Supplementary Material (ESI) for Chemical Communications

Supporting Information:

C_{sp3}–F bond activation by nucleophilic attack of the {Pt_2S_2} core assisted by non-covalent interactions

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I) Computational Details:

The calculations were performed using the Gaussian03 package.[1] The geometries of the minima and transition states were fully optimized at B3LYP level. The reaction mechanism involves a S_N2 reaction step (see text). It is well known that for this type of processes DFT calculations underestimate the reaction barriers.[2] Therefore, the energies here presented were obtained from single point calculations at MP2 level. The solvent effects (toluene, $\varepsilon = 2.379$) were included by means of PCM calculation using the CPCM[3] polarizable conductor calculation model.[4]

For the Pt, P and S atoms, the lanl2dz effective core potential was used to describe the innermost electrons,[5] whereas their associated double-ζ basis set was employed for the rest of the electrons. An extra series of d-polarization functions were also added for P (exp. 0.387) and S (exp. 0.503) atoms.[6] The carbon and oxygen atoms of 1,3-difluoro-2-propanol were described by the 6-31G(d) basis set.[7] The rest of the C and H atoms was described by the 6-31G basis set. The fluorine atoms were described by the 6-31G+(d) basis set.[8]

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[5]Hay, P. J.; Wadt, W. R., *J. Chem. Phys.* **1985**, *82*, 299.
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[7] Hehre, W. J.; Ditchfield, R.; Pople, J. A., *J. Phys. Chem.* **1972**, *56*, 2257.
[8] Frisch, M. J.; Pople, J. A.; Binkley, J. S., *J. Chem. Phys.* **1984**, *80*, 3265.

II) Optimized Geometries (Cartesian coordinates) for all Calculated Species

1: $FCH_2CH(OH)CH_2F$

C	3.280696	-0.282307	-2.159425
C	2.187257	-0.443137	-3.209166
H	1.262979	-0.722491	-2.687844
C	2.523848	-1.553207	-4.203000
H	3.362831	-1.274755	-4.849075
H	2.758025	-2.490768	-3.686262
F	1.421491	-1.795410	-5.030803
H	3.019386	0.510681	-1.454608
H	3.497443	-1.212547	-1.624534
O	1.908080	0.787954	-3.846224
H	2.716528	1.076638	-4.301690
F	4.474845	0.116324	-2.803816

2: $[Pt_2(\mu\text{-}S)_2(dppp)_2]$

Pt	-1.646038	0.000044	-0.520642
Pt	1.645912	0.000109	-0.520103
S	0.000015	1.613559	-1.210873
S	0.000071	-1.613168	-1.211384
P	-3.040714	1.700411	0.130143
P	-3.040397	-1.700448	0.130470
P	3.040490	-1.700345	0.130653
P	3.040575	1.700507	0.130658
H	-2.767861	2.314457	1.386836
C	-4.860276	1.306867	0.320008
H	-3.086450	2.877783	-0.664988
H	-3.086067	-2.878068	-0.664305
H	-2.767286	-2.314091	1.387302
C	-4.860016	-1.307167	0.320387
H	3.085761	-2.877936	-0.664179
C	4.860189	-1.307012	0.319710
H	2.768030	-2.314029	1.387618
H	2.768318	2.314297	1.387617
H	3.085843	2.878044	-0.664251
C	4.860255	1.307030	0.319543
H	-5.352331	2.152462	0.814875
H	-5.281583	1.231175	-0.691038
H	-5.281395	-1.231861	-0.690660
H	-5.351881	-2.152711	0.815532
H	5.352324	-2.152571	0.814560
H	5.281069	-1.231623	-0.691538
H	5.281005	1.231441	-0.691743
H	5.352546	2.152606	0.814210
C	5.145723	0.000051	1.102642

C	-5.145248	-0.000064	1.103367
H	-6.208467	-0.000142	1.377643
H	-4.589457	0.000124	2.052587
H	6.209082	0.000037	1.376369
H	4.590419	0.000125	2.052146

1···2: $[Pt_2(\mu\text{-}S)_2(dppp)_2]\cdot FCH_2CH(OH)CH_2F$ (van der Waals complex)

