

Searching for Hidden Descriptors in the Metal-Ligand Bond through Statistical Analysis of Density Functional Theory (DFT) Results

Oier Lakuntza^[a], Maria Besora^[a] and Feliu Maseras^[a,b]

^[a] *Institute of Chemical Research of Catalonia (ICIQ), The Barcelona Institute of Science and Technology, Avda. Països Catalans, 16, 43007 Tarragona, Catalonia, Spain*

^[b] *Universitat Autònoma de Barcelona (UAB), Departament de Química, 08193 Bellaterra, Catalonia, Spain*

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1 More details on the statistical analysis: matrix decomposition

In this section we extend the information available in the "Statistical analysis: matrix decomposition" section of the main text. We describe here in detail our procedure to extract information from the **BDE** matrix.

This procedure starts with a singular value decomposition analysis (SVD).^{1,2} SVD is a statistical procedure, based on the factorization of a matrix. It is the generalization of the eigendecomposition of a positive semidefinite normal matrix. Formally, the singular value decomposition of an $m \times n$ **BDE** matrix is a factorization of the form $\mathbf{M} \times \mathbf{W} \times \mathbf{L}^T$ where $\mathbf{M}$ is an $m \times m$ unitary matrix, $\mathbf{W}$ is a $m \times n$ diagonal matrix and $\mathbf{L}$ is a $n \times n$ unitary matrix ($\mathbf{L}^T = \mathbf{L}^*$ is the transposed form of the $\mathbf{L}$ matrix). The diagonal entries $\mathbf{W}$ are known as the singular values of **BDE**. The columns of $\mathbf{M}$ and the columns of $\mathbf{L}$ are called the left-singular vectors and right-singular vectors of **BDE** and are a set of orthonormal eigenvectors. The value for any element of BDE can be obtained from the expression in equation 1.

$$\mathbf{BDE}_{i,j} = \mathbf{M}_i \cdot \mathbf{W} \cdot \mathbf{L}_j^T \quad (1)$$

For the purposes of this study, equation 1 has the desired form, providing the binding energy $\mathbf{BDE}_{i,j}$ between a metal fragment i and a ligand j as a function of a vector $\mathbf{M}_i$ related to the metal fragment and a vector $\mathbf{L}_j$ related to the ligand, thus separating the contribution of ligands and metal fragments. The number of elements in the vectors is the number of singular values used in the singular value decomposition from where these equations derive. Please note that exactly equal results are obtained if we use the transposed **BDE** matrix (ligands in rows and metal fragments in columns).

The key feature of the SVD is that the importance of the weights in matrix $\mathbf{W}$ is hierarchical with the first one being the largest, thus most important. So, SVD can be used to reduce a high-dimensional dataset into fewer dimensions while retaining the most important information. This is done by reducing the number of hidden descriptors from m (or n) to a smaller number k . The $\mathbf{M}$ matrix is pruned from an $m \times m$ matrix to $m \times k$, we will call this smaller matrix $\mathbf{HD}_M$. The $\mathbf{L}$ matrix, originally $n \times n$ will be reduced to $n \times k$, and will be called $\mathbf{HD}_L$. Similarly the rectangular diagonal matrix $\mathbf{W}$ will become square, with dimensions $k \times k$, and w will be labeled as $\mathbf{HD}_W$. As the weights are ordered by their importance taking the firsts k weights/hidden descriptors results in taking the most relevant information. With that, the recovered **BDE** matrix will have the original $m \times n$ size but will be less accurate. The loss of accuracy comes from the dimension reduction in matrices $\mathbf{M}$, $\mathbf{W}$ and $\mathbf{L}$, that will be smaller, see Figure 1 of the main text.

SVD follows a procedure similar to that used in the popular Principal Components Analysis (PCA),³ in fact SVD is sometimes used to find a fast solution for PCA. Both are eigenvalue methods used to reduce a high-dimensional dataset into fewer dimensions and both usually work with the covariance matrix.⁴ However there are important

differences, PCA works only on centered data while SVD can work on centered and not centered data. When the data is centered, the covariance matrix equals to $\mathbf{X}^T\mathbf{X}/(n-1)$ and the PCA loadings will be the same as $\mathbf{L}$ and the PCA scores are the result of the $\mathbf{MW}$ product. The PCA scores will be descriptors for our metal fragments but their shape will not be the nice unitary matrix $\mathbf{M}$. We believe matrices $\mathbf{M}$ and $\mathbf{W}$ are easier to understand separately, the first giving the contribution of the metal fragments and the second the importance of each weight/hidden descriptor.

References

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2 Initial set (B3LYP-D3 in vacuum)

2.1 Multiplicity and geometrical structure associated to each metal fragment

We considered an initial training set constituted by 22 ligands: Br^- , CH_3^- , Cl^- , CN^- , CO , F^- , C_6H_5^- , H_2 , H_2O , H^- , I^- , NCH , NCS^- , NH_3 , NHC , O^{2-} , OH^- , PH_3 , $\text{C}_5\text{H}_5\text{N}$, S^{2-} , SCN^- , SH^- and 23 metal fragments: AlCl_3 , AuPH_3^+ , $\text{Co}(\text{NH}_3)_5^{3+}$, CrO_3 , $\text{Cu}(\text{NH}_3)_3^{2+}$, FeCl_2^+ , $\text{Fe}(\text{CO})_4$, $\text{IrCO}(\text{PH}_3)_2^+$, K^+ , MnO_3^+ , $\text{Mo}(\text{SH})_3^+$, $\text{Nb}(\text{NH}_2)_4^+$, OsO_3^{2+} , $\text{PdH}(\text{PH}_3)_2^+$, PdPH_3 , PtF_5^- , $\text{Rh}(\text{H}_2\text{O})_5^{3+}$, $\text{Ru}(\text{SH})_4$, TaMe_4^+ , TiCl_3^+ , $\text{W}(\text{CO})_5$, ZnCH_3^+ and ZrCl_5^- . We computed the bond dissociation energies (BDEs) for all combinations between these 23 metal fragments and 22 ligands. Some of the resulting metal fragments may have different stable forms with different multiplicities and geometrical arrangements. These variations would interfere in our study, and for this reason we chose a single arrangement for each metal fragment. This arrangement was the one most common in the metal fragments where it was involved. The favored multiplicity and geometry for each metallic fragment is collected in Table S1.

Such a problem did not exist for the ligands, which were on the singlet state and bound to the metal through its donor atom.

Table S1: Geometry structure and multiplicity state of the metal fragments, L-[M].

Metal fragment	Geometry	Multiplicity	Metal fragment	Geometry	Multiplicity
L- AlCl_3	Trigonal pyramid	Singlet	L- OsO_3^{2+}	Trigonal pyramid	Singlet
L- AuPH_3^+	Linear	Singlet	L- $\text{PdH}(\text{PH}_3)_2^+$	Planar (trans)	Singlet
L- $\text{Co}(\text{NH}_3)_5^{3+}$	Octahedral	Singlet	L- PdPH_3	Linear	Singlet
L- CrO_3	Trigonal pyramid	Singlet	L- PtF_5^-	Octahedral	Singlet
L- $\text{Cu}(\text{NH}_3)_3^{2+}$	Planar	Doublet	L- $\text{Rh}(\text{H}_2\text{O})_5^{3+}$	Octahedral	Singlet
L- FeCl_2^+	Planar	Sextet	L- $\text{Ru}(\text{SH})_4$	Trigonal bipyramid	Singlet
L- $\text{Fe}(\text{CO})_4$	Trigonal bipyramid	Singlet	L- TaMe_4^+	Tetragonal pyramid	Singlet
L- $\text{IrCO}(\text{PH}_3)_2^+$	Planar (trans)	Singlet	L- TiCl_3^+	Trigonal pyramid	Singlet
L- K^+		Singlet	L- $\text{W}(\text{CO})_5$	Octahedral	Singlet
L- MnO_3^+	Trigonal pyramid	Singlet	L- ZnCH_3^+	Linear	Singlet
L- $\text{Mo}(\text{SH})_3^+$	Trigonal pyramid	Singlet	L- ZrCl_5^-	Octahedral	Singlet
L- $\text{Nb}(\text{NH}_2)_4^+$	Tetragonal pyramid	Singlet			

2.2 BDE matrix of the Initial Training Set

The matrix of bond dissociation energies in vacuum and B3LYP-D3 for the Initial Training Set is presented in Table S2. This is the matrix **BDE**, the starting point of the statistical analysis.

Table S2: Bond dissociation energies (kcal/mol) for the Initial Training Set. Calculations in vacuum with the B3LYP-D3 functional. Results are split in two separate tables, part A and part B.

