Supplementary Materials

*Table S1***.** The most important bond lengths, bond and non-bond angles in the molecular structures of complexes of [M**SP**] type, obtained using the DFT M06/TZVP method.

Structural parameter	3*d*-element (M)								
	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
M–N bond lengths in chelate node MN_3, *pm*									
M1N2	193.2	195.6	198.3	196.5	192.0	186.7	184.9	189.5	187.4
M1N3	194.1	195.6	189.0	196.5	192.1	189.7	184.9	182.9	187.4
M1N5	193.2	195.8	198.8	196.5	190.3	186.7	185.0	189.5	187.5
C–N bond lengths in 6-numbered chelate rings, *pm*									
N1C1	132.1	133.5	133.5	133.5	133.4	133.2	133.4	133.4	133.5
C1N2	138.7	136.7	136.2	136.7	136.5	137.0	136.6	136.0	136.9
N2C4	138.6	136.7	136.7	136.7	136.9	136.7	136.6	136.7	136.9
C4N6	132.6	133.5	133.5	133.5	133.3	133.4	133.4	133.4	133.5
N6C12	133.0	133.5	133.6	133.5	133.6	133.4	133.4	133.4	133.5
C12N5	138.6	136.7	136.6	136.7	136.9	136.7	136.6	136.7	136.8
N5C9	138.6	136.7	136.2	136.7	136.9	137.0	136.6	136.0	136.8
C9N4	132.3	133.5	133.5	133.6	133.6	133.2	133.4	133.4	133.5
N4C8	134.3	133.5	133.3	133.5	133.3	133.6	133.4	133.0	133.5
C8N3	137.9	136.7	137.3	136.7	136.8	136.4	136.6	137.4	136.9
N3C5	137.9	136.7	137.2	136.7	136.5	136.4	136.6	137.4	136.9
C5N1	134.3	133.5	133.4	133.5	133.4	133.6	133.4	133.0	133.5
C–C bond lengths in 5-numbered non-chelate rings, *pm*									
C1C2	144.7	144.6	144.7	144.6	144.8	144.5	144.6	144.8	144.7
C2C3	136.2	136.2	136.0	136.2	136.1	136.3	136.2	136.0	136.1
C3C4	144.3	144.6	144.9	144.6	144.8	144.5	144.6	145.1	144.7
C5C6	142.9	144.6	144.1	144.6	144.8	144.8	144.6	143.9	144.7
C6C7	137.4	136.2	136.5	136.2	136.1	136.0	136.2	136.9	136.1
C7C8	143.0	144.6	144.1	144.6	144.8	144.8	144.6	143.9	144.7
C9C10	144.6	144.6	144.7	144.6	144.2	144.5	144.6	144.8	144.7
C10C11	136.3	136.2	136.0	136.2	136.5	136.3	136.2	136.0	136.1
C11C12	144.2	144.6	144.9	144.6	144.2	144.5	144.6	145.1	144.7
Bond angles in chelate node MN_3, *deg*									
N2M1N5	85.5	82.8	85.9	85.3	87.9	88.8	90.9	95.1	94.8
N5M1N3	84.2	82.8	83.1	85.3	87.9	89.5	90.9	89.2	94.8
N3M1N2	84.2	82.8	83.1	85.3	85.5	89.5	91.0	89.2	94.9
Bond angles sum (BAS), *deg*	**253.9**	**248.4**	**252.1**	**255.9**	**261.3**	**267.8**	**272.8**	**273.5**	**284.5**
Non-bond angles between N atoms in N3 grouping, *deg*									
N2N3N5	60.6	60.0	63.5	60.0	60.6	59.0	60.0	64.6	60.0
N3N5N2	59.7	60.0	58.2	60.0	58.8	60.5	60.0	57.7	60.0
N5N2N3	59.7	60.0	58.3	60.0	60.6	60.5	60.0	57.7	60.0
Non-bond angles sum (NBAS), *deg*	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
Bond angles in 6-numbered chelate ring (M1N2C1N1C5N3), *deg*									
M1N2C1	124.7	124.8	124.8	124.0	125.3	123.7	123.1	124.6	121.0
N2C1N1	124.6	124.8	124.3	125.4	125.0	125.4	125.4	124.6	126.1
C1N1C5	121.7	120.3	119.9	121.4	120.7	121.3	121.0	120.3	123.1
N1C5N3	123.6	124.8	125.1	125.4	124.9	125.4	125.4	126.1	126.1
C5N3M1	125.1	124.8	125.0	124.0	125.3	123.2	123.1	123.7	121.0
N3M1N2	84.2	82.8	83.1	85.3	85.5	89.5	91.0	89.2	94.9
Bond angles sum (BAS[61]), *deg*	703.9	702.3	702.2	705.5	706.7	708.5	709.0	708.5	712.2
Bond angles in 6-numbered chelate ring (M1N2C4N6C12N5), *deg*									
M1N2C4	124.8	124.8	123.2	124.0	122.7	123.6	123.1	119.3	121.1
N2C4N6	124.6	124.8	125.9	125.4	125.4	124.8	125.4	126.8	126.1
C4N6C12	122.2	120.3	121.9	121.4	121.5	121.1	120.9	123.2	123.1
N6C12N5	124.5	124.8	125.9	125.4	125.2	124.9	125.4	126.8	126.1
C12N5M1	124.8	124.8	123.1	124.0	123.6	123.6	123.1	119.3	121.1
N5M1N2	85.5	82.8	85.9	85.3	87.9	88.8	90.9	95.1	94.8
Bond angles sum (BAS[62]), *deg*	706.4	702.3	705.9	705.5	706.3	706.8	708.8	710.5	712.3

