Supporting Information for

The influence of the composition of eight-atom Pt–Ir clusters on the magnetic properties

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Supplemental materials:

1. **Table S1.** Geometries, total magnetic moments, binding energies per atom and relative energies of four most stable isomers in the clusters.
2. **Table S2.** In $\text{Pt}_{8-n}\text{Ir}_n$ clusters, electron distribution numbers and charge numbers of all the atoms after the optimization are summarized as follows.
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4. **Figure S1.** Most favorable geometrical structures of the low-lying isomers for different compositions at a given size.

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Table S1. Geometries, total magnetic moments (unit: μ_B), binding energies (unit: eV/atom) and relative energies (unit: eV) of four most stable isomers in the clusters.

Notation	Structure	Total Moment	Binding Energy	Relative Energy
1T_0		4.37	3.490	0
2P_0		4.00	3.464	0.210
3P_0		3.99	3.460	0.243
4T_0		8.00	3.447	0.343
1T_1		3.62	3.704	0
2T_1		3.00	3.683	0.164
3T_1		6.99	3.669	0.282
4T_1		2.99	3.667	0.294
1T_2		4.03	3.902	0

2T_2		4.02	3.892	0.080
3P_2		3.95	3.876	0.206
4P_2		3.96	3.852	0.401
1T_3		5.24	4.058	0
2T_3		7.01	4.053	0.042
3T_3		4.89	4.051	0.057
4P_3		1.05	4.047	0.088
1T_4		4.06	4.251	0
2T_4		8.00	4.245	0.050
3T_4		4.58	4.214	0.301

4T_4		2.57	4.205	0.367
1T_5		6.52	4.411	0
2T_5		5.01	4.406	0.040
3T_5		5.00	4.393	0.139
4T_5		5.05	4.385	0.207
1T_6		5.99	4.613	0
2T_6		4.12	4.605	0.060
3T_6		5.95	4.569	0.348
4T_6		8.00	4.567	0.364
1T_7		4.52	4.828	0

2T_7		4.84	4.720	0.868
3T_7		10.69	4.700	1.027
4T_7		7.23	4.668	1.283
1T_8		0	5.114	0
2T_8		8.00	4.895	1.759
3T_8		0.20	4.876	1.906
4T_8		11.83	4.846	2.147

Notes: Notation iP_j or iT_j represents the corresponding geometry of clusters, where superscript i shows energy order of clusters, and subscript j means the atomic number of iridium atoms among the cluster as well, what's more, notation P and T represent the planar and three-dimensional structures, respectively.

Table S2. In $\text{Pt}_{8-n}\text{Ir}_n$ clusters, electron distribution numbers and charge numbers of all the atoms after the optimization are summarized as follows.

Clusters	Atoms (no.)	Electron distribution numbers	Q (e)
Pt_8	Pt 1	9.964	0.036
	Pt 2	9.947	0.053
	Pt 3	9.925	0.075
	Pt 4	9.922	0.078
	Pt 5	10.064	-0.064
	Pt 6	10.059	-0.059
	Pt 7	10.042	-0.042
	Pt 8	10.077	-0.077
Pt_7Ir	Ir 1	8.568	0.432
	Pt 2	10.250	-0.250
	Pt 3	9.941	0.059
	Pt 4	10.063	-0.063
	Pt 5	10.051	-0.051
	Pt 6	9.972	0.028
	Pt 7	9.959	0.041
	Pt 8	10.196	-0.196
Pt_6Ir_2	Ir 1	8.708	0.292
	Ir 2	8.731	0.269
	Pt 3	10.049	-0.049
	Pt 4	10.104	-0.104
	Pt 5	10.115	-0.115
	Pt 6	10.062	-0.062
	Pt 7	10.096	-0.096
	Pt 8	10.135	-0.135
Pt_5Ir_3	Ir 1	8.792	0.208
	Ir 2	8.676	0.324
	Ir 3	8.918	0.082
	Pt 4	10.046	-0.046
	Pt 5	10.108	-0.108
	Pt 6	10.139	-0.139
	Pt 7	10.151	-0.151
	Pt 8	10.169	-0.169
Pt_4Ir_4	Ir 1	8.762	0.238
	Ir 2	8.915	0.085
	Ir 3	8.835	0.165
	Ir 4	8.842	0.158
	Pt 5	10.125	-0.125
	Pt 6	10.180	-0.180
	Pt 7	10.143	-0.143
	Pt 8	10.198	-0.198
Pt_3Ir_5	Ir 1	8.891	0.109

	Ir 2	8.887	0.114
	Ir 3	8.998	0.002
	Ir 4	8.909	0.091
	Ir 5	8.937	0.063
	Pt 6	10.134	-0.134
	Pt 7	10.120	-0.120
	Pt 8	10.124	-0.124
Pt ₂ Ir ₆	Ir 1	8.942	0.058
	Ir 2	8.988	0.012
	Ir 3	8.933	0.067
	Ir 4	8.990	0.010
	Ir 5	8.957	0.043
	Ir 6	8.950	0.050
	Pt 7	10.119	-0.119
	Pt 8	10.124	-0.124
PtIr ₇	Ir 1	8.997	0.003
	Ir 2	9.003	-0.003
	Ir 3	8.994	0.006
	Ir 4	8.954	0.046
	Ir 5	8.954	0.046
	Ir 6	8.989	0.011
	Ir 7	8.955	0.045
	Pt 8	10.153	-0.153
Ir ₈	Ir 1	8.984	0.016
	Ir 2	8.969	0.031
	Ir 3	9.021	-0.021
	Ir 4	8.996	0.004
	Ir 5	9.025	-0.025
	Ir 6	9.011	-0.011
	Ir 7	8.998	0.002
	Ir 8	8.995	0.005

Table S3. Local magnetic moments in the PAW sphere of both Pt and Ir atoms along with the spin population numbers in different orbitals are provided below.

