Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Metallaaromaticity – A Protean World

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cforoutan–nejad@icho.edu.pl

The HOMOs of complexes and contributions of each MO in the magnetically induced current density.

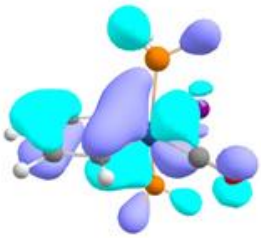
HOMO
0.02

HOMO -1
1.50

HOMO -2
3.70

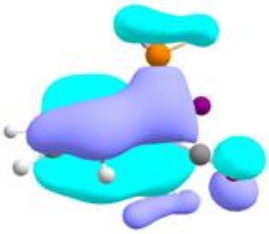
HOMO -3
0.84

HOMO -4
0.52



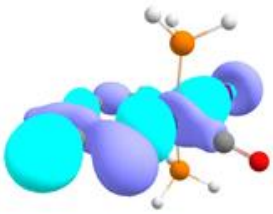
HOMO -5
5.28

HOMO -6
14.80



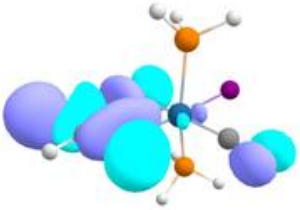
HOMO -7
-1.46

HOMO -8
0.34

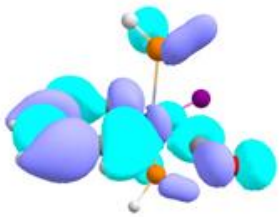


HOMO -9
0.84

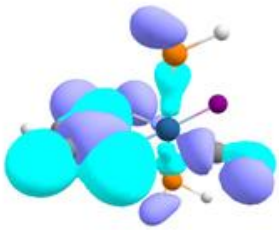
HOMO -10
-4.34



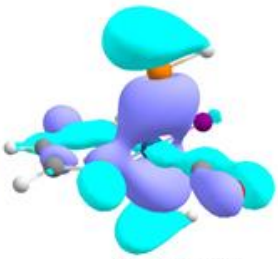
HOMO -11
-1.36



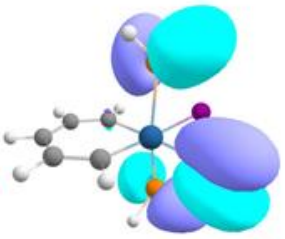
HOMO -12
3.74



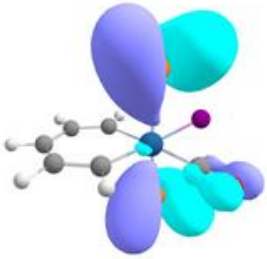
HOMO -13
-3.94



HOMO -14
-0.52



HOMO -15
-0.76



HOMO -16
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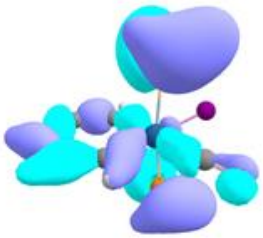
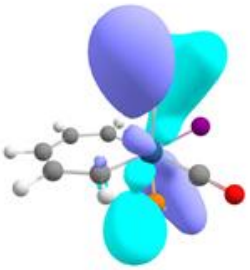
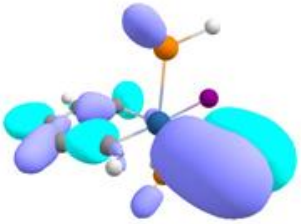


HOMO -17
1.54



HOMO -18
-0.06



HOMO -19
0.66

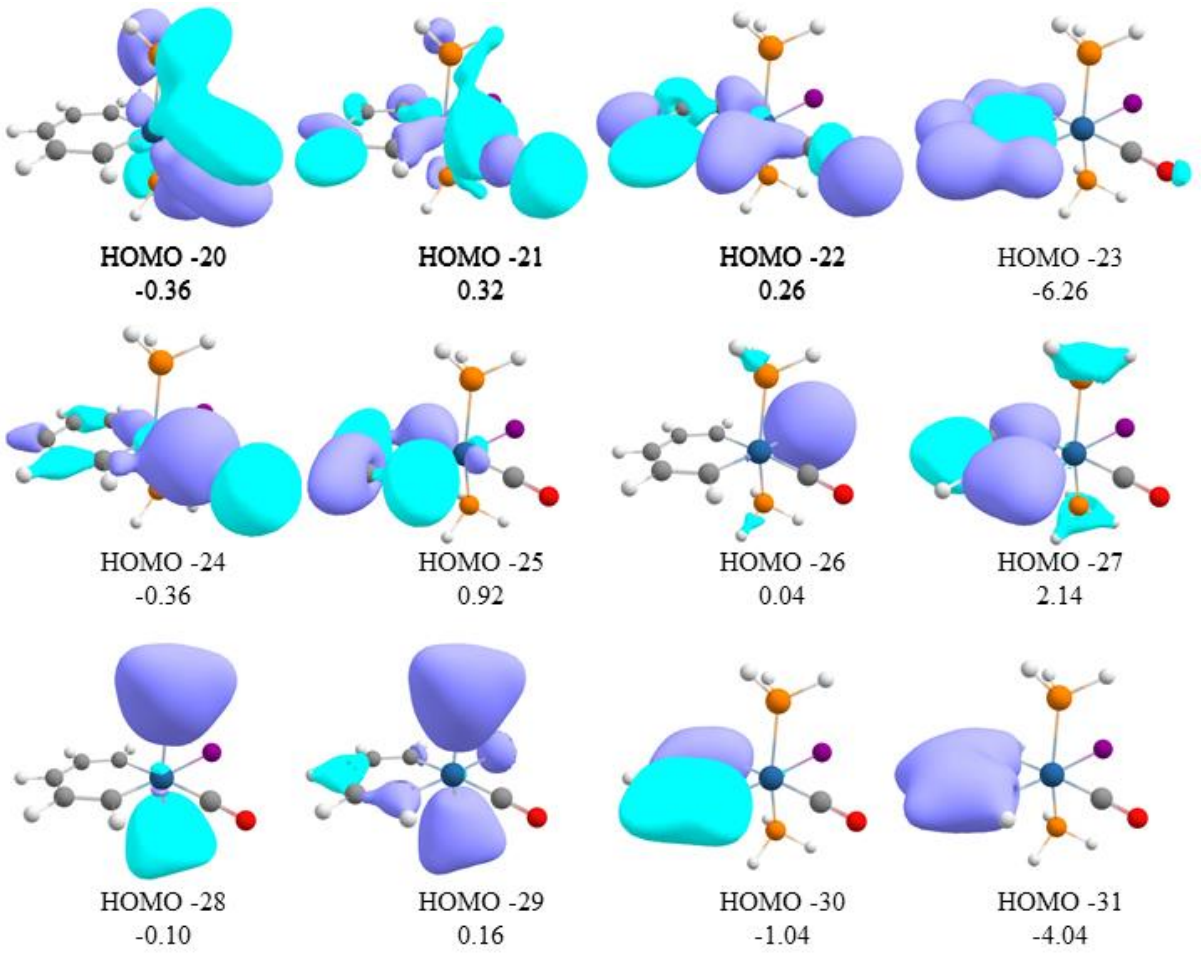
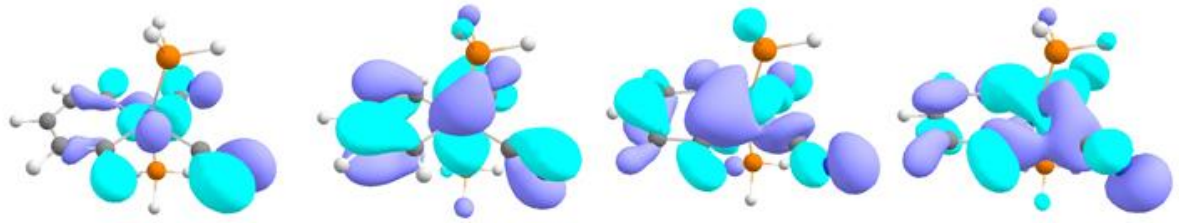


Figure S1. Valence molecular orbitals of molecule **1** and their contribution to the magnetically induced current intensity in $nA.T^{-1}$.

