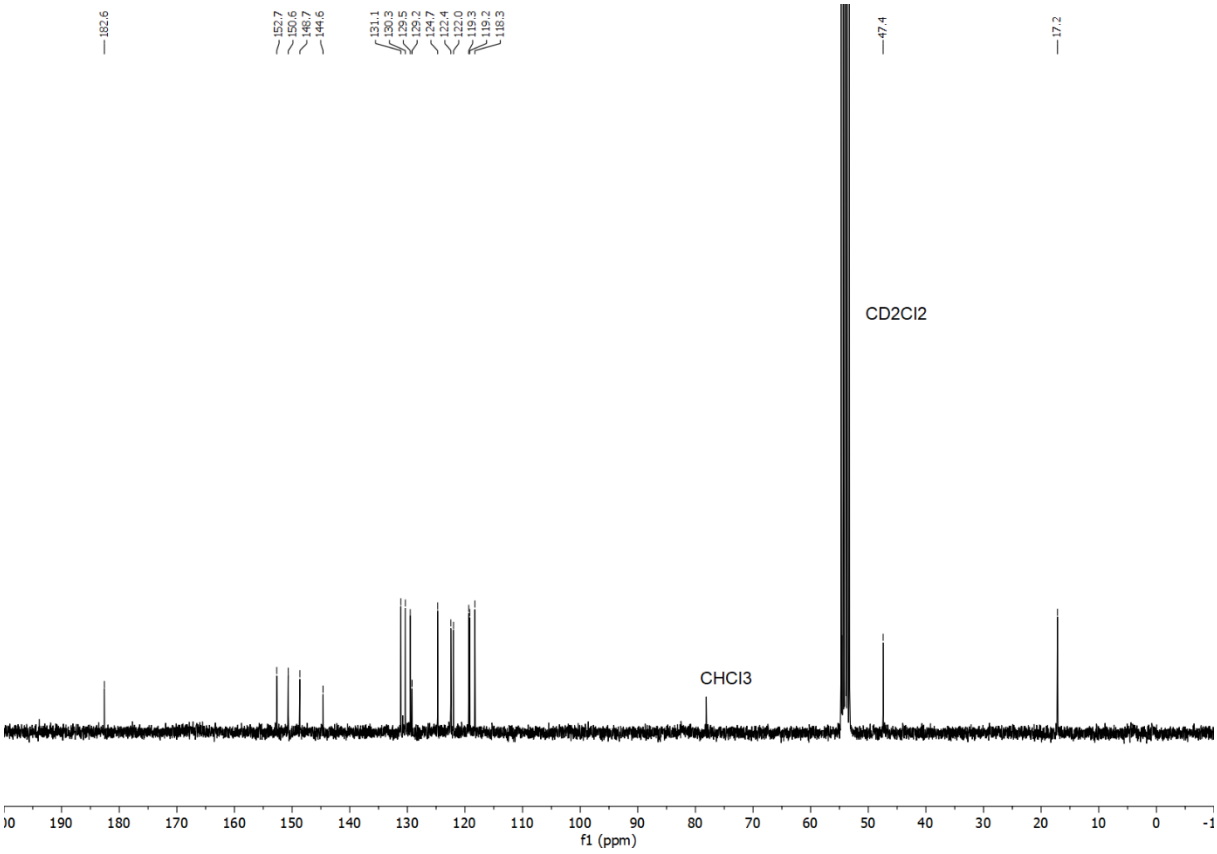


Figure S 21. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of **23**.

S 5. **Coordinates of Quantum Chemical Calculations**

Given in xyz format.

Table 1: Pyridine, No Ligand, I

30

H	4.0540948	-0.2114109	-2.5296731
H	4.2352090	2.2695573	-2.6445060
H	2.3328910	-3.3221303	-1.1563306
H	0.3734173	-4.3085504	0.0440141
H	2.8414310	3.7214236	-1.2713916
H	-1.3683090	-2.9116593	0.9747477
H	1.2804236	2.7654468	0.4181381
C	3.3743560	0.4080813	-1.9593041
C	3.4775224	1.8266326	-2.0110709
C	1.6227874	-2.6886646	-0.6421276
C	2.3982673	-0.1040114	-1.1525661
C	1.7101140	-1.3203582	-0.6136495
C	2.6819544	2.6514525	-1.2491951
C	0.5036044	-3.2343114	0.0197580
C	1.5187000	0.7302655	-0.4008851
C	1.6691714	2.1329322	-0.3769024
C	0.7665320	-0.5066515	0.0650322
C	-0.4823760	-2.4341644	0.5758110
C	-0.4178709	-1.0135270	0.5733236
C	-1.6455534	-0.2649655	0.9412919
C	-2.4466135	-0.6932350	1.9985562
C	-3.6633189	-0.0775402	2.2538844
C	-4.0786976	0.9647379	1.4351590
C	-3.2437474	1.3713900	0.4102258
N	-2.0583348	0.7817795	0.1698754
H	-2.0995578	-1.5064225	2.6207651
H	-4.2787624	-0.4097902	3.0799249
H	-5.0246374	1.4659802	1.5855559
H	-3.5140617	2.1839969	-0.2489308
Au	-0.5186351	1.7337166	-0.9095304

Table 1: Pyridine, No Ligand, TS

30

H	-0.5750825	-4.5753819	1.0003913
H	0.3157348	-5.5609425	-1.1024009
H	-0.9846714	-2.1735579	3.2509483
H	-0.8163574	0.1353984	4.1735210
H	1.2273089	-4.1452187	-2.8806895
H	-0.3192678	2.0353407	2.7350956
H	1.2157284	-1.6705902	-2.6794774
C	-0.2857042	-3.9343260	0.1777655
C	0.2550734	-4.4845272	-1.0034796
C	-0.7547137	-1.3376704	2.6031002
C	-0.3685188	-2.5668930	0.2527068
C	-0.5351288	-1.4998327	1.2516103
C	0.7741639	-3.6865300	-2.0114119
C	-0.6359616	-0.0373829	3.1206251
C	0.0794902	-1.7493946	-0.8191712
C	0.7476548	-2.2810982	-1.9177239
C	-0.1669083	-0.4097933	0.4452673
C	-0.3197136	1.0395331	2.3094863
C	-0.0838239	0.8967847	0.9190375
Au	-0.8615635	-0.0075332	-1.6419758
C	0.0449863	2.0974428	0.0630767
N	-0.5073610	2.0558919	-1.1823265
C	-0.4577304	3.1308229	-1.9829322
C	0.1299658	4.3181860	-1.5803650
C	0.7027428	4.3814750	-0.3157260
C	0.6606781	3.2646083	0.5073636
H	-0.9186093	3.0252599	-2.9549553
H	0.1334195	5.1683219	-2.2482841
H	1.1834613	5.2892670	0.0252722
H	1.1207079	3.2823399	1.4856516

Table 1: Pyridine, No Ligand, II

30

C	-0.4348352	-0.0150856	0.0000000
C	-0.9726377	1.2559161	0.0000000
C	-2.3774076	1.2939780	0.0000000
C	-3.0988587	0.1034907	0.0000000
C	-2.4781613	-1.1469839	0.0000000
C	-1.0795390	-1.2399252	0.0000000
H	-2.8993162	2.2422931	0.0000000
H	-4.1800046	0.1497786	0.0000000
H	-3.0794214	-2.0477052	0.0000000
C	-0.1881498	-2.4015597	0.0000000
C	-0.5766227	-3.7374602	0.0000000
C	1.1915136	-2.0862147	0.0000000
C	0.3902742	-4.7405590	0.0000000
H	-1.6275041	-4.0006872	0.0000000
C	2.1516208	-3.0797097	0.0000000
C	1.7418248	-4.4184203	0.0000000
H	0.0849496	-5.7788489	0.0000000
H	3.2098730	-2.8451564	0.0000000
H	2.4877569	-5.2030764	0.0000000
C	-0.0420748	2.3897236	0.0000000
C	-0.4220125	3.7267112	0.0000000
N	1.2809198	2.0553553	0.0000000
C	0.5506853	4.7174801	0.0000000
H	-1.4714092	3.9856487	0.0000000
C	2.2177201	3.0121433	0.0000000
C	1.8940068	4.3586267	0.0000000
H	0.2620892	5.7606093	0.0000000
H	3.2477506	2.6793713	0.0000000
H	2.6798276	5.1007963	0.0000000
Au	1.5371426	-0.0905299	0.0000000

Table 1: NHC, MeCN, I

37

H	4.7088146	-0.5815215	-0.7492755
H	4.8109903	1.9080891	-0.6036872
H	2.7269997	-3.8291492	-0.1183900
H	0.6238222	-4.9281431	0.6590037
H	2.9389362	3.2182047	0.2378165
H	-1.2956047	-3.6215638	1.4144779
H	0.8155164	2.1372778	0.9825988
C	3.8590474	-0.0170580	-0.3879473
C	3.9074001	1.3942297	-0.2998684
C	1.8906715	-3.2319103	0.2196751
C	2.6854952	-0.5940891	0.0209159
C	1.9064183	-1.8632820	0.2513734
C	2.8400369	2.1414010	0.1780132
C	0.6967237	-3.8481653	0.6681595
C	1.5896075	0.1719256	0.4997528
C	1.6323682	1.5384205	0.6008143
C	0.8050326	-1.0930758	0.7158051
C	-0.3899043	-3.1139247	1.1068514
C	-0.3473228	-1.7000761	1.1357335
Au	-1.4612072	0.7278478	-0.8913560
N	-1.4879218	-0.9606536	1.5785486
C	-2.0575571	0.0590389	0.8842649
N	-3.0965232	0.4674829	1.6459403

C	-3.1848112	-0.2897048	2.7987058
C	-2.1744181	-1.1907856	2.7569755
C	-4.0161616	1.5476104	1.2989080
H	-3.9451450	-0.1171478	3.5396062
H	-1.8681775	-1.9498601	3.4539076
H	-5.0301810	1.1570405	1.2263985
H	-3.9721051	2.3254044	2.0600354
H	-3.7102444	1.9550293	0.3386101
N	-0.8229914	1.3788139	-2.6844911
C	-0.4109638	1.7344881	-3.6959540
C	0.1098671	2.1824852	-4.9701718
H	-0.3434111	3.1392469	-5.2336931
H	-0.1252575	1.4455617	-5.7396158
H	1.1921609	2.3005125	-4.8984417

Table 1: NHC, MeCN, TS

37

H	-0.7441813	-3.9029126	-2.3288431
H	0.6907007	-3.2729873	-4.2693766
H	-1.6622352	-4.1038720	0.4738975
H	-1.8384757	-3.7486871	2.9354607
H	2.1011108	-1.2476576	-4.1855373
H	-0.9486863	-1.7048238	3.9819433
H	2.0436047	0.2748950	-2.2229177
C	-0.1893441	-2.9684678	-2.3239878
C	0.6397767	-2.6220274	-3.4014817
C	-1.3018854	-3.1836811	0.9244597
C	-0.2321344	-2.1125695	-1.2287970
C	-0.7077143	-2.1921807	0.1477631
C	1.4387473	-1.4802465	-3.3555564
C	-1.3705386	-2.9942700	2.3105946
C	0.5243356	-0.9309229	-1.2454555
C	1.4118712	-0.6076585	-2.2443351
C	-0.1955944	-1.0275738	0.7496175
C	-0.8440312	-1.8524695	2.9111566
C	-0.2312455	-0.8582710	2.1286025
Au	-0.0434828	1.1727835	-0.0889681
C	1.1620033	3.7904846	2.2953407
H	2.2394879	3.9698278	2.3404310
C	1.0433673	1.9300671	3.9982036
N	0.2448453	0.3553141	2.6903996
C	0.6488591	0.6276289	3.9888912
H	0.6440511	4.4924607	2.9532685
H	0.6460377	-0.1122578	4.7724454
C	0.3713349	1.4615438	1.8988520
H	0.8102992	3.9152760	1.2709322
H	1.4277217	2.5425368	4.7989622
N	0.8673010	2.4207645	2.7087535
N	-0.7004965	1.8763083	-1.9704492
C	-1.1057343	2.1246703	-3.0226547
C	-1.6116241	2.4328389	-4.3441839
H	-1.4209003	1.5926478	-5.0200063
H	-1.1170308	3.3285461	-4.7338610
H	-2.6901206	2.6149430	-4.2935645

Table 1: NHC, MeCN, II

37

C	0.0383151	1.5078075	-0.0290714
C	1.2559722	2.1611304	-0.0540555
C	1.2980901	3.5491753	-0.0824795
C	0.0806926	4.2344615	-0.0846512
C	-1.1443165	3.5708365	-0.0595577
C	-1.1834820	2.1718229	-0.0308785
H	2.2337667	4.0923364	-0.1023047
H	0.0944367	5.3164073	-0.1065831
H	-2.0615857	4.1459371	-0.0624206
C	-2.3321375	1.2619232	-0.0014312
C	-3.6698627	1.6464402	0.0038804
C	-1.9969472	-0.1154558	0.0235506
C	-4.6740626	0.6822636	0.0338445
H	-3.9330910	2.6973683	-0.0151911
C	-3.0048895	-1.0655891	0.0537771
C	-4.3451631	-0.6668948	0.0588976
H	-5.7129398	0.9865669	0.0378028
H	-2.7723114	-2.1229675	0.0745917
H	-5.1276569	-1.4154870	0.0826610
Au	0.0391432	-0.4663480	0.0099728
N	2.3717419	1.2775854	-0.0471134
C	3.7258121	1.5322008	-0.0649131
C	2.1264321	-0.0645903	-0.0180351
C	4.3396302	0.3222370	-0.0465066
H	4.1344893	2.5259741	-0.0886203
N	3.3419328	-0.6401552	-0.0179897
H	5.3837504	0.0637289	-0.0510987
C	3.5864644	-2.0780059	0.0091149
H	4.1425772	-2.3733561	-0.8796502
H	2.6253071	-2.5822400	0.0253969
H	4.1539862	-2.3380023	0.9017075
N	-0.0937856	-2.5709344	0.0503549
C	-0.3108862	-3.6991001	0.0701917
C	-0.5966010	-5.1188615	0.0965655
H	-0.6823890	-5.4529092	1.1317309
H	-1.5368524	-5.3078327	-0.4239570
H	0.2064197	-5.6674733	-0.3975322

