Electronic Supplementary Information (ESI)

Copper activation of C–X bonds: Bimolecular vs unimolecular reaction mechanism.

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Table Of Contents

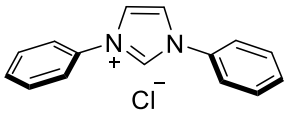
General Information

All the manipulations that were performed under N_2 atmosphere were run inside a Glove Box or using standard Schlenk techniques. Solvents were dried using a solvent purification system SPS PS-MD-5 or were distilled from appropriate drying agents.[1] Anhydrous, oxygen-free, N,N-Dimethylformamide, anhydrous, amine free, 99.9% obtained by Alfa Aesar. Diethylether (Et_2O) and n-hexane were obtained oxygen- and water-free from an SPS PS–MD–5 solvent purification apparatus. Tetrahydrofuran (THF) were dried by the usual procedures and distilled under argon prior to being used. Solvents for experiments in an inert atmosphere were stored into Schlenk flasks over freshly activated 3 or 4 Å molecular sieves. Commercially available chemicals were purchased from Sigma Aldrich, Alfa Aesar, Fluorochem and Acros Organics companies and were used without further purification. $[PdRfCl(PPh_3)_2]$[2], RfI[3], [Cu(Bipy)(Pf)][4], $[PdRf_2(PPh_3)_2]$[5], [PdClRf(dppf)][6], RfH[7],$[Cu(IPr)(C_6F_5)]$[8], RfBr[9].

NMR spectra were recorded with Bruker Avance 400 Ultrashield and Varian 500/54 Premium Shielded instruments equipped with variable-temperature probes. Chemical shifts are reported in ppm referenced to tetramethylsilane (^1H), CCl_3F (^{19}F), with positive shifts downfield, at 298 K unless otherwise stated. The temperature for the NMR probe was calibrated with an ethylene glycol standard (high temperature) and with a methanol standard (low temperature).[2] In the ^{19}F spectra registered in non-deuterated solvents, a coaxial tube containing acetone-d_6 was used to maintain the ^2H lock signal. In the kinetic experiments trilfuorotoluene was used as internal standard. Elemental analysis were performed with a Carlo Erba 1108 Elemental Analyser at the services of Vigo University

Synthesis and characterization of compounds

1,3-Bisphenylimidazolium chloride DPI·HCl



General procedure: Modified procedure from reference 10

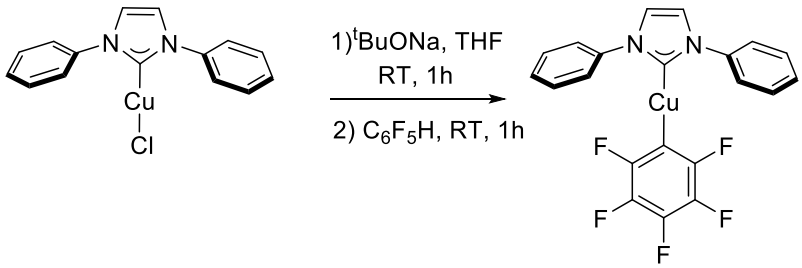
Aniline (1.17 mL, 12.86 mmol, 2.00 eq), 40% glyoxal in (0.73 mL, 6.43 mmol, 1.00 eq) and few drops of formic acid were introduced in a 10 mL Schlenk tube and the mixture was stirred for 2 hours. Then a solution of paraformaldehyde in 4M hydrochloric acid in dioxane (1.00 eq) was introduced. The solution was stirred for 5 hours at room temperature. Then, ethyl acetate (5mL) was added and the resulting suspension was filtrated. The solid was washed three times with ethyl acetate (5x3 mL) and then dried under vacuum to afford 1,3-bisphenylimidazolium chloride DPI·HCl (1.46 g, 6.43 mmol, 88%) as a light orange powder.

^{1}H NMR (499.73 MHz, DMSO-*d*$_6$) δ 10.45 (s, 1H), 8.62 (d, J = 1.4 Hz, 2H), 7.94 (d, J = 7.5 Hz, 4H), 7.70 (t, J = 7.7 Hz, 4H), 7.65 – 7.60 (m, 2H)

^{13}C NMR (125.67 MHz, DMSO-*d*$_6$) δ 134.9, 134.1, 130.1, 130.0, 129.6, 122.0, 121.8.

All the resonances of ^{1}H and ^{13}C NMR spectra were consistent with reported values.[10]

[Cu(DPI)(C_6F_5)]



In the glovebox, to a suspension of [Cu(DPI)Cl] (504 mg, 1.57 mmol) in anhydrous THF (25 mL) was added sodium tert-butoxide (151 mg, 1.0 equiv). The mixture was stirred at room temperature for 1 h. Pentafluorobenzene (288 mg, 1.1 equiv) was subsequently

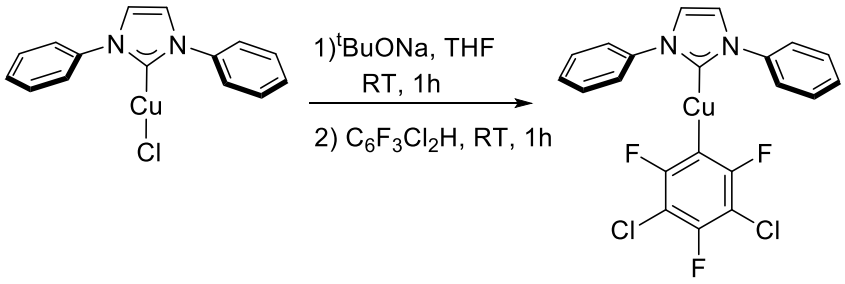
added to the solution and stirred for another 1 h. The suspension was filtered and volatile materials were removed in vacuo. The residue was then washed with anhydrous n-hexane affording off-white solid [Cu(DPI)(C_6F_5)] (483 mg, 68%). Calcd. for $C_{21}H_{12}CuF_5N_2$ (M.W.= 450,88 g mol^{-1}): C, 55.94; H, 2.68; N 6.21; Found: C, 55.96; H, 2.69; N, 6.22.

^{1}H NMR (499.73 MHz, DMF-*d*$_7$) δ 8.78 (t, $^3J_{HH}$ = 1.9 Hz, 2H), 8.23 – 8.19 (m, 4H), 7.75 – 7.62 (m, 6H).

^{19}F NMR (**470.17 MHz, DMF-*d*$_7$**) δ -110.0 (m, 2F), -160.9 (t, J = 19.5 Hz, 1F), -162.9 (m, 2F).

^{13}C NMR (150 MHz, DMF-*d*$_7$) δ 183.2, 139.1, 135.1, 134.3, 129.2, 121.4.

[Cu(DPI)($C_6F_3Cl_2$)]



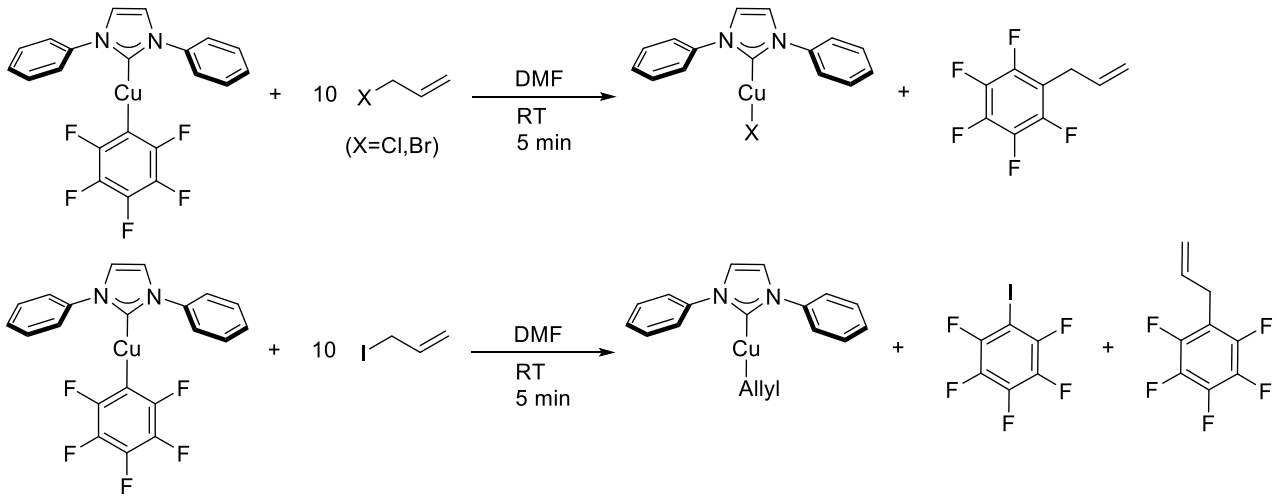
In the glovebox, to a suspension of [Cu(DPI)Cl] (504 mg, 1.57 mmol) in anhydrous THF (25 mL) was added sodium tert-butoxide (151 mg, 1.0 equiv). The mixture was stirred at room temperature for 1 h. ($C_6HCl_2F_3$) (314 mg, 1.1 equiv) was subsequently added to the solution and stirred for 1 h. The reaction mixture was filtered through a plug of celite and volatile materials were removed in vacuo. The residue was then washed with anhydrous n-hexane affording off-white solid [Cu(DPI)($C_6F_3Cl_2$)] 446 mg, 72%). Calcd. for $C_{21}H_{13}Cl_2CuF_3N_2$ (M.W.= 484,79 g mol^{-1}): C, 52.03; H, 2.70; N 5.78; Found: C, 52.11; H, 2.72; N, 5.76.

^{1}H NMR (500 MHz, DMF-*d*$_7$) δ 8.81 (d, $^3J_{HH}$ = 1.7 Hz, 2H), 8.24 – 8.22 (m, 4H), 7.76 – 7.63 (m, 6H).

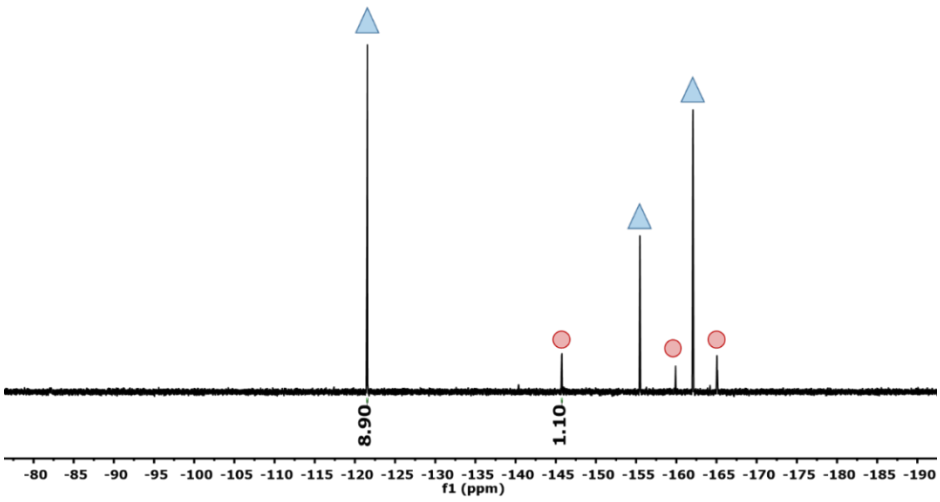
^{19}F NMR (**470.17 MHz, DMF-*d*$_7$**) δ -84.23 (s, 2F), -122.35 (s, 1F).

^{13}C NMR (150 MHz, DMF-*d*$_7$) δ 184.4, 138.5, 135.3, 134.6, 129.4, 121.7.

Reaction of [Cu(DPI)(Pf)] (Pf = C_6F_5) with allyl halides.



Weighted amounts of complex [Cu(DPI)(C_6F_5)] (10.21 mg, 0.0125 mmol) and Allyl-X (X = Cl,Br,I) (0.0123 mmol) were added inside a screw cap NMR tube with the aid of a Schlenk NMR tube adaptor along with a flame sealed coaxial capillary containing acetone-d_6 to the lock the deuterium signal. The tube was cooled to 195 K in an isopropanol/N_2 (liq) bath and subsequently, 0.50 mL of dry DMF with dissolved trifluorotoluene as internal standard (0.025 mol × L^{-1}) were added with a microsyringe. The tube was closed inside the adaptor and then, taken out of the cool bath and mechanically shaken until total dissolution of the solids. The products were confirmed by NMR and GC–MS.



Spectrum ESI1: Final ^{19}F NMR (DMF/acetone-d_6) of **[Cu(DPI)(C_6F_5)] + allyl iodide** (298K). Blue triangles represent the metathesis product Pf-I, and red dots represent the cross-coupling product Pf-Allyl.

Kinetic experiments

Weighted amounts of complex ***[Cu(DPI)(C_6F_5)]*** **(1-Pf)** were added inside a screw cap NMR tube with the aid of a Schlenk NMR tube adaptor along with a flame sealed coaxial capillary containing acetone-d_6 to the lock deuterium signal. The tube was cooled to 195 K in an isopropanol bath and a weighted amount the allyl halide and a volume and DMF taken with a syringe. The tube was closed inside the adaptor and then, taken out of the cool bath, manually shaken until total dissolution of solids and transferred to the NMR probe, which had been preheated to the monitoring temperature.

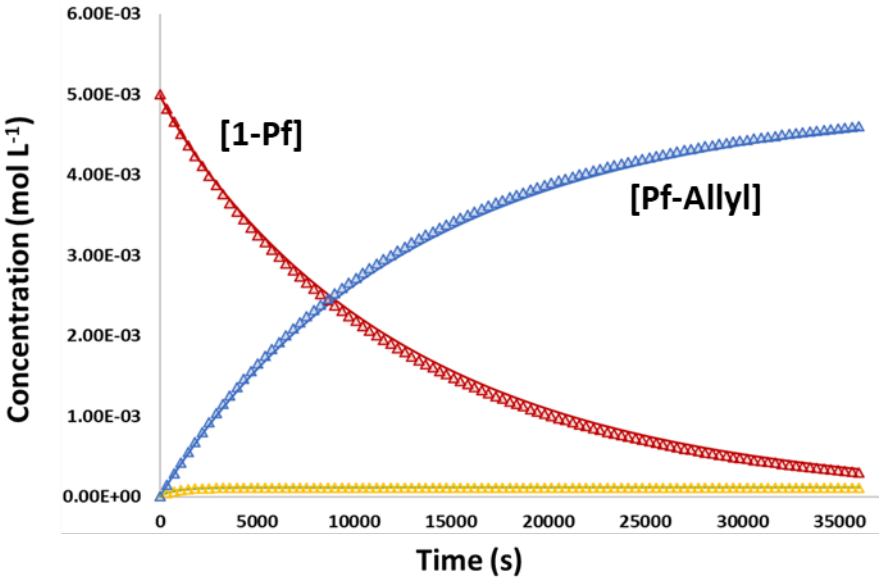


Figure ESI1. ^{19}F NMR monitoring of the reaction between [Cu(DPI)(Pf)] and Cl-Allyl (1:10) in dry DMF at 253 K. Lines represent kinetic fitting of data using COPASI software.

Oxidative addition: $CuPf + Allyl\text{-}Cl \xrightarrow{k_1} CuCl + Allyl\text{-}Pf$

Hydrolysis 1: $CuPf + H_2O \xrightarrow{k_2} CuOH + PfH$

Traces of water have been included in the kinetic fit to maintain material balance.

Parameter	Value s^{-1}; $M^{-1}\cdot s^{-1}$	Std. Deviation
k_1	1.65E-3	6.56E-4
k_2	2.37E-1	2.99E-6

Table ESI 1. Values of kinetic simulations constants.

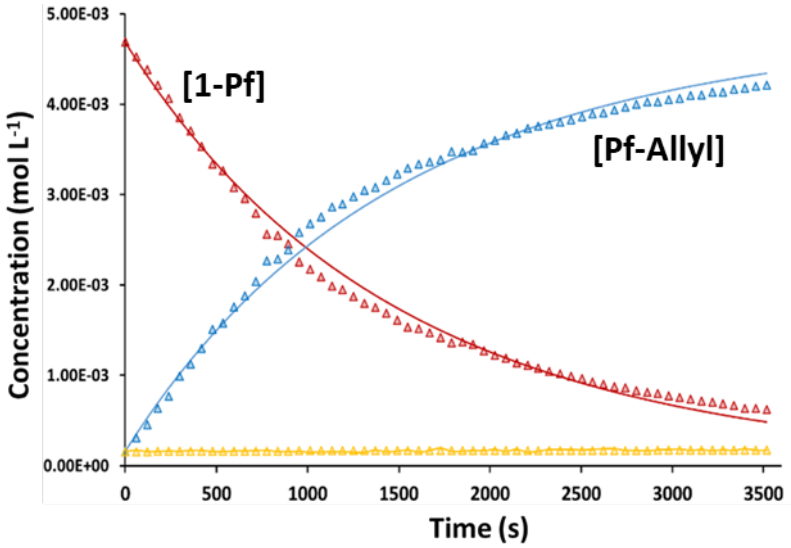


Figure *ESI*2. ^{19}F NMR monitoring of the reaction between [Cu(DPI)(Pf)] and Br-Allyl (1:10) in dry DMF at 253 K. Lines represent kinetic fitting of data using COPASI software

Oxidative addition: $CuPf + Allyl\text{-}Br \xrightarrow{k_1} CuBr + Allyl\text{-}Pf$

Hydrolysis 1: $CuPf + H_2O \xrightarrow{k_2} CuOH + PfH$

Parameter	Value s^{-1}; $M^{-1}\cdot s^{-1}$	Std. Deviation
k_1	1.51E-2	2.40E-4
k_2	3.12E-2	1.50E-5

Table *ESI* 2. Values of kinetic simulations constants.

Table *ESI* 3. Experimental and best least square fitted concentration vs time plot of the formed species in the reaction of [Cu(DPI)(Pf)] (**X**) ($4.7\cdot10^{-3}$M) with Br-Allyl ($4.7\cdot10^{-2}$M) in DMF at 253K

Time	CuPf	Pf-Allyl	PfH	CuPf fit	Pf-Allyl fir	PfH fit
0	0.00468688	0.0001565	0.00015662	0.00468688	0.0001565	0.00015662
59.6029	0.00452157	0.00030773	0.0001707	0.00449912	0.00034359	0.00015729
119.206	0.00438565	0.00045673	0.00015762	0.00431957	0.00052249	0.00015794
178.809	0.0042109	0.00063194	0.00015716	0.00414782	0.00069362	0.00015856
238.412	0.00406716	0.00076872	0.00016412	0.00398349	0.00085736	0.00015915
298.015	0.00385097	0.00098987	0.00015917	0.0038262	0.00101409	0.00015972
357.618	0.00370731	0.00112394	0.00016875	0.00367561	0.00116413	0.00016026
417.221	0.00353299	0.00129868	0.00016833	0.0035314	0.00130782	0.00016078
476.823	0.00333604	0.00150707	0.00015689	0.00339327	0.00144545	0.00016128
536.426	0.00326555	0.00157858	0.00015586	0.00326092	0.00157732	0.00016175
596.029	0.00307925	0.00175735	0.00016339	0.00313409	0.00170369	0.00016221
655.632	0.00295803	0.00187948	0.00016249	0.00301252	0.00182483	0.00016265

715.235	0.00279421	0.00203928	0.00016651	0.00289597	0.00194096	0.00016307
774.838	0.00256101	0.00226884	0.00017015	0.0027842	0.00205233	0.00016347
834.441	0.00255272	0.00229036	0.00015693	0.002677	0.00215914	0.00016386
894.044	0.00245305	0.00239235	0.0001546	0.00257416	0.00226161	0.00016423
953.647	0.0022584	0.00258189	0.00015971	0.00247549	0.00235992	0.00016459
1013.25	0.00217173	0.00267976	0.00014851	0.0023808	0.00245427	0.00016493
1072.85	0.00209317	0.0027544	0.00015243	0.00228992	0.00254482	0.00016526
1132.46	0.00198533	0.00286239	0.00015229	0.00220268	0.00263175	0.00016557
1192.06	0.0019487	0.00289625	0.00015505	0.00211892	0.0027152	0.00016588
1251.66	0.00187096	0.00298105	0.000148	0.00203849	0.00279534	0.00016617
1311.26	0.00179941	0.00305158	0.000149	0.00196125	0.0028723	0.00016645
1370.87	0.0017492	0.00307967	0.00017113	0.00188706	0.00294622	0.00016672
1430.47	0.00168735	0.00315748	0.00015517	0.00181579	0.00301724	0.00016697
1490.07	0.00161088	0.00322891	0.00016021	0.00174732	0.00308546	0.00016722
1549.68	0.00153193	0.00329342	0.00017465	0.00168153	0.00315101	0.00016746
1609.28	0.00151633	0.00333347	0.0001502	0.00161831	0.00321401	0.00016769
1668.88	0.00146938	0.0033625	0.00016811	0.00155754	0.00327455	0.00016791
1728.49	0.00142043	0.00338562	0.00019395	0.00149914	0.00333274	0.00016812
1788.09	0.00136482	0.00347461	0.00016057	0.001443	0.00338868	0.00016832
1847.69	0.00137078	0.00346899	0.00016023	0.00138903	0.00344245	0.00016852
1907.29	0.00134189	0.00349183	0.00016628	0.00133714	0.00349415	0.00016871
1966.9	0.00127022	0.00356385	0.00016593	0.00128724	0.00354387	0.00016889
2026.5	0.0012225	0.00359831	0.0001792	0.00123926	0.00359168	0.00016906
2086.1	0.0011882	0.00365369	0.0001581	0.00119312	0.00363765	0.00016923
2145.71	0.00114054	0.00367956	0.0001799	0.00114874	0.00368187	0.00016939
2205.31	0.00111592	0.00373365	0.00015043	0.00110605	0.00372441	0.00016954
2264.91	0.00107962	0.00376065	0.00015973	0.00106499	0.00376532	0.00016969
2324.51	0.00104471	0.00377681	0.00017847	0.00102549	0.00380468	0.00016984
2384.12	0.00102006	0.00380117	0.00017877	0.00098748	0.00384254	0.00016997
2443.72	0.00099382	0.00382852	0.00017766	0.00095092	0.00387898	0.00017011
2503.32	0.00096604	0.00386023	0.00017372	0.00091574	0.00391403	0.00017023
2562.93	0.00092847	0.00389209	0.00017945	0.00088188	0.00394776	0.00017036
2622.53	0.00090539	0.0039063	0.0001883	0.0008493	0.00398022	0.00017047
2682.13	0.00087735	0.00393433	0.00018832	0.00081795	0.00401146	0.00017059
2741.73	0.00086429	0.00396659	0.00016912	0.00078778	0.00404152	0.0001707
2801.34	0.00083446	0.00399768	0.00016786	0.00075874	0.00407046	0.0001708
2860.94	0.00081331	0.00402338	0.00016331	0.00073079	0.00409831	0.0001709
2920.54	0.00079864	0.00402606	0.00017529	0.00070388	0.00412512	0.000171
2980.15	0.00077298	0.00404952	0.0001775	0.00067798	0.00415092	0.0001711
3039.75	0.00075533	0.00406091	0.00018376	0.00065305	0.00417576	0.00017119
3099.35	0.00073553	0.00409537	0.0001691	0.00062905	0.00419968	0.00017127
3158.96	0.00071774	0.00410467	0.00017759	0.00060594	0.0042227	0.00017136
3218.56	0.00070129	0.0041331	0.0001656	0.0005837	0.00424487	0.00017144
3278.16	0.00068638	0.00413726	0.00017635	0.00056228	0.00426621	0.00017151
3337.76	0.00066355	0.00416782	0.00016863	0.00054165	0.00428676	0.00017159

3397.37	0.00063242	0.00418028	0.0001873	0.0005218	0.00430654	0.00017166
3456.97	0.0006309	0.00419805	0.00017105	0.00050268	0.00432559	0.00017173
3516.57	0.00061809	0.00421165	0.00017026	0.00048426	0.00434394	0.0001718

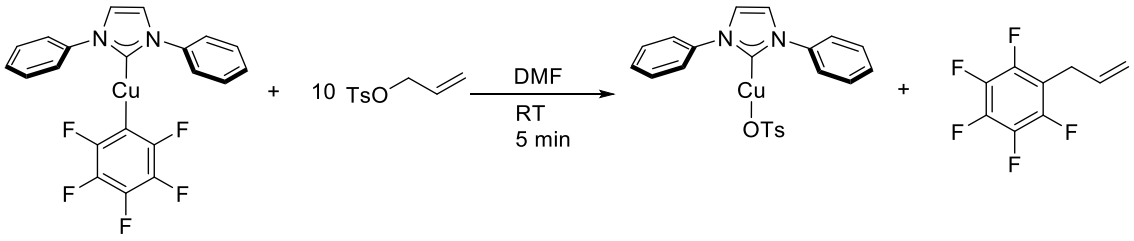
Table S4. Experimental and best least square fitted concentration vs time plot of the formed species in the reaction of [Cu(DPI)(Pf)] ($5.0\cdot10^{-3}$M) with Cl-Allyl ($5.0\cdot10^{-2}$M) in DMF at 253K

Time	CuPf fit	Pf-Allyl fit	PfH fit	CuPf	Pf-Allyl	PfH
0	0.005	8.27E-06	1.19E-05	0.005	8.27E-06	1.19E-05
360	0.00482629	0.00014765	4.62E-05	0.00481969	0.00015383	4.66E-05
720	0.00466987	0.00028198	6.83E-05	0.0046574	0.00029392	6.88E-05
1080	0.0045257	0.00041173	8.27E-05	0.00450789	0.00042904	8.32E-05
1440	0.00439066	0.00053722	9.23E-05	0.0043679	0.00055954	9.27E-05
1800	0.00426277	0.00065871	9.87E-05	0.00423541	0.00068571	9.90E-05
2160	0.00414073	0.0007764	0.00010299	0.00410907	0.00080778	0.00010327
2520	0.00402368	0.00089048	0.00010597	0.003988	0.00092595	0.00010618
2880	0.003911	0.0010011	0.00010803	0.00387156	0.00104038	0.00010819
3240	0.00380227	0.00110839	0.00010947	0.00375932	0.00115122	0.00010959
3600	0.00369716	0.00121249	0.00011048	0.00365094	0.00125862	0.00011058
3960	0.00359543	0.0013135	0.0001112	0.00354615	0.0013627	0.00011128
4320	0.00349687	0.00141153	0.00011172	0.00344476	0.00146359	0.00011178
4680	0.00340133	0.0015067	0.0001121	0.00334659	0.0015614	0.00011214
5040	0.00330867	0.00159908	0.00011238	0.00325148	0.00165624	0.00011241
5400	0.00321876	0.00168879	0.00011258	0.00315932	0.00174821	0.0001126
5760	0.0031315	0.0017759	0.00011273	0.00306998	0.00183741	0.00011274
6120	0.00304679	0.0018605	0.00011284	0.00298335	0.00192393	0.00011285
6480	0.00296453	0.00194268	0.00011292	0.00289934	0.00200786	0.00011293
6840	0.00288464	0.0020225	0.00011299	0.00281785	0.00208929	0.00011299
7200	0.00280705	0.00210004	0.00011304	0.00273879	0.0021683	0.00011304
7560	0.00273167	0.00217539	0.00011307	0.00266208	0.00224497	0.00011308
7920	0.00265844	0.00224859	0.0001131	0.00258765	0.00231938	0.00011311
8280	0.00258728	0.00231973	0.00011313	0.00251541	0.0023916	0.00011313
8640	0.00251813	0.00238886	0.00011314	0.00244529	0.00246169	0.00011314
9000	0.00245092	0.00245605	0.00011316	0.00237723	0.00252974	0.00011316
9360	0.0023856	0.00252136	0.00011317	0.00231116	0.0025958	0.00011317
9720	0.00232211	0.00258484	0.00011318	0.00224701	0.00265994	0.00011318
10080	0.00226039	0.00264655	0.00011318	0.00218473	0.00272222	0.00011318
10440	0.00220039	0.00270655	0.00011319	0.00212425	0.00278269	0.00011319
10800	0.00214206	0.00276488	0.00011319	0.00206552	0.00284141	0.00011319
11160	0.00208534	0.0028216	0.0001132	0.00200849	0.00289845	0.0001132
11520	0.00203018	0.00287675	0.0001132	0.00195309	0.00295384	0.0001132
11880	0.00197655	0.00293038	0.0001132	0.00189929	0.00300764	0.0001132
12240	0.00192439	0.00298253	0.00011321	0.00184702	0.0030599	0.00011321
12600	0.00187367	0.00303326	0.00011321	0.00179625	0.00311067	0.00011321
12960	0.00182433	0.00308259	0.00011321	0.00174693	0.00316	0.00011321

13320	0.00177634	0.00313058	0.00011321	0.00169901	0.00320792	0.00011321
13680	0.00172966	0.00317726	0.00011321	0.00165245	0.00325447	0.00011321
14040	0.00168425	0.00322267	0.00011321	0.00160721	0.00329971	0.00011321
14400	0.00164008	0.00326684	0.00011321	0.00156325	0.00334367	0.00011321
14760	0.0015971	0.00330982	0.00011321	0.00152053	0.00338639	0.00011321
15120	0.00155529	0.00335163	0.00011321	0.00147902	0.0034279	0.00011321
15480	0.00151461	0.00339231	0.00011321	0.00143867	0.00346824	0.00011321
15840	0.00147502	0.0034319	0.00011321	0.00139946	0.00350745	0.00011321
16200	0.0014365	0.00347041	0.00011321	0.00136135	0.00354557	0.00011321
16560	0.00139902	0.0035079	0.00011321	0.00132431	0.00358261	0.00011321
16920	0.00136255	0.00354437	0.00011321	0.0012883	0.00361862	0.00011321
17280	0.00132705	0.00357987	0.00011322	0.0012533	0.00365362	0.00011322
17640	0.0012925	0.00361442	0.00011322	0.00121927	0.00368764	0.00011322
18000	0.00125888	0.00364804	0.00011322	0.00118619	0.00372072	0.00011322
18360	0.00122615	0.00368076	0.00011322	0.00115403	0.00375288	0.00011322
18720	0.0011943	0.00371262	0.00011322	0.00112277	0.00378415	0.00011322
19080	0.0011633	0.00374362	0.00011322	0.00109237	0.00381455	0.00011322
19440	0.00113312	0.0037738	0.00011322	0.00106281	0.0038441	0.00011322
19800	0.00110374	0.00380318	0.00011322	0.00103407	0.00387284	0.00011322
20160	0.00107514	0.00383178	0.00011322	0.00100613	0.00390079	0.00011322
20520	0.0010473	0.00385962	0.00011322	0.00097895	0.00392796	0.00011322
20880	0.00102019	0.00388672	0.00011322	0.00095253	0.00395439	0.00011322
21240	0.00099381	0.00391311	0.00011322	0.00092683	0.00398008	0.00011322
21600	0.00096812	0.0039388	0.00011322	0.00090184	0.00400507	0.00011322
21960	0.0009431	0.00396381	0.00011322	0.00087754	0.00402938	0.00011322
22320	0.00091875	0.00398817	0.00011322	0.0008539	0.00405301	0.00011322
22680	0.00089504	0.00401188	0.00011322	0.00083091	0.004076	0.00011322
23040	0.00087195	0.00403497	0.00011322	0.00080855	0.00409836	0.00011322
23400	0.00084947	0.00405745	0.00011322	0.00078681	0.00412011	0.00011322
23760	0.00082757	0.00407934	0.00011322	0.00076566	0.00414126	0.00011322
24120	0.00080625	0.00410066	0.00011322	0.00074508	0.00416183	0.00011322
24480	0.0007855	0.00412142	0.00011322	0.00072507	0.00418185	0.00011322
24840	0.00076528	0.00414164	0.00011322	0.0007056	0.00420131	0.00011322
25200	0.00074559	0.00416132	0.00011322	0.00068667	0.00422025	0.00011322
25560	0.00072642	0.0041805	0.00011322	0.00066825	0.00423867	0.00011322
25920	0.00070775	0.00419917	0.00011322	0.00065033	0.00425659	0.00011322
26280	0.00068956	0.00421735	0.00011322	0.00063289	0.00427402	0.00011322
26640	0.00067185	0.00423506	0.00011322	0.00061594	0.00429098	0.00011322
27000	0.0006546	0.00425231	0.00011322	0.00059944	0.00430748	0.00011322
27360	0.0006378	0.00426911	0.00011322	0.00058339	0.00432353	0.00011322
27720	0.00062144	0.00428548	0.00011322	0.00056777	0.00433914	0.00011322
28080	0.0006055	0.00430142	0.00011322	0.00055258	0.00435434	0.00011322
28440	0.00058997	0.00431694	0.00011322	0.0005378	0.00436912	0.00011322
28800	0.00057485	0.00433206	0.00011322	0.00052342	0.0043835	0.00011322
29160	0.00056012	0.00434679	0.00011322	0.00050942	0.00439749	0.00011322

29520	0.00054578	0.00436114	0.00011322	0.00049581	0.00441111	0.00011322
29880	0.0005318	0.00437511	0.00011322	0.00048256	0.00442435	0.00011322
30240	0.00051819	0.00438873	0.00011322	0.00046967	0.00443724	0.00011322
30600	0.00050493	0.00440199	0.00011322	0.00045713	0.00444978	0.00011322
30960	0.00049201	0.0044149	0.00011322	0.00044493	0.00446199	0.00011322
31320	0.00047943	0.00442749	0.00011322	0.00043305	0.00447386	0.00011322
31680	0.00046717	0.00443975	0.00011322	0.0004215	0.00448542	0.00011322
32040	0.00045523	0.00445169	0.00011322	0.00041026	0.00449666	0.00011322
32400	0.00044359	0.00446332	0.00011322	0.00039931	0.0045076	0.00011322
32760	0.00043226	0.00447466	0.00011322	0.00038867	0.00451825	0.00011322
33120	0.00042122	0.0044857	0.00011322	0.00037831	0.00452861	0.00011322
33480	0.00041046	0.00449646	0.00011322	0.00036823	0.00453869	0.00011322
33840	0.00039998	0.00450693	0.00011322	0.00035841	0.0045485	0.00011322
34200	0.00038977	0.00451714	0.00011322	0.00034887	0.00455805	0.00011322
34560	0.00037982	0.00452709	0.00011322	0.00033957	0.00456734	0.00011322
34920	0.00037013	0.00453678	0.00011322	0.00033053	0.00457638	0.00011322
35280	0.00036069	0.00454623	0.00011322	0.00032173	0.00458518	0.00011322
35640	0.00035149	0.00455542	0.00011322	0.00031317	0.00459375	0.00011322
36000	0.00034253	0.00456439	0.00011322	0.00030483	0.00460208	0.00011322

Reaction of [Cu(DPI)(Pf)] (Pf = C_6F_5) with Allyl p-toluenesulfonate.