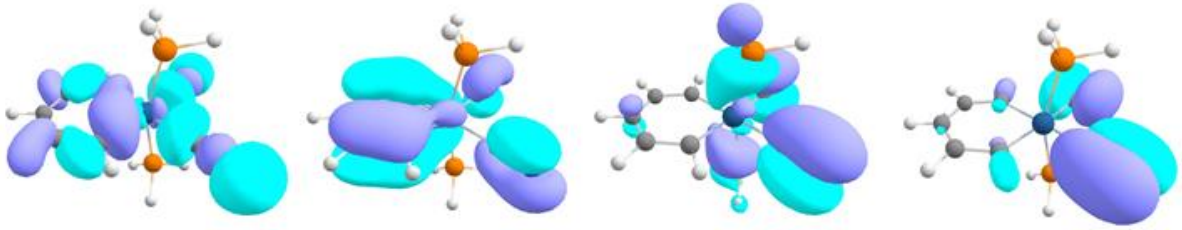


HOMO
-0.10

HOMO -1
0.16

HOMO -2
-1.04

HOMO -3
-4.04

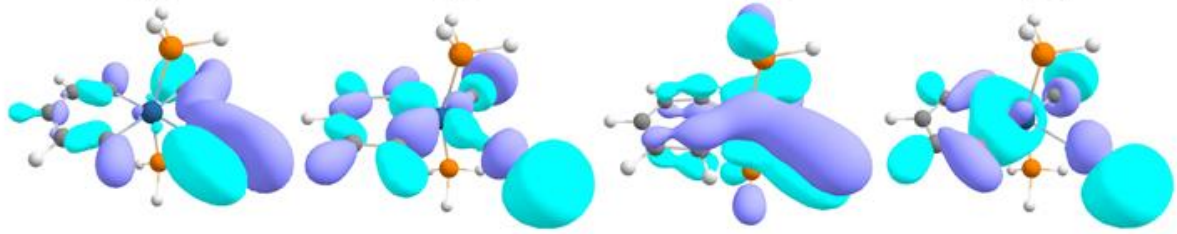


HOMO -4
-0.10

HOMO -5
0.16

HOMO -6
-1.04

HOMO -7
-4.04

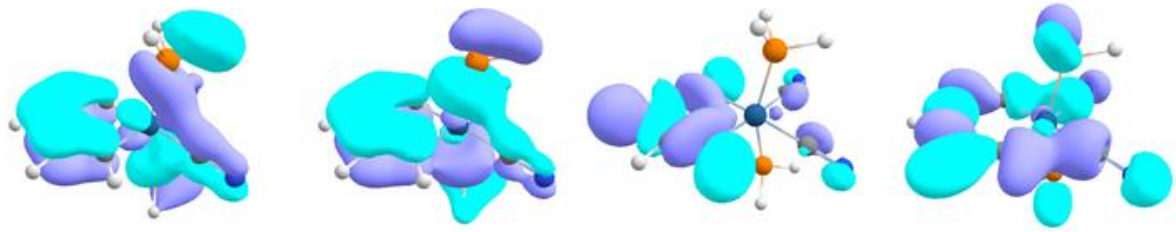


HOMO -8
-0.10

HOMO -9
0.16

HOMO -10
-1.04

HOMO -11
-4.04

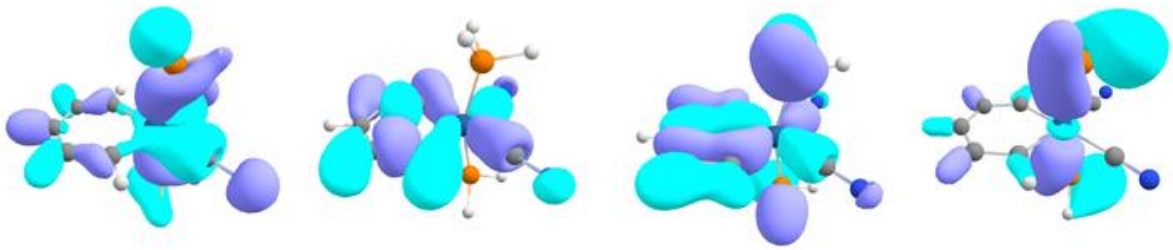


HOMO -12
3.74

HOMO -13
-3.94

HOMO -14
-0.52

HOMO -15
-0.76



HOMO -16
0.22

HOMO -17
1.54

HOMO -18
-0.06

HOMO -19
0.66

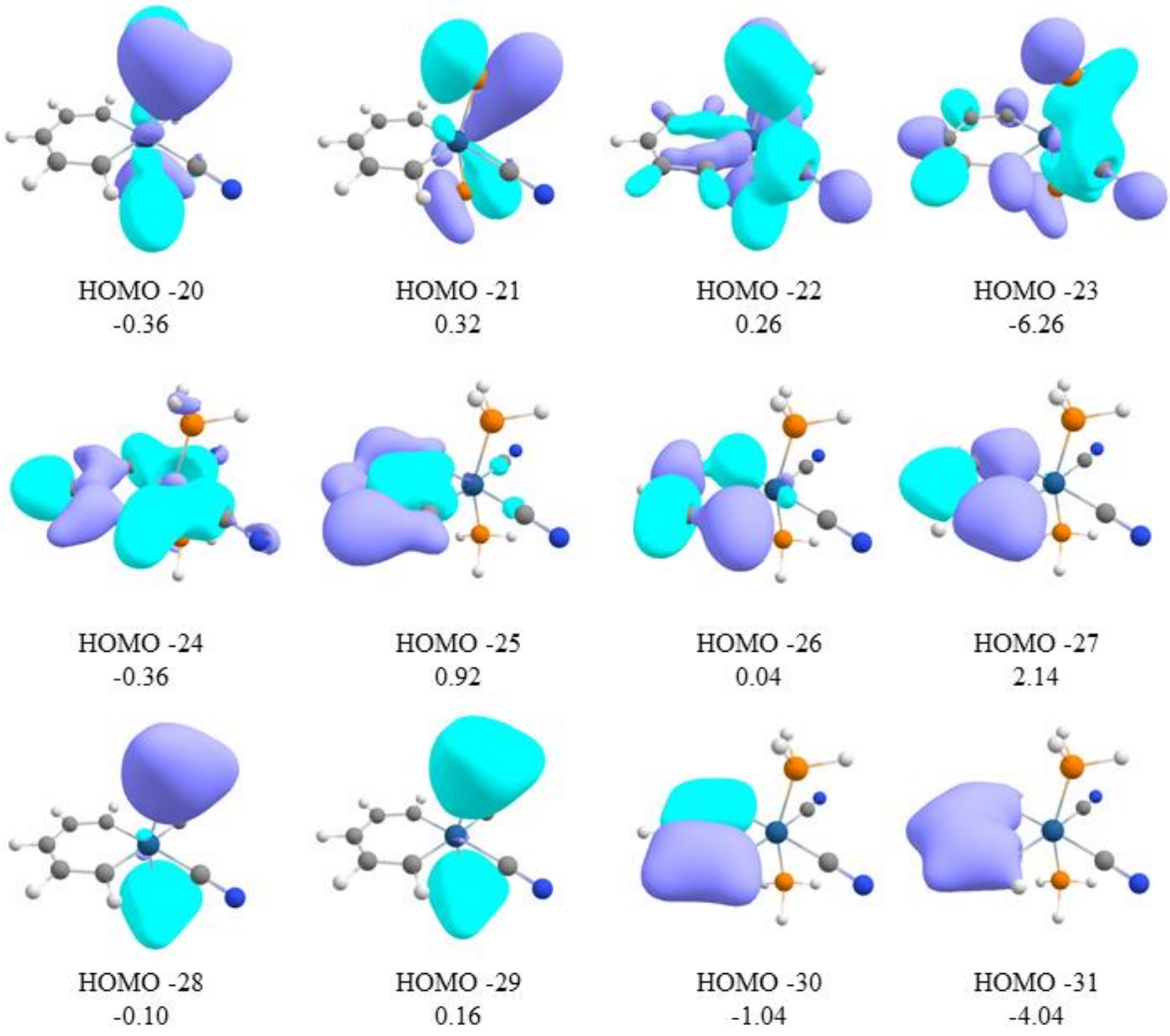
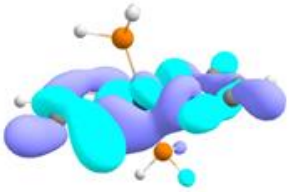