Pt	0.146959	-0.077649	2.153717
Pt	-0.725895	0.160254	-1.069665
S	-0.269427	-1.682581	0.413993
S	0.819770	1.356208	0.344978
P	-0.594340	-1.581171	3.721642
P	0.534056	1.617629	3.653754
P	-0.942212	1.994610	-2.446745
P	-2.139594	-1.146680	-2.325772
H	-2.004702	-1.710839	3.877910
C	-0.065692	-1.315366	5.495782
H	-0.282895	-2.954898	3.531468
H	1.638549	2.482187	3.422936
H	-0.480292	2.610998	3.773862
C	0.789821	1.155837	5.448950
H	0.161638	2.883510	-2.504731
C	-1.268047	1.648126	-4.249739
H	-1.967272	2.940275	-2.147054
H	-3.529723	-1.137084	-2.005514
H	-1.926024	-2.550629	-2.289566
C	-2.185478	-0.800740	-4.158576
H	-0.631009	-2.001705	6.137120
H	0.991838	-1.602456	5.563363
H	1.800463	0.735093	5.533556
H	0.767875	2.071060	6.052157
H	-1.446011	2.601680	-4.761054
H	-0.336727	1.224116	-4.644069
H	-1.213909	-1.111374	-4.563547
H	-2.953813	-1.435812	-4.615114
C	-2.453100	0.684934	-4.511741
C	-0.245864	0.140772	5.996499
H	-0.156400	0.130922	7.090791
H	-1.266578	0.489749	5.781656
H	-2.685451	0.731796	-5.583858
H	-3.356168	1.040932	-3.993501
C	3.395863	-0.168419	-2.157050
C	2.258012	-0.457818	-3.119927
H	1.359095	-0.611448	-2.510557
C	2.504911	-1.704119	-3.958015
H	3.324641	-1.570791	-4.671106
H	2.700849	-2.574579	-3.323757
F	1.350694	-1.997918	-4.715460
H	3.146605	0.675976	-1.511815
H	3.666055	-1.036422	-1.550139
O	1.983532	0.676230	-3.939239
H	2.824217	0.951487	-4.342424
F	4.547892	0.190379	-2.917091

TS1

Pt	-0.114817	-0.026318	2.026855
Pt	-0.910130	-0.321768	-1.323536
S	1.032310	-0.816604	0.052773
S	-1.425812	1.200550	0.454873
P	1.247401	-1.257812	3.435443
P	-1.398572	0.817476	3.733868
P	-2.557502	0.591566	-2.629227
P	-0.261768	-1.691923	-3.078645
H	0.909667	-2.626478	3.644532
C	1.429768	-0.654493	5.194078
H	2.602387	-1.438115	3.046551
H	-1.947645	2.111518	3.537420
H	-2.596116	0.108424	4.031397
C	-0.619591	0.954621	5.424131
H	-3.138424	1.788768	-2.135608
C	-1.937051	1.074871	-4.318595
H	-3.746052	-0.130989	-2.944781
H	-1.099159	-2.784429	-3.454480
H	0.968193	-2.391173	-2.964830
C	-0.085388	-0.759517	-4.679306
H	1.981381	-1.410274	5.764781
H	2.053575	0.248113	5.160655
H	0.102439	1.780219	5.380184
H	-1.397427	1.239778	6.141954
H	-2.747887	1.579271	-4.857348
H	-1.135589	1.805769	-4.155129
H	0.682058	0.005618	-4.495796
H	0.290696	-1.443496	-5.448592
C	-1.405458	-0.109001	-5.166795
C	0.087548	-0.339479	5.901114
H	0.296022	-0.227291	6.972834
H	-0.595616	-1.197264	5.817382
H	-1.221790	0.276339	-6.177925
H	-2.189174	-0.873673	-5.274173
C	2.194673	1.035131	-0.784050
C	2.669989	0.449484	-2.112315
H	2.270745	-0.558325	-2.257769
C	4.191157	0.307826	-2.134090
H	4.676790	1.275553	-2.255661
H	4.557812	-0.199781	-1.234848
F	4.559380	-0.505793	-3.231691
H	1.289243	1.615769	-0.751922
H	2.856858	1.100030	0.066531
O	2.190272	1.235192	-3.183940
H	2.417497	2.146560	-2.852502
F	2.994141	2.803520	-1.399305

3: $[Pt_2(dppp)_2(\mu\text{-}S)(\mu\text{-}SCH_2CH(OH)CH_2F)]F$

Pt	0.036434	-0.064790	-2.047764
Pt	-0.693305	0.217087	1.256043
S	1.225241	0.887014	-0.123938
S	-0.959616	-1.499584	-0.433736

P	1.043269	1.368407	-3.579705
P	-1.353694	-1.043083	-3.567328
P	-2.080842	-0.937222	2.673401
P	-0.338884	1.897238	2.797653
H	0.559052	2.708196	-3.631973
C	0.964238	0.886122	-5.383615
H	2.425955	1.666351	-3.426946
H	-1.640487	-2.415863	-3.363190
H	-2.674887	-0.521851	-3.598811
C	-0.873797	-0.972444	-5.369236
H	-1.987201	-2.336995	2.538065
C	-2.081712	-0.621343	4.506336
H	-3.466883	-0.760816	2.364247
H	-1.241109	3.002372	2.728057
H	0.886842	2.599200	2.713325
C	-0.493879	1.443368	4.588804
H	1.302902	1.737059	-5.985236
H	1.687570	0.074082	-5.533499
H	-0.054724	-1.688379	-5.516477
H	-1.724743	-1.326635	-5.963004
H	-3.034002	-0.995543	4.902605
H	-1.259526	-1.234218	4.883766
H	0.298825	0.718727	4.798894
H	-0.310351	2.344643	5.185317
C	-1.884128	0.851305	4.931494
C	-0.439686	0.432729	-5.857466
H	-0.429671	0.415155	-6.954741
H	-1.194245	1.181452	-5.576157
H	-2.006229	0.894180	6.021924
H	-2.681549	1.486401	4.515814
C	2.332786	-0.490497	0.475944
C	2.948751	-0.186850	1.865698
H	3.611149	0.684835	1.764398
C	3.825959	-1.380544	2.257366
H	3.207488	-2.211705	2.608699
H	4.471923	-1.708445	1.434477
F	4.680509	-1.017109	3.315498
H	1.730400	-1.401744	0.488451
H	3.128712	-0.591966	-0.270420
O	2.026774	0.119048	2.871206
H	1.385511	-0.665535	3.060694
F	0.313058	-1.620060	3.414146