Complex ***[Cu(DPI)(C_6F_5)]*** (10.0 mg) was added inside a screw cap NMR tube with the aid of a Schlenk NMR tube adaptor along with a flame sealed coaxial capillary containing acetone-d_6 to keep the lock signal. A weighted amount of Allyl p-toluensulfonate (10 Eq.), DMF (0.50 mL) were added. After 5 minutes, the reaction was finish and the product was recording in ^{19}F NMR.

Kinetic experiments

Weighted amounts of complex ***[Cu(DPI)(C_6F_5)]*** were added inside a screw cap NMR tube with the aid of a Schlenk NMR tube adaptor along with a flame sealed coaxial capillary containing acetone-d_6 to the lock deuterium signal. The tube was cooled to 195 K in an isopropanol/N_2 (liq) bath and a weighted amount the Allyl p-toluenesulfonate and a volume and DMF taken with a syringe. The tube was closed inside the adaptor and then, taken out of the cool bath, manually shaken until total dissolution of solids and transferred to the NMR probe, which had been preheated to the monitoring temperature.

Parameter	Value s^{-1}; $M^{-1}\cdot s^{-1}$	Std. Deviation
k_1	2.75E-4	3.25E-5
k_2	1.03E-1	2.99E-3

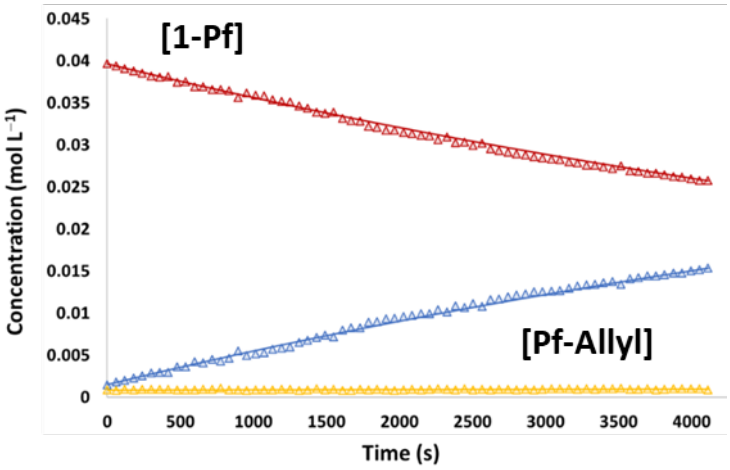


Figure *ESI* 3. ^{19}F NMR monitoring of the reaction between [Cu(DPI)(Pf)] and TsO-Allyl (1:10) in dry DMF at 243 K. Lines represent kinetic fitting of data using COPASI software.

Table *ESI* 5. Experimental and best least square fitted concentration vs time plot of the formed species in the reaction of [Cu(DPI)(Pf)] ($4.0 \cdot 10^{-3}$M) with TsO-Allyl ($4.0 \cdot 10^{-2}$M) in DMF at 243K

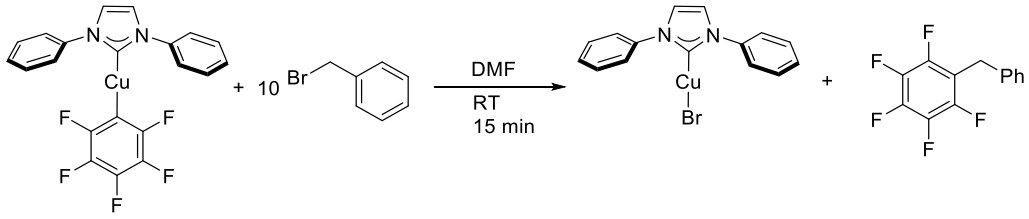
Time	CuPf	PfAllyl	PfH	CuPf Fit	AllylPf Fit	PfH Fit
0	0.03963595	0.00150547	0.00085858	0.03963595	0.00150547	0.00085858
59.6029	0.03937928	0.00184158	0.00077914	0.03938341	0.00175575	0.00086084
119.206	0.03908483	0.00200101	0.00091416	0.03913264	0.00200428	0.00086308
178.809	0.0387792	0.00230866	0.00091214	0.03888363	0.00225107	0.0008653
238.412	0.03854196	0.00254111	0.00091693	0.03863636	0.00249613	0.00086751
298.015	0.03817688	0.0028628	0.00096032	0.03839081	0.00273949	0.00086969
357.618	0.03805921	0.00296753	0.00097326	0.03814698	0.00298116	0.00087186
417.221	0.03811082	0.00297526	0.00091392	0.03790485	0.00322115	0.000874
476.823	0.03746857	0.00362928	0.00090215	0.0376644	0.00345946	0.00087613
536.426	0.03748701	0.00365542	0.00085757	0.03742563	0.00369613	0.00087824
596.029	0.03691506	0.00420318	0.00088176	0.03718851	0.00393115	0.00088033
655.632	0.03691884	0.00412673	0.00095443	0.03695304	0.00416455	0.00088241
715.235	0.0365623	0.00450041	0.00093729	0.03671921	0.00439633	0.00088447
774.838	0.03659885	0.00432081	0.00108034	0.03648699	0.00462651	0.0008865
834.441	0.03647182	0.00461761	0.00091057	0.03625637	0.0048551	0.00088853
894.044	0.03563387	0.00551908	0.00084705	0.03602735	0.00508211	0.00089053
953.647	0.03619736	0.00496531	0.00083733	0.03579991	0.00530757	0.00089252
1013.25	0.03592792	0.00518952	0.00088256	0.03557404	0.00553147	0.00089449
1072.85	0.03581204	0.00533793	0.00085003	0.03534973	0.00575383	0.00089644
1132.46	0.03540282	0.00568516	0.00091201	0.03512695	0.00597467	0.00089838
1192.06	0.03514564	0.00587594	0.00097842	0.03490571	0.00619399	0.0009003
1251.66	0.03508592	0.00597043	0.00094365	0.03468598	0.00641181	0.00090221
1311.26	0.03461689	0.00654448	0.00083863	0.03446777	0.00662813	0.0009041
1370.87	0.034334	0.00675786	0.00090814	0.03425104	0.00684298	0.00090597
1430.47	0.03389403	0.00708672	0.00101925	0.0340358	0.00705636	0.00090783
1490.07	0.03376415	0.0073746	0.00086125	0.03382204	0.00726829	0.00090968
1549.68	0.03386354	0.00721795	0.00091851	0.03360973	0.00747877	0.0009115

1609.28	0.0331517	0.00802272	0.00082558	0.03339887	0.00768782	0.00091332
1668.88	0.03291864	0.0082368	0.00084456	0.03318944	0.00789544	0.00091511
1728.49	0.0328123	0.00824162	0.00094608	0.03298145	0.00810166	0.0009169
1788.09	0.03223063	0.00891389	0.00085548	0.03277486	0.00830647	0.00091866
1847.69	0.03211373	0.00897106	0.0009152	0.03256968	0.0085099	0.00092042
1907.29	0.03176054	0.00935589	0.00088357	0.0323659	0.00871195	0.00092216
1966.9	0.03176238	0.00941757	0.00082005	0.03216349	0.00891263	0.00092388
2026.5	0.03149537	0.00959745	0.00090718	0.03196246	0.00911195	0.00092559
2086.1	0.03135353	0.00973035	0.00091612	0.03176279	0.00930992	0.00092729
2145.71	0.03112819	0.00996133	0.00091048	0.03156446	0.00950656	0.00092897
2205.31	0.03110632	0.00995802	0.00093567	0.03136748	0.00970188	0.00093064
2264.91	0.03060305	0.01040033	0.00099662	0.03117183	0.00989587	0.0009323
2324.51	0.0309094	0.01015906	0.00093154	0.03097749	0.01008857	0.00093394
2384.12	0.03026141	0.01086351	0.00087508	0.03078447	0.01027996	0.00093557
2443.72	0.03033932	0.01064957	0.00101112	0.03059274	0.01047007	0.00093719
2503.32	0.02995736	0.01116739	0.00087525	0.0304023	0.0106589	0.00093879
2562.93	0.03021842	0.01083996	0.00094162	0.03021315	0.01084647	0.00094038
2622.53	0.02954576	0.01158949	0.00086475	0.03002526	0.01103278	0.00094196
2682.13	0.02932409	0.01170706	0.00096886	0.02983863	0.01121785	0.00094352
2741.73	0.02913524	0.01194775	0.00091701	0.02965325	0.01140167	0.00094508
2801.34	0.02895107	0.01214636	0.00090257	0.02946911	0.01158427	0.00094662
2860.94	0.02876252	0.01230844	0.00092904	0.02928621	0.01176565	0.00094814
2920.54	0.02860186	0.01252225	0.00087589	0.02910452	0.01194582	0.00094966
2980.15	0.02848843	0.01256105	0.00095051	0.02892405	0.01212478	0.00095116
3039.75	0.02834485	0.01261937	0.00103578	0.02874478	0.01230256	0.00095266
3099.35	0.02828777	0.01271931	0.00099292	0.02856671	0.01247915	0.00095414
3158.96	0.0280038	0.01298156	0.00101464	0.02838982	0.01265457	0.0009556
3218.56	0.02786145	0.01320692	0.00093164	0.02821411	0.01282883	0.00095706
3278.16	0.02757949	0.01339003	0.00103048	0.02803957	0.01300192	0.00095851
3337.76	0.02761915	0.01344139	0.00093946	0.02786618	0.01317387	0.00095994
3397.37	0.02741103	0.01359858	0.00099039	0.02769395	0.01334469	0.00096136
3456.97	0.02715844	0.01379458	0.00104698	0.02752286	0.01351437	0.00096277
3516.57	0.02752628	0.01342101	0.00105271	0.0273529	0.01368292	0.00096418
3576.18	0.02693074	0.01410174	0.00096753	0.02718407	0.01385037	0.00096557
3635.78	0.02682258	0.01422994	0.00094747	0.02701635	0.01401671	0.00096694
3695.38	0.02661731	0.01440211	0.00098058	0.02684974	0.01418195	0.00096831
3754.98	0.0266671	0.01443006	0.00090284	0.02668423	0.0143461	0.00096967
3814.59	0.02643635	0.01458792	0.00097573	0.02651981	0.01450917	0.00097102
3874.19	0.02623737	0.01474505	0.00101758	0.02635648	0.01467117	0.00097235
3933.79	0.02619317	0.01479679	0.00101004	0.02619422	0.0148321	0.00097368
3993.4	0.02598536	0.01502776	0.00098688	0.02603303	0.01499198	0.000975
4053	0.02580748	0.01515247	0.00104005	0.0258729	0.0151508	0.0009763
4112.6	0.02575944	0.01539078	0.00084978	0.02571382	0.01530858	0.0009776

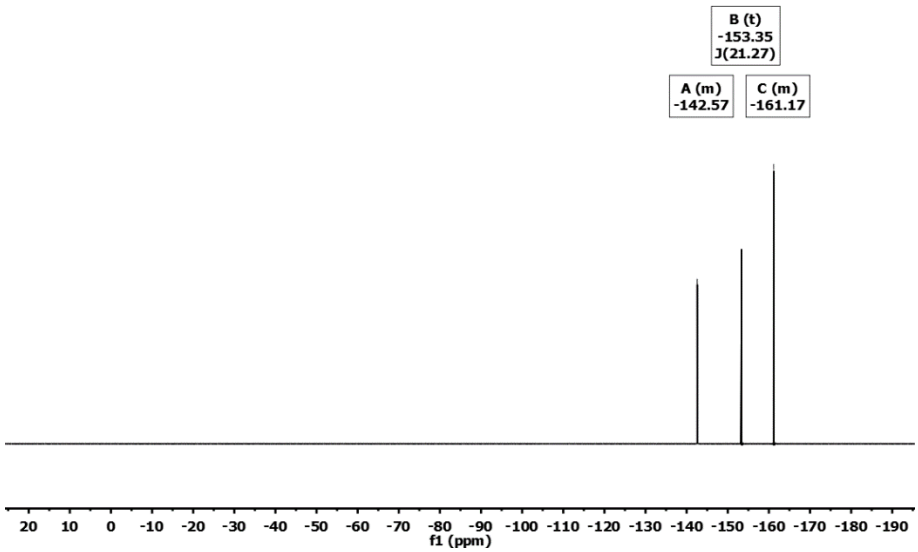
Under the same conditions, the reaction with allyl iodide lasts less than 5 minutes. Therefore, it is assumed to compare the constants of the oxidative addition step a simulated constant with the copasi software.

Parameter	Value s^{-1}; $M^{-1}{\cdot}s^{-1}$
k_1 (I-Allyl)	>3.0E-1
k_1 (Br-Allyl)	1.51E-2
k_1 (Cl-Allyl)	1.65E-3
k_1(OTs-Allyl)	2.75E-4

Reaction of [Cu(DPI)(Pf)] (Pf = C_6F_5) with Benzyl bromide.



Complex ***[Cu(DPI)(C_6F_5)]*** (10.0 mg) was added inside a screw cap NMR tube with the aid of a Schlenk NMR tube adaptor along with a flame sealed coaxial capillary containing acetone-d_6 to keep the lock signal. A weighted amount of Benzyl bromide (10 Eq.), DMF (0.50 mL) were added. After 15 minutes, the reaction was finish (full conversion) and the product was recording in ^{19}F NMR.



Spectrum ESI2: Final ^{19}F NMR (DMF/acetone-d_6) of **[Cu(DPI)(C_6F_5)] + benzyl bromide** (298K). Full conversion to the cross coupling product.

Kinetic data analysis

Determination of the kinetic order of reaction of compound [Cu(DPI)(C_6F_5)] in oxidative addition reactions with Rf-I (Rf = $C_6F_3Cl_2$)

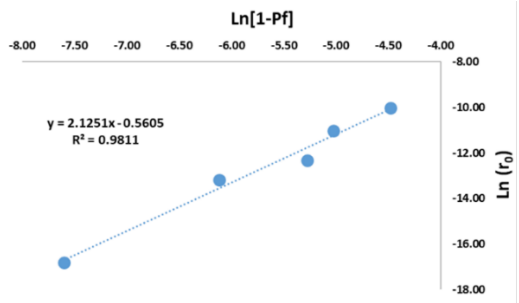
Weighted amounts of complex ***[Cu(DPI)(C_6F_5)]*** were added inside a screw cap NMR tube with the aid of a Schlenk NMR tube adaptor along with a flame sealed coaxial capillary containing acetone-d_6 to the lock deuterium signal. The tube was cooled to 195 K in an isopropanol bath and a weighted amount $C_6F_3Cl_2I$ (RfI) and a volume and DMF taken with a syringe. The tube was closed inside the adaptor and then, taken out of the cool bath, manually shaken until total dissolution of solids and transferred to the NMR probe, which had been preheated to the monitoring temperature (273 K).

Table ESI 6: Amounts of reagents used in the monitoring experiments of the reaction of compound [Cu(DPI)(C_6F_5)] and $C_6F_3Cl_2I$.

Exp.	Compound *[Cu(DPI)(C_6F_5)]*	Rf-I	*[Cu(DPI)(C_6F_5)]*$_0$ (mol L^{-1})	DMF (mL)
1	1.55 mg	26.30 mg	5.00E-4	0.5
2	6.82 mg	26.30 mg	2.20E-3	0.5
3	15.50 mg	26.30 mg	5.10E-3	0.5
4	25.10 mg	26.30 mg	6.58E-3	0.5
5	35.04 mg	26.30 mg	1.13E-2	0.5

Recording started after about 1 min used for the setup of the experiment, time zero for the measurements is taken at that moment. ^{19}F NMR spectra parameters are 1 scan, relaxation delay of 1 s, pulse angle of 90°. Spectra were collected every 58 s.

Order of reaction for compound ***[Cu(DPI)(C_6F_5)]*** in the reaction of ***[Cu(DPI)(C_6F_5)]*** and $C_6F_3Cl_2I$ was determined by initial rates method, measuring the linear rates for the formation of C_6F_5–I up to 15% of total conversion.



r_0	[1-Pf]	Ln(r0)	Ln[1-Pf]
4.47E-05	1.13E-02	-10.02	-4.48
1.61E-05	6.58E-03	-11.04	-5.02
4.40E-06	5.10E-03	-12.33	-5.28
1.90E-06	2.20E-03	-13.17	-6.12
5.00E-08	5.00E-04	-16.81	-7.60

Figure ESI 4: Correlation of the found initial reaction rates and initial concentrations of compound **[Cu(DPI)(C_6F_5)].**

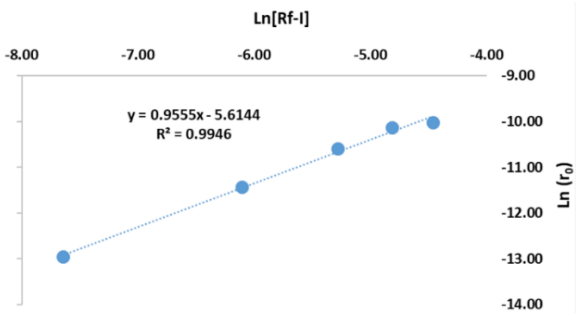
Weighted amounts of compound **Rf-I** were added inside a screw cap NMR tube with the aid of a Schlenk NMR tube adaptor along with a flame sealed coaxial capillary containing acetone-d_6 to the lock deuterium signal. The tube was cooled to 195 K in an isopropanol bath and a weighted amount ***[Cu(DPI)(C_6F_5)]*** and a volume and DMF taken with a syringe. The tube was closed inside the adaptor and then, taken out of the cool bath, manually shaken until total dissolution of solids and transferred to the NMR probe, which had been preheated to the monitoring temperature (273 K). Triflurotoluene was used as internal standard.

Table ESI 7: Amounts of reagents used in the monitoring experiments of the reaction of compound **[Cu(DPI)(C_6F_5)]** and $C_6F_3Cl_2I$.

Exp.	Compound Rf-I	*[Cu(DPI)(C_6F_5)]*	$[RfI]_0$	DMF (mL)
1	0.79 mg	13.20 mg	4.80 × 10-4	0.5
2	3.64 mg	13.20 mg	2.23 × 10-3	0.5
3	8.32 mg	13.20 mg	5.09 × 10-3	0.5
4	13.27 mg	13.20 mg	8.12 × 10-3	0.5
5	18.14 mg	13.20 mg	1.11 × 10-2	0.5

Recording started after about 1 min used for the setup of the experiment, time zero for the measurements is taken at that moment. ^{19}F NMR spectra parameters are 1 scan, relaxation delay of 1 s, pulse angle of 90°. Spectra were collected every 58 s.

Order of reaction for compound Rf-I in the reaction of ***[Cu(DPI)(C_6F_5)]*** and Rf-I was determined by initial rates method, measuring the linear rates for the formation of Pf–I up to 15% of total conversion.



r_0 (mol s^{-1})	[Rf-I] mol L^{-1}	Ln(r0)	Ln[Rf-I]
4.47E-05	1.15E-02	-10.02	-4.46
3.99E-05	8.12E-03	-10.13	-4.81
2.51E-05	5.09E-03	-10.59	-5.28
1.09E-05	2.23E-03	-11.43	-6.11
2.36E-06	4.79E-04	-12.96	-7.64

Figure ESI 5: Correlation of the found initial reaction rates and initial concentrations of compound **Rf-I.**

Determination of the kinetic order of reaction of compound [Cu(DPI)(C_6F_5)] in oxidative addition reactions with Rf-Br (Rf = $C_6F_3Cl_2$)

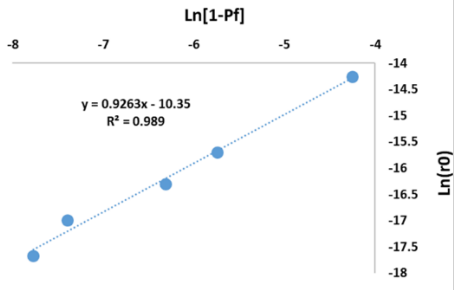
Weighted amounts of complex ***[Cu(DPI)(C_6F_5)]*** were added inside a screw cap NMR tube with the aid of a Schlenk NMR tube adaptor along with a flame sealed coaxial capillary containing acetone-d_6 to the lock deuterium signal. The tube was cooled to 273 K in an isopropanol bath and a weighted amount **Rf-Br** and a volume and DMF taken with a syringe. The tube was closed inside the adaptor and then, taken out of the cool bath, manually shaken until total dissolution of solids and transferred to the NMR probe, which had been preheated to the monitoring temperature (323 K). Triflurotoluene was used as internal standard.

Table ESI 8: Amounts of reagents used in the monitoring experiments of the reaction of compound [Cu(DPI)(C6F5)] and $C_6F_3Cl_2I$.

Exp.	Compound [Cu(DPI)(C_6F_5)]	Rf-Br	[Cu(DPI)(C_6F_5)]$_0$ (mol L^{-1})	DMF (mL)
1	1.00 mg	26.30 mg	4.21E-4	0.5
2	1.38 mg	26.30 mg	6.13E-4	0.5
3	4.08 mg	26.30 mg	1.81E-3	0.5
4	7.19 mg	26.30 mg	3.19E-3	0.5
5	32.01 mg	26.30 mg	1.42E-2	0.5

Recording started after about 1 min used for the setup of the experiment, time zero for the measurements is taken at that moment. ^{19}F NMR spectra parameters are 1 scan, relaxation delay of 1 s, pulse angle of 90°. Spectra were collected every 58 s.

Order of reaction for compound ***[Cu(DPI)(C_6F_5)]*** in the reaction of ***[Cu(DPI)(C_6F_5)]*** and Rf-I was determined by initial rates method, measuring the linear rates for the formation of Pf–Rf up to 15% of total conversion.



r_0	[1-Pf]	Ln(r0)	Ln[1-Pf]
6.42E-07	1.42E-02	-1.43E+01	-4.25E+00
1.53E-07	3.19E-03	-1.57E+01	-5.75E+00
8.30E-08	1.81E-03	-1.63E+01	-6.31E+00
4.20E-08	6.13E-04	-1.70E+01	-7.40E+00
2.11E-08	4.21E-04	-1.77E+01	-7.77E+00

Figure ESI 6: Correlation of the found initial reaction rates and initial concentrations of compound **[Cu(DPI)(C_6F_5)]** with Rf-Br

Kinetic models used for non-linear fitting of the concentration / time data for the reaction between [Cu(DPI)(C_6F_5)] and Rf-I (Rf = $C_6Cl_2F_3$)

Complex ***[Cu(DPI)(C_6F_5)]*** reacts with $C_6Cl_2F_3I$ in dry DMF at 298 K producing the aryl methatesis product C_6F_5–I and the complex **[Cu(DPI)($C_6F_3Cl_2$)]**, and residual amounts of the hydrolysis products C_6F_5H and $C_6Cl_2F_3H$. (Pf = C_6F_5, Rf = $C_6F_3Cl_2$)

A 500 MHz NMR spectrometer was preheated to the appropriate reaction temperature. Shimming and 90° pulse calibration were performed according to the ^{19}F signals of a dummy sample (500 µL of dry DMF, Trifluorotoluene was used as internal standard). The cold sample was then quickly warmed to room temperature and transferred to the NMR. After letting the sample thermally equilibrate for ~30 s, single-scan ^{19}F NMR spectra were collected.

Initial conditions: $[Cu(DPI)Pf]_0 = 4.2\cdot10^{-2}$ M; $[RfI]_0 = 4.2\cdot10^{-1}$ M

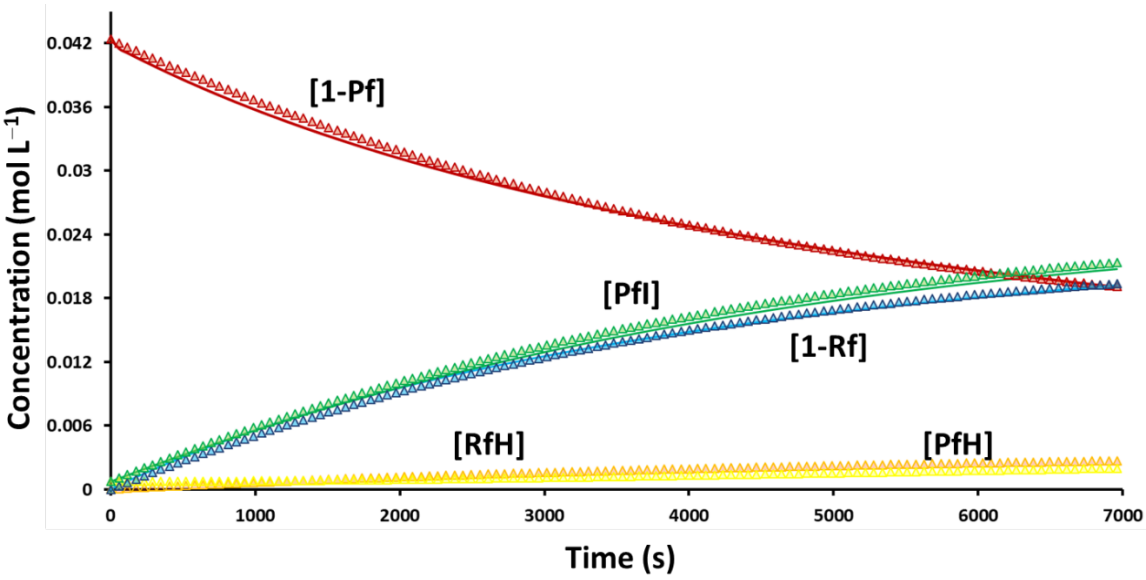


Figure *ESI* 7. Experimental (Triangles) and best least square fitted (continuous line) concentration vs time plot of the formed species in the reaction of **1**–**Pf** ($4.2\cdot10^{-2}$M) with RfI (**3**) ($4.2\cdot10^{-1}$M) in DMF at 298K

Kinetic model

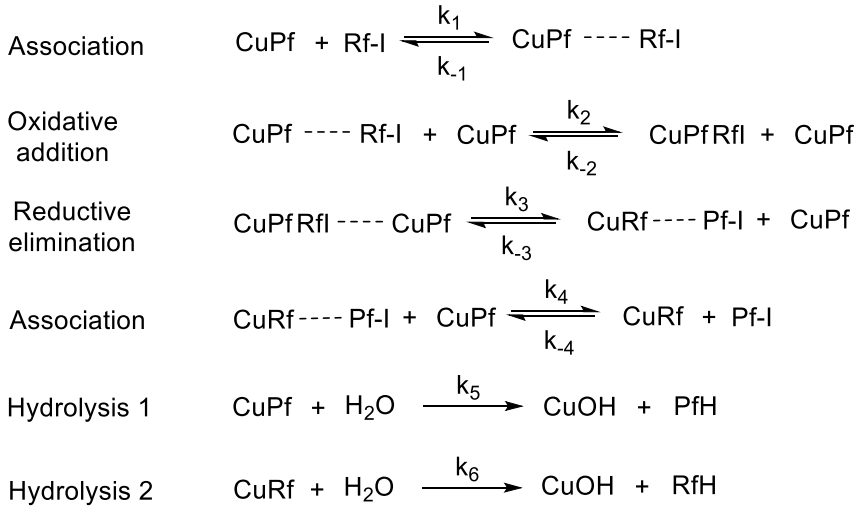


Figure *ESI* 8. Kinetic equations for the fitting of Figure S7.

For kinetic simulations, a series of simplifications are made. The fluorinated aryls Rf and Pf are considered electronically identical, so the hydrolysis constants are considered virtually the same. In addition, the constants k_1/k_{-4} and k_4/k_{-1} are considered equal to simplify the system.

Parameter	Value s^{-1}; $M^{-1}\cdot s^{-1}$	Std. Deviation
k_1	49.95	6.92E+03
k_{-1}	1000	3.54E+02
k_2	0.01	0.01861
k_{-2}	1.21E-06	6.21E-06
k_3	0.01	0.0140906
k_{-3}	1.32e-6	0.00253619
k_4	1000	6.92E+03
k_{-4}	49.95	3.54E+02
k_5	1.65 e-3	3.28E-06
k_6	1.88 e-3	8.00E-06

Table *ESI* 9. Values of kinetic simulations constants.

