Electronic Supplementary Information

Structural and electrochemical aspects of tris(ferrocenyl/phenyl-ethynyl)phosphine ligated chalcogen bridged iron carbonyl clusters

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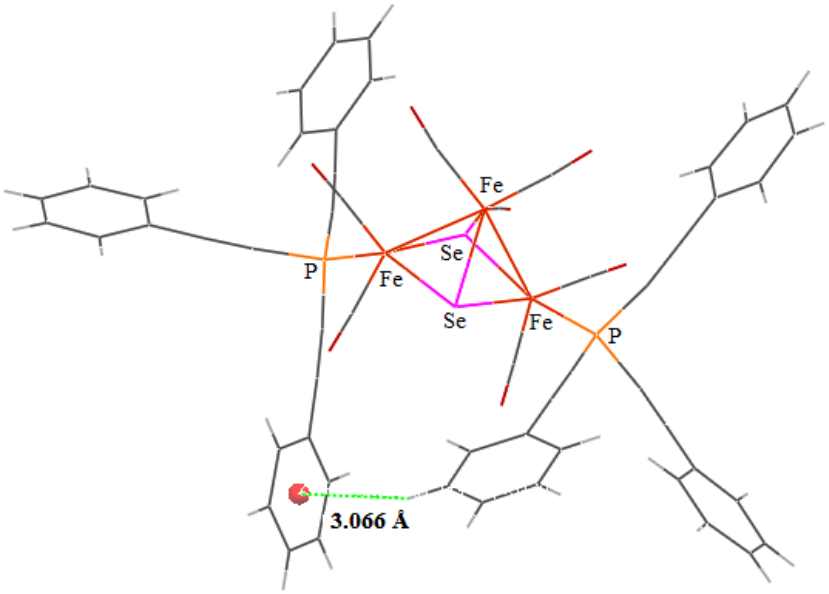


Figure S1. Molecular structure of **3** showing CH..π interaction between two phenyl rings

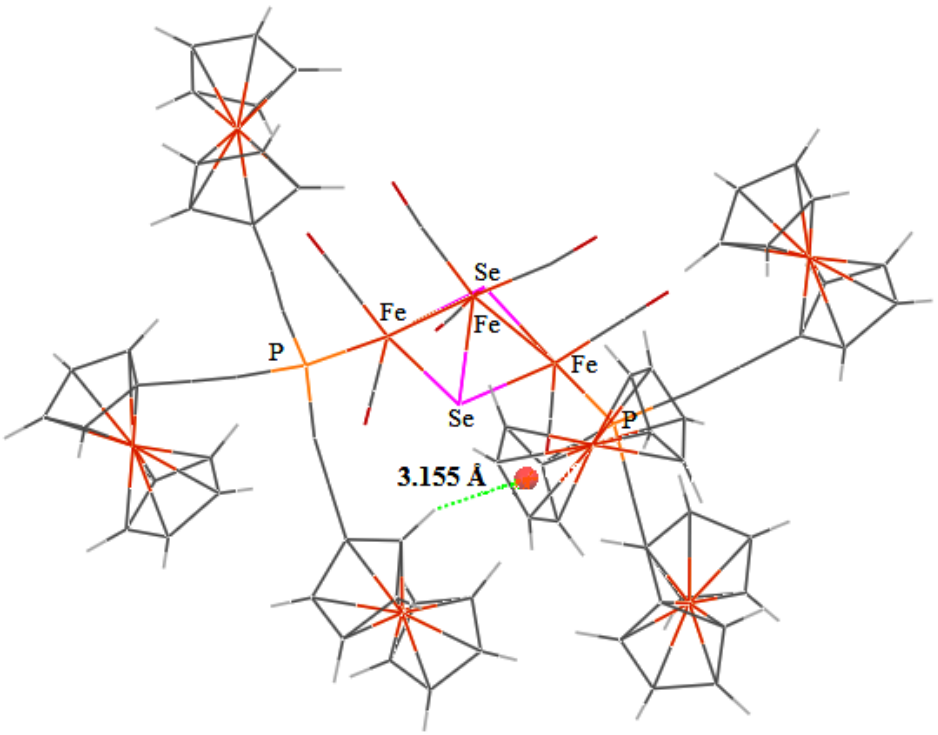


Figure S2. Molecular structure of **4** showing CH..π interaction between two ferrocenyl rings

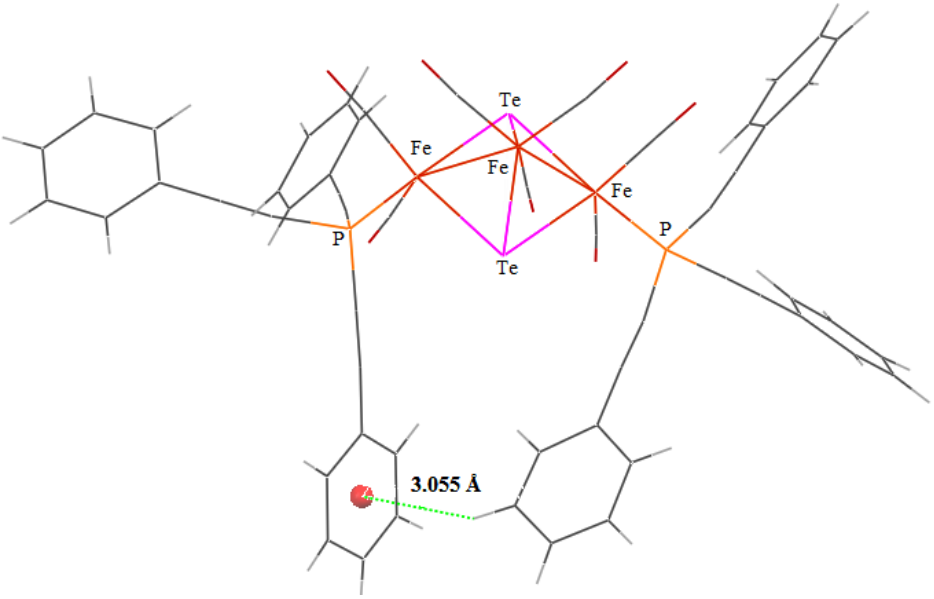


Figure S3. Molecular structure of **4** showing CH..π interaction between two phenyl rings