4: $FCH_2CH_2CH_2F$

C	0.885089	0.134345	-0.915158
C	0.773228	-0.192823	0.564200
H	1.920577	0.070363	-1.262469
H	0.249862	-0.511691	-1.527412
C	-0.654554	-0.191835	1.083325
H	1.220613	-1.179874	0.739382
H	1.355986	0.537334	1.140719
H	-0.689185	-0.377427	2.160967
H	-1.174300	0.742213	0.852786
F	0.458961	1.461211	-1.140727

F	-1.384296	-1.230467	0.465460

2···4: $[Pt_2(\mu\text{-}S)_2(dppp)_2]\cdot FCH_2CH_2CH_2F$ (van der Waals complex)

Pt	0.201068	-0.014674	2.033205
Pt	-0.587696	0.051899	-1.178251
S	0.467713	-1.590987	0.236649
S	0.459388	1.637081	0.304181
P	-0.105184	-1.742177	3.511709
P	-0.106256	1.653920	3.576570
P	-1.518628	1.750954	-2.406070
P	-1.456537	-1.622604	-2.490816
H	-1.391586	-2.354383	3.518175
C	0.126757	-1.387086	5.334017
H	0.677822	-2.917483	3.350013
H	0.678783	2.832827	3.458614
H	-1.391987	2.266612	3.606164
C	0.126628	1.228164	5.383485
H	-0.817621	2.985708	-2.469225
C	-1.850833	1.403065	-4.210894
H	-2.785645	2.255096	-1.989008
H	-2.684682	-2.215624	-2.074238
H	-0.686470	-2.807902	-2.622654
C	-1.835584	-1.210091	-4.271703
H	-0.246578	-2.243986	5.907072
H	1.207500	-1.321009	5.516255
H	1.207618	1.154749	5.561269
H	-0.245689	2.062384	5.989715
H	-2.388741	2.256602	-4.639950
H	-0.874323	1.344085	-4.708359
H	-0.868749	-1.132818	-4.783205
H	-2.378994	-2.052155	-4.716471
C	-2.645212	0.096489	-4.464848
C	-0.565467	-0.088216	5.820898
H	-0.578368	-0.109093	6.918647
H	-1.620105	-0.082416	5.508756
H	-2.996487	0.118518	-5.504872
H	-3.552387	0.077895	-3.842463
C	3.086850	0.919800	-2.589257
H	2.117049	1.253627	-2.964376
H	3.252884	1.349398	-1.599467
F	4.071300	1.463817	-3.460652
C	3.201490	-0.591980	-2.566734
H	2.505151	-0.975646	-1.810123
H	4.215700	-0.871461	-2.249612
C	2.942543	-1.253394	-3.907344
H	3.561163	-0.833800	-4.705316
H	3.087454	-2.336498	-3.856021
F	1.591222	-1.054887	-4.312355

TS2

Pt	1.826657	-0.708686	-0.427081
Pt	-1.721431	-0.569986	-0.327195
S	0.056587	0.599151	-1.486807
S	0.019408	-2.093603	0.281275
P	3.575304	0.686438	-1.086337
P	3.251937	-1.671853	1.090011
P	-3.218749	-1.791007	0.913844
P	-3.365737	0.932502	-0.978413
H	4.659552	0.081803	-1.788308
C	4.426257	1.533342	0.334799
H	3.308661	1.748126	-1.992600
H	2.648263	-2.531422	2.044783
H	4.357415	-2.488853	0.704514
C	4.090247	-0.371564	2.131568
H	-2.667917	-2.560886	1.971443
C	-4.585565	-0.841853	1.755233
H	-3.960207	-2.814112	0.253972
H	-4.121304	0.561125	-2.129512
H	-2.983557	2.232749	-1.396252
C	-4.735390	1.287496	0.237447
H	5.206999	2.191472	-0.064637
H	3.663726	2.176049	0.808999
H	3.290461	0.229011	2.581104
H	4.634065	-0.871471	2.942006
H	-5.230815	-1.555565	2.280698
H	-4.112452	-0.203244	2.511721
H	-4.284831	1.862727	1.054284
H	-5.474808	1.931634	-0.252622
C	-5.436212	0.021719	0.789835
C	5.063142	0.549242	1.348750
H	5.595819	1.156780	2.091511
H	5.831129	-0.063046	0.852397
H	-6.326874	0.351450	1.340384
H	-5.809495	-0.597855	-0.038895
C	0.724372	2.420464	-0.122497
C	-0.255394	3.558732	-0.271089
H	-0.956145	3.390738	-1.097009
H	0.331369	4.449715	-0.521116
C	-1.017709	3.875561	0.999445
H	-0.355564	3.856611	1.865577
H	-1.535810	4.836742	0.929193
F	-2.040898	2.902997	1.227832
H	0.699215	1.770643	0.731880
H	1.601829	2.444455	-0.736976
F	1.961336	3.488368	1.090828