Table *ESI* 10. Experimental and best least square fitted concentration vs time plot of the formed species in the reaction of **1**–**Pf** ($4.2\cdot10^{-2}$M) with RfI (3) ($4.2\cdot10^{-1}$M) in DMF at 298K

Time	CuPf fit	CuRf fit	PfI fit	PfH fit	RfH fit
0	0.042393	2.04E-05	0.00075422	3.90E-05	0.00075071
58	0.04147931	0.00040034	0.00105543	7.99E-05	0.00075095
116	0.0410719	0.00077205	0.00135395	0.00012015	0.0007516
174	0.04067248	0.00113581	0.00164977	0.00015989	0.00075267
232	0.04028081	0.00149186	0.00194289	0.00019908	0.00075413
290	0.03989666	0.00184042	0.00223331	0.00023775	0.00075598
348	0.03951982	0.00218172	0.00252103	0.00027589	0.0007582

406	0.03915008	0.00251597	0.00280606	0.00031353	0.00076078
464	0.03878724	0.00284338	0.00308839	0.00035067	0.00076371
522	0.0384311	0.00316413	0.00336803	0.00038731	0.00076698
580	0.03808148	0.00347843	0.00364498	0.00042348	0.00077059
638	0.03773819	0.00378645	0.00391925	0.00045918	0.00077452
696	0.03740107	0.00408837	0.00419084	0.00049442	0.00077876
754	0.03706995	0.00438436	0.00445976	0.0005292	0.0007833
812	0.03674467	0.00467458	0.004726	0.00056354	0.00078814
870	0.03642508	0.00495919	0.00498959	0.00059745	0.00079327
928	0.03611102	0.00523833	0.00525052	0.00063093	0.00079868
986	0.03580235	0.00551216	0.00550881	0.00066398	0.00080435
1044	0.03549893	0.00578082	0.00576445	0.00069663	0.00081029
1102	0.03520063	0.00604444	0.00601747	0.00072887	0.00081648
1160	0.03490732	0.00630316	0.00626786	0.00076071	0.00082292
1218	0.03461887	0.00655709	0.00651565	0.00079217	0.0008296
1276	0.03433517	0.00680637	0.00676083	0.00082324	0.00083652
1334	0.03405609	0.00705111	0.00700342	0.00085393	0.00084366
1392	0.03378152	0.00729143	0.00724344	0.00088425	0.00085102
1450	0.03351136	0.00752743	0.00748088	0.00091421	0.00085859
1508	0.03324549	0.00775923	0.00771577	0.00094382	0.00086638
1566	0.03298382	0.00798693	0.00794812	0.00097307	0.00087436
1624	0.03272625	0.00821062	0.00817793	0.00100197	0.00088255
1682	0.03247267	0.00843041	0.00840523	0.00103054	0.00089092
1740	0.032223	0.00864639	0.00863002	0.00105878	0.00089948
1798	0.03197715	0.00885865	0.00885232	0.00108668	0.00090821
1856	0.03173503	0.00906729	0.00907214	0.00111426	0.00091713
1914	0.03149656	0.00927237	0.0092895	0.00114153	0.00092621
1972	0.03126164	0.00947399	0.00950441	0.00116848	0.00093545
2030	0.03103021	0.00967224	0.00971689	0.00119513	0.00094486
2088	0.03080219	0.00986718	0.00992695	0.00122147	0.00095442
2146	0.0305775	0.01005889	0.01013461	0.00124752	0.00096413
2204	0.03035606	0.01024744	0.01033988	0.00127328	0.00097398
2262	0.03013782	0.01043292	0.01054278	0.00129874	0.00098398
2320	0.02992269	0.01061537	0.01074333	0.00132393	0.00099411
2378	0.02971062	0.01079489	0.01094154	0.00134883	0.00100438
2436	0.02950153	0.01097152	0.01113743	0.00137346	0.00101478
2494	0.02929537	0.01114533	0.01133101	0.00139782	0.0010253
2552	0.02909207	0.01131638	0.01152231	0.00142192	0.00103594
2610	0.02889158	0.01148474	0.01171134	0.00144575	0.0010467
2668	0.02869383	0.01165046	0.01189811	0.00146933	0.00105758
2726	0.02849878	0.0118136	0.01208265	0.00149265	0.00106857
2784	0.02830636	0.01197421	0.01226497	0.00151572	0.00107966
2842	0.02811652	0.01213235	0.01244509	0.00153854	0.00109086
2900	0.02792922	0.01228806	0.01262303	0.00156112	0.00110215
2958	0.0277444	0.0124414	0.01279881	0.00158346	0.00111355

3016	0.027562	0.01259242	0.01297244	0.00160557	0.00112504
3074	0.027382	0.01274117	0.01314395	0.00162744	0.00113662
3132	0.02720433	0.01288769	0.01331334	0.00164909	0.00114829
3190	0.02702895	0.01303203	0.01348065	0.00167051	0.00116004
3248	0.02685582	0.01317423	0.01364588	0.00169171	0.00117188
3306	0.0266849	0.01331434	0.01380906	0.00171269	0.0011838
3364	0.02651614	0.01345239	0.0139702	0.00173345	0.00119579
3422	0.0263495	0.01358843	0.01412933	0.001754	0.00120786
3480	0.02618495	0.0137225	0.01428646	0.00177434	0.00122001
3538	0.02602244	0.01385463	0.01444161	0.00179447	0.00123222
3596	0.02586194	0.01398487	0.0145948	0.0018144	0.0012445
3654	0.0257034	0.01411325	0.01474605	0.00183413	0.00125684
3712	0.02554681	0.01423981	0.01489538	0.00185366	0.00126924
3770	0.02539211	0.01436458	0.0150428	0.00187299	0.00128171
3828	0.02523927	0.0144876	0.01518834	0.00189213	0.00129424
3886	0.02508827	0.0146089	0.01533201	0.00191108	0.00130682
3944	0.02493906	0.01472851	0.01547383	0.00192985	0.00131945
4002	0.02479162	0.01484647	0.01561383	0.00194842	0.00133214
4060	0.02464591	0.0149628	0.01575201	0.00196682	0.00134487
4118	0.02450191	0.01507753	0.0158884	0.00198503	0.00135766
4176	0.02435959	0.0151907	0.01602302	0.00200307	0.00137049
4234	0.02421891	0.01530234	0.01615588	0.00202093	0.00138336
4292	0.02407985	0.01541247	0.01628701	0.00203862	0.00139628
4350	0.02394238	0.01552111	0.01641642	0.00205614	0.00140924
4408	0.02380648	0.01562831	0.01654413	0.00207349	0.00142223
4466	0.02367211	0.01573408	0.01667015	0.00209067	0.00143526
4524	0.02353925	0.01583844	0.01679452	0.00210769	0.00144833
4582	0.02340788	0.01594143	0.01691724	0.00212455	0.00146144
4640	0.02327797	0.01604307	0.01703833	0.00214124	0.00147457
4698	0.0231495	0.01614338	0.01715781	0.00215778	0.00148774
4756	0.02302244	0.01624238	0.01727571	0.00217416	0.00150093
4814	0.02289677	0.0163401	0.01739203	0.00219039	0.00151415
4872	0.02277246	0.01643657	0.01750679	0.00220647	0.0015274
4930	0.02264951	0.01653179	0.01762002	0.0022224	0.00154068
4988	0.02252788	0.0166258	0.01773172	0.00223817	0.00155397
5046	0.02240755	0.01671862	0.01784193	0.00225381	0.00156729
5104	0.0222885	0.01681026	0.01795064	0.00226929	0.00158063
5162	0.02217072	0.01690075	0.01805789	0.00228464	0.00159399
5220	0.02205417	0.0169901	0.01816369	0.00229984	0.00160737
5278	0.02193885	0.01707833	0.01826806	0.00231491	0.00162077
5336	0.02182474	0.01716547	0.018371	0.00232984	0.00163418
5394	0.02171181	0.01725153	0.01847255	0.00234463	0.00164761
5452	0.02160004	0.01733653	0.01857271	0.00235928	0.00166105
5510	0.02148943	0.01742048	0.01867151	0.00237381	0.0016745
5568	0.02137994	0.01750341	0.01876895	0.0023882	0.00168796

5626	0.02127157	0.01758533	0.01886506	0.00240247	0.00170144
5684	0.0211643	0.01766626	0.01895986	0.0024166	0.00171492
5742	0.02105811	0.01774621	0.01905334	0.00243061	0.00172842
5800	0.02095298	0.0178252	0.01914555	0.0024445	0.00174192
5858	0.0208489	0.01790325	0.01923648	0.00245826	0.00175542
5916	0.02074586	0.01798036	0.01932616	0.0024719	0.00176893
5974	0.02064383	0.01805656	0.0194146	0.00248542	0.00178245
6032	0.02054281	0.01813186	0.01950181	0.00249882	0.00179597
6090	0.02044277	0.01820628	0.01958781	0.00251211	0.00180949
6148	0.02034371	0.01827982	0.01967263	0.00252527	0.00182302
6206	0.02024561	0.0183525	0.01975626	0.00253832	0.00183654
6264	0.02014846	0.01842434	0.01983873	0.00255126	0.00185007
6322	0.02005224	0.01849535	0.01992005	0.00256409	0.0018636
6380	0.01995694	0.01856554	0.02000023	0.0025768	0.00187712
6438	0.01986255	0.01863492	0.0200793	0.00258941	0.00189064
6496	0.01976905	0.01870351	0.02015726	0.00260191	0.00190416
6554	0.01967643	0.01877132	0.02023413	0.0026143	0.00191768
6612	0.01958468	0.01883835	0.02030992	0.00262658	0.00193119
6670	0.01949379	0.01890463	0.02038465	0.00263876	0.0019447
6728	0.01940374	0.01897017	0.02045833	0.00265083	0.0019582
6786	0.01931453	0.01903497	0.02053097	0.00266281	0.00197169
6844	0.01922614	0.01909904	0.02060259	0.00267468	0.00198518
6902	0.01913856	0.0191624	0.0206732	0.00268645	0.00199866
6960	0.01905178	0.01922506	0.02074282	0.00269812	0.00201213
7018	0.01896579	0.01928703	0.02081145	0.0027097	0.00202559
7076	0.01888058	0.01934831	0.02087911	0.00272117	0.00203904
7134	0.01879613	0.01940893	0.02094582	0.00273255	0.00205249
Time	**CuPf**	**CuRf**	**PfI**	**PfH**	**RfH**
0	0.042393	2.04E-05	0.00075422	3.90E-05	0.00075071
58	0.04203029	0.0003422	0.0010762	7.97E-05	0.00075092
116	0.04167115	0.00066055	0.00139512	0.00011996	0.00075149
174	0.04131558	0.00097548	0.00171098	0.00015968	0.00075242
232	0.04096357	0.00128698	0.00202376	0.0001989	0.0007537
290	0.04061512	0.00159508	0.00233348	0.00023763	0.00075532
348	0.04027021	0.00189978	0.00264014	0.00027589	0.00075728
406	0.03992883	0.00220108	0.00294374	0.00031366	0.00075958
464	0.03959098	0.002499	0.00324428	0.00035097	0.00076219
522	0.03925665	0.00279355	0.00354176	0.00038782	0.00076513
580	0.03892582	0.00308474	0.0038362	0.00042421	0.00076837
638	0.03859849	0.00337259	0.00412759	0.00046016	0.00077192
696	0.03827463	0.00365709	0.00441595	0.00049565	0.00077578
754	0.03795424	0.00393828	0.00470128	0.00053072	0.00077992
812	0.0376373	0.00421616	0.00498359	0.00056535	0.00078435
870	0.0373238	0.00449074	0.00526289	0.00059955	0.00078907
928	0.03701372	0.00476205	0.00553918	0.00063334	0.00079405

986	0.03670704	0.00503009	0.00581248	0.00066671	0.00079931
1044	0.03640376	0.00529489	0.0060828	0.00069967	0.00080484
1102	0.03610384	0.00555646	0.00635016	0.00073224	0.00081062
1160	0.03580728	0.00581482	0.00661455	0.0007644	0.00081665
1218	0.03551406	0.00606998	0.006876	0.00079618	0.00082293
1276	0.03522416	0.00632197	0.00713451	0.00082757	0.00082946
1334	0.03493755	0.00657081	0.00739011	0.00085858	0.00083622
1392	0.03465422	0.00681651	0.0076428	0.00088921	0.00084321
1450	0.03437416	0.00705909	0.0078926	0.00091948	0.00085043
1508	0.03409733	0.00729858	0.00813953	0.00094938	0.00085787
1566	0.03382372	0.00753499	0.00838359	0.00097893	0.00086552
1624	0.0335533	0.00776835	0.00862482	0.00100812	0.00087339
1682	0.03328606	0.00799867	0.00886321	0.00103696	0.00088146
1740	0.03302198	0.00822599	0.0090988	0.00106546	0.00088973
1798	0.03276102	0.00845031	0.00933159	0.00109362	0.0008982
1856	0.03250317	0.00867167	0.00956161	0.00112145	0.00090686
1914	0.03224841	0.00889009	0.00978888	0.00114895	0.00091571
1972	0.03199671	0.00910558	0.0100134	0.00117612	0.00092474
2030	0.03174805	0.00931818	0.01023521	0.00120298	0.00093395
2088	0.03150241	0.0095279	0.01045431	0.00122952	0.00094333
2146	0.03125975	0.00973477	0.01067073	0.00125575	0.00095288
2204	0.03102006	0.00993882	0.0108845	0.00128167	0.0009626
2262	0.03078332	0.01014006	0.01109562	0.0013073	0.00097247
2320	0.03054949	0.01033853	0.01130411	0.00133263	0.00098251
2378	0.03031856	0.01053424	0.01151001	0.00135766	0.00099269
2436	0.0300905	0.01072722	0.01171333	0.00138241	0.00100303
2494	0.02986528	0.0109175	0.01191409	0.00140687	0.0010135
2552	0.02964287	0.0111051	0.0121123	0.00143106	0.00102412
2610	0.02942326	0.01129005	0.012308	0.00145497	0.00103488
2668	0.02920642	0.01147236	0.01250121	0.00147861	0.00104576
2726	0.02899232	0.01165208	0.01269194	0.00150198	0.00105678
2784	0.02878094	0.01182921	0.01288021	0.00152508	0.00106792
2842	0.02857225	0.01200379	0.01306606	0.00154793	0.00107919
2900	0.02836622	0.01217585	0.01324949	0.00157052	0.00109057
2958	0.02816283	0.0123454	0.01343054	0.00159286	0.00110206
3016	0.02796206	0.01251247	0.01360922	0.00161495	0.00111367
3074	0.02776387	0.0126771	0.01378556	0.0016368	0.00112539
3132	0.02756824	0.01283929	0.01395958	0.00165841	0.00113721
3190	0.02737516	0.01299909	0.0141313	0.00167978	0.00114913
3248	0.02718458	0.01315651	0.01430075	0.00170091	0.00116115
3306	0.02699648	0.01331159	0.01446794	0.00172182	0.00117327
3364	0.02681085	0.01346434	0.01463289	0.00174249	0.00118547
3422	0.02662765	0.01361479	0.01479564	0.00176295	0.00119777
3480	0.02644685	0.01376297	0.0149562	0.00178318	0.00121015
3538	0.02626844	0.0139089	0.0151146	0.0018032	0.00122262

3596	0.02609238	0.01405261	0.01527086	0.001823	0.00123516
3654	0.02591865	0.01419413	0.01542499	0.00184259	0.00124779
3712	0.02574722	0.01433347	0.01557703	0.00186198	0.00126048
3770	0.02557808	0.01447067	0.015727	0.00188116	0.00127325
3828	0.02541118	0.01460574	0.01587491	0.00190014	0.00128609
3886	0.02524652	0.01473872	0.0160208	0.00191892	0.001299
3944	0.02508406	0.01486962	0.01616467	0.0019375	0.00131197
4002	0.02492378	0.01499848	0.01630656	0.00195589	0.001325
4060	0.02476565	0.01512532	0.01644649	0.00197409	0.00133809
4118	0.02460965	0.01525015	0.01658447	0.00199211	0.00135124
4176	0.02445576	0.01537301	0.01672054	0.00200994	0.00136444
4234	0.02430394	0.01549393	0.01685471	0.00202759	0.0013777
4292	0.02415418	0.01561291	0.016987	0.00204506	0.001391
4350	0.02400645	0.01573	0.01711743	0.00206235	0.00140435
4408	0.02386072	0.01584521	0.01724604	0.00207947	0.00141775
4466	0.02371698	0.01595856	0.01737283	0.00209642	0.00143119
4524	0.02357519	0.01607008	0.01749784	0.0021132	0.00144467
4582	0.02343534	0.0161798	0.01762108	0.00212982	0.0014582
4640	0.0232974	0.01628773	0.01774256	0.00214627	0.00147175
4698	0.02316135	0.0163939	0.01786233	0.00216255	0.00148535
4756	0.02302717	0.01649833	0.01798039	0.00217868	0.00149897
4814	0.02289482	0.01660105	0.01809676	0.00219466	0.00151263
4872	0.02276429	0.01670207	0.01821147	0.00221048	0.00152632
4930	0.02263556	0.01680142	0.01832453	0.00222614	0.00154004
4988	0.0225086	0.01689912	0.01843598	0.00224166	0.00155378
5046	0.02238339	0.01699519	0.01854582	0.00225703	0.00156754
5104	0.02225991	0.01708966	0.01865408	0.00227225	0.00158133
5162	0.02213814	0.01718255	0.01876077	0.00228733	0.00159514
5220	0.02201805	0.01727387	0.01886592	0.00230227	0.00160897
5278	0.02189962	0.01736365	0.01896955	0.00231706	0.00162281
5336	0.02178284	0.01745192	0.01907167	0.00233172	0.00163668
5394	0.02166767	0.01753868	0.01917231	0.00234625	0.00165055
5452	0.02155411	0.01762396	0.01927149	0.00236064	0.00166444
5510	0.02144212	0.01770779	0.01936921	0.0023749	0.00167834
5568	0.02133169	0.01779018	0.01946551	0.00238903	0.00169225
5626	0.0212228	0.01787115	0.0195604	0.00240303	0.00170617
5684	0.02111543	0.01795072	0.0196539	0.0024169	0.0017201
5742	0.02100955	0.01802891	0.01974603	0.00243066	0.00173403
5800	0.02090515	0.01810575	0.0198368	0.00244428	0.00174797
5858	0.02080221	0.01818124	0.01992624	0.00245779	0.00176191
5916	0.0207007	0.01825542	0.02001436	0.00247118	0.00177586
5974	0.02060061	0.01832829	0.02010117	0.00248445	0.0017898
6032	0.02050193	0.01839988	0.02018671	0.0024976	0.00180375
6090	0.02040462	0.0184702	0.02027097	0.00251064	0.00181769
6148	0.02030867	0.01853928	0.02035399	0.00252357	0.00183163

6206	0.02021407	0.01860713	0.02043578	0.00253638	0.00184557
6264	0.02012079	0.01867377	0.02051635	0.00254909	0.0018595
6322	0.02002882	0.01873922	0.02059572	0.00256169	0.00187343
6380	0.01993814	0.01880349	0.02067392	0.00257418	0.00188735
6438	0.01984873	0.0188666	0.02075094	0.00258657	0.00190126
6496	0.01976057	0.01892857	0.02082682	0.00259885	0.00191516
6554	0.01967365	0.01898942	0.02090156	0.00261103	0.00192906
6612	0.01958795	0.01904916	0.02097518	0.00262311	0.00194294
6670	0.01950345	0.01910781	0.0210477	0.00263509	0.00195681
6728	0.01942013	0.01916538	0.02111913	0.00264697	0.00197067
6786	0.01933799	0.0192219	0.0211895	0.00265875	0.00198452
6844	0.019257	0.01927737	0.0212588	0.00267044	0.00199835
6902	0.01917714	0.01933182	0.02132706	0.00268203	0.00201217
6960	0.0190984	0.01938525	0.0213943	0.00269353	0.00202597
7018	0.01902077	0.01943769	0.02146052	0.00270494	0.00203975
7076	0.01894423	0.01948914	0.02152574	0.00271626	0.00205352
7134	0.01886877	0.01953963	0.02158998	0.00272749	0.00206727

NMR DOSY – Diffusion experiments

NMR experiments were recorded with a Variant spectrometer (11.7 T). All spectra were acquired in a 5 mm observe probehead at 273.15 K in 5 mm tubes.

All DOSY experiments were performed using DOSY Bipolar Pulse Pair Simulated Echo with convection compensation (dbppste_cc) pulse sequence. The total diffusion-encoding pulse duration δ and the diffusion delay Δ were optimized in order to obtain a 1 - 5% residual signal with the maximum gradient strength. Typically, in each NMR experiment ''dbppste_cc'' using 20 spectra on 16 K data points were collected, the value of d was of 1.0 ms duration, the diffusion delay (D) was set to 50 ms in all experiments and relaxation time (t1) between acquisition was set to 2 s. The experiments were performed without sample spinning.

Resonance frequency [MHz]: 470.17 Fitted function: $f(x) = Io*\exp(-D*x^2*\gamma^2*\delta^2(\Delta-\delta/3)*10^4$

Used γ: 26752 rad/(s*Gauss) used δ: 0.0017200 s used Δ: 0.099900 s. Used gradient strength: variable. Random error estimation of data: RMS per spectrum (or trace/plane) Systematic error estimation of data: worst case per peak scenario

Fit parameter Error estimation method: from fit using arbitrary uncertainties

Confidence level: 95 %

Dosy experiments were processed in NMR Varian Software.

For the calibration line, different tubes were charged with similar quantities of the standard substances (0.0199 mmol) in dry DMF (0.5 mL). When the substance got dissolved, the sample was placed into the NMR probe thermostated at 273.15 K. An empirical relation between diffusion coefficient and molecular weight was established and its expressed as: $D = K \cdot M_W^{\alpha}$ where K is a molecule-dependent constant and α is a parameter that depends highly on the particle shape.[11–15] This equation was transformed into a linear equation in order to obtain the parameter α.

$$\mathbf{\ln D = \ln K + \alpha \cdot \ln M_W}$$

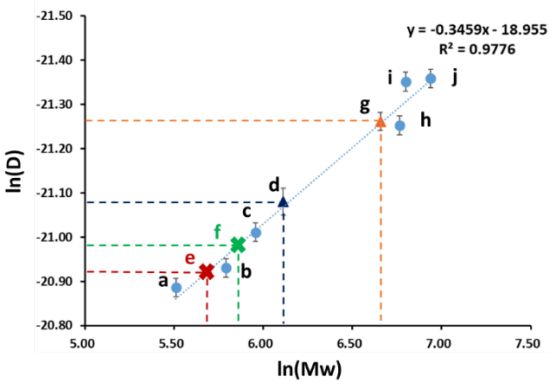


Figure *ESI* 9. Plot of lnD versus lnMw. Blue dots represent experimental values obtained for known complexes for the calibration line.

Table *ESI* 11. Results of diffusion experiments of different compounds in DMF for the calibration line.

Name	Compound	Signal Measured	Mw (calc) / g mol^{-1}	ln Mw	lnD
a	**PfBr**	F_{ortho}	246.93	5.51	-20.89
b	**RfI**	F_{ortho}	326.87	5.79	-20.93
c	**[Cu(bipy)(Pf)]**	F_{ortho}	385.99	5.96	-21.01
d	**[Cu(DPI)(Pf)]**	F_{ortho}	450.88	6.11	-21.08
e	**[Cu(DPI)(Pf)] + PfBr**	F_{ortho} of PfBr	**284.62**	**5.65**	-20.91
f	**[Cu(bipy)(Pf)] + RfI**	F_{ortho} of RfI	**337.71**	**5.82**	-20.97
g	**[Cu(DPI)(Pf)] + RfI**	F_{ortho} of RfI	**777.75**	**6.66**	-21.26
h	**[PdCl(Rf)(PPh_3)$_2$]**	F_{ortho}	866.41	6.76	-21.25
i	**[PdCl(Rf)(dppf)]**	F_{ortho}	896.22	6.80	-21.35
j	**[Pd(Rf)$_2$(PPh_3)$_2$]**	F_{ortho}	1030.93	6.94	-21.36

Table *ESI* 12. Results of diffusion experiments of different compounds in DMF at 273K.

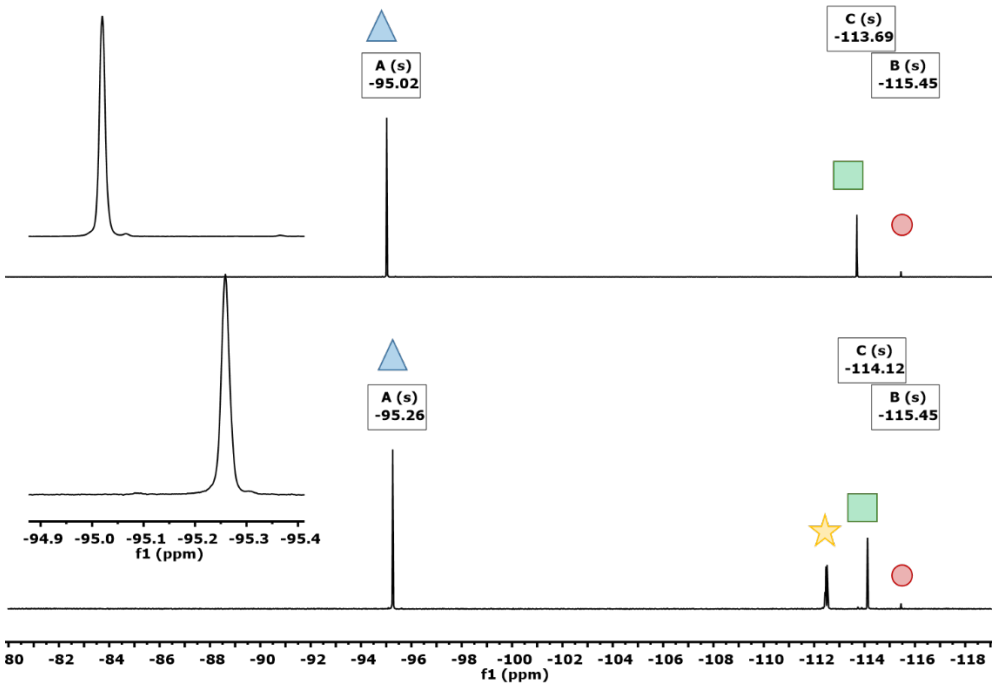
Compound	D (m^2s^{-1})	1/D^3
[PdRfCl(PPh_3)$_2$]	5.9 ± 0.12E-10	4.9E+27
RfI	8.3 ± 0.19E-10	1.7E+27
[Cu(DPI)(Pf)]	7.0 ± 0.10E-10	2.9E+27
[Cu(Bipy)(Pf)]	7.5 ± 0.16E-10	2.3E+27
[Pd(Rf)$_2$(PPh_3)$_2$]	5.3 ± 0.09E-10	6.7E+27
Pf-Br	8.5 ± 0.17E-10	1.6E+27
[PdCl(Rf)(dppf)]	5.3 ± 0.21E-10	6.5E+27
[Cu(DPI)(Pf)] + RfI	5.8 ± 0.11E-10	5.0E+27
[Cu(DPI)(Pf)] + BrPf	8.2 ± 0.10E-10	1.7E+27

[Cu(Bipy)(Pf)] + RfI	7.8 ± 0.14E-10	2.1E+27

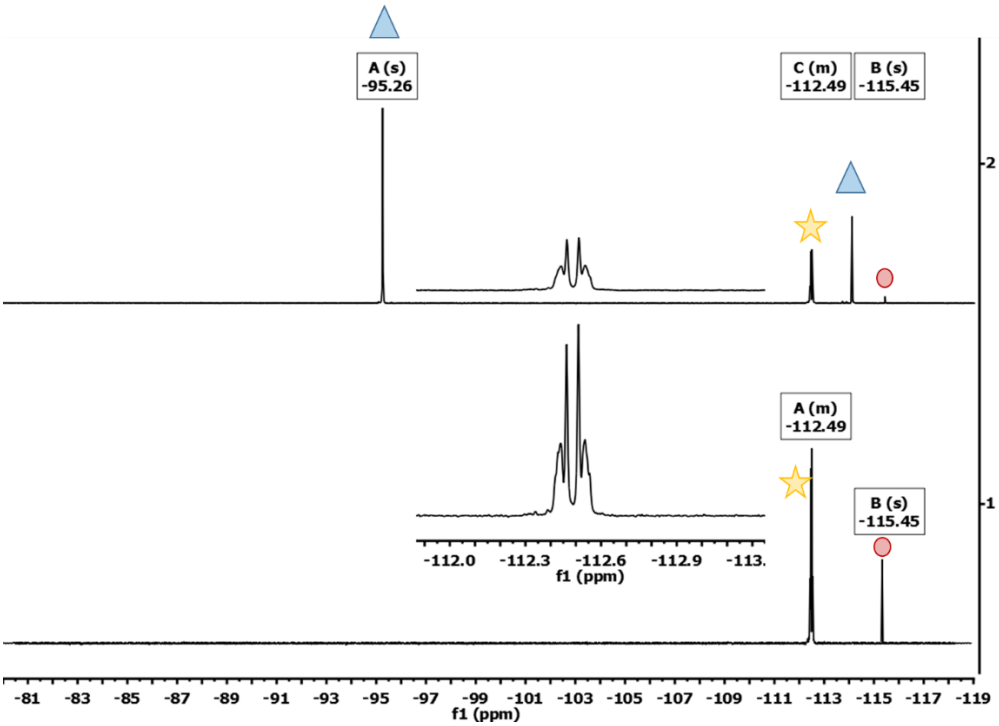
Table *ESI* 13. Results of MW in diffusion experiments and MW theoretical in DMF at 273K.

Aggregate	MW_{det} (DOSY)	MW (theoretical)
[Cu(DPI)(Pf)] + RfI	783	777.8
[Cu(DPI)(Pf)] + BrPf	254	247.0
[Cu(Bipy)(Pf)] + RfI	336	326.9
Rf-I	327	326.9
Pf-Br	247	246.9

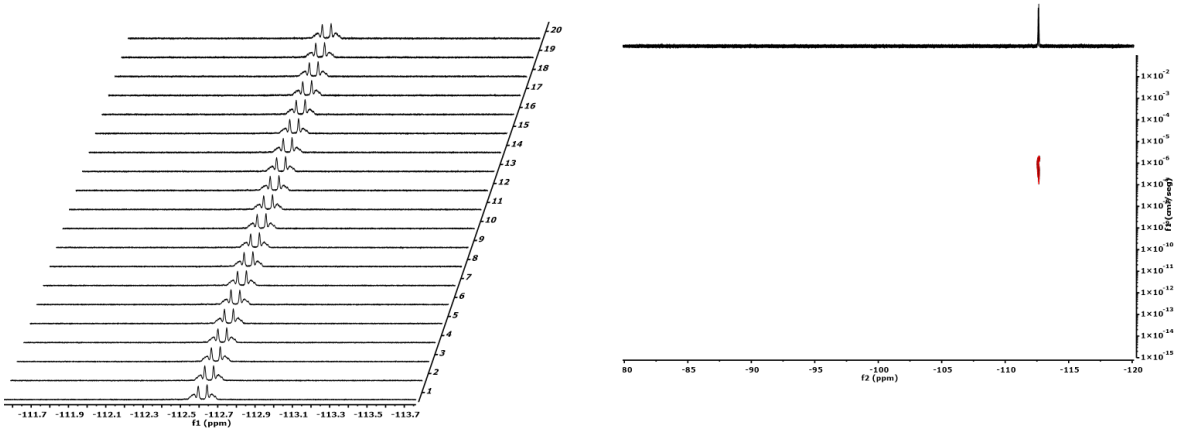
Weighted amounts of $C_6F_3Cl_2$–I ($4.2\cdot10^{-2}$ M) and [Cu(DPI)(Pf)] (**1-Pf**) ($4.2\cdot10^{-2}$ M) were added inside a screw cap NMR tube with the aid of a Schlenk NMR tube adaptor along with a flame sealed coaxial capillary containing acetone-d_6 to the lock deuterium signal. The tube was cooled to 273 K in an isopropanol bath and a volume and DMF taken with a syringe. The tube was closed inside the adaptor and then, taken out of the cool bath, manually shaken until total dissolution of solids and transferred to the NMR probe, which had been preheated to the monitoring temperature (273 K). C_6F_6 was used as internal standard.



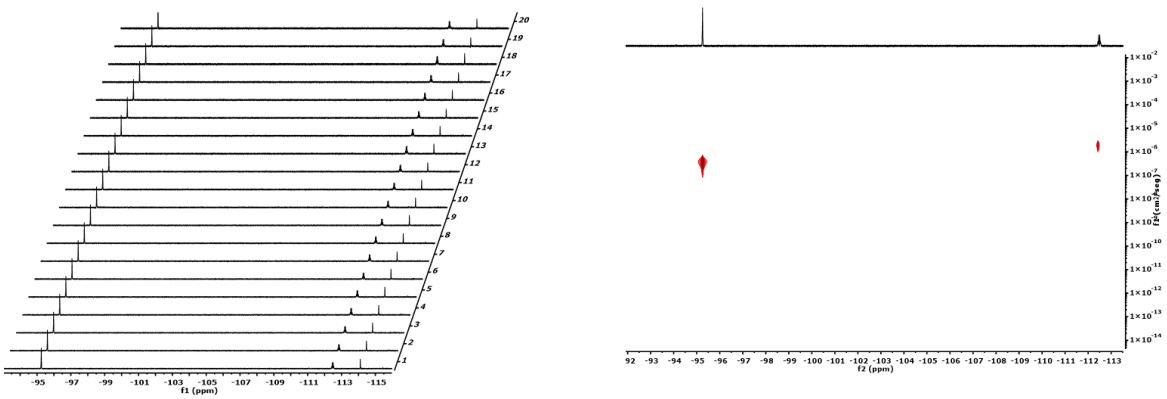
Spectrum ESI3. First spectra represents the ^{19}F NMR spectra of $C_6F_3Cl_2$–I (blue triangles F_{ortho} and green square F_{para}) and C_6F_6 (red circle, internal standar) in DMF at 273 K. Second one represents the ^{19}F NMR of $C_6F_3Cl_2$–I (blue triangles F_{ortho} and green square F_{para}) with [Cu(DPI)(Pf)] (yellow star) and C_6F_6 (red circle, internal standar) in DMF at 273 K.



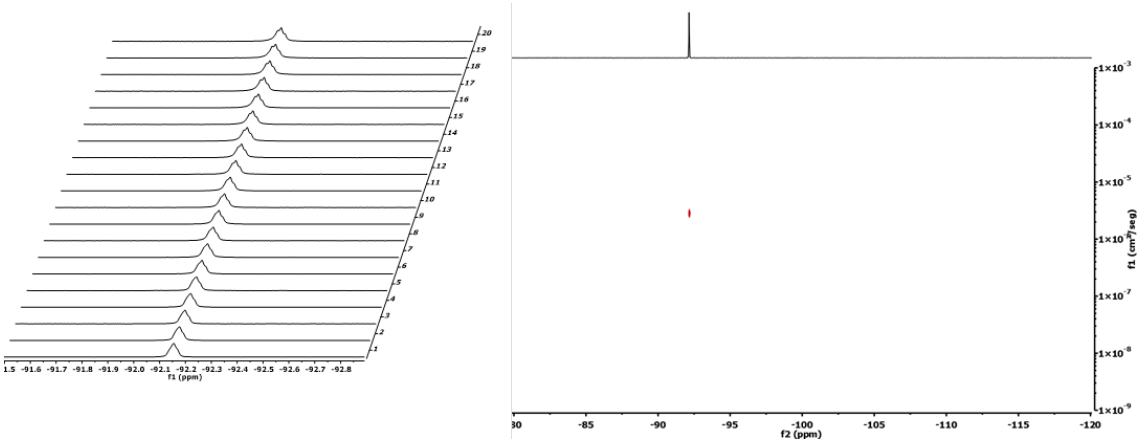
Spectrum ESI4. First spectra represents the ^{19}F NMR spectra of $C_6F_3Cl_2$–I (blue triangles F_{ortho} and F_{para}) , C_6F_6 (red circle, internal standar) and [Cu(DPI)(Pf)] (yellow star) in DMF at 273 K. Second one represents the ^{19}F NMR of [(DPI)Cu(Pf)] (yellow star) and C_6F_6 (red circle, internal standar) in DMF at 273 K.