Bond angles in 6-numbered chelate ring (M1N5C9N4C8N3), *deg*									
M1N5C9	124.7	124.8	124.7	124.0	123.6	123.7	123.1	124.6	121.1
N5C9N4	124.5	124.8	124.3	125.4	125.2	125.4	125.4	124.6	126.1
C9N4C8	121.7	120.3	120.0	121.4	121.5	121.3	120.9	120.3	123.1
N4C8N3	123.7	124.8	125.1	125.4	125.4	125.4	125.4	126.1	126.1
C8N3M1	124.9	124.8	125.0	124.0	122.7	123.2	123.1	123.7	121.1
N3M1N5	84.2	82.8	83.1	85.3	87.9	89.5	90.9	89.2	94.8
Bond angles sum (BAS[63]), *deg*	703.6	702.3	702.2	705.5	706.3	708.5	708.8	708.5	712.3
Bond angles in 5-numbered ring (N2C1C2C3C4), *deg*									
N2C1C2	106.8	107.3	107.8	107.2	107.0	106.7	106.7	107.6	106.7
C1C2C3	107.4	107.2	106.8	107.2	107.3	107.4	107.3	106.7	107.3
C2C3C4	107.8	107.2	107.2	107.2	107.2	107.4	107.3	107.2	107.3
C3C4N2	106.9	107.3	107.3	107.2	107.0	106.7	106.7	106.9	106.7
C4N2C1	107.4	108.3	108.0	108.2	108.6	108.8	108.8	107.9	108.4
Bond angles sum (BAS[51]), *deg*	536.3	537.3	537.1	537.0	537.1	537.0	536.8	536.3	536.4
Bond angles in 5-numbered ring (N3C5C6C7C8), *deg*									
N3C5C6	107.1	107.3	106.4	107.2	107.1	107.4	106.7	105.3	106.7
C5C6C7	107.5	107.2	107.6	107.2	107.3	107.0	107.3	107.9	107.3
C6C7C8	107.5	107.2	107.7	107.2	107.2	107.0	107.3	107.9	107.3
C7C8N3	107.1	107.3	106.4	107.2	107.0	107.4	106.7	105.3	106.7
C8N3C5	108.2	108.3	108.3	108.2	108.6	108.0	108.8	110.2	108.4
Bond angles sum (BAS[52]), *deg*	537.4	537.3	537.4	537.0	537.2	536.8	536.8	536.6	536.4
Bond angles in 5-numbered ring (N5C9C10C11C12), *deg*									
N5C9C10	106.8	107.3	107.8	107.2	107.2	106.7	106.7	107.6	106.7
C9C10C11	107.3	107.2	106.8	107.2	107.2	107.4	107.3	106.7	107.3
C10C11C12	107.8	107.2	107.1	107.2	107.2	107.4	107.3	107.2	107.3
C11C12N5	106.9	107.3	107.3	107.2	107.2	106.7	106.7	106.9	106.7
C12N5C9	107.5	108.3	107.9	108.2	108.1	108.8	108.8	107.9	108.4
Bond angles sum (BAS[53]), *deg*	536.3	537.3	536.9	537.0	536.9	537.0	536.8	536.3	536.4

*Table S2***.** The most important bond lengths, bond and non-bond angles in the molecular structures of complexes of [M**SP**] type, obtained using the DFT OPBE/TZVP method.

Structural parameter	3*d*-element (M)								
	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
M–N bond lengths in chelate node MN_3, *pm*									
M1N2	190.8	190.3	194.3	195.4	187.7	184.0	182.9	188.7	187.5
M1N3	190.8	190.3	185.9	195.4	189.0	184.0	182.9	183.2	187.5
M1N5	190.9	190.5	194.3	195.4	189.2	184.1	182.9	188.7	187.6
C–N bond lengths in 6-numbered chelate rings, *pm*									
N1C1	134.0	134.2	134.2	134.5	134.6	134.2	134.2	134.5	134.5
C1N2	139.0	137.7	137.0	137.2	137.6	137.5	137.2	136.6	137.3
N2C4	139.0	137.7	137.9	137.2	137.6	137.5	137.2	137.5	137.3
C4N6	134.0	134.2	134.3	134.5	134.6	134.2	134.2	134.2	134.5
N6C12	134.0	134.2	134.3	134.5	134.1	134.2	134.2	134.2	134.5
C12N5	139.0	137.7	137.9	137.2	137.6	137.5	137.2	137.5	137.3
N5C9	139.0	137.7	137.0	137.2	137.3	137.5	137.2	136.6	137.3
C9N4	134.0	134.2	134.2	134.5	134.3	134.2	134.2	134.5	134.5
N4C8	134.0	134.2	134.4	134.5	134.3	134.2	134.2	134.0	134.5
C8N3	139.0	137.7	137.8	137.2	137.3	137.5	137.2	137.7	137.3
N3C5	139.0	137.7	137.8	137.2	137.6	137.5	137.2	137.8	137.3
C5N1	134.0	134.2	134.4	134.5	134.1	134.2	134.2	133.9	134.5

