Electronic Supplementary Information (ESI) for

Universal Spectrochemical Series of Six-Coordinate Octahedral Metal Complexes for Modifying the Ligand Field Splitting

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Table S1. Effective charge of each atom on $[Co(NH_3)_6]^{3+}$ metal complex.

Atom	Effective Charge
Co	+1.84
N(1)	–1.39
N(2)	–1.37
N(3)	–1.43
N(4)	–1.39
N(5)	–1.36
N(6)	–1.34
H(11)	+0.53
H(12)	+0.52
H(13)	+0.54
H(21)	+0.52
H(22)	+0.52
H(23)	+0.52
H(31)	+0.55
H(32)	+0.52
H(33)	+0.53
H(41)	+0.52
H(42)	+0.53
H(43)	+0.53
H(51)	+0.51
H(52)	+0.53
H(53)	+0.53
H(61)	+0.51
H(62)	+0.53
H(63)	+0.52

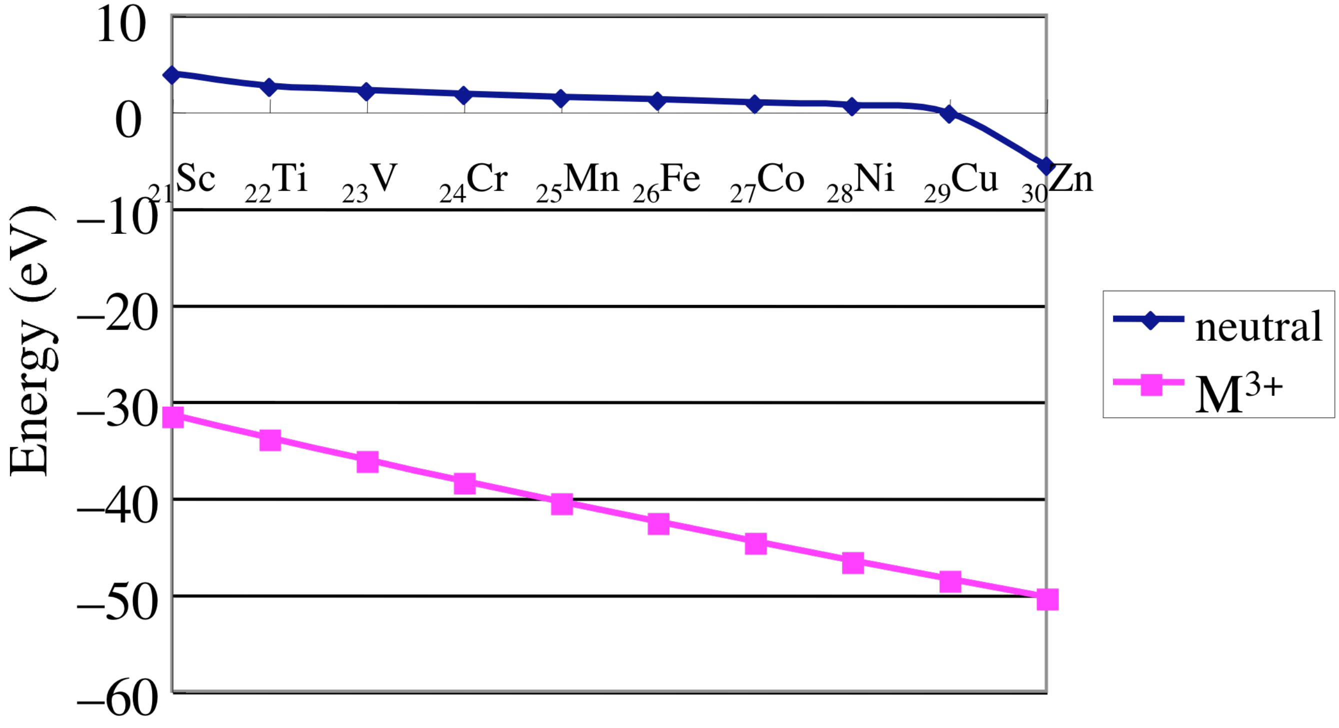


Figure S2. Metal dependences of the relative *3d* atomic orbital energy levels of neutral (blue line) and trivalent ion (purple line). The numbers shown on the horizontal axis denote the atomic number (*Z*) of the metal.

Table S3. Calculated energy level of each atomic orbital of chrome atom.

Orbital	Energy (eV)	Occupancy (electrons)
1s	–5821.13	2.00
2s	–652.18	2.00
2p(0)	–554.67	2.00
2p(1)	–554.67	2.00
2p(–1)	–554.67	2.00
3s	–67.23	2.00
3p(–1)	–40.18	2.00
3p(1)	–40.18	2.00
3p(0)	–40.18	2.00
3d(–1)	1.63	2.00
3d(1)	1.63	2.00
4s	1.63	2.00
3d(2)	1.63	0.00
3d(–2)	1.64	0.00
3d(0)	1.65	0.00
4p(1)	6.47	0.00
4p(–1)	6.47	0.00
4p(0)	6.49	0.00

Table S4. Calculated energy level of each atomic orbital of chrome atom including the Gaussian distribution among *4s* and five *3d* atomic orbitals.