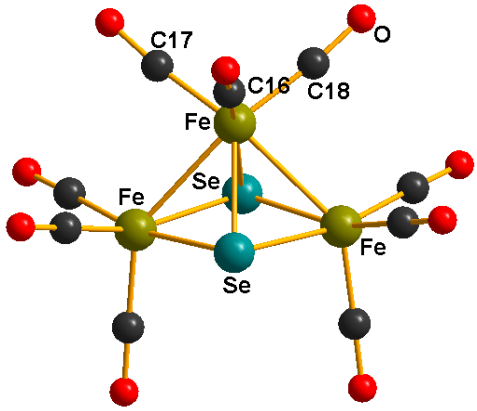


Figure S4. Calculated structure of $[Fe_3Se_2(CO)_9]$

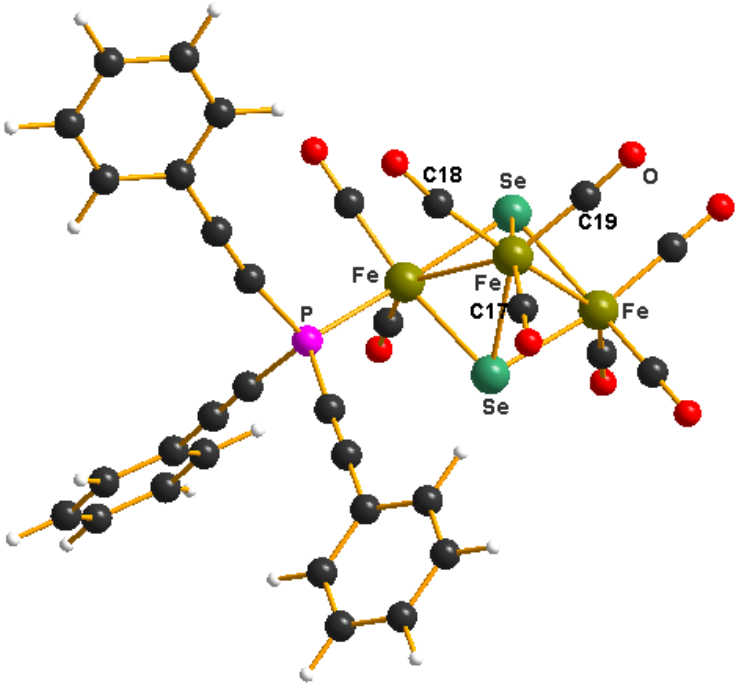


Figure S5. Calculated structure of **1**

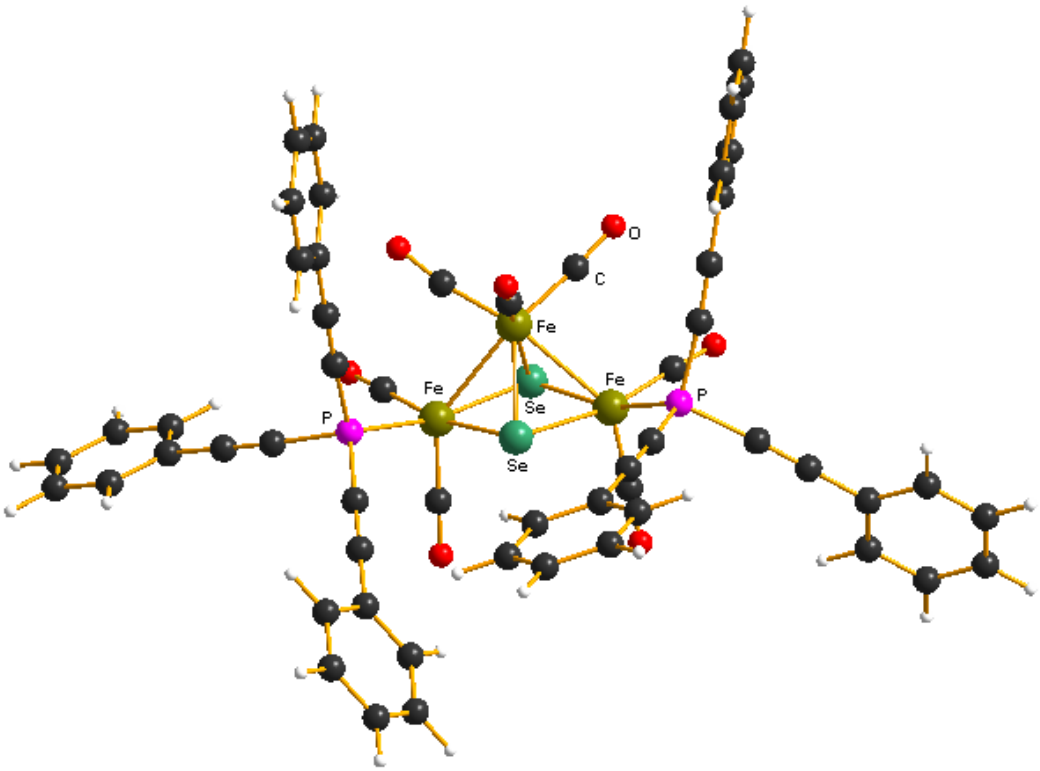