Figure S2. Valence molecular orbitals of molecule **2** and their contribution to the magnetically induced current intensity in $nA.T^{-1}$.

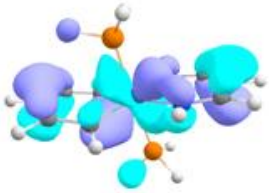
HOMO
-0.10

HOMO -1
0.16

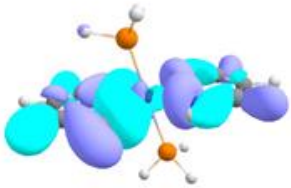
HOMO -2
-1.04



HOMO -3
-4.04

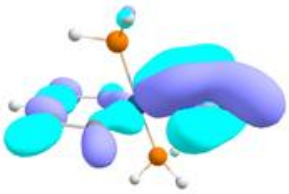


HOMO -4
-0.10



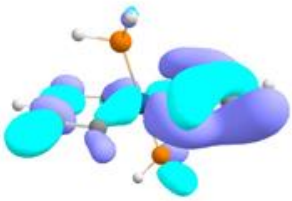
HOMO -5
0.16

HOMO -6
-1.04

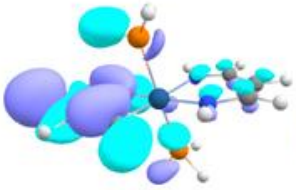


HOMO -7
-4.04

HOMO -8
-0.10



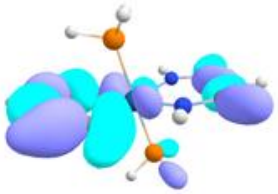
HOMO -9
0.16



HOMO -10
-1.04

HOMO -11
-4.04

HOMO -12
3.74

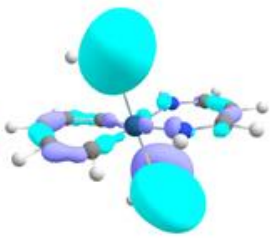


HOMO -13
-3.94

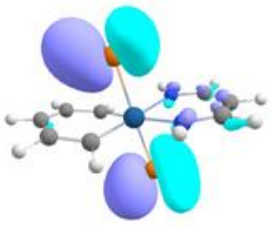
HOMO -14
-0.52

HOMO -15
-0.76

HOMO -16
0.22



HOMO -17
1.54



HOMO -18
-0.06

HOMO -19
0.66

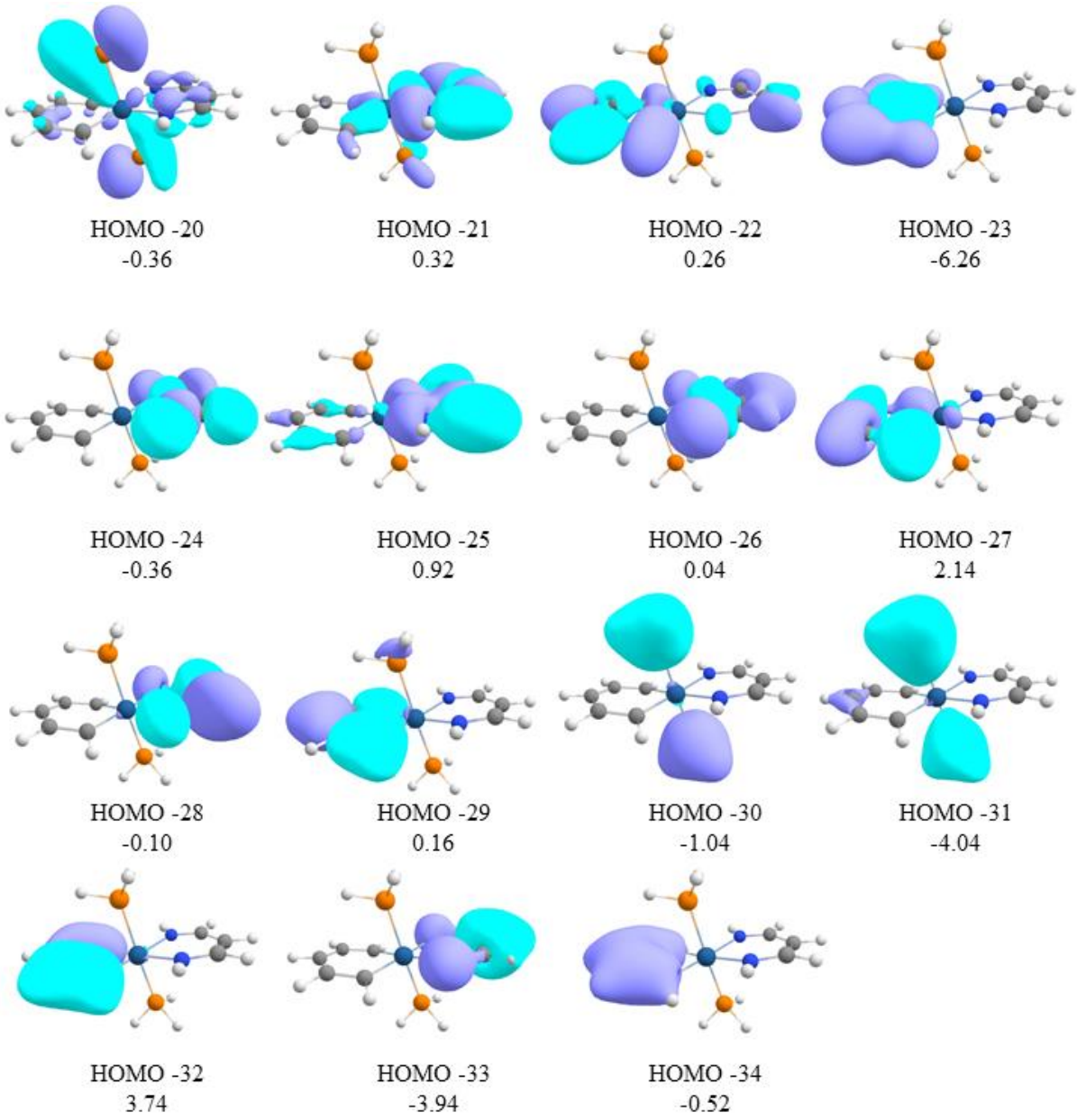
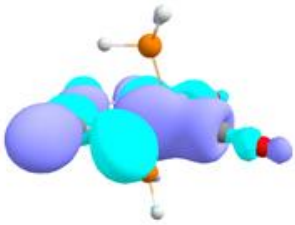


Figure S3. Valence molecular orbitals of molecule **3** and their contribution to the magnetically induced current intensity in $nA.T^{-1}$.