5: $[Pt_2(dppp)_2(\mu\text{-}S)(\mu\text{-}SCH_2CH_2CH_2F)]F$

Pt	-0.410458	-0.313228	1.715348
Pt	-0.313510	-0.337710	-1.900362
S	0.972483	-1.279243	-0.055629
S	-1.837609	0.285147	-0.181591
P	0.954273	-0.963441	3.535407
P	-1.883296	0.571070	3.191501

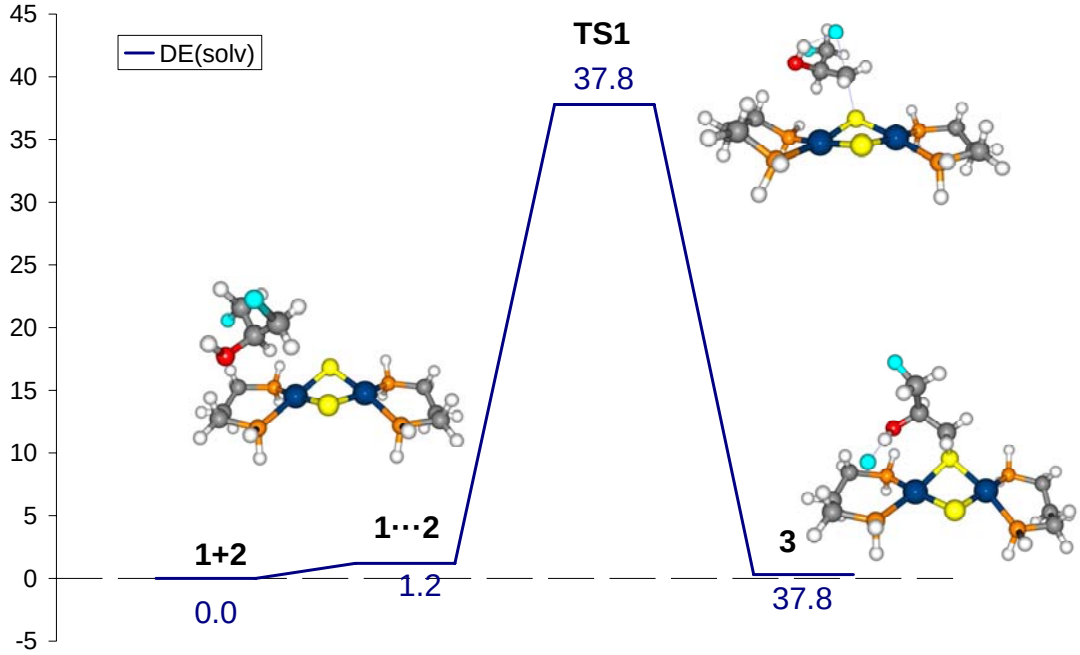
P	-1.757341	0.632977	-3.391380
P	1.166921	-0.992364	-3.579470
H	0.009855	-1.931144	4.119598
C	0.966142	0.052340	5.108823
H	1.966674	-1.951638	3.462264
H	-2.730786	1.581500	2.662731
H	-2.873602	-0.331841	3.669415
C	-1.274215	1.332248	4.776221
H	-2.554094	1.684288	-2.873459
C	-1.023853	1.365505	-4.939689
H	-2.777419	-0.202413	-3.927648
H	0.971152	-2.280929	-4.157069
H	2.547549	-1.128620	-3.265449
C	1.243960	0.071273	-5.115250
H	1.527376	-0.525418	5.854375
H	1.526742	0.968591	4.911073
H	-0.669413	2.205824	4.501013
H	-2.149609	1.693513	5.329531
H	-1.843253	1.728739	-5.570816
H	-0.433130	2.238040	-4.632876
H	1.741832	1.007942	-4.833012
H	1.881844	-0.428762	-5.852825
C	-0.138103	0.380574	-5.743638
C	-0.439585	0.369033	5.658547
H	-0.326684	0.841376	6.643956
H	-0.997721	-0.562604	5.826597
H	0.040571	0.825029	-6.731052
H	-0.686615	-0.554074	-5.930804
C	2.638640	-0.436605	-0.030231
C	2.730880	1.014640	-0.513117
H	2.330432	1.110572	-1.530883
H	3.798718	1.270941	-0.561577
C	2.045407	2.036243	0.378815
H	0.960281	1.913428	0.392621
H	2.434363	2.015999	1.398221
F	2.304978	3.329056	-0.157666
H	2.957289	-0.508729	1.012844
H	3.282773	-1.071286	-0.648106
F	2.436215	0.141603	2.950105