Figure S6. Calculated structure of *equatorial-equatorial-syn* (**3)**

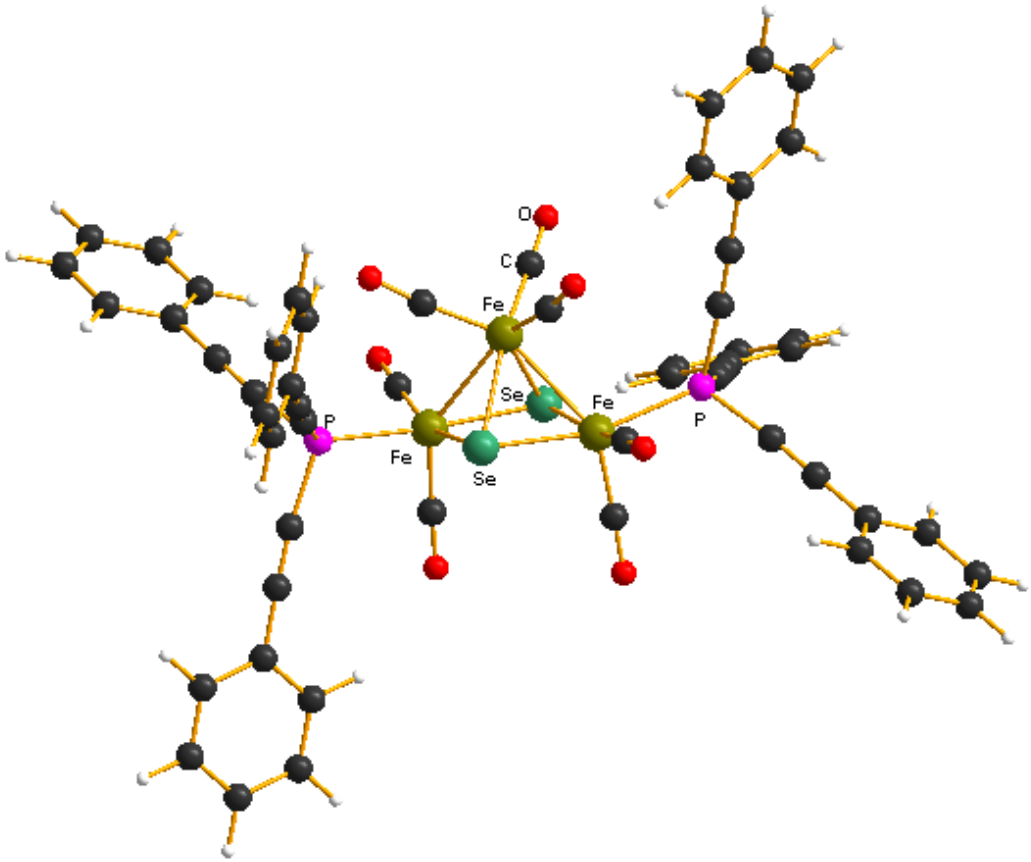


Figure S7. Calculated structure of *equatorial-equatorial-anti* orientation of **3**