Orbital	Energy (eV)	Occupancy (electrons)
1s	–5820.99	2.00
2s	–652.04	2.00
2p(0)	–554.53	2.00
2p(1)	–554.53	2.00
2p(–1)	–554.53	2.00
3s	–67.14	2.00
3p(–1)	–40.10	2.00
3p(1)	–40.10	2.00
3p(0)	–40.10	2.00
4s	1.65	1.60
3d(–1)	1.70	0.95
3d(1)	1.70	0.95
3d(2)	1.70	0.90
3d(–1)	1.70	0.88
3d(0)	1.71	0.72
4p(1)	6.48	0.00
4p(–1)	6.49	0.00
4p(0)	6.51	0.00

Table S5. Averaged energy level of the five *3d* (and *4s*) atomic orbitals.

Z	21	22	23	24	25
Atom	Sc	Ti	V	Cr	Mn
4s	2	2	2	1	2
3d	1	2	3	5	5
Energy (eV)	3.75	2.49	2.05	1.69	1.36
Orbital	3d	4s+3d			

Z	26	27	28	29	30
Atom	Fe	Co	Ni	Cu	Zn
4s	2	2	2	1	2
3d	6	7	8	10	10
Energy (eV)	1.06	0.79	0.52	-0.25	-5.68
Orbital	4s+3d			3d	

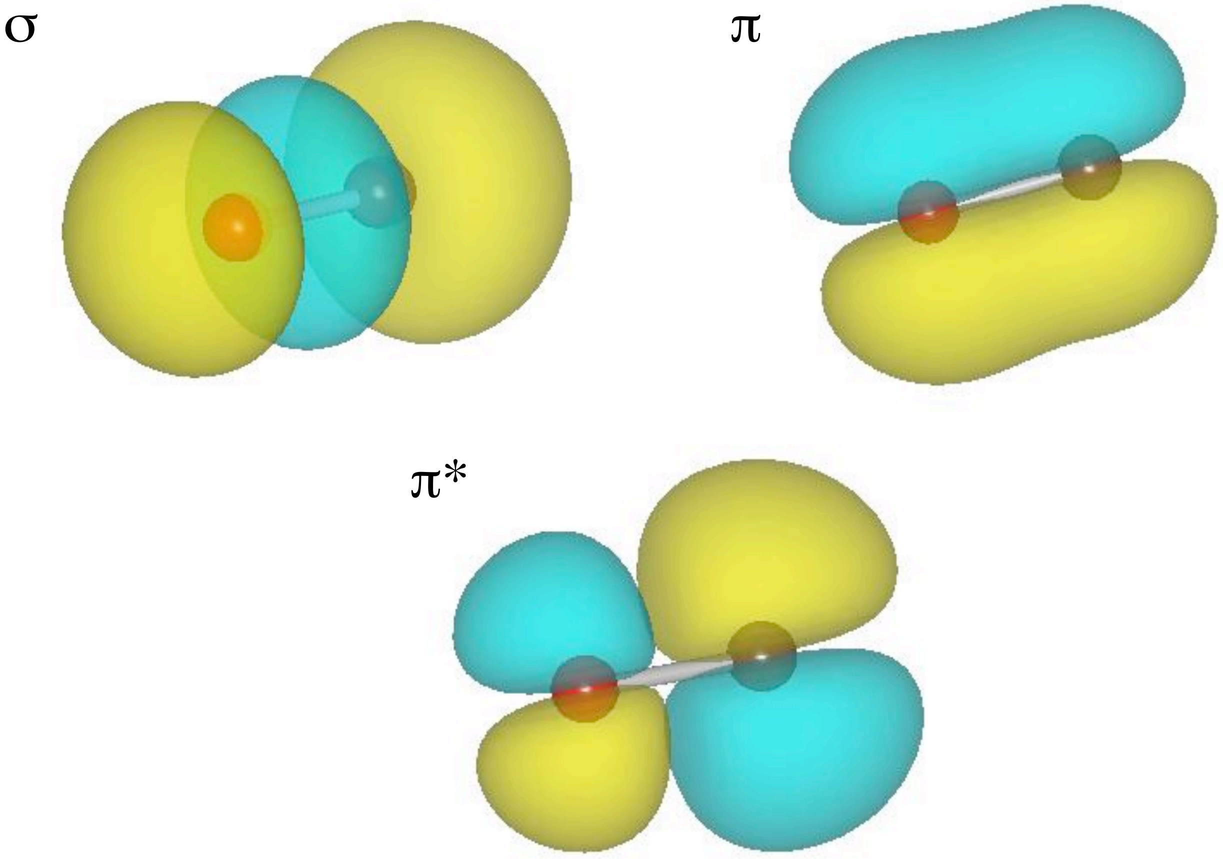


Figure S6. 3D Visualizations of σ-, π- and π*-molecular orbitals of carbonyl CO ligand.

