Supplementary Material for New Journal of Chemistry

Electronic Supplementary Information

Synthesis of triester-functionalized molecular motors incorporating bis-acetylide *trans*-platinum insulating fragments

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Parameters used in the calculations for the atoms C, H, Fe and Pt (Hückel constant of 1.75)

Atom	H_{ii}(s) (eV)	H_{ii}(p) (eV)	H_{ii}(d) (eV)	ζ_{i1}(s)	ζ_{i1}(p)	ζ_{i1}(d)	C_1	ζ_{i2}(d)	C_2
H	-13.600	-	-	1.300	-	-	-	-	-
C	-21.400	-11.400	-	1.625	1.625	-	-	-	-
Fe	-9.910	-5.070	-11.000	1.575	0.975	5.350	0.5380	1.800	0.6678
Pt	-9.077	-5.475	-12.590	2.554	2.554	6.013	0.6334	2.996	0.5513

Energy of the orbitals and V_{ab} of 1, 1b and 2b as a function of the energy of the iron 3d orbitals

As shown in the table below, V_{ab} varies strongly with the energy of the iron 3d orbitals (from 10.5 to 11.5eV instead of the usual value of 11eV) but the results remain consistent, the value for the platinum-containing complex being always significantly lower than for the fully-conjugated complex.

Composé	E_{3d}(Fe)	E(u)	E(g)	ΔE (eV)	V_{ab} (eV)
1	-10,500	-10.904	-10.742	0.162	0.081
1	-11,000	-11.277	-11.098	0.179	0.090
1	-11,500	-11.656	-11.390	0.266	0.133
1b	-10,500	-10,767	-10,903	0,136	0,068
1b	-11,000	-11,117	-11,272	0,155	0,077
1b	-11,500	-11,390	-11,649	0,259	0,129
2b	-10,500	-10,849	-10,813	0,036	0,018
2b	-11,000	-11,231	-11,186	0,045	0,022
2b	-11,500	-11,612	-11,522	0,090	0,045

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Molecular modeling coordinates