Table 1: NHC, No Ligand, I

31

H	4.4851755	-0.2152822	-2.0562704
H	4.5517897	2.2755054	-2.1517297
H	2.7393011	-3.4041242	-0.8959621
H	0.7370522	-4.4964732	0.1264684
H	2.8504521	3.6423693	-1.0662219
H	-1.1590185	-3.1912987	0.9093198
H	0.9906062	2.6156680	0.2310375
C	3.6969774	0.3704119	-1.6018297
C	3.7287255	1.7861239	-1.6469015
C	1.9345150	-2.8072123	-0.4889252
C	2.6276337	-0.1848157	-0.9514183
C	1.9272683	-1.4378979	-0.5081922
C	2.7581025	2.5642911	-1.0410794
C	0.7957016	-3.4166395	0.0834376
C	1.6029678	0.6027701	-0.3624963
C	1.6556851	1.9878321	-0.3547825
C	0.8702532	-0.6599555	0.0374881
C	-0.2777082	-2.6768189	0.5484236
C	-0.2668007	-1.2635021	0.5173415
Au	-0.8697571	1.5043393	-1.1360453
N	-1.4540757	-0.5522854	0.8856948
C	-1.9519874	0.5173562	0.2091078
N	-3.1315474	0.8067626	0.7856065
C	-3.3868046	-0.0759028	1.8209969
C	-2.3380168	-0.9297242	1.8837806
C	-4.0170064	1.9012704	0.3908781
H	-4.2797767	-0.0120674	2.4172028
H	-2.1340616	-1.7510239	2.5464582
H	-5.0124112	1.5065553	0.1955507
H	-4.0598669	2.6439548	1.1862595
H	-3.6133677	2.3498136	-0.5131981

Table 1: NHC, No Ligand, TS

31

H	-0.6778019	-4.7400749	0.5410966
H	0.2667951	-5.4878432	-1.6337812
H	-1.1302636	-2.7062334	3.0462936
H	-1.0276293	-0.5724437	4.3253464
H	1.3281726	-3.9001824	-3.1691387

H	-0.4564117	1.5323009	3.2255219
H	1.4443690	-1.4811539	-2.6297555
C	-0.3069552	-4.0140893	-0.1709330
C	0.2580330	-4.4326967	-1.3916894
C	-0.8495773	-1.7839242	2.5549951
C	-0.3203548	-2.6644309	0.0884231
C	-0.5272613	-1.7428579	1.2125395
C	0.8597813	-3.5379235	-2.2630148
C	-0.7726610	-0.5834267	3.2738726
C	0.2194913	-1.7454809	-0.8427737
C	0.9050795	-2.1577717	-1.9773343
C	-0.0984156	-0.5521207	0.6031797
C	-0.4131228	0.6087920	2.6619295
C	-0.0724235	0.6512369	1.2994235
Au	-0.4673351	0.2176853	-1.4884451
C	-0.1544475	3.9875108	-2.2603601
H	0.8016332	4.3353507	-2.6487527
C	0.5051811	4.0126387	0.1784724
N	0.1100379	1.9036398	0.6366907
C	0.5451090	3.1003643	1.1795143
H	-0.8414983	4.8260864	-2.1597055
H	0.8579827	3.1959385	2.2033322
C	-0.2125910	2.0723523	-0.6849638
H	-0.5763584	3.2408858	-2.9274515
H	0.7586869	5.0581429	0.1727376
N	0.0447558	3.3597289	-0.9552696

Table 1: NHC, No Ligand, II

31

C	-0.0548558	0.6735113	-0.0021581
C	1.1997008	1.2441799	-0.0132364
C	1.2640490	2.6346017	-0.0188032
C	0.0632001	3.3490046	-0.0128147
C	-1.1829925	2.7260597	-0.0015636
C	-1.2753500	1.3255845	0.0042129
H	2.2141030	3.1524363	-0.0275436
H	0.1077305	4.4301588	-0.0171290
H	-2.0844039	3.3256583	0.0028283
C	-2.4353706	0.4323629	0.0158308
C	-3.7695238	0.8262777	0.0239314
C	-2.1104200	-0.9465168	0.0185086
C	-4.7745957	-0.1384017	0.0346703
H	-4.0308945	1.8777252	0.0218749
C	-3.1140640	-1.8995184	0.0292602
C	-4.4526618	-1.4901652	0.0373509
H	-5.8126205	0.1680773	0.0409278
H	-2.8848224	-2.9595829	0.0316656
H	-5.2385527	-2.2350117	0.0457659
Au	-0.0940074	-1.3061350	0.0053834
N	2.2817219	0.3268577	-0.0176236
C	3.6444453	0.5471823	-0.0282258
C	2.0042511	-1.0120755	-0.0106816
C	4.2235655	-0.6789772	-0.0277665
H	4.0803449	1.5296228	-0.0350857
N	3.2014585	-1.6167576	-0.0169554
H	5.2607853	-0.9643157	-0.0341060
C	3.4087189	-3.0639863	-0.0129007
H	3.9562463	-3.3576628	-0.9070376
H	2.4365402	-3.5492341	-0.0045281
H	3.9682744	-3.3509602	0.8759485

Table 1: PPh2, Chloride, I

47

H	1.6658800	-0.0392436	-3.3445038
H	1.7988756	2.4254281	-3.1269527
H	0.0413029	-1.3147518	-1.9863745
H	0.2996038	3.6097225	-1.5511440
H	-4.4996021	-0.0625274	-0.6161501
H	5.5077766	-0.9029581	-1.0468903
H	5.7548383	1.5546380	-0.6787073
H	-6.2189134	1.5006650	0.2351018
H	3.3079362	-4.0779027	-0.7397949
H	-1.2903761	2.3354952	-0.1599527
H	1.1292253	-5.0893060	-0.0455419
H	4.0030003	2.8678245	0.3876048
H	-0.6240029	-3.7630949	0.9836529
H	1.8689249	1.8241215	1.1512514
H	-5.7085932	2.9725896	2.1635768
H	-0.2924474	-0.1540401	1.9816977
H	-1.2843732	-1.6089309	2.2194352
H	-1.7539854	1.3539556	2.3665212
H	-3.4731873	2.8837080	3.2269835
C	1.0191744	0.4813661	-2.6495453
C	1.0922760	1.8655619	-2.5268283
C	0.1131818	-0.2385680	-1.8815988
C	0.2541837	2.5308164	-1.6376606
C	-0.7090729	0.4228433	-0.9623193
C	-0.6406441	1.8134193	-0.8513925
C	4.7192817	-0.3382512	-0.5653168
C	4.8490368	1.0560764	-0.3549764
C	-4.2751839	0.5965817	0.2146917
C	2.5491293	-3.4722656	-0.2608869
C	3.5501244	-0.8991582	-0.1233856
C	-5.2404539	1.4713791	0.6982125
C	2.6985104	-2.1362076	-0.0001165
C	3.8523624	1.8033701	0.2530544
C	1.3105951	-4.0366169	0.1323889
C	2.5257841	-0.1302929	0.4951051
C	2.6426590	1.2186980	0.6976657
C	-3.0076325	0.5476642	0.8034084
C	1.6736171	-1.3648433	0.6115070
C	0.3115066	-3.2820496	0.7227361
C	0.4616761	-1.8928897	0.9800871
C	-4.9533343	2.2967258	1.7814427
C	-0.6689170	-1.0594540	1.5044487
C	-2.7271387	1.3791296	1.8925781
C	-3.6977255	2.2473992	2.3796732
Cl	-3.5086504	-4.2280398	-1.9410987
Au	-2.6431731	-2.3780148	-0.9280533
P	-1.7830556	-0.5897723	0.0963667

Table 1: PPh2, Chloride, TS

47

H	-0.2751123	-6.0294805	0.6447153
H	-0.2775429	-6.7994811	-1.7249103
H	0.4467381	-4.1451686	3.0486064
H	1.5133974	-2.2042846	4.1998276
H	0.0981857	-5.2134162	-3.5596281
H	2.0797643	-0.1738346	2.9479804
H	0.3501827	-2.7843208	-3.1259094
H	2.2016634	0.2763950	-0.5104051
H	2.0199487	1.1864571	0.9940392
C	-0.1896354	-5.3149021	-0.1651342
C	-0.1595718	-5.7463182	-1.5014868
C	0.6198827	-3.2162821	2.5190897
C	-0.0538865	-3.9629767	0.0701502
C	0.2868684	-3.0758893	1.1867780
C	0.0582789	-4.8512151	-2.5392611
C	1.2499311	-2.1364486	3.1515532
C	0.0847704	-3.0571525	-0.9960780
C	0.2078681	-3.4711299	-2.3026076
C	0.5374868	-1.8725200	0.4848290
C	1.5767110	-0.9898291	2.4412359
C	1.2561423	-0.8347905	1.0787973
C	1.5476045	0.4444282	0.3492080
Au	-0.9852950	-1.0222524	-0.9461410
P	-0.0690385	1.0313497	-0.3416038

C	-0.9195543	1.8112951	1.0559934
C	-2.2709317	1.5163957	1.2534520
C	-2.9616350	2.0881390	2.3171134
C	-2.3066418	2.9501833	3.1901186
C	-0.9583708	3.2463088	2.9999006
C	-0.2667943	2.6807318	1.9365126
H	-2.7711789	0.8350148	0.5739059
H	-4.0084182	1.8536176	2.4650522
H	-2.8436872	3.3905423	4.0215124
H	-0.4475421	3.9167817	3.6803768
H	0.7796000	2.9214677	1.7895748
C	0.3534253	2.3642275	-1.4966633
C	-0.0726709	3.6829981	-1.3224649
C	0.2453276	4.6499549	-2.2711804
C	0.9892002	4.3108280	-3.3959903
C	1.4080782	2.9946421	-3.5805480
C	1.0841685	2.0249341	-2.6424502
H	-0.6547955	3.9521610	-0.4505087
H	-0.0914196	5.6697759	-2.1296527
H	1.2345798	5.0658096	-4.1327891
H	1.9760684	2.7228178	-4.4618419
H	1.3849436	0.9954369	-2.8052864
Cl	-3.0070932	-1.6810007	-1.9977816

Table 1: PPh2, Chloride, II

47

C	-1.3964206	-1.2574759	0.2775500
C	-2.1645693	-0.0959901	0.2209617
C	-3.4547782	-0.1196736	0.7660031
C	-3.9524767	-1.2897207	1.3283932
C	-3.1876641	-2.4543182	1.3501540
C	-1.8968047	-2.4541517	0.8215692
H	-4.0681396	0.7743460	0.7422364
H	-4.9514305	-1.2973546	1.7477621
H	-3.6012439	-3.3586597	1.7808263
C	-0.9742739	-3.5912264	0.7455068
C	-1.2467632	-4.8857482	1.1888370
C	0.2760851	-3.3120915	0.1519623
C	-0.2934643	-5.8887201	1.0420356
H	-2.2023535	-5.1154154	1.6470233
C	1.2229853	-4.3133393	0.0078192
C	0.9349228	-5.6060034	0.4534026
H	-0.5109591	-6.8924488	1.3874903
H	2.1806997	-4.0885807	-0.4444318
H	1.6749775	-6.3899632	0.3403594
C	-1.6160620	1.1334074	-0.4658602
P	0.2219766	1.0014032	-0.5675107
Au	0.5111389	-1.3342928	-0.3776576
H	-1.9719529	1.1805289	-1.4999330
H	-1.9156320	2.0613422	0.0263344
Cl	2.7533065	-1.4751411	-1.1298932
C	0.8530243	1.8574242	0.8948452
C	2.0842252	2.5168419	0.8449064
C	2.5980739	3.1142626	1.9894853
C	1.8937350	3.0515254	3.1882327
C	0.6733776	2.3838935	3.2439932
C	0.1536682	1.7828740	2.1042765
H	2.6354939	2.5616812	-0.0860643
H	3.5509767	3.6270451	1.9444808
H	2.2972261	3.5175349	4.0788233
H	0.1265148	2.3261251	4.1771202
H	-0.7871138	1.2478458	2.1582849
C	0.7583919	1.9722600	-1.9909964
C	0.4144030	3.3251696	-2.1019975
C	0.8139268	4.0514500	-3.2150964
C	1.5631949	3.4348070	-4.2163381
C	1.9139477	2.0941834	-4.1030909
C	1.5129764	1.3572289	-2.9921720
H	-0.1555845	3.8080893	-1.3166094
H	0.5460103	5.0973668	-3.3019919
H	1.8765570	4.0050684	-5.0825160
H	2.5042599	1.6182347	-4.8761877
H	1.8016109	0.3183759	-2.8823283