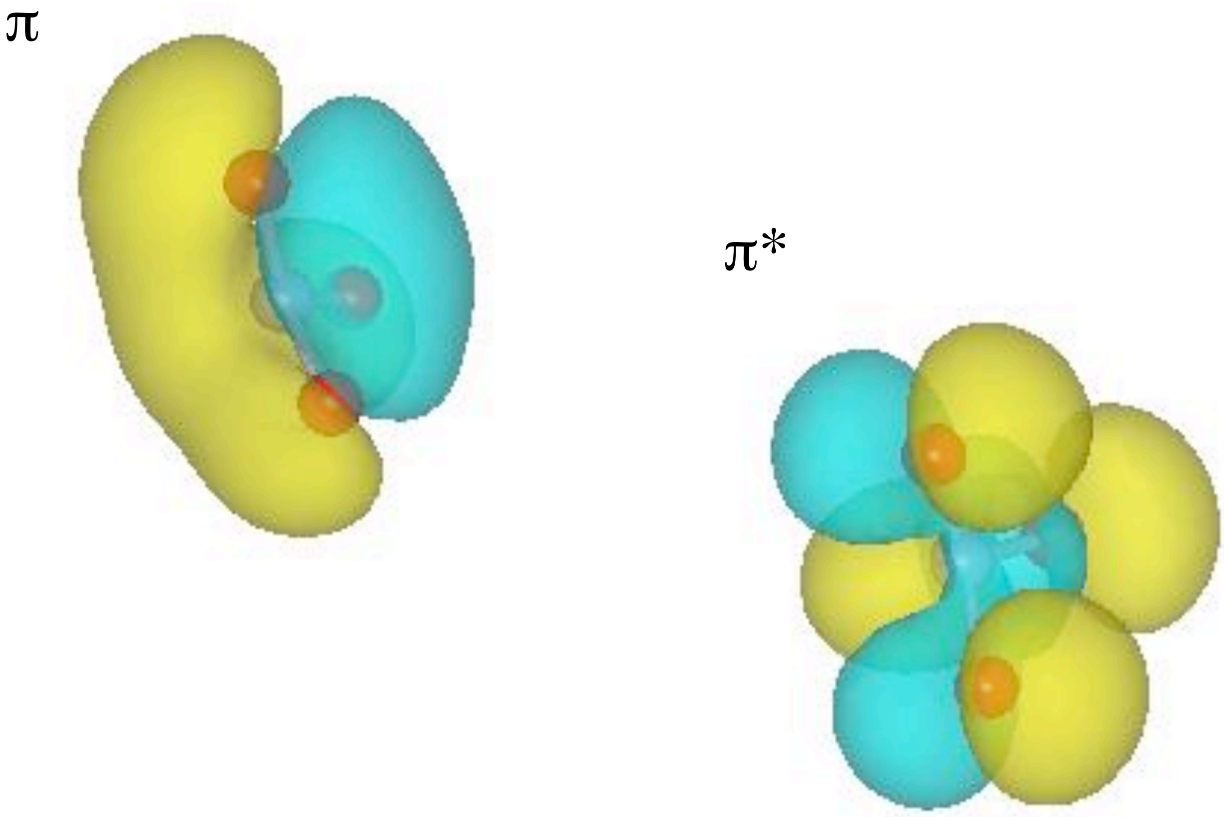


Figure S7. 3D Visualizations of π- and π*-molecular orbitals of nitrate NO_3^- ligand.