Table S2, PART A										
	Br ⁻	CH ₃ ⁻	Cl ⁻	CN ⁻	CO	F ⁻	C ₆ H ₅ ⁻	H ₂	H ₂ O	H ⁻
AlCl ₃	-62.3	-118.6	-73.3	-80.8	-11.5	-116.2	-107.9	0.9	-25.8	-149.1
AuPH ₃ ⁺	-154.0	-218.7	-159.6	-174.5	-37.8	-176.7	-205.5	-12.8	-35.9	-255.9
Co(NH ₃) ₅ ³⁺	-333.75	-410.35	-341.65	-346.75	-31.45	-376.35	-405.05	-8.85	-49.25	-445.75
CrO ₃	-80.0	-142.1	-88.2	-101.2	-34.1	-122.4	-131.3	-12.0	-39.2	-175.8
Cu(NH ₃) ₃ ²⁺	-231.4	-295.0	-238.4	-240.5	-16.3	-268.1	-283.0	-3.4	-34.6	-327.5
FeCl ₂ ⁺	-192.9	-254.8	-201.2	-197.4	-26.0	-233.7	-243.4	-8.2	-48.5	-280.9
Fe(CO) ₄	-47.1	-102.1	-51.2	-72.2	-36.6	-70.6	-93.1	-10.0	-17.7	-148.2
IrCO(PH ₃) ₂ ⁺	-148.3	-205.3	-154.8	-170.7	-44.8	-178.4	-198.6	-15.5	-33.0	-246.7
K ⁺	-102.6	-125.4	-107.8	-105.8	-6.1	-128.1	-114.3	-1.2	-17.7	-164.5
MnO ₃ ⁺	-233.1	-325.2	-240.4	-247.7	-54.4	-271.8	-309.5	-23.8	-70.0	-352.0
Mo(SH) ₃ ⁺	-174.9	-240.6	-185.3	-185.7	-41.4	-222.5	-228.6	-15.1	-42.8	-265.7
Nb(NH ₂) ₄ ⁺	-116.5	-169.4	-126.6	-129.3	-4.8	-168.3	-157.8	6.6	-16.9	-205.5
OsO ₃ ²⁺	-413.8	-517.8	-419.4	-418.3	-82.1	-439.7	-522.5	-35.5	-110.0	-529.8
PdH(PH ₃) ₂ ⁺	-128.0	-179.0	-133.0	-144.2	-25.1	-151.6	-170.1	-6.3	-22.7	-219.4
PdPH ₃	-32.4	-64.3	-35.9	-49.5	-36.1	-47.9	-60.3	-10.6	-13.9	-103.1
PtF ₅ ⁻	25.9	-44.1	21.6	-10.8	-39.1	0.7	-45.2	-7.4	-29.9	-78.3
Rh(H ₂ O) ₅ ³⁺	-375.0	-465.5	-381.6	-392.0	-58.7	-405.1	-466.3	-24.6	-67.7	-498.7
Ru(SH) ₄	-47.3	-99.7	-52.2	-70.4	-28.3	-74.7	-89.5	-1.4	-18.2	-140.6
TaMe ₄ ⁺	-180.8	-238.9	-193.0	-189.3	-27.6	-236.2	-225.9	-6.3	-46.4	-264.4
TiCl ₃ ⁺	-197.7	-262.9	-210.5	-202.9	-31.6	-255.0	-249.5	-10.0	-55.2	-285.1
W(CO) ₅	-55.6	-101.8	-60.2	-77.3	-41.7	-81.9	-95.7	-12.7	-21.2	-144.6
ZnCH ₃ ⁺	-175.3	-235.0	-183.2	-186.2	-21.7	-210.1	-219.5	-5.9	-41.0	-267.1
ZrCl ₅ ⁻	38.5	-5.1	30.5	21.4	-6.5	-10.1	2.0	-0.3	-13.6	-36.1

Table S2, PART B

	I ⁻	NCH	NCS ⁻	NH ₃	NHC	O ²⁻	OH ⁻	PH ₃	C ₅ H ₅ N	S ²⁻	SCN ⁻	SH ⁻
AlCl ₃	-52.6	-21.9	-72.2	-37.4	-56.4	-252.0	-121.1	-18.8	-41.0	-151.3	-54.3	-78.2
AuPH ₃ ⁺	-151.5	-43.5	-147.2	-55.7	-91.3	-391.2	-191.5	-53.8	-62.2	-315.1	-146.0	-174.9
Co(NH ₃) ₅ ³⁺	-327.75	-63.05	-331.45	-64.85	-117.65	-783.75	-390.55	-56.15	-95.35	-678.15	-321.15	-356.35
CrO ₃	-73.8	-39.5	-85.7	-56.4	-81.5	-267.8	-131.4	-44.4	-59.7	-159.0	-75.9	-98.0
Cu(NH ₃) ₃ ²⁺	-226.0	-40.6	-226.9	-47.7	-85.0	-572.9	-279.8	-36.8	-65.9	-482.9	-219.9	-251.0
FeCl ₂ ⁺	-187.2	-49.1	-195.8	-62.2	-98.5	-514.9	-251.6	-48.0	-77.4	-408.3	-179.7	-217.5
Fe(CO) ₄	-44.1	-24.5	-49.5	-31.0	-56.8	-179.2	-79.4	-30.6	-32.0	-116.1	-45.5	-62.5
IrCO(PH ₃) ₂ ⁺	-143.3	-42.7	-146.8	-47.7	-83.7	-396.0	-189.4	-45.2	-58.4	-313.2	-141.3	-165.8
K ⁺	-96.9	-18.9	-98.9	-19.3	-28.3	-285.1	-133.5	-10.6	-22.4	-218.4	-91.7	-107.9
MnO ₃ ⁺	-229.9	-76.4	-234.0	-98.5	-149.1	-573.8	-293.8	-94.8	-117.6	-453.6	-225.4	-263.3
Mo(SH) ₃ ⁺	-167.5	-48.0	-179.8	-54.8	-93.9	-521.4	-240.5	-47.6	-69.9	-392.5	-167.3	-199.5
Nb(NH ₂) ₄ ⁺	-107.3	-16.9	-120.6	-23.9	-44.2	-422.2	-176.2	-9.9	-30.1	-294.1	-105.6	-131.4
OsO ₃ ²⁺	-417.9	-129.0	-434.0	-147.2	-245.5	-912.0	-478.4	-159.3	-203.4	-795.0	-403.5	-453.9
PdH(PH ₃) ₂ ⁺	-124.1	-28.5	-121.6	-34.0	-61.2	-346.1	-161.4	-30.5	-41.1	-278.8	-122.0	-143.0
PdPH ₃	-30.5	-21.1	-34.9	-24.3	-43.5	-146.5	-54.5	-29.1	-24.7	-80.2	-31.7	-43.0
PtF ₅ ⁻	27.8	-23.7	11.2	-46.3	-77.1	-32.7	-13.5	-39.6	-48.9	34.5	16.1	5.1
Rh(H ₂ O) ₅ ³⁺	-374.6	-86.2	-374.3	-94.2	-166.2	-846.9	-429.1	-97.1	-132.2	-749.0	-367.8	-405.5
Ru(SH) ₄	-42.1	-23.0	-50.4	-28.5	-54.1	-226.1	-81.3	-28.7	-31.1	-130.8	-44.8	-60.6
TaMe ₄ ⁺	-170.7	-49.6	-186.8	-58.5	-88.5	-515.0	-248.8	-41.7	-71.9	-385.1	-163.7	-198.4
TiCl ₃ ⁺	-188.1	-56.2	-205.8	-69.7	-103.4	-557.7	-270.8	-52.5	-84.4	-418.8	-181.7	-218.8
W(CO) ₅	-52.3	-30.5	-59.3	-33.2	-58.0	-202.4	-87.8	-34.0	-36.8	-125.8	-52.4	-68.9
ZnCH ₃ ⁺	-169.0	-43.4	-170.1	-56.7	-87.8	-427.4	-222.5	-43.2	-66.8	-345.2	-160.3	-193.1
ZrCl ₅ ⁻	45.3	-3.9	24.3	-21.2	-32.8	-108.0	-15.5	-7.0	-18.3	14.9	39.1	25.9

2.3 Hidden descriptor tables of the Initial Training Set

We performed a Singular Value Decomposition analysis of the BDE matrix resulting in the Left and right-singular vectors as explained in the main text, we will call hidden descriptors $\mathbf{HD}_{Lk}$ for the ligands and hidden descriptors $\mathbf{HD}_{Mk}$ for the metal fragments. Please note that $\mathbf{HD}_{Lk} = \mathbf{L}_k$ and $\mathbf{HD}_{Mk} = \mathbf{M}_k$ for $n=1-6$. Tables S3 and S4 report the values for the first seven hidden descriptors for each ligand and metal fragment, respectively. In the Tables S5 and S6 the same values appear ordered in decreasing order and with the corresponding name of the ligand next to it. This arrangement allows for an easier visualization of the ligands having larger and lower values for a given k .