C–C bond lengths in 5-numbered non-chelate rings, *pm*									
C1C2	144.4	144.9	145.1	145.2	144.5	145.2	145.2	145.3	145.3
C2C3	137.9	137.4	137.2	137.3	137.8	137.3	137.4	137.2	137.2
C3C4	144.4	144.9	145.2	145.2	144.5	145.2	145.2	145.7	145.3
C5C6	144.4	144.9	144.5	145.2	145.3	145.2	145.2	144.6	145.3
C6C7	137.9	137.4	137.8	137.3	137.3	137.3	137.4	138.0	137.2
C7C8	144.4	144.9	144.5	145.2	145.3	145.2	145.2	144.6	145.3
C9C10	144.4	144.9	145.1	145.2	145.3	145.2	145.2	145.3	145.3
C10C11	137.9	137.4	137.2	137.3	137.3	137.3	137.4	137.2	137.2
C11C12	144.4	144.9	145.2	145.2	145.3	145.2	145.2	145.7	145.3
Bond angles in chelate node MN_3, *deg*									
N2M1N5	85.1	85.0	89.0	84.9	88.8	91.2	91.7	96.5	94.9
N5M1N3	85.1	85.0	84.0	84.9	86.6	91.2	91.7	89.2	94.9
N3M1N2	85.1	85.0	84.0	84.9	88.9	91.2	91.8	89.1	95.0
Bond angles sum (BAS), *deg*	**255.3**	**255.0**	**257.0**	**254.7**	**264.3**	**273.6**	**275.2**	**274.8**	**284.8**
Non-bond angles between N atoms in N3 grouping, *deg*									
N2N3N5	60.0	60.0	64.7	60.0	60.6	60.0	60.0	65.2	60.0
N3N5N2	60.0	60.0	57.6	60.0	60.5	60.0	60.0	57.4	60.0
N5N2N3	60.0	60.0	57.7	60.0	58.9	60.0	60.0	57.4	60.0
Non-bond angles sum (NBAS), *deg*	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
Bond angles in 6-numbered chelate ring (M1N2C1N1C5N3), *deg*									
M1N2C1	124.9	124.7	125.4	124.3	123.7	123.4	123.1	125.1	121.1
N2C1N1	124.2	124.7	124.4	125.4	125.1	125.1	125.6	124.7	126.3
C1N1C5	121.0	119.8	118.6	120.2	120.7	120.9	120.0	119.4	122.4
N1C5N3	124.2	124.7	125.1	125.4	125.4	125.1	125.6	126.4	126.3
C5N3M1	124.9	124.7	124.8	124.3	122.8	123.4	123.1	123.8	121.1
N3M1N2	85.1	85.0	84.0	84.9	88.9	91.2	91.8	89.1	95.0
Bond angles sum (BAS[61]), *deg*									
Bond angles in 6-numbered chelate ring (M1N2C4N6C12N5), *deg*									
M1N2C4	125.0	124.8	122.0	124.3	123.8	123.4	123.2	118.6	121.2
N2C4N6	124.2	124.7	126.2	125.4	125.0	125.1	125.6	127.1	126.3
C4N6C12	121.0	119.8	121.6	120.2	120.7	120.9	120.0	122.7	122.3
N6C12N5	124.2	124.7	126.2	125.4	125.4	125.1	125.6	127.1	126.3
C12N5M1	125.0	124.8	122.0	124.3	122.8	123.4	123.2	118.6	121.2
N5M1N2	85.1	85.0	89.0	84.9	88.8	91.2	91.7	96.5	94.9
Bond angles sum (BAS[62]), *deg*									
Bond angles in 6-numbered chelate ring (M1N5C9N4C8N3), *deg*									
M1N5C9	125.0	124.8	125.4	124.3	125.4	123.4	123.2	125.1	121.2
N5C9N4	124.2	124.7	124.4	125.4	125.0	125.1	125.6	124.8	126.3
C9N4C8	121.0	119.8	118.6	120.2	120.1	120.9	120.0	119.4	122.3
N4C8N3	124.2	124.7	125.1	125.4	124.9	125.1	125.6	126.4	126.3
C8N3M1	125.0	124.8	124.8	124.3	125.5	123.4	123.2	123.8	121.2
N3M1N5	85.1	85.0	84.0	84.9	86.6	91.2	91.7	89.2	94.9
Bond angles sum (BAS[63]), *deg*									
Bond angles in 5-numbered ring (N2C1C2C3C4), *deg*									
N2C1C2	106.8	107.1	107.7	107.3	107.3	106.9	106.7	107.9	106.8
C1C2C3	107.5	107.3	106.7	107.0	107.1	107.2	107.2	106.5	107.1
C2C3C4	107.5	107.3	107.3	107.0	107.1	107.2	107.2	107.1	107.1
C3C4N2	106.8	107.1	107.2	107.3	107.3	106.9	106.7	107.0	106.8
C4N2C1	107.9	108.4	107.8	108.3	108.1	108.5	108.9	107.7	108.5
Bond angles sum (BAS[51]), *deg*									

Bond angles in 5-numbered ring (N3C5C6C7C8), *deg*									
N3C5C6	106.8	107.1	106.0	107.3	107.0	106.9	106.7	105.3	106.8
C5C6C7	107.5	107.3	107.8	107.0	107.0	107.2	107.2	107.8	107.1
C6C7C8	107.5	107.3	107.8	107.0	107.3	107.2	107.2	107.8	107.1
C7C8N3	106.8	107.1	106.0	107.3	107.0	106.9	106.7	105.3	106.8
C8N3C5	107.9	108.4	110.1	108.3	108.6	108.5	108.9	110.4	108.5
Bond angles sum (BAS[52]), *deg*									
Bond angles in 5-numbered ring (N5C9C10C11C12), *deg*									
N5C9C10	106.8	107.1	107.7	107.3	107.0	106.9	106.7	107.9	106.8
C9C10C11	107.5	107.3	106.7	107.0	107.0	107.2	107.2	106.5	107.1
C10C11C12	107.5	107.3	107.3	107.0	107.3	107.2	107.2	107.1	107.1
C11C12N5	106.8	107.1	107.2	107.3	107.0	106.9	106.7	107.0	106.8
C12N5C9	107.9	108.4	107.8	108.3	108.5	108.5	108.9	107.7	108.5
Bond angles sum (BAS[53]), *deg*									

Table S3. Electric dipole moments (◎) for M**SP**] compounds of various M calculated by DFT B3PW91/TZVP, DFT OPBE/TZVP *и* DFT M06/TZVP chemical models.

DFT method	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
B3PW91/TZVP	4.59	3.02	2.72	3.12	2.65	2.07	1.61	1.12	1.73
OPBE/TZVP	4.81	2.28	2.22	2.73	2.16	1.64	1.14	0.89	1.70
M06/TZVP	5.02	3.63	2.88	3.08	2.61	1.86	1.43	0.98	1.64

Table S4. Energy distances between the ground and nearest excited states with spin multiplicity different from the multiplicity of the ground state for various [M**SP**] complexes in the framework of various versions of the DFT method.

Complex	DFT method	ΔE, kJ/mol					
		M = 1	*M* = 2	*M* = 3	*M* = 4	*M* = 5	*M* = 6
[Ti**SP**]	B3PW91/TZVP	78.7	-	0.0	-	-	-
	M06/TZVP	23.1	-	0.0	-	-	-
	OPBE/TZVP	43.0	-	0.0	-	-	-
[V**SP**]	B3PW91/TZVP	-	81.8	-	0.0	-	-
	M06/TZVP	-	95.3	-	0.0	-	-
	OPBE/TZVP	-	60.6	-	0.0	-	-
[Cr**SP**]	B3PW91/TZVP	233.6	-	49.2	-	0.0	-
	M06/TZVP	279.3	-	71.2	-	0.0	-
	OPBE/TZVP	107.2	-	15.5	-	0.0	-
[Mn**SP**]	B3PW91/TZVP	-	146.2	-	127.1	-	0.0
	M06/TZVP	-	211.9	-	139.7	-	0.0
	OPBE/TZVP	-	95.8	-	98.0	-	0.0
[Fe**SP**]	B3PW91/TZVP	57.4	-	81.4	-	0.0	-
	M06/TZVP	82.7	-	100.8	-	0.0	-
	OPBE/TZVP	17.0	-	36.7	-	0.0	-
[Co**SP**]	B3PW91/TZVP	-	39.2	-	0.0	-	156.2
	M06/TZVP	-	28.9	-	0.0	-	146.7
	OPBE/TZVP	-	12.7	-	0.0	-	160.5
[Ni**SP**]	B3PW91/TZVP	123.1	-	0.0	-	-	-
	M06/TZVP	106.6	-	0.0	-	-	-
	OPBE/TZVP	76.7	-	0.0	-	-	-
[Cu**SP**]	B3PW91/TZVP	-	0.0	-	148.9	-	-
	M06/TZVP	-	0.0	-	140.6	-	-
	OPBE/TZVP	-	0.0	-	115.2	-	-