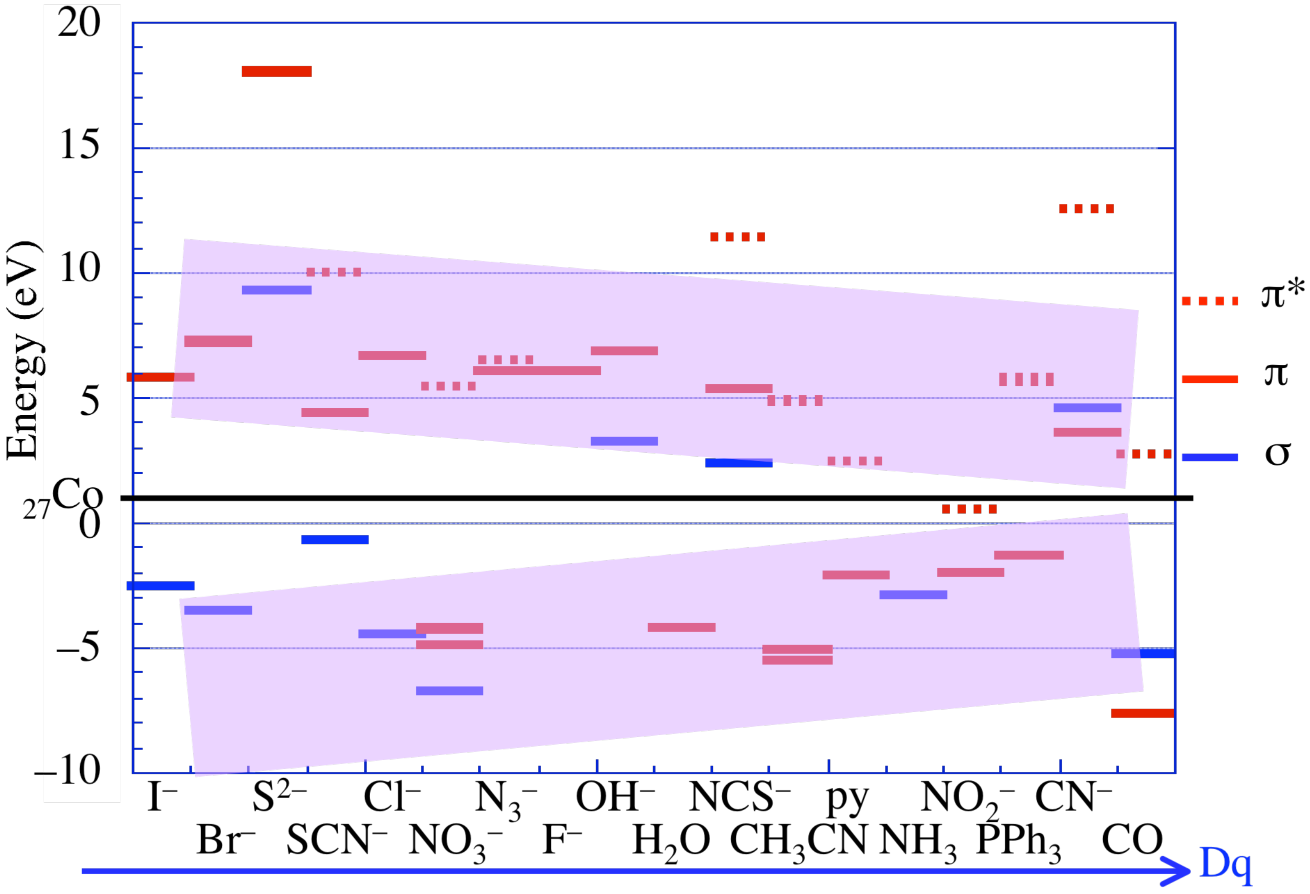


Figure S8. Ligand molecule dependence of relative energy levels of σ-, π- and π*-molecular orbitals. Two purple rectangles denote their relationship.

