

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 _{il} (s)	ζ _{il} (p)	ζ _{il} (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

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

Coordinates of **1b**

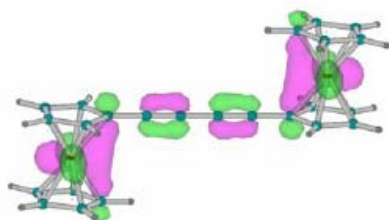
C	2.8729	-1.1712	8.1511
C	3.8277	-0.7195	9.1227
C	0.5415	-1.1641	10.3963
C	1.4991	-0.7197	11.3758
C	-5.5095	0.7195	-0.9053
C	-5.5095	-0.7195	-0.9053
C	-4.5552	-1.1712	0.0667
C	-2.2250	-1.1641	-2.1815
C	-3.1851	0.7198	-3.1588
C	-3.1851	-0.7198	-3.1588
C	-2.2250	1.1641	-2.1815
Fe	-3.6530	-0.0000	-1.3151
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

Coordinates of 2

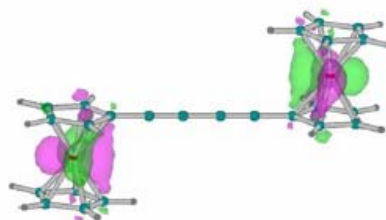
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Pt  0.0409  0.0106 -0.0615
P  -0.0916 -2.3129  0.0399
C  -1.4138 -2.9969 -1.0503
H  -1.1656 -2.7752 -2.1000
H  -1.5220 -4.0867 -0.9187
H  -2.3549 -2.4842 -0.7973
C  -0.5451 -2.9110  1.7254
H  -1.4743 -2.4020  2.0250
H  -0.6856 -4.0050  1.7418
H   0.2500 -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

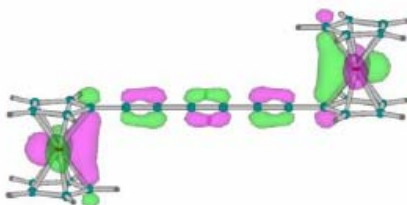
Orbitals and energy levels of complex 1 (top), 1b (middle) and 2b (bottom) involved in the electronic coupling (with an orbital contour value of 0.05).



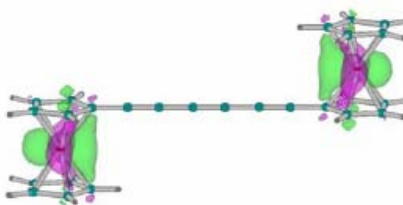
$$E(g) = -11.098 \text{ eV}$$



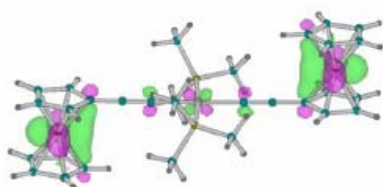
$$E(u) = -11.277 \text{ eV}$$



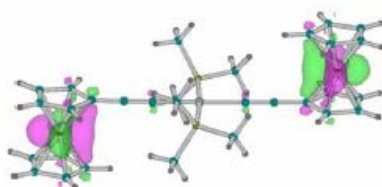
$$E(u) = -11.117 \text{ eV}$$



$$E(g) = -11.272 \text{ eV}$$



$$E(g) = -11.186 \text{ eV}$$



$$E(u) = -11.231 \text{ eV}$$