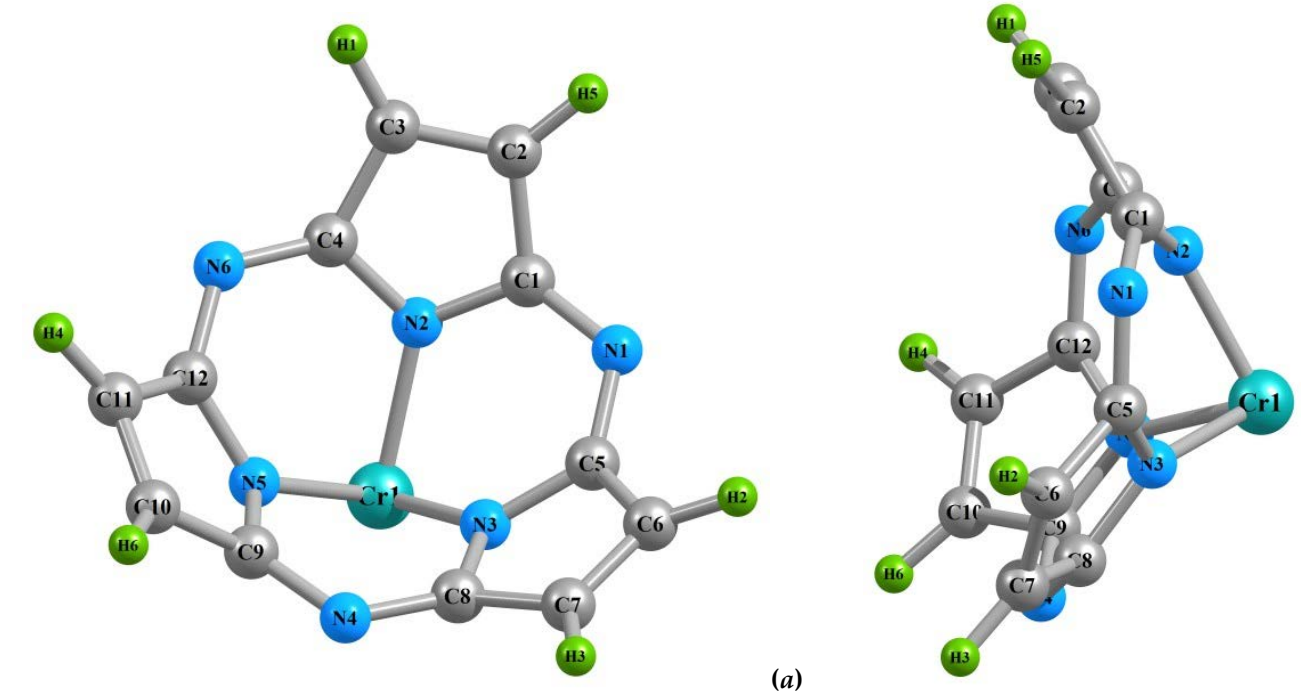
[Zn**SP**]	B3PW91/TZVP	0.0	-	150.9	-	-	-
	M06/TZVP	0.0	-	142.5	-	-	-
	OPBE/TZVP	0.0	-	162.2	-	-	-

Table S5. NBO analysis data for the [M**SP**] compounds calculated by the DFT OPBE/TZVP method.

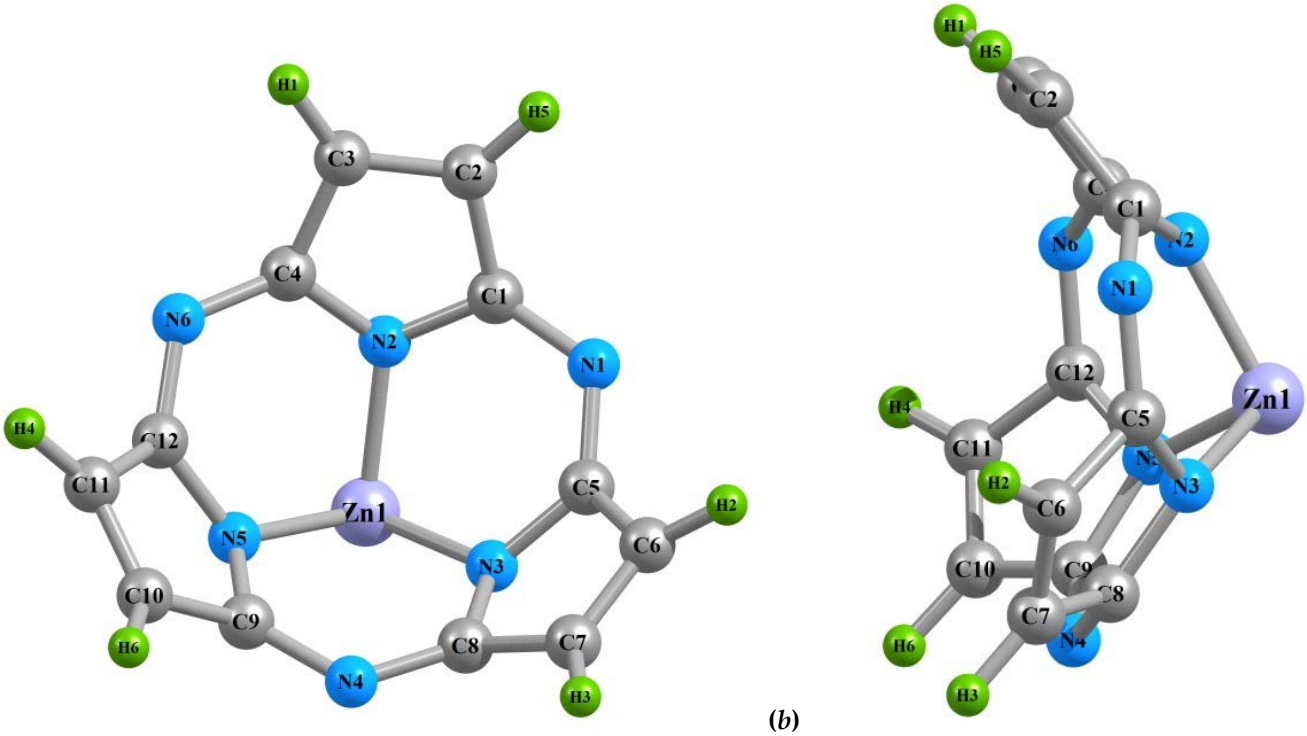
Complex	Effective charge on atom, in electron charge units (ē)							<S**2>
	M1	N1	N2	N3	N4	N5	N6	
[Ti**SP**]	+1.1298	-0.3850	-0.5382	-0.5382	-0.3849	-0.5380	-0.3849	2.0002
[V**SP**]	+0.8762	-0.3844	-0.5084	-0.5084	-0.3844	-0.5084	-0.3844	3.7503
[Cr**SP**]	+0.9720	-0.3844	-0.5661	-0.4944	-0.3844	-0.5660	-0.3844	6.0007
[Mn**SP**]	+1.1443	-0.3892	-0.6021	-0.6021	-0.3891	-0.6021	-0.3891	8.7501
[Fe**SP**]	+1.0125	-0.3848	-0.5593	-0.5611	-0.3797	-0.5610	-0.3848	6.0003
[Co**SP**]	+0.8973	-0.3782	-0.5228	-0.5228	-0.3781	-0.3781	-0.5228	3.7502
[Ni**SP**]	+0.8690	-0.3862	-0.5224	-0.5224	-0.3860	-0.5223	-0.3860	2.0000
[Cu**SP**]	+0.9319	-0.3826	-0.5754	-0.4972	-0.3827	-0.5760	-0.3955	0.7500
[Zn**SP**]	+1.2766	-0.3946	-0.6579	-0.6579	-0.3945	-0.6576	-0.3945	0.0000