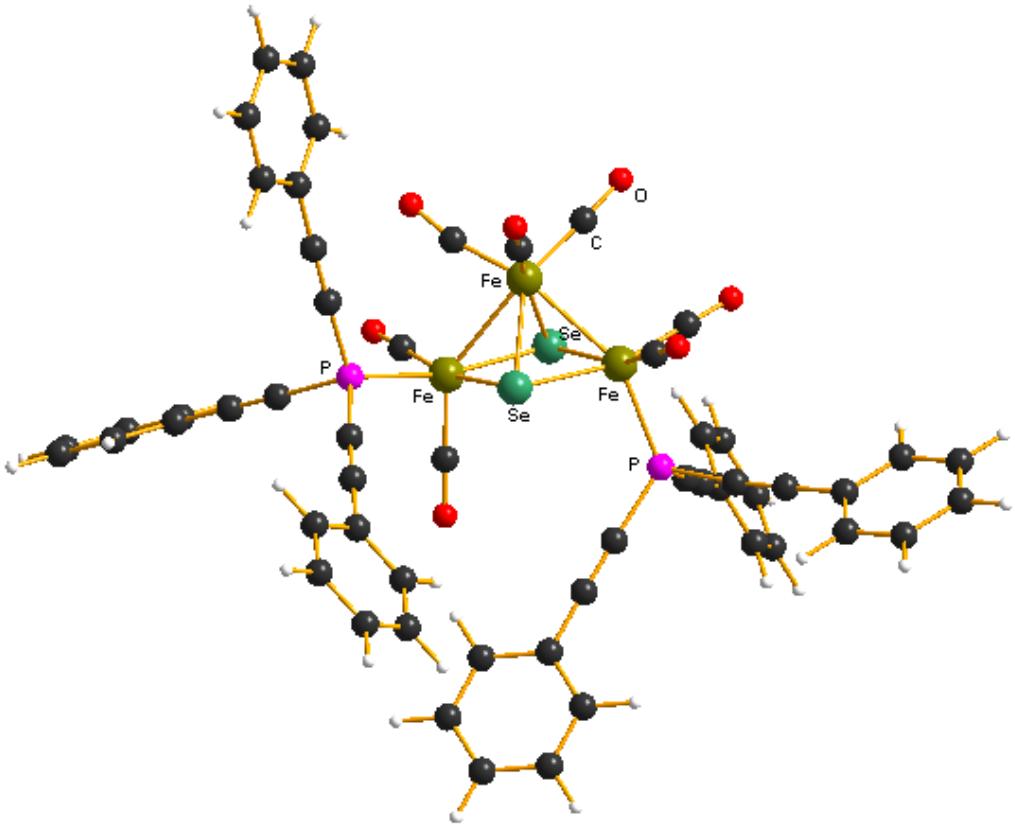


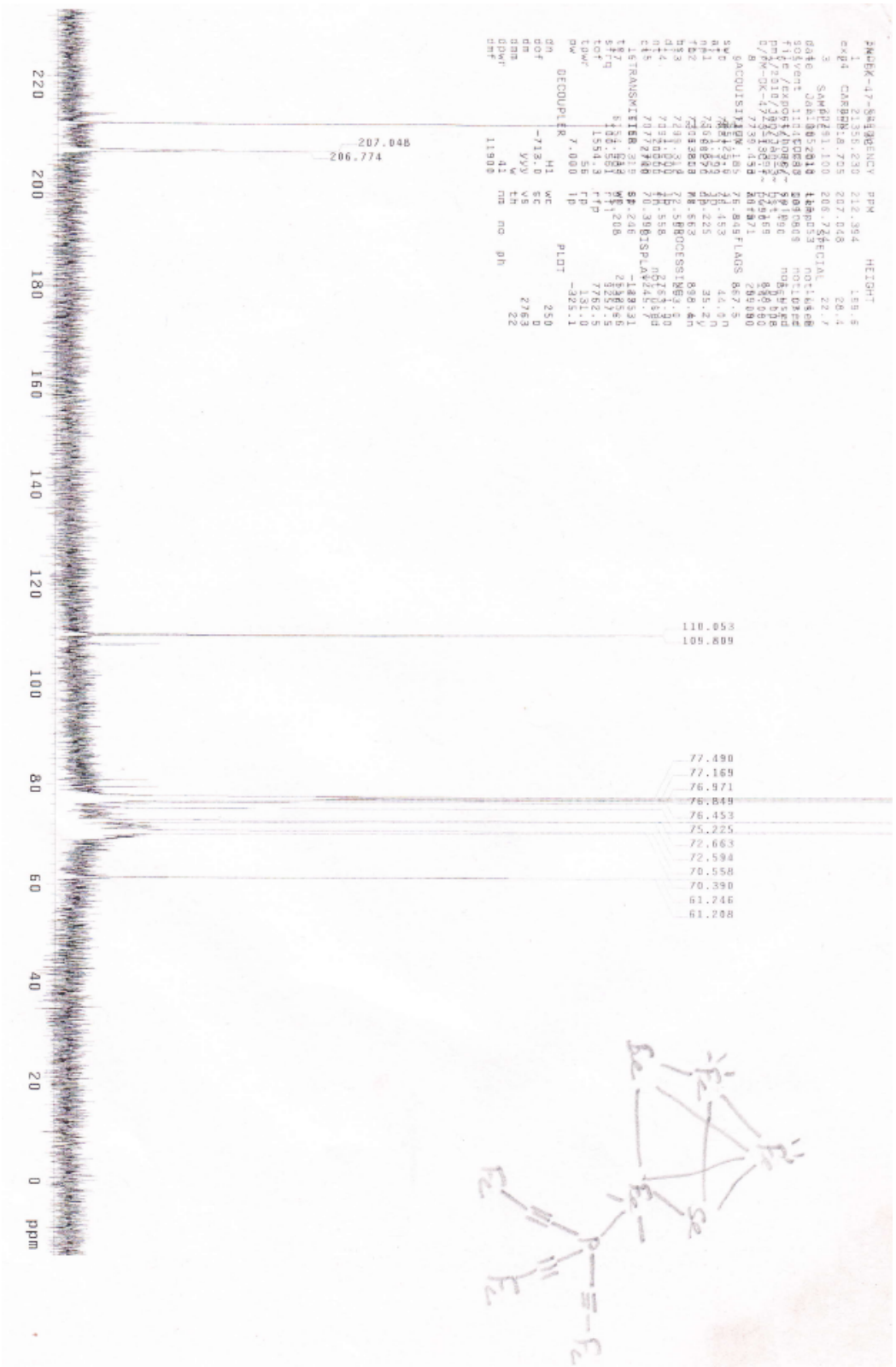
Figure S8. Calculated structure of *equatorial-axial* orientation of **3**

Table S1. Comparison of calculated and experimental bonds lengths (Å) and bond angles (°) of **1** and **3**