III) Table of Energies

E (Hartees)	1	2	1···2(vdw)	TS1	3
B3lyp	-525,43241	-392,82563	-918,27495	-918,22533	-918,27615
B3lyp Solvent	-525,44876	-392,83111	-918,28184	-918,24267	-918,29183
MP2	-520,58323	-390,81785	-911,41724	-911,34593	-911,41041
MP2 Solvent	-520,60721	-390,82490	-911,43016	-911,37180	-911,43158

E (Hartees)	4	2	2···4(vdw)	TS2	5
B3lyp	-317,62147	-392,82563	-843,0648	-843,0036	-843,0557
B3lyp Solvent	-317,62589	-392,83111	-843,0690	-843,0186	-843,0651
MP2	-315,97205	-390,81785	-836,5670	-836,4843	-836,5478
MP2 Solvent	-315,97352	-390,82490	-836,5778	-836,5068	-836,5622

IV) Graphic representation of relative energies (kcal/mol)



V) Experimental details

a) Materials and methods.

All the manipulations were carried out at room temperature under an atmosphere of pure nitrogen, and conventionally dried and degassed solvents were used throughout. These were Purex Analytical Grade from SDS. The synthesis of $[Pt_2(\mu\text{-}S)_2(dppp)_2]$ (**2**) has already been reported.[9] The high purity level of 1,3-difluoro-2-propanol was confirmed by NMR analysis.

Elemental analyses were performed on a Carlo-Erba CHNS EA-1108 analyzer. The FAB-MS measurement was performed on a VG-QUATTRO (Micromass, UK) instrument in the positive ion mode using 3-nitrobenzil alcohol (NBA) as matrix. ESI MS measurements were performed using the same instrument under the following conditions: 10 μL of sample was injected at 15 μL/min; capillary counter electrode voltage, 4.5 kV; lens-counter electrode voltage,1.0 kV; cone potential, 55 V; source temperature, 90 °C. in a 1:1 mixture of methanol and water containing 1% formic acid

$^{31}P\{^1H\}$, ^1H, ^{19}F, ^{13}C DEPT-135 NMR spectra were recorded from samples in $CDCl_3$ solution at room temperature using a Bruker AVANCE360 spectrometer. ^1H and ^{13}C chemical shifts are relative to TMS, and ^{19}F chemical shift to $CFCl_3$. $^{31}P\{H\}$ NMR spectra were referenced to external 85% H_3PO_4 (0.00 ppm). Multiplicities are abbreviated as follows: singlet (s), doublet (d)

[9] Mas-Ballesté, R.; Capdevila, M.; Champkin, P. A.; Clegg, W.; Coxall, R. A.; Lledós, A.; Mégret, C.; González-Duarte, P., *Inorg. Chem.* **2002**, *41*, 3218

and broad (br). Protons of the $FCH_2CH(OH)CH_2S^-$ ligand were assigned according to ^1H-^1H COSY and $^1H\{^{19}F\}$ NMR spectral data.

b) Experimental Procedures and Characterization Data for 3.

1,3-difluoro-2-propanol (200 μl, 2.6 mmol) was added to a solution of $[Pt_2(\mu\text{-}S)_2(dppp)_2]$ (300 mg, 0.2 mmol) in dry toluene (30 ml). After refluxing for 24 h the solvent was removed under vacuum. The remaining yellow solid was dissolved in CH_2Cl_2 (20 ml) and the excess of 1,3-difluoro-2-propanol was removed with 5 successive extractions with water (20 ml each extraction). The resulting CH_2Cl_2 solution was dried over Na_2SO_4 anhydride and concentrated to about 5 mL. Addition of diethyl ether to the organic solution caused precipitation of a yellow solid. Yield: 111 mg (34.4%). Anal. Calcd for $C_{57}F_2H_{58}OP_4Pt_2S_2{\cdot}CHCl_3$ (1494.63): C, 46.61; H, 3.98; S, 4.29. Found: C, 46.59; H, 4.02; S, 4.12. MS (FAB+): m/z = 1354.6 Da. NMR data are presented in Tables S1-S6.