The SVD analysis was performed with the script presented in Section 9.1 of this Supporting Information.

Table S3: First seven hidden descriptors of the ligands for the Initial Training Set. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

Ligand	$\mathbf{HD}_{L1} = \mathbf{L}_1$	$\mathbf{HD}_{L2} = \mathbf{L}_2$	$\mathbf{HD}_{L3} = \mathbf{L}_3$	$\mathbf{HD}_{L4} = \mathbf{L}_4$	$\mathbf{HD}_{L5} = \mathbf{L}_5$	$\mathbf{HD}_{L6} = \mathbf{L}_6$	$\mathbf{L}_7$
Br^-	0.193	-0.275	-0.077	0.008	0.042	0.195	-0.172
CH_3^-	0.253	0.083	-0.142	-0.179	0.218	-0.176	-0.022
Cl^-	0.199	-0.223	-0.038	0.040	0.123	0.250	-0.072
CN^-	0.204	-0.093	-0.098	-0.278	0.020	0.059	0.243
CO	0.034	0.176	-0.211	-0.142	-0.457	0.431	0.459
F^-	0.225	0.005	0.119	0.142	0.429	0.253	0.309
C_6H_5^-	0.246	0.011	-0.214	-0.137	0.034	-0.489	0.415
H_2	0.012	0.023	-0.116	-0.006	-0.180	0.282	0.136
H_2O	0.044	0.114	-0.157	0.223	0.145	0.093	-0.105
H^-	0.280	0.366	-0.035	-0.671	0.155	0.116	-0.290
I^-	0.189	-0.323	-0.139	0.000	-0.063	0.114	-0.260
NCH	0.050	0.083	-0.192	0.121	-0.074	0.259	0.012
NCS^-	0.195	-0.212	-0.121	0.197	-0.010	-0.058	0.195
NH_3	0.059	0.189	-0.238	0.190	0.164	0.067	-0.189
NHC	0.099	0.284	-0.378	0.148	-0.069	-0.237	-0.039
O^{2-}	0.484	0.430	0.507	0.290	-0.274	0.001	-0.057
OH^-	0.239	0.048	0.059	0.192	0.359	0.172	0.157
PH_3	0.054	0.117	-0.350	0.119	-0.257	0.082	-0.305
$\text{C}_5\text{H}_5\text{N}$	0.077	0.140	-0.310	0.285	0.051	-0.189	0.013
S^{2-}	0.394	-0.283	0.189	-0.003	-0.372	-0.221	-0.112
SCN^-	0.184	-0.278	-0.142	-0.043	-0.102	-0.055	0.073
SH^-	0.213	-0.176	-0.117	0.005	0.038	0.076	-0.178

Table S4: First seven hidden descriptors of the metal fragments for the Initial Training Set. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

Metal Frag.	$\text{HD}_{M1} = \text{M}_1$	$\text{HD}_{M2} = \text{M}_2$	$\text{HD}_{M3} = \text{M}_3$	$\text{HD}_{M4} = \text{M}_4$	$\text{HD}_{M5} = \text{M}_5$	$\text{HD}_{M6} = \text{M}_6$	M_7
AlCl_3	-0.095	-0.237	-0.097	-0.054	-0.419	0.092	-0.222
AuPH_3^+	-0.177	-0.077	0.075	0.245	0.012	-0.067	0.305
$\text{Co}(\text{NH}_3)_5^{3+}$	-0.355	0.254	-0.207	0.223	-0.106	0.171	-0.331
CrO_3	-0.110	-0.274	0.120	-0.021	-0.296	-0.231	-0.137
$\text{Cu}(\text{NH}_3)_3^{2+}$	-0.253	0.118	-0.215	0.178	-0.135	0.221	0.137
FeCl_2^+	-0.220	-0.032	-0.098	-0.151	-0.051	0.038	0.242
$\text{Fe}(\text{CO})_4$	-0.075	-0.238	0.075	0.326	0.067	-0.052	-0.016
$\text{IrCO}(\text{PH}_3)_2^+$	-0.173	-0.084	0.003	0.197	0.158	-0.218	-0.232
K^+	-0.116	-0.005	-0.220	0.095	-0.094	-0.281	0.327
MnO_3^+	-0.262	-0.105	0.256	-0.059	-0.164	-0.145	0.244
$\text{Mo}(\text{SH})_3^+$	-0.211	-0.110	-0.175	-0.197	0.334	-0.124	-0.226
$\text{Nb}(\text{NH}_2)_4^+$	-0.154	-0.130	-0.440	-0.051	0.109	0.282	0.079
OsO_3^{2+}	-0.437	0.151	0.538	-0.383	0.192	0.153	0.152
$\text{PdH}(\text{PH}_3)_2^+$	-0.150	-0.048	-0.088	0.276	0.072	0.046	0.192
PdPH_3	-0.054	-0.212	0.038	0.130	0.320	-0.272	0.034
PtF_5^-	-0.011	-0.451	0.352	0.164	-0.167	0.415	-0.234
$\text{Rh}(\text{H}_2\text{O})_5^{3+}$	-0.397	0.248	0.085	0.195	0.166	0.163	-0.230
$\text{Ru}(\text{SH})_4$	-0.080	-0.272	-0.068	0.126	0.274	0.117	0.222
TaMe_4^+	-0.211	-0.080	-0.184	-0.263	-0.106	-0.235	-0.193
TiCl_3^+	-0.231	-0.092	-0.141	-0.350	-0.083	-0.203	-0.106
$\text{W}(\text{CO})_5$	-0.081	-0.229	0.063	0.176	0.160	-0.292	-0.183
ZnCH_3^+	-0.194	-0.014	0.002	0.115	-0.424	-0.106	0.236
ZrCl_5^-	-0.006	-0.451	-0.191	-0.279	0.136	0.324	0.133

Table S5: First seven hidden descriptors of the ligands for the Initial Training Set, ordered by their values in decreasing order. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

$\text{HD}_{L1} = \mathbf{L}_1$	$\text{HD}_{L2} = \mathbf{L}_2$	$\text{HD}_{L3} = \mathbf{L}_3$	$\text{HD}_{L4} = \mathbf{L}_4$	$\text{HD}_{L5} = \mathbf{L}_5$	$\text{HD}_{L6} = \mathbf{L}_6$	$\mathbf{L}_7$
O^{2-} 0.484	O^{2-} 0.430	O^{2-} 0.507	O^{2-} 0.290	F^- 0.429	CO 0.431	CO 0.459
S^{2-} 0.394	H^- 0.366	S^{2-} 0.189	$\text{C}_5\text{H}_5\text{N}$ 0.285	OH^- 0.359	H_2 0.282	C_6H_5^- 0.415
H^- 0.280	NHC 0.284	F^- 0.119	H_2O 0.223	CH_3^- 0.218	NCH 0.259	F^- 0.309
CH_3^- 0.253	NH_3 0.189	OH^- 0.059	NCS^- 0.197	NH_3 0.164	F^- 0.253	CN^- 0.243
C_6H_5^- 0.246	CO 0.176	H^- -0.035	OH^- 0.192	H^- 0.155	Cl^- 0.250	NCS^- 0.195
OH^- 0.239	$\text{C}_5\text{H}_5\text{N}$ 0.140	Cl^- -0.038	NH_3 0.190	H_2O 0.145	Br^- 0.195	OH^- 0.157
F^- 0.225	PH_3 0.117	Br^- -0.077	NHC 0.148	Cl^- 0.123	OH^- 0.172	H_2 0.136
SH^- 0.213	H_2O 0.114	CN^- -0.098	F^- 0.142	$\text{C}_5\text{H}_5\text{N}$ 0.051	H^- 0.116	SCN^- 0.073
CN^- 0.204	CH_3^- 0.083	H_2 -0.116	NCH 0.121	Br^- 0.042	I^- 0.114	$\text{C}_5\text{H}_5\text{N}$ 0.013
Cl^- 0.199	NCH 0.083	SH^- -0.117	PH_3 0.119	SH^- 0.038	H_2O 0.093	NCH 0.012
NCS^- 0.195	OH^- 0.048	NCS^- -0.121	Cl^- 0.040	C_6H_5^- 0.034	PH_3 0.082	CH_3^- -0.022
Br^- 0.193	H_2 0.023	I^- -0.139	Br^- 0.008	CN^- 0.020	SH^- 0.076	NHC -0.039
I^- 0.189	C_6H_5^- 0.011	CH_3^- -0.142	SH^- 0.005	NCS^- -0.010	NH_3 0.067	O^{2-} -0.057
SCN^- 0.184	F^- 0.005	SCN^- -0.142	I^- 0.000	I^- -0.063	CN^- 0.059	Cl^- -0.072
NHC 0.099	CN^- -0.093	H_2O -0.157	S^{2-} -0.003	NHC -0.069	O^{2-} 0.001	H_2O -0.105
$\text{C}_5\text{H}_5\text{N}$ 0.077	SH^- -0.176	NCH -0.192	H_2 -0.006	NCH -0.074	SCN^- -0.055	S^{2-} -0.112
NH_3 0.059	NCS^- -0.212	CO -0.211	SCN^- -0.043	SCN^- -0.102	NCS^- -0.058	Br^- -0.172
PH_3 0.054	Cl^- -0.223	C_6H_5^- -0.214	C_6H_5^- -0.137	H_2 -0.180	CH_3^- -0.176	SH^- -0.178
NCH 0.050	Br^- -0.275	NH_3 -0.238	CO -0.142	PH_3 -0.257	$\text{C}_5\text{H}_5\text{N}$ -0.189	NH_3 -0.189
H_2O 0.044	SCN^- -0.278	$\text{C}_5\text{H}_5\text{N}$ -0.310	CH_3^- -0.179	O^{2-} -0.274	S^{2-} -0.221	I^- -0.260
CO 0.034	S^{2-} -0.283	PH_3 -0.350	CN^- -0.278	S^{2-} -0.372	NHC -0.237	H^- -0.290
H_2 0.012	I^- -0.323	NHC -0.378	H^- -0.671	CO -0.457	C_6H_5^- -0.489	PH_3 -0.305