Coordinates of **1**

```
C -3.7075  2.8599  8.0235
C -4.5375  3.8033  7.3767
C -3.7615  4.5008  6.4117
C -3.0167  5.1294 10.2621
C -2.9336  6.7340  8.6632
C -3.7863  6.0814  9.5662
C -1.6460  6.1982  8.7986
Fe -2.9671  4.7390  8.2693
C -1.6989  5.2136  9.7921
H  3.2013  2.1088  0.7386
H  4.7620  3.3077 -0.9269
C -2.4080  2.9517  7.4672
H  3.3513  5.0643 -2.1996
C -2.4404  3.9631  6.4520
C -1.3708  4.3448  5.5954
C -0.4954  4.6233  4.8260
Fe  2.9671  4.8290  0.4977
C  2.4404  5.6049  2.3150
C  2.4080  6.6163  1.2998
C  3.7075  6.7081  0.7435
C  4.5375  5.7647  1.3903
C  3.7615  5.0672  2.3553
C  1.6460  3.3698 -0.0316
C  1.6989  4.3544 -1.0251
C  3.0167  4.4386 -1.4951
C  3.7863  3.4866 -0.7992
C  2.9336  2.8340  0.1038
C  1.3708  5.2232  3.1716
C  0.4954  4.9447  3.9410
H  1.6125  7.1588  1.0330
H  3.9903  7.3339  0.0171
H  5.5078  5.6145  1.2015
H  4.0831  4.3333  2.9538
H  0.8365  3.0972  0.4875
H  0.9271  4.9046 -1.3445
H -1.6125  2.4092  7.7340
H -0.9271  4.6634 10.1115
H -0.8365  6.4708  8.2795
H -4.7620  6.2603  9.6939
H -3.2013  7.4592  8.0284
H -3.3513  4.5037 10.9666
H -4.0831  5.2347  5.8132
H -5.5078  3.9535  7.5655
H -3.9903  2.2341  8.7499
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Coordinates of **1b**

C	2.8729	-1.1712	8.1511
C	3.8277	-0.7195	9.1227
C	0.5415	-1.1641	10.3963
C	1.4991	-0.7197	11.3758
C	-5.5095	0.7195	-0.9053
C	-5.5095	-0.7195	-0.9053
C	-4.5552	-1.1712	0.0667
C	-2.2250	-1.1641	-2.1815
C	-3.1851	0.7198	-3.1588
C	-3.1851	-0.7198	-3.1588
C	-2.2250	1.1641	-2.1815
Fe	-3.6530	-0.0000	-1.3151
C	-1.6312	0.0000	-1.5817
H	4.4398	-1.3594	9.7593
H	-0.7893	-0.0000	8.9924
C	-4.5552	1.1712	0.0667
H	2.6348	2.2042	7.8982
C	-0.4200	0.0000	4.5689
C	-3.9640	-0.0000	0.7026
C	-3.0184	-0.0000	1.7483
C	-1.2632	-0.0000	3.6497
C	-2.1713	-0.0000	2.6555
Fe	1.9713	0.0000	9.5329
C	2.2815	0.0000	7.5154
C	2.8729	1.1712	8.1511
C	3.8277	0.7195	9.1227
C	-0.0510	-0.0000	9.7951
C	0.5415	1.1641	10.3963
C	1.4991	0.7197	11.3758
C	1.3355	0.0000	6.4701
C	0.4881	0.0000	5.5631
H	2.6348	-2.2042	7.8982
H	4.4398	1.3594	9.7593
H	2.1185	1.3610	12.0042
H	0.3098	2.2006	10.1490
H	-4.3172	2.2042	0.3198
H	-0.8907	0.0000	-0.7810
H	-1.9929	2.2007	-1.9349
H	-3.8060	-1.3611	-3.7854
H	-3.8060	1.3611	-3.7854
H	-1.9929	-2.2007	-1.9349
H	-4.3172	-2.2042	0.3198
H	-6.1211	-1.3594	-1.5425
H	-6.1211	1.3594	-1.5425
H	2.1185	-1.3610	12.0042
H	0.3098	-2.2006	10.1490

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Coordinates of **2**

Pt	0.0409	0.0106	-0.0615
P	-0.0916	-2.3129	0.0399
C	-1.4138	-2.9969	-1.0503
H	-1.1656	-2.7752	-2.1000
H	-1.5220	-4.0867	-0.9187
H	-2.3549	-2.4842	-0.7973
C	-0.5451	-2.9110	1.7254
H	-1.4743	-2.4020	2.0250
H	-0.6856	-4.0050	1.7418
H	0.2500	-2.6301	2.4337
C	1.4142	-3.2786	-0.4039
H	2.2478	-2.9519	0.2355
H	1.2389	-4.3607	-0.2820
H	1.6883	-3.0551	-1.4460
P	-0.0011	2.3385	-0.1049
C	1.5456	3.2116	-0.5973
H	1.4184	4.3056	-0.5397
H	2.3634	2.8853	0.0625
H	1.8102	2.9162	-1.6238
C	-1.2888	3.0062	-1.2455
H	-1.0446	2.7118	-2.2782
H	-2.2510	2.5477	-0.9689
H	-1.3541	4.1054	-1.1804
C	-0.4395	3.0640	1.5343
H	-1.3892	2.6129	1.8608
H	0.3409	2.8031	2.2662
H	-0.5384	4.1610	1.4745
C	-1.9041	0.0611	0.4566
C	-3.1004	0.0855	0.7926
C	-4.4659	0.1084	1.1872
Fe	-6.1765	0.0004	0.0610
C	-5.2830	-1.0379	1.5568
C	-6.5782	-0.5694	1.9676
C	-6.5913	0.8663	1.8496
C	-5.3039	1.2850	1.3661
H	-4.9885	2.3100	1.1685
H	-7.4325	1.5209	2.0825
H	-7.4074	-1.1928	2.3055
H	-4.9491	-2.0757	1.5279
C	-7.6661	0.5708	-1.2034
C	-6.3862	1.0356	-1.6755
C	-5.5373	-0.1117	-1.8661
C	-6.2902	-1.2857	-1.5076
C	-7.6069	-0.8644	-1.0995
H	-8.4150	-1.5175	-0.7674
H	-5.9271	-2.3139	-1.5354
H	-4.4918	-0.0907	-2.1772
H	-6.1076	2.0750	-1.8538
H	-8.5272	1.1961	-0.9636
C	1.9808	-0.0437	-0.5540
C	3.1856	-0.0794	-0.8512
C	4.5637	-0.1238	-1.1939
Fe	6.2210	-0.0235	0.0109
C	5.4870	0.1129	1.9016
C	6.3379	-1.0409	1.7661

C	7.6428	-0.5881	1.3541
C	7.5971	0.8462	1.2317
C	6.2638	1.2789	1.5687
H	5.9057	2.3091	1.5667
H	8.4249	1.4913	0.9342
H	8.5109	-1.2208	1.1640
H	6.0442	-2.0768	1.9402
H	4.4263	0.1008	2.1573
C	5.4140	1.0060	-1.5399
C	6.7208	0.5145	-1.8818
C	6.7082	-0.9197	-1.7440
C	5.3934	-1.3136	-1.3175
H	5.0547	-2.3311	-1.1205
H	7.5502	-1.5886	-1.9280
H	7.5738	1.1219	-2.1883
H	5.0944	2.0485	-1.5401

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Orbitals and energy levels of complex 1 (top), 1b (middle) and 2b (bottom) involved in the electronic coupling (with an orbital contour value of 0.05).