Table S6. NBO analysis data for the [M**SP**] compounds calculated by the DFT M06/TZVP method.

Complex	Effective charge on atom, in electron charge units (ē)							<S**2>
	M1	N1	N2	N3	N4	N5	N6	
[Ti**SP**]	+1.2081	-0.4330	-0.6159	-0.6033	-0.4350	-0.6151	-0.4283	2.0001
[V**SP**]	+1.0229	-0.4385	-0.5943	-0.5943	-0.4388	-0.5944	-0.4388	3.7501
[Cr**SP**]	+1.0742	-0.4346	-0.6429	-0.5839	-0.4342	-0.6433	-0.4452	6.0002
[Mn**SP**]	+1.2299	-0.4409	-0.6719	-0.6719	-0.4409	-0.6719	-0.4409	8.7500
[Fe**SP**]	+1.1194	-0.4339	-0.6377	-0.6375	-0.4366	-0.6372	-0.4365	6.0002
[Co**SP**]	+1.0215	-0.4353	-0.6144	-0.6074	-0.4355	-0.6144	-0.4306	3.7502
[Ni**SP**]	+0.9639	-0.4360	-0.5971	-0.5971	-0.4359	-0.5970	-0.4359	2.0000
[Cu**SP**]	+0.9536	-0.4309	-0.6285	-0.5409	-0.4309	-0.6286	-0.4471	0.7500
[Zn**SP**]	+1.2579	-0.4434	-0.6972	-0.6972	-0.4433	-0.6971	-0.4433	0.0000



(*a*)



(*b*)

Fig. S1. The images of molecular structures of the complexes with subporphyrazine obtained by using quantum-chemical calculation by DFT M06/TZVP method: *a*: [Cr**SP**], *b*: [Zn**SP**] (*left* **–** front view, *right* **–** side view).