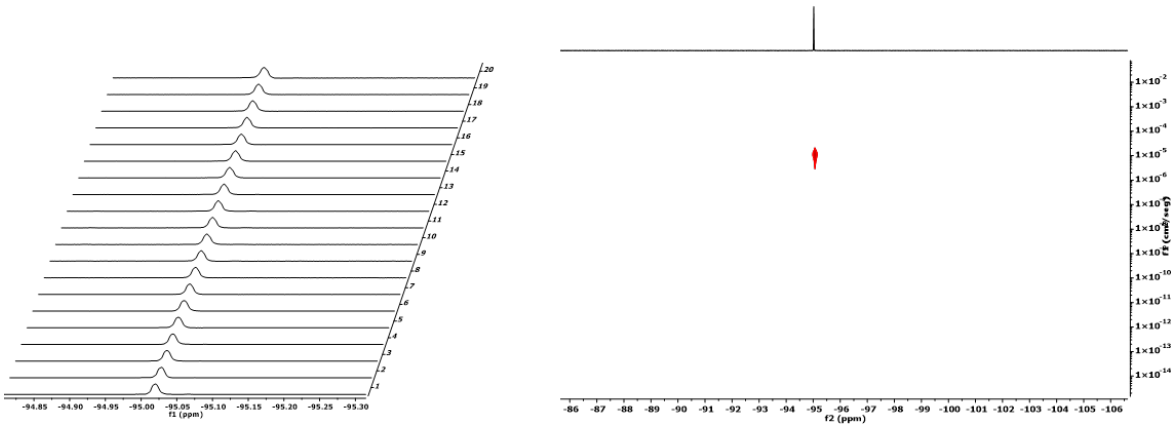
Spectrum ESI5. ^{19}F DOSY NMR spectrum of 1-Pf in DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s



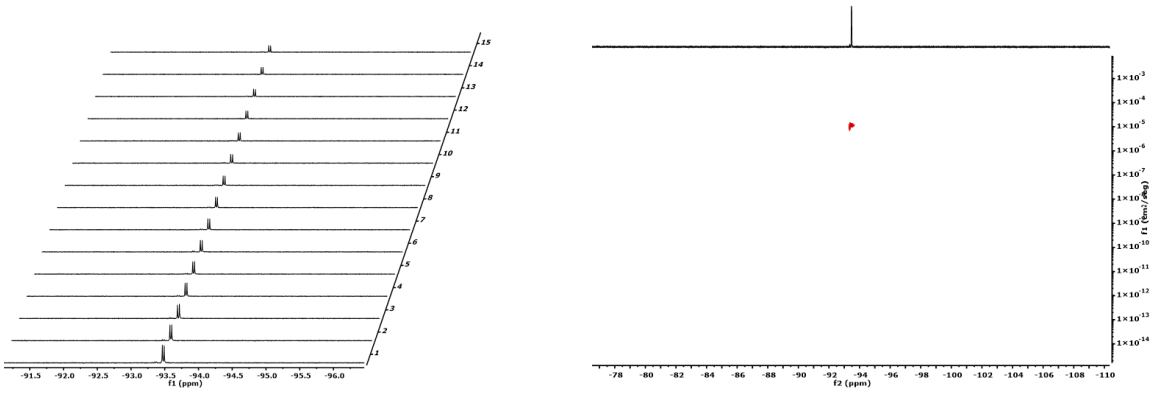
Spectrum ESI6. ^{19}F DOSY NMR spectrum of 1-Pf + Rf-I in DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s



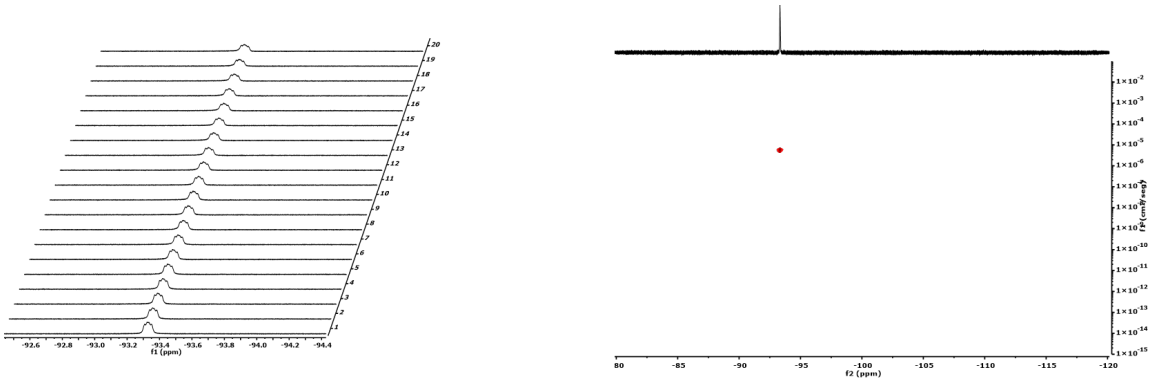
Spectrum ESI7. ^{19}F DOSY NMR spectrum of $[Pd(Rf)I(PPh_3)_2]$ in DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s



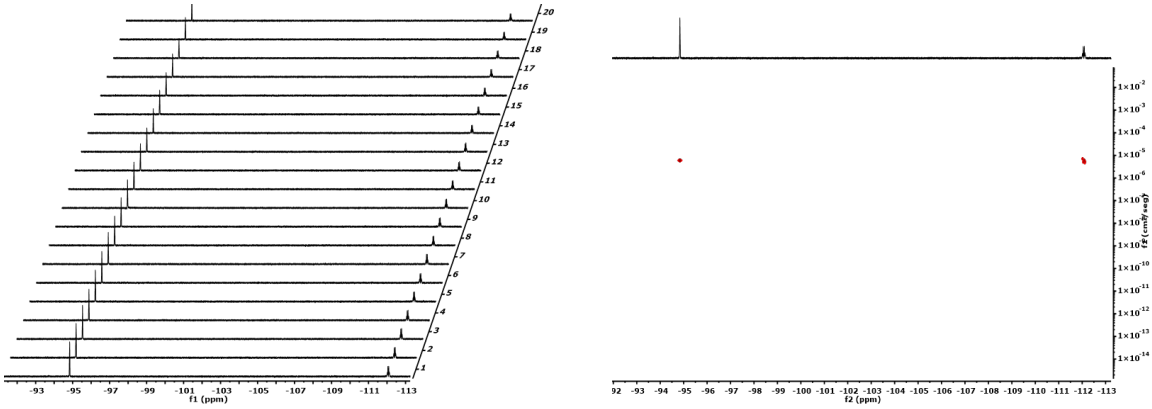
Spectrum ESI8 ^{19}F DOSY NMR spectrum of Rf-I in DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s



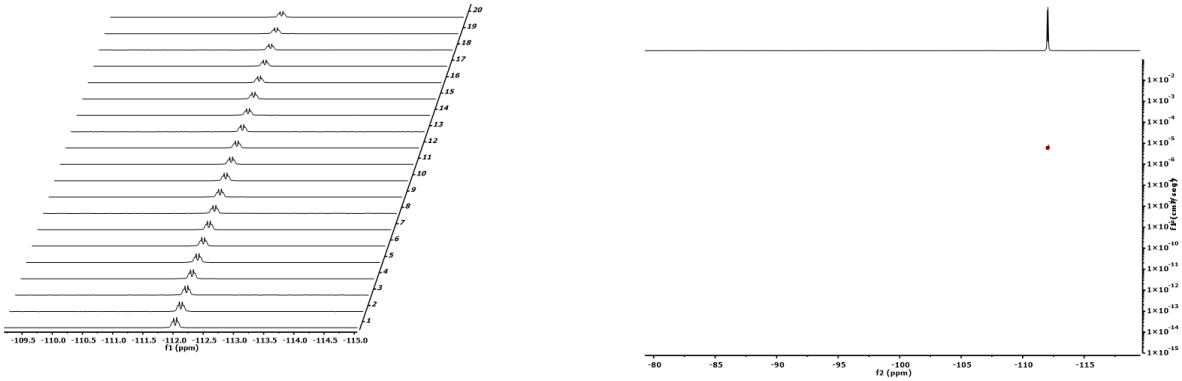
Spectrum ESI9. ^{19}F DOSY NMR spectrum of $[PdRf_2(PPh_3)_2]$ DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s



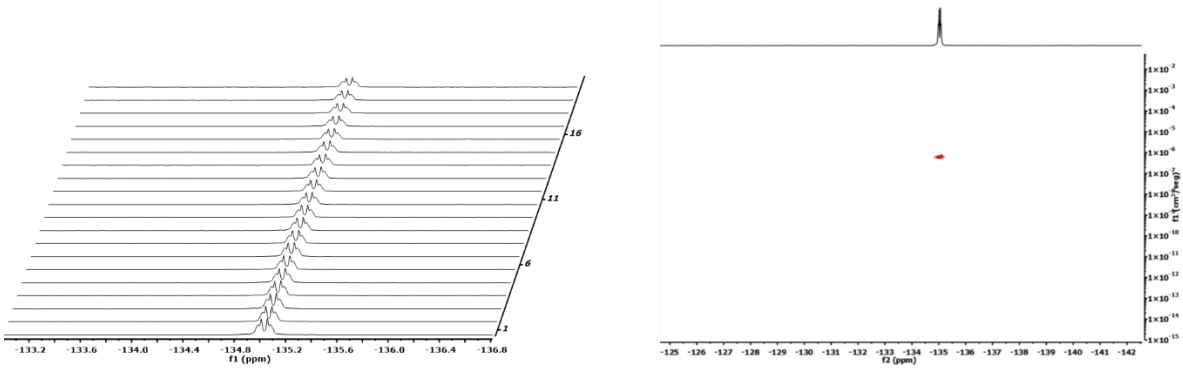
Spectrum ESI10. ^{19}F DOSY NMR spectrum of [Pd(Rf)Cl(Dppf)] in DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s



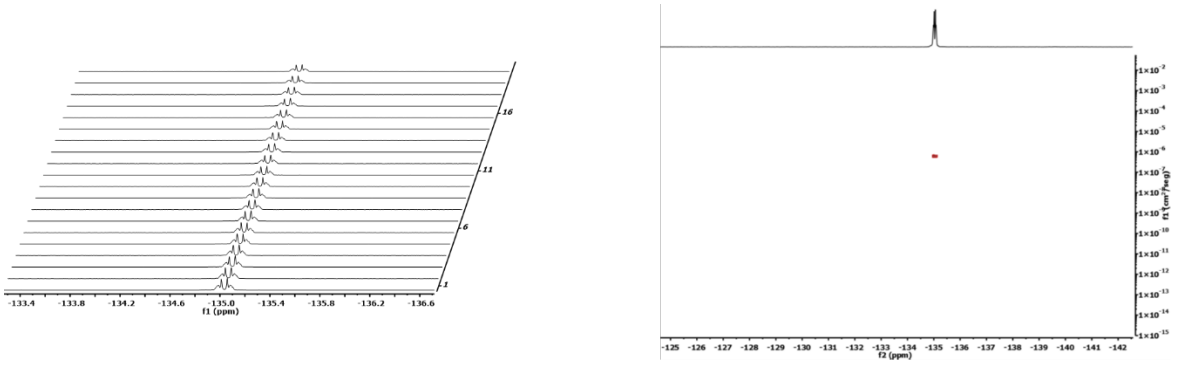
Spectrum ESI11. ^{19}F DOSY NMR spectrum of [Cu(Bipy)Pf] + RfI in DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s



Spectrum ESI12. ^{19}F DOSY NMR spectrum of [Cu(Bipy)Pf] in DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s



Spectrum ESI13. ^{19}F DOSY NMR spectrum of Pf-Br in DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s



Spectrum ESI14. ^{19}F DOSY NMR spectrum of [Cu(DPI)Pf] + Pf-Br in DMF/acetone cap.at 273 K . F1 chemical shift; F2 Diffusion coefficient (cm^2/s

Computational Section

Theoretical calculations were performed at DFT level of theory using Gaussian16 software.[15] The structures of all the intermediates and transition states were optimized in tetrahydrofuran solvent (DMF, ε= 37.219) with the SMD continuum model[16] using the B3LYP functional[17] combined with the Grimme's D3 correction for dispersion.[18] Basis set BS1 was used for the optimizations. BS1 includes the 6-31G(d,p) basis set for the main group elements,[19] excluding iodine, and the scalar relativistic Stuttgart-Dresden SDD pseudopotential and its associated double-ζ basis set,[20] complemented with a set of polarization functions, for the copper (*f* polarization functions)[21] and iodine (*d* polarization functions)[22] atoms. Frequency calculations were carried out for all the optimized geometries in order to characterize the stationary points as either minima or transition states.

Gibbs energies in DMF were calculated at 298.15 K adding to the potential energies in DMF, obtained with single point calculations using an extended basis set (BS2) at the BS1 optimized geometries, the thermal and entropic corrections obtained with BS1. BS2 consists in the def2-TZVP basis set for the main group elements, and the quadruple-ζ def2-QZVP basis set for Cu.[23] A correction of 1.9 kcal mol^{-1} was applied to all Gibbs values to change the standard state from the gas phase (1 atm) to solution (1 M) at 298.15 K.[24] In this way, all the energy values in the energy profiles are Gibbs energies in THF solution calculated using the formula:

$$G = E(BS2) + G(BS1) - E(BS1) + \Delta G^{1atm \rightarrow 1M}$$

where $\Delta G^{1atm \rightarrow 1M}$ = 1.9 kcal mol^{-1} is the Gibbs energy change for compression of 1 mol of an ideal gas from 1 atm to the 1 M solution phase standard state.

3D-structures were generated using CYLview. [26]

Optimized structures of all the intermediates and transition states in the reaction of [Cu(DPI)(C_6F_5)] with Rf–I

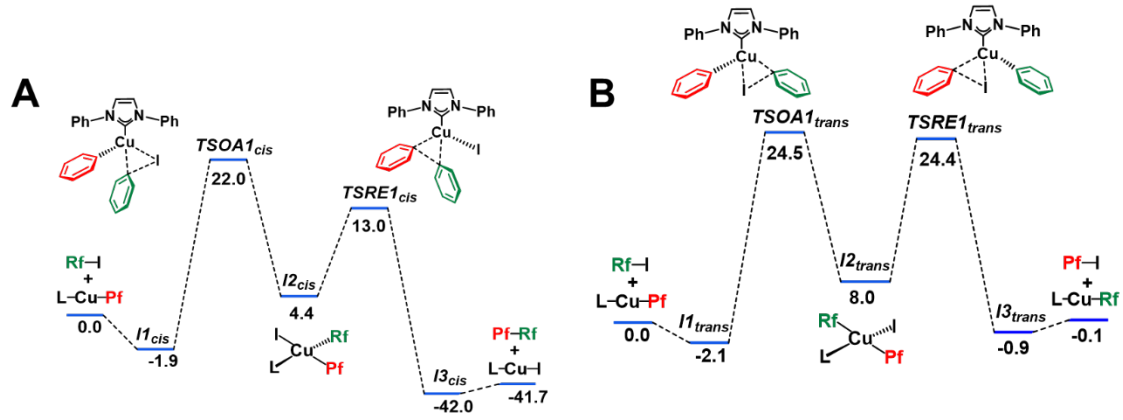


Figure *ESI* 10 .

Pathway A

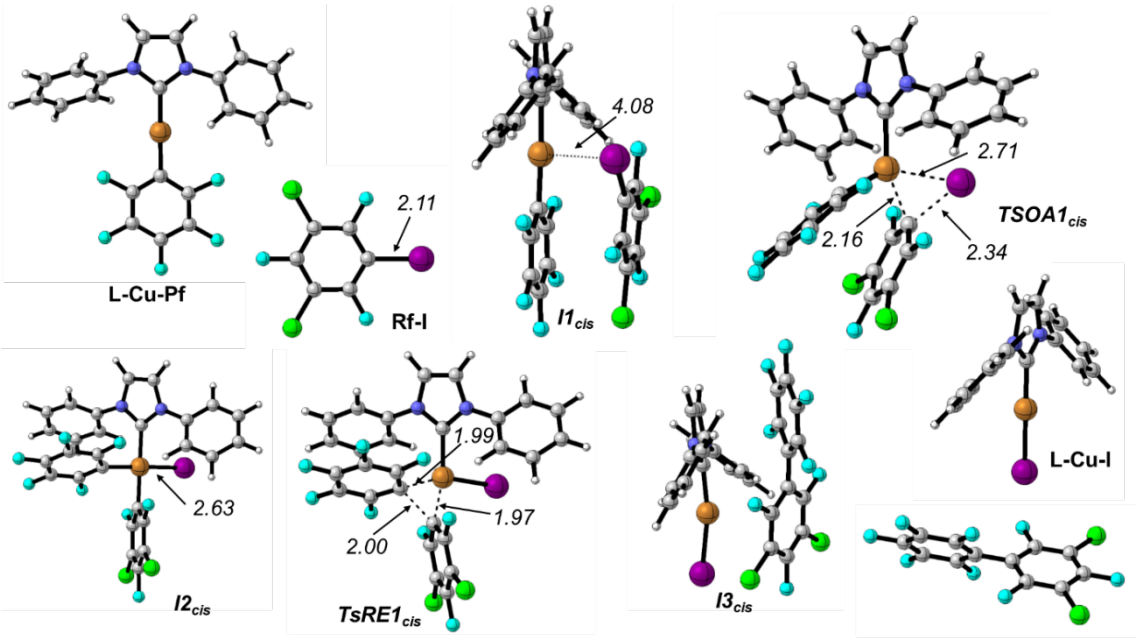


Figure *ESI* 11. Optimized structures of all the intermediates and transition states in the pathway for the formation of the aryl methatesis product, **Pf-I**.

Pathway B

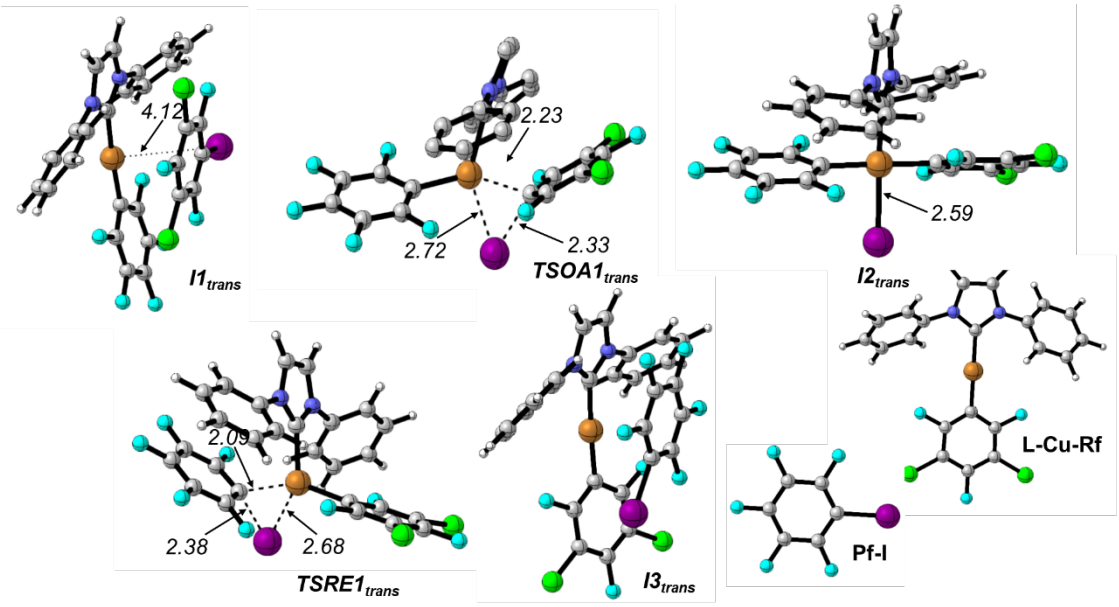


Figure *ESI* 12. Optimized structures of all the intermediates and transition states in the pathway for the formation of the heterocoupling product, **Pf-Rf**.

Second order pathway calculations

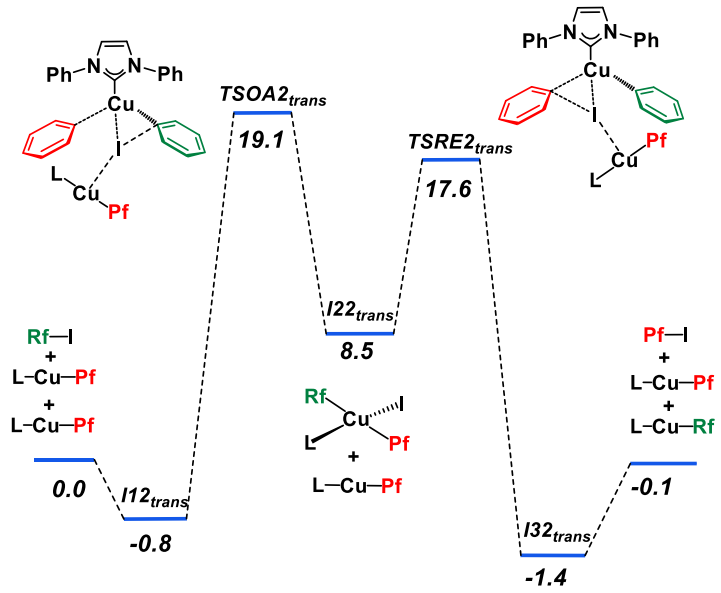


Figure *ESI* 13. (also Fig. 3 in main text) DFT-computed (B3LYP-D3/BS2 in DMF) pathway for the formation of the product **Ar^F–I** in the reaction of **1–Pf** with $C_6F_3Cl_2$–*I*. Relative Gibbs energies are given in kcal mol^{-1}.

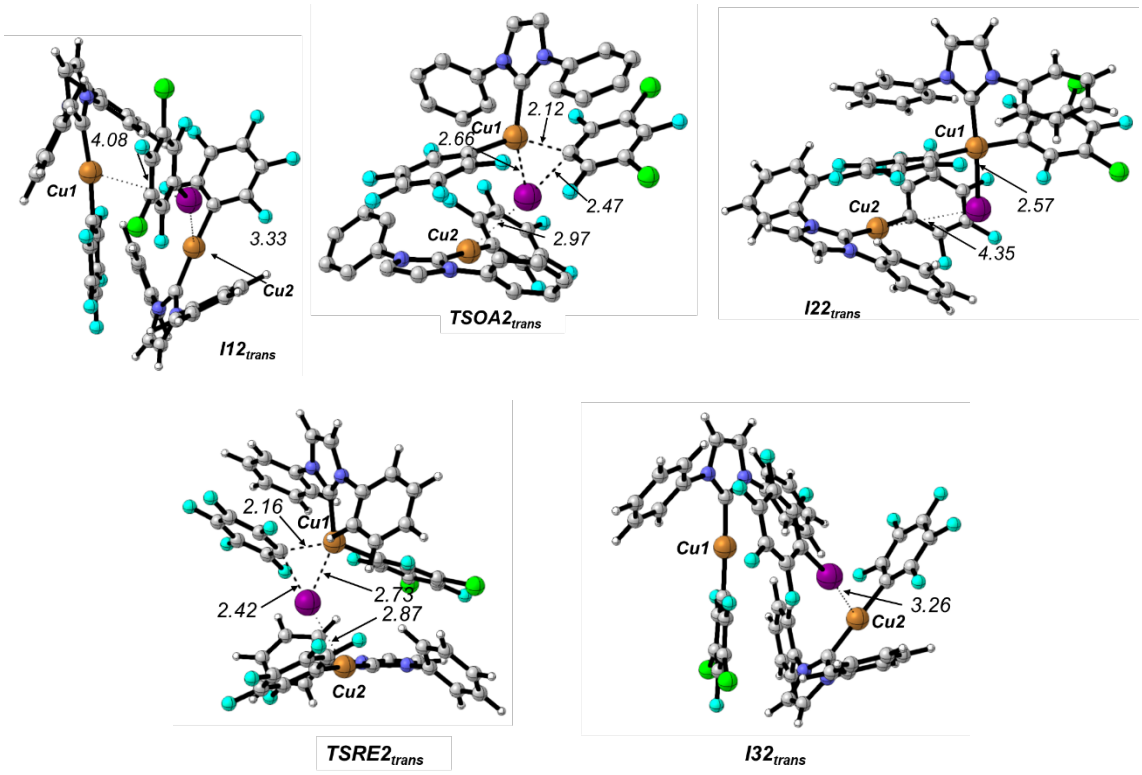


Figure *ESI* 14. Optimized structures of all the intermediates and transition states in the pathway for the formation of the aryl methatesis product, **Pf-I**.

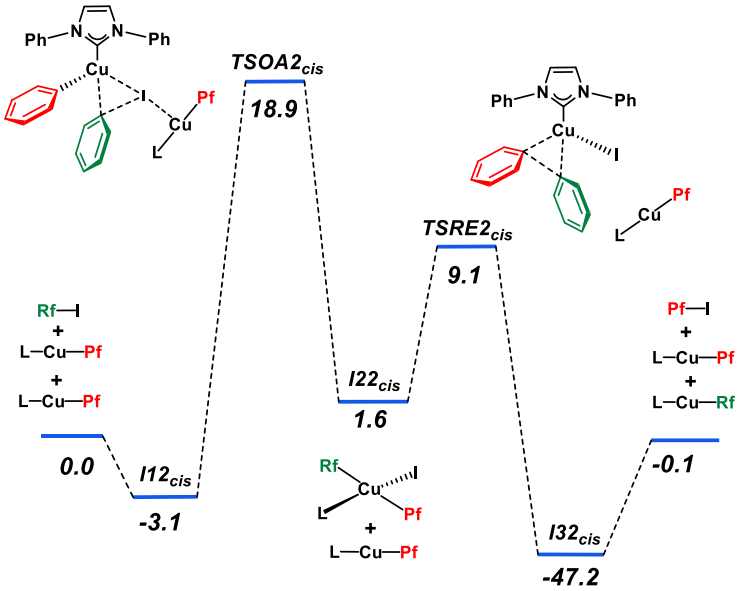
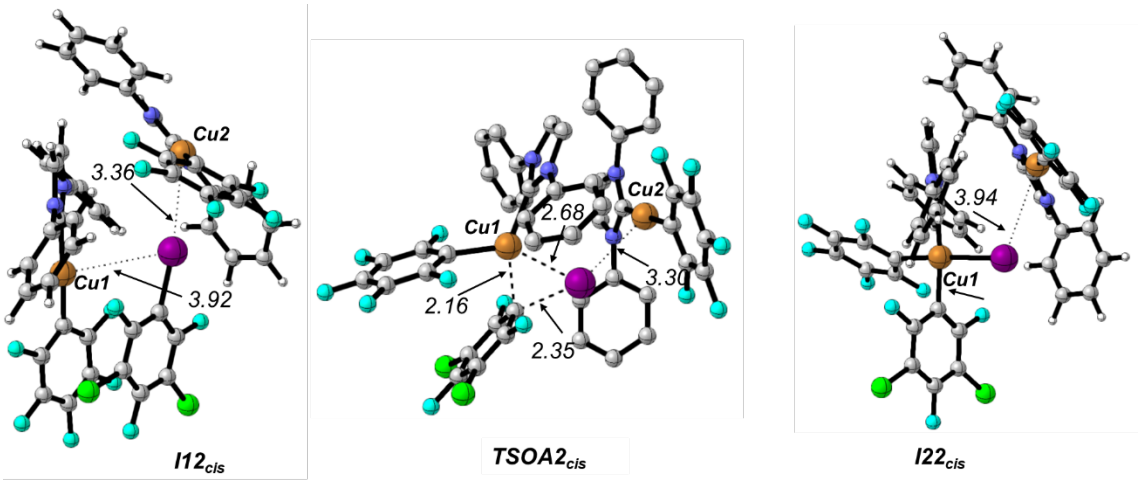


Figure *ESI* 15. DFT-computed (B3LYP-D3/BS2 in DMF) pathway for the formation of the product $Ar^F–Ar^F$ in the reaction of **1–Pf** with $C_6F_3Cl_2–I$. Relative Gibbs energies are given in kcal mol^{-1}.



Optimized structures of all the intermediates and transition states in the reaction of [Cu(DPI)(C_6F_5)] with Rf–Br

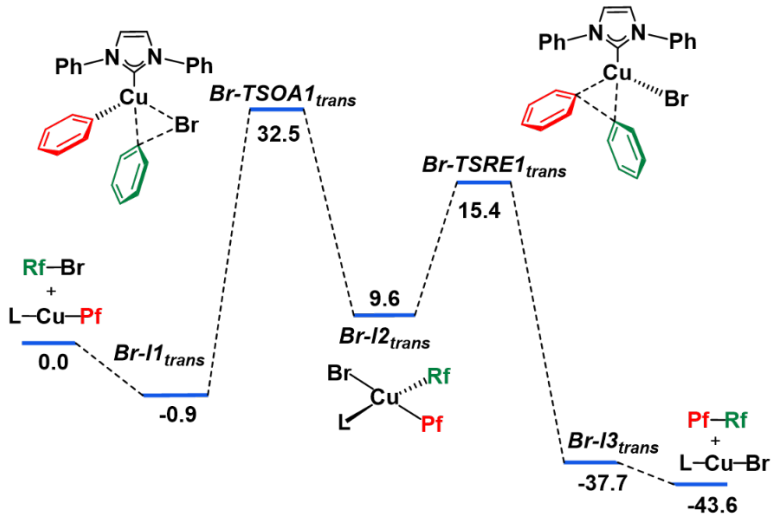


Figure *ESI* 16. DFT-computed (B3LYP-D3/BS2 in DMF) pathway for the formation of the product **cross-coupling** in the reaction of **1–Pf** with $C_6F_3Cl_2$–*Br*. Relative Gibbs energies are given in kcal mol^{-1}.

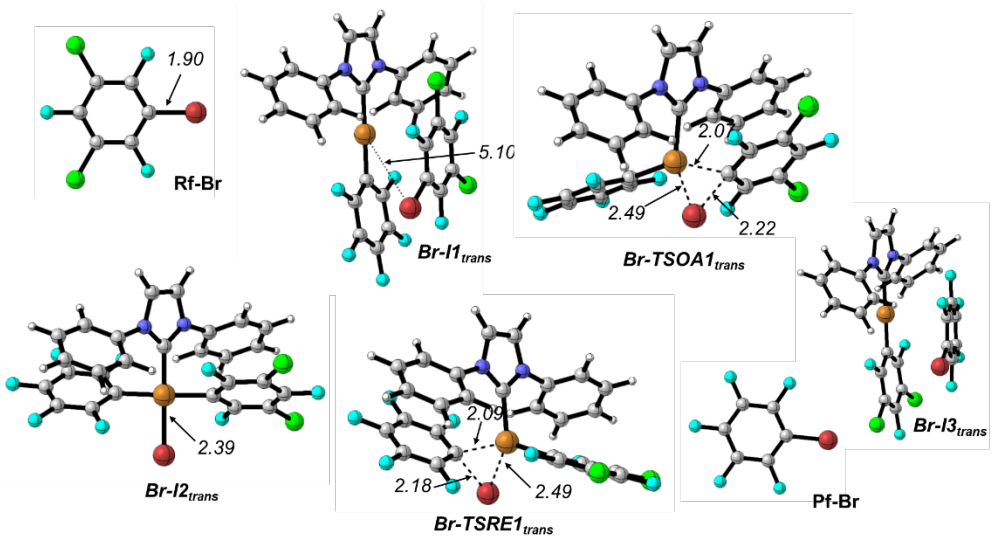


Figure *ESI* 17. DFT-computed (B3LYP-D3/BS2 in DMF) pathway for the formation of the product $Ar^F–Ar^F$ in the reaction of **1–Pf** with $C_6F_3Cl_2–Br$. Relative Gibbs energies are given in kcal mol^{-1}.

Second order pathway calculations

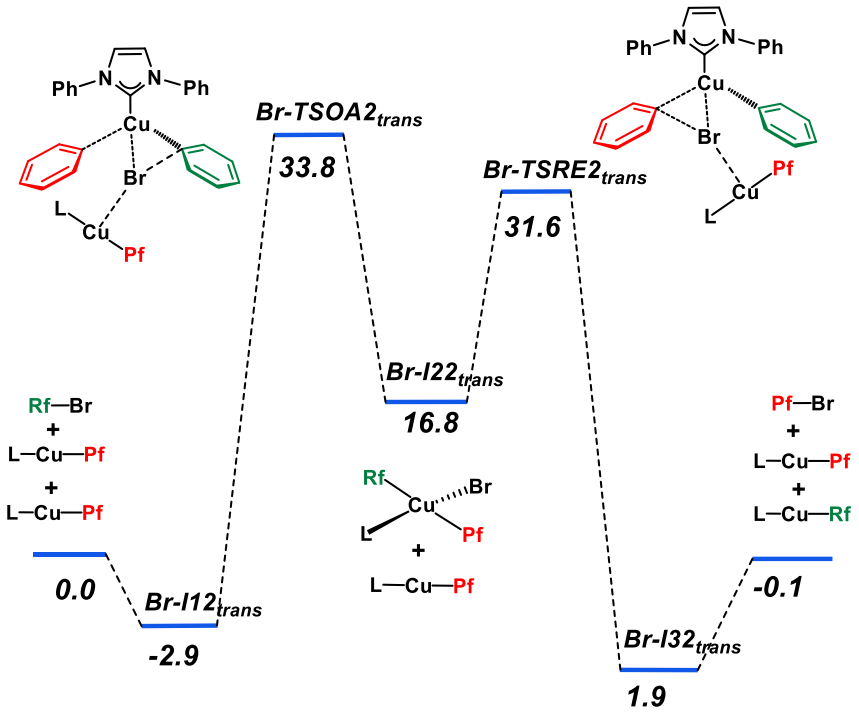


Figure *ESI* 18. DFT-computed (B3LYP-D3/BS2 in DMF) pathway for the formation of the product $Ar^F–Ar^F$ in the reaction of **1–Pf** with $C_6F_3Cl_2–Br$. Relative Gibbs energies are given in kcal mol^{-1}. The Rf-Br/(NHC)CuPf adduct ***Br-I12***$_{trans}$ at -2.9 kcal/mol is found in the second order pathway for the formation of the $Ar^F–Ar^F$ product that has a barrier of 36.7 kcal mol^{-1} and is not the favored one for Rf-Br. In this intermediate the Br···Cu2 distance is 4.34 Å, precluding any Cu2···Br interaction. Its stabilization is due to dispersive interactions between Rf and Ph_{NHC} rings.

