Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information (ESI):

A large perturbation on geometry structures, excited state properties, charge-injection and -transporting abilities of Ir(III) complexes by different substituents on ligands: a DFT/TDDFT study

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1. Computational methods and basis sets

Table S1 The calculated geometry parameters obtained by different computational methods and basis sets together with the experimental results of complex **5**

	PBE1PBE			B3LYP			
Complex **5**	6-31G(d)	6-31+G(d)	6-311+G(d)	6-31G(d)	6-31+G(d)	6-311+G(d)	exp
Ir-N	2.079	2.078	2.078	2.110	2.108	2.108	2.082(3)
	2.079	2.078	2.078	2.110	2.108	2.108	2.086(3)
Ir-O	2.186	2.186	2.185	2.219	2.219	2.218	2.147(3)
	2.186	2.186	2.185	2.219	2.219	2.218	2.164(2)
Ir-C	1.976	1.974	1.977	1.994	1.992	1.997	1.981(3)
	1.976	1.974	1.977	1.994	1.992	1.997	1.984(3)
N-Ir-N	176.79	176.56	176.41	176.59	176.45	176.32	172.4(11)
C- Ir-C	94.63	94.04	93.86	94.54	93.92	93.69	92.5(13)
O-Ir-O	86.19	85.99	85.45	85.20	84.97	84.48	85.9(10)
C- Ir-N	97.45	97.25	97.28	97.52	97.38	97.45	95.5 (1)
	97.45	97.25	97.28	97.52	97.38	97.44	93.2(12)
	80.35	80.38	80.24	80.14	80.17	80.01	80.2(13)
	80.35	80.38	80.24	80.14	80.17	80.01	80.8(13)
N- Ir-O	101.26	101.51	101.35	101.33	101.50	101.38	104.0(1)
	101.25	101.51	101.35	101.31	101.50	101.38	103.4(1)
	81.12	81.05	81.33	81.23	81.17	81.39	82.6(1)
	81.12	81.05	81.33	81.22	81.17	81.39	80.9(1)
C- Ir-O	175.23	175.26	175.25	174.86	174.95	174.94	175.6(1)
	175.23	175.26	175.25	174.86	174.95	174.94	172.0(1)
	89.63	90.04	90.39	90.17	90.60	90.95	87.9(1)
	89.63	90.04	90.39	90.17	90.60	90.96	93.9(1)

2. Geometries in the ground and excited state

Table S2 Main optimized geometry parameters of **1**-**4** in the ground and the lowest lying triplet states.

	1		**2**		**3**		**4**	
	S_0	T_1	S_0	T_1	S_0	T_1	S_0	T_1
Ir-N	2.110	2.109	2.109	2.138	2.110	2.143	2.104	2.128
	2.110	2.100	2.112	2.052	2.110	2.077	2.117	2.098
Ir-O	2.220	2.202	2.214	2.210	2.215	2.211	2.225	2.222
	2.220	2.201	2.209	2.202	2.215	2.209	2.218	2.206
Ir-C	1.993	1.979	1.996	2.000	1.993	1.994	1.998	1.995
	1.993	1.975	1.992	1.980	1.993	1.969	1.994	1,960
O-Ir-O	84.95	83.53	85.24	85.26	85.31	84.51	85.00	83.47
N-Ir-N	176.05	177.68	176.39	176.38	175.98	176.74	176.44	177.75
C-Ir-C	94.66	97.35	94.26	94.12	94.52	95.61	94.57	96.43

3. Geometries in the ground and excited state of 4-F^-

Table S3 Main optimized geometry parameters of **4**-F^- in the ground and the lowest lying triplet states.

	Ir-N		Ir-O		Ir-C		O-Ir-O	N-Ir-N	C-Ir-C
S0	2.110	2.113	2.268	2.268	2.002	1.999	83.14	174.98	96.27
T1	2.103	2.107	2.251	2.253	1.981	1.977	81.93	178.75	98.81