Table S6: First seven hidden descriptors of the metal fragments for the Initial Training Set, ordered by their values in decreasing order. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

$HD_{M1} = \mathbf{M}_1$	$HD_{M2} = \mathbf{M}_2$	$HD_{M3} = \mathbf{M}_3$	$HD_{M4} = \mathbf{M}_4$
AlCl_3 -0.095	AlCl_3 -0.237	AlCl_3 -0.097	AlCl_3 -0.054
AuPH_3^+ -0.177	AuPH_3^+ -0.077	AuPH_3^+ 0.075	AuPH_3^+ 0.245
$\text{Co}(\text{NH}_3)_5^{3+}$ -0.355	$\text{Co}(\text{NH}_3)_5^{3+}$ 0.254	$\text{Co}(\text{NH}_3)_5^{3+}$ -0.207	$\text{Co}(\text{NH}_3)_5^{3+}$ 0.223
CrO_3 -0.110	CrO_3 -0.274	CrO_3 0.120	CrO_3 -0.021
$\text{Cu}(\text{NH}_3)_3^{2+}$ -0.253	$\text{Cu}(\text{NH}_3)_3^{2+}$ 0.118	$\text{Cu}(\text{NH}_3)_3^{2+}$ -0.215	$\text{Cu}(\text{NH}_3)_3^{2+}$ 0.178
FeCl_2^+ -0.220	FeCl_2^+ -0.032	FeCl_2^+ -0.098	FeCl_2^+ -0.151
$\text{Fe}(\text{CO})_4$ -0.075	$\text{Fe}(\text{CO})_4$ -0.238	$\text{Fe}(\text{CO})_4$ 0.075	$\text{Fe}(\text{CO})_4$ 0.326
$\text{IrCO}(\text{PH}_3)_2^+$ -0.173	$\text{IrCO}(\text{PH}_3)_2^+$ -0.084	$\text{IrCO}(\text{PH}_3)_2^+$ 0.003	$\text{IrCO}(\text{PH}_3)_2^+$ 0.197
K^+ -0.116	K^+ -0.005	K^+ -0.220	K^+ 0.095
MnO_3^+ -0.262	MnO_3^+ -0.105	MnO_3^+ 0.256	MnO_3^+ -0.059
$\text{Mo}(\text{SH})_3^+$ -0.211	$\text{Mo}(\text{SH})_3^+$ -0.110	$\text{Mo}(\text{SH})_3^+$ -0.175	$\text{Mo}(\text{SH})_3^+$ -0.197
$\text{Nb}(\text{NH}_2)_4^+$ -0.154	$\text{Nb}(\text{NH}_2)_4^+$ -0.130	$\text{Nb}(\text{NH}_2)_4^+$ -0.440	$\text{Nb}(\text{NH}_2)_4^+$ -0.051
OsO_3^{2+} -0.437	OsO_3^{2+} 0.151	OsO_3^{2+} 0.538	OsO_3^{2+} -0.383
$\text{PdH}(\text{PH}_3)_2^+$ -0.150	$\text{PdH}(\text{PH}_3)_2^+$ -0.048	$\text{PdH}(\text{PH}_3)_2^+$ -0.088	$\text{PdH}(\text{PH}_3)_2^+$ 0.276
PdPH_3 -0.054	PdPH_3 -0.212	PdPH_3 0.038	PdPH_3 0.130
PtF_5^- -0.011	PtF_5^- -0.451	PtF_5^- 0.352	PtF_5^- 0.164
$\text{Rh}(\text{H}_2\text{O})_5^{3+}$ -0.397	$\text{Rh}(\text{H}_2\text{O})_5^{3+}$ 0.248	$\text{Rh}(\text{H}_2\text{O})_5^{3+}$ 0.085	$\text{Rh}(\text{H}_2\text{O})_5^{3+}$ 0.195
$\text{Ru}(\text{SH})_4$ -0.080	$\text{Ru}(\text{SH})_4$ -0.272	$\text{Ru}(\text{SH})_4$ -0.068	$\text{Ru}(\text{SH})_4$ 0.126
TaMe_4^+ -0.211	TaMe_4^+ -0.080	TaMe_4^+ -0.184	TaMe_4^+ -0.263
TiCl_3^+ -0.231	TiCl_3^+ -0.092	TiCl_3^+ -0.141	TiCl_3^+ -0.350
$\text{W}(\text{CO})_5$ -0.081	$\text{W}(\text{CO})_5$ -0.229	$\text{W}(\text{CO})_5$ 0.063	$\text{W}(\text{CO})_5$ 0.176
ZnCH_3^+ -0.194	ZnCH_3^+ -0.014	ZnCH_3^+ 0.002	ZnCH_3^+ 0.115
ZrCl_5^- -0.006	ZrCl_5^- -0.451	ZrCl_5^- -0.191	ZrCl_5^- -0.279

$HD_{M5} = \mathbf{M}_5$	$HD_{M6} = \mathbf{M}_6$	$\mathbf{M}_7$
AlCl_3 -0.419	AlCl_3 0.092	AlCl_3 -0.222
AuPH_3^+ 0.012	AuPH_3^+ -0.067	AuPH_3^+ 0.305
$\text{Co}(\text{NH}_3)_5^{3+}$ -0.106	$\text{Co}(\text{NH}_3)_5^{3+}$ 0.171	$\text{Co}(\text{NH}_3)_5^{3+}$ -0.331
CrO_3 -0.296	CrO_3 -0.231	CrO_3 -0.137
$\text{Cu}(\text{NH}_3)_3^{2+}$ -0.135	$\text{Cu}(\text{NH}_3)_3^{2+}$ 0.221	$\text{Cu}(\text{NH}_3)_3^{2+}$ 0.137
FeCl_2^+ -0.051	FeCl_2^+ 0.038	FeCl_2^+ 0.242
$\text{Fe}(\text{CO})_4$ 0.067	$\text{Fe}(\text{CO})_4$ -0.052	$\text{Fe}(\text{CO})_4$ -0.016
$\text{IrCO}(\text{PH}_3)_2^+$ 0.158	$\text{IrCO}(\text{PH}_3)_2^+$ -0.218	$\text{IrCO}(\text{PH}_3)_2^+$ -0.232
K^+ -0.094	K^+ -0.281	K^+ 0.327
MnO_3^+ -0.164	MnO_3^+ -0.145	MnO_3^+ 0.244
$\text{Mo}(\text{SH})_3^+$ 0.334	$\text{Mo}(\text{SH})_3^+$ -0.124	$\text{Mo}(\text{SH})_3^+$ -0.226
$\text{Nb}(\text{NH}_2)_4^+$ 0.109	$\text{Nb}(\text{NH}_2)_4^+$ 0.282	$\text{Nb}(\text{NH}_2)_4^+$ 0.079
OsO_3^{2+} 0.192	OsO_3^{2+} 0.153	OsO_3^{2+} 0.152
$\text{PdH}(\text{PH}_3)_2^+$ 0.072	$\text{PdH}(\text{PH}_3)_2^+$ 0.046	$\text{PdH}(\text{PH}_3)_2^+$ 0.192
PdPH_3 0.320	PdPH_3 -0.272	PdPH_3 0.034
PtF_5^- -0.167	PtF_5^- 0.415	PtF_5^- -0.234
$\text{Rh}(\text{H}_2\text{O})_5^{3+}$ 0.166	$\text{Rh}(\text{H}_2\text{O})_5^{3+}$ 0.163	$\text{Rh}(\text{H}_2\text{O})_5^{3+}$ -0.230
$\text{Ru}(\text{SH})_4$ 0.274	$\text{Ru}(\text{SH})_4$ 0.117	$\text{Ru}(\text{SH})_4$ 0.222
TaMe_4^+ -0.106	TaMe_4^+ -0.235	TaMe_4^+ -0.193
TiCl_3^+ -0.083	TiCl_3^+ -0.203	TiCl_3^+ -0.106
$\text{W}(\text{CO})_5$ 0.160	$\text{W}(\text{CO})_5$ -0.292	$\text{W}(\text{CO})_5$ -0.183
ZnCH_3^+ -0.424	ZnCH_3^+ -0.106	ZnCH_3^+ 0.236
ZrCl_5^- 0.136	ZrCl_5^- 0.324	ZrCl_5^- 0.133