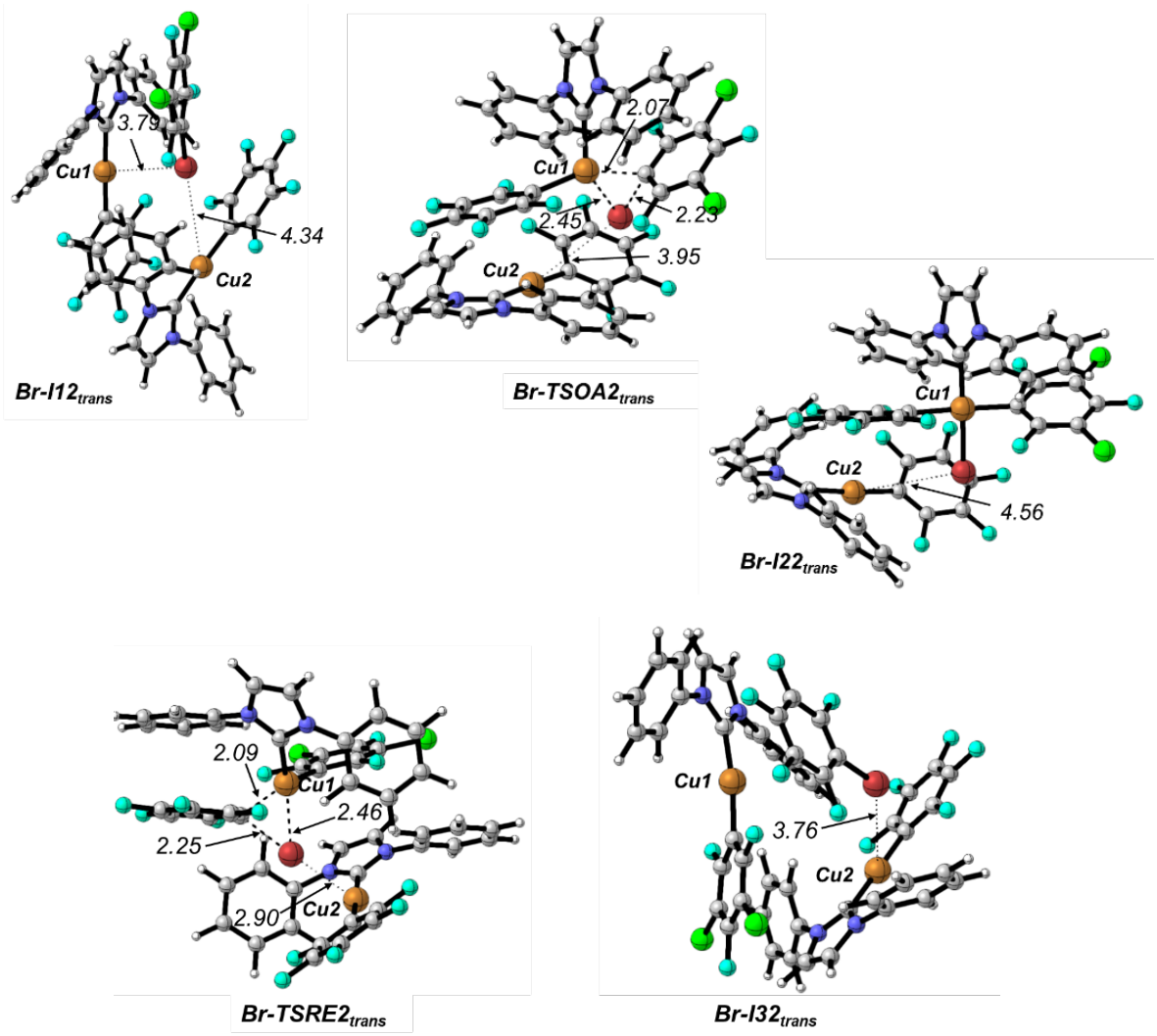


Figure *ESI* 19. DFT-computed (B3LYP-D3/BS2 in DMF) pathway for the formation of the product $\mathbf{Ar^F–Ar^F}$ in the reaction of **1–Pf** with $C_6F_3Cl_2$–*Br*. Relative Gibbs energies are given in kcal mol^{-1}

Cartesian coordinates and absolute E and G energies in DMF of the optimized structures

[Cu(DPI)Pf]

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-1613.56600617
Thermal and entropic correction, BS1 (a.u.)	0.224632
Electronic Energy, BS2 (a.u.)	-3057.405017
Gibbs Energy, BS2 (a.u.)	-3057.180385
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	-2.082530000	0.000761000	0.000135000	6	4.631081000	-0.002098000	0.000106000
6	-4.260024000	-0.675311000	-0.005747000	6	3.928960000	-1.201912000	-0.066113000
6	-4.259181000	0.679551000	0.006566000	6	2.537020000	-1.167286000	-0.063812000
1	-5.072269000	-1.384473000	-0.022866000	9	1.912600000	2.378095000	0.127850000
1	-5.070564000	1.389700000	0.023928000	9	1.910101000	-2.379413000	-0.128145000
7	-2.925774000	-1.072924000	-0.014184000	9	5.975943000	-0.002796000	0.000224000
7	-2.924464000	1.075529000	0.014667000	9	4.610255000	2.361583000	0.129986000
6	-2.683431000	-4.683004000	0.838557000	9	4.607777000	-2.365758000	-0.129716000
6	-1.642004000	-5.090853000	0.000740000	6	-2.492042000	2.440357000	0.021111000
6	-1.033850000	-4.166690000	-0.853053000	6	-3.106833000	3.356616000	-0.836526000
6	-1.464718000	-2.839762000	-0.876679000	6	-1.461131000	2.840933000	0.876479000
6	-2.494952000	-2.438232000	-0.020951000	6	-2.678230000	4.685175000	-0.838824000
6	-3.110557000	-3.353970000	0.836655000	6	-1.028784000	4.167375000	0.852460000
1	-3.158817000	-5.395437000	1.506120000	6	-1.636129000	5.092037000	-0.001366000
1	-1.307528000	-6.123925000	0.011836000	1	-3.898229000	3.028296000	-1.503047000
29	-0.150516000	0.000085000	-0.000031000	1	-1.007405000	2.119720000	1.547620000
1	-3.901411000	-3.024921000	1.503456000	1	-3.152977000	5.398006000	-1.506418000
1	-1.010385000	-2.118907000	-1.547803000	1	-0.221677000	4.476454000	1.509877000
6	1.784817000	-0.000582000	-0.000161000	1	-1.300516000	6.124740000	-0.012785000
6	2.538241000	1.165318000	0.063632000	1	-0.227282000	-4.476554000	-1.510765000
6	3.930212000	1.198446000	0.066216000				

Rf-I

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-1459.931777
Thermal and entropic correction, BS1 (a.u.)	0.007407
Electronic Energy, BS2 (a.u.)	-1746.619008
Gibbs Energy, BS2 (a.u.)	-1746.611601
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	0.190568000	1.197034000	0.000000000	9	-0.461049000	-2.362470000	-0.000001000
6	1.586829000	1.214004000	0.000002000	9	3.606958000	0.000000000	0.000005000
6	2.273729000	0.000000000	0.000003000	9	-0.461049000	2.362470000	-0.000001000
6	1.586829000	-1.214004000	0.000002000	53	-2.633002000	0.000000000	-0.000003000
6	0.190568000	-1.197034000	0.000000000	17	2.457672000	-2.716397000	0.000003000
6	-0.524438000	0.000000000	-0.000001000	17	2.457672000	2.716397000	0.000003000

I1cis

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.530501
Thermal and entropic correction, BS1 (a.u.)	0.255036
Electronic Energy, BS2 (a.u.)	-4804.046964
Gibbs Energy, BS2 (a.u.)	-4803.791928
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	2.917436000	0.576933000	0.533103000	1	1.781824000	6.560686000	-0.449623000
6	5.006062000	1.284479000	-0.050488000	29	1.036407000	0.579635000	0.966161000
6	5.088952000	-0.042567000	0.209691000	6	-2.229070000	-1.652565000	-1.125342000
1	5.753121000	1.995562000	-0.365084000	6	-3.280103000	-0.733708000	-1.105049000
1	5.928643000	-0.718730000	0.188565000	6	-3.031034000	0.577664000	-1.507322000
7	3.675628000	1.644007000	0.145595000	6	-1.765356000	0.969099000	-1.943470000
7	3.808937000	-0.458313000	0.567811000	6	-0.741001000	0.022782000	-1.957414000
6	3.359235000	5.340249000	0.372131000	6	-0.950734000	-1.293404000	-1.548452000
6	2.172047000	5.553906000	-0.333589000	9	0.479954000	0.412033000	-2.349755000
6	1.490200000	4.469942000	-0.892591000	9	-4.013872000	1.478228000	-1.453232000
6	1.989119000	3.174452000	-0.753245000	9	-2.466030000	-2.897261000	-0.701302000
6	3.167737000	2.971112000	-0.029316000	1	4.768503000	3.869296000	1.099008000
6	3.859852000	4.047061000	0.532443000	1	1.478363000	2.329021000	-1.199794000
1	3.893150000	6.178116000	0.810397000	6	-0.830987000	0.646006000	1.463885000

6	-1.539200000	-0.468909000	1.892809000	6	3.464245000	-1.809245000	0.889927000
6	-2.899201000	-0.467446000	2.189648000	6	3.964328000	-2.848697000	0.100517000
6	-3.616807000	0.715963000	2.048557000	6	2.606858000	-2.074917000	1.960793000
6	-2.962146000	1.865013000	1.615033000	6	3.589009000	-4.163917000	0.382076000
6	-1.596226000	1.800248000	1.352242000	6	2.225067000	-3.391070000	2.223128000
9	-0.906939000	-1.675659000	2.005705000	6	2.712843000	-4.437601000	1.436584000
9	-1.016044000	2.961485000	0.926765000	1	4.616014000	-2.628793000	-0.738948000
9	-4.938213000	0.739893000	2.295802000	1	2.241016000	-1.257802000	2.573078000
53	0.638449000	-2.672415000	-1.462120000	1	3.974368000	-4.972022000	-0.232441000
17	-4.861746000	-1.203575000	-0.567143000	1	1.549472000	-3.594945000	3.048425000
17	-1.474926000	2.609628000	-2.427290000	1	2.416519000	-5.461060000	1.646124000
9	-3.541026000	-1.591710000	2.567306000	1	0.570590000	4.630057000	-1.446448000
9	-3.660104000	3.007573000	1.454733000				

TSOA1$_{cis}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.491067
Thermal and entropic correction, BS1 (a.u.)	0.254020
Electronic Energy, BS2 (a.u.)	-4804.007894
Gibbs Energy, BS2 (a.u.)	-4803.753874
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	2.441445000	1.138808000	0.610492000	29	0.762784000	0.157675000	0.079262000
6	3.922639000	2.801960000	1.094152000	6	-1.222777000	-1.887671000	-0.851696000
6	4.584572000	1.625565000	1.213053000	6	-2.607556000	-1.975244000	-0.892578000
1	4.252133000	3.820973000	1.220613000	6	-3.328781000	-0.956358000	-1.524782000
1	5.604387000	1.406182000	1.486990000	6	-2.668822000	0.121990000	-2.113244000
7	2.617712000	2.484957000	0.721203000	6	-1.278090000	0.175643000	-2.050088000
7	3.664135000	0.622302000	0.917662000	6	-0.528386000	-0.789162000	-1.372611000
6	0.399554000	5.453811000	1.019767000	9	-0.652698000	1.230933000	-2.599612000
6	-0.398640000	5.305258000	-0.118815000	9	-4.662486000	-1.022640000	-1.569392000
6	-0.187930000	4.226510000	-0.980478000	9	-0.533710000	-2.831484000	-0.192540000
6	0.821654000	3.301794000	-0.713828000	1	2.008202000	4.618404000	2.200671000
6	1.601806000	3.450492000	0.434841000	1	0.997757000	2.465891000	-1.380230000
6	1.400273000	4.523965000	1.306406000	6	-0.787812000	0.146735000	1.367603000
1	0.236824000	6.288197000	1.695447000	6	-0.937872000	-0.845077000	2.323455000
1	-1.182250000	6.026712000	-0.330519000	6	-2.110095000	-1.061246000	3.043147000

6	-3.204109000	-0.233119000	2.811504000	6	5.106135000	-1.212660000	0.200173000
6	-3.102581000	0.785275000	1.868808000	6	3.104850000	-1.682907000	1.497588000
6	-1.900920000	0.952801000	1.185835000	6	5.370783000	-2.581452000	0.125415000
9	0.084223000	-1.718222000	2.577931000	6	3.370535000	-3.049351000	1.403611000
9	-1.879126000	1.949293000	0.252624000	6	4.501600000	-3.502017000	0.718800000
9	-4.350120000	-0.417777000	3.490572000	1	5.759545000	-0.493303000	-0.283504000
53	1.655707000	-1.148675000	-2.120943000	1	2.232989000	-1.321977000	2.028325000
17	-3.442563000	-3.295926000	-0.128264000	1	6.251120000	-2.926997000	-0.408299000
17	-3.574548000	1.393456000	-2.878345000	1	2.693574000	-3.757194000	1.872947000
9	-2.208013000	-2.052123000	3.952362000	1	4.707967000	-4.566037000	0.650652000
9	-4.164283000	1.582627000	1.634485000	1	-0.807621000	4.096255000	-1.862413000
6	3.969534000	-0.775049000	0.883995000				

$I2_{cis}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.532168
Thermal and entropic correction, BS1 (a.u.)	0.259860
Electronic Energy, BS2 (a.u.)	-4804.041862
Gibbs Energy, BS2 (a.u.)	-4803.782002
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	1.887727000	-1.274417000	-0.256745000	6	-2.280790000	0.204875000	1.164019000
6	4.131960000	-1.545505000	-0.317698000	6	-3.570688000	0.680680000	1.412904000
6	3.606756000	-2.638489000	0.286408000	6	-4.250084000	1.319954000	0.376376000
1	5.149258000	-1.280241000	-0.557186000	6	-3.654375000	1.475942000	-0.875858000
1	4.076559000	-3.515054000	0.702457000	6	-2.365474000	0.972962000	-1.069243000
7	3.060802000	-0.719390000	-0.645694000	6	-1.658284000	0.321082000	-0.068877000
7	2.224654000	-2.457845000	0.318742000	9	-1.814199000	1.119571000	-2.288845000
6	4.153842000	2.755465000	-1.348184000	9	-5.485296000	1.788681000	0.584501000
6	3.338339000	3.076008000	-2.438074000	9	-1.622495000	-0.385847000	2.186682000
6	2.451953000	2.126231000	-2.951562000	1	4.681817000	1.241341000	0.105318000
6	2.371354000	0.856988000	-2.377708000	1	1.677207000	0.111829000	-2.753252000
6	3.181882000	0.557201000	-1.281918000	6	0.748257000	1.072310000	0.678808000
6	4.078887000	1.492159000	-0.761402000	6	1.387912000	0.941229000	1.902868000
1	4.837992000	3.494156000	-0.941854000	6	2.002885000	2.018489000	2.536478000
1	3.392928000	4.064719000	-2.883555000	6	1.973146000	3.273800000	1.938610000
29	0.102289000	-0.454801000	-0.332388000	6	1.328598000	3.435814000	0.717476000

6	0.712200000	2.342034000	0.116775000	6	0.234015000	-2.980660000	1.648957000
9	1.492918000	-0.262390000	2.509763000	6	0.582396000	-5.698364000	1.094832000
9	0.100585000	2.562797000	-1.064206000	6	-0.676197000	-3.916947000	2.138513000
9	2.570999000	4.316907000	2.530163000	6	-0.504025000	-5.276423000	1.866865000
53	-0.764409000	-2.263515000	-2.029536000	1	2.315168000	-5.089706000	-0.042312000
17	-4.320632000	0.496420000	2.973893000	1	0.112968000	-1.928253000	1.866865000
17	-4.516009000	2.274019000	-2.162413000	1	0.720698000	-6.752953000	0.876435000
9	2.633807000	1.852756000	3.710038000	1	-1.515378000	-3.576622000	2.738001000
9	1.309749000	4.640183000	0.124895000	1	-1.210782000	-6.003985000	2.254579000
6	1.305718000	-3.412554000	0.865342000	1	1.815849000	2.371744000	-3.796325000
6	1.489275000	-4.768570000	0.584049000				

TSRE1$_{cis}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.522386
Thermal and entropic correction, BS1 (a.u.)	0.260560
Electronic Energy, BS2 (a.u.)	-4804.028830
Gibbs Energy, BS2 (a.u.)	-4803.768270
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	-1.243758000	1.987634000	-0.245631000	6	3.263136000	-2.855942000	0.424799000
6	-3.212548000	3.121812000	-0.224035000	6	2.619377000	-2.754261000	-0.809515000
6	-2.271373000	3.933991000	0.314467000	6	1.524732000	-1.900722000	-0.933040000
1	-4.263862000	3.272394000	-0.411059000	6	1.034294000	-1.145297000	0.143552000
1	-2.339133000	4.932777000	0.714815000	9	1.002643000	-1.747643000	-2.158554000
7	-2.564209000	1.937543000	-0.563577000	9	4.308360000	-3.672912000	0.559275000
7	-1.071592000	3.223894000	0.295775000	9	1.343245000	-0.532338000	2.407185000
6	-4.991119000	-0.805048000	-1.178642000	1	-4.815684000	0.797791000	0.264235000
6	-4.409816000	-1.434863000	-2.282792000	1	-1.695809000	0.592689000	-2.685352000
6	-3.226205000	-0.932324000	-2.829484000	6	-0.917290000	-0.960142000	0.560913000
6	-2.619254000	0.195680000	-2.276345000	6	-1.446202000	-0.531115000	1.788500000
6	-3.204077000	0.807618000	-1.165123000	6	-2.566888000	-1.117732000	2.363719000
6	-4.388723000	0.318522000	-0.610810000	6	-3.203546000	-2.178374000	1.729626000
1	-5.904054000	-1.199386000	-0.742898000	6	-2.711125000	-2.626760000	0.512073000
1	-4.875251000	-2.316827000	-2.711984000	6	-1.587471000	-2.028898000	-0.047041000
29	0.070189000	0.498396000	-0.363468000	9	-0.974667000	0.562554000	2.418744000
6	1.735743000	-1.255965000	1.347995000	9	-1.174563000	-2.532740000	-1.219454000
6	2.835173000	-2.097146000	1.513014000	9	-4.292909000	-2.735522000	2.268218000

53	1.965785000	1.668652000	-1.930823000	6	2.216865000	3.469924000	2.028375000
17	3.658864000	-2.206270000	3.039769000	6	2.588934000	4.777270000	1.705671000
17	3.218587000	-3.643097000	-2.179262000	1	-0.117527000	5.653867000	-0.172490000
9	-3.067000000	-0.630666000	3.508664000	1	0.708201000	1.939919000	1.834895000
9	-3.324939000	-3.629453000	-0.131235000	1	2.025358000	6.582578000	0.664008000
6	0.168959000	3.745158000	0.788846000	1	2.867455000	2.849476000	2.637692000
6	0.530773000	5.053186000	0.457258000	1	3.532647000	5.179369000	2.061909000
6	1.002633000	2.950041000	1.579646000	1	-2.769115000	-1.418823000	-3.685504000
6	1.741621000	5.567050000	0.923396000				

$I3_{cis}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.522386
Thermal and entropic correction, BS1 (a.u.)	0.260560
Electronic Energy, BS2 (a.u.)	-4804.028830
Gibbs Energy, BS2 (a.u.)	-4803.768270
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	0.142320000	1.260611000	-1.473324000	6	-0.579074000	-1.983096000	0.815311000
6	-1.807500000	2.168973000	-2.227240000	6	-0.969999000	-0.833530000	1.512698000
6	-1.052601000	3.182650000	-1.739872000	9	-1.411693000	-2.509270000	-0.086434000
1	-2.784894000	2.169458000	-2.681763000	9	2.732329000	-2.601565000	2.125942000
1	-1.249827000	4.239432000	-1.656850000	9	-0.365522000	0.792244000	3.111824000
7	-1.063532000	1.001475000	-2.059961000	1	-3.519077000	0.069507000	-1.696659000
7	0.131036000	2.611793000	-1.284320000	1	0.371888000	-0.934830000	-3.226887000
6	-3.314852000	-1.918313000	-2.509935000	6	-2.291699000	-0.213161000	1.285571000
6	-2.446861000	-2.849822000	-3.084305000	6	-2.427556000	1.153825000	1.022645000
6	-1.118204000	-2.497347000	-3.335392000	6	-3.657749000	1.736889000	0.743773000
6	-0.654197000	-1.219856000	-3.019495000	6	-4.805299000	0.950446000	0.739649000
6	-1.527504000	-0.301330000	-2.429375000	6	-4.708387000	-0.411046000	1.012938000
6	-2.857927000	-0.643759000	-2.175092000	6	-3.467497000	-0.973415000	1.288529000
1	-4.346761000	-2.185116000	-2.301594000	9	-1.347993000	1.948865000	1.005507000
1	-2.802822000	-3.844741000	-3.334873000	9	-3.422400000	-2.283348000	1.568006000
29	1.604719000	0.095176000	-1.065299000	9	-5.993945000	1.497934000	0.474213000
6	-0.040423000	-0.299539000	2.410882000	53	3.863686000	-1.015475000	-0.909143000
6	1.219562000	-0.862866000	2.610100000	17	2.352622000	-0.142485000	3.709855000
6	1.549189000	-2.027376000	1.916793000	17	1.081719000	-4.027258000	0.124322000
6	0.656778000	-2.597626000	1.008813000	9	-3.736285000	3.044289000	0.467484000

9	-5.810830000	-1.170711000	1.019933000	1	1.264495000	4.860249000	-2.133769000
6	1.166177000	3.337378000	-0.614413000	1	1.242585000	1.967735000	1.044357000
6	1.659455000	4.512938000	-1.184115000	1	3.058771000	6.130467000	-0.968339000
6	1.662014000	2.865434000	0.605538000	1	3.069916000	3.204899000	2.191783000
6	2.669834000	5.217772000	-0.526961000	1	3.976425000	5.294747000	1.187237000
6	2.681525000	3.570502000	1.245849000	1	-0.438768000	-3.213253000	-3.788475000
6	3.186575000	4.746047000	0.682899000				

[(BPI)CuI]

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-897.263594
Thermal and entropic correction, BS1 (a.u.)	0.186787
Electronic Energy, BS2 (a.u.)	-2627.150779
Gibbs Energy, BS2 (a.u.)	-2626.963992
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	0.134147000	-1.245228000	0.002544000	1	3.300601000	-2.857201000	1.458116000
6	0.972206000	-3.364082000	-0.020446000	1	2.158258000	0.002358000	-1.543595000
6	-0.378597000	-3.465719000	0.000453000	53	-0.334056000	3.161313000	-0.002359000
1	1.741143000	-4.119651000	-0.048844000	6	-2.268971000	-1.839566000	0.041148000
1	-1.026530000	-4.327548000	0.016632000	6	-3.138301000	-2.502649000	-0.828836000
7	1.268679000	-2.003298000	-0.023133000	6	-2.744770000	-0.867555000	0.926798000
7	-0.874586000	-2.165067000	0.019262000	6	-4.497200000	-2.182962000	-0.812771000
6	4.864610000	-1.526092000	0.783604000	6	-4.102736000	-0.546158000	0.923668000
6	5.191012000	-0.453223000	-0.049901000	6	-4.981221000	-1.202594000	0.057284000
6	4.215446000	0.102901000	-0.881918000	1	-2.752217000	-3.246756000	-1.518342000
6	2.917815000	-0.410619000	-0.888291000	1	-2.057181000	-0.376127000	1.606886000
6	2.599013000	-1.475161000	-0.039622000	1	-5.174048000	-2.694861000	-1.490244000
6	3.566208000	-2.038443000	0.796961000	1	-4.473503000	0.209909000	1.609305000
1	5.616836000	-1.961611000	1.434482000	1	-6.038117000	-0.953264000	0.062184000
1	6.201101000	-0.054587000	-0.053379000	1	4.464471000	0.930734000	-1.539077000
29	-0.038154000	0.661395000	0.003239000				

Pf-Rf

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-2176.310777
Thermal and entropic correction, BS1 (a.u.)	0.049475
Electronic Energy, BS2 (a.u.)	-2176.943852
Gibbs Energy, BS2 (a.u.)	-2176.894377
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	1.114456000	-1.135503000	-0.362434000	6	-3.907512000	-0.000081000	-0.000252000
6	2.508406000	-1.158961000	-0.363726000	6	-3.210710000	0.985932000	-0.692319000
6	3.194721000	0.000100000	0.000318000	6	-1.820695000	0.973197000	-0.691720000
6	2.508046000	1.159006000	0.364207000	9	-1.178393000	-1.923233000	1.386411000
6	1.114121000	1.135123000	0.362874000	9	-1.178218000	1.922813000	-1.386627000
6	0.384206000	-0.000294000	0.000132000	9	-5.243212000	0.000023000	0.000015000
9	0.452222000	2.236759000	0.731597000	17	3.376458000	-2.591263000	-0.819582000
9	4.527308000	0.000406000	0.000013000	17	3.375622000	2.591701000	0.819679000
9	0.452862000	-2.236997000	-0.732181000	9	-3.880304000	-1.930782000	1.364584000
6	-1.092978000	-0.000264000	-0.000163000	9	-3.879782000	1.931200000	-1.364370000
6	-1.820898000	-0.973701000	0.691495000				
6	-3.210781000	-0.986076000	0.692149000				

Pf-I

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-739.192929
Thermal and entropic correction, BS1 (a.u.)	0.011378
Electronic Energy, BS2 (a.u.)	-1025.914694
Gibbs Energy, BS2 (a.u.)	-1025.903316
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	0.206970000	0.000006000	0.000315000	9	0.123090000	-2.379766000	0.000301000
6	-0.507297000	1.197962000	0.000234000	9	-3.933783000	-0.000001000	-0.000342000
6	-1.899403000	1.203567000	0.000046000	9	-2.568193000	2.364009000	-0.000054000
6	-2.597129000	-0.000006000	-0.000094000	9	-2.568168000	-2.364029000	-0.000040000
6	-1.899397000	-1.203575000	0.000042000	53	2.313907000	0.000002000	-0.000117000
6	-0.507289000	-1.197954000	0.000230000				
9	0.123074000	2.379774000	0.000312000				

[Cu(DPI)($C_6F_3Cl_2$)]

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-2334.306132
Thermal and entropic correction, BS1 (a.u.)	0.220075
Electronic Energy, BS2 (a.u.)	-3778.108982
Gibbs Energy, BS2 (a.u.)	-3777.888907
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	2.416320000	-0.000197000	0.000038000	6	-1.452899000	0.000183000	0.000004000
6	4.593060000	-0.678000000	0.000566000	9	-1.561083000	-2.360108000	0.142636000
6	4.593259000	0.676962000	-0.000649000	9	-5.638039000	0.000426000	-0.000006000
1	5.404797000	-1.387873000	0.011926000	9	-1.560800000	2.360481000	-0.142631000
1	5.405202000	1.386596000	-0.012065000	1	4.231188000	-3.014275000	-1.529786000
7	3.258561000	-1.074698000	0.005724000	1	1.343053000	-2.132467000	1.531344000
7	3.258876000	1.074054000	-0.005702000	17	-4.483498000	2.715751000	-0.168602000
6	3.010887000	-4.676558000	-0.879835000	17	-4.483819000	-2.715031000	0.168601000
6	1.969104000	-5.090587000	-0.045479000	6	2.827039000	2.439130000	-0.000704000
6	1.362905000	-4.173573000	0.817354000	6	3.441148000	3.347623000	0.865629000
6	1.796041000	-2.847661000	0.853316000	6	1.796826000	2.847405000	-0.853281000
6	2.826339000	-2.439653000	0.000717000	6	3.012251000	4.676012000	0.879769000
6	3.440157000	-3.348289000	-0.865673000	6	1.364065000	4.173441000	-0.817342000
1	3.484786000	-5.383433000	-1.554323000	6	1.970552000	5.090310000	0.045443000
1	1.632843000	-6.122931000	-0.066323000	1	4.232114000	3.013411000	1.529719000
29	0.484751000	0.000012000	0.000038000	1	1.343615000	2.132324000	-1.531280000
6	-2.206566000	1.165147000	-0.071397000	1	3.486378000	5.382773000	1.554219000
6	-3.603685000	1.208107000	-0.074761000	1	0.557242000	4.488323000	-1.472355000
6	-4.297604000	0.000348000	-0.000009000	1	1.634580000	6.122749000	0.066269000
6	-3.603826000	-1.207492000	0.074747000	1	0.556012000	-4.488245000	1.472382000
6	-2.206701000	-1.164699000	0.071390000				

$I1_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.531095
Thermal and entropic correction, BS1 (a.u.)	0.254965
Electronic Energy, BS2 (a.u.)	-4804.047348
Gibbs Energy, BS2 (a.u.)	-4803.792383
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	-1.629914000	0.637675000	-1.604610000	6	-3.349688000	2.134999000	-1.582434000
6	-3.895816000	0.895692000	-1.609406000	1	-4.924683000	0.575106000	-1.639671000

1	-3.808118000	3.110811000	-1.588367000	6	0.027370000	0.706025000	1.811562000
7	-2.834909000	-0.006075000	-1.627053000	6	-1.325107000	1.042654000	1.836184000
7	-1.967224000	1.961509000	-1.583609000	6	-2.321733000	0.072015000	1.948440000
6	-4.034476000	-3.395861000	-0.683815000	6	-1.946425000	-1.268954000	2.025984000
6	-3.206255000	-4.205164000	-1.464939000	6	-0.602081000	-1.641885000	1.998497000
6	-2.273678000	-3.618796000	-2.324991000	6	0.369972000	-0.643696000	1.902258000
6	-2.163964000	-2.230360000	-2.404891000	53	1.504174000	2.190867000	1.592610000
6	-2.981131000	-1.429621000	-1.600357000	9	-1.695618000	2.324108000	1.747490000
6	-3.924185000	-2.006015000	-0.745791000	9	1.655808000	-1.005292000	1.899892000
1	-4.758876000	-3.842560000	-0.009532000	9	-2.886122000	-2.208561000	2.139895000
1	-3.288742000	-5.286380000	-1.406373000	17	-3.995568000	0.528138000	2.021107000
29	0.118033000	-0.158578000	-1.498035000	17	-0.154602000	-3.314162000	2.112269000
6	1.979783000	-2.306927000	-0.893682000	1	-1.632530000	-4.240226000	-2.943021000
6	3.165309000	-2.893584000	-0.462413000	6	-1.020015000	3.031812000	-1.511918000
6	4.310366000	-2.107174000	-0.377630000	6	0.155598000	2.975392000	-2.266538000
6	4.244282000	-0.761614000	-0.727467000	6	-1.273304000	4.115876000	-0.666797000
6	3.027348000	-0.235508000	-1.151317000	6	1.095957000	3.999155000	-2.148317000
6	1.849546000	-0.966655000	-1.233139000	6	-0.335947000	5.144910000	-0.573263000
9	3.031584000	1.091708000	-1.476172000	6	0.853576000	5.086262000	-1.304494000
9	5.354158000	0.001801000	-0.643704000	1	0.329374000	2.136896000	-2.932216000
9	5.473029000	-2.644105000	0.034309000	1	-2.177031000	4.137380000	-0.068268000
9	3.227169000	-4.197401000	-0.121286000	1	2.013576000	3.948505000	-2.726688000
9	0.888839000	-3.128046000	-0.938504000	1	-0.531249000	5.985149000	0.086311000
1	-4.544873000	-1.377139000	-0.117909000	1	1.584461000	5.885130000	-1.220824000
1	-1.449618000	-1.767362000	-3.077078000				

TSOA1$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.488061
Thermal and entropic correction, BS1 (a.u.)	0.255719
Electronic Energy, BS2 (a.u.)	-4804.005688
Gibbs Energy, BS2 (a.u.)	-4803.749969
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	-0.378574000	-0.129143000	1.630355000	1	-2.500132000	-0.777593000	4.064716000
6	-1.223857000	0.930235000	3.460532000	7	-0.354198000	1.009459000	2.375372000
6	-1.799347000	-0.293877000	3.403473000	7	-1.270680000	-0.930267000	2.280137000
1	-1.325391000	1.734753000	4.171589000	6	0.545094000	4.526718000	1.589534000

6	1.920032000	4.408197000	1.365452000	6	-3.701720000	0.029832000	-0.580101000
6	2.545384000	3.166096000	1.501688000	6	-3.760410000	1.417877000	-0.431110000
6	1.801649000	2.042811000	1.864154000	6	-2.640379000	2.212361000	-0.685068000
6	0.425461000	2.168271000	2.056965000	6	-1.455873000	1.594223000	-1.078207000
6	-0.210783000	3.404880000	1.932127000	53	0.102761000	-0.620829000	-2.821616000
1	0.054339000	5.489394000	1.482431000	9	-2.449492000	-1.881104000	-1.138489000
1	2.501402000	5.281834000	1.085693000	9	-0.380108000	2.361247000	-1.316664000
29	0.516851000	-0.414012000	-0.144747000	9	-4.907728000	1.993524000	-0.061401000
6	3.326362000	0.384883000	-0.568749000	17	-5.122326000	-0.934775000	-0.308385000
6	4.712183000	0.411565000	-0.449866000	17	-2.744975000	3.941673000	-0.534222000
6	5.356680000	-0.676502000	0.131868000	1	3.611479000	3.064442000	1.321660000
6	4.601066000	-1.753197000	0.584514000	6	-1.659611000	-2.234097000	1.838722000
6	3.215259000	-1.707049000	0.447453000	6	-0.707980000	-3.087043000	1.274082000
6	2.520391000	-0.651992000	-0.119351000	6	-2.994453000	-2.629311000	1.955129000
9	2.537984000	-2.792957000	0.936267000	6	-1.105169000	-4.338834000	0.804223000
9	5.221958000	-2.811108000	1.146455000	6	-3.376640000	-3.890206000	1.495645000
9	6.696320000	-0.686626000	0.255221000	6	-2.437900000	-4.745164000	0.913455000
9	5.438004000	1.468121000	-0.872070000	1	0.326582000	-2.775388000	1.208199000
9	2.759842000	1.488278000	-1.143994000	1	-3.730683000	-1.951759000	2.373199000
1	-1.282456000	3.478320000	2.082381000	1	-0.365154000	-5.000059000	0.362682000
1	2.271465000	1.073137000	1.973069000	1	-4.415771000	-4.194099000	1.579158000
6	-1.345071000	0.204758000	-1.198661000	1	-2.742299000	-5.722122000	0.549817000
6	-2.500324000	-0.552389000	-0.975496000				