HOMO
-3.00

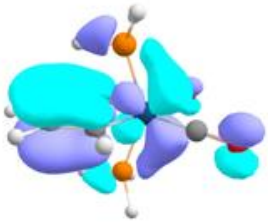
HOMO -1
8.42



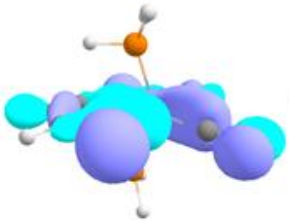
HOMO -2
-2.34

HOMO -3
0.54

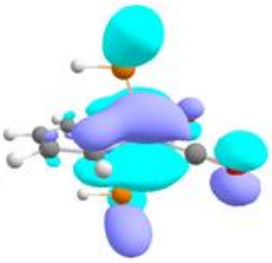
HOMO -4
-3.48



HOMO -5
-2.44



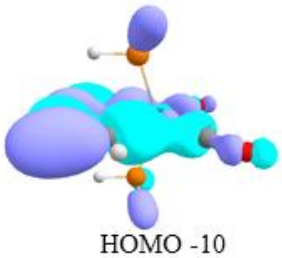
HOMO -6
-0.42



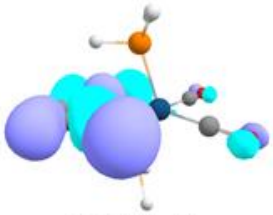
HOMO -7
0.14

HOMO -8
2.10

HOMO -9
2.38

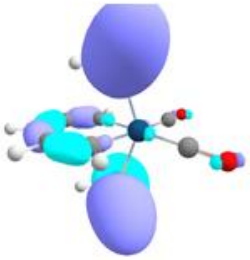


HOMO -10
3.20

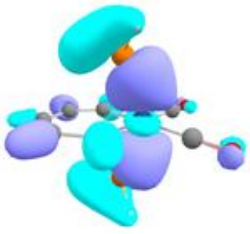


HOMO -11
0.34

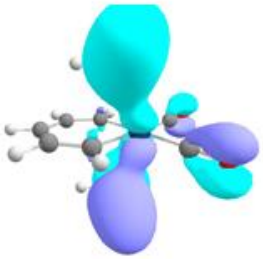
HOMO -12
2.90



HOMO -13
1.08

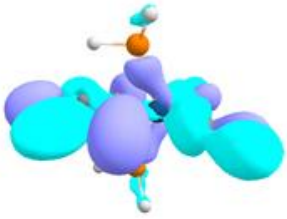


HOMO -14
0.46

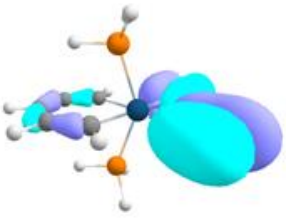


HOMO -15
0.28

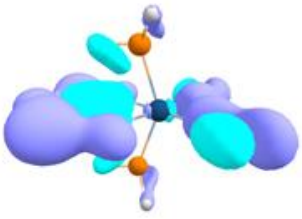
HOMO -16
1.28



HOMO -17
-0.44



HOMO -18
0.30



HOMO -19
-0.22

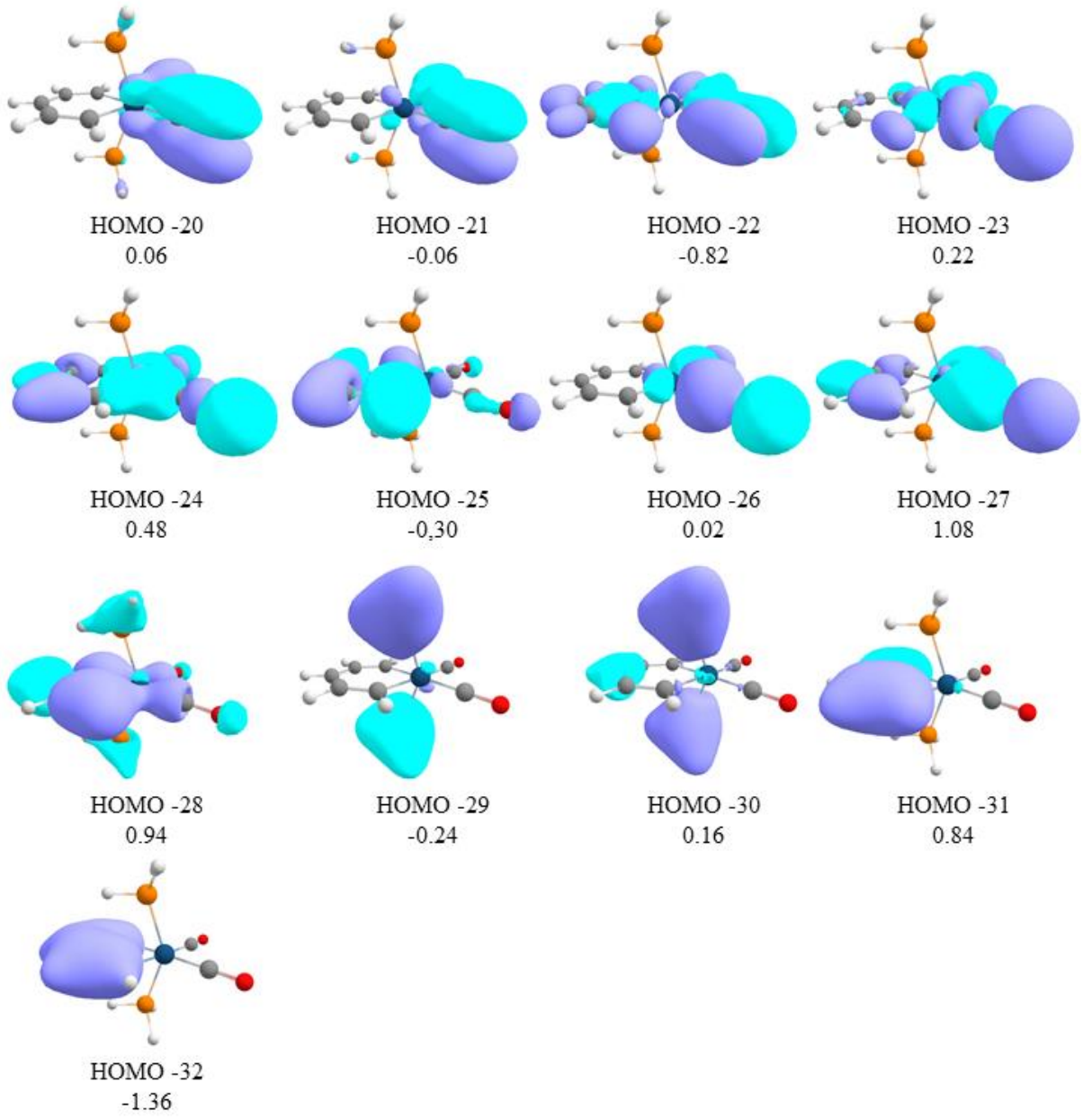
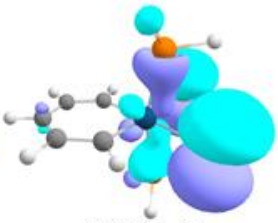


Figure S4. Valence molecular orbitals of molecule **4** and their contribution to the magnetically induced current intensity in $nA.T^{-1}$.