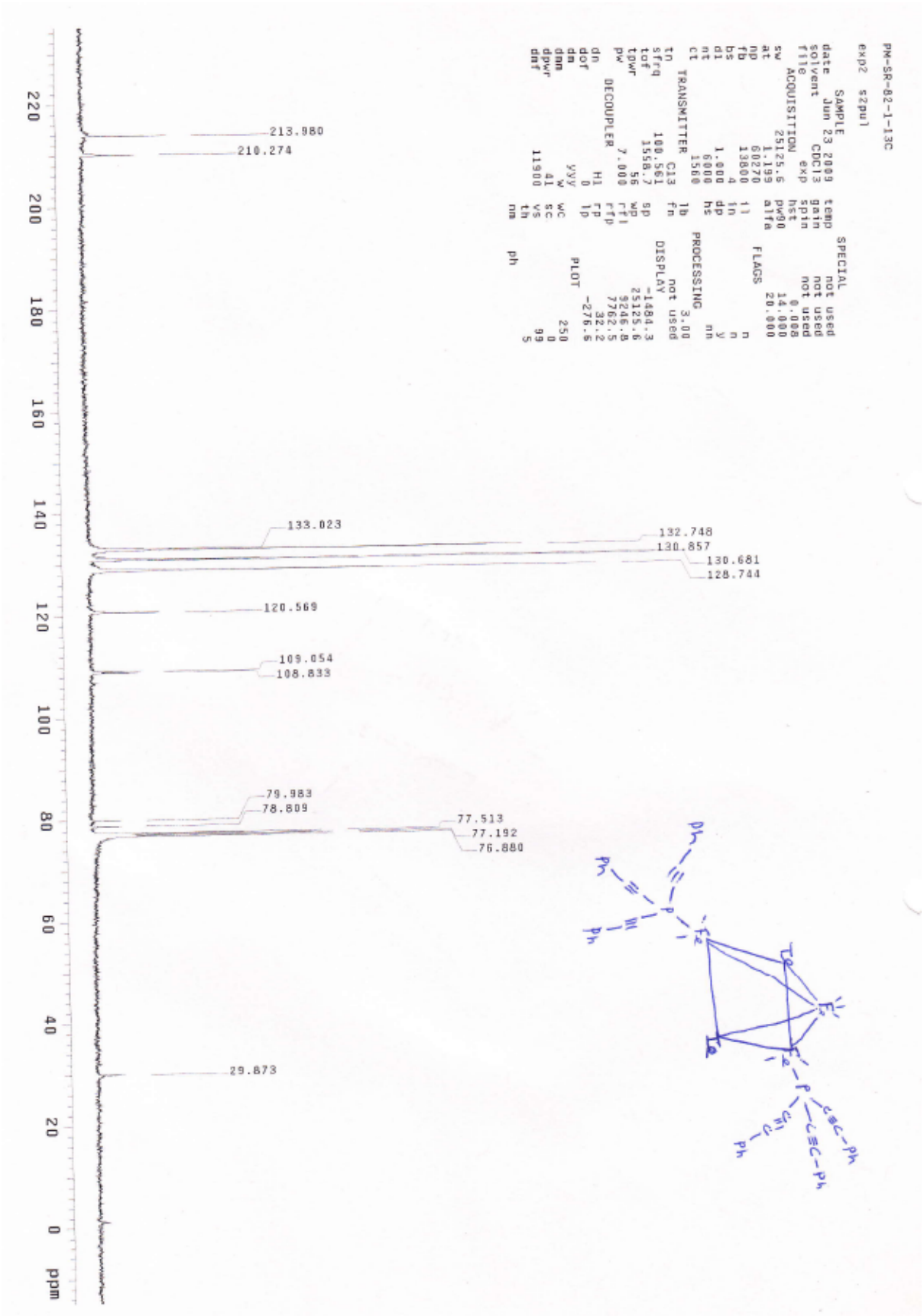
$[Fe_3Se_2(CO)_8P(C_2Ph)_3]$ (**1**)	Experimental	Calculated
P(1)-C(25)	1.756	1.7920
C(25)-C(26)	1.2034	1.2270
Fe(1)-C(2)	1.7892	1.8010
Fe(1)-C(1)	1.7415	1.7581
Fe(3)-C(6)	1.8055	1.7992
Fe(3)-C(8)	1.7699	1.7726
Fe(1)-Se(1)	2.3505	2.4166
Fe(1)-Se(2)	2.3530	2.4182
Fe(3)-Se(1)	2.3478	2.4351
Fe(3)-Se(2)	2.3556	2.4327
Fe(2)-Se(1)	2.3627	2.4635
Fe(2)-Se(2)	2.3811	2.4723
Fe(1)-P(1)	2.2023	2.3764
Fe(1)-Se(1)-Fe(3)	97.727	95.786
Se(1)-Fe(3)-Se(2)	81.942	83.687
Fe(3)-Se(2)-Fe(1)	97.439	95.807
Se(2)-Fe(1)-Se(1)	91.939	84.391
C(17)-P(1)-C(25)	103.839	104.888
$[Fe_3Se_2(CO)_7\{P(C_2Ph)_3\}_2]$ (**3**)		
P(1)-C(8)	1.7592	1.7973
P(2)-C(32)	1.7511	1.7930
C(8)-C(9)	1.1831	1.2263
C(32)-C(33)	1.1897	1.2264
Fe(1)-C(2)	1.7975	1.7923
Fe(3)-C(6)	1.8006	1.7924
Fe(1)-C(1)	1.7898	1.7582
Fe(3)-C(7)	1.7823	1.7574
Fe(2)-Fe(1)	2.6500	2.6683
Fe(2)-Fe(3)	2.6365	2.6562
Fe(2)-Se(1)	2.3664	2.4632
Fe(2)-Se(2)	2.3967	2.4733
Fe(1)-Se(1)	2.3530	2.4223
Fe(3)-Se(1)	2.3508	2.4256
Fe(3)-Se(2)	2.3515	2.4167
Fe(1)-P(1)	2.1876	2.3545
Fe(3)-P(2)	2.2072	2.3535
C(16)-P(1)-C(24)	102.813	103.758
C(40)-P(2)-C(48)	103.030	103.912
Fe(1)-Se(1)-Fe(3)	97.606	96.009
Se(1)-Fe(3)-Se(2)	81.716	83.547
Fe(3)-Se(2)-Fe(1)	97.913	96.447
Se(2)-Fe(1)-Se(1)	81.882	83.665