$I2_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.523145
Thermal and entropic correction, BS1 (a.u.)	0.257940
Electronic Energy, BS2 (a.u.)	-4804.034175
Gibbs Energy, BS2 (a.u.)	-4803.776235
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	0.229204000	0.093076000	1.594880000	7	-0.551812000	-0.542138000	2.505528000
6	0.690700000	0.852486000	3.673212000	6	2.659206000	3.951611000	0.874827000
6	-0.278747000	-0.084153000	3.790765000	6	4.002625000	3.597120000	1.018791000
1	1.196666000	1.459226000	4.407142000	6	4.348729000	2.371187000	1.594443000
1	-0.795478000	-0.480560000	4.650174000	6	3.352197000	1.491718000	2.018220000
7	0.994475000	0.949891000	2.318682000	6	2.014841000	1.850337000	1.844384000

6	1.653888000	3.077780000	1.292942000	6	-3.358864000	2.206016000	-0.294146000
1	2.389817000	4.909198000	0.439442000	6	-2.038054000	1.750846000	-0.261911000
1	4.781261000	4.277634000	0.686932000	53	0.141027000	-0.438972000	-2.919848000
29	0.196945000	-0.147458000	-0.343175000	9	-2.451213000	-1.784217000	-0.749190000
6	3.060611000	0.234735000	-0.764747000	9	-1.058850000	2.675599000	-0.129913000
6	4.416845000	-0.073034000	-0.771337000	9	-5.649904000	1.669400000	-0.509600000
6	4.829389000	-1.340789000	-0.373026000	17	-5.347451000	-1.245432000	-0.876554000
6	3.879449000	-2.282231000	0.011704000	17	-3.742434000	3.897805000	-0.128492000
6	2.532179000	-1.927875000	0.007362000	1	5.392139000	2.093346000	1.705608000
6	2.091001000	-0.668432000	-0.358772000	6	-1.547033000	-1.551509000	2.261709000
9	1.642671000	-2.891702000	0.358002000	6	-1.158963000	-2.820142000	1.837306000
9	4.270546000	-3.516476000	0.374678000	6	-2.883513000	-1.244749000	2.524555000
9	6.134034000	-1.655507000	-0.364122000	6	-2.137095000	-3.799313000	1.653707000
9	5.330851000	0.848229000	-1.122825000	6	-3.851397000	-2.231797000	2.340812000
9	2.709730000	1.478088000	-1.165112000	6	-3.479342000	-3.507047000	1.904088000
1	0.607650000	3.339303000	1.202845000	1	-0.111620000	-3.030077000	1.665472000
1	3.598845000	0.529030000	2.454252000	1	-3.153347000	-0.245222000	2.850420000
6	-1.690709000	0.417473000	-0.383046000	1	-1.845712000	-4.791239000	1.321514000
6	-2.731034000	-0.477254000	-0.579383000	1	-4.894753000	-2.002253000	2.532727000
6	-4.071381000	-0.086471000	-0.629575000	1	-4.237158000	-4.271617000	1.760572000
6	-4.373991000	1.267026000	-0.475097000				

TSRE1$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.492555
Thermal and entropic correction, BS1 (a.u.)	0.256328
Electronic Energy, BS2 (a.u.)	-4804.006414
Gibbs Energy, BS2 (a.u.)	-4803.750086
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	0.519986000	-0.976137000	1.522495000	6	3.830510000	2.905317000	1.893590000
6	1.568799000	-1.402510000	3.498918000	6	4.422929000	1.710781000	2.311796000
6	0.642466000	-2.373411000	3.316906000	6	3.649222000	0.560114000	2.475175000
1	2.262848000	-1.221206000	4.303974000	6	2.275513000	0.620749000	2.228559000
1	0.378018000	-3.230006000	3.916409000	6	1.670246000	1.812688000	1.825896000
7	1.478292000	-0.555635000	2.394543000	1	1.986176000	3.875090000	1.322091000
7	0.015074000	-2.098296000	2.103440000	1	4.438779000	3.793587000	1.753069000
6	2.455318000	2.952058000	1.649349000	29	-0.090035000	-0.171218000	-0.218794000

6	2.257931000	1.002718000	-1.368778000
6	3.589769000	1.297430000	-1.099313000
6	4.449381000	0.287139000	-0.689885000
6	3.969932000	-1.015995000	-0.553211000
6	2.645187000	-1.294255000	-0.842298000
6	1.745893000	-0.290886000	-1.219743000
9	2.213029000	-2.557585000	-0.673250000
9	4.787968000	-1.978065000	-0.100496000
9	5.719762000	0.568236000	-0.379522000
9	4.040654000	2.554710000	-1.211630000
9	1.467138000	2.018232000	-1.765238000
1	0.603202000	1.843609000	1.647623000
1	4.108392000	-0.380026000	2.763997000
6	-1.854726000	0.803566000	-0.073791000
6	-3.089635000	0.173182000	-0.093437000
6	-4.316836000	0.825649000	0.056811000
6	-4.307948000	2.209009000	0.235040000
6	-3.100554000	2.907026000	0.255753000
6	-1.918387000	2.177257000	0.100723000
53	0.061214000	-0.843422000	-2.806507000
9	-3.135246000	-1.172439000	-0.277401000
9	-0.756935000	2.893147000	0.114679000
9	-5.464512000	2.870955000	0.383609000
17	-5.834905000	-0.042524000	0.028368000
17	-3.098008000	4.642904000	0.469931000
1	5.492505000	1.664278000	2.491076000
6	-1.019992000	-2.909594000	1.536060000
6	-0.902086000	-3.357186000	0.219209000
6	-2.134386000	-3.233885000	2.312549000
6	-1.924878000	-4.130401000	-0.330487000
6	-3.146764000	-4.016427000	1.755379000
6	-3.045999000	-4.461987000	0.434177000
1	-0.023581000	-3.096090000	-0.357416000
1	-2.208594000	-2.866507000	3.331375000
1	-1.840160000	-4.476605000	-1.356398000
1	-4.018089000	-4.268846000	2.352282000
1	-3.838946000	-5.066303000	0.003446000

$I3_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3073.534623
Thermal and entropic correction, BS1 (a.u.)	0.254865
Electronic Energy, BS2 (a.u.)	-4804.045304
Gibbs Energy, BS2 (a.u.)	-4803.790439
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	-2.273501000	0.093903000	-1.325833000
6	-4.523602000	0.273819000	-1.010055000
6	-4.250939000	-1.035345000	-1.228272000
1	-5.457835000	0.783804000	-0.838079000
1	-4.900389000	-1.893894000	-1.286386000
7	-3.308658000	0.951314000	-1.081488000
7	-2.875466000	-1.127126000	-1.429660000
6	-2.067672000	4.439974000	-1.455821000
6	-2.779994000	5.089842000	-0.444486000
6	-3.683792000	4.368809000	0.339806000
6	-3.867120000	3.001170000	0.131103000
6	-3.147521000	2.359576000	-0.880624000
6	-2.257069000	3.077157000	-1.686743000
1	-1.370474000	4.993664000	-2.077696000
1	-2.634200000	6.151919000	-0.271065000
29	-0.393944000	0.488536000	-1.276985000
1	-1.720305000	2.569831000	-2.481051000
1	-4.538794000	2.434200000	0.764263000
6	0.038185000	-1.084071000	1.878292000
6	-1.098391000	-1.891140000	1.815881000

6	-2.373560000	-1.339199000	1.888165000	1	-2.062771000	-5.570270000	-0.617791000
6	-2.528138000	0.035515000	2.024175000	1	0.418492000	-3.559158000	-3.505180000
6	-1.407726000	0.855922000	2.083172000	1	-0.178918000	-5.621727000	-2.243310000
6	-0.135994000	0.292967000	2.021753000	1	-4.239522000	4.865669000	1.129465000
9	-0.995491000	-3.219977000	1.685812000	6	1.485380000	0.880113000	-1.102043000
9	0.915316000	1.119136000	2.099135000	6	1.939946000	2.048820000	-0.506908000
9	-3.757407000	0.561124000	2.079470000	6	2.484216000	-0.028297000	-1.422384000
9	-3.458931000	-2.124038000	1.813198000	6	3.279096000	2.320329000	-0.216458000
9	-1.551073000	2.184430000	2.175060000	6	3.843408000	0.164992000	-1.163250000
6	-2.167126000	-2.346759000	-1.669977000	6	4.231331000	1.357337000	-0.552616000
6	-2.514343000	-3.498761000	-0.959996000	9	1.031758000	2.997166000	-0.150100000
6	-1.119497000	-2.367291000	-2.596877000	9	2.135002000	-1.210323000	-1.999395000
6	-1.798566000	-4.677371000	-1.176358000	9	5.526404000	1.578447000	-0.283864000
6	-0.400060000	-3.546398000	-2.791627000	17	3.776578000	3.808170000	0.555442000
6	-0.737761000	-4.704162000	-2.084816000	17	5.041874000	-1.045311000	-1.556950000
1	-3.305869000	-3.463342000	-0.220542000	53	1.963005000	-1.923576000	1.739988000
1	-0.874457000	-1.469044000	-3.152812000				

$I12_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.139308
Thermal and entropic correction, BS1 (a.u.)	0.507444
Electronic Energy, BS2 (a.u.)	-7861.475108
Gibbs Energy, BS2 (a.u.)	-7860.967664
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	3.511138000	1.701600000	1.775524000	6	6.791248000	0.596454000	0.711699000
6	5.395543000	2.973597000	1.944883000	1	8.410342000	-0.495968000	-0.180848000
6	4.334534000	3.805765000	2.083660000	1	7.768991000	-2.663354000	0.859833000
1	6.455741000	3.167254000	1.974398000	29	2.269209000	0.230258000	1.661352000
1	4.281106000	4.871999000	2.236518000	6	-0.286428000	-1.174851000	2.143785000
7	4.877172000	1.693581000	1.759370000	6	-1.139202000	-2.268540000	2.256350000
7	3.195262000	3.015090000	1.971563000	6	-0.660589000	-3.532240000	1.929072000
6	7.548805000	-0.552117000	0.477500000	6	0.655402000	-3.677867000	1.505319000
6	7.185795000	-1.769061000	1.058233000	6	1.471049000	-2.552235000	1.461622000
6	6.069566000	-1.831183000	1.896932000	6	1.046560000	-1.264918000	1.764333000
6	5.318480000	-0.684927000	2.156762000	9	2.761539000	-2.766033000	1.066797000
6	5.673768000	0.522868000	1.547313000	9	-1.472033000	-4.606044000	1.989655000

9	-0.841255000	0.045738000	2.422483000
1	7.049133000	1.532712000	0.229061000
1	4.463524000	-0.722445000	2.822986000
6	1.768680000	-0.034284000	-1.679864000
6	2.652018000	1.030790000	-1.843077000
6	4.031147000	0.843908000	-1.942653000
6	4.532647000	-0.457295000	-1.904041000
6	3.680369000	-1.549860000	-1.742033000
6	2.307477000	-1.319532000	-1.629724000
9	2.178290000	2.284538000	-1.898399000
9	1.498246000	-2.371510000	-1.472997000
9	5.843827000	-0.660040000	-2.036636000
53	-0.321069000	0.296132000	-1.487116000
6	1.850919000	3.505071000	2.008534000
6	1.446534000	4.384799000	3.014742000
6	0.951593000	3.077486000	1.029461000
6	0.120814000	4.827958000	3.037878000
6	-0.369995000	3.512890000	1.070840000
6	-0.791953000	4.389997000	2.073389000
1	2.153883000	4.704467000	3.773719000
1	1.288568000	2.416938000	0.243323000
1	-0.198610000	5.509502000	3.820770000
1	-1.053411000	3.173317000	0.302423000
1	-1.821986000	4.729982000	2.092372000
1	5.783154000	-2.770833000	2.359798000
6	-3.863627000	-1.980481000	-0.008404000
6	-4.810885000	-3.675588000	1.185484000
6	-3.964465000	-4.238114000	0.290046000
1	-5.438922000	-4.115864000	1.943449000
1	-3.719619000	-5.269617000	0.095656000
7	-4.735735000	-2.300400000	0.991087000
7	-3.396897000	-3.191298000	-0.433117000
6	-7.544643000	-0.568359000	2.700627000
6	-6.897380000	0.562836000	3.205828000
6	-5.526837000	0.733593000	2.993271000
6	-4.798968000	-0.221706000	2.282991000
6	-5.461983000	-1.336964000	1.760880000
6	-6.831263000	-1.519996000	1.969547000
1	-8.609559000	-0.706741000	2.862220000
1	-7.458377000	1.305952000	3.764931000
29	-3.501616000	-0.185569000	-0.624358000
1	-7.331258000	-2.387353000	1.549954000
1	-3.731035000	-0.114528000	2.139715000
6	-3.445266000	1.663004000	-1.190219000
6	-3.429909000	2.045455000	-2.525739000
6	-3.433583000	3.366995000	-2.961872000
6	-3.466719000	4.386903000	-2.014791000
6	-3.493913000	4.061589000	-0.661936000
6	-3.481646000	2.720918000	-0.289416000
9	-3.385831000	1.091758000	-3.504104000
9	-3.463975000	2.478113000	1.054466000
9	-3.469752000	5.673149000	-2.403173000
9	-3.402143000	3.678993000	-4.272943000
9	-3.503755000	5.048033000	0.259500000
6	-2.453356000	-3.372843000	-1.494204000
6	-1.410907000	-4.291069000	-1.334618000
6	-2.580413000	-2.634946000	-2.674040000
6	-0.485571000	-4.461653000	-2.364427000
6	-1.642610000	-2.807062000	-3.693414000
6	-0.595348000	-3.719393000	-3.543225000
1	-1.313686000	-4.850025000	-0.411584000
1	-3.398057000	-1.930465000	-2.783771000
1	0.333050000	-5.162506000	-2.232103000
1	-1.738093000	-2.229267000	-4.608006000
1	0.132487000	-3.849652000	-4.338597000
1	-5.015581000	1.607381000	3.385548000
17	4.322369000	-3.162479000	-1.710568000
17	5.100602000	2.199546000	-2.130541000
9	1.101058000	-4.897256000	1.138702000
9	-2.418015000	-2.132236000	2.666228000

$TSOA2_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.105787
Thermal and entropic correction, BS1 (a.u.)	0.507630
Electronic Energy, BS2 (a.u.)	-7861.443535
Gibbs Energy, BS2 (a.u.)	-7860.935905
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	2.510361000	0.005182000	2.493211000	6	3.147617000	1.757324000	-0.103954000
6	4.259306000	0.270426000	3.928950000	6	4.462387000	1.964555000	-0.507885000
6	3.167385000	0.813219000	4.519035000	6	5.029456000	1.073930000	-1.424624000
1	5.276762000	0.168935000	4.271225000	6	4.292023000	0.004402000	-1.926536000
1	3.038924000	1.304830000	5.470432000	6	2.987736000	-0.181255000	-1.465016000
7	3.838768000	-0.221358000	2.692542000	9	2.612997000	2.617440000	0.782610000
7	2.111246000	0.645420000	3.625466000	9	2.298777000	-1.229111000	-1.949447000
6	6.804960000	-1.040785000	0.607548000	9	6.296362000	1.245282000	-1.812032000
6	6.362425000	-2.190546000	-0.051187000	53	-0.038401000	0.944864000	-0.866373000
6	5.079755000	-2.685139000	0.199223000	6	0.775771000	1.112342000	3.859976000
6	4.242560000	-2.044170000	1.111998000	6	0.091268000	0.681650000	4.998289000
6	4.693994000	-0.892974000	1.762846000	6	0.180361000	1.984977000	2.946711000
6	5.971388000	-0.384203000	1.514650000	6	-1.213013000	1.129172000	5.217180000
1	7.793863000	-0.640646000	0.405797000	6	-1.124021000	2.425793000	3.173636000
1	7.009737000	-2.692249000	-0.763688000	6	-1.821872000	1.997099000	4.305773000
29	1.338631000	-0.451748000	0.924922000	1	0.572449000	-0.002362000	5.690629000
6	-1.143324000	-1.966121000	1.732097000	1	0.734751000	2.303202000	2.073377000
6	-2.045020000	-3.024284000	1.792916000	1	-1.753904000	0.793240000	6.096910000
6	-1.698074000	-4.236188000	1.205070000	1	-1.593764000	3.104170000	2.470752000
6	-0.461268000	-4.361019000	0.583768000	1	-2.837499000	2.341207000	4.479145000
6	0.401153000	-3.268797000	0.571895000	1	4.723737000	-3.572720000	-0.315149000
6	0.103249000	-2.036881000	1.130655000	6	-3.272527000	-1.475889000	-1.254874000
9	1.591532000	-3.457336000	-0.078726000	6	-4.252763000	-3.466333000	-0.730905000
9	-2.567051000	-5.262871000	1.206018000	6	-3.250185000	-3.727484000	-1.604117000
9	-1.563541000	-0.788044000	2.289345000	1	-4.935506000	-4.123096000	-0.217091000
1	6.298897000	0.524788000	2.008543000	1	-2.905137000	-4.656594000	-2.027882000
1	3.248976000	-2.427031000	1.311029000	7	-4.246640000	-2.090867000	-0.522388000
6	2.391340000	0.666088000	-0.530204000	7	-2.662959000	-2.503455000	-1.916112000

6	-7.395507000	-1.021007000	1.138730000	9	-1.868454000	5.174135000	-3.520552000
6	-6.918047000	-0.043910000	2.016708000	9	-2.956015000	5.126720000	1.090941000
6	-5.550928000	0.243552000	2.061394000	6	-1.553816000	-2.351458000	-2.808699000
6	-4.659743000	-0.443176000	1.237160000	6	-0.507441000	-3.278386000	-2.767175000
6	-5.151360000	-1.403800000	0.348944000	6	-1.519963000	-1.278510000	-3.703667000
6	-6.514804000	-1.701712000	0.295357000	6	0.583470000	-3.116758000	-3.621803000
1	-8.456628000	-1.248338000	1.098550000	6	-0.416281000	-1.119274000	-4.542714000
1	-7.608034000	0.487776000	2.665409000	6	0.637668000	-2.035349000	-4.504492000
29	-2.933772000	0.436074000	-1.310998000	1	-0.533441000	-4.105758000	-2.068106000
1	-6.880628000	-2.444986000	-0.406216000	1	-2.344642000	-0.574481000	-3.734488000
1	-3.595838000	-0.253413000	1.290688000	1	1.401177000	-3.829892000	-3.580054000
6	-2.817541000	2.367326000	-1.337873000	1	-0.388708000	-0.280346000	-5.231934000
6	-2.443713000	3.117480000	-2.446280000	1	1.496337000	-1.907413000	-5.156765000
6	-2.246300000	4.494822000	-2.420102000	1	-5.168901000	0.995001000	2.745803000
6	-2.425414000	5.178115000	-1.219910000	17	4.986039000	-1.069091000	-3.105719000
6	-2.805281000	4.474473000	-0.079362000	17	5.412427000	3.270068000	0.142903000
6	-2.998344000	3.101595000	-0.170803000	9	-0.152721000	-5.511766000	-0.056180000
9	-2.204970000	2.494281000	-3.636642000	9	-3.259322000	-2.897446000	2.369028000
9	-3.346576000	2.467349000	0.985284000				
9	-2.233243000	6.505750000	-1.163075000				

I22$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.131798
Thermal and entropic correction, BS1 (a.u.)	0.509148
Electronic Energy, BS2 (a.u.)	-7861.461927
Gibbs Energy, BS2 (a.u.)	-7860.952779
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	2.216310000	-0.855168000	2.156062000	6	5.360806000	-3.383239000	0.121806000
6	3.448333000	-1.407309000	3.969360000	6	4.286816000	-2.956723000	0.905702000
6	2.304645000	-0.836802000	4.414614000	6	4.467909000	-1.874885000	1.763073000
1	4.297558000	-1.817750000	4.491820000	6	5.701148000	-1.228117000	1.875290000
1	1.946402000	-0.627961000	5.409980000	1	7.726443000	-1.162976000	1.161193000
7	3.380995000	-1.409511000	2.579406000	1	7.428416000	-3.074886000	-0.401009000
7	1.558217000	-0.499911000	3.289096000	29	1.614745000	-0.534141000	0.323389000
6	6.767975000	-1.668366000	1.093754000	6	-1.224028000	-1.255216000	0.951946000
6	6.597778000	-2.742081000	0.213747000	6	-2.272198000	-2.130586000	1.216846000

6	-2.094121000	-3.493653000	1.014247000	1	-5.021652000	-3.961950000	-1.415200000
6	-0.860860000	-3.962870000	0.576082000	7	-5.566235000	-1.004472000	-0.144704000
6	0.177999000	-3.057264000	0.380446000	7	-4.246848000	-1.939483000	-1.560402000
6	0.038844000	-1.693438000	0.584783000	6	-8.121499000	0.982389000	1.683903000
9	1.353356000	-3.564877000	-0.076393000	6	-7.310994000	1.828911000	2.445671000
9	-3.121348000	-4.343436000	1.175913000	6	-5.919874000	1.725461000	2.357833000
9	-1.493945000	0.064246000	1.044972000	6	-5.334329000	0.778386000	1.517117000
1	5.808074000	-0.382641000	2.546962000	6	-6.155757000	-0.047625000	0.742029000
1	3.322852000	-3.444902000	0.853886000	6	-7.547437000	0.044411000	0.823519000
6	3.310971000	0.375201000	-0.080429000	1	-9.203047000	1.057967000	1.747502000
6	3.795532000	1.487811000	0.583449000	1	-7.761969000	2.563207000	3.106810000
6	5.047978000	2.052371000	0.324655000	29	-3.592718000	0.941754000	-1.163315000
6	5.845440000	1.469500000	-0.658672000	1	-8.168803000	-0.600699000	0.209909000
6	5.401369000	0.348301000	-1.359632000	1	-4.257960000	0.671234000	1.466669000
6	4.146374000	-0.175425000	-1.044782000	6	-2.558968000	2.576774000	-1.210958000
9	3.051835000	2.055303000	1.560428000	6	-1.737239000	2.904381000	-2.280953000
9	3.752187000	-1.280900000	-1.713039000	6	-0.744878000	3.877927000	-2.237833000
9	7.050860000	1.984759000	-0.926869000	6	-0.555620000	4.594045000	-1.059988000
53	0.627908000	0.206049000	-1.926884000	6	-1.374782000	4.333155000	0.034426000
6	0.300172000	0.190725000	3.395454000	6	-2.348162000	3.344148000	-0.072073000
6	-0.770071000	-0.461303000	4.010083000	9	-1.841264000	2.212452000	-3.456868000
6	0.187403000	1.502792000	2.936983000	9	-3.104546000	3.130636000	1.046830000
6	-1.982764000	0.214732000	4.151064000	9	0.405741000	5.531204000	-0.981845000
6	-1.026364000	2.172819000	3.093361000	9	0.063458000	4.111276000	-3.293594000
6	-2.110121000	1.530241000	3.696070000	9	-1.194178000	5.027591000	1.180469000
1	-0.653228000	-1.484477000	4.352784000	6	-3.197016000	-2.158616000	-2.508440000
1	1.032963000	1.982574000	2.462074000	6	-2.411861000	-3.311402000	-2.409958000
1	-2.827469000	-0.289010000	4.610894000	6	-2.955776000	-1.217082000	-3.514070000
1	-1.126841000	3.188726000	2.730077000	6	-1.370358000	-3.512229000	-3.317700000
1	-3.055951000	2.051519000	3.807189000	6	-1.907438000	-1.424452000	-4.411011000
1	5.227166000	-4.218532000	-0.558865000	6	-1.111363000	-2.569569000	-4.315934000
6	-4.529456000	-0.730421000	-0.988049000	1	-2.602053000	-4.038113000	-1.628608000
6	-5.920073000	-2.349430000	-0.186683000	1	-3.582234000	-0.334859000	-3.587111000
6	-5.086440000	-2.940768000	-1.075810000	1	-0.757142000	-4.404730000	-3.233184000
1	-6.711973000	-2.754642000	0.422881000	1	-1.718675000	-0.689360000	-5.187941000

1	-0.297032000	-2.726921000	-5.016908000	17	5.619613000	3.440818000	1.209158000
1	-5.282768000	2.376508000	2.949019000	9	-0.706225000	-5.271013000	0.303173000
17	6.407584000	-0.373015000	-2.584130000	9	-3.461259000	-1.672837000	1.649073000

$TsRE2_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.101363
Thermal and entropic correction, BS1 (a.u.)	0.504783
Electronic Energy, BS2 (a.u.)	-7861.443142
Gibbs Energy, BS2 (a.u.)	-7860.938359
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	2.892744000	-0.642650000	2.231361000	1	3.489802000	-2.492603000	0.224370000
6	4.884077000	-0.602020000	3.343729000	6	2.365893000	1.073091000	-0.230699000
6	3.909015000	-0.378809000	4.255957000	6	3.004801000	2.048327000	0.536865000
1	5.954531000	-0.678539000	3.452261000	6	4.236403000	2.579816000	0.186458000
1	3.957168000	-0.194172000	5.317416000	6	4.849915000	2.169880000	-0.997211000
7	4.246692000	-0.766563000	2.113979000	6	4.229739000	1.221158000	-1.799880000
7	2.700268000	-0.405688000	3.559778000	6	3.010736000	0.683861000	-1.405344000
6	6.782709000	-0.613047000	-0.600019000	9	2.441555000	2.474633000	1.688422000
6	6.256213000	-1.528656000	-1.514740000	9	2.461662000	-0.246508000	-2.209991000
6	5.068841000	-2.202979000	-1.217351000	9	6.054997000	2.650117000	-1.332313000
6	4.409848000	-1.970497000	-0.010260000	53	-0.033368000	1.249983000	-0.453395000
6	4.934844000	-1.039574000	0.890011000	17	-2.904785000	-4.101091000	2.118948000
6	6.121554000	-0.359427000	0.602980000	17	0.152823000	-5.354781000	-2.195232000
1	7.694768000	-0.070979000	-0.831444000	9	4.857001000	3.467051000	0.982401000
1	6.764214000	-1.708772000	-2.457320000	9	4.824293000	0.810111000	-2.931600000
29	1.514984000	-0.642857000	0.767858000	6	1.419576000	-0.226220000	4.175148000
6	-0.756396000	-2.598446000	1.245625000	6	1.131609000	-0.913740000	5.357951000
6	-1.564322000	-3.725527000	1.061482000	6	0.472797000	0.615315000	3.585867000
6	-1.268526000	-4.572890000	-0.005284000	6	-0.123014000	-0.757512000	5.949146000
6	-0.184377000	-4.303813000	-0.838585000	6	-0.786844000	0.747224000	4.172881000
6	0.586208000	-3.170133000	-0.567027000	6	-1.085892000	0.064967000	5.355411000
6	0.342166000	-2.273237000	0.462633000	1	1.874453000	-1.572791000	5.797487000
9	1.639144000	-2.941682000	-1.406856000	1	0.721913000	1.148575000	2.676740000
9	-2.049964000	-5.637223000	-0.248639000	1	-0.349745000	-1.291415000	6.867708000
9	-1.102135000	-1.766740000	2.268202000	1	-1.531667000	1.380171000	3.697628000
1	6.505488000	0.382155000	1.296004000	1	-2.064255000	0.171863000	5.815014000

1	4.648496000	-2.914079000	-1.922224000	6	-2.621334000	5.241933000	-0.873498000
6	-2.871447000	-0.802236000	-1.802559000	6	-2.890870000	5.509376000	0.466535000
6	-3.315461000	-3.027255000	-2.002460000	6	-3.126996000	4.455499000	1.346591000
6	-2.408783000	-2.708325000	-2.958960000	6	-3.088930000	3.152553000	0.859904000
1	-3.758473000	-3.971564000	-1.729883000	9	-2.313481000	3.715158000	-2.621131000
1	-1.927831000	-3.311066000	-3.712140000	9	-3.293236000	2.159698000	1.775921000
7	-3.579841000	-1.853213000	-1.302288000	9	-2.921743000	6.777348000	0.908013000
7	-2.151808000	-1.346481000	-2.824319000	9	-2.380111000	6.262352000	-1.719869000
6	-6.645349000	-2.194234000	0.769338000	9	-3.382073000	4.717254000	2.643552000
6	-6.277687000	-1.477743000	1.912018000	6	-1.233320000	-0.610950000	-3.638541000
6	-5.005136000	-0.905947000	1.996924000	6	0.031706000	-1.142707000	-3.894831000
6	-4.098423000	-1.049428000	0.946856000	6	-1.602480000	0.640929000	-4.139546000
6	-4.487892000	-1.743995000	-0.202004000	6	0.932159000	-0.411733000	-4.672172000
6	-5.754317000	-2.324594000	-0.297431000	6	-0.685252000	1.372821000	-4.893642000
1	-7.632429000	-2.641358000	0.698250000	6	0.581031000	0.846346000	-5.166617000
1	-6.979082000	-1.370218000	2.734143000	1	0.322374000	-2.091842000	-3.457129000
29	-2.816059000	1.017596000	-1.122125000	1	-2.592057000	1.032980000	-3.931532000
1	-6.040773000	-2.855615000	-1.199989000	1	1.921429000	-0.815323000	-4.862030000
1	-3.093791000	-0.649884000	1.021995000	1	-0.966566000	2.349890000	-5.275269000
6	-2.842726000	2.831902000	-0.470266000	1	1.291027000	1.415653000	-5.759379000
6	-2.603899000	3.918774000	-1.303136000	1	-4.705749000	-0.360922000	2.887113000

$I32_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.137722
Thermal and entropic correction, BS1 (a.u.)	0.507365
Electronic Energy, BS2 (a.u.)	-7861.475988
Gibbs Energy, BS2 (a.u.)	-7860.968623
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	3.021721000	1.751701000	1.872499000	6	7.458947000	-0.472445000	0.684102000
6	4.468636000	3.511162000	1.963383000	6	6.516096000	-0.857830000	1.641750000
6	3.237723000	3.985956000	2.270394000	6	5.487021000	0.010414000	2.006776000
1	5.424624000	4.005687000	1.900427000	6	5.395587000	1.263730000	1.391149000
1	2.904355000	4.984120000	2.504711000	6	6.336554000	1.661090000	0.438828000
7	4.320847000	2.146896000	1.731007000	1	8.092149000	1.093046000	-0.659647000
7	2.364555000	2.901676000	2.211992000	1	8.260135000	-1.150300000	0.405027000
6	7.369069000	0.788269000	0.090554000	29	2.305643000	-0.011986000	1.547624000

6	0.693279000	-2.308033000	2.322019000	1	-2.855424000	3.215428000	3.153838000
6	0.145345000	-3.592934000	2.276372000	1	6.585828000	-1.831588000	2.117497000
6	0.433733000	-4.387477000	1.166318000	6	-2.981229000	-2.048547000	-0.414065000
6	1.261279000	-3.908853000	0.151036000	6	-2.724521000	-4.135528000	0.464659000
6	1.796679000	-2.625583000	0.290795000	6	-2.426900000	-4.214495000	-0.855726000
6	1.535177000	-1.773753000	1.354676000	1	-2.707341000	-4.882045000	1.241193000
9	2.646374000	-2.209433000	-0.687718000	1	-2.119282000	-5.049142000	-1.465009000
9	-0.089176000	-5.619306000	1.074535000	7	-3.047069000	-2.805515000	0.718090000
9	0.377592000	-1.548270000	3.406594000	7	-2.592193000	-2.934120000	-1.377478000
1	6.240981000	2.623591000	-0.048855000	6	-4.471005000	-2.368250000	4.125431000
1	4.761397000	-0.274504000	2.760778000	6	-3.798102000	-1.217410000	4.547326000
6	1.640071000	0.786887000	-1.992479000	6	-2.877791000	-0.595943000	3.698833000
6	2.267510000	1.934895000	-1.511952000	6	-2.623130000	-1.125706000	2.434071000
6	3.631304000	2.142900000	-1.687411000	6	-3.314966000	-2.266240000	2.016714000
6	4.395824000	1.189798000	-2.351670000	6	-4.236054000	-2.896497000	2.854564000
6	3.789297000	0.033567000	-2.833108000	1	-5.187116000	-2.853290000	4.782037000
6	2.421206000	-0.154567000	-2.660645000	1	-3.988767000	-0.808886000	5.535395000
9	1.576352000	2.884268000	-0.859843000	29	-3.422215000	-0.175329000	-0.569833000
9	1.878358000	-1.278957000	-3.148758000	1	-4.762092000	-3.782071000	2.511679000
9	5.707289000	1.381639000	-2.530111000	1	-1.893614000	-0.668794000	1.775626000
53	-0.429774000	0.459225000	-1.691100000	6	-3.887334000	1.696547000	-0.707757000
17	-0.848827000	-4.222074000	3.566110000	6	-3.780906000	2.433187000	-1.881057000
17	1.620045000	-4.916724000	-1.231307000	6	-3.976158000	3.809473000	-1.959652000
9	4.206125000	3.257895000	-1.209389000	6	-4.305860000	4.511831000	-0.803464000
9	4.524804000	-0.891382000	-3.465411000	6	-4.439930000	3.823274000	0.398553000
6	0.959246000	2.987927000	2.475611000	6	-4.242952000	2.446625000	0.406001000
6	0.487307000	3.829303000	3.487438000	9	-3.451979000	1.809259000	-3.051388000
6	0.064665000	2.230005000	1.716369000	9	-4.372160000	1.836117000	1.624876000
6	-0.887816000	3.911912000	3.724982000	9	-4.495717000	5.841787000	-0.849139000
6	-1.300336000	2.297043000	1.979779000	9	-3.848015000	4.474398000	-3.125820000
6	-1.787078000	3.146586000	2.977226000	9	-4.743474000	4.496942000	1.526768000
1	1.183019000	4.404584000	4.089615000	6	-2.297404000	-2.564060000	-2.727828000
1	0.431161000	1.604568000	0.915770000	6	-1.103444000	-3.002279000	-3.305139000
1	-1.251628000	4.572033000	4.506883000	6	-3.164891000	-1.720893000	-3.426542000
1	-1.975990000	1.692697000	1.387760000	6	-0.771063000	-2.580034000	-4.592640000