Clusters	Atoms (no.)	s (μ_B)	p (μ_B)	d (μ_B)	Total (μ_B)
Pt ₈	Pt 1	0.048	0.024	0.477	0.549
	Pt 2	0.048	0.024	0.477	0.549
	Pt 3	0.048	0.024	0.477	0.549
	Pt 4	0.048	0.024	0.477	0.549
	Pt 5	0.018	0.009	0.172	0.198
	Pt 6	0.018	0.009	0.172	0.198
	Pt 7	0.018	0.009	0.172	0.198
	Pt 8	0.018	0.009	0.172	0.198
Pt ₇ Ir	Ir 1	0.045	0.016	0.538	0.598
	Pt 2	-0.008	0.004	0.161	0.158
	Pt 3	0.008	0.002	0.309	0.320
	Pt 4	0.012	0.009	0.356	0.376
	Pt 5	0.011	0.008	0.353	0.373
	Pt 6	0.034	0.015	0.391	0.440
	Pt 7	0.035	0.015	0.394	0.443
	Pt 8	-0.008	0.001	0.110	0.103
Pt ₆ Ir ₂	Ir 1	0.003	0.000	0.429	0.432
	Ir 2	0.003	0.000	0.429	0.432
	Pt 3	0.019	0.012	0.443	0.475
	Pt 4	0.019	0.012	0.443	0.475
	Pt 5	0.033	0.014	0.258	0.305
	Pt 6	0.019	0.012	0.443	0.475
	Pt 7	0.019	0.012	0.443	0.475
	Pt 8	0.033	0.014	0.258	0.305
Pt ₅ Ir ₃	Ir 1	0.007	0.004	0.437	0.448
	Ir 2	0.009	0.004	0.427	0.440
	Ir 3	0.069	0.036	1.043	1.148
	Pt 4	0.029	0.013	0.465	0.507
	Pt 5	0.033	0.014	0.248	0.296
	Pt 6	0.024	0.014	0.407	0.445
	Pt 7	0.040	0.023	0.514	0.576
	Pt 8	0.032	0.014	0.230	0.276
Pt ₄ Ir ₄	Ir 1	0.047	0.036	0.684	0.767
	Ir 2	0.047	0.036	0.683	0.766
	Ir 3	0.047	0.036	0.683	0.766
	Ir 4	0.047	0.036	0.683	0.766
	Pt 5	0.021	0.008	0.201	0.229
	Pt 6	0.021	0.008	0.201	0.229
	Pt 7	-0.018	-0.008	-0.122	-0.148
	Pt 8	-0.018	-0.008	-0.122	-0.148
Pt ₃ Ir ₅	Ir 1	0.029	0.031	0.614	0.674

	Ir 2	0.030	0.031	0.621	0.682
	Ir 3	0.038	0.051	0.901	0.991
	Ir 4	-0.003	-0.005	0.019	0.011
	Ir 5	0.005	0.012	0.388	0.405
	Pt 6	0.012	0.018	0.396	0.426
	Pt 7	0.015	0.009	0.390	0.414
	Pt 8	0.012	0.018	0.394	0.424
Pt ₂ Ir ₆	Ir 1	0.035	0.044	0.858	0.938
	Ir 2	0.005	-0.002	0.027	0.031
	Ir 3	0.018	0.031	0.686	0.735
	Ir 4	0.014	0.015	0.270	0.300
	Ir 5	0.035	0.044	0.859	0.938
	Ir 6	0.018	0.030	0.684	0.733
	Pt 7	0.018	0.014	0.404	0.436
	Pt 8	0.021	0.016	0.477	0.513
PtIr ₇	Ir 1	0.003	0.011	0.298	0.311
	Ir 2	-0.003	-0.013	-0.081	-0.097
	Ir 3	0.003	0.011	0.297	0.310
	Ir 4	0.034	0.024	0.585	0.644
	Ir 5	0.035	0.024	0.586	0.645
	Ir 6	0.003	0.011	0.296	0.310
	Ir 7	0.035	0.024	0.585	0.644
	Pt 8	0.018	0.020	0.444	0.482
Ir ₈	Ir 1	0.000	0.000	-0.002	-0.003
	Ir 2	0.000	0.000	0.001	0.001
	Ir 3	-0.001	-0.001	-0.005	-0.007
	Ir 4	0.001	0.001	0.007	0.008
	Ir 5	0.000	0.000	0.000	0.000
	Ir 6	0.001	0.000	0.005	0.006
	Ir 7	0.000	0.000	-0.001	-0.001
	Ir 8	-0.001	-0.001	-0.005	-0.006

Figure S1. Most favorable geometrical structures of the low-lying isomers for different compositions at a given size.