^{13}C, ^{31}P and ^{77}Se NMR spectra of some of the compounds

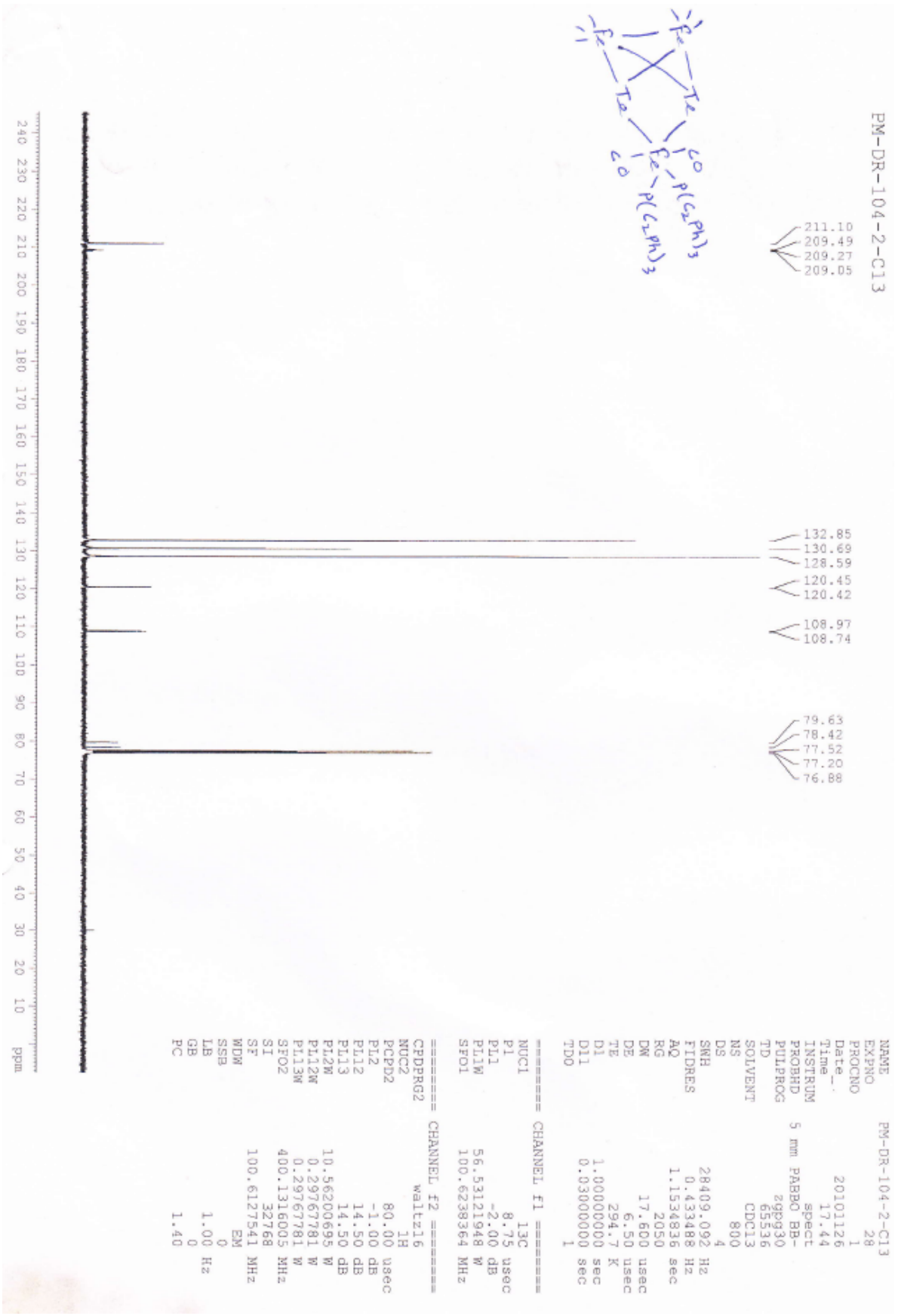
^{13}C NMR of compound **2**



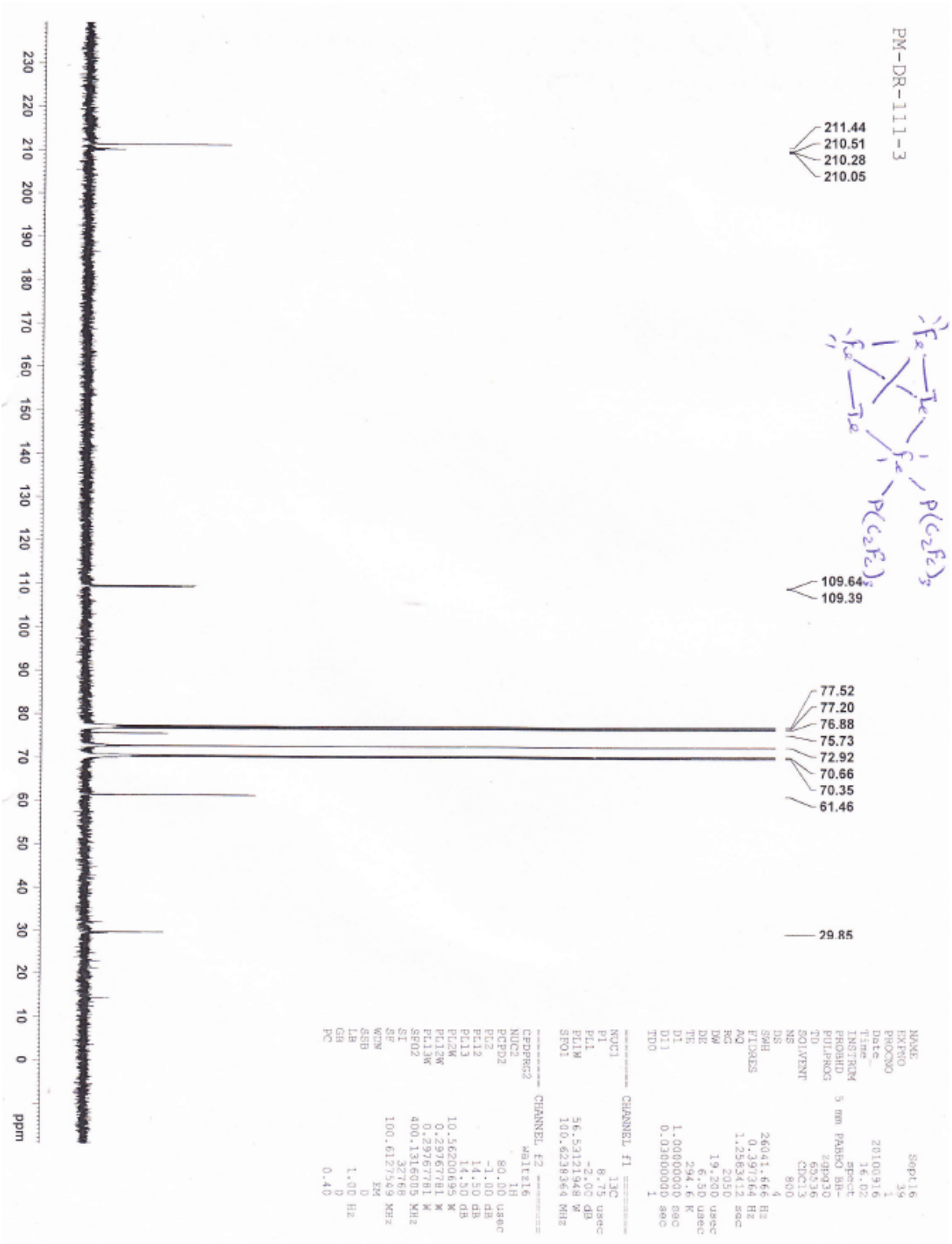