Table 1: PPh2, No Ligand, I

46

H	3.7625142	4.2966372	-1.4623027
H	2.5008643	5.2783102	-3.3518299
H	2.8614789	2.3608540	-0.2445373
H	0.3228116	4.3096641	-4.0267427
H	-2.0388860	-0.7186672	-0.0866920
H	-0.9244002	-5.8013406	0.4465694
H	0.2173206	-6.2691109	-1.7171860
H	-4.1897690	-0.1185510	0.9782095
H	-1.5805158	-3.4047955	3.3786385
H	-0.5903747	2.3600341	-2.8222958
H	-1.2854053	-1.1241651	4.3539525
H	1.8481514	-4.7267928	-2.6667849
H	0.0604755	0.5693607	3.2486545
H	2.5245793	-2.6528795	-1.4522002
H	-4.6083176	2.2161656	1.6894472
H	2.4106480	0.1693912	0.5250380
H	1.4831991	1.3356760	1.4897440
H	-0.7267997	3.3602954	0.2800611
H	-2.8791395	3.9517141	1.3374792
C	2.8112567	3.8736484	-1.7588742
C	2.1006793	4.4248203	-2.8194782
C	2.3007968	2.7776085	-1.0710741
C	0.8750818	3.8807367	-3.2004455
C	1.0712874	2.2319798	-1.4499856
C	0.3611289	2.7846198	-2.5238913
C	-0.2350810	-5.0789338	0.0292347
C	0.4228746	-5.3392813	-1.2025510
C	-2.2245929	0.3010798	0.2311182
C	-0.9100009	-2.6909929	2.9191139
C	0.0614384	-3.8902156	0.6373485
C	-3.4307534	0.6389702	0.8304597
C	-0.1849065	-2.9519410	1.7848383
C	1.3376734	-4.4631654	-1.7497136
C	-0.7506925	-1.3929920	3.4517838
C	0.9716624	-2.9533606	0.0684917
C	1.6602677	-3.2215147	-1.1198658
C	-1.2448673	1.2789423	0.0389706
C	0.6810691	-1.9919932	1.2002697
C	0.0289311	-0.4289195	2.8285279
C	0.7622755	-0.6882764	1.6458366
C	-3.6640088	1.9518253	1.2303814
C	1.4125787	0.4333826	0.8796171
C	-1.4806098	2.5988088	0.4392439
C	-2.6921253	2.9298921	1.0327184
Au	0.4262289	-1.2142896	-1.6361505
P	0.3639731	0.8077613	-0.6131472

Table 1: PPh2, No Ligand, TS

46

H	-1.0582935	-5.9767348	0.6020134
H	-1.7324444	-6.5987821	-1.7075477
H	0.4759864	-4.2635708	2.8943053
H	1.9016020	-2.4423524	3.8188112
H	-1.4120135	-5.0555759	-3.5840456
H	2.4149811	-0.4469394	2.5043599
H	-0.4730083	-2.7839485	-3.2246197
H	2.0918308	0.0479872	-0.9559104
H	2.2229962	0.9150408	0.5746276
C	-1.0046429	-5.2479703	-0.1965317
C	-1.3537167	-5.6032164	-1.5134914
C	0.6785486	-3.3731304	2.3133625

C	-0.5486550	-3.9676702	0.0143076
C	0.1726264	-3.2035969	1.0392659
C	-1.1711992	-4.7335285	-2.5790142
C	1.4979496	-2.3546641	2.8184221
C	-0.4416379	-3.0555926	-1.0647873
C	-0.6568673	-3.4376576	-2.3811108
C	0.5033411	-2.0614625	0.2942802
C	1.8072814	-1.2293916	2.0649470
C	1.3318514	-1.0428972	0.7501423
C	1.5918774	0.2396131	-0.0037910
Au	-0.9599001	-0.9515049	-0.9907630
P	-0.0316650	1.0726553	-0.4165130
C	-0.6337315	1.7671537	1.1292154
C	-1.9143073	1.4404500	1.5811254
C	-2.3788756	1.9567230	2.7856990
C	-1.5664605	2.7965814	3.5400482
C	-0.2878256	3.1259340	3.0929463
C	0.1810607	2.6149190	1.8908323
H	-2.5420390	0.7857839	0.9877288
H	-3.3721667	1.7031953	3.1331586
H	-1.9283037	3.1978891	4.4782767
H	0.3413188	3.7822678	3.6807138
H	1.1717047	2.8828728	1.5423904
C	0.3415810	2.4146379	-1.5564207
C	-0.1040799	3.7161644	-1.3082477
C	0.1644023	4.7242148	-2.2277204
C	0.8713554	4.4402281	-3.3912386
C	1.3076477	3.1413118	-3.6460401
C	1.0390005	2.1284523	-2.7371089
H	-0.6557490	3.9400604	-0.4045496
H	-0.1801366	5.7317605	-2.0327330
H	1.0796561	5.2284339	-4.1035266
H	1.8526697	2.9188275	-4.5544981
H	1.3664500	1.1170290	-2.9507703

Table 1: PPh2, No Ligand, II

46

C	-1.3891292	-1.3150406	0.2759177
C	-2.1061296	-0.1382854	0.1873544
C	-3.4093354	-0.1944040	0.7085216
C	-3.9070132	-1.3766058	1.2425313
C	-3.1414313	-2.5396831	1.2737353
C	-1.8344378	-2.5400164	0.7790513
H	-4.0245391	0.6971913	0.6805466
H	-4.9155074	-1.3950971	1.6353401
H	-3.5572957	-3.4527512	1.6813021
C	-0.8885958	-3.6509946	0.7025734
C	-1.1260178	-4.9613678	1.1100626
C	0.3587933	-3.3176652	0.1390092
C	-0.1319365	-5.9239312	0.9529828
H	-2.0785294	-5.2378824	1.5461509
C	1.3449196	-4.2747075	-0.0225219
C	1.0943107	-5.5881975	0.3905684
H	-0.3173438	-6.9422829	1.2695852
H	2.3069908	-4.0287651	-0.4591519
H	1.8616641	-6.3426301	0.2696804
C	-1.5503079	1.0998130	-0.4721887
P	0.2931687	1.0442116	-0.5277624
Au	0.5381531	-1.3244079	-0.3264826
H	-1.8764059	1.1401282	-1.5156417
H	-1.8958311	2.0134055	0.0143858
C	0.8928001	1.9055941	0.9357030
C	2.1754413	2.4664678	0.9332360
C	2.6700215	3.0646993	2.0850275
C	1.8973677	3.0976538	3.2428494
C	0.6269123	2.5288653	3.2516643
C	0.1231540	1.9292635	2.1040562
H	2.7773311	2.4473562	0.0327487
H	3.6580304	3.5070300	2.0774762
H	2.2856576	3.5659057	4.1383135
H	0.0265534	2.5521434	4.1521509
H	-0.8622292	1.4795037	2.1251792
C	0.8385041	1.9429381	-1.9840621
C	0.8605693	3.3432027	-2.0004912
C	1.2379366	4.0108049	-3.1576426
C	1.5946544	3.2907002	-4.2962664
C	1.5748912	1.8993492	-4.2830966
C	1.1985553	1.2238277	-3.1284389
H	0.5919044	3.9033984	-1.1132832
H	1.2557898	5.0930950	-3.1719500
H	1.8912573	3.8168124	-5.1948041
H	1.8551991	1.3418379	-5.1674949
H	1.1814854	0.1395170	-3.1164246

Table 1: PMe2, Chloride, I

33

H	0.1136582	-4.7598875	-0.9684109
H	1.4092013	-4.4166433	-3.0753727
H	-1.2945312	-3.2714103	2.3130500
H	-1.5372953	-1.2836389	3.8098468
H	2.3580936	-2.2492792	-3.6517679
H	-0.5945751	0.8771226	3.2257490
H	2.0808537	-0.2637158	-2.1689098
H	1.6936049	1.5328008	0.3604993
H	1.0549469	2.1946289	1.8574352
C	-1.8809924	2.7674926	1.0212079
C	0.5244590	-3.7872232	-1.2079127
C	1.2610448	-3.5831547	-2.3995704
C	-0.8722610	-2.3156650	2.0306141
C	0.3797218	-2.6873051	-0.4046100
C	-0.1741623	-2.1074455	0.8713212
C	1.8008897	-2.3492290	-2.7282994
C	-1.0064170	-1.1832187	2.8709014
C	0.9306932	-1.4211224	-0.7426654
C	1.6464329	-1.2167077	-1.8933047
C	-0.8842597	1.6541002	-1.4135918
C	0.3729785	-0.8410699	0.5304212
C	-0.4723645	0.0492243	2.5361007
C	0.2468825	0.2696152	1.3293607
C	0.7908389	1.6178514	0.9683218
Au	0.5156075	4.6567857	-0.5376714
P	-0.3726348	2.6842032	0.0000379
H	-1.6525529	2.1908628	-1.9710944
H	-0.0349033	1.4855778	-2.0744574
H	-1.2788232	0.6948183	-1.0754349
H	-2.6423465	3.3208327	0.4706178
H	-1.6682311	3.3045581	1.9456659
H	-2.2501647	1.7672173	1.2530526
Cl	1.4366075	6.6690243	-1.0811295

Table 1: PMe2, Chloride, TS

33

H	-1.1720617	-4.4876305	-0.2744654
H	0.0753146	-5.1870084	-2.3151446
H	-1.7011828	-2.8071980	2.3049247
H	-1.2525818	-1.0775532	4.0478582
H	1.5563340	-3.6134081	-3.4795532
H	0.0916149	0.9026484	3.5156448
H	1.7425951	-1.2502564	-2.7564177
H	2.0783359	1.4978208	0.7031372
H	1.1903884	2.3537294	1.9775152
C	1.1124166	3.9234472	-0.8235390
C	-0.5824763	-3.7693350	-0.8315127
C	0.1467129	-4.1648655	-1.9642605
C	-1.1851940	-1.8892572	2.0511196
C	-0.4735183	-2.4534169	-0.4324777
C	-0.7249374	-1.6550662	0.7711597

C	0.9884776	-3.2773950	-2.6201839
C	-0.9007273	-0.9314820	3.0340709
C	0.3185997	-1.5443541	-1.1545085
C	1.1071006	-1.9353188	-2.2123862
C	-1.2886986	3.2729103	0.6289795
C	-0.0233072	-0.4703714	0.4398352
C	-0.1353865	0.1861695	2.7336763
C	0.3460900	0.4379897	1.4333360
C	1.0823285	1.7061031	1.1046196
Au	-0.4005564	0.6295133	-1.5118300
P	0.1135632	2.5058506	-0.2518292
H	-1.9410550	3.7663463	-0.0916772
H	-1.8559520	2.4872429	1.1291140
H	-0.9429195	3.9995213	1.3677292
H	0.5490741	4.4703908	-1.5805970
H	2.0317859	3.5555826	-1.2799172
H	1.3582122	4.5966787	0.0011269
Cl	-1.3083893	0.2219717	-3.6635469

Table 1: PMe2, Chloride, II

33

C	-0.7326777	0.0348204	0.0614142
C	-1.4964847	1.1997130	0.0031289
C	-2.8148070	1.1553301	0.4748991
C	-3.3396055	-0.0336649	0.9682714
C	-2.5741434	-1.1981746	0.9961624
C	-1.2559920	-1.1797626	0.5414048
H	-3.4297375	2.0482958	0.4483929
H	-4.3604196	-0.0559051	1.3305647
H	-3.0088377	-2.1155258	1.3755086
C	-0.3217797	-2.3103438	0.4881953
C	-0.6122148	-3.6177473	0.8786798
C	0.9615967	-2.0071123	-0.0191035
C	0.3560510	-4.6110256	0.7651603
H	-1.5926849	-3.8658178	1.2699112
C	1.9226465	-2.9997367	-0.1283263
C	1.6172403	-4.3058467	0.2633434
H	0.1244660	-5.6250300	1.0689879
H	2.9055789	-2.7578295	-0.5135804
H	2.3681614	-5.0827711	0.1763405
C	-0.9178172	2.4561171	-0.6143853
P	0.9174913	2.3005540	-0.7008526
Au	1.2048934	-0.0162095	-0.4872846
H	-1.2776183	2.5665103	-1.6431561
H	-1.2130736	3.3603039	-0.0755482
C	1.5818873	3.2192724	0.7216588
C	1.4888467	3.2007709	-2.1712658
H	1.2255205	4.2591017	-2.1216600
H	1.0447020	2.7526367	-3.0602584
H	2.5720172	3.0899041	-2.2361402
H	1.3269232	4.2791564	0.6617050
H	2.6657427	3.1000660	0.7390863
H	1.1708247	2.7954927	1.6383257
Cl	3.4933038	-0.0355422	-1.0995800

Table 1: PMe2, Pyridine, I

43

H	0.3399865	-4.5221900	-0.0760671
H	1.8223263	-4.1150951	-2.0443956
H	-1.2425526	-3.1720187	3.1981370
H	-1.5048951	-1.2740373	4.7983056
H	2.9290620	-1.9738912	-2.3906355
H	-0.4329565	0.8740838	4.4244159
H	2.6353970	-0.0773322	-0.7967834
H	2.1112537	1.5967436	1.8276982
H	1.2274336	2.2792969	3.2003629
C	0.9042061	4.1984306	0.8186383
C	0.8096328	-3.5574398	-0.2188316
C	1.6537919	-3.3170801	-1.3317554
C	-0.7548881	-2.2246619	3.0099483
C	0.6550639	-2.5060211	0.6468528
C	0.0395484	-1.9821603	1.9206260
C	2.2852431	-2.0983257	-1.5289339
C	-0.9004518	-1.1417126	3.9097299
C	1.2971666	-1.2517065	0.4405925
C	2.1220788	-1.0160123	-0.6299822
C	-1.4333348	3.0350506	2.0691369
C	0.6713252	-0.7293821	1.7068163
C	-0.2907701	0.0842060	3.6952277
C	0.5275383	0.3347020	2.5634783
C	1.1253358	1.6853238	2.2887331
Au	-0.4113311	1.4187620	-0.7347855
P	0.0566886	2.6172778	1.1166265
H	-2.1056205	3.6301706	1.4512102
H	-1.9426309	2.1171452	2.3621910
H	-1.1633705	3.6030645	2.9614295
H	0.2797085	4.8351971	0.1915715
H	1.8481137	4.0187119	0.3039939
H	1.0982914	4.7057371	1.7653919
N	-0.9079038	0.3024793	-2.4415468
C	-1.2764754	0.9125125	-3.5854669
C	-1.6209510	0.1979916	-4.7182371
C	-1.5886891	-1.1919176	-4.6746194
C	-1.2089937	-1.8175680	-3.4939625
C	-0.8733793	-1.0429208	-2.3970371
H	-1.2886288	1.9933650	-3.5711295
H	-1.9093379	0.7280704	-5.6154919
H	-1.8541059	-1.7751381	-5.5470656
H	-1.1648119	-2.8947034	-3.4128732
H	-0.5631132	-1.4870075	-1.4615138