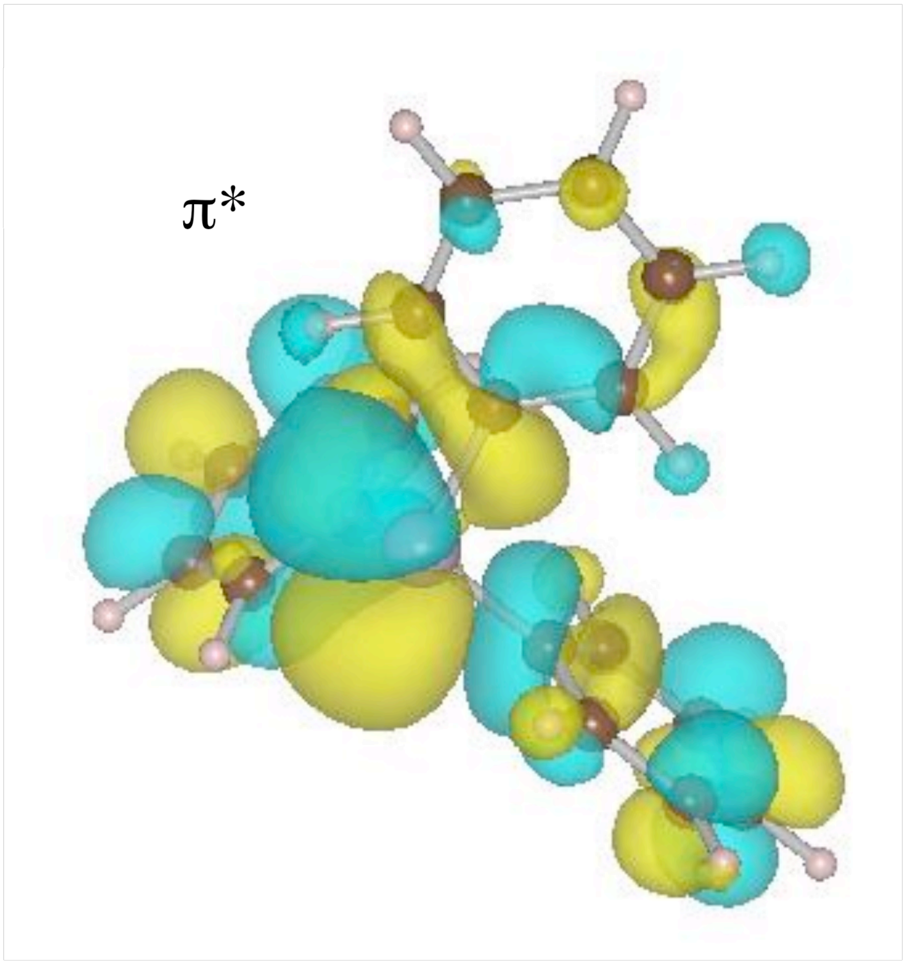
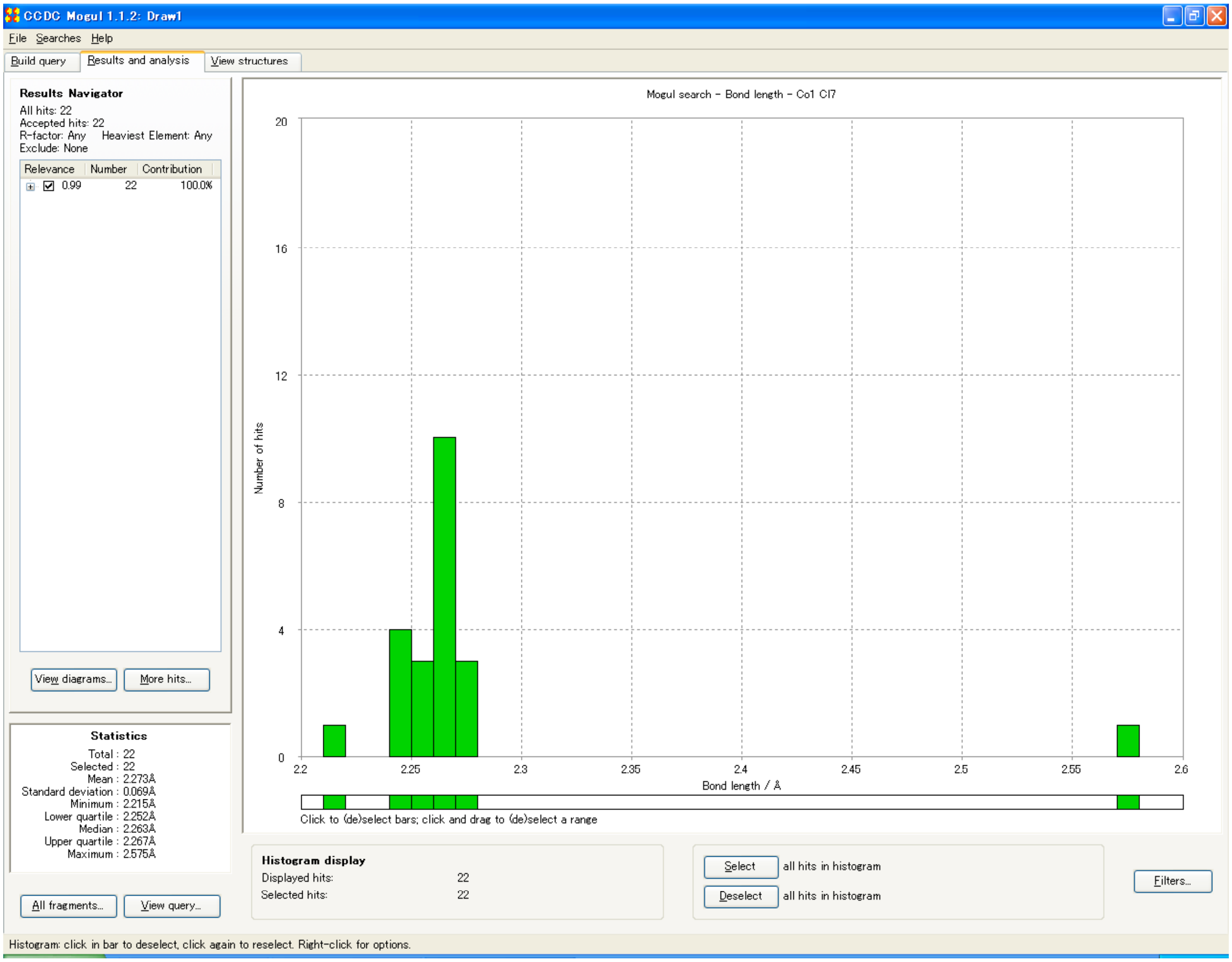


Figure S9. 3D Visualization of π*-molecular orbital of triphenylphosphine ligand PPh_3.