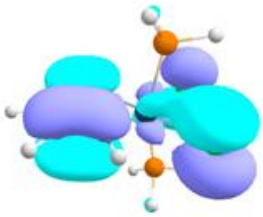
HOMO
-0.54

HOMO -1
-2.0

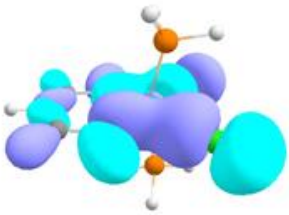
HOMO -2
-0.04



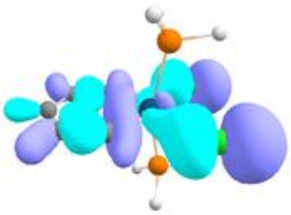
HOMO -3
0.54



HOMO -4
1.98

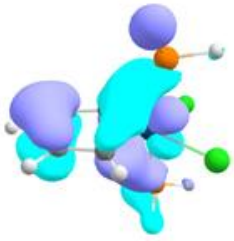


HOMO -5
-1.48

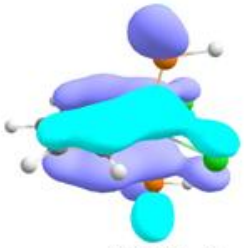


HOMO -6
-2.26

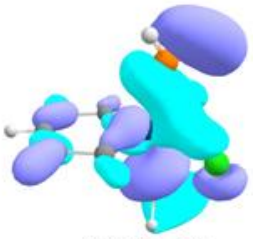
HOMO -7
0.22



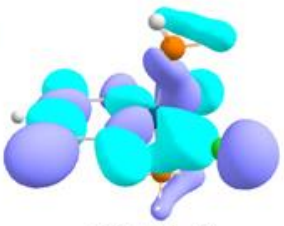
HOMO -8
3.42



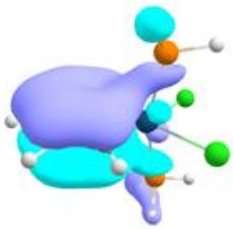
HOMO -9
0.66



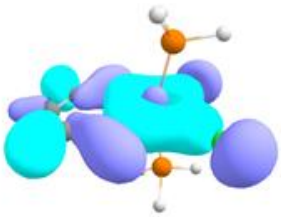
HOMO -10
0.10



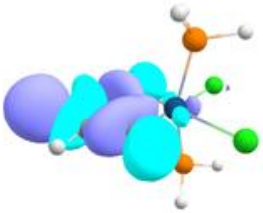
HOMO -11
0.28



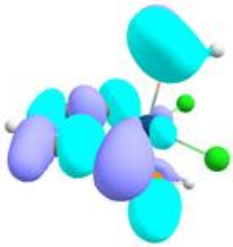
HOMO -12
-0.12



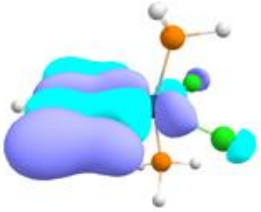
HOMO -13
-0.54



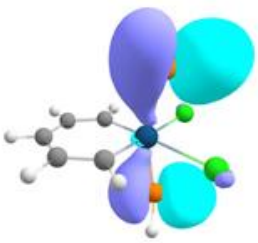
HOMO -14
1.60



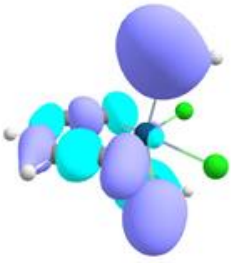
HOMO -15
1.20



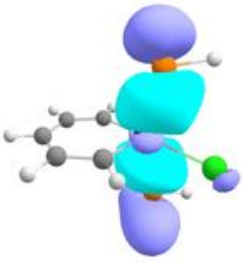
HOMO -16
1.26



HOMO -17
0.04



HOMO -18
0.86



HOMO -19
0.04

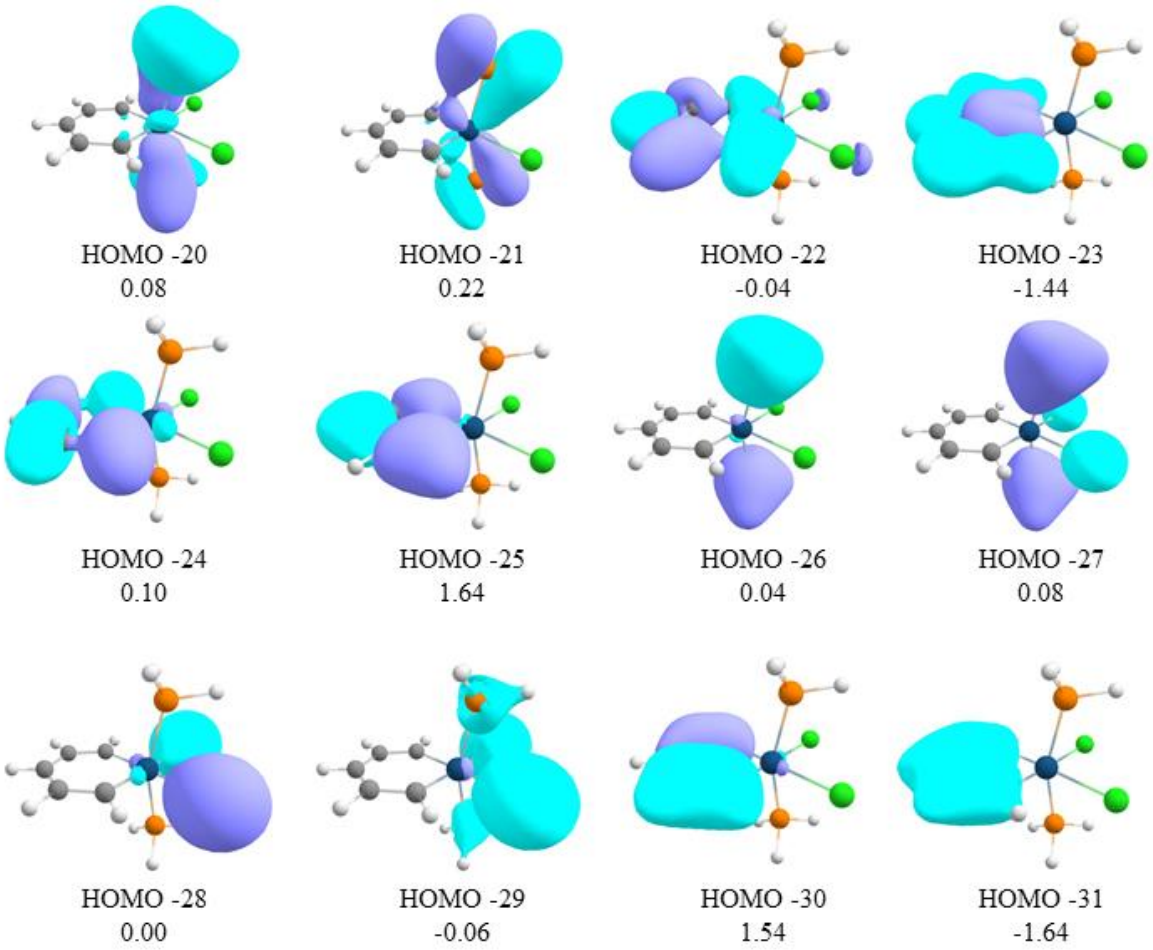
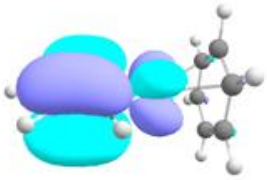
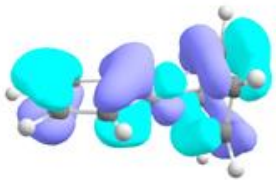


Figure S5. Valence molecular orbitals of molecule **5** and their contribution to the magnetically induced current intensity in $nA.T^{-1}$.