Table 1: PMe2, Pyridine, TS

43

H	-1.0504567	-3.9833692	1.9376595
H	0.6598976	-5.2095030	0.6097814
H	-2.1888434	-1.6352887	3.6616380
H	-2.1669343	0.5565095	4.8442325
H	2.4804883	-4.0042613	-0.5133258
H	-0.6733426	2.3567045	4.1221650
H	2.5870125	-1.5245761	-0.4808143
H	2.0674156	2.1506889	1.9853810
H	0.8815903	3.3282960	2.5671812
C	1.8465500	3.8650764	-0.4677447
C	-0.3118589	-3.4398969	1.3616585
C	0.6764274	-4.1273442	0.6364889
C	-1.5879126	-0.8152710	3.2894512
C	-0.2611741	-2.0601719	1.3633629
C	-0.7890134	-0.9543449	2.1712217
C	1.7082396	-3.4478626	0.0033538
C	-1.5468335	0.4086983	3.9694132
C	0.7380100	-1.3808720	0.6393290
C	1.7749140	-2.0398784	0.0155903
C	-0.9477886	3.7339778	0.2796921
C	0.0211758	0.1111332	1.7264799
C	-0.6951444	1.4277526	3.5640149
C	0.1397104	1.3014687	2.4358883
C	1.0105343	2.4310839	1.9591886
Au	0.2731913	0.5332464	-0.4840424
P	0.5755609	2.7399888	0.1908524
H	-1.2953330	3.9658940	-0.7270089
H	-1.7190129	3.1571333	0.7911915
H	-0.7686013	4.6628162	0.8246872
H	1.5887820	4.1423239	-1.4904664
H	2.8128338	3.3605457	-0.4763953
H	1.9147341	4.7687939	0.1412219
N	-0.2700475	-0.5446414	-2.3522290
C	-0.6871025	-1.8209354	-2.3012791

C	-1.0779304	-2.5159897	-3.4343678
C	-1.0294247	-1.8771132	-4.6673283
C	-0.5951153	-0.5574954	-4.7209894
C	-0.2292021	0.0750463	-3.5445514
H	-0.6991353	-2.2829728	-1.3231093
H	-1.4110880	-3.5409033	-3.3434626
H	-1.3244817	-2.3968310	-5.5699307
H	-0.5400779	-0.0197717	-5.6578005
H	0.1087870	1.1021157	-3.5362789

Table 1: PMe2, Pyridine, II

43

C	-1.8624888	0.0748573	0.3928482
C	-2.6639281	1.2096682	0.2983916
C	-3.9659895	1.1427690	0.8091857
C	-4.4351766	-0.0383704	1.3706357
C	-3.6314092	-1.1751368	1.4265365
C	-2.3279847	-1.1355770	0.9345467
H	-4.6105710	2.0123827	0.7578609
H	-5.4439855	-0.0779363	1.7615916
H	-4.0260613	-2.0892185	1.8525693
C	-1.3710406	-2.2443425	0.8819245
C	-1.6140512	-3.5455158	1.3174947
C	-0.1212712	-1.9331099	0.3045092
C	-0.6364965	-4.5265107	1.1739410
H	-2.5670090	-3.8011321	1.7652272
C	0.8455310	-2.9148510	0.1545534
C	0.5860649	-4.2177322	0.5908094
H	-0.8343206	-5.5354582	1.5130727
H	1.8021640	-2.6956884	-0.3038745
H	1.3407065	-4.9852639	0.4699638
C	-2.1457070	2.4482862	-0.3944370
P	-0.3115844	2.4064307	-0.3785136
Au	0.0636849	0.0622388	-0.1908747
H	-2.4600967	2.4540885	-1.4434947
H	-2.5173817	3.3702410	0.0586742
C	0.1956505	3.2849598	1.1316225
C	0.2776595	3.4208212	-1.7679064
H	-0.1174428	4.4360097	-1.6964252
H	-0.0463216	2.9764100	-2.7093655
H	1.3675707	3.4626429	-1.7540972
H	-0.1430676	4.3220898	1.1019613
H	1.2815645	3.2640702	1.2287731
H	-0.2443977	2.7852253	1.9951266
N	2.1405061	-0.0615078	-0.7500981
C	2.5160693	0.0184503	-2.0377050
C	3.8404626	-0.0966223	-2.4240865
C	4.8113831	-0.2969611	-1.4489010
C	4.4192160	-0.3797868	-0.1178461
C	3.0752408	-0.2626035	0.1947308
H	1.7248389	0.1683223	-2.7601193
H	4.0986537	-0.0332855	-3.4723197
H	5.8543598	-0.3914442	-1.7223423
H	5.1386087	-0.5410693	0.6732964
H	2.7178475	-0.3408395	1.2125599

Table 1: PMe2, OTf, I

40

H	0.0339879	-4.9611516	0.2569752
H	0.4697710	-4.7005263	-2.1877910
H	-0.1000866	-3.3341796	3.7703283
H	0.1699866	-1.2816077	5.1712673
H	1.1965174	-2.5775050	-3.1377356
H	0.8490557	0.8430843	4.2043673
H	1.5556095	-0.5704525	-1.7267241
H	2.1188481	1.3715156	0.7851116
H	1.7514062	2.1542332	2.3311878
C	0.4235788	3.8933748	0.3130845
C	0.3687188	-4.0125066	-0.1434602
C	0.6210310	-3.8557923	-1.5270584
C	0.2162581	-2.4013669	3.3215161
C	0.5643392	-2.8944971	0.6237430
C	0.4972932	-2.2599800	1.9888546
C	1.0426210	-2.6511216	-2.0691573
C	0.3649225	-1.2309420	4.1067961
C	0.9882250	-1.6582435	0.0662904
C	1.2453872	-1.5013411	-1.2713113
C	-1.2565592	2.5010935	2.2024764
C	0.9070817	-1.0198718	1.4266213
C	0.7506095	-0.0213853	3.5563655
C	1.0337167	0.1267207	2.1710692
C	1.3697371	1.4632049	1.5743733
Au	-0.9722650	1.0500940	-0.8580789
P	-0.1213441	2.2266943	0.8078772
H	-2.1532928	3.0045463	1.8413824
H	-1.5388386	1.5380123	2.6270792
H	-0.7789175	3.1118146	2.9713949
H	-0.4268842	4.4512937	-0.0791306
H	1.1721888	3.8088240	-0.4748791
H	0.8480324	4.4273913	1.1657250
O	-1.8042447	-0.0305091	-2.4203692
S	-1.0996098	-0.0414948	-3.7614153
C	-2.1188529	1.2028473	-4.6941615
O	0.2217609	0.5417224	-3.6951969
O	-1.2913504	-1.2854190	-4.4500315
F	-2.0832787	2.3983856	-4.0759107
F	-3.3967074	0.8159849	-4.7784162
F	-1.6384522	1.3590562	-5.9330586

Table 1: PMe2, OTf, TS

40

Energy =

H	-0.0119755	-5.0028145	0.7924356
H	1.6510919	-5.3662589	-1.0280955
H	-1.3507614	-3.3645580	3.2394286
H	-1.6192837	-1.4535947	4.8241994
H	2.8335667	-3.4745253	-2.0489626
H	-0.7729082	0.7711532	4.2504412
H	2.3241275	-1.1343579	-1.3941928
H	1.3887656	1.6823307	1.6234780
H	0.1722281	2.3474141	2.7272424
C	0.1192482	3.6373260	-0.2513842
C	0.4409930	-4.1588335	0.2867080
C	1.4065462	-4.3575282	-0.7189584
C	-1.0486386	-2.3645864	2.9537009
C	0.1425258	-2.8593880	0.6249475
C	-0.4790525	-2.1055110	1.7264588
C	2.0801617	-3.2906081	-1.2930777
C	-1.1653827	-1.2936406	3.8542215
C	0.7795474	-1.7776035	-0.0182748
C	1.7975461	-1.9580897	-0.9303248
C	-2.2654342	2.5859324	1.0269121
C	-0.0395073	-0.8078767	1.3714309
C	-0.6773834	-0.0356154	3.5319853
C	-0.0784329	0.2451532	2.2869199
C	0.3337175	1.6419614	1.9093338
Au	-0.3382445	0.0787437	-0.6685992
P	-0.6260509	2.1074634	0.3896978
H	-2.9120478	2.8548290	0.1914381
H	-2.7030496	1.7336836	1.5479555
H	-2.1874278	3.4316914	1.7136196
H	-0.4873195	4.0002554	-1.0813271
H	1.1111948	3.4032002	-0.6383749
H	0.1830979	4.4060411	0.5216674
O	-0.2522862	-0.3278577	-2.8933034
S	0.8013717	0.5189767	-3.5283522
C	-0.2110213	1.8803841	-4.2903662
O	1.4596218	-0.1172242	-4.6362727

O	1.6241148	1.2089766	-2.5446461
F	-0.9343241	2.5258019	-3.3450574
F	0.5779479	2.7859901	-4.8840616
F	-1.0668826	1.4031641	-5.2005910

Table 1: PMe2, OTf, II

40

C	-1.5071221	0.0156053	0.3845768
C	-2.1831483	1.2145458	0.1774003
C	-3.5176398	1.3013160	0.5949632
C	-4.1429234	0.2061690	1.1779189
C	-3.4621059	-0.9969996	1.3495114
C	-2.1302063	-1.1110773	0.9537180
H	-4.0644865	2.2267103	0.4533199
H	-5.1751461	0.2873870	1.4961870
H	-3.9708436	-1.8438928	1.7941959
C	-1.2819376	-2.3013954	1.0484289
C	-1.6696359	-3.5455054	1.5448220
C	0.0325480	-2.1290352	0.5703938
C	-0.7614863	-4.6002843	1.5618125
H	-2.6766772	-3.6966195	1.9169334
C	0.9371759	-3.1775372	0.5905313
C	0.5336951	-4.4202350	1.0874695
H	-1.0666752	-5.5655709	1.9474598
H	1.9477207	-3.0349659	0.2295362
H	1.2367292	-5.2447401	1.1039334
C	-1.4989749	2.3543532	-0.5359404
P	0.3298534	2.1321573	-0.4717991
Au	0.4306442	-0.2128080	-0.0627427
H	-1.7807715	2.3491684	-1.5944802
H	-1.7882792	3.3288885	-0.1344613
C	0.8751019	3.0894523	0.9744622
C	0.9554155	3.0186231	-1.9289238
H	0.5591750	4.0365346	-1.9351469
H	0.6396479	2.4996311	-2.8335082
H	2.0419473	3.0391427	-1.8896689
H	0.6222242	4.1442453	0.8499406
H	1.9524779	2.9728914	1.0795472
H	0.3799025	2.7000862	1.8646355
O	2.4576687	-0.7177323	-0.4225129
S	3.6134682	0.2054257	-0.6961401
C	3.7336036	0.0686440	-2.5455027
O	4.8485840	-0.3156668	-0.1909989
O	3.2876734	1.5974823	-0.4576862
F	2.5591714	0.4125143	-3.1163642
F	4.6774950	0.8918856	-3.0160369
F	4.0261368	-1.1787939	-2.9197845

Table 1: PMe2, MeCN, I

38

H	-0.0166956	-4.2558869	-1.1123948
H	1.0904714	-3.6051042	-3.2545677
H	-0.9267886	-3.3360966	2.5437705
H	-0.8896703	-1.6375398	4.3720980
H	2.1828706	-1.4436746	-3.5251131
H	0.0917504	0.5630659	4.0567485
H	2.2311145	0.2348338	-1.6812476
H	2.1029602	1.6502760	1.1354607
H	1.4556735	2.1633910	2.7010032
C	0.6313397	4.2344989	0.5178129
C	0.4428540	-3.2813877	-1.2180870
C	1.0714084	-2.9011030	-2.4310100
C	-0.4683930	-2.3690728	2.3842765
C	0.4886070	-2.3544707	-0.2108577
C	0.1288209	-1.9959152	1.2089967
C	1.6946925	-1.6719479	-2.5854837
C	-0.4494384	-1.3967744	3.4125945
C	1.1095076	-1.0846806	-0.3759879
C	1.7302461	-0.7151271	-1.5420687
C	-1.3788736	2.9110540	2.1343855
C	0.7257684	-0.7202644	1.0346916
C	0.1103426	-0.1416027	3.2328020
C	0.7182674	0.2469701	2.0113019
C	1.2141308	1.6452031	1.7698025
Au	-0.8435673	1.4332348	-0.8723297
P	-0.0883522	2.6089507	0.8931553
H	-2.1842001	3.4946277	1.6885653
H	-1.7798566	1.9567442	2.4754938
H	-0.9620500	3.4563479	2.9832186
H	-0.1255313	4.8704019	0.0579105
H	1.4613538	4.1179823	-0.1789140
H	0.9899126	4.7062603	1.4344238
N	-1.4928672	0.2389072	-2.4039579
C	-1.7285702	-0.5647741	-3.1897022
C	-2.0300559	-1.5735550	-4.1816043
H	-1.1977962	-1.6488260	-4.8824551
H	-2.1697411	-2.5340158	-3.6840422
H	-2.9396448	-1.3009301	-4.7186890

Table 1: PMe2, MeCN, TS

38

H	-0.8392354	-3.0035071	-3.2872406
H	0.7338829	-1.9970510	-4.9311284
H	-1.8369293	-3.8976265	-0.4638279
H	-1.7343834	-4.2123320	2.0050870
H	2.3633883	-0.2983820	-4.2358156
H	-0.3830541	-2.7249906	3.4034650
H	2.4019109	0.5637164	-1.9069404
H	2.0937636	-0.4997364	2.4002742
H	0.9608804	-0.7686395	3.7320985
C	1.5716211	2.3590512	3.1442484
C	-0.1950689	-2.1829715	-2.9968739
C	0.7183231	-1.6325941	-3.9117660
C	-1.3101583	-3.1869253	0.1602207
C	-0.1899622	-1.6837425	-1.7107695
C	-0.6505870	-2.1012115	-0.3817390
C	1.6421842	-0.6737710	-3.5201736
C	-1.2201379	-3.3783205	1.5449837
C	0.6956418	-0.6517196	-1.3523626
C	1.6687833	-0.1762339	-2.2012460
C	-1.1191851	1.3072784	3.3647787
C	0.0696166	-1.2110462	0.4426775
C	-0.4487576	-2.5390958	2.3376202
C	0.2481681	-1.4366994	1.8040273
C	1.0356572	-0.4984755	2.6773320
Au	0.0603190	1.0118689	0.0707021
P	0.3989231	1.2063883	2.3651066
H	-1.5812323	2.2855352	3.2327028
H	-1.8184725	0.5412628	3.0280741
H	-0.8926915	1.1521585	4.4214405
H	1.1965047	3.3777711	3.0408147
H	2.5382838	2.2911316	2.6449941
H	1.6932585	2.1272211	4.2042742
N	-0.6395597	2.2929615	-1.5390945
C	-1.0061581	2.9089022	-2.4385902
C	-1.4679174	3.6855561	-3.5723604
H	-1.0443129	4.6897857	-3.5274123
H	-1.1568094	3.2016554	-4.4991439
H	-2.5564974	3.7528273	-3.5484373