c) NMR data for compound 3 (below) and corresponding labeling scheme

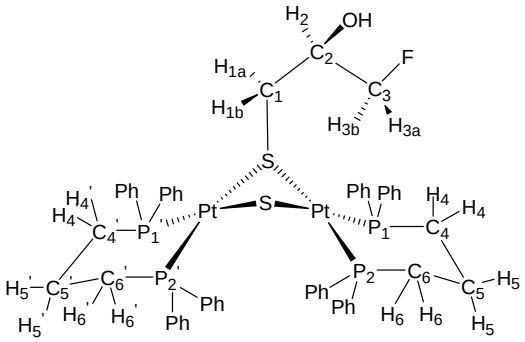


Table S1: $^{31}P\{^{1}H\}$NMR data observed for **3** at +50ºC

^{31}**P NMR (+50ºC)**	$\delta(^{31}P)$ **(ppm)**	$^{1}J_{P\text{-}Pt}$ **(Hz)**
P_1, P_1'	2.98	2405
P_2, P_2'	2.45	3010

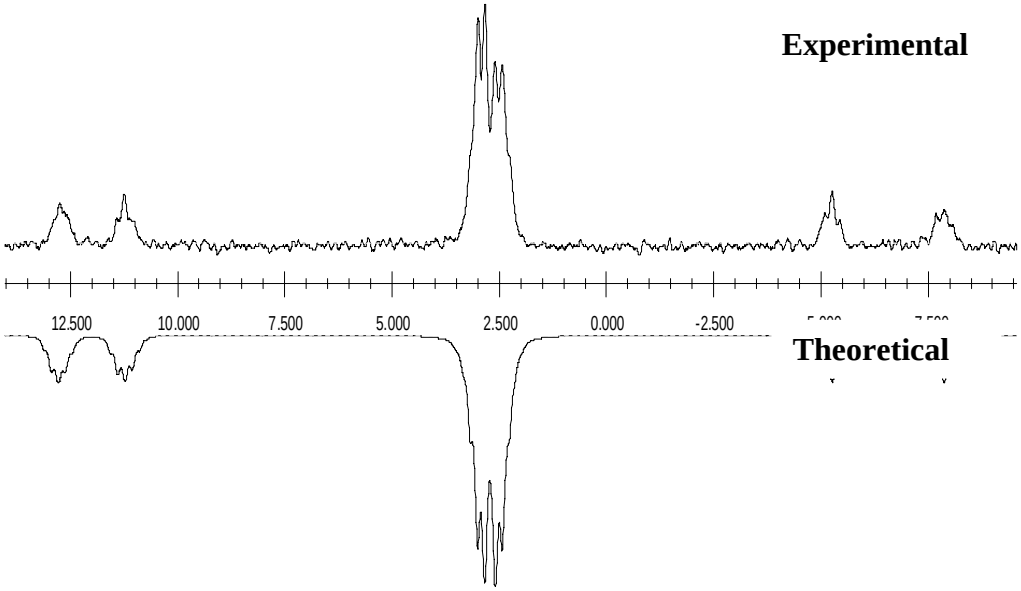


Figure S1. Comparison between experimental $^{31}P\{^{1}H\}$NMR spectrum obtained for product **3** at +50ºC and the simulation carried out using the parameters shown in table S1

Table S2: $^{31}P\{^{1}H\}$NMR data observed for product **3** at -40ºC

^{31}**P NMR (-50ºC)**	$\delta(^{31}$**P) (ppm)**	$^{1}J_{\text{P-Pt}}$ **(Hz)**
$\mathbf{P_1}$	3.69	2417
$\mathbf{P_1'}$	3.00	2370
$\mathbf{P_2}$	3.21	2960
$\mathbf{P_2'}$	2.54	2985