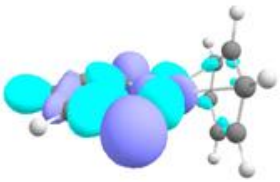


HOMO
0.16

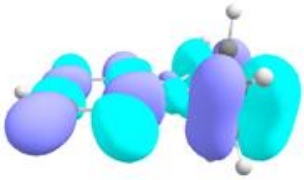


HOMO -1
3.56

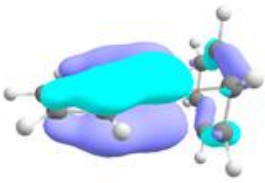
HOMO -2
-0.20



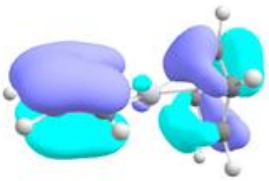
HOMO -3
-2.80



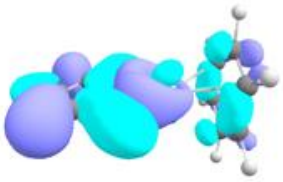
HOMO -4
-0.66



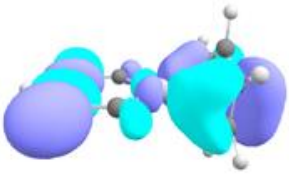
HOMO -5
0.64



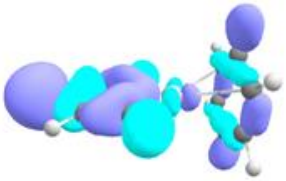
HOMO -6
-1.54



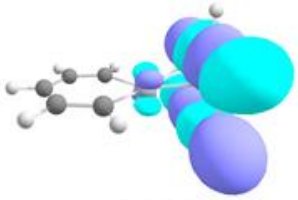
HOMO -7
-1.40



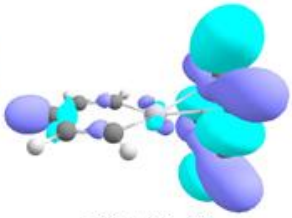
HOMO -8
0.62



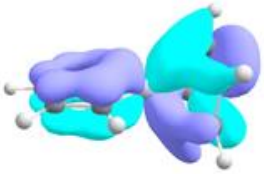
HOMO -9
1.94



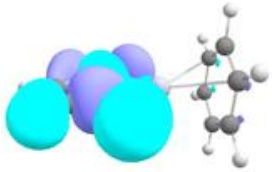
HOMO -10
0.00



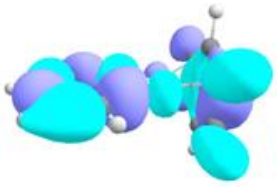
HOMO -11
0.36



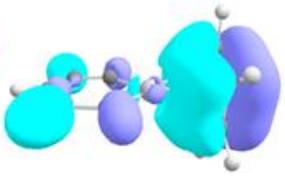
HOMO -12
1.08



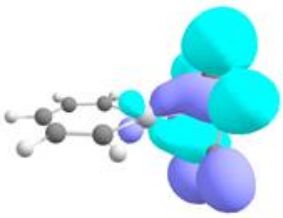
HOMO -13
-0.94



HOMO -14
2.94

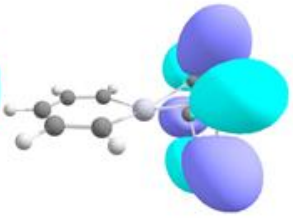


HOMO -15
-0.20

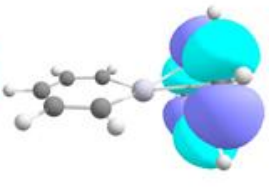


HOMO -16
0.04

HOMO -17
1.04



HOMO -18
0.00



HOMO -19
0.00

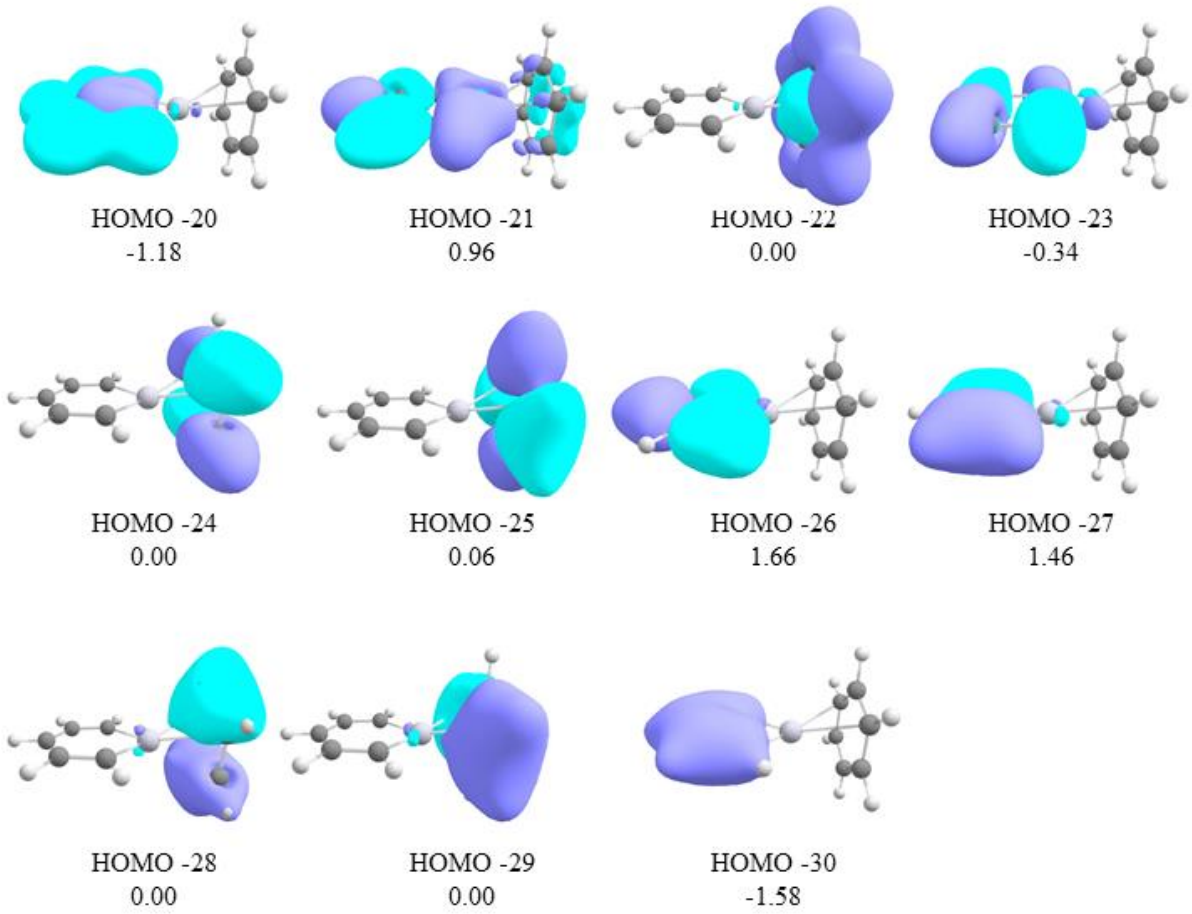
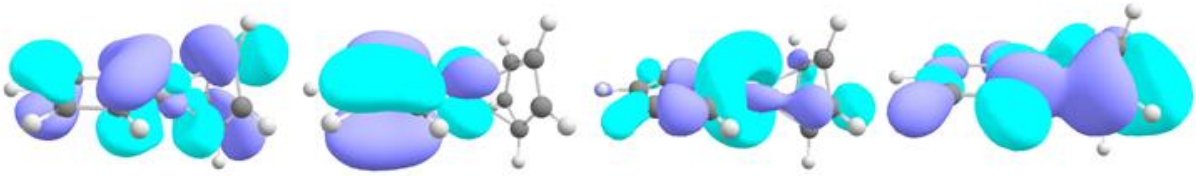


Figure S6. Valence molecular orbitals of molecule **6** and their contribution to the magnetically induced current intensity in $nA.T^{-1}$.