Results Navigator

All hits: 22
Accepted hits: 22
R-factor: Any Heaviest Element: Any
Exclude: None

Relevance	Number	Contribution
⊞ ☑ 0.99	22	100.0%

Statistics

Total : 22
Selected : 22
Mean : 2.273Å
Standard deviation : 0.069Å
Minimum : 2.215Å
Lower quartile : 2.252Å
Median : 2.263Å
Upper quartile : 2.267Å
Maximum : 2.575Å

Click to (de)select bars; click and drag to (de)select a range

Histogram display

Displayed hits: 22
Selected hits: 22

Select all hits in histogram
Deselect all hits in histogram

Histogram: click in bar to deselect, click again to reselect. Right-click for options.

Figure S10. Example of statistical analysis of a coordination bond distance between cobalt metal and cyanide ligand in $[M(CN)(NH_3)_5]^{3+}$ metal complex by *The MOGUL* application.

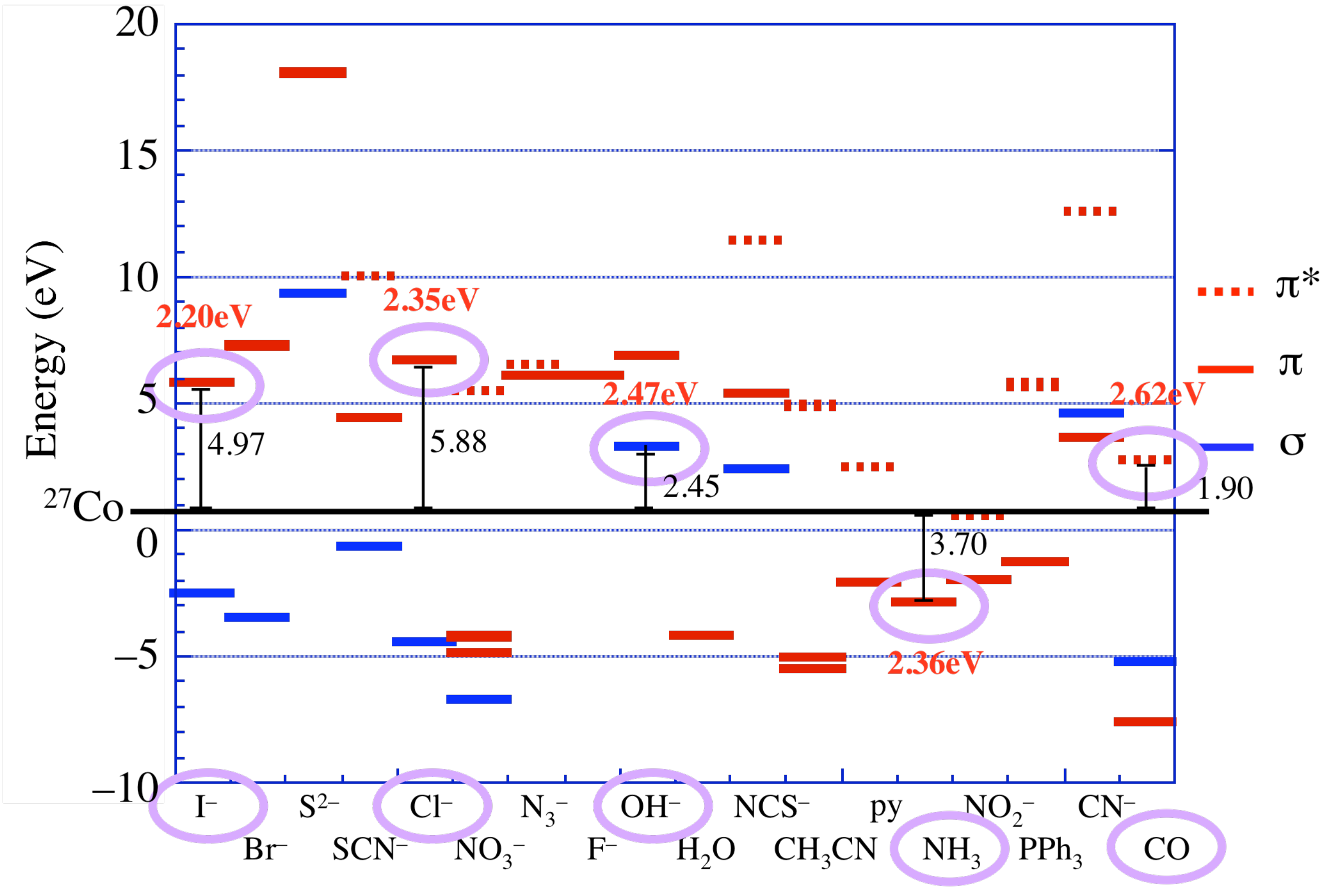


Figure S11. Relative energy differences of *3d* atomic orbitals of a cobalt ion and the σ-, π- and π*-molecular orbitals of ligands. Black values written in this figure denote the energy differences. Red values are calculated Δ_0 of the ligands marked by purple ellipsoids discussed in Fig. 3.