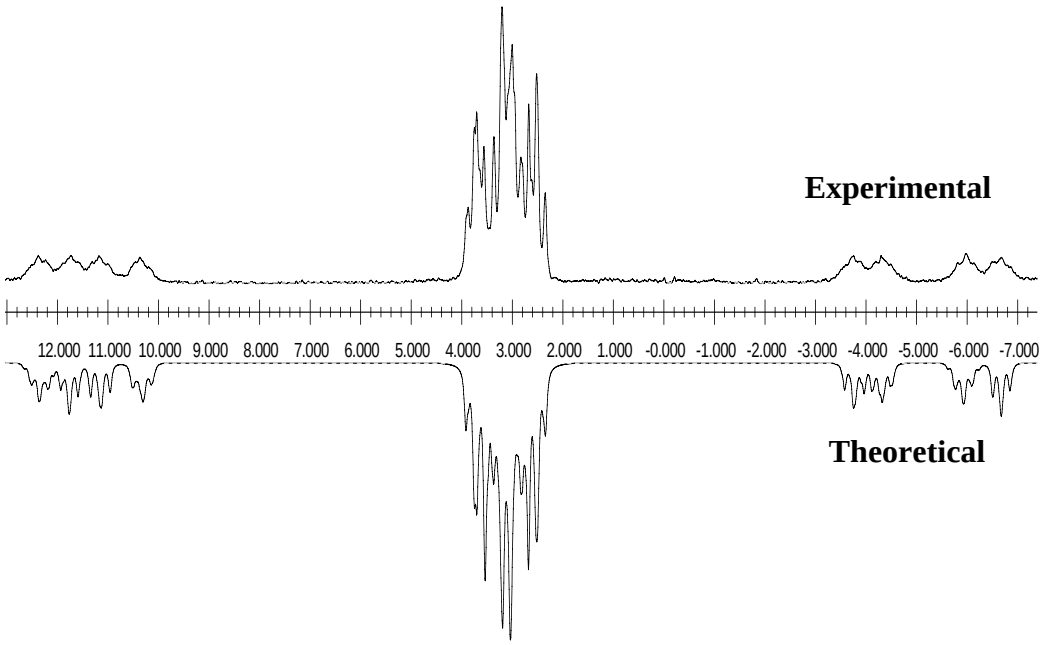


Figure S2. Comparison between experimental $^{31}P\{^{1}H\}$NMR spectrum obtained for product **3** at -40ºC and the simulation carried out using the parameters shown in table S2

Table S3: ^{19}F-NMR data observed for product **3** at room temperature

^{19}**F NMR**	$\delta(^{19}$**F) (ppm)**	$^{2}J_{\text{F-H}}$ **(Hz)**	$^{3}J_{\text{F-H}}$ **(Hz)**
F	-229.1	47.30	19.30
$\mathbf{F^-}$	-161.8		

Table S4: ^{13}C DEPT-135 NMR data observed for product **3** at room temperature

^{13}**C NMR**	$\delta(^{13}$**C) (ppm)**	$^{1}J_{\text{C-F}}$ **(Hz)**
$\mathbf{C_1}$	37.14	
$\mathbf{C_5}$	18.63	
$\mathbf{C_4,C_6}$	24.55	
$\mathbf{C_3}$	84.95	
$\mathbf{C_2}$	70.13	171
$\mathbf{C_{arom}}$	133.10, 130.54, 128.17, 127.92	

Table S5: ^{1}H-NMR data observed for product **3** at room temperature

^{1}H NMR	$\delta(^{1}H)$ (ppm)	$^{2}J_{H-H}$ (Hz)	$^{3}J_{H-H}$ (Hz)	$^{2}J_{F-H}$ (Hz)	$^{3}J_{F-H}$ (Hz)
H_{1a}	1.39	12.86	0		
H_{1b}	1.71	12.86	9.60		
H_5,H_5'	1.94				
H_4,H_4',H_6,H_6'	2.73				
H_{3a}	3.88	8.98	5.13	47.30	
H_{3b}	3.99	8.98	4.70	47.30	
OH	4.13				
H_2	4.15		4.70, 5.13, 9.60		19.30
H_{arom}	7.00-7.86				