2.4 Errors by number of hidden descriptors (k) used and weights $\mathbf{W}$ for the Initial Training Set.

We present in Table S7 the maximum absolute and average errors obtained when a given number of hidden descriptors is used for the calculation of the estimated BDE. The errors are the subtraction between the computational BDEs and the BDEs estimated from the use of a given number of hidden descriptors (k) (using the corresponding hidden descriptors $\mathbf{L}_k$, $\mathbf{M}_k$ and $\mathbf{W}$) for the Initial Training Set. Please note that as the weights matrix $\mathbf{W}$ is diagonal, only the elements of the diagonal are presented in a single column.

Table S7: Maximum absolute and average error (in kcal/mol) of the estimated BDE with respect to the number of hidden descriptors (k) considered for the Initial Training Set. The diagonal term in matrix, $\mathbf{W}_{k,k}$, is also provided.

Initial Training Set			
k	Max error	Aver error	Weight, $\mathbf{W}_{k,k}$
1	94.9	13.5	4646.2
2	58.7	8.7	309.1
3	26.1	4.3	243.5
4	14.4	2.6	105.5
5	10.0	1.8	56.7
6	6.0	1.3	39.0
7	5.0	0.9	22.8
8	4.2	0.7	17.9
9	3.3	0.5	14.8
10	2.2	0.4	9.7
11	1.9	0.4	7.5
12	1.7	0.3	7.1
13	1.0	0.2	5.2
14	0.9	0.2	3.6
15	0.6	0.1	3.1
16	0.5	0.1	2.2
17	0.4	0.1	2.1
18	0.4	0.0	1.6
19	0.2	0.0	1.2
20	0.1	0.0	0.7
21	0.1	0.0	0.3
22	0.0	0.0	0.3

3 Extended and Full Set (B3LYP-D3 in vacuum)

3.1 Multiplicity and geometrical structure associated to each metal fragment

We considered an Extended Set with 19 new metal fragments and 21 new ligands at the B3LYP-D3 level in vacuum. We will call Extended Set the BDEs of these 21 new ligands with the 19 new metal fragments but also the BDEs of these new ligands with the metal fragments of the Initial Training Set and the new metal fragments with the ligands of the Initial Training Set. We will call Full Set of data, all BDEs between all ligands and all metal fragments (42x43) wich is constituted by the Initial Training Set and the Extended Set. The favored multiplicity and geometry for each of the new metallic fragment is collected in Table S8. The Full set of ligands include: Br^- , CH_3^- , Cl^- , CN^- , CO , F^- , C_6H_5^- , H_2 , H_2O , H^- , I^- , NCH , NCS^- , NH_3 , NHC , O^{2-} , OH^- , PH_3 , $\text{C}_5\text{H}_5\text{N}$, S^{2-} , SCN^- , SH^- , $\text{C}_2\text{H}_4\text{O}_2\text{B}^-$ (Bpin^-), CCH^- , CHCH_2^- , $\text{C}_6\text{H}_4\text{Cl}^-$, $\text{C}_6\text{H}_4\text{NO}_2^-$, $\text{C}_6\text{H}_4\text{OMe}^-$, H_2S , He , $\text{C}_3\text{H}_4\text{N}_2$ (Imidazol), NH_2^- , NMe_3 , $\text{C}_4\text{H}_4\text{O}$ (THF), OMe^- , PCl_3 , PF_3 , SiH_3^- , SiMe_3^- , SMe^- , $\text{C}_4\text{H}_4\text{S}$ (thiophene) and Xe . And the Full Set of metal fragments is: AlCl_3 , AuPH_3^+ , $\text{Co}(\text{NH}_3)_5^{3+}$, CrO_3 , $\text{Cu}(\text{NH}_3)_3^{2+}$, FeCl_2^+ , $\text{Fe}(\text{CO})_4$, $\text{IrCO}(\text{PH}_3)_2^+$, K^+ , MnO_3^+ , $\text{Mo}(\text{SH})_3^+$, $\text{Nb}(\text{NH}_2)_4^+$, OsO_3^{2+} , $\text{PdH}(\text{PH}_3)_2^+$, PdPH_3 , PtF_5^- , $\text{Rh}(\text{H}_2\text{O})_5^{3+}$, $\text{Ru}(\text{SH})_4$, TaMe_4^+ , TiCl_3^+ , $\text{W}(\text{CO})_5$, ZnCH_3^+ and ZrCl_5^- , $\text{Ag}(\text{NHC})^+$, AuCl_3 , AuCN , $\text{Cr}(\text{H}_2\text{O})_5^{2+}$, CuCH_3 , CuCN , FeCl_3 , FeCl_3^- , GaCl_3 , HgI_2 , InCl_2^+ , $\text{Ni}(\text{PF}_3)_3$, NiPH_3 , PtPH_3 , SnMe_3^+ , $\text{Y}(\text{H}_2\text{O})_5^{3+}$, ZnCl_3^- , ZnNH_3^{2+} and $\text{Zr}(\text{OMe})_3^+$.

Table S8: Geometry structure and multiplicity state of the structures related to each new metal fragment

Metal Fragment	Geometry	Multiplicity	Metal Fragment	Geometry	Multiplicity
L-Ag(NHC) ⁺	Linear	Singlet	L-InCl ₂ ⁺	Trigonal	Singlet
L-AuCl ₃	Planar	Singlet	L-Ni(PF ₃) ₃	Trigonal pyramid	Singlet
L-AuCN	Linear	Singlet	L-NiPH ₃	Linear	Singlet
L-Cr(H ₂ O) ₅ ²⁺	Octahedral	Triplet	L-PtPH ₃	Linear	Singlet
L-CuCH ₃	Linear	Singlet	L-SnMe ₃ ⁺	Trigonal pyramid	Singlet
L-CuCN	Linear	Singlet	L-Y(H ₂ O) ₅ ³⁺	Octahedral	Singlet
L-FeCl ₃ ⁻	Trigonal pyramid	Quintet	L-ZnCl ₃ ⁻	Trigonal pyramid	Singlet
L-FeCl ₃	Trigonal pyramid	Sextet	L-ZnNH ₃ ²⁺	Linear	Singlet
L-GaCl ₃	Trigonal pyramid	Singlet	L-Zr(OMe) ₃ ⁺	Trigonal pyramid	Singlet
L-HgI ₂	T shape	Singlet			

3.2 BDE matrices for the Full Set of data.

The inclusion of the 19 new metal fragments and 21 new ligands together with the 23 metal fragments and 22 new ligands generates an overall table of 42 metal fragments and 43 ligands. This Table of 42x43 data can not fit on a page and we will divide the matrix in four groups:

- BDEs for metal fragments and ligands on the the Initial Training Set. This data is presented in the previous section in Tables S2 part A and part B, and it will not be repeated here.
- BDEs for metal fragments from the Initial Training Set and new ligands. This data is presented in this section on Tables S9 part A and part B.
- BDEs for new metal fragments and ligands from the Initial Training Set. This data is presented in this section on Tables S10 part A and part B.
- BDEs for new metal fragments and new ligands. This data is presented in this section on Tables S11 part A and part B.