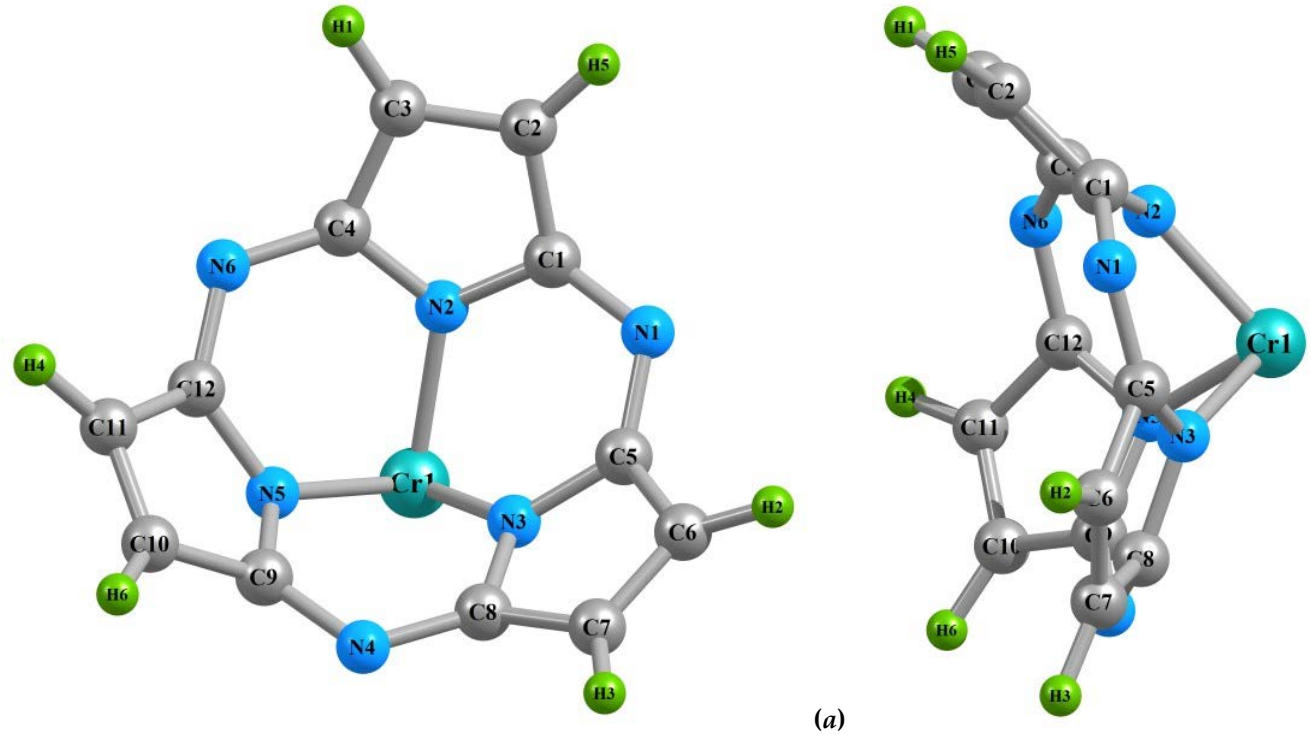


Fig. S2. The images of molecular structures of the complexes with subporphyrazine obtained by using quantum-chemical calculation by DFT OPBE/TZVP method: *a*: [Cr**SP**], *b*: [Zn**SP**] (*left* – front view, *right* – side view).

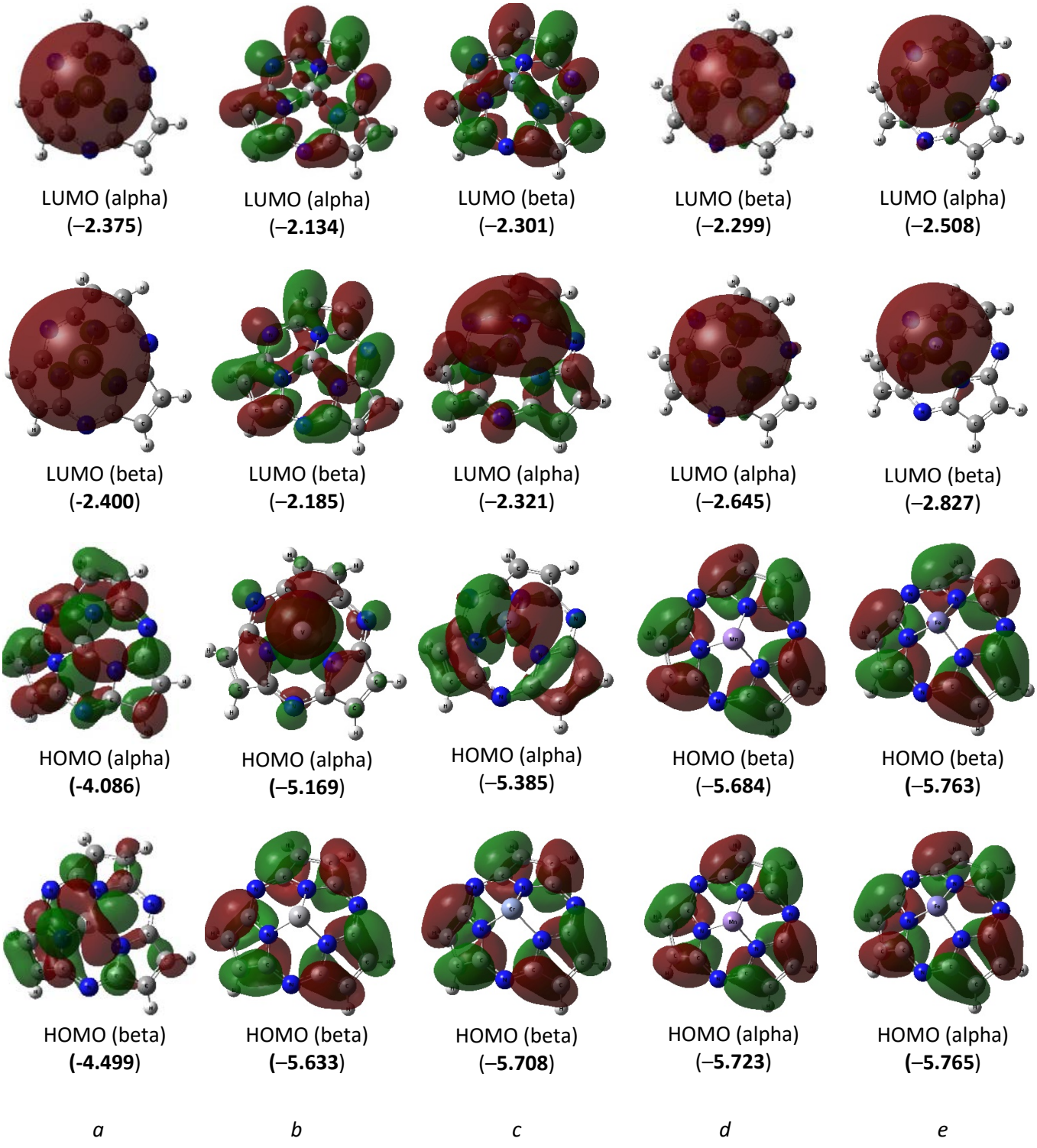


Fig. S3*, A*. Images of the highest occupied (HOMO) and lowest vacant (LUMO) molecular orbitals of complexes [Ti**SP**] with *M* = 3 (*a*), [V**SP**] with *M* = 4 (*b*), [Cr**SP**] with *M* = 5 (*c*), [Mn**SP**] with *M* = 6 (*d*) and [Fe**SP**] with *M* = 5 (*e*) obtained within the DFT M06/TZVP method. The energies values of the given MOs (in brackets) are expressed in eV. The symbol “alpha” belongs to electron having spin (+1/2), symbol “beta”, to electron having spin (-l/2).