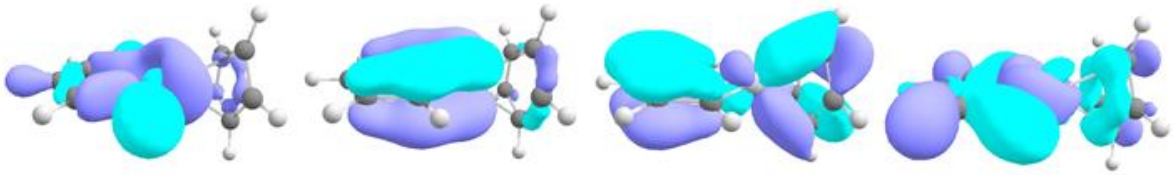


HOMO
4.76

HOMO -1
2.84

HOMO -2
-1.20

HOMO -3
-0.48

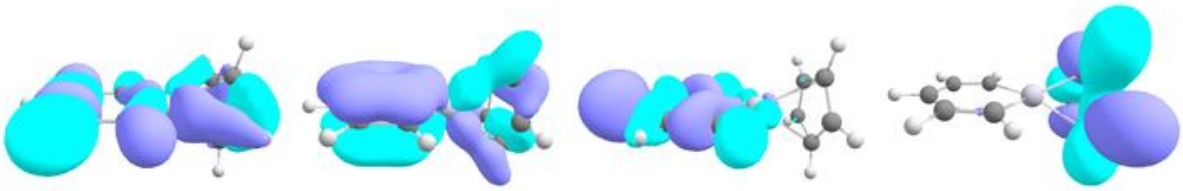


HOMO -4
-1.46

HOMO -5
0.66

HOMO -6
-2.10

HOMO -7
-1.26

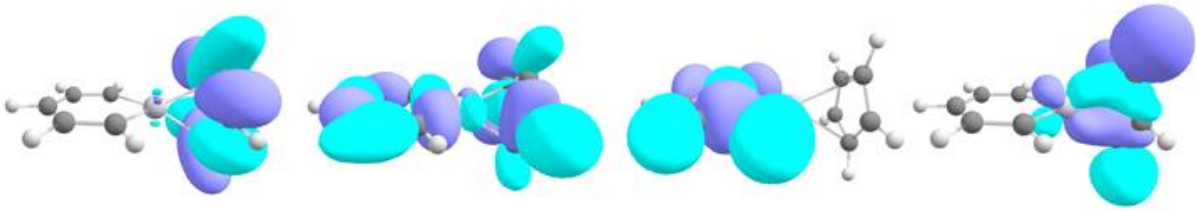


HOMO -8
0.20

HOMO -9
1.06

HOMO -10
2.22

HOMO -11
0.08

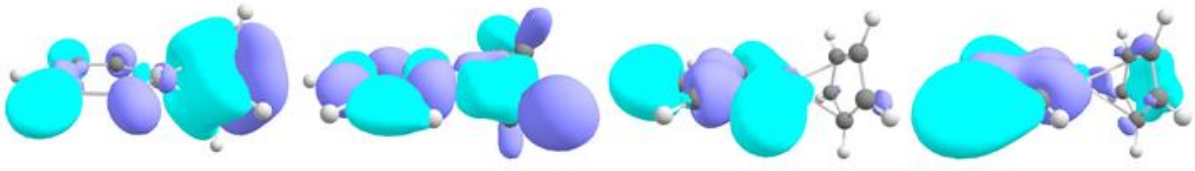


HOMO -12
0.00

HOMO -13
1.66

HOMO -14
1.28

HOMO -15
0.16



HOMO -16
-0.24

HOMO -17
2.48

HOMO -18
-2.06

HOMO -19
1.58

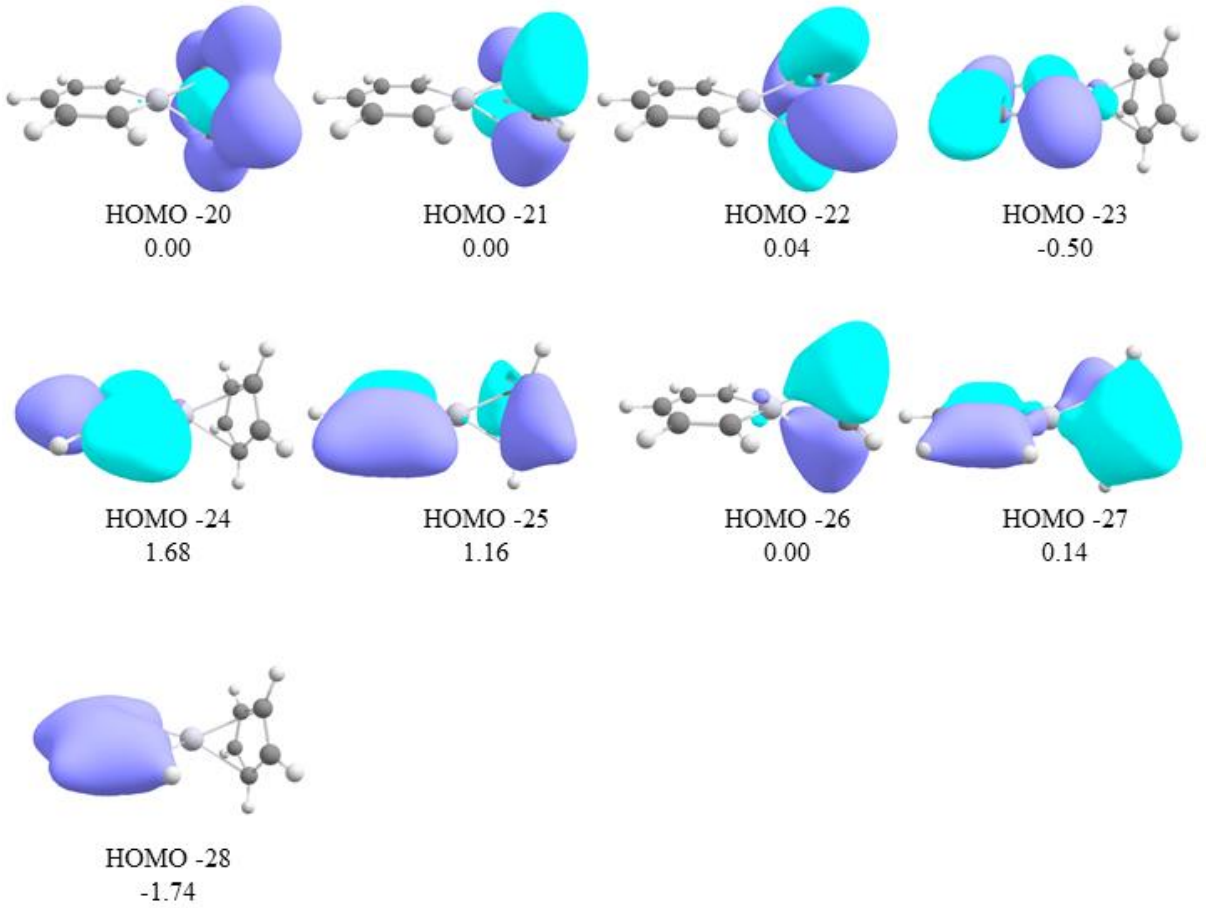


Figure S7. Valence molecular orbitals of molecule **7** and their contribution to the magnetically induced current intensity in $nA.T^{-1}$.