Table 1: PMe2, MeCN, II

38

C	-1.4426219	0.0899365	0.2593009
C	-2.2216948	1.2400221	0.1555785
C	-3.5330139	1.1922642	0.6440306
C	-4.0338424	0.0173228	1.1901966

C	-3.2524071	-1.1340555	1.2509791
C	-1.9401392	-1.1161140	0.7821529
H	-4.1600006	2.0740498	0.5852200
H	-5.0497683	-0.0058618	1.5634754
H	-3.6700462	-2.0444668	1.6624386
C	-1.0049828	-2.2409189	0.7384745
C	-1.2742193	-3.5389062	1.1680619
C	0.2572908	-1.9467415	0.1837557
C	-0.3063643	-4.5315809	1.0436952
H	-2.2386350	-3.7815703	1.5979796
C	1.2178624	-2.9369119	0.0596236
C	0.9332111	-4.2362066	0.4899671
H	-0.5229734	-5.5381329	1.3782265
H	2.1894445	-2.7241066	-0.3682184
H	1.6829300	-5.0115633	0.3904800
C	-1.6774541	2.4729061	-0.5247988
P	0.1534506	2.4110187	-0.4736408
Au	0.4836947	0.0500520	-0.3063151
H	-1.9716207	2.4817679	-1.5796042
H	-2.0491928	3.3975408	-0.0775466
C	0.6399547	3.2609683	1.0588421
C	0.7803344	3.4299733	-1.8416527
H	0.3835465	4.4448456	-1.7745884
H	0.4823147	2.9883404	-2.7927326
H	1.8692583	3.4710167	-1.7982636
H	0.3170986	4.3033273	1.0346666
H	1.7226443	3.2216009	1.1811226
H	0.1732422	2.7563899	1.9053423
N	2.5100055	-0.1018352	-0.8892362
C	3.6021025	-0.2684583	-1.2046844
C	4.9778749	-0.4925019	-1.5990957
H	5.3217784	0.3310292	-2.2262980
H	5.6047502	-0.5575884	-0.7083903
H	5.0461878	-1.4268512	-2.1585447

Table 1: PMe2, No Ligand, I

32

C	-4.2852885	0.1560913	-0.6030198
C	-3.4318408	0.8116151	-1.5304191
C	-2.1459782	1.0346859	-1.1212116
C	-1.6755317	0.6286152	0.1600427
C	-2.5228289	0.0289010	1.1006388
C	-3.8620897	-0.2076478	0.6584675
H	-5.3110178	-0.0405185	-0.8872753
H	-3.8046765	1.1142187	-2.5002063
H	-2.2802260	-0.0555924	2.1568666
H	-4.5627838	-0.6591301	1.3485691
C	-0.7805464	1.5653428	-1.4535167
C	0.0322681	2.1199841	-2.4082497
C	1.4009618	2.1879626	-2.0686141
C	1.8942244	1.6634180	-0.8815053
C	1.0600577	1.0703815	0.0976242
C	-0.2871455	1.1138253	-0.2021011
H	-0.3226773	2.4665846	-3.3694312
H	2.0972285	2.6305361	-2.7696651
H	2.9621601	1.7006175	-0.6991734
C	1.6536693	0.3307365	1.2702587
H	1.1649577	0.5869499	2.2128950
P	1.4405586	-1.4979049	1.0384929
H	2.7192268	0.5502709	1.3726812
C	2.4428016	-1.9369049	-0.4070938
C	2.2073430	-2.2954987	2.4764004
Au	-0.8073677	-1.6083480	0.8070901
H	2.1393814	-3.3781742	2.3683020
H	1.6831974	-1.9996338	3.3849216
H	3.2569970	-2.0035494	2.5491139
H	3.4907687	-1.6922709	-0.2220872
H	2.0863671	-1.3811120	-1.2741714
H	2.3478294	-3.0044513	-0.6046239

Table 1: PMe2, No Ligand, TS

32

H	-1.1110177	-4.3922448	1.2459461
H	-0.3676844	-5.6433251	-0.7686541
H	-1.1656780	-1.9327009	3.3612132
H	-0.5671898	0.2998350	4.2888996
H	0.8551633	-4.5293364	-2.5766299
H	0.4690474	2.0143957	2.8909276
H	1.3231893	-2.0918565	-2.4909531
H	2.0526918	1.6658964	-0.2046309
H	1.2498649	2.8558798	0.8233820
C	0.8271485	3.3980784	-2.3311090
C	-0.6662019	-3.8664709	0.4109431
C	-0.2121074	-4.5730285	-0.7192665
C	-0.7289316	-1.1716514	2.7276353
C	-0.4716454	-2.5053620	0.4263381
C	-0.4693533	-1.3978670	1.3897949
C	0.4830777	-3.9466597	-1.7437331
C	-0.3702465	0.0790506	3.2478270
C	0.1629088	-1.8572301	-0.6622473
C	0.7351710	-2.5616429	-1.7123358
C	-1.4348238	3.2421113	-0.5019467
C	0.1522436	-0.4088591	0.6122332
C	0.2355836	1.0482962	2.4580361
C	0.5360530	0.8370400	1.0957021
C	1.0921526	1.9505614	0.2340333
Au	-0.4081234	0.0473364	-1.5169648
P	-0.0530653	2.2902266	-1.1947875
H	-2.1664795	3.4452371	-1.2840125
H	-1.9135703	2.6588001	0.2849404
H	-1.0730894	4.1855538	-0.0886750
H	0.1704992	3.6476446	-3.1651952
H	1.7133662	2.8971393	-2.7201021
H	1.1210468	4.3151523	-1.8166084

Table 1: PMe2, No Ligand, II

32

C	-0.6679054	-0.0091594	0.0416950
C	-1.3645273	1.1773928	-0.0732736
C	-2.6767747	1.1469594	0.4263538
C	-3.2020242	-0.0217907	0.9631821
C	-2.4566118	-1.1972643	1.0171718
C	-1.1414534	-1.2230390	0.5459946
H	-3.2770078	2.0479901	0.3804705
H	-4.2169652	-0.0201377	1.3392189
H	-2.8954054	-2.1007494	1.4220986
C	-0.2139078	-2.3490501	0.4827734
C	-0.4716231	-3.6552927	0.8902880
C	1.0410642	-2.0370905	-0.0754118
C	0.5095254	-4.6320081	0.7373910
H	-1.4295546	-3.9174881	1.3231249
C	2.0145721	-3.0063201	-0.2356355
C	1.7422739	-4.3156016	0.1782365
H	0.3083278	-5.6472564	1.0541410
H	2.9806084	-2.7754982	-0.6716198
H	2.4984002	-5.0814360	0.0592267
C	-0.7806339	2.3977315	-0.7450080
P	1.0590306	2.3268204	-0.7418934
Au	1.2718094	-0.0502996	-0.5260744
H	-1.0962543	2.4223127	-1.7929107
H	-1.1333298	3.3200130	-0.2791769
C	1.5965781	3.2368640	0.7370721
C	1.6294975	3.2839763	-2.1751492
H	1.2424151	4.3037230	-2.1289055
H	1.2889034	2.8075523	-3.0946011
H	2.7196747	3.3171359	-2.1795981
H	1.2652869	4.2754300	0.6834069

H	2.6840198	3.2098669	0.8132888
H	1.1719910	2.7657133	1.6241232

Scheme 9: 6* @ RI-TPSSh-D3(BJ)/def2-TZVPP

113

C	0.6956567	0.9720421	-0.0442224
N	1.4364881	0.8147427	1.0112089
C	1.5415991	1.0409720	-1.2990078
C	0.8570657	0.8153857	2.3448461
C	2.9200706	0.6144644	0.7443975
C	2.9672466	0.6609553	-0.7982442
C	1.4972809	2.5197451	-1.7291912
C	1.0266456	-0.0555933	-2.2613220
C	0.3461184	-0.3913889	2.8497279
C	0.7474053	2.0320604	3.0388555
C	3.3844504	-0.7242866	1.3064037
C	3.7461885	1.7280447	1.3828474
H	3.7032490	1.3887320	-1.1379579
H	3.2638654	-0.3112384	-1.1849614
H	1.8217502	3.1372970	-0.8883872
H	2.1699825	2.7185297	-2.5608461
H	0.4889180	2.8305530	-1.9989939
N	0.5001036	-1.0109009	-1.5985121
C	1.2658432	0.0633566	-3.7721712
C	0.3358629	-1.6905488	2.0648845
C	-0.2517919	-0.3577477	4.1097064
C	0.1441489	2.0019757	4.2959928
C	1.1706684	3.3713585	2.4631986
H	4.4547896	-0.8245429	1.1198087
H	3.2237200	-0.7719988	2.3842230
H	2.8773951	-1.5589678	0.8299570
H	3.5777251	1.7730306	2.4587567
H	4.8010580	1.5050872	1.2166770
H	3.5369127	2.7029715	0.9450469
C	0.0435655	-2.2756078	-2.0337666
C	0.4129658	1.2226454	-4.3422749
C	0.8885989	-1.1934655	-4.5692701
C	2.7609726	0.3361895	-4.0339565
H	0.9045785	-1.5498411	1.1473443
C	0.9514266	-2.8469166	2.8612092
C	-1.0926442	-2.0385450	1.6334711
H	-0.6651586	-1.2700917	4.5204078
C	-0.3446527	0.8209086	4.8323588
H	0.0431285	2.9249609	4.8533064
H	1.6918617	3.1906146	1.5249995
C	-0.0578116	4.2262368	2.1293496
C	2.1160784	4.1349492	3.3988948
C	0.9515091	-3.3549475	-2.0888789
C	-1.3306830	-2.4887124	-2.2608910
H	0.7905670	2.2053566	-4.0752156
H	0.4222334	1.1511073	-5.4313785
H	-0.6243311	1.1484483	-4.0112422
H	-0.1689875	-1.4349854	-4.4914127
H	1.1145881	-0.9995723	-5.6201890
H	1.4528844	-2.0681311	-4.2588647
H	3.3730300	-0.5073109	-3.7091477
H	2.9131939	0.4659053	-5.1070477
H	3.1249778	1.2352998	-3.5379941
H	0.3923870	-3.0338657	3.7799268
H	0.9253041	-3.7649992	2.2717398
H	1.9874191	-2.6445883	3.1363903
H	-1.5210814	-1.2222245	1.0482262
H	-1.0893897	-2.9382495	1.0155426
H	-1.7340117	-2.2103309	2.5001070
H	-0.8154190	0.8224938	5.8074296
H	-0.6589135	4.4128484	3.0217730
H	0.2508574	5.1896578	1.7172632
H	-0.6916402	3.7242857	1.3965355
H	2.9892435	3.5406382	3.6706455
H	2.4610236	5.0516245	2.9163824
H	1.6081270	4.4201445	4.3221647
C	0.4731976	-4.6102452	-2.4564700
C	2.4203539	-3.2055396	-1.7343229
C	-1.7543352	-3.7619440	-2.6382788
C	-2.3580596	-1.3819688	-2.1135630
H	1.1686489	-5.4392989	-2.5161454
C	-0.8655789	-4.8201940	-2.7514344
H	2.6087833	-2.1500754	-1.5331571
C	3.3603042	-3.6457132	-2.8647316
C	2.7410896	-3.9935392	-0.4561696
H	-2.8047143	-3.9267871	-2.8464912
H	-1.8579671	-0.5395720	-1.6206221
C	-3.5309084	-1.8261777	-1.2284754
C	-2.8869791	-0.9002368	-3.4714734
H	-1.2147591	-5.8002103	-3.0504985
H	4.4013244	-3.4967068	-2.5685778
H	3.2303857	-4.7056943	-3.0913444
H	3.1860014	-3.0866669	-3.7848405
H	2.0933944	-3.6917648	0.3671131
H	2.5928316	-5.0632315	-0.6179976
H	3.7807637	-3.8407635	-0.1564682
H	-4.1027134	-2.6239342	-1.7054372
H	-3.1816593	-2.1949907	-0.2645869
H	-4.2251993	-0.9997591	-1.0545823
H	-2.0864100	-0.5317686	-4.1123436
H	-3.3851297	-1.7173042	-3.9978644
H	-3.6169697	-0.0955284	-3.3441135
H	-3.8896002	2.8979789	4.8474751
C	-3.9190160	2.0299482	4.2018731
C	-4.2841423	-0.3758298	3.9041191
C	-3.4456677	1.7780505	0.8143379
H	-3.3055380	3.3536474	-2.1735133
C	-3.4367112	2.9497888	1.6553790
Au	-1.2803504	1.3735163	0.0136179
C	-3.7545007	0.9317859	2.0261839
C	-4.2096744	0.7499607	4.7170266
C	-3.6918811	2.0835271	2.8487754
C	-4.0631348	-0.3122223	2.5123466
H	-4.1393475	-1.1948420	1.8928564
C	-3.4251247	1.8828601	-0.5787198
H	-3.4604269	5.1008537	1.7597271
C	-3.4051613	4.2122628	1.1447809
H	-3.6424089	1.0543111	-1.2394175
C	-3.3383290	3.2211837	-1.0999691
H	-3.2764945	5.3068015	-0.7191335
H	-4.5261768	-1.3305259	4.3542805
C	-3.3247791	4.3208118	-0.2743836
H	-4.3934441	0.6397267	5.7785750