^{13}C NMR of compound **5**



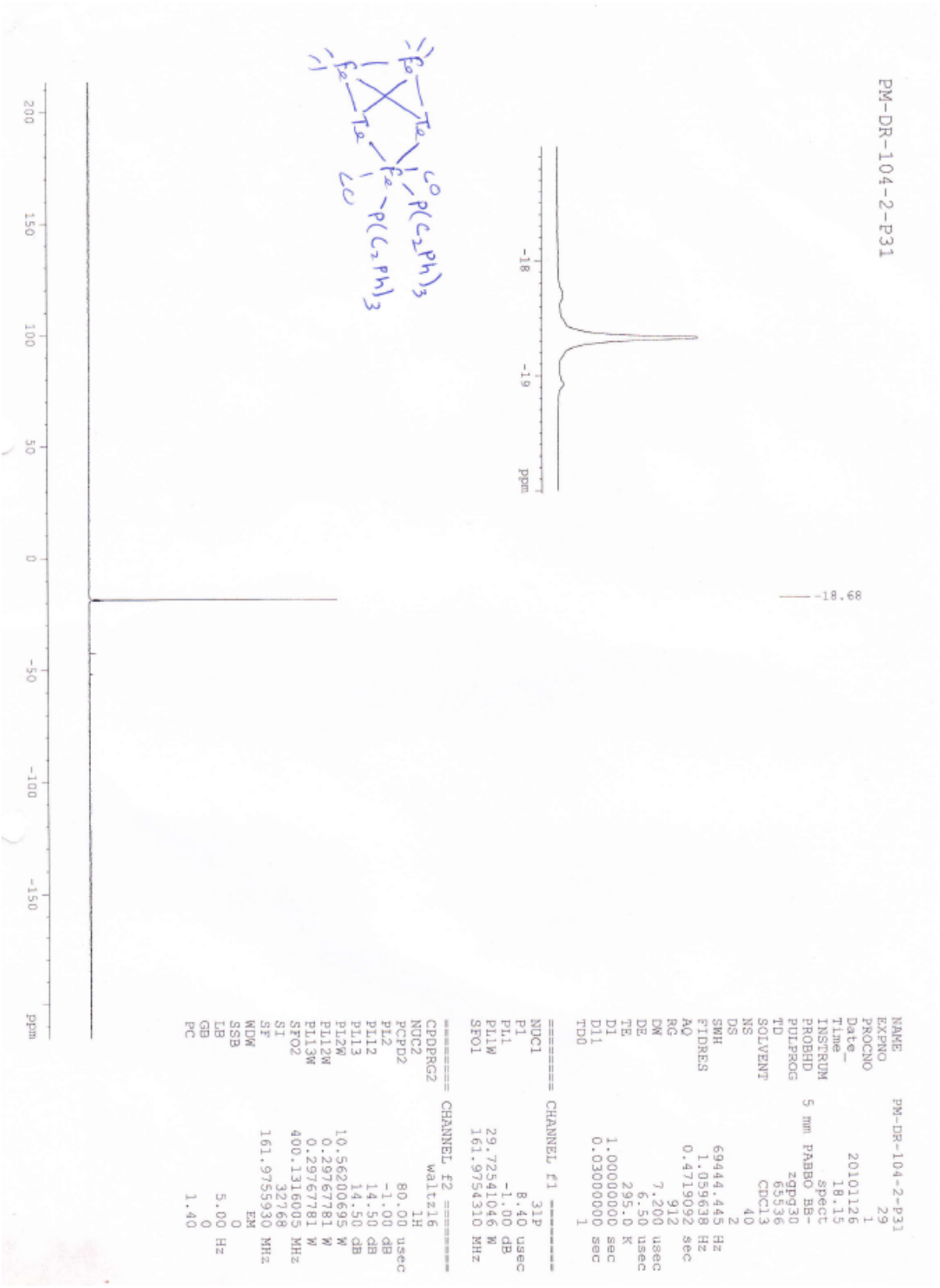
^{13}C NMR of compound **7**



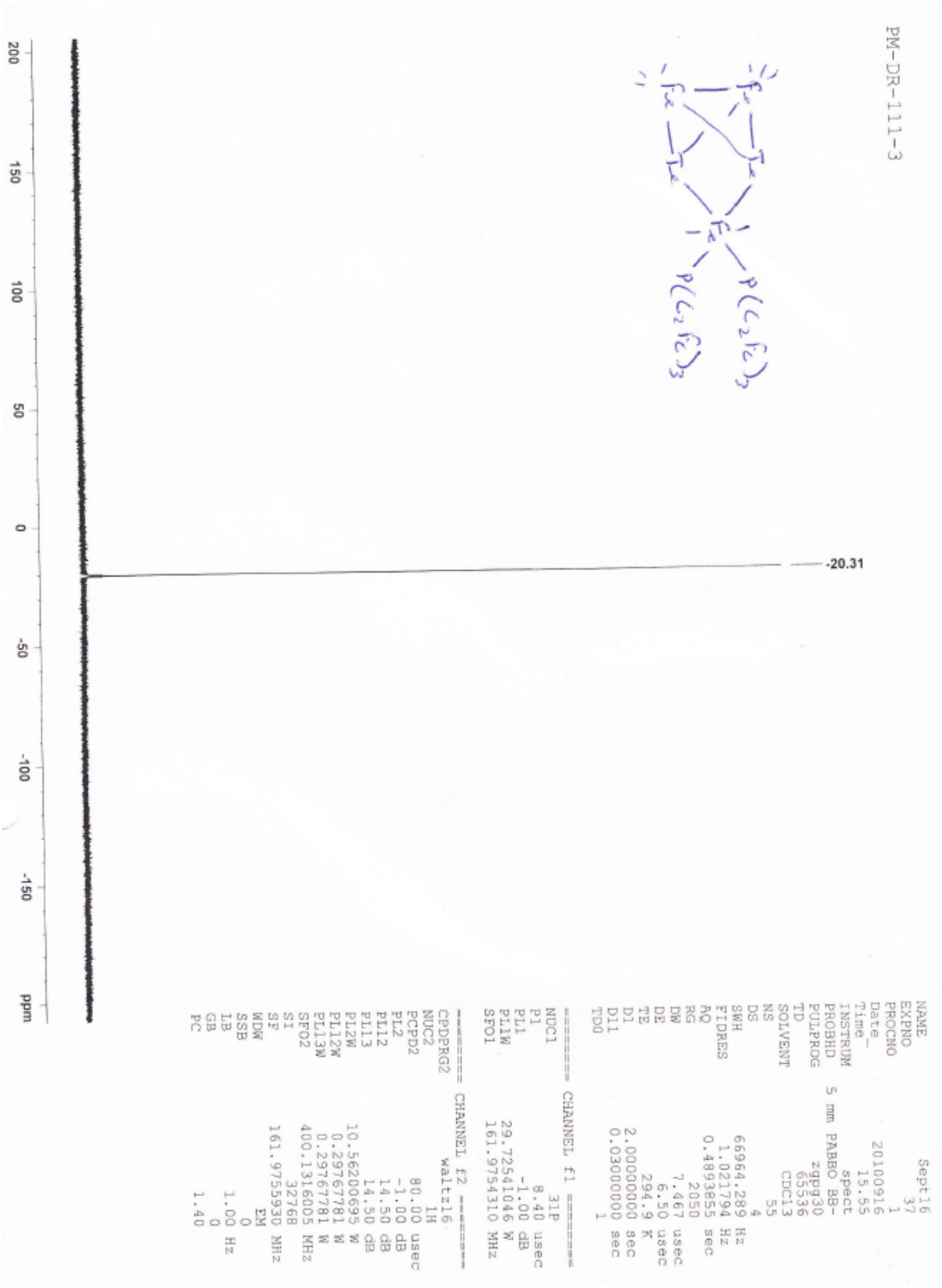
^{13}C NMR of compound **8**