Cartesian Coordinates (Å)

1

Os	-1.50799	0.11623	1.24714
I	-3.82740	0.29195	2.87008
P	-1.99064	-2.14753	1.50346
P	-1.80768	2.42553	1.26976
O	0.52087	0.15252	3.54562
C	0.04798	-0.08085	-1.39137
C	-1.06582	-0.07780	-2.20358
C	0.01947	-0.00836	0.00497
C	-2.39889	-0.00164	-1.75690
C	-2.73711	0.07942	-0.43529
C	-0.27420	0.14223	2.72183
H	-0.90121	-0.13918	-3.27584
H	1.02979	-0.02745	0.42244
H	-3.17351	-0.00963	-2.51957
H	-3.81610	0.13154	-0.26010
H	1.01615	-0.14458	-1.88038
H	-1.19530	-3.11747	0.85260
H	-1.98930	-2.67937	2.80437
H	-3.25982	-2.55763	1.06362
H	-1.75868	3.08520	2.50978
H	-0.94026	3.25773	0.52682
H	-3.04195	2.88854	0.78531

2

C	-0.04129	0.00000	-0.04343
C	-1.22627	-0.00071	-0.77553
C	-2.51126	0.00000	-0.23795
C	-2.77868	0.01165	1.12584
C	0.00932	-0.00933	1.34544
H	0.88570	0.00645	-0.61633
H	-1.14079	-0.00137	-1.86110
H	-3.33714	-0.00632	-0.94890
H	-3.85691	-0.00509	1.32734
H	1.04268	0.00990	1.71323
Os	-1.50000	0.00000	2.70000
P	-1.80413	-2.23800	3.11235
H	-0.98989	-3.22882	2.51270
H	-1.66263	-2.64537	4.45129
H	-3.05456	-2.83281	2.83614
P	-1.26456	2.23676	3.16095
H	-1.61422	2.64056	4.46225
H	0.01366	2.83193	3.08584
H	-1.97471	3.22958	2.44378
C	-0.03556	-0.11569	4.18785
N	0.83493	-0.17373	4.95777
C	-3.17960	0.11251	3.94017
N	-4.16006	0.16904	4.56419

3

C	0.00438	-0.01099	-0.00892
C	-1.17145	-0.10009	-0.75772
C	-2.46482	-0.22401	-0.24501
C	-2.74338	-0.23558	1.11739
C	0.01950	0.00248	1.38149
H	0.93995	-0.05772	-0.56200
H	-1.06214	-0.17115	-1.83700
H	-3.25786	-0.42013	-0.96333
H	-3.77872	-0.54395	1.33031
H	1.03348	-0.12821	1.79031
Os	-1.52603	0.29441	2.59455
P	-1.62276	2.43067	1.70243
H	-1.50147	2.53026	0.30212
H	-2.78246	3.21756	1.88715
H	-0.66267	3.39572	2.08330
P	-1.44103	-1.81372	3.57884

H	-0.43422	-2.07597	4.53677
H	-2.55404	-2.25825	4.32966
H	-1.26445	-2.96699	2.78541
H	0.72778	1.10410	4.02148
H	-4.11059	0.69476	3.55929
C	-3.08874	0.99904	5.18443
C	-0.61748	1.20803	5.42062
H	0.16477	1.48949	6.12691
H	-4.02559	1.13546	5.72636
C	-1.91906	1.17548	5.92870
H	-2.03814	1.39505	6.98031
N	-0.25854	0.95544	4.18587
N	-3.16202	0.70948	3.90846

4

C	-0.04239	0.04354	-0.05292
C	-1.11234	0.00000	-0.96633
C	-2.47318	-0.04354	-0.60965
C	-3.02706	-0.05265	0.64005
C	-0.08763	0.05265	1.31327
H	0.95206	0.07393	-0.49700
H	-0.87073	0.00000	-2.02127
H	-3.17523	-0.07393	-1.44227
H	-4.10575	-0.08865	0.73304
H	0.84306	0.08865	1.86647
Ir	-1.88573	0.00000	2.41048
P	-1.65448	-2.20001	1.74491
H	-0.62844	-2.99531	2.30428
H	-2.76496	-3.07185	1.81496
H	-1.33985	-2.25117	0.37917
P	-1.80426	2.20001	1.71061
H	-2.97148	2.99531	1.76766
H	-0.83496	3.07185	2.25698
H	-1.49311	2.25117	0.34407
C	-3.59420	-0.05094	3.33603
C	-0.75040	0.05094	3.98735
O	-4.60937	-0.08154	3.84286
O	-0.05701	0.08154	4.88549

5

C	0.01186	-0.03161	-0.05758
C	-1.15078	-0.10000	-0.82263
C	-2.44707	-0.16839	-0.31603
C	-2.73577	-0.17645	1.03207
C	0.01396	-0.02355	1.32108
H	0.95890	0.01630	-0.58628
H	-1.03722	-0.10000	-1.90304
H	-3.26350	-0.21630	-1.03007
H	-3.79708	-0.23541	1.28496
H	0.99951	0.03541	1.78910
Ir	-1.50528	-0.10000	2.55024
P	-1.54971	-2.35779	2.97295
H	-1.41877	-2.63296	4.33933
H	-2.72057	-3.05330	2.63059
H	-0.57006	-3.20479	2.41594
P	-1.54971	2.15779	2.97295
H	-1.96187	2.43296	4.28225
H	-0.33326	2.85330	2.88150
H	-2.39214	3.00479	2.22443
Cl	-3.44921	-0.24634	4.05473
Cl	0.08337	0.04634	4.42602

6

C	-0.58484	0.77296	4.61260
C	-1.80140	1.45551	4.44284
C	-2.99190	0.72648	4.28185
C	-2.96519	-0.67617	4.28514
C	-1.74801	-1.35880	4.44980
C	-0.55828	-0.62969	4.61587
H	0.33459	1.33156	4.72506
H	-1.82019	2.53664	4.42763
H	-3.92809	1.24924	4.13932
H	-3.88088	-1.23477	4.14535
H	-1.72574	-2.43991	4.43972
H	0.38168	-1.15246	4.73108
Pt	-1.50616	0.04952	2.49187
C	-2.64718	0.02477	0.92981
C	0.01387	0.07616	1.29546
H	0.96882	0.09462	1.82158
H	-3.70861	0.00429	1.17885
C	-2.34610	0.02879	-0.40118
C	0.08289	0.07570	-0.06741
H	-3.16168	0.01199	-1.11552
H	1.06089	0.09353	-0.53529
C	-1.04158	0.05316	-0.88959
H	-0.89398	0.05468	-1.96399

7

C	-1.24389	1.22585	4.66248
C	-2.61479	0.85696	4.52533
C	-2.68842	-0.55403	4.51785
C	-1.36344	-1.06504	4.65032
C	-0.47662	0.03676	4.74743
H	-0.86173	2.23309	4.70149
H	-3.44557	1.53911	4.44267
H	-3.58565	-1.14509	4.42843
H	-1.08823	-2.10695	4.67846
H	0.59470	-0.01972	4.85553
C	-0.00495	0.02995	1.41671
C	-2.66759	0.17003	1.15040
H	0.97810	-0.02374	1.88784
H	-3.72402	0.22363	1.41993
C	0.01250	0.03631	0.04165
C	-2.41366	0.16395	-0.20135
H	0.97213	-0.01100	-0.46467
H	-3.25432	0.21136	-0.88727
C	-1.13455	0.10018	-0.74111
Pt	-1.47512	0.09992	2.66342
H	-1.02642	0.10026	-1.82074