Scheme 9: 6_{TS} @ RI-TPSSh-D3(BJ)/def2-TZVPP

113

C	0.8908554	-0.2997882	0.8586536
N	0.6436674	-0.1832230	2.1305295
C	1.9869145	-1.3168141	0.6101515
C	-0.2765461	0.8370962	2.6131954
C	1.4041906	-1.1402256	3.0343687
C	2.1734193	-1.9923480	2.0009761
C	3.2279781	-0.4886786	0.2263198
C	1.4212545	-2.3453393	-0.3923944
C	-1.6409474	0.5151235	2.7044262
C	0.2084518	2.1351597	2.8563631
C	0.4484267	-1.9701844	3.8849373
C	2.3386226	-0.3671078	3.9618799
H	3.2278326	-2.0600085	2.2659601
H	1.7700314	-3.0028827	1.9888375
H	3.4302373	0.2326487	1.0211181
H	4.1128170	-1.1120922	0.1164351
H	3.0660185	0.0705263	-0.6943672

N	0.1502444	-2.3862437	-0.2961896
C	2.3551028	-3.1990377	-1.2571420
C	-2.2101315	-0.8418516	2.3309683
C	-2.5173851	1.5284887	3.0933966
C	-0.7163617	3.1048433	3.2445772
C	1.6552441	2.5575334	2.6679597
H	1.0398163	-2.5981253	4.5531913
H	-0.1859202	-1.3295937	4.4991505
H	-0.1775364	-2.6195667	3.2775775
H	1.7784395	0.3295354	4.5852955
H	2.8366445	-1.0814155	4.6188570
H	3.1061284	0.1790379	3.4156875
C	-0.7920795	-3.2351169	-0.9145023
C	3.0039394	-2.3111210	-2.3442141
C	1.6491610	-4.3495089	-1.9879727
C	3.4458094	-3.8306420	-0.3684939
H	-1.3844508	-1.5331159	2.1765690
C	-3.1189157	-1.3944794	3.4355459
C	-2.9566991	-0.7700260	0.9933881
H	-3.5751874	1.3097658	3.1659513
C	-2.0639119	2.8085359	3.3697519
H	-0.3702267	4.1127447	3.4366433
H	2.2354232	1.6798992	2.3864242
C	1.7934866	3.5731195	1.5255843
C	2.2513551	3.1398327	3.9573073
C	-1.2272795	-4.3842479	-0.2222002
C	-1.3994381	-2.8552199	-2.1269307
H	3.7104004	-1.5884471	-1.9456920
H	3.5452850	-2.9574837	-3.0378942
H	2.2417885	-1.7753700	-2.9125534
H	0.9177485	-3.9968997	-2.7107473
H	2.4099271	-4.9195255	-2.5260209
H	1.1416218	-5.0248977	-1.3042741
H	3.0063068	-4.5239389	0.3513267
H	4.1314804	-4.3968546	-1.0013457
H	4.0336940	-3.0956719	0.1795020
H	-3.9823564	-0.7473176	3.5984653
H	-3.4997798	-2.3781013	3.1575770
H	-2.5880375	-1.4879302	4.3842556
H	-2.2724512	-0.4648268	0.2000863
H	-3.3561506	-1.7505933	0.7285600
H	-3.7856393	-0.0597266	1.0407064
H	-2.7631968	3.5794634	3.6688899
H	1.2031594	4.4699521	1.7221626
H	2.8382337	3.8702073	1.4125261
H	1.4539530	3.1493335	0.5791318
H	2.1502019	2.4572498	4.8013459
H	3.3119398	3.3571912	3.8155345
H	1.7552053	4.0745309	4.2257890
C	-2.2326420	-5.1623857	-0.7903275
C	-0.6411706	-4.7909668	1.1180749
C	-2.4065565	-3.6652673	-2.6484647
C	-0.9997693	-1.5995980	-2.8789159
H	-2.5589286	-6.0578947	-0.2742120
C	-2.8223254	-4.8173066	-1.9980172
H	0.1079757	-4.0450268	1.3894157
C	0.0484334	-6.1614879	1.0724725
C	-1.7210838	-4.7886832	2.2076719
H	-2.8712795	-3.3871058	-3.5872959
H	-0.1993823	-1.1161430	-2.3096138
C	-2.1734409	-0.6144171	-2.9667122
C	-0.4784230	-1.9165996	-4.2878165
H	-3.6012382	-5.4364711	-2.4243546
H	0.4589368	-6.4115637	2.0537293
H	-0.6620995	-6.9444127	0.7998473
H	0.8633216	-6.1870369	0.3480959
H	-2.2215424	-3.8224166	2.2610502
H	-2.4812000	-5.5453649	2.0031404
H	-1.2854485	-5.0101489	3.1850823
H	-2.9855164	-1.0332482	-3.5642969
H	-2.5729116	-0.3940159	-1.9766150
H	-1.8624180	0.3224071	-3.4354368
H	0.3937897	-2.5708957	-4.2627485
H	-1.2486195	-2.4142653	-4.8799714
H	-0.2049381	-0.9998828	-4.8171939
H	-0.7980385	6.0905746	-0.9878998
C	-1.1978786	5.0927399	-0.8596359
C	-3.0629846	3.6359676	-0.2948816
C	0.4365732	2.2618339	-2.2702221
H	2.4671392	1.6576131	-4.8647693
C	0.6406448	3.6506668	-2.1262611
Au	0.1786734	1.0348280	-0.5040568
C	-1.0683019	2.6916116	-1.1384728
C	-2.4838916	4.8963838	-0.3313219
C	-0.4987833	3.9759107	-1.2633340
C	-2.3739374	2.4935516	-0.7428954
H	-2.8439033	1.5226849	-0.7212815
C	1.0093299	1.5307729	-3.2910827
H	1.6745171	5.3851113	-2.8760014
C	1.5359676	4.3133307	-2.9393682
H	0.7976770	0.4846520	-3.4540973
C	1.9470202	2.2088178	-4.0912482
H	2.9413496	4.0451552	-4.5479487
H	-4.0676492	3.5171230	0.0909955
C	2.2188507	3.5579940	-3.9055492
H	-3.0527258	5.7502613	0.0142651

Scheme 9: 7 @ RI-TPSSh-D3(BJ)/def2-TZVPP

113

Au	0.5652977	0.8636761	0.6485143
N	1.1975450	-1.2189380	0.0522753
C	-1.1979013	-0.2065659	0.2903659
C	0.0006480	2.5859172	1.5825598
C	2.3902993	1.8567611	0.7462569
C	0.3314308	-2.1767224	0.1062763
C	2.5946803	-1.4141242	-0.1882030
N	-2.2749273	0.0219089	-0.3990448
C	-1.0616118	-1.7029488	0.5366643
C	-1.3106823	2.9221184	1.8607285
C	1.0592711	3.3860971	2.0477272
C	2.3809981	2.9968753	1.5743925
C	3.5562074	1.5346630	0.0659006
C	0.5807095	-3.6817188	-0.1630855
C	3.0650832	-1.4424239	-1.5097754
C	3.4527541	-1.4363184	0.9231716
C	-2.8124346	-1.2327510	-1.1009435
C	-2.9179645	1.3125535	-0.5515911
C	-2.3290668	-2.2995687	-0.1235375
C	-1.1431577	-1.8116033	2.0890607
H	-2.1242801	2.3335795	1.4764711
C	-1.5916508	4.0520885	2.6310533
C	0.7637009	4.5057490	2.8262581
C	3.5549369	3.7163213	1.7935788
H	3.5958829	0.7116820	-0.6290811
C	4.7236915	2.2754175	0.2679730
C	0.1469718	-4.0073579	-1.6145905
C	-0.2324649	-4.5639007	0.8103596
C	2.0345207	-4.1863000	-0.0451263
C	2.1458961	-1.2002298	-2.6925899
C	4.4355417	-1.6193955	-1.6991181
C	2.9455649	-1.1943821	2.3364066
C	4.8103694	-1.6305283	0.6767015
C	-2.0831829	-1.3116503	-2.4434645
C	-4.3116433	-1.2281893	-1.3412657
C	-2.4348881	2.2658997	-1.4572281
C	-4.0196624	1.5555601	0.2946233
H	-2.1779316	-3.2470751	-0.6250014
H	-3.0843312	-2.4553824	0.6497275
H	-0.2583331	-1.3767916	2.5521177

H	-1.2432629	-2.8475163	2.4021059
H	-2.0186860	-1.2605485	2.4353524
H	-2.6226578	4.3102123	2.8399531
C	-0.5546957	4.8350416	3.1214364
H	1.5682417	5.1312616	3.1935879
H	3.5475748	4.5820485	2.4449758
C	4.7317048	3.3459249	1.1523568
H	5.6241054	2.0015159	-0.2682861
H	-0.8975846	-3.7950566	-1.8252438
H	0.3065592	-5.0756677	-1.7708629
H	0.7580143	-3.4697838	-2.3359362
H	0.1453129	-4.4736892	1.8296824
H	-0.1000681	-5.6020998	0.5035274
H	-1.3002275	-4.3598557	0.8158276
H	2.6829344	-3.8095403	-0.8298228
H	1.9918442	-5.2734212	-0.1403553
H	2.4840640	-3.9544968	0.9155780
H	1.1311583	-1.4599248	-2.3860496
C	2.4969670	-2.0484919	-3.9181425
C	2.1353808	0.2930235	-3.0529052
H	4.8326093	-1.6580587	-2.7051076
C	5.2981760	-1.7418625	-0.6180009
H	2.0297543	-0.6004183	2.2454188
C	3.9284287	-0.3604504	3.1656856
C	2.5830357	-2.4841108	3.0851884
H	5.4995693	-1.6694239	1.5096537
H	-2.3537672	-0.4715126	-3.0800690
H	-2.3702420	-2.2305396	-2.9562512
H	-1.0005138	-1.3085417	-2.3100835
H	-4.8839333	-1.3278505	-0.4233091
H	-4.5550912	-2.0773878	-1.9815770
H	-4.6227670	-0.3200471	-1.8588097
C	-1.2283806	2.0676399	-2.3546469
C	-3.1108798	3.4873030	-1.5163993
C	-4.5068255	0.5740796	1.3524675
C	-4.6475612	2.7944564	0.1913538
H	5.6415726	3.9080090	1.3222359
H	3.4473432	-1.7402228	-4.3574822
H	1.7312664	-1.9278845	-4.6871323
H	2.5727301	-3.1092037	-3.6706261
H	1.8237724	0.9042427	-2.2046612
H	1.4508168	0.4783313	-3.8836630
H	3.1324261	0.6227787	-3.3518020
H	6.3572180	-1.8918878	-0.7860220
H	4.8241900	-0.9307006	3.4208913
H	3.4533890	-0.0640246	4.1026359
H	4.2292295	0.5405924	2.6313715
H	1.7549125	-3.0137356	2.6118537
H	2.2855654	-2.2484713	4.1091845
H	3.4377036	-3.1628488	3.1300282
H	-0.7742470	1.1024384	-2.1198611
C	-0.1736589	3.1582153	-2.1120147
C	-1.6394004	2.0675097	-3.8351346
H	-2.7614285	4.2453737	-2.2054861
C	-4.2030659	3.7524743	-0.7086459
H	-4.0380023	-0.3934443	1.1684018
C	-6.0290700	0.3822196	1.2955408
C	-4.0936025	1.0063651	2.7687252
H	-5.4890642	3.0154693	0.8352844
H	-0.5647428	4.1416409	-2.3787766
H	0.7051362	2.9730861	-2.7312290
H	0.1381661	3.1917544	-1.0686094
H	-2.4205964	1.3359839	-4.0494285
H	-0.7768076	1.8479819	-4.4672017
H	-2.0231319	3.0479924	-4.1240830
H	-4.7042868	4.7100843	-0.7722370
H	-6.5499612	1.2839545	1.6216874
H	-6.3281672	-0.4262153	1.9655512
H	-6.3750193	0.1457521	0.2885371
H	-3.0108462	1.0240571	2.8936253
H	-4.5121167	0.3141582	3.5024922
H	-4.4725264	2.0051975	2.9944190
H	-0.7698729	5.7087645	3.7238202

H2O @ RIJCOSX-TPSSh-D3(BJ)/def2-TZVPP + C-PCM

3

O	-0.0250421	-0.0000000	-0.1694490
H	0.1881183	0.0000000	0.7719108
H	0.8369240	0.0000000	-0.6024618

Biphenylene @ RIJCOSX-TPSSh-D3(BJ)/def2-TZVPP + C-PCM

20

H	3.1822368	0.0108748	-0.00000658
H	3.4259430	2.4979109	-0.00000011
H	0.8448414	-3.0680996	-0.00000843
H	-1.4851294	-3.9712264	-0.00000288
H	1.4851325	3.9712277	0.00000205
H	-3.4259449	-2.4979125	0.00000611
H	-0.8448379	3.0681020	0.00000018
C	2.3070514	0.6485165	0.00000818
C	2.4346030	2.0599209	0.00000371
C	-0.0042372	-2.3960221	0.00000679
C	1.0221015	0.1707873	0.00000536
C	0.1108515	-1.0300311	0.00000394
C	1.3292346	2.8985925	-0.00000580
C	-1.3292336	-2.8985911	0.00000367
C	-0.1108523	1.0300308	-0.00000143
C	0.0042389	2.3960217	-0.00001197
C	-1.0221032	-0.1707887	-0.00000303
C	-2.4346050	-2.0599218	-0.00000236
C	-2.3070532	-0.6485174	-0.00000912
H	-3.1822377	-0.0108743	0.00001193