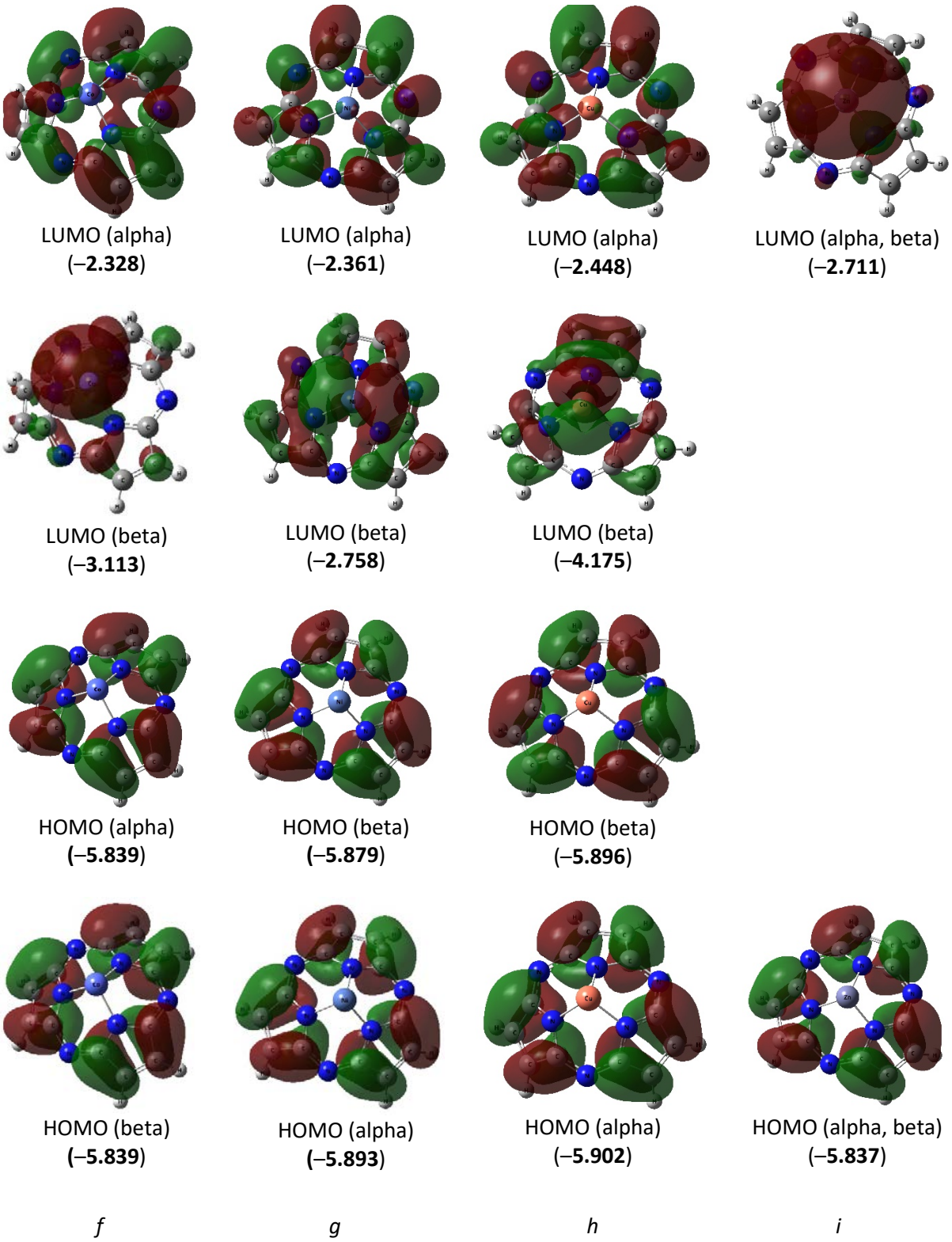


***Fig. S3**, B.* Images of the highest occupied (HOMO) and lowest vacant (LUMO) molecular orbitals of complexes [Co**SP**] with *M* = 4 (*f*), [Ni**SP** with *M* = 3 (*g*), [Cu**SP**] with *M* = 2 (*h*), and [Zn**SP**] with *M* = 1 (*i*) obtained within the DFT M06/TZVP method. The energies values of the given MOs (in brackets) are expressed in eV. The symbol "alpha" belongs to electron having spin (+1/2), symbol "beta", to electron having spin (-l/2).