Please note, that if considering the Actual Training Set instead of the Initial Training Set some ligands and metal fragments on the Extended Set will move to this training set and although the BDEs will not change the organization of the data will. Data will have to be re-organized to be compared with the Actual Training Set.

Table S9: Bond dissociation energies (in kcal/mol) between the 21 new ligands and 23 metal fragments of the Initial Training Set calculated using B3LYP-D3 in vacuum. Results are split in two separate tables, part A and part B.

Table S9, PART A										
	CCH ⁻	CHCH ₂ ⁻	C ₆ H ₄ Cl ⁻	C ₆ H ₄ NO ₂ ⁻	C ₆ H ₄ OMe ⁻	H ₂ S	He C ₃ H ₄ N ₂	NH ₂ ⁻	NMe ₃	
Bpin ⁻	-102.7	-96.2	-112.6	-103.9	-97.2	-108.5	-16.0	-1.0	-44.5	-121.7
AlCl ₃	-221.6	-193.2	-212.1	-199.0	-188.7	-206.2	-42.4	-2.5	-66.7	-205.3
AuPH ₃ ⁺	-425.85	-380.05	-407.15	-392.65	-371.95	-408.95	-46.55	-2.55	-101.15	-400.15
Co(NH ₃) ₅ ³⁺	-134.9	-114.3	-135.8	-127.4	-121.5	-131.4	-37.6	-4.1	-62.3	-136.6
CrO ₃	-296.1	-265.6	-288.0	-273.1	-257.7	-284.2	-30.5	-1.5	-70.5	-295.2
Cu(NH ₃) ₃ ²⁺	-242.5	-226.3	-248.5	-235.4	-220.7	-247.2	-42.6	-2.0	-83.0	-266.9
FeCl ₂ ⁺	-110.4	-81.9	-98.3	-89.7	-85.4	-93.0	-20.1	1.0	-34.3	-88.8
Fe(CO) ₄	-211.0	-188.6	-203.9	-191.9	-181.7	-199.0	-34.8	-2.9	-61.9	-199.9
IrCO(PH ₃) ₂ ⁺	-119.4	-114.6	-120.4	-109.4	-101.8	-114.4	-10.8	-1.0	-26.4	-130.0
K ⁺	-323.4	-277.6	-315.5	-300.6	-286.3	-311.6	-78.8	-6.7	-121.8	-310.2
MnO ₃ ⁺	-231.0	-212.8	-236.0	-220.5	-207.2	-231.2	-41.4	-1.0	-75.4	-249.9
Mo(SH) ₃ ⁺	-162.3	-147.1	-164.2	-151.1	-140.6	-158.5	-8.6	-1.1	-34.9	-177.8
Nb(NH ₂) ₄ ⁺	-525.0	-475.7	-516.2	-513.4	-486.7	-536.5	-131.3	-7.3	-208.7	-508.5
OsO ₃ ²⁺	-184.2	-159.2	-175.3	-163.6	-153.7	-170.3	-23.5	-1.4	-44.4	-169.7
PdH(PH ₃) ₂ ⁺	-65.6	-55.6	-63.0	-58.6	-56.7	-60.3	-20.6	-1.8	-25.7	-60.2
PdPH ₃	-46.7	-17.7	-42.5	-45.7	-47.6	-45.3	-31.0	-1.3	-45.5	-27.8
PtF ₅ ⁻	-490.7	-429.4	-463.6	-453.5	-431.7	-470.9	-78.3	-6.0	-136.4	-448.0
Rh(H ₂ O) ₅ ³⁺	-103.8	-81.5	-97.2	-85.6	-84.8	-89.4	-12.4	-4.5	-31.9	-91.0
Ru(SH) ₄	-219.3	-215.2	-232.5	-218.1	-204.9	-228.0	-36.5	-1.5	-77.4	-251.9
TaMe ₄ ⁺	-244.4	-232.0	-255.3	-241.3	-226.9	-252.4	-46.6	-3.5	-90.5	-274.7
TiCl ₃ ⁺	-105.3	-87.0	-99.5	-92.3	-88.1	-95.6	-24.4	-3.0	-38.8	-93.7
W(CO) ₅	-225.8	-208.8	-226.5	-212.2	-200.3	-220.6	-37.5	-1.4	-72.0	-231.0
ZnCH ₃ ⁺	10.7	13.8	-0.4	0.2	0.7	-0.6	-7.0	1.3	-18.1	-15.0
ZrCl ₅ ⁻										

Table S9, PART B

	C ₄ H ₄ O	OMe	PF ₃	PCl ₃	PMe ₃	SiH ₃ ⁻	SiMe ₃ ⁻	SMe ⁻	C ₄ H ₄ S	Xe
AlCl ₃	-21.2	-112.7	-10.8	-6.7	-37.0	-80.4	-89.6	-83.7	-15.1	-1.2
AuPH ₃ ⁺	-32.6	-181.8	-42.2	-34.0	-76.5	-195.1	-206.3	-179.6	-43.7	-20.2
Co(NH ₃) ₅ ³⁺	-57.45	-386.35	-54.25	-29.15	-98.05	-376.55	-399.65	-367.95	-68.15	-24.85
CrO ₃	-35.2	-125.3	-36.1	-30.8	-66.6	-113.1	-126.2	-104.7	-35.8	-15.1
Cu(NH ₃) ₃ ²⁺	-37.0	-273.1	-29.1	-12.4	-66.2	-263.9	-281.0	-254.1	-42.6	-13.1
FeCl ₂ ⁺	-47.8	-247.4	-35.2	-21.5	-76.8	-216.8	-234.0	-227.7	-47.8	-20.9
Fe(CO) ₄	-14.8	-72.9	-30.5	-30.8	-47.5	-88.7	-101.3	-68.5	-18.9	-3.3
IrCO(PH ₃) ₂ ⁺	-32.3	-180.4	-40.8	-36.3	-64.3	-180.3	-189.4	-171.5	-38.3	-15.1
K ⁺	-13.2	-125.3	-3.8	-0.4	-17.8	-105.4	-108.4	-108.8	-7.7	3.9
MnO ₃ ⁺	-75.3	-293.1	-81.7	-59.9	-139.5	-298.3	-323.3	-276.6	-89.8	-44.1
Mo(SH) ₃ ⁺	-41.1	-236.7	-41.7	-32.0	-73.1	-198.8	-215.9	-210.7	-46.1	-16.0
Nb(NH ₂) ₄ ⁺	-14.4	-171.0	-6.2	0.3	-24.9	-133.8	-143.3	-137.5	-12.3	7.1
OsO ₃ ²⁺	-143.6	-486.4	-156.6	-105.3	-234.8	-494.0	-535.4	-477.3	-173.6	-92.0
PdH(PH ₃) ₂ ⁺	-21.4	-153.8	-26.0	-20.0	-47.2	-157.1	-166.6	-147.5	-27.4	-9.8
PdPH ₃	-11.6	-46.9	-33.2	-33.0	-36.4	-51.8	-56.9	-44.9	-19.7	-7.8
PtF ₅ ⁻	-23.8	-7.7	-38.2	-36.2	-62.4	-24.7	-42.4	-3.2	-25.7	-5.9
Rh(H ₂ O) ₅ ³⁺	-81.2	-428.2	-96.8	-64.2	-150.2	-440.1	-470.1	-420.2	-105.1	-46.4
Ru(SH) ₄	-16.3	-77.2	-29.3	-26.2	-38.7	-79.8	-92.1	-65.3	-13.6	-6.9
TaMe ₄ ⁺	-44.4	-242.9	-29.9	-18.2	-65.6	-191.3	-201.8	-205.6	-40.6	-17.1
TiCl ₃ ⁺	-55.0	-268.5	-39.8	-26.2	-82.7	-217.5	-234.6	-228.9	-54.3	-23.7
W(CO) ₅	-19.8	-82.6	-35.9	-35.2	-48.4	-85.2	-95.3	-73.7	-23.9	-8.0
ZnCH ₃ ⁺	-37.2	-211.8	-29.4	-16.8	-68.3	-198.8	-208.7	-197.2	-41.8	-16.9
ZrCl ₅ ⁻	-9.1	-11.1	-9.5	-7.4	-19.0	24.4	14.8	20.4	-5.1	10.9

Table S10: Bond dissociation energies (in kcal/mol) between the 22 ligands of the Initial Training Set and 19 new metal fragments calculated using B3LYP-D3 in vacuum. Results are split in two separate tables, part A and part B.