1 water complex @ RIJCOSX-TPSSh-D3(BJ)/def2-TZVPP + C-PCM

76

N	-1.7574355	0.3364677	-0.8110312
C	-0.5499805	-0.1914392	-0.4869495
N	-0.1809416	-0.9251132	-1.5676526
C	-1.1469161	-0.8552614	-2.5576877
C	-2.1393837	-0.0690380	-2.0806935
Au	0.5548973	0.1526407	1.0980382
H	-1.0375995	-1.3798486	-3.4895870
H	-3.0793011	0.2271837	-2.5084817
C	-2.5824793	1.1315134	0.0701539
C	-3.2974724	0.4706610	1.0782069
C	-4.0999206	1.2521058	1.9122064
C	-4.1965087	2.6235280	1.7320040
C	-3.4882138	3.2465823	0.7121255
C	-2.6602725	2.5168027	-0.1417242
C	-3.2685397	-1.0329282	1.2764280
H	-4.6625396	0.7724239	2.7041719
H	-4.8283400	3.2114877	2.3871332
H	-3.5736425	4.3178827	0.5807970
C	-1.9042162	3.2133058	-1.2575655
C	0.9488657	-1.8247947	-1.6102869
C	0.6916309	-3.1824198	-1.3712569
C	1.7704675	-4.0638894	-1.4380246
C	3.0494739	-3.6051058	-1.7241938
C	3.2709373	-2.2549531	-1.9525146
C	2.2249631	-1.3304290	-1.9024316
C	-0.6951769	-3.7117114	-1.0616756
H	1.6044329	-5.1197608	-1.2605130
H	3.8768820	-4.3031462	-1.7711276
H	4.2704189	-1.9074749	-2.1810143

C	2.5044541	0.1306277	-2.1866443
C	-4.6551297	-1.6352487	1.0006638
C	-2.7892241	-1.4007367	2.6870962
H	-2.5682949	-1.4669934	0.5633693
H	-1.0486006	2.5892156	-1.5238914
C	-2.7928508	3.3778615	-2.5024829
C	-1.3761635	4.5897561	-0.8342718
C	2.8507522	0.3270647	-3.6701943
C	3.6298412	0.6595205	-1.2903282
H	1.6035344	0.7050220	-1.9685185
C	-0.7214058	-4.4578769	0.2789483
C	-1.1973456	-4.6008230	-2.2088727
H	-1.3785830	-2.8668685	-0.9763002
H	-2.1933175	5.3101049	-0.7447519
H	-0.8496144	4.5452535	0.1180890
H	-0.6841395	4.9662890	-1.5894660
H	-2.7543985	-2.4871265	2.7974057
H	-3.4692156	-1.0063181	3.4453165
H	-1.7922417	-0.9972333	2.8787046
H	-4.9769521	-1.4292877	-0.0227422
H	-5.4002735	-1.2181506	1.6821093
H	-4.6308019	-2.7178883	1.1481218
H	-3.1761284	2.4245442	-2.8669879
H	-2.2230109	3.8495291	-3.3068184
H	-3.6464746	4.0191060	-2.2678994
H	-0.0768404	-5.3390111	0.2540500
H	-1.7379761	-4.7893289	0.5017898
H	-0.3837320	-3.8088052	1.0892489
H	3.3748216	0.5426281	-0.2358369
H	4.5652412	0.1283958	-1.4797051
H	3.7965271	1.7193857	-1.4847596
H	3.7481629	-0.2386784	-3.9326006
H	2.0355116	-0.0095315	-4.3141435
H	3.0433189	1.3829613	-3.8743545
H	-1.2142019	-4.0493061	-3.1514205
H	-2.2080070	-4.9573532	-1.9982059
H	-0.5481109	-5.4699477	-2.3375074
F	3.5981583	5.2327065	1.9204215
F	3.8824973	4.1723792	-0.5286569
Sb	2.5150549	4.1623788	0.7909768
F	1.1648414	4.0572056	2.1276591
F	3.3056383	2.5895566	1.5877658
F	1.4534410	3.0620387	-0.3282328
F	1.7444158	5.7269896	0.0465417
O	1.8252208	0.6398268	2.7087795
H	2.4145220	1.3692133	2.4082870
H	2.4053621	-0.0965357	2.9513957

1 SbF6 complex @ RIJCOSX-TPSSh-D3(BJ)/def2-TZVPP + C-PCM

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N	0.6715191	1.0179172	-1.1661589
C	0.1272523	0.1206303	-0.3163999
N	0.2224709	-1.0741495	-0.9411919
C	0.8266083	-0.9294351	-2.1785628
C	1.1105580	0.3890186	-2.3206265
Au	-0.6342963	0.4222262	1.4520802
H	0.9932739	-1.7707640	-2.8273014
H	1.5766144	0.9382902	-3.1192095
F	-1.4784758	0.6915934	3.3894702
C	-0.2342969	-2.3051660	-0.3472336
C	-1.5550349	-2.7029878	-0.5814163
C	-1.9863633	-3.8713441	0.0480571
C	-1.1337096	-4.5928012	0.8742274
C	0.1722732	-4.1672170	1.0841878
C	0.6551184	-3.0093407	0.4724772
C	-2.5002547	-1.8999435	-1.4537591
H	-3.0042270	-4.2104329	-0.1008406
H	-1.4913701	-5.4916772	1.3617504
H	0.8248496	-4.7366926	1.7351827
C	2.0807490	-2.5486585	0.7062317
C	0.7867753	2.4232882	-0.8728213
C	-0.2542173	3.2698766	-1.2706784
C	-0.1286847	4.6230497	-0.9530121
C	0.9867625	5.0949071	-0.2708006
C	1.9987616	4.2236713	0.1133723
C	1.9197552	2.8607450	-0.1772197
C	-1.4926375	2.7514603	-1.9752807
H	-0.9155090	5.3112457	-1.2376203
H	1.0653226	6.1489376	-0.0316992
H	2.8590204	4.6030224	0.6516178
C	3.0133616	1.9117818	0.2722008
C	2.3172737	-2.2037563	2.1822465
H	2.2460843	-1.6399408	0.1261224
C	3.0849997	-3.6000965	0.2145112
H	-1.3280906	1.7036897	-2.2308723
C	-1.7638573	3.5093176	-3.2804294
C	-2.7058992	2.8137396	-1.0352870
H	2.7587739	0.9077295	-0.0687970
C	4.3641233	2.2833804	-0.3540943
C	3.1033391	1.8706360	1.8035788
C	-3.0327156	-2.7429515	-2.6200152
H	-1.9461985	-1.0615399	-1.8784689
C	-3.6501444	-1.3166829	-0.6207573
H	-3.6196457	-3.5898561	-2.2570689
H	-3.6778909	-2.1329798	-3.2567297
H	-2.2132116	-3.1311982	-3.2286094
H	-4.3017061	-0.7108189	-1.2550957
H	-4.2496503	-2.1136636	-0.1751234
H	-3.2678018	-0.6866494	0.1849598
H	-2.9162712	3.8457671	-0.7446033
H	-3.5898469	2.4098413	-1.5334739
H	-2.5260333	2.2319823	-0.1285647
H	4.3043327	2.2788478	-1.4445948
H	5.1282706	1.5664991	-0.0454100
H	4.6830737	3.2774507	-0.0326219
H	-2.6280511	3.0746227	-3.7876899
H	-0.9041906	3.4539166	-3.9518179
H	-1.9813788	4.5627972	-3.0893873
H	2.9387184	-3.8170951	-0.8456297
H	2.9791239	-4.5334779	0.7721117
H	4.1055091	-3.2362756	0.3558014
H	3.3395305	-1.8445444	2.3222004
H	2.1745278	-3.0812483	2.8166816
H	1.6270203	-1.4270112	2.5159903
H	2.1482427	1.5719535	2.2407777
H	3.8640026	1.1512469	2.1143816
H	3.3733887	2.8499587	2.2053499
Sb	-2.1343701	-0.8033999	4.5210071
F	-0.4019088	-1.5547586	4.4015091
F	-3.8161631	0.0582941	4.5361840
F	-2.7570889	-2.2187731	5.6024530
F	-1.5911711	0.2272407	6.0081542
F	-2.6190181	-1.6932458	2.9220990

Scheme 10: 1* @ RIJCOSX-TPSSh-D3(BJ)/def2-TZVPP + C-PCM

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N	-3.9953477	-2.6746583	-1.5885918
C	-2.6600052	-2.7541721	-1.3988711
N	-2.2878059	-3.9253211	-1.9635950
C	-3.3856468	-4.5794928	-2.4982625
C	-4.4625528	-3.7885531	-2.2659034
Au	-1.4945246	-1.4242657	-0.4561149
H	-3.2964327	-5.5378341	-2.9769723
H	-5.5028120	-3.9075042	-2.5112828
H	4.3065605	-3.8855883	0.9443150
H	4.2259414	-2.7286464	-1.1991962

C	1.5592150	-1.3302236	0.2369625
C	0.3884056	-1.2542775	1.9539981
C	-1.3739059	0.1152535	2.7483446
H	-0.3577117	-1.3832648	3.9721140
C	3.4747020	-2.5002080	-0.4529739
C	1.5991908	-2.0020821	1.4848369
C	-0.5834861	0.4540924	0.4401368
C	3.5198161	-3.1612582	0.7704856
C	-0.4243190	-0.9202531	2.9961275
C	2.4767901	-1.5494859	-0.7586183
H	2.6209357	-3.4496569	2.7337346
C	2.5705467	-2.9251915	1.7882558
H	-2.1792096	1.5641086	1.4066693
H	2.4494581	-1.0486310	-1.7158904
H	-0.5406784	1.0953412	-0.4300465
C	0.3172954	-0.5896325	0.6745085
C	-1.4522908	0.7738312	1.5425882
H	-2.0503813	0.4007260	3.5442680
C	-4.7881803	-1.5749525	-1.0989892
C	-5.2962544	-1.6586428	0.2030602
C	-6.0127774	-0.5595958	0.6784859
C	-6.2082423	0.5624596	-0.1179142
C	-5.6919824	0.6098346	-1.4069325
C	-4.9662617	-0.4626080	-1.9287152
C	-5.0574436	-2.8647013	1.0907236
H	-6.4142380	-0.5819001	1.6840069
H	-6.7649901	1.4074879	0.2698808
H	-5.8460220	1.4924458	-2.0160644
C	-4.3796337	-0.3891953	-3.3240957
C	-0.9416247	-4.4398063	-1.9062992
C	-0.5675070	-5.1620024	-0.7669234
C	0.7416761	-5.6448615	-0.7194353
C	1.6241938	-5.4118830	-1.7646175
C	1.2220970	-4.6827628	-2.8777130
C	-0.0727036	-4.1729654	-2.9737349
C	-1.5237352	-5.4346942	0.3784459
H	1.0702735	-6.2036677	0.1485552
H	2.6379654	-5.7891778	-1.7075865
H	1.9285614	-4.4959548	-3.6761308
C	-0.5210524	-3.3841136	-4.1894443
C	-6.3720792	-3.4367203	1.6359956
C	-4.0933682	-2.5083464	2.2306357
H	-4.5852978	-3.6441163	0.4904969
H	-3.9005246	-1.3442211	-3.5446626
C	-5.4704859	-0.1633814	-4.3784193
C	-3.3000077	0.6980089	-3.3976822
C	-1.0587761	-4.3302786	-5.2757643
C	0.5906386	-2.4991727	-4.7603965
H	-1.3385187	-2.7291532	-3.8788853
C	-0.9818381	-4.8812007	1.7019082
C	-1.8254259	-6.9359635	0.4868705
H	-2.4644262	-4.9229795	0.1729453
H	-3.7258530	1.6842575	-3.1968186
H	-2.5106004	0.5121513	-2.6680782
H	-2.8503105	0.7173362	-4.3921979
H	-3.8975248	-3.3870057	2.8493560
H	-4.5167979	-1.7258077	2.8653685
H	-3.1425808	-2.1465798	1.8349524
H	-7.0494850	-3.7067956	0.8234469
H	-6.8803457	-2.7147254	2.2796763
H	-6.1685709	-4.3307398	2.2298931
H	-6.2235012	-0.9539380	-4.3413604
H	-5.0266984	-0.1548869	-5.3763864
H	-5.9733901	0.7943934	-4.2251635
H	-0.0352599	-5.3554873	1.9701351
H	-1.6973151	-5.0699225	2.5051233
H	-0.8176792	-3.8047231	1.6321044
H	1.0233670	-1.8597233	-3.9915634
H	1.3877146	-3.0988914	-5.2054811
H	0.1821641	-1.8587152	-5.5450290
H	-0.2642653	-4.9959885	-5.6217930
H	-1.8801618	-4.9461453	-4.9060212
H	-1.4201716	-3.7533931	-6.1301102
H	-2.2435657	-7.3202137	-0.4458614
H	-2.5451222	-7.1165173	1.2891405
H	-0.9164466	-7.4997848	0.7105194
F	0.2943791	0.2184003	-2.7057734
F	2.4157406	1.0061183	-4.1591838
Sb	1.0038791	1.9003914	-3.2495376
F	-0.4117577	2.7750551	-2.3203127
F	-0.0555276	1.8420715	-4.8287133
F	1.7046299	3.5863922	-3.7789631
F	2.0561154	1.9505770	-1.6631672