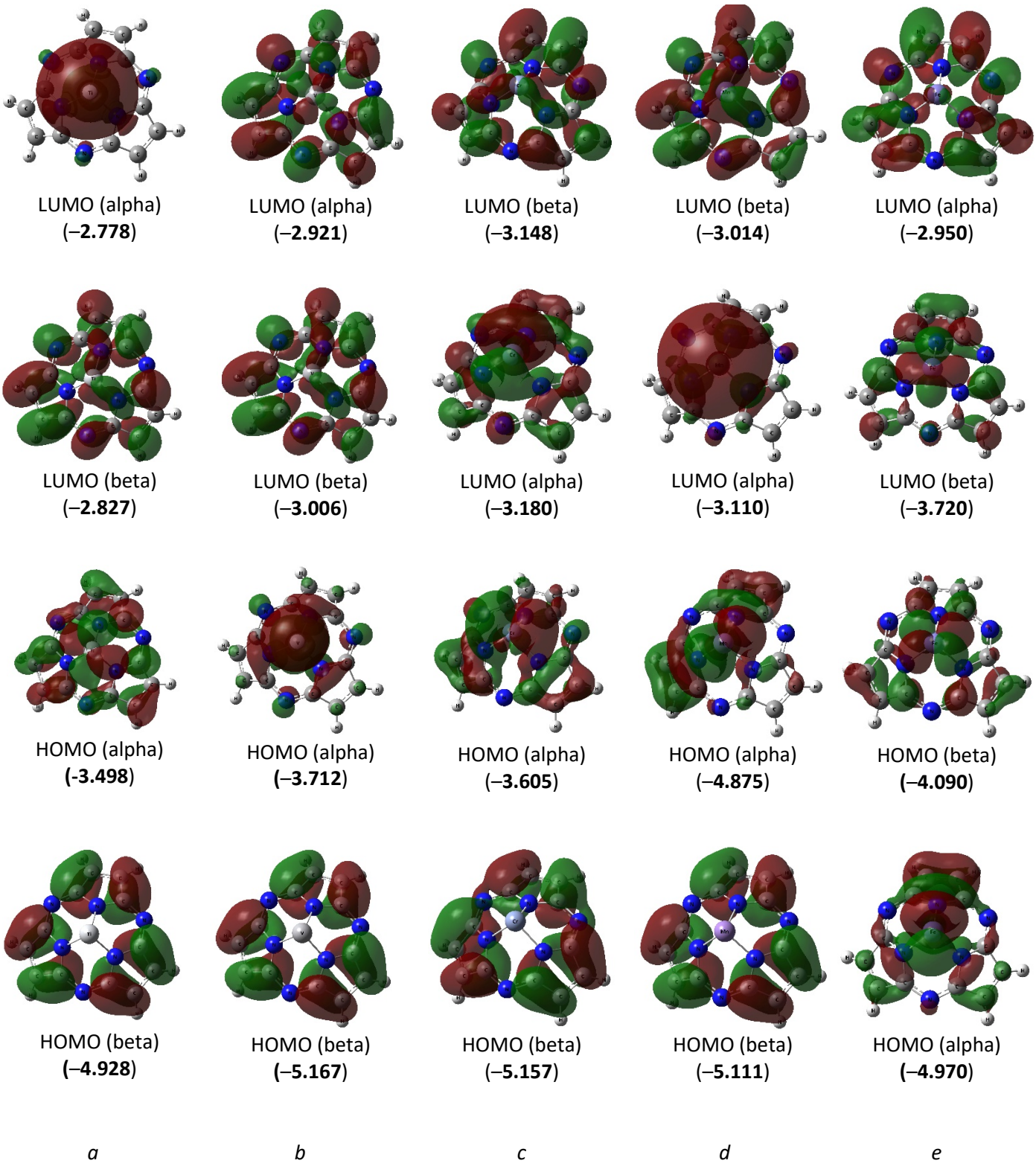


Fig. S4*, A.* Images of the highest occupied (HOMO) and lowest vacant (LUMO) molecular orbitals of complexes [Ti**SP**] with *M* = 3 (*a*), [V**SP**] with *M* = 4 (*b*), [Cr**SP**] with *M* = 5 (*c*), [Mn**SP**] with *M* = 6 (*d*) and [Fe**SP**] with *M* = 5 (*e*) obtained within the DFT OPBE/TZVP method. The energies values of the given MOs (in brackets) are expressed in eV. The symbol “alpha” belongs to electron having spin (+1/2), symbol “beta”, to electron having spin (-l/2).

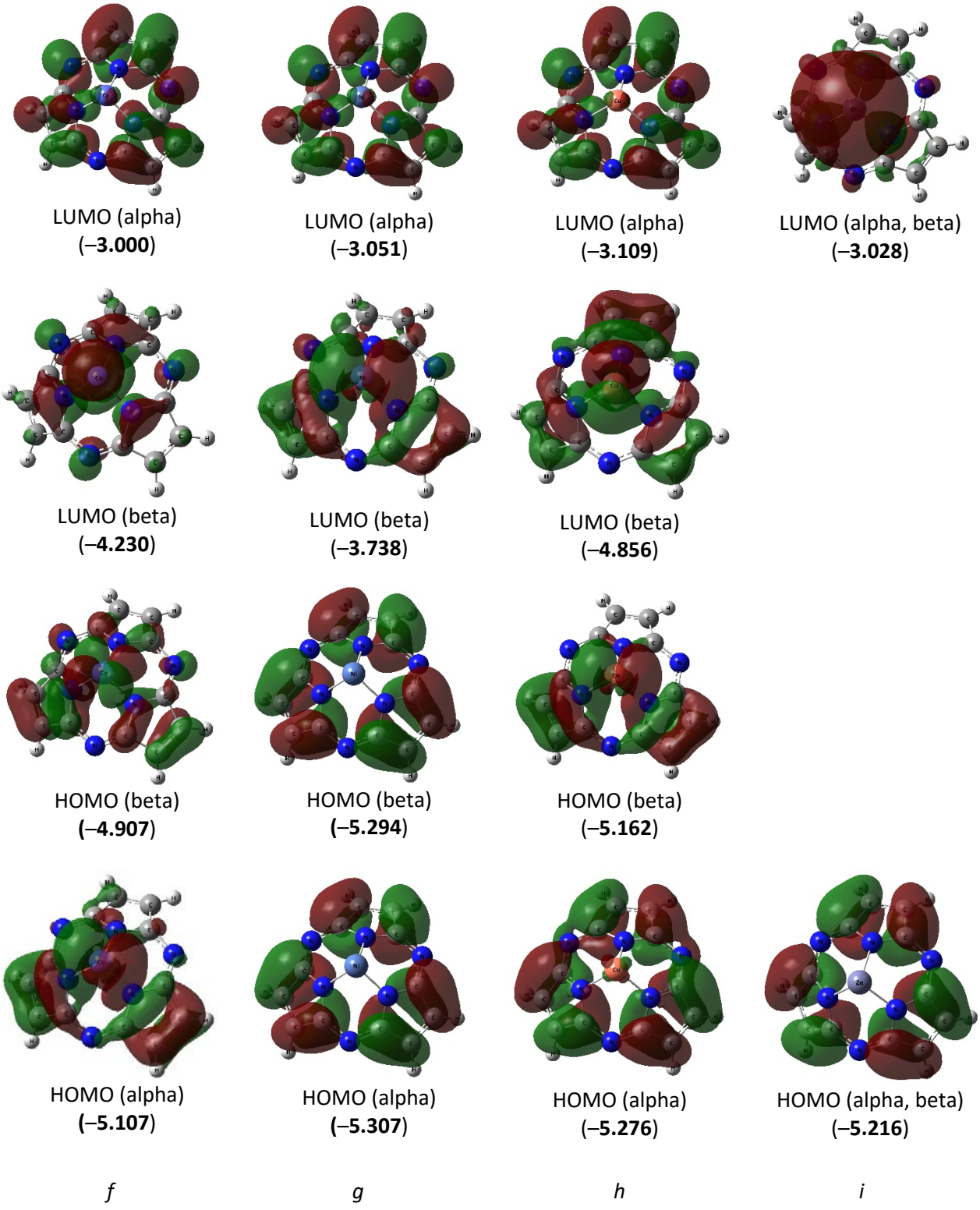


***Fig. S4**, B.* Images of the highest occupied (HOMO) and lowest vacant (LUMO) molecular orbitals of complexes [Co**SP**] with *M* = 4 (*f*), [Ni**SP** with *M* = 3 (*g*), [Cu**SP**] with *M* = 2 (*h*), and [Zn**SP**] with *M* = 1 (*i*) obtained within the DFT B3PW91/TZVP method. The energies values of the given MOs (in brackets) are expressed in eV. The symbol “alpha” belongs to electron having spin (+1/2), symbol “beta”, to electron having spin (-l/2).