Table S10, PART A												
	Br ⁻	CH ₃ ⁻	Cl ⁻	CN ⁻	CO	F ⁻	C ₆ H ₅ ⁻	H ₂	H ₂ O	H ⁻	I ⁻	
Ag(NHC) ⁺	-129.6	-177.3	-134.8	-144.0	-25.5	-151.5	-165.4	-8.2	-28.1	-216.1	-126.2	
AuCl ₃	-72.9	-154.2	-77.3	-101.2	-26.9	-97.1	-141.2	-2.2	-26.3	-191.9	-71.1	
AuCN	-70.2	-121.2	-75.3	-94.8	-38.5	-91.6	-114.0	-12.6	-26.2	-159.7	-67.1	
Cr(H ₂ O) ₅ ²⁺	-207.5	-252.8	-215.1	-217.1	-21.8	-248.9	-245.0	-1.5	-26.9	-284.6	-197.9	
CuCH ₃	-40.5	-76.0	-46.0	-58.6	-23.3	-63.2	-70.9	-3.9	-18.1	-110.2	-36.3	
CuCN	-67.6	-108.8	-74.1	-86.2	-31.9	-93.0	-101.2	-10.2	-28.3	-142.9	-62.7	
FeCl ₃ ⁻	49.6	15.9	45.2	34.1	-3.0	21.6	17.7	4.7	-7.9	-15.3	53.4	
FeCl ₃	-64.8	-118.5	-72.3	-76.7	-13.2	-104.8	-106.3	-2.0	-24.0	-148.4	-57.8	
GaCl ₃	-59.3	-123.2	-67.8	-78.2	-7.1	-102.4	-111.5	-0.6	-19.9	-154.1	-52.1	
HgI ₂	-39.4	-96.8	-42.6	-52.2	-2.6	-58.5	-84.7	-0.5	-7.2	-133.5	-37.0	
InCl ₂ ⁺	-182.6	-255.2	-192.0	-195.4	-18.3	-226.1	-242.7	-2.4	-42.1	-284.6	-176.4	
Ni(PF ₃) ₃	-48.8	-95.5	-52.9	-68.5	-29.2	-67.6	-88.8	-4.4	-13.8	-136.1	-45.9	
NiPH ₃	-39.9	-74.1	-45.8	-58.2	-48.8	-62.9	-69.5	-15.8	-24.0	-106.6	-35.8	
PtPH ₃	-40.7	-84.5	-45.4	-65.5	-49.6	-60.2	-81.6	-15.1	-19.9	-121.1	-38.4	
SnMe ₃ ⁺	-144.3	-211.2	-153.2	-160.2	-11.8	-187.2	-196.7	-1.5	-27.5	-245.4	-137.2	
Y(H ₂ O) ₅ ³⁺	-319.6	-368.2	-330.9	-316.5	-21.8	-374.3	-362.0	-5.2	-51.0	-395.7	-310.3	
ZnCl ₃ ⁻	48.3	10.3	44.3	32.4	-2.6	24.4	13.3	-0.4	-9.8	-21.6	51.7	
ZnNH ₃ ²⁺	-327.7	-407.7	-333.8	-333.4	-60.3	-354.9	-392.7	-26.8	-84.4	-433.5	-325.7	
Zr(OMe) ₃ ⁺	-155.5	-206.4	-166.4	-163.7	-21.4	-208.0	-193.0	-5.4	-40.4	-236.2	-146.0	

Table S10, PART B

	NCH	NCS ⁻	NH ₃	NHC	O ²⁻	OH ⁻	PH ₃	C ₅ H ₅ N	S ²⁻	SCN ⁻	SH ⁻
Ag(NHC) ⁺	-33.3	-123.1	-41.5	-67.4	-335.7	-161.4	-36.5	-45.7	-265.1	-120.7	-144.2
AuCl ₃	-24.8	-70.1	-45.8	-84.3	-255.8	-116.9	-42.0	-48.2	-176.9	-73.6	-100.0
AuCN	-33.1	-71.5	-42.5	-70.3	-206.9	-101.6	-41.6	-44.7	-141.6	-67.2	-86.4
Cr(H ₂ O) ₅ ²⁺	-36.3	-202.9	-36.7	-66.9	-559.2	-259.7	-25.1	-50.5	-451.7	-198.5	-219.7
CuCH ₃	-21.6	-46.0	-28.7	-44.2	-152.0	-69.4	-21.6	-29.0	-86.9	-38.2	-51.8
CuCN	-34.0	-71.5	-41.8	-61.4	-196.9	-100.6	-33.7	-43.2	-130.2	-62.8	-80.8
FeCl ₃ ⁻	2.4	39.2	-11.3	-21.6	-49.7	16.2	-2.6	-10.5	54.4	46.8	39.7
FeCl ₃	-20.5	-67.7	-36.3	-54.7	-271.6	-114.5	-22.5	-38.8	-168.6	-57.1	-81.1
GaCl ₃	-15.4	-63.1	-31.7	-53.1	-248.6	-110.6	-16.3	-36.1	-158.3	-52.6	-77.6
HgI ₂	-4.5	-30.9	-11.8	-27.3	-200.6	-71.1	-5.1	-15.1	-133.1	-33.6	-56.6
InCl ₂ ⁺	-42.1	-182.3	-54.3	-93.8	-480.0	-239.5	-40.8	-72.6	-388.4	-168.9	-206.9
Ni(PF ₃) ₃	-20.2	-48.7	-25.6	-50.9	-193.6	-77.0	-26.0	-28.5	-124.5	-45.6	-62.7
NiPH ₃	-35.5	-47.7	-35.3	-53.1	-167.2	-70.0	-34.2	-37.0	-90.8	-39.2	-52.0
PtPH ₃	-30.1	-46.5	-33.9	-60.3	-170.0	-69.3	-39.9	-36.2	-98.4	-42.1	-55.6
SnMe ₃ ⁺	-28.0	-142.5	-39.3	-66.6	-408.8	-196.4	-26.2	-48.1	-317.7	-133.5	-163.4
Y(H ₂ O) ₅ ³⁺	-57.2	-323.8	-58.0	-99.8	-782.9	-391.2	-42.9	-85.4	-659.2	-296.3	-334.1
ZnCl ₃ ⁻	1.6	39.3	-12.8	-21.6	-2.7	18.5	-3.4	-11.8	62.8	46.3	38.1
ZnNH ₃ ²⁺	-96.9	-318.7	-110.9	-169.7	-697.9	-377.9	-106.9	-138.5	-610.6	-309.6	-353.8
Zr(Ome) ₃ ⁺	-40.3	-158.0	-50.7	-73.9	-455.5	-216.6	-34.0	-59.2	-334.5	-140.9	-170.0

Table S11: Bond dissociation energies (in kcal/mol) between the 21 new ligands and 19 new metal fragments calculated using B3LYP-D3 in vacuum. Results are split in two separate tables, part A and part B.