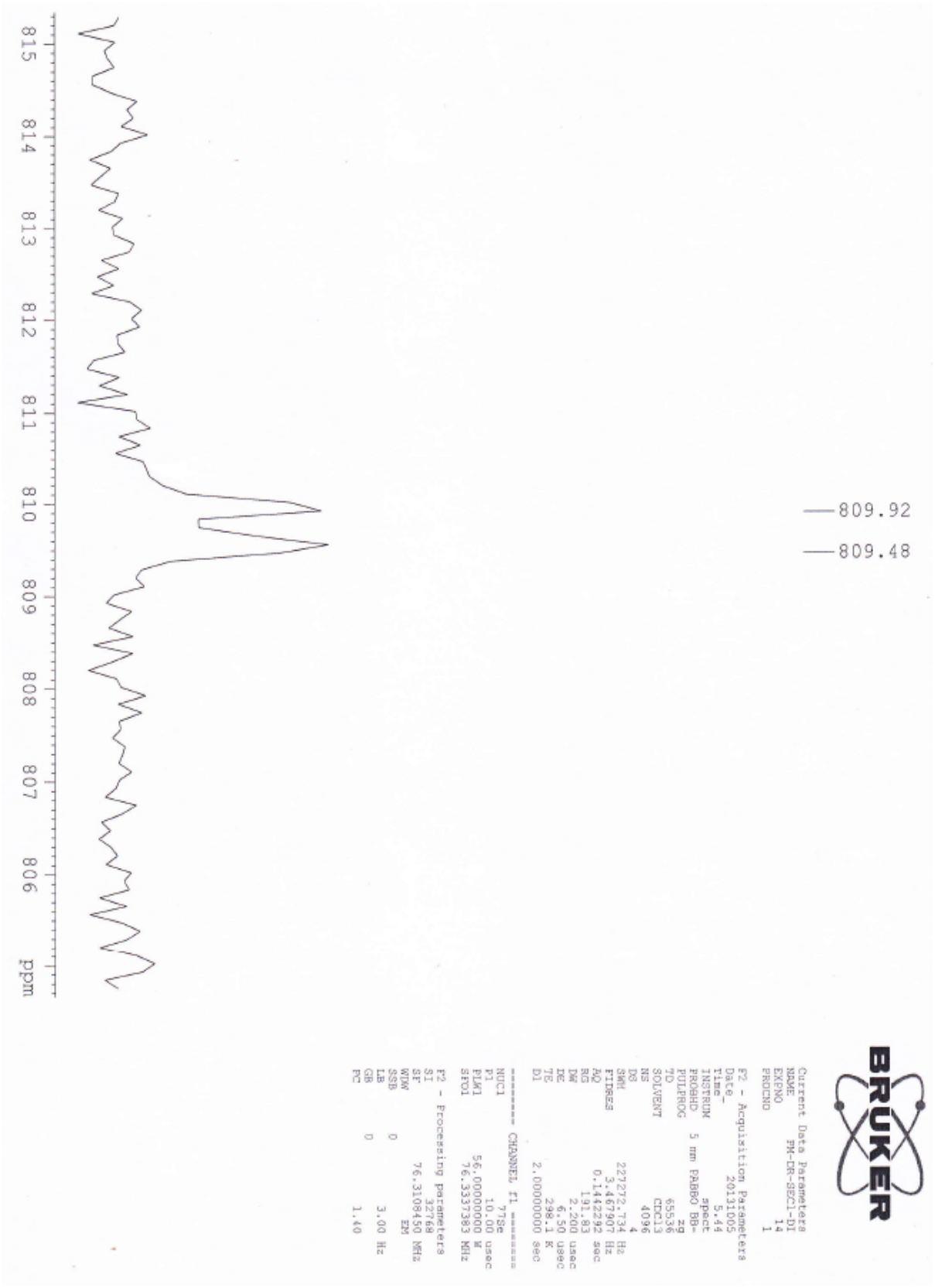
^{31}P NMR of compound **7**



^{31}P NMR of compound **8**



^{77}Se NMR of compound **1**



^{77}Se NMR of compound **2**