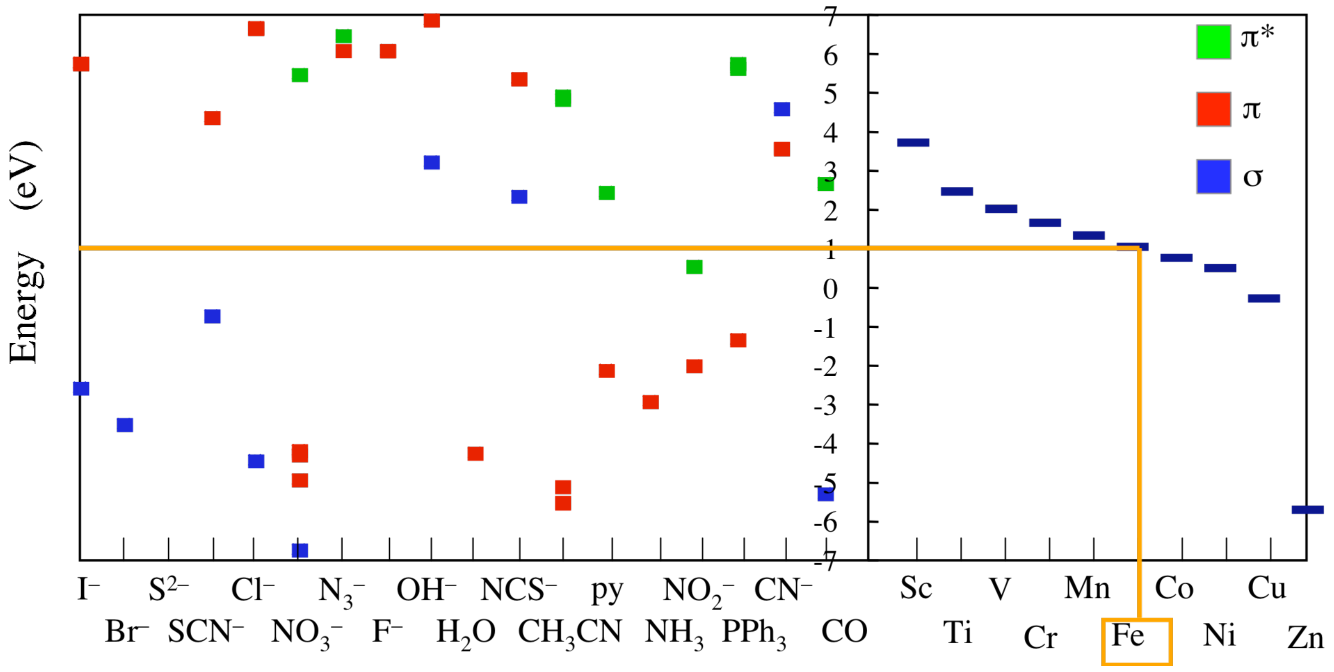


Figure S12. Relative energy levels of both the *3d* orbitals of an iron ion and the σ-, π- and π*-molecular orbitals of the ligands. Orange horizontal line denote their relative energy level relationship.