6	-2.815541000	-1.292029000	-4.707904000	1	-3.483560000	-0.628085000	-5.248426000
6	-1.619711000	-1.718019000	-5.292981000	1	-1.352854000	-1.383661000	-6.291178000
1	-0.427986000	-3.635260000	-2.740082000	1	-2.346543000	0.295529000	4.017863000
1	-4.091678000	-1.398303000	-2.964172000				
1	0.162929000	-2.909799000	-5.037198000				

$I12_{cis}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.141123
Thermal and entropic correction, BS1 (a.u.)	0.509194
Electronic Energy, BS2 (a.u.)	-7861.480402
Gibbs Energy, BS2 (a.u.)	-7860.971208
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	-3.623784000	1.745987000	1.036127000	9	-2.783843000	-2.054701000	3.508587000
6	-4.242642000	3.894476000	0.580641000	9	-3.597731000	-2.403619000	-1.173144000
6	-3.404053000	3.933680000	1.642691000	9	-2.132291000	-6.149801000	1.277688000
1	-4.769592000	4.684838000	0.071877000	9	-2.101458000	-4.655623000	3.569817000
1	-3.051112000	4.759768000	2.238812000	9	-2.875975000	-4.998032000	-1.090607000
7	-4.370532000	2.553857000	0.221323000	6	-2.145922000	2.234600000	2.959174000
7	-3.042610000	2.617880000	1.911499000	6	-0.940285000	2.923946000	3.113268000
6	-6.516262000	0.414113000	-1.947082000	6	-2.475051000	1.169233000	3.799825000
6	-6.584466000	1.189998000	-3.107129000	6	-0.052898000	2.531674000	4.115298000
6	-5.947042000	2.432578000	-3.144673000	6	-1.571932000	0.773751000	4.787732000
6	-5.222860000	2.888922000	-2.042025000	6	-0.361542000	1.452180000	4.947970000
6	-5.148595000	2.098922000	-0.889650000	1	-0.695524000	3.742230000	2.445221000
6	-5.813257000	0.869481000	-0.831176000	1	-3.419787000	0.653845000	3.670444000
1	-7.023080000	-0.545199000	-1.899862000	1	0.889971000	3.057164000	4.229635000
1	-7.136290000	0.832860000	-3.971410000	1	-1.820770000	-0.063638000	5.432303000
29	-3.418588000	-0.179210000	1.036993000	1	0.339374000	1.141721000	5.717023000
1	-5.781470000	0.276375000	0.076582000	1	-5.994014000	3.045638000	-4.039653000
1	-4.691566000	3.831746000	-2.092345000	6	-0.348827000	0.395635000	-2.506818000
6	-3.218376000	-2.102160000	1.161658000	6	-2.577073000	0.606536000	-2.952110000
6	-2.851445000	-2.751075000	2.335475000	6	-2.225232000	-0.667674000	-3.246996000
6	-2.484478000	-4.091382000	2.406763000	1	-3.525772000	1.113333000	-3.014154000
6	-2.490401000	-4.855448000	1.243320000	1	-2.807913000	-1.492439000	-3.622682000
6	-2.882068000	-4.266419000	0.045242000	7	-1.422031000	1.239599000	-2.496123000
6	-3.240610000	-2.922278000	0.042319000	7	-0.864778000	-0.780893000	-2.972509000

6	-1.914002000	4.924280000	-2.438420000	6	4.897245000	2.349317000	-0.041081000
6	-1.216678000	5.272583000	-1.279053000	6	3.598881000	2.062385000	-0.453441000
6	-0.600429000	4.278624000	-0.513490000	9	4.199766000	-0.201933000	-3.190845000
6	-0.684932000	2.939058000	-0.895591000	9	2.598855000	2.643070000	0.279021000
6	-1.364117000	2.604987000	-2.072246000	9	7.225037000	1.970837000	-0.303754000
6	-1.983284000	3.589915000	-2.845175000	53	-0.103665000	-0.644627000	1.311594000
1	-2.395589000	5.690528000	-3.038461000	17	4.852495000	-2.613321000	-0.893463000
1	-1.156603000	6.312152000	-0.971154000	17	5.134501000	0.866274000	3.268258000
29	1.466056000	0.783339000	-1.986656000	9	6.732464000	0.273769000	-2.390740000
6	2.669433000	-1.552544000	0.356831000	9	5.142845000	3.178855000	0.993213000
6	4.061651000	-1.624918000	0.294353000	6	-0.118962000	-1.997564000	-3.089659000
6	4.809411000	-0.868546000	1.195607000	6	-0.693815000	-3.188013000	-2.638702000
6	4.186435000	-0.060734000	2.147187000	6	1.175405000	-1.984569000	-3.616270000
6	2.791478000	-0.007315000	2.172827000	6	0.043372000	-4.371249000	-2.693100000
6	2.013525000	-0.743439000	1.282170000	6	1.908331000	-3.171253000	-3.655903000
9	2.202670000	0.786855000	3.074261000	6	1.348735000	-4.365145000	-3.192024000
9	6.142771000	-0.898208000	1.131608000	1	-1.699855000	-3.184792000	-2.242621000
9	1.956405000	-2.270421000	-0.519625000	1	1.604316000	-1.055845000	-3.975904000
1	-2.502702000	3.315157000	-3.757306000	1	-0.406597000	-5.289802000	-2.328467000
1	-0.233905000	2.158039000	-0.293771000	1	2.919662000	-3.157494000	-4.051174000
6	3.283033000	1.218087000	-1.509011000	1	1.925700000	-5.284698000	-3.222408000
6	4.383805000	0.656241000	-2.143270000	1	-0.055834000	4.540922000	0.387964000
6	5.703906000	0.878669000	-1.762844000				
6	5.960963000	1.738589000	-0.698361000				

TSOA2$_{cis}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.105213
Thermal and entropic correction, BS1 (a.u.)	0.509194
Electronic Energy, BS2 (a.u.)	-7861.446035
Gibbs Energy, BS2 (a.u.)	-7860.936282
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	-2.890528000	2.140022000	1.473459000	7	-3.333997000	3.275292000	0.851746000
6	-2.903356000	4.421369000	1.515672000	7	-2.177996000	2.613531000	2.538163000
6	-2.172753000	4.003635000	2.576930000	6	-5.749330000	2.359834000	-1.832848000
1	-3.166198000	5.413476000	1.186052000	6	-5.450806000	3.324020000	-2.799588000
1	-1.669626000	4.553362000	3.356216000	6	-4.463121000	4.278836000	-2.543475000

6	-3.761617000	4.262247000	-1.336793000
6	-4.070441000	3.295922000	-0.374635000
6	-5.073017000	2.350345000	-0.612397000
1	-6.520627000	1.618369000	-2.018739000
1	-5.985894000	3.332579000	-3.744423000
29	-3.222124000	0.283300000	1.040143000
1	-5.317440000	1.618746000	0.150659000
1	-2.963935000	4.974029000	-1.157269000
6	-3.685396000	-1.567742000	0.706284000
6	-3.452044000	-2.600141000	1.607890000
6	-3.660638000	-3.947810000	1.329493000
6	-4.147112000	-4.308167000	0.076164000
6	-4.430405000	-3.313800000	-0.853029000
6	-4.191157000	-1.985479000	-0.516789000
9	-2.953202000	-2.321620000	2.850688000
9	-4.443138000	-1.068478000	-1.502047000
9	-4.332298000	-5.601261000	-0.239476000
9	-3.382307000	-4.906193000	2.236073000
9	-4.864726000	-3.660810000	-2.084422000
6	-1.455247000	1.782402000	3.452210000
6	-0.108573000	2.055676000	3.700187000
6	-2.086310000	0.684964000	4.042283000
6	0.616492000	1.210603000	4.541554000
6	-1.349895000	-0.160312000	4.873147000
6	0.000647000	0.099641000	5.124003000
1	0.370814000	2.900362000	3.217652000
1	-3.134129000	0.494846000	3.837344000
1	1.667749000	1.412215000	4.722911000
1	-1.835061000	-1.020069000	5.324972000
1	0.569970000	-0.560234000	5.772035000
1	-4.219471000	5.028794000	-3.289977000
6	-0.327864000	0.435327000	-2.074643000
6	-2.068281000	1.509798000	-3.082568000
6	-2.154084000	0.202123000	-3.419906000
1	-2.700401000	2.348809000	-3.323516000
1	-2.861442000	-0.318931000	-4.043892000
7	-0.947298000	1.633368000	-2.261210000
7	-1.082321000	-0.441894000	-2.800180000
6	-0.082272000	5.229377000	-1.906183000
6	0.315709000	5.281703000	-0.567176000
6	0.294323000	4.120711000	0.209645000
6	-0.132562000	2.912077000	-0.340042000
6	-0.516537000	2.868840000	-1.682408000
6	-0.494223000	4.021556000	-2.471787000
1	-0.063553000	6.126459000	-2.517779000
1	0.641575000	6.222047000	-0.132588000
29	1.249564000	0.026489000	-0.876024000
6	2.835908000	-2.008423000	0.707877000
6	4.168174000	-2.179237000	1.073496000
6	4.833167000	-1.128007000	1.707705000
6	4.170510000	0.073040000	1.977640000
6	2.841138000	0.204987000	1.594380000
6	2.159423000	-0.801677000	0.903543000
9	2.228432000	1.385930000	1.795849000
9	6.112649000	-1.273084000	2.067520000
9	2.204267000	-3.018449000	0.086532000
1	-0.788476000	3.970542000	-3.515152000
1	-0.163847000	2.010164000	0.258953000
6	3.099665000	0.451930000	-1.551909000
6	3.976832000	-0.539044000	-1.962676000
6	5.332105000	-0.333130000	-2.205115000
6	5.853332000	0.947663000	-2.051133000
6	5.013231000	1.983311000	-1.653914000
6	3.667076000	1.710162000	-1.424470000
9	3.535880000	-1.827704000	-2.102454000
9	2.906544000	2.765405000	-1.010996000
9	7.158099000	1.181642000	-2.279968000
53	-0.170220000	-0.965397000	1.168252000
17	5.006035000	-3.664232000	0.727117000
17	5.014152000	1.388478000	2.744733000

9	6.144608000	-1.342759000	-2.578402000	1	-2.954103000	-2.325682000	-2.904459000
9	5.518218000	3.224316000	-1.497221000	1	1.296880000	-1.682926000	-2.843809000
6	-0.853372000	-1.853729000	-2.854259000	1	-2.594345000	-4.765036000	-2.856848000
6	-1.947771000	-2.721568000	-2.886952000	1	1.667442000	-4.122004000	-2.780570000
6	0.450065000	-2.357868000	-2.841253000	1	-0.274923000	-5.687316000	-2.783888000
6	-1.735584000	-4.100588000	-2.863580000	1	0.604499000	4.151370000	1.248625000
6	0.652157000	-3.737850000	-2.808972000				
6	-0.437103000	-4.613977000	-2.814304000				

$I22_{cis}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.142069
Thermal and entropic correction, BS1 (a.u.)	0.512496
Electronic Energy, BS2 (a.u.)	-7861.476232
Gibbs Energy, BS2 (a.u.)	-7860.963736
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	2.579270000	-1.849601000	2.119864000	6	4.748252000	3.614714000	-1.113530000
6	2.147926000	-3.953937000	2.890575000	6	4.923251000	2.365514000	-1.695155000
6	1.585859000	-3.082922000	3.762564000	6	4.531609000	1.230266000	-0.992096000
1	2.191092000	-5.031026000	2.895380000	9	3.326013000	2.683448000	2.072985000
1	1.036455000	-3.245697000	4.675914000	9	4.664786000	0.045242000	-1.666670000
7	2.747845000	-3.188626000	1.893865000	9	5.068560000	4.729537000	-1.793666000
7	1.858966000	-1.807571000	3.280207000	9	4.034557000	4.903946000	0.740630000
6	5.040650000	-3.666491000	-1.002432000	9	5.373908000	2.282809000	-2.966758000
6	4.461885000	-4.779427000	-1.618815000	6	1.345732000	-0.603935000	3.862477000
6	3.333010000	-5.376514000	-1.051135000	6	-0.018352000	-0.519340000	4.155678000
6	2.769765000	-4.855097000	0.114985000	6	2.197497000	0.477360000	4.094855000
6	3.355715000	-3.740171000	0.722594000	6	-0.531940000	0.664609000	4.686220000
6	4.500097000	-3.151048000	0.176006000	6	1.671983000	1.660956000	4.614957000
1	5.923106000	-3.200652000	-1.430862000	6	0.309883000	1.756890000	4.912673000
1	4.889391000	-5.180362000	-2.532929000	1	-0.669997000	-1.361075000	3.949669000
29	3.250655000	-0.333751000	1.133838000	1	3.252254000	0.388599000	3.859364000
1	4.955850000	-2.298384000	0.668082000	1	-1.593716000	0.737756000	4.898751000
1	1.865558000	-5.288497000	0.527275000	1	2.330692000	2.506588000	4.786276000
6	3.969566000	1.247475000	0.275720000	1	-0.094182000	2.679591000	5.318639000
6	3.855610000	2.520900000	0.824227000	1	2.872835000	-6.238525000	-1.524688000
6	4.215812000	3.694837000	0.169648000	6	0.137461000	-0.587339000	-1.377988000

6	1.592363000	-2.194598000	-2.029934000
6	1.869891000	-1.081654000	-2.746341000
1	2.055689000	-3.167458000	-2.016608000
1	2.613600000	-0.907191000	-3.504903000
7	0.521612000	-1.875725000	-1.198648000
7	0.966903000	-0.096606000	-2.340176000
6	-1.133949000	-4.995722000	-0.072435000
6	-1.476089000	-4.663682000	1.241954000
6	-1.140227000	-3.408559000	1.753839000
6	-0.462154000	-2.480469000	0.962783000
6	-0.134719000	-2.823033000	-0.349330000
6	-0.463573000	-4.074421000	-0.876589000
1	-1.400968000	-5.966244000	-0.479301000
1	-2.005479000	-5.379749000	1.863187000
29	-1.411016000	0.280355000	-0.513101000
6	-3.775024000	1.910688000	-0.729708000
6	-4.913282000	2.612589000	-0.324490000
6	-5.289631000	2.541271000	1.016782000
6	-4.543843000	1.790721000	1.927445000
6	-3.413953000	1.112423000	1.465598000
6	-3.002517000	1.162105000	0.142087000
9	-2.694511000	0.406164000	2.359787000
9	-6.376112000	3.200374000	1.435549000
9	-3.422127000	1.975236000	-2.034336000
1	-0.216906000	-4.311309000	-1.906067000
1	-0.207297000	-1.498001000	1.343379000
6	-2.605323000	-1.061567000	-1.267151000
6	-2.614915000	-1.332019000	-2.628444000
6	-3.310265000	-2.410098000	-3.170469000
6	-4.037747000	-3.246638000	-2.330972000
6	-4.064144000	-2.989290000	-0.965008000
6	-3.368351000	-1.894897000	-0.458215000
9	-1.892883000	-0.580731000	-3.490963000
9	-3.440470000	-1.702814000	0.875104000
9	-4.703299000	-4.295408000	-2.834216000
53	0.093061000	1.997641000	0.767378000
17	-5.851718000	3.550520000	-1.453007000
17	-5.020105000	1.717331000	3.601786000
9	-3.275931000	-2.654641000	-4.490667000
9	-4.754844000	-3.798343000	-0.145354000
6	0.966963000	1.237344000	-2.868664000
6	2.183214000	1.804094000	-3.258575000
6	-0.218138000	1.969211000	-2.982744000
6	2.221036000	3.121519000	-3.714094000
6	-0.170885000	3.286316000	-3.439684000
6	1.046086000	3.872046000	-3.797442000
1	3.098345000	1.233380000	-3.189312000
1	-1.169427000	1.524945000	-2.728022000
1	3.179118000	3.558852000	-3.978126000
1	-1.096035000	3.850109000	-3.515323000
1	1.077215000	4.900511000	-4.144299000
1	-1.412265000	-3.148105000	2.770779000

TSRE2$_{cis}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.131376
Thermal and entropic correction, BS1 (a.u.)	0.512527
Electronic Energy, BS2 (a.u.)	-7861.464293
Gibbs Energy, BS2 (a.u.)	--7860.951766
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	-2.574181000	1.825998000	2.065574000	1	0.771752000	1.685023000	3.804278000
6	-2.274911000	3.984639000	2.743389000	1	-2.980556000	-0.409867000	3.866724000
6	-1.605491000	3.192403000	3.614905000	1	1.891674000	-0.276142000	4.841659000
1	-2.401617000	5.054727000	2.710972000	1	-1.859918000	-2.389037000	4.881843000
1	-1.029768000	3.429876000	4.495031000	1	0.574791000	-2.316386000	5.386158000
7	-2.859896000	3.138927000	1.805732000	1	-3.255024000	5.925792000	-1.809637000
7	-1.799187000	1.882402000	3.188662000	6	-0.233777000	0.308017000	-1.288031000
6	-5.326870000	3.356172000	-0.974999000	6	-1.950944000	1.627263000	-1.981787000
6	-4.809586000	4.430056000	-1.704399000	6	-2.166956000	0.385021000	-2.478545000
6	-3.667338000	5.093504000	-1.247064000	1	-2.531054000	2.534005000	-2.047274000
6	-3.031098000	4.676241000	-0.077214000	1	-2.969259000	-0.004096000	-3.083884000
6	-3.553777000	3.596763000	0.641068000	7	-0.760819000	1.560147000	-1.260334000
6	-4.709431000	2.943346000	0.206092000	7	-1.101549000	-0.409687000	-2.053759000
1	-6.214801000	2.835385000	-1.319750000	6	0.608129000	4.961709000	-0.681753000
1	-5.294690000	4.749633000	-2.621974000	6	1.042666000	4.855586000	0.642647000
29	-3.214198000	0.261337000	1.138865000	6	0.881113000	3.652502000	1.335178000
1	-5.109214000	2.114943000	0.779605000	6	0.284055000	2.556771000	0.711929000
1	-2.119091000	5.158747000	0.255329000	6	-0.151428000	2.678228000	-0.608368000
6	-4.075706000	-1.248607000	0.287345000	6	0.009192000	3.871524000	-1.314974000
6	-3.821851000	-2.565320000	0.652618000	1	0.744608000	5.889239000	-1.229333000
6	-4.344384000	-3.675245000	-0.004745000	1	1.512992000	5.704165000	1.129728000
6	-5.213383000	-3.477529000	-1.072845000	29	1.449956000	-0.312090000	-0.436716000
6	-5.539178000	-2.179857000	-1.458922000	6	4.135092000	-1.398254000	-1.038185000
6	-4.964436000	-1.111197000	-0.773594000	6	5.263612000	-2.113485000	-0.639810000
9	-2.992345000	-2.832875000	1.702945000	6	5.640910000	-2.072277000	0.701929000
9	-5.293903000	0.132049000	-1.234400000	6	4.888621000	-1.349757000	1.629679000
9	-5.708417000	-4.532335000	-1.744667000	6	3.767344000	-0.650314000	1.190065000
9	-4.009531000	-4.931971000	0.351476000	6	3.367194000	-0.635994000	-0.154197000
9	-6.382523000	-1.985654000	-2.493018000	9	3.006578000	-0.059660000	2.123118000
6	-1.168792000	0.746919000	3.789715000	9	6.721486000	-2.742068000	1.105528000
6	0.201960000	0.797432000	4.060389000	9	3.781696000	-1.456339000	-2.331212000
6	-1.917626000	-0.394977000	4.083544000	1	-0.322157000	3.938631000	-2.345988000
6	0.825199000	-0.308194000	4.640946000	1	0.164251000	1.613317000	1.231173000
6	-1.281903000	-1.498305000	4.654665000	6	2.768664000	1.038897000	-1.091056000
6	0.086114000	-1.456079000	4.938653000	6	2.676955000	1.206658000	-2.480751000

6	3.030873000	2.390421000	-3.116989000	6	-2.074257000	-2.618949000	-2.373156000
6	3.510778000	3.463821000	-2.376224000	6	0.305684000	-2.313699000	-2.722247000
6	3.624748000	3.331492000	-0.999526000	6	-1.945138000	-3.977307000	-2.660514000
6	3.270226000	2.137211000	-0.382418000	6	0.427585000	-3.675018000	-3.003850000
9	2.112280000	0.271721000	-3.269770000	6	-0.691967000	-4.511426000	-2.971839000
9	3.424735000	2.097809000	0.950002000	1	-3.035789000	-2.204426000	-2.109806000
9	3.834940000	4.613468000	-2.976941000	1	1.174576000	-1.670114000	-2.745257000
53	0.489285000	-2.356761000	1.058258000	1	-2.826461000	-4.611220000	-2.620288000
17	6.189279000	-3.037477000	-1.785225000	1	1.405179000	-4.078842000	-3.250787000
17	5.320545000	-1.376543000	3.314727000	1	-0.588293000	-5.570085000	-3.190608000
9	2.862108000	2.517930000	-4.441439000	1	1.225273000	3.560289000	2.359642000
9	4.070560000	4.358595000	-0.262580000	+			
6	-0.949355000	-1.794066000	-2.394418000				

I32$_{cis}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4687.223169
Thermal and entropic correction, BS1 (a.u.)	0.512584
Electronic Energy, BS2 (a.u.)	-7861.554195
Gibbs Energy, BS2 (a.u.)	-7861.041611
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	-2.340613000	1.849859000	2.275973000	1	-4.885852000	2.012034000	1.069093000
6	-2.030133000	4.021299000	2.899046000	1	-2.090952000	5.220844000	0.433076000
6	-1.319497000	3.250767000	3.757383000	6	-3.693027000	-1.397457000	0.730193000
1	-2.168770000	5.089469000	2.855911000	6	-3.022285000	-2.611873000	0.785990000
1	-0.713156000	3.511244000	4.610008000	6	-3.542518000	-3.816839000	0.328024000
7	-2.649595000	3.153166000	2.003655000	6	-4.828845000	-3.831871000	-0.200924000
7	-1.523335000	1.930519000	3.367802000	6	-5.555499000	-2.647972000	-0.271142000
6	-5.266219000	3.268718000	-0.644011000	6	-4.970572000	-1.472945000	0.191321000
6	-4.853671000	4.384376000	-1.377727000	9	-1.753570000	-2.664426000	1.297121000
6	-3.722598000	5.099100000	-0.974323000	9	-5.723241000	-0.337059000	0.060048000
6	-2.994753000	4.694951000	0.146331000	9	-5.343850000	-4.971793000	-0.695647000
6	-3.418095000	3.579560000	0.875048000	9	-2.820013000	-4.955687000	0.351124000
6	-4.560297000	2.869678000	0.491294000	9	-6.787286000	-2.658412000	-0.821852000
1	-6.146014000	2.708075000	-0.945769000	6	-0.864252000	0.805867000	3.959368000
1	-5.409876000	4.694863000	-2.257216000	6	0.503757000	0.885290000	4.236457000
29	-2.930446000	0.246690000	1.390599000	6	-1.581940000	-0.362198000	4.234443000

6	1.155798000	-0.217688000	4.789696000
6	-0.915850000	-1.464566000	4.771369000
6	0.451337000	-1.395323000	5.052217000
1	1.052322000	1.792676000	4.008867000
1	-2.645997000	-0.401487000	4.027142000
1	2.219208000	-0.158330000	5.000177000
1	-1.471747000	-2.373872000	4.979739000
1	0.964663000	-2.253694000	5.474983000
1	-3.390261000	5.963493000	-1.541357000
6	-0.795736000	0.300805000	-1.210064000
6	-2.017878000	1.996087000	-2.126897000
6	-2.484477000	0.838627000	-2.646433000
1	-2.345383000	3.011626000	-2.272941000
1	-3.263729000	0.660142000	-3.368822000
7	-0.981665000	1.658032000	-1.258010000
7	-1.726854000	-0.188254000	-2.087515000
6	0.825526000	4.834892000	-0.589060000
6	1.353018000	4.599948000	0.682114000
6	1.106551000	3.379498000	1.314207000
6	0.334210000	2.398587000	0.691483000
6	-0.189494000	2.640979000	-0.581165000
6	0.057594000	3.858871000	-1.223876000
1	1.024530000	5.770295000	-1.102503000
1	1.955180000	5.358156000	1.173713000
29	0.420082000	-0.711206000	-0.122235000
6	5.060353000	-0.865161000	-1.332342000
6	5.880283000	-1.488051000	-0.392527000
6	5.849982000	-1.032039000	0.925910000
6	5.017799000	0.020899000	1.304183000
6	4.203424000	0.601648000	0.335686000
6	4.202739000	0.184352000	-0.996942000
9	3.350373000	1.562338000	0.707945000
9	6.614784000	-1.625509000	1.842467000
9	5.091077000	-1.293161000	-2.599300000
1	-0.308608000	4.029913000	-2.229624000
1	0.138880000	1.458417000	1.191271000
6	3.280522000	0.786100000	-1.980357000
6	2.387507000	-0.001887000	-2.712239000
6	1.452564000	0.554861000	-3.575083000
6	1.406456000	1.935221000	-3.737073000
6	2.310289000	2.743750000	-3.055737000
6	3.219703000	2.169197000	-2.176734000
9	2.387615000	-1.336947000	-2.553854000
9	4.045655000	2.979995000	-1.500541000
9	0.475353000	2.488092000	-4.520456000
53	1.913903000	-2.199674000	1.262129000
17	6.920764000	-2.801004000	-0.847761000
17	4.947210000	0.544602000	2.956371000
9	0.561899000	-0.221828000	-4.206113000
9	2.275301000	4.071372000	-3.223934000
6	-1.926832000	-1.568798000	-2.412327000
6	-3.221227000	-2.023295000	-2.680164000
6	-0.842884000	-2.450994000	-2.472196000
6	-3.429914000	-3.366990000	-2.992640000
6	-1.066871000	-3.797381000	-2.761302000
6	-2.358433000	-4.261909000	-3.021299000
1	-4.064972000	-1.346825000	-2.610342000
1	0.162626000	-2.087082000	-2.309333000
1	-4.440779000	-3.717767000	-3.175676000
1	-0.221918000	-4.478837000	-2.796763000
1	-2.528295000	-5.310598000	-3.245725000
1	1.520293000	3.181456000	2.296839000

Rf-Br

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-1461.896717
Thermal and entropic correction, BS1 (a.u.)	0.008419

Electronic Energy, BS2 (a.u.)	-4022.998884
Gibbs Energy, BS2 (a.u.)	-4022.990465
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	-1.171191000	1.214786000	-0.000051000	9	0.883183000	2.359726000	0.000039000
6	0.224616000	1.201184000	-0.000107000	9	-3.189274000	-0.000029000	0.000027000
6	0.934199000	0.000016000	-0.000055000	17	-2.039820000	2.716535000	0.000021000
6	0.224611000	-1.201194000	-0.000068000	17	-2.039819000	-2.716534000	0.000022000
6	-1.171156000	-1.214799000	-0.000060000	35	2.830228000	0.000002000	0.000015000
6	-1.857473000	0.000006000	-0.000005000				
9	0.883231000	-2.359702000	0.000026000				

Br-I1$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3075.494834
Thermal and entropic correction, BS1 (a.u.)	0.256677
Electronic Energy, BS2 (a.u.)	-7080.425833
Gibbs Energy, BS2 (a.u.)	-7080.169156
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	-2.674468000	0.350981000	0.733253000	6	-0.560200000	-0.559322000	-2.170769000
6	-4.843399000	-0.163739000	0.253711000	6	0.323687000	0.517257000	-2.257907000
6	-4.742284000	1.187446000	0.258761000	6	1.666959000	0.384728000	-1.910154000
1	-5.691145000	-0.808718000	0.087750000	9	-0.138357000	1.699943000	-2.674340000
1	-5.476050000	1.956634000	0.077938000	9	-0.907573000	-2.822557000	-1.615779000
7	-3.576150000	-0.659443000	0.548479000	9	3.404249000	-1.004149000	-1.122404000
7	-3.413530000	1.483467000	0.548062000	1	-1.967291000	-1.872026000	2.304230000
6	-2.012723000	-3.890769000	1.535862000	1	-4.460484000	-2.511179000	-1.140961000
6	-2.553844000	-4.752365000	0.578251000	6	1.079695000	0.105313000	1.580460000
6	-3.452005000	-4.257961000	-0.370848000	6	1.955105000	1.175454000	1.447331000
6	-3.795556000	-2.905720000	-0.379791000	6	3.338316000	1.071948000	1.565035000
6	-3.248509000	-2.052177000	0.582389000	6	3.897975000	-0.170100000	1.847724000
6	-2.368710000	-2.541854000	1.552051000	6	3.067248000	-1.274252000	2.013071000
1	-1.317582000	-4.265965000	2.280942000	6	1.691870000	-1.103754000	1.886217000
1	-2.278209000	-5.802761000	0.572531000	9	1.470929000	2.415614000	1.143614000
29	-0.795869000	0.231167000	1.146887000	9	0.933863000	-2.229833000	2.039206000
6	2.124062000	-0.855810000	-1.466650000	9	5.232357000	-0.304868000	1.945880000
6	1.264372000	-1.950077000	-1.365772000	1	-3.873891000	-4.920122000	-1.121089000
6	-0.075930000	-1.787420000	-1.717726000	6	-2.887172000	2.811853000	0.632633000

6	-1.697072000	3.128779000	-0.028165000	1	-3.581651000	5.820047000	2.040354000
6	-3.572541000	3.776031000	1.375918000	1	-1.450658000	6.397513000	0.894357000
6	-1.178297000	4.419572000	0.076923000	35	2.845118000	1.861519000	-2.024238000
6	-3.052623000	5.068992000	1.461315000	17	1.848521000	-3.483667000	-0.808605000
6	-1.853901000	5.391989000	0.819139000	17	-2.220822000	-0.375869000	-2.631619000
1	-1.193542000	2.375368000	-0.620588000	9	4.145412000	2.137724000	1.387073000
1	-4.491243000	3.511853000	1.890304000	9	3.609109000	-2.481585000	2.271140000
1	-0.250505000	4.663517000	-0.432231000				

Br-TSOA1$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3075.442081
Thermal and entropic correction, BS1 (a.u.)	0.257875
Electronic Energy, BS2 (a.u.)	-7080.373883
Gibbs Energy, BS2 (a.u.)	-7080.116008
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	-0.021897000	1.170449000	1.267410000	6	-1.295030000	0.112202000	-1.267425000
6	-1.040520000	2.068314000	3.090005000	9	-1.570358000	2.447489000	-1.091864000
6	-0.016692000	2.888973000	2.754629000	9	-5.351916000	-0.317201000	-0.577667000
1	-1.754702000	2.113605000	3.896532000	9	-1.153568000	-2.239693000	-1.504595000
1	0.331557000	3.812060000	3.190069000	1	-0.408262000	-1.559086000	1.885813000
7	-1.028201000	1.019841000	2.170751000	1	-3.654504000	1.184827000	2.538963000
7	0.591827000	2.325737000	1.635941000	6	2.222254000	-1.029165000	-0.011620000
6	-2.363021000	-2.449201000	2.101927000	6	3.495136000	-0.537612000	-0.262066000
6	-3.721975000	-2.216677000	2.328976000	6	4.661937000	-1.279767000	-0.095718000
6	-4.186780000	-0.909549000	2.494070000	6	4.567627000	-2.594428000	0.351237000
6	-3.298348000	0.165282000	2.434265000	6	3.314689000	-3.137300000	0.619635000
6	-1.941145000	-0.081907000	2.214139000	6	2.187269000	-2.342034000	0.432540000
6	-1.464118000	-1.383938000	2.050506000	9	3.659189000	0.740680000	-0.704257000
1	-1.996082000	-3.461995000	1.965887000	9	0.985001000	-2.940083000	0.701482000
1	-4.417150000	-3.049469000	2.367959000	9	5.677455000	-3.335031000	0.518743000
29	0.523890000	0.017142000	-0.273691000	1	-5.243390000	-0.720046000	2.655577000
6	-1.901632000	-1.148153000	-1.283932000	6	1.710987000	2.910125000	0.956120000
6	-3.270282000	-1.310405000	-1.068684000	6	1.621200000	3.192172000	-0.407678000
6	-4.049547000	-0.180191000	-0.831205000	6	2.873854000	3.187273000	1.677614000
6	-3.481347000	1.098712000	-0.841024000	6	2.720579000	3.750521000	-1.060291000
6	-2.121281000	1.225685000	-1.091674000	6	3.964492000	3.753307000	1.016032000

6	3.890821000	4.032190000	-0.351873000	35	0.353020000	0.277353000	-2.743416000
1	0.703693000	2.976591000	-0.940851000	17	-3.993589000	-2.887502000	-1.105864000
1	2.921329000	2.952307000	2.736353000	17	-4.456948000	2.492367000	-0.491054000
1	2.657541000	3.968530000	-2.122331000	9	5.875832000	-0.753360000	-0.357484000
1	4.873615000	3.968596000	1.569538000	9	3.218865000	-4.412872000	1.046884000
1	4.743714000	4.469213000	-0.862799000				