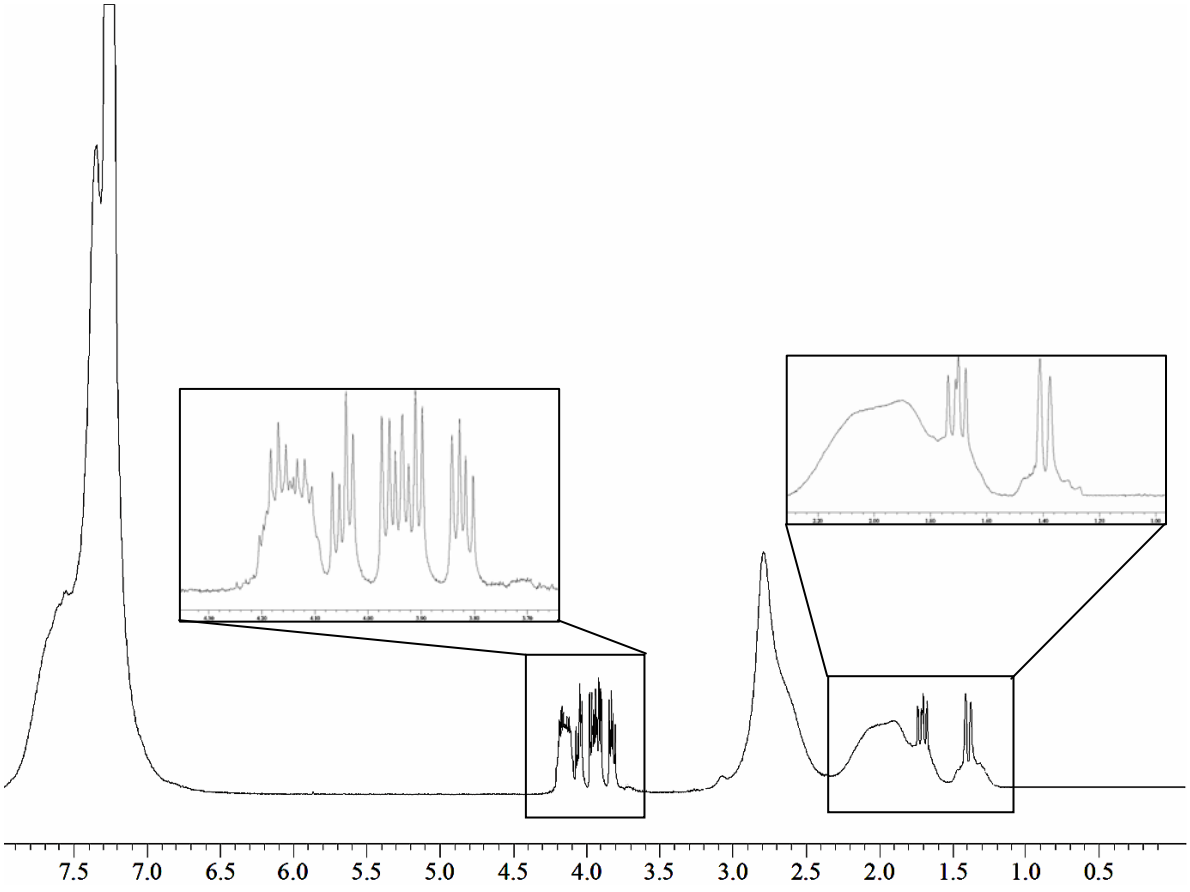


Figure S3 - ^{1}H NMR spectrum of **3** recorded in $CDCl_3$ solution at room temperature.

d) FAB-MS data for compound 3

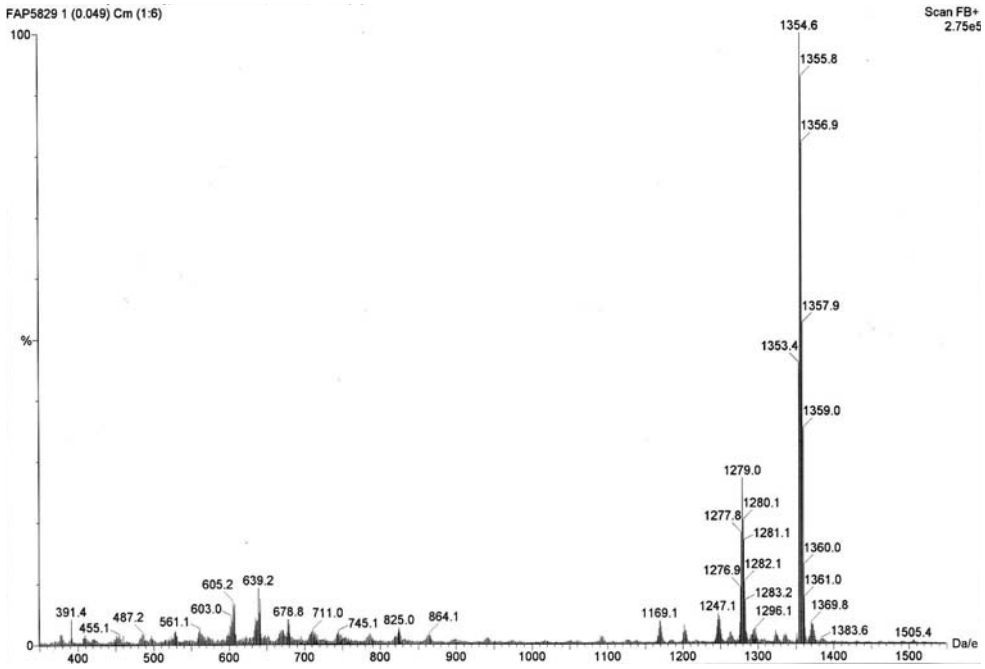
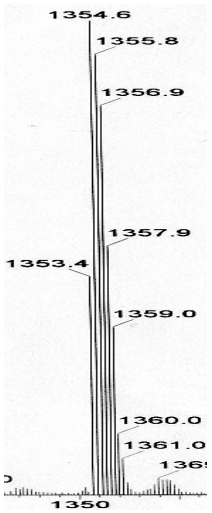


Figure S4 - FABS$^+$ spectrum of **3** using 3-nitrobenzil alcohol (NBA) as matrix.



(a)

mass	%
1349	0.0
1350	0.0
1351	1.1
1352	1.9
1353	25.7
1354	64.8
1355	100.0
1356	93.4
1357	71.6
1358	44.6
1359	27.5
1360	12.0
1361	5.5
1362	2.0
1363	0.6
1364	0.2
1365	0.0
1366	0.0

(b)

Figure S5 - (a) Region of the FABS$^+$ spectrum corresponding to $[Pt_2(dppp)_2(\mu\text{-}S)(\mu\text{-}SCH_2CH(OH)CH_2F)]^+$ cation. (b) Simulation of the isotopic distribution for the $[Pt_2(dppp)_2(\mu\text{-}S)(\mu\text{-}SCH_2CH(OH)CH_2F)]^+$ cation.