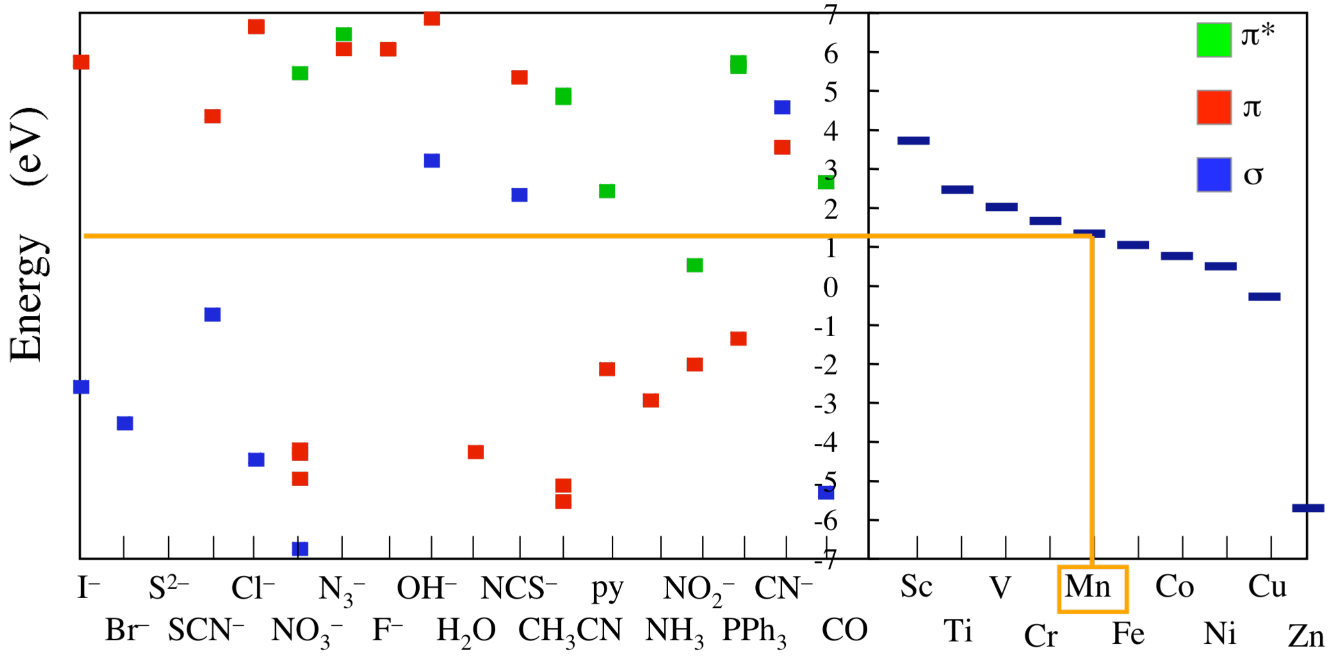


Figure S13. Relative energy levels of both the *3d* orbitals of a manganese ion and the σ-, π- and π*-molecular orbitals of the ligands. Orange horizontal line denote their relative energy level relationship.

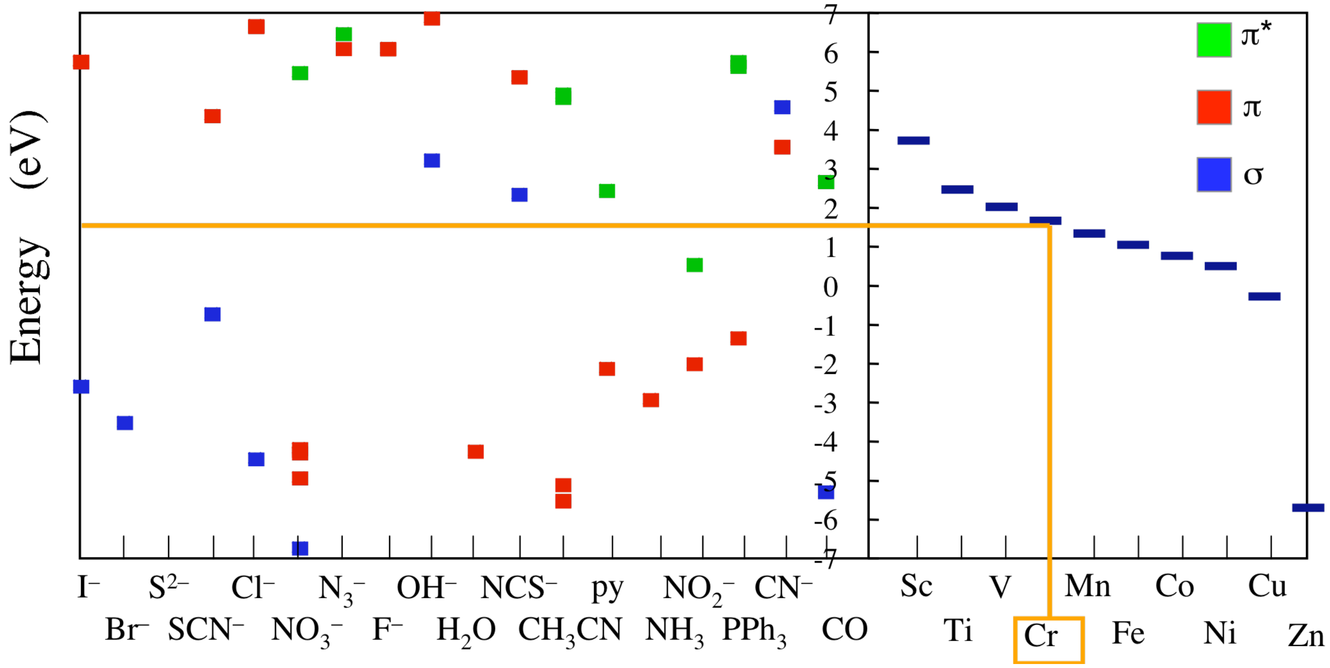


Figure S14. Relative energy levels of both the *3d* orbitals of a chrome ion and the σ-, π- and π*-molecular orbitals of the ligands. Orange horizontal line denote their relative energy level relationship.