Br-I2$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3075.481891
Thermal and entropic correction, BS1 (a.u.)	0.261816
Electronic Energy, BS2 (a.u.)	-7080.409692
Gibbs Energy, BS2 (a.u.)	-7080.147876
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	0.268864000	0.256538000	1.312068000	9	-5.715033000	1.339821000	-0.612013000
6	-0.224881000	0.414253000	3.508163000	9	-2.344173000	-1.881564000	-1.241640000
6	0.860841000	1.189319000	3.279537000	1	-0.586592000	-2.643514000	1.312333000
1	-0.775579000	0.198943000	4.409723000	1	-3.051561000	0.469732000	2.948897000
1	1.449207000	1.810806000	3.935212000	6	2.102902000	-0.726437000	-0.459165000
7	-0.579324000	-0.153137000	2.287872000	6	3.088782000	-0.078257000	-1.194871000
7	1.153507000	1.083618000	1.923463000	6	4.441367000	-0.373379000	-1.055127000
6	-2.686940000	-3.125940000	1.528553000	6	4.839532000	-1.366069000	-0.166046000
6	-3.939213000	-2.664403000	1.938033000	6	3.879268000	-2.044113000	0.575802000
6	-4.074930000	-1.372771000	2.457080000	6	2.536382000	-1.711816000	0.413633000
6	-2.961348000	-0.542038000	2.567130000	9	2.777901000	0.913608000	-2.054784000
6	-1.716090000	-1.019581000	2.150577000	9	1.651490000	-2.379170000	1.198761000
6	-1.562898000	-2.305072000	1.635888000	9	6.140177000	-1.658908000	-0.017647000
1	-2.580007000	-4.125483000	1.118783000	1	-5.049374000	-1.006464000	2.765096000
1	-4.810292000	-3.306084000	1.847780000	6	2.260976000	1.774312000	1.323860000
29	0.212198000	-0.208581000	-0.576236000	6	2.048329000	2.657273000	0.266823000
6	-2.680270000	-0.612314000	-0.947823000	6	3.538191000	1.548172000	1.842566000
6	-4.039630000	-0.291569000	-0.954680000	6	3.145744000	3.312259000	-0.294597000
6	-4.418840000	1.008751000	-0.621083000	6	4.625243000	2.209144000	1.272898000
6	-3.459301000	1.965191000	-0.294548000	6	4.431144000	3.087712000	0.201867000
6	-2.114013000	1.585320000	-0.313171000	1	1.047253000	2.809025000	-0.116928000
6	-1.687603000	0.307042000	-0.629929000	1	3.672979000	0.846950000	2.659538000
9	-1.202453000	2.524952000	0.030518000	1	2.992324000	3.991723000	-1.127205000

1	5.624200000	2.027961000	1.657473000	17	-3.942225000	3.584620000	0.130284000
1	5.281679000	3.593874000	-0.244647000	9	5.367950000	0.304559000	-1.754859000
35	0.156381000	-0.711722000	-2.915288000	9	4.255635000	-2.999694000	1.443421000
17	-5.249169000	-1.477756000	-1.358868000				

Br-TSOA1$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3075.443771
Thermal and entropic correction, BS1 (a.u.)	0.256516
Electronic Energy, BS2 (a.u.)	-7080.372565
Gibbs Energy, BS2 (a.u.)	-7080.116049
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	0.523416000	-0.924582000	1.370747000	9	4.275025000	2.361324000	-1.370584000
6	1.541734000	-1.397434000	3.348599000	9	1.638837000	2.023705000	-1.827742000
6	0.533232000	-2.288123000	3.190326000	1	0.822924000	1.890482000	1.488319000
1	2.252350000	-1.259237000	4.147827000	1	4.158575000	-0.598079000	2.562900000
1	0.194756000	-3.104355000	3.808756000	6	-1.861062000	0.758464000	-0.249877000
7	1.519599000	-0.568083000	2.227908000	6	-3.045938000	0.079592000	-0.494014000
7	-0.074967000	-1.983632000	1.975584000	6	-4.320148000	0.635058000	-0.346727000
6	2.755473000	2.856693000	1.479077000	6	-4.414685000	1.966299000	0.059209000
6	4.125467000	2.702914000	1.708142000	6	-3.261010000	2.710746000	0.305278000
6	4.629457000	1.463843000	2.112008000	6	-2.025920000	2.076325000	0.143619000
6	3.771312000	0.375387000	2.279831000	9	-2.988713000	-1.210698000	-0.907061000
6	2.404240000	0.542830000	2.047493000	9	-0.916534000	2.833339000	0.385978000
6	1.887192000	1.778978000	1.655159000	9	-5.619634000	2.534435000	0.208698000
1	2.357115000	3.815965000	1.162669000	17	-5.770718000	-0.293127000	-0.649295000
1	4.798485000	3.542757000	1.565772000	17	-3.388933000	4.382470000	0.802097000
29	-0.053595000	-0.117190000	-0.362384000	1	5.694260000	1.334490000	2.278519000
6	2.378385000	0.951368000	-1.489740000	6	-1.182576000	-2.713395000	1.428009000
6	3.736753000	1.139461000	-1.265186000	6	-1.025376000	-3.401185000	0.224399000
6	4.532485000	0.059746000	-0.904645000	6	-2.396628000	-2.722309000	2.117002000
6	3.963222000	-1.208045000	-0.774639000	6	-2.108120000	-4.109728000	-0.297967000
6	2.613172000	-1.385730000	-1.022647000	6	-3.472367000	-3.435296000	1.585871000
6	1.782960000	-0.306157000	-1.344704000	6	-3.329132000	-4.128133000	0.380309000
9	2.088266000	-2.613351000	-0.866861000	1	-0.069274000	-3.375516000	-0.284671000
9	4.721853000	-2.236525000	-0.370402000	1	-2.491803000	-2.172859000	3.048476000
9	5.829325000	0.240938000	-0.633731000	1	-1.994523000	-4.647607000	-1.234503000

1	-4.422057000	-3.444264000	2.112242000
1	-4.169521000	-4.680418000	-0.029862000
35	0.181587000	-0.669249000	-2.776389000

Br-I3$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-3075.498021
Thermal and entropic correction, BS1 (a.u.)	0.256902
Electronic Energy, BS2 (a.u.)	-7080.423305
Gibbs Energy, BS2 (a.u.)	-7080.166403
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	2.736226000	0.348841000	-0.730547000	9	-3.094537000	-0.668734000	1.664841000
6	4.946610000	-0.057055000	-0.346674000	1	2.135915000	-1.955398000	-2.247342000
6	4.792270000	1.286837000	-0.426436000	1	4.645778000	-2.362167000	1.219557000
1	5.825057000	-0.661977000	-0.188181000	6	-1.047922000	-0.125108000	-1.310350000
1	5.503601000	2.091840000	-0.332560000	6	-1.942144000	0.937659000	-1.287020000
7	3.685023000	-0.614203000	-0.537209000	6	-3.332602000	0.804712000	-1.331856000
7	3.438591000	1.517191000	-0.655391000	6	-3.865574000	-0.480962000	-1.424640000
6	2.298448000	-3.950752000	-1.432260000	6	-3.024916000	-1.593258000	-1.468729000
6	2.884942000	-4.754844000	-0.451980000	6	-1.646123000	-1.374295000	-1.410814000
6	3.743199000	-4.184712000	0.491766000	9	-1.452288000	2.202580000	-1.190335000
6	4.007550000	-2.815053000	0.468216000	9	-0.852266000	-2.480590000	-1.406378000
6	3.419561000	-2.020650000	-0.519216000	9	-5.194878000	-0.649513000	-1.463562000
6	2.573199000	-2.583407000	-1.478844000	17	-4.398145000	2.187560000	-1.265112000
1	1.632156000	-4.385357000	-2.171481000	17	-3.707698000	-3.198135000	-1.568068000
1	2.673713000	-5.819717000	-0.423120000	1	4.197780000	-4.802390000	1.260605000
29	0.846593000	0.112172000	-1.020075000	6	2.857967000	2.817615000	-0.803390000
6	-1.770866000	-0.712770000	1.848505000	6	1.690169000	3.138918000	-0.105458000
6	-1.114330000	-1.921406000	1.641598000	6	3.465879000	3.748695000	-1.649108000
6	0.267005000	-1.997524000	1.780687000	6	1.115211000	4.398445000	-0.275451000
6	0.987744000	-0.865431000	2.146768000	6	2.890553000	5.011876000	-1.799565000
6	0.324692000	0.339147000	2.357681000	6	1.712884000	5.337115000	-1.120821000
6	-1.058332000	0.431966000	2.204896000	1	1.253013000	2.412314000	0.567524000
9	1.054179000	1.416110000	2.680900000	1	4.367570000	3.481083000	-2.190989000
9	2.319121000	-0.923585000	2.272442000	1	0.204913000	4.646488000	0.262459000
9	0.898231000	-3.148891000	1.542220000	1	3.359123000	5.736721000	-2.458516000
9	-1.806213000	-3.000311000	1.258608000	1	1.265377000	6.318465000	-1.247414000

35 -1.942603000 2.091278000 2.411814000

Br-I12$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4689.101138
Thermal and entropic correction, BS1 (a.u.)	0.510425
Electronic Energy, BS2 (a.u.)	-10137.860182
Gibbs Energy, BS2 (a.u.)	-10137.349757
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	-2.501960000	0.423461000	2.358241000	6	-4.036561000	-1.094460000	-0.782075000
6	-4.741209000	0.741497000	2.060538000	6	-5.413322000	-0.954936000	-0.959870000
6	-4.567979000	-0.534547000	2.481129000	6	-5.886610000	0.110221000	-1.726459000
1	-5.635981000	1.289796000	1.813454000	6	-5.007975000	1.024382000	-2.309876000
1	-5.277303000	-1.327815000	2.651418000	6	-3.636873000	0.860121000	-2.109963000
7	-3.472395000	1.313034000	1.990813000	9	-3.578622000	-2.111919000	-0.047443000
7	-3.197537000	-0.714977000	2.649215000	9	-2.795951000	1.739780000	-2.661403000
6	-3.662302000	4.456896000	0.015897000	9	-7.199437000	0.260555000	-1.900692000
6	-2.696610000	5.239956000	0.653705000	6	-2.598737000	-1.951861000	3.053318000
6	-2.001881000	4.725784000	1.752285000	6	-3.150357000	-2.661147000	4.123679000
6	-2.264108000	3.435626000	2.213981000	6	-1.479362000	-2.440065000	2.372807000
6	-3.217290000	2.652528000	1.555864000	6	-2.566151000	-3.866064000	4.518081000
6	-3.924994000	3.161055000	0.463270000	6	-0.889682000	-3.634157000	2.788921000
1	-4.208909000	4.846335000	-0.837640000	6	-1.433298000	-4.350703000	3.857993000
1	-2.488222000	6.244917000	0.299311000	1	-4.015016000	-2.266676000	4.648117000
29	-0.596801000	0.683851000	2.450807000	1	-1.074647000	-1.888577000	1.533203000
6	2.144077000	-0.254353000	2.553519000	1	-2.991820000	-4.418082000	5.350745000
6	3.528127000	-0.215042000	2.422431000	1	-0.016946000	-4.000158000	2.261051000
6	4.152013000	1.010627000	2.215698000	1	-0.977578000	-5.284201000	4.174959000
6	3.380959000	2.168131000	2.178606000	1	-1.256160000	5.330373000	2.259477000
6	2.000065000	2.065493000	2.323695000	6	4.195514000	0.929169000	-1.105327000
6	1.322886000	0.864881000	2.492159000	6	5.961942000	2.358801000	-0.915545000
9	1.304047000	3.239829000	2.289136000	6	4.846379000	3.114237000	-1.049176000
9	5.484446000	1.076525000	2.045372000	1	6.994240000	2.638130000	-0.779603000
9	1.601177000	-1.486436000	2.764756000	1	4.712142000	4.183529000	-1.075942000
1	-4.664416000	2.545652000	-0.035148000	7	5.549371000	1.029015000	-0.955097000
1	-1.739029000	3.037161000	3.075384000	7	3.779176000	2.229044000	-1.174461000
6	-3.134088000	-0.193368000	-1.346202000	6	8.539075000	-1.100929000	-1.536527000

6	8.203647000	-2.249103000	-0.814762000	9	-0.355079000	-4.647171000	-0.094154000
6	6.985198000	-2.306903000	-0.132969000	6	2.420389000	2.640023000	-1.371721000
6	6.106104000	-1.223915000	-0.163777000	6	1.898663000	3.668889000	-0.585505000
6	6.446157000	-0.084083000	-0.897785000	6	1.632014000	2.010350000	-2.341117000
6	7.660897000	-0.016988000	-1.586645000	6	0.565644000	4.049079000	-0.751689000
1	9.481539000	-1.048217000	-2.073403000	6	0.300281000	2.394859000	-2.491827000
1	8.887991000	-3.091696000	-0.782308000	6	-0.239828000	3.407239000	-1.694068000
29	3.059049000	-0.635404000	-1.164379000	1	2.512993000	4.133207000	0.176155000
1	7.909342000	0.864744000	-2.168318000	1	2.050050000	1.218428000	-2.952035000
1	5.172844000	-1.255166000	0.381733000	1	0.151816000	4.831060000	-0.124237000
6	1.773107000	-2.026674000	-1.573673000	1	-0.319752000	1.893786000	-3.226912000
6	1.200289000	-2.043407000	-2.841452000	1	-1.283887000	3.684604000	-1.798201000
6	0.151242000	-2.874547000	-3.219875000	1	6.719031000	-3.191176000	0.438813000
6	-0.374569000	-3.758194000	-2.284251000	17	-5.611707000	2.352799000	-3.248822000
6	0.170905000	-3.802684000	-1.005928000	17	-6.518740000	-2.078632000	-0.237484000
6	1.221023000	-2.945635000	-0.688806000	9	3.983134000	3.360259000	1.971857000
9	1.634953000	-1.168321000	-3.800068000	9	4.268038000	-1.345531000	2.465665000
9	1.695248000	-3.030015000	0.588236000	35	-1.275364000	-0.416790000	-1.114419000
9	-1.423086000	-4.538481000	-2.600964000				
9	-0.406381000	-2.795533000	-4.446030000				

Br-TSOA2$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4689.054288
Thermal and entropic correction, BS1 (a.u.)	0.511794
Electronic Energy, BS2 (a.u.)	-10137.803206
Gibbs Energy, BS2 (a.u.)	-10137.291412
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

6	2.320562000	-0.077264000	2.382112000	6	4.565078000	-3.292364000	0.372984000
6	3.885077000	-0.250879000	4.022672000	6	3.760856000	-2.487699000	1.180135000
6	2.873378000	0.506984000	4.508609000	6	4.341401000	-1.428291000	1.879389000
1	4.803703000	-0.589336000	4.474513000	6	5.710897000	-1.168524000	1.786557000
1	2.735720000	0.991717000	5.462135000	1	7.570066000	-1.779790000	0.899810000
7	3.530343000	-0.600722000	2.720025000	1	6.558691000	-3.676394000	-0.354136000
7	1.928605000	0.605353000	3.490331000	29	1.251029000	-0.216263000	0.695122000
6	6.507399000	-1.985771000	0.982879000	6	-1.538874000	-1.049996000	1.642699000
6	5.937509000	-3.047898000	0.276312000	6	-2.525069000	-1.959479000	2.017032000

6	-2.368508000	-3.302087000	1.693767000	7	-4.790886000	-1.800143000	-0.441510000
6	-1.216189000	-3.707675000	1.032041000	7	-3.169267000	-2.447566000	-1.700727000
6	-0.247490000	-2.757472000	0.726084000	6	-8.002037000	-0.472872000	0.884262000
6	-0.355492000	-1.404346000	1.011261000	6	-7.563936000	0.644908000	1.598304000
9	0.862415000	-3.235531000	0.080810000	6	-6.199564000	0.944398000	1.647604000
9	-3.330828000	-4.189670000	1.998647000	6	-5.273511000	0.133020000	0.992741000
9	-1.802218000	0.257287000	1.926122000	6	-5.723938000	-0.974421000	0.265859000
1	6.141260000	-0.328322000	2.321602000	6	-7.086027000	-1.282091000	0.208903000
1	2.698248000	-2.674937000	1.265771000	1	-9.060127000	-0.712965000	0.838542000
6	2.726604000	0.526316000	-0.544136000	1	-8.280199000	1.276006000	2.116086000
6	3.659190000	1.442842000	-0.052015000	29	-3.141417000	0.503299000	-1.332448000
6	5.011207000	1.358404000	-0.358705000	1	-7.427510000	-2.134073000	-0.370117000
6	5.443191000	0.353771000	-1.231413000	1	-4.213542000	0.341573000	1.064695000
6	4.537045000	-0.548678000	-1.784532000	6	-2.482743000	2.303815000	-1.553235000
6	3.191585000	-0.449506000	-1.430874000	6	-1.812373000	2.705059000	-2.704251000
9	3.242690000	2.397284000	0.795446000	6	-1.130254000	3.912951000	-2.831149000
9	2.324841000	-1.328470000	-1.959937000	6	-1.122069000	4.795595000	-1.756334000
9	6.742481000	0.247836000	-1.519399000	6	-1.809409000	4.461229000	-0.593630000
6	0.717028000	1.365511000	3.597162000	6	-2.460733000	3.233835000	-0.521270000
6	-0.169833000	1.088320000	4.639004000	9	-1.765811000	1.879614000	-3.792320000
6	0.449309000	2.371014000	2.666640000	9	-3.085114000	2.955734000	0.660828000
6	-1.347633000	1.829634000	4.743274000	9	-0.455407000	5.959791000	-1.839535000
6	-0.732949000	3.102709000	2.777820000	9	-0.451897000	4.226308000	-3.954246000
6	-1.631396000	2.832995000	3.812803000	9	-1.801050000	5.321825000	0.448324000
1	0.058985000	0.297188000	5.346297000	6	-2.019941000	-2.451462000	-2.557183000
1	1.159963000	2.573103000	1.874431000	6	-1.043968000	-3.439728000	-2.397561000
1	-2.045085000	1.616109000	5.547813000	6	-1.875343000	-1.464030000	-3.536458000
1	-0.947947000	3.886180000	2.061748000	6	0.090212000	-3.421868000	-3.210987000
1	-2.551912000	3.403837000	3.892859000	6	-0.730461000	-1.447120000	-4.333362000
1	4.114422000	-4.111329000	-0.179433000	6	0.255829000	-2.423783000	-4.174140000
6	-3.737280000	-1.323444000	-1.169904000	1	-1.152538000	-4.200271000	-1.633898000
6	-4.875834000	-3.188312000	-0.518787000	1	-2.646247000	-0.713411000	-3.665532000
6	-3.852202000	-3.596014000	-1.306593000	1	0.852114000	-4.183804000	-3.076856000
1	-5.629810000	-3.750133000	0.007917000	1	-0.618658000	-0.671102000	-5.084740000
1	-3.554217000	-4.582088000	-1.624486000	1	1.146806000	-2.407299000	-4.794715000

1	-5.846299000	1.805049000	2.208128000	9	-3.640889000	-1.568745000	2.666833000
17	5.074777000	-1.771597000	-2.893934000	35	0.723900000	1.314508000	-1.140060000
17	6.162322000	2.437371000	0.370254000				
9	-1.082897000	-4.999415000	0.657037000				

Br-I22$_{trans}$

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4689.085245
Thermal and entropic correction, BS1 (a.u.)	0.511999
Electronic Energy, BS2 (a.u.)	-10137.830512
Gibbs Energy, BS2 (a.u.)	-10137.318513
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

6	2.264082000	-0.633223000	2.127996000	1	5.838525000	-0.310764000	2.475899000
6	3.445181000	-1.169728000	3.974912000	1	3.254282000	-3.411709000	1.017561000
6	2.349366000	-0.485874000	4.379120000	6	3.416135000	0.398011000	-0.147026000
1	4.260366000	-1.610668000	4.525878000	6	4.005023000	1.503902000	0.437703000
1	2.009895000	-0.187595000	5.358055000	6	5.284734000	1.956867000	0.102751000
7	3.382558000	-1.248731000	2.586718000	6	5.999386000	1.259825000	-0.869599000
7	1.633371000	-0.157528000	3.231346000	6	5.449683000	0.135164000	-1.485463000
6	6.752744000	-1.727699000	1.118586000	6	4.172343000	-0.273492000	-1.099254000
6	6.545568000	-2.857106000	0.319942000	9	3.347186000	2.174112000	1.411242000
6	5.289748000	-3.466047000	0.279790000	9	3.675263000	-1.389414000	-1.671510000
6	4.232228000	-2.950353000	1.032315000	9	7.228509000	1.665859000	-1.207727000
6	4.450005000	-1.813764000	1.805662000	35	0.797626000	0.279209000	-1.804253000
6	5.703463000	-1.199648000	1.868548000	6	0.444324000	0.649428000	3.278586000
1	7.726246000	-1.248050000	1.146273000	6	-0.630368000	0.211336000	4.054556000
1	7.362575000	-3.259053000	-0.271312000	6	0.400110000	1.863910000	2.593622000
29	1.662871000	-0.361818000	0.299279000	6	-1.772675000	1.008400000	4.138396000
6	-1.199386000	-1.016643000	1.022935000	6	-0.745448000	2.654256000	2.689172000
6	-2.233472000	-1.895331000	1.334831000	6	-1.829707000	2.229035000	3.459713000
6	-2.052979000	-3.260723000	1.158479000	1	-0.572659000	-0.742243000	4.569705000
6	-0.835722000	-3.732320000	0.682127000	1	1.244452000	2.175195000	1.993116000
6	0.191397000	-2.824579000	0.443661000	1	-2.619172000	0.671244000	4.728949000
6	0.057135000	-1.457099000	0.633435000	1	-0.794565000	3.590827000	2.146400000
9	1.356354000	-3.335264000	-0.037383000	1	-2.721078000	2.845180000	3.527042000
9	-3.071086000	-4.111778000	1.372334000	1	5.127971000	-4.345541000	-0.335962000
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Br-TSRE2$_{trans}$

Charge	0
Spin State	Singlet
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Thermal and entropic correction, BS1 (a.u.)	0.509730
Electronic Energy, BS2 (a.u.)	-10137.804552
Gibbs Energy, BS2 (a.u.)	-10137.294822
Number of Imaginary Frequencies	1

Molecular Geometry in Cartesian Coordinates

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Br-I32$_{trans}$

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Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-4689.097807
Thermal and entropic correction, BS1 (a.u.)	0.506971
Electronic Energy, BS2 (a.u.)	-10137.849138
Gibbs Energy, BS2 (a.u.)	-10137.342167
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

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6	-3.091558000	2.486702000	-2.003521000	1	-4.056145000	1.402830000	2.881714000
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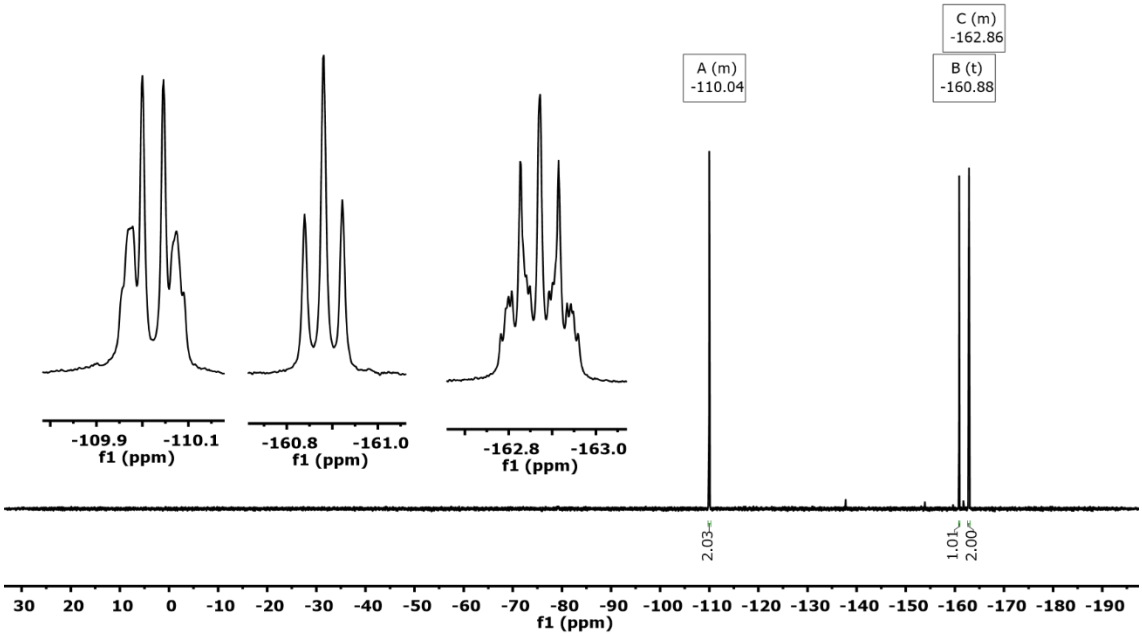
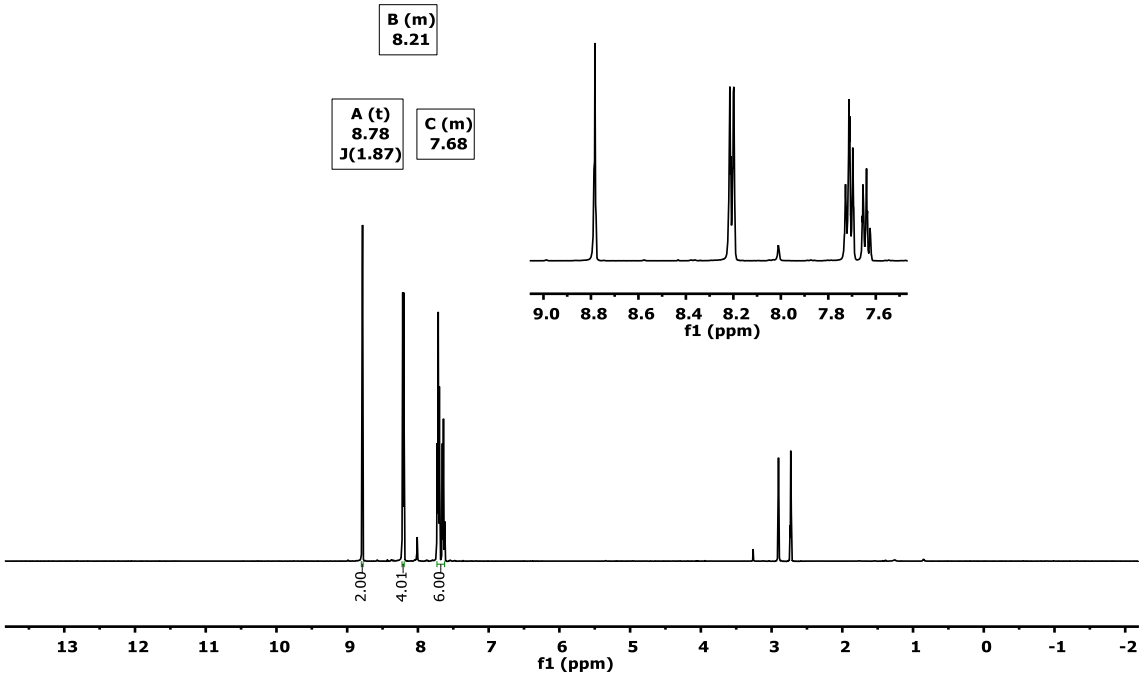
NMR spectra

^{19}F NMR (470 MHz, DMF-d_7) δ -110.04 (m), -160.88 (t, J = 19.5 Hz), -162.86 (m).



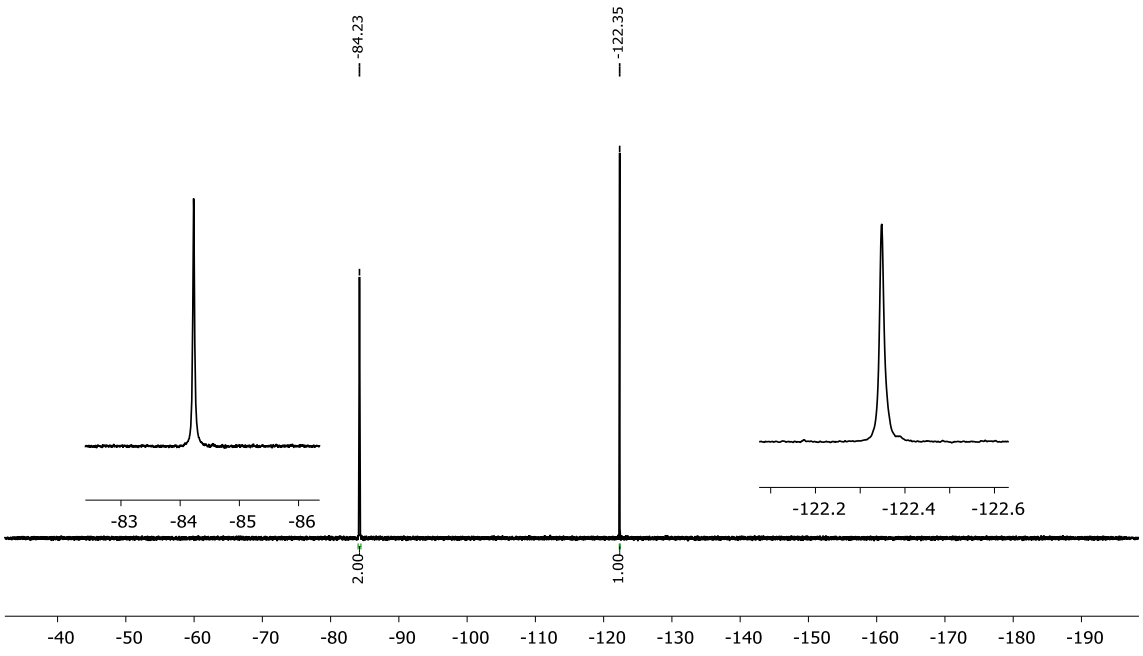
Spectrum ESI 15: ^{19}F NMR (DMF-d_7) of **[Cu(DPI)(C_6F_5)]** (298K)

^{1}H NMR (500 MHz, DMF-d_7) δ 8.78 (t, J = 1.9 Hz, 2H), 8.23 – 8.19 (m, 4H), 7.75 – 7.62 (m, 6H).



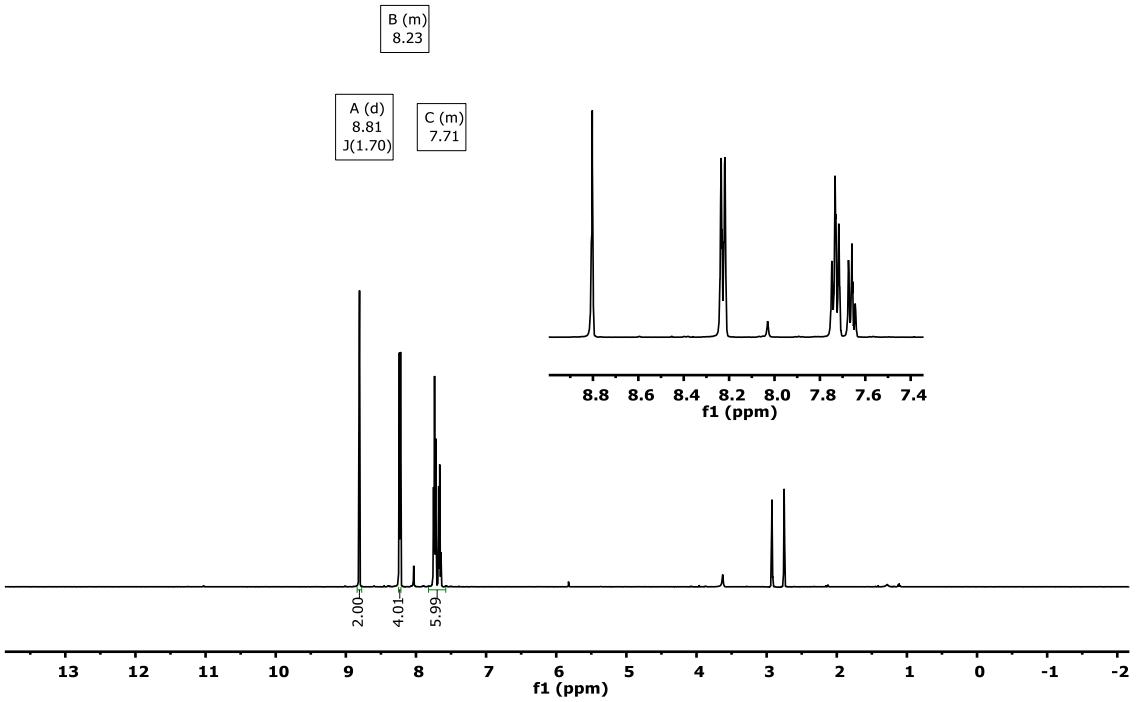
Spectrum ESI 16: ^{1}H NMR (DMF-d_7) of **[Cu(DPI)(C_6F_5)]** (298K)

^{19}F NMR (470 MHz, DMF-d_7) δ -84.23 (s), -122.35 (s).



Spectrum ESI 17: ^{19}F NMR (DMF-d_7) of **[Cu(DPI)($C_6F_3Cl_2$)]** (298K)

^{1}H NMR (500 MHz, DMF-d_7) δ 8.81 (d, J = 1.7 Hz, 1H), 8.24 – 8.22 (m, 3H), 7.76 – 7.63 (m, 4H).



Spectrum ESI 18: ^{1}H NMR (DMF-d_7) of **[Cu(DPI)($C_6F_3Cl_2$)]** (298K)

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