1_{TS} @ RIJCOSX-TPSSh-D3(BJ)/def2-TZVPP + C-PCM

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H	5.1857459	-1.4518540	1.5297436
H	4.7764876	-3.7632208	0.6901928
H	5.0550605	1.7810494	1.4765605
H	4.4514505	4.0264732	0.5811638
H	3.0776067	-4.1968647	-1.0317590
H	2.7034271	4.2755460	-1.1284962
H	1.6450998	-2.3674581	-1.9107534
C	4.3735740	-1.6526871	0.8423534
C	4.1600394	-2.9466195	0.3355966
C	4.2228395	1.8960099	0.7933541
C	3.5365145	-0.6509551	0.3980721
C	3.4707424	0.8161265	0.3817141
C	3.2051724	-3.1942345	-0.6423108
C	3.8992513	3.1537540	0.2554951
C	2.5186741	-0.9410130	-0.5334693
C	2.3755827	-2.1704724	-1.1396281
C	2.4265769	0.9943238	-0.5495302
C	2.9165202	3.2969267	-0.7161483
C	2.1726595	2.1949127	-1.1793385
Au	0.5740176	-0.0545421	-0.2722029
H	1.4167177	2.3092754	-1.9433869
C	-1.3761252	-0.1748358	0.2450243
N	-2.2659407	0.8363886	0.3337036
C	-3.4667568	0.3853048	0.8564913
C	-3.3150627	-0.9431882	1.0888956
N	-2.0237905	-1.2665140	0.7072458
H	-3.9931783	-1.6809852	1.4787834
H	-4.3003439	1.0460306	1.0148544
C	-1.3983585	-2.5658123	0.7400725
C	-1.5502567	-3.3881705	-0.3831073
C	-0.8500671	-4.5949331	-0.3864425
C	-0.0528120	-4.9585829	0.6922904
C	0.0618331	-4.1246532	1.7970254
C	-0.6066655	-2.8998946	1.8449769
C	-2.3873112	-2.9649240	-1.5750303
H	-0.9216167	-5.2496081	-1.2464406
H	0.4869516	-5.8975871	0.6692131
H	0.6876824	-4.4211815	2.6301572
C	-0.4539936	-1.9873609	3.0478572
C	-1.9270641	2.1976426	-0.0006190
C	-2.1687076	2.6456354	-1.3061849
C	-1.8177071	3.9648838	-1.5945816
C	-1.2441987	4.7814477	-0.6262667
C	-0.9893482	4.2922515	0.6480384
C	-1.3179708	2.9788388	0.9877673
C	-2.7813404	1.7387593	-2.3570823
H	-1.9865161	4.3556473	-2.5896521
H	-0.9781461	5.8020725	-0.8743379
H	-0.5207260	4.9308914	1.3868968
C	-0.9995229	2.4367605	2.3679349
H	-3.0085611	-2.1201142	-1.2723529
C	-3.3300724	-4.0770405	-2.0487679

C	-1.4819895	-2.4864698	-2.7176162
C	0.4877135	2.6156759	2.6993992
C	-1.8946806	3.0772012	3.4365983
H	-1.2060572	1.3661291	2.3709930
C	-4.3083205	1.9064793	-2.4030931
C	-2.1826074	1.9597519	-3.7490781
H	-2.5662822	0.7075354	-2.0688836
C	-0.9763924	-2.6644740	4.3226234
H	-1.0524300	-1.0917787	2.8757711
C	1.0045753	-1.5448009	3.2301591
H	-0.4038976	-3.5683484	4.5441145
H	-2.0273545	-2.9426545	4.2216586
H	-0.8754073	-1.9849905	5.1722246
H	1.3779716	-1.0507782	2.3317528
H	1.6493217	-2.4014506	3.4398048
H	1.0833674	-0.8454556	4.0660902
H	-3.9684498	-3.6969778	-2.8497221
H	-2.7743233	-4.9306732	-2.4429194
H	-3.9688353	-4.4294943	-1.2359624
H	-2.0830874	-2.1374162	-3.5591723
H	-0.8415413	-3.2994738	-3.0680454
H	-0.8411470	-1.6651663	-2.3954466
H	0.7102282	2.1683643	3.6707058
H	1.1126135	2.1319187	1.9467738
H	0.7596649	3.6723512	2.7422633
H	-1.6718155	2.6470546	4.4162318
H	-1.7264384	4.1559572	3.4893115
H	-2.9507068	2.9035744	3.2166242
H	-4.5690622	2.9259164	-2.6989399
H	-4.7358142	1.2186646	-3.1357560
H	-4.7660427	1.7020947	-1.4334928
H	-2.5784672	1.2121739	-4.4382038
H	-1.0965079	1.8671630	-3.7343417
H	-2.4432900	2.9440790	-4.1447808
F	1.6895528	-2.1363596	-4.6500916
F	0.7863731	0.0626274	-3.3749866
Sb	1.3154579	-0.3403896	-5.1586217
F	-0.4730698	-0.8243372	-5.5963018
F	3.1026335	0.1471933	-4.7152322
F	0.9381487	1.4574193	-5.6585573
F	1.8468115	-0.7423177	-6.9399795

3* @ RIJCOSX-TPSSh-D3(BJ)/def2-TZVPP + C-PCM

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C	0.5333731	1.7037059	-1.8416785
C	1.8152603	1.8913263	-1.3633357
C	2.6423965	2.8248449	-1.9948530
C	2.1823468	3.5344835	-3.0969756
C	0.8947101	3.3215892	-3.5801452
C	0.0441736	2.4051748	-2.9589115
H	3.6452206	2.9808132	-1.6175204
H	2.8262782	4.2562846	-3.5843416
H	0.5411673	3.8769796	-4.4406299
C	-1.3246189	2.0861921	-3.3487252
C	-1.9914145	2.5511101	-4.4827026
C	-1.9619447	1.1837377	-2.4803030
C	-3.2768101	2.0943310	-4.7616960
H	-1.5097317	3.2530644	-5.1535545
C	-3.2285597	0.7045411	-2.7806486
C	-3.8874294	1.1642238	-3.9247808
H	-3.7964979	2.4557873	-5.6408352
H	-3.7225328	-0.0107669	-2.1362083
H	-4.8797637	0.7950269	-4.1549350
Au	-0.8408118	0.5685539	-0.8878393
N	1.3677409	-1.2580213	0.1010919
C	2.2480619	-1.5929847	1.1177939
C	0.4914415	-0.3009359	0.5137173
C	1.9158553	-0.8307458	2.1825202
H	2.9997884	-2.3505145	0.9938608
N	0.8282451	-0.0562916	1.8042686
H	2.3246677	-0.7775556	3.1752427
H	2.1923681	1.3430120	-0.5142434
C	1.2842890	-1.9565129	-1.1610364
C	0.1318634	-2.7264406	-1.4125444
C	0.0710372	-3.4078470	-2.6277874
C	1.1230800	-3.3615390	-3.5330146
C	2.2611679	-2.6267306	-3.2392780
C	2.3655344	-1.8966720	-2.0526616
C	-0.9657517	-2.9282915	-0.3807739
H	-0.8043334	-3.9990632	-2.8599572
H	1.0564246	-3.9069329	-4.4667217
H	3.0849259	-2.6100761	-3.9421749
C	3.6346891	-1.1127389	-1.7762775
C	0.0461703	0.6679129	2.7835615
C	-0.6784515	-0.1036241	3.7083417
C	-1.3772225	0.5827448	4.7015963
C	-1.3570448	1.9692762	4.7669672
C	-0.6359926	2.7007820	3.8349904
C	0.0862019	2.0657427	2.8230706
C	-0.7073480	-1.6242381	3.6927353
H	-1.9463649	0.0194617	5.4310769
H	-1.9103082	2.4813267	5.5453256
H	-0.6286007	3.7829947	3.8897874
C	0.8804605	2.8903009	1.8335018
H	3.4460784	-0.4392071	-0.9406165
C	4.7809684	-2.0567934	-1.3777164
C	4.0562952	-0.2626179	-2.9829224
C	-0.0378860	3.7900799	0.9963723
H	1.3861455	2.2048114	1.1560916
C	1.9641080	3.7192023	2.5328369
C	0.0087249	-2.1919905	4.9287408
C	-2.1369080	-2.1706673	3.6105539
H	-0.1776520	-1.9778804	2.8080999
H	-0.5463212	4.5201402	1.6301574
H	0.5486785	4.3302599	0.2499239
H	-0.7978451	3.2037829	0.4773287
H	5.0245576	-2.7244790	-2.2073186
H	5.6743403	-1.4794347	-1.1291895
H	4.5215169	-2.6747429	-0.5166753
H	-2.1160337	-3.2628877	3.6422404
H	-2.6237211	-1.8582940	2.6888254
H	-2.7435877	-1.8224441	4.4492687
H	0.0273964	-3.2832636	4.8805756
H	1.0366916	-1.8308728	5.0016331
H	-0.5169444	-1.9001537	5.8409053
H	3.2323378	0.3532049	-3.3423929
H	4.8801493	0.3959643	-2.6999830
H	4.4018792	-0.8932013	-3.8049954
H	2.6489542	3.0784289	3.0929149
H	2.5408284	4.2774787	1.7906188
H	1.5222371	4.4372634	3.2280459
C	-0.6182408	-4.1356529	0.5058191
C	-2.3575244	-3.0918336	-0.9969273
H	-1.0071737	-2.0539005	0.2687516
H	-1.3761421	-4.2615524	1.2812213
H	0.3515628	-4.0075148	0.9914822
H	-0.5840714	-5.0466667	-0.0971731
H	-3.1044177	-3.0979402	-0.2010364
H	-2.4494284	-4.0311787	-1.5465847
H	-2.5894698	-2.2702260	-1.6763522
Sb	-4.3577251	0.8498667	0.9752806
F	-3.2468004	1.8735595	2.1063256
F	-2.7624819	-0.0709999	0.2852469
F	-4.1454067	2.1863726	-0.3483530
F	-5.9158303	1.6832189	1.6636311
F	-5.3937268	-0.2122222	-0.2042137
F	-4.5272438	-0.4995127	2.2916626

3 @ RIJCOSX-TPSSh-D3(BJ)/def2-TZVPP + C-PCM

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C	-1.8697428	1.6774050	-0.5516564
C	-0.9406395	2.6754156	-0.7855911
C	-1.3777377	3.9477348	-1.1640589
C	-2.7342607	4.2036845	-1.3207456
C	-3.6665119	3.1947453	-1.0966542
C	-3.2501497	1.9228634	-0.7003886
H	-0.6498485	4.7314085	-1.3331063
H	-3.0700820	5.1907058	-1.6147077
H	-4.7241666	3.4020207	-1.2134209
C	-4.1204791	0.7884623	-0.3991054
C	-5.4986766	0.7301246	-0.6060189
C	-3.4397683	-0.3359022	0.1040249
C	-6.1907054	-0.4490009	-0.3394925
H	-6.0321291	1.5918139	-0.9906851
C	-4.1321564	-1.5133280	0.3498169
C	-5.5111155	-1.5691475	0.1269001
H	-7.2602562	-0.4951404	-0.5070604
H	-3.6245679	-2.3994237	0.7105044
H	-6.0494350	-2.4881194	0.3275079
Au	-1.4137633	-0.1174891	0.2505903
N	1.4090705	-0.0205008	-1.0434164
C	2.7684539	0.0688701	-0.7826496
C	0.6959709	0.0256231	0.1110403
C	2.9038855	0.1736298	0.5586419
H	3.5035951	0.0323462	-1.5646619
N	1.6249793	0.1267594	1.0902419
H	3.7736470	0.2743147	1.1819591
H	0.1179498	2.4947035	-0.6668913
O	-1.2009339	-1.9151218	1.5076358
H	-0.3929439	-1.7926599	2.0356215
H	-1.9183113	-1.9037096	2.1808465
C	1.3217832	-0.0029795	2.4947690
C	0.7370714	1.0781952	3.1659491
C	0.4289200	0.8969665	4.5145526
C	0.6943343	-0.3059528	5.1543693
C	1.2839412	-1.3566329	4.4634558
C	1.6175707	-1.2341478	3.1128732
C	0.4904128	2.4126633	2.4904269
H	-0.0252757	1.7097160	5.0672390
H	0.4368376	-0.4284268	6.1990015
H	1.4895012	-2.2861764	4.9786027
C	2.3130083	-2.3759828	2.3822938
C	0.8167658	-0.2830847	-2.3340911
C	0.8757508	0.6995614	-3.3322635
C	0.2262434	0.4249623	-4.5374788
C	-0.4322240	-0.7795982	-4.7396125
C	-0.4244806	-1.7544243	-3.7516624
C	0.2093753	-1.5360177	-2.5286737
C	1.6723432	1.9810302	-3.1750255
H	0.2365414	1.1675386	-5.3252414
H	-0.9403375	-0.9677491	-5.6777453
H	-0.9109041	-2.7032477	-3.9342533
C	0.3189048	-2.6652118	-1.5185320
C	3.0573941	1.8145666	-3.8291559
H	1.8192219	2.1663062	-2.1085747
C	0.9722931	3.2062641	-3.7765152
H	2.2425428	-2.1879217	1.3096548
C	3.8047555	-2.4313738	2.7561876
C	1.6764385	-3.7460178	2.6525284
C	-0.9343482	2.9294785	2.7197502
H	0.6225213	2.2754590	1.4185102
C	1.5323107	3.4438744	2.9502082
C	1.5731345	-3.5033560	-1.8167057
H	0.4548867	-2.2368228	-0.5263097
C	-0.9282114	-3.5498073	-1.4633348
H	1.5047320	-3.9556242	-2.8092401
H	1.6711424	-4.3028645	-1.0789690
H	2.4750709	-2.8887565	-1.7802250
H	1.4453445	3.6287815	4.0237502
H	1.3757513	4.3888581	2.4248726
H	2.5472581	3.0975402	2.7416162
H	-1.6756037	2.1943795	2.4068862
H	-1.1086030	3.1624517	3.7725188
H	-1.0901669	3.8422622	2.1412588
H	3.9202446	-2.6803245	3.8141395
H	4.3068710	-1.4805001	2.5730932
H	4.3037469	-3.2037052	2.1676594
H	0.9682869	3.1615362	-4.8676190
H	1.5094969	4.1106262	-3.4823992
H	-0.0571423	3.2908006	-3.4305156
H	1.7822333	-4.0315019	3.7012413
H	2.1829480	-4.5013070	2.0489991
H	0.6149444	-3.7675488	2.3965964
H	3.6620913	2.7085534	-3.6590457
H	3.5987776	0.9531138	-3.4374583
H	2.9452932	1.6724298	-4.9070977
H	-1.0503329	-4.1341807	-2.3778665
H	-0.8370713	-4.2515057	-0.6323191
H	-1.8303161	-2.9549526	-1.3119004
F	-2.6773462	-0.9912588	6.0029423
F	-5.0930076	0.2389653	5.8334760
F	-3.2159550	0.6802362	3.9401456
F	-5.3966590	-0.7444906	3.3653276
F	-4.8373683	-2.4249393	5.4015017
F	-2.9693502	-1.9676224	3.5405989
Sb	-4.0444599	-0.8536214	4.6901179