Table S11, PART A												
	Bpin ⁻	CCH ⁻	CHCH ₂ ⁻	C ₆ H ₄ Cl ⁻	C ₆ H ₄ NO ₂ ⁻	C ₆ H ₄ OMe ⁻	H ₂ S	He	C ₃ H ₄ N ₂	NH ₂ ⁻	NMe ₃	
Ag(NHC) ⁺	-176.9	-158.7	-171.6	-159.7	-150.9	-165.7	-29.7	-2.1	-50.1	-170.0	-43.2	
AuCl ₃	-161.9	-116.4	-146.6	-136.3	-129.1	-141.2	-31.2	-1.0	-50.9	-135.6	-48.6	
AuCN	-123.9	-105.6	-118.3	-110.7	-105.8	-114.0	-31.7	-2.1	-47.2	-111.4	-44.7	
Cr(H ₂ O) ₅ ²⁺	-251.9	-241.0	-250.0	-235.1	-222.2	-246.4	-20.5	-1.7	-56.1	-262.3	-40.3	
CuCH ₃	-70.3	-66.0	-73.9	-68.8	-66.0	-70.9	-17.8	-0.9	-30.2	-74.2	-29.3	
CuCN	-102.4	-96.0	-105.3	-98.2	-93.6	-101.2	-28.7	-2.1	-45.7	-106.3	-43.3	
FeCl ₃ ⁻	26.2	29.5	18.9	18.0	14.0	17.1	-3.6	-0.8	-9.2	14.9	-16.5	
FeCl ₃	-104.3	-91.8	-110.9	-102.0	-95.2	-106.9	-20.1	-0.4	-41.1	-120.2	-43.8	
GaCl ₃	-112.1	-94.5	-116.0	-107.0	-99.5	-112.1	-13.5	-0.7	-38.5	-116.5	-39.9	
HgI ₂	-96.3	-66.8	-89.4	-79.9	-72.1	-85.3	-5.5	-0.7	-15.7	-82.9	-16.6	
InCl ₂ ⁺	-249.6	-222.8	-247.3	-234.4	-220.7	-244.8	-33.5	-0.8	-78.4	-250.6	-67.1	
Ni(PF ₃) ₃	-99.0	-78.8	-92.6	-85.3	-80.2	-88.8	-18.1	-1.5	-30.6	-85.9	-28.8	
NiPH ₃	-67.4	-65.3	-72.3	-67.9	-67.1	-69.5	-28.5	-3.3	-36.4	-74.6	-34.3	
PtPH ₃	-87.2	-74.0	-84.0	-79.6	-77.7	-81.5	-28.3	-2.2	-36.9	-77.7	-35.5	
SnMe ₃ ⁺	-204.9	-182.1	-203.4	-189.3	-177.6	-197.9	-21.1	-1.1	-52.7	-203.8	-45.9	
Y(H ₂ O) ₅ ³⁺	-367.2	-352.1	-366.6	-351.0	-331.5	-367.6	-38.0	-2.1	-92.9	-388.1	-71.6	
ZnCl ₃ ⁻	19.6	27.3	14.1	12.8	12.7	12.8	-5.3	-0.5	-9.6	14.0	-18.2	
ZnNH ₃ ²⁺	-406.7	-370.0	-397.8	-382.4	-364.5	-396.2	-91.7	-6.7	-145.0	-394.9	-132.6	
Zr(OMe) ₃ ⁺	-190.0	-184.5	-199.8	-186.2	-174.8	-194.3	-30.4	-2.3	-64.2	-217.0	-58.4	

Table S11, PART B

	C ₄ H ₄ O	OMe	PF ₃	PCl ₃	PMe ₃	SiH ₃ ⁻	SiMe ₃ ⁻	SMe ⁻	C ₄ H ₄ S	Xe
Ag(NHC) ⁺	-24.1	-151.4	-26.9	-20.5	-53.3	-154.4	-161.6	-147.0	-30.2	-13.3
AuCl ₃	-20.0	-108.6	-31.9	-25.5	-67.0	-133.1	-149.4	-106.1	-29.5	-6.6
AuCN	-22.4	-92.8	-35.1	-32.8	-57.2	-102.2	-109.9	-89.7	-29.6	-12.5
Cr(H ₂ O) ₅ ²⁺	-26.7	-250.1	-24.0	-11.9	-45.6	-216.0	-223.2	-225.7	-28.1	-13.5
CuCH ₃	-13.7	-61.5	-18.8	-16.4	-31.5	-55.6	-60.1	-53.7	-15.2	-4.1
CuCN	-23.6	-91.7	-26.2	-23.8	-46.6	-85.1	-90.3	-82.8	-26.4	-10.9
FeCl ₃ ⁻	-3.5	22.3	-7.2	-4.6	-11.8	36.5	29.9	35.4	-1.2	4.9
FeCl ₃	-20.3	-108.6	-15.9	-11.1	-41.1	-86.4	-98.4	-88.0	-19.3	-4.7
GaCl ₃	-16.6	-102.3	-8.6	-3.8	-36.4	-88.7	-100.8	-83.9	-13.2	-0.2
HgI ₂	-7.0	-62.7	-4.6	-2.7	-16.1	-74.7	-87.4	-62.2	-5.8	6.2
InCl ₂ ⁺	-41.9	-231.1	-26.4	-12.3	-71.7	-219.9	-236.2	-214.4	-40.4	-13.7
Ni(PF ₃) ₃	-12.8	-70.3	-27.1	-25.6	-40.4	-78.2	-89.4	-67.4	-19.8	-5.4
NiPH ₃	-19.0	-61.6	-40.2	-39.7	-41.0	-53.7	-58.3	-53.6	-25.9	-10.2
PtPH ₃	-17.5	-61.4	-43.1	-43.5	-51.0	-69.2	-76.9	-59.0	-26.8	-10.2
SnMe ₃ ⁺	-24.0	-187.5	-15.4	-5.8	-48.9	-176.5	-188.6	-169.4	-24.4	-5.4
Y(H ₂ O) ₅ ³⁺	-55.7	-386.5	-34.1	-14.2	-72.3	-322.6	-339.0	-344.5	-53.0	-20.8
ZnCl ₃ ⁻	-6.2	24.7	-10.1	-8.5	-12.1	31.6	23.7	33.7	-4.7	2.5
ZnNH ₃ ²⁺	-90.9	-369.6	-92.4	-64.3	-151.6	-374.7	-395.4	-362.4	-109.4	-60.5
Zr(OMe) ₃ ⁺	-36.6	-209.6	-22.5	-13.8	-54.1	-165.7	-174.6	-175.3	-33.8	-13.2

3.3 Hidden descriptor tables for the Full Set of data.

We performed a SVD analysis for the Full Set of data as explained in the main text. We obtained hidden descriptors HD_{Lk} for the ligands and hidden descriptors HD_{Mk} for the metal fragments. Tables S12 and S13 report the values for the first seven hidden descriptors for each ligand and metal fragment, respectively.

In the Table S14 part A and part B the same values for the ligands appear ordered in decreasing order and with the corresponding name of the ligand next to it. Also in Table S15 part A and part B the hidden descriptors of the metal fragments appear ordered in the same way. This arrangement allows for an easier visualization of the ligands having larger and lower values for a given SV.

The SVD analysis was performed with the script presented in Section 9.1 of this Supporting Information.

Please note that this are not estimated hidden descriptors for the Extended Set but just the results of the application of the SVD analysis to the Full Set of data.

Table S12: First seven hidden descriptors of the ligands for the Full Set of data. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

Ligand	$\text{HD}_{L1} = \mathbf{L}_1$	$\text{HD}_{L2} = \mathbf{L}_2$	$\text{HD}_{L3} = \mathbf{L}_3$	$\text{HD}_{L4} = \mathbf{L}_4$	$\text{HD}_{L5} = \mathbf{L}_5$	$\text{HD}_{L6} = \mathbf{L}_6$	$\mathbf{L}_7$
Br^-	-0.149	0.173	0.205	-0.066	0.076	-0.135	0.140
CH_3^-	-0.197	-0.081	-0.039	0.143	-0.181	-0.099	0.164
Cl^-	-0.155	0.160	0.150	-0.093	0.055	-0.198	0.085
CN^-	-0.158	0.045	0.085	0.114	0.161	-0.239	-0.162
CO	-0.025	-0.197	0.003	0.030	0.495	-0.196	-0.145
F^-	-0.176	0.109	-0.083	-0.179	-0.080	-0.306	-0.162
C_6H_5^-	-0.191	-0.065	0.040	0.108	-0.108	0.082	-0.238
H_2	-0.008	-0.065	0.049	-0.019	0.170	-0.073	0.067
H_2O	-0.034	-0.121	0.006	-0.157	-0.093	-0.119	0.066
H^-	-0.220	-0.225	-0.302	0.406	0.062	-0.354	0.218
I^-	-0.146	0.171	0.267	-0.048	0.089	-0.053	0.187
NCH	-0.039	-0.122	0.051	-0.112	0.146	-0.171	0.026
NCS^-	-0.150	0.126	0.182	-0.194	0.071	-0.016	-0.288
NH_3	-0.046	-0.204	-0.006	-0.125	-0.089	-0.168	0.101
NHC	-0.076	-0.320	-0.016	-0.065	-0.053	-0.016	-0.072
O^{2-}	-0.379	0.042	-0.658	-0.254	0.237	0.319	0.099
OH^-	-0.187	0.057	-0.094	-0.178	-0.108	-0.220	-0.069
PH_3	-0.041	-0.216	0.102	-0.072	0.131	-0.013	0.168
$\text{C}_5\text{H}_5\text{N}$	-0.059	-0.199	0.051	-0.173	-0.120	0.017	-0.085
S^{2-}	-0.307	0.323	0.014	-0.029	0.155	0.300	0.174
SCN^-	-0.142	0.142	0.236	-0.023	0.127	0.000	-0.051
SH^-	-0.165	0.089	0.146	-0.023	0.001	-0.089	0.191
Bpin^-	-0.197	-0.074	0.054	0.347	-0.017	0.076	-0.069
CCH^-	-0.177	0.020	0.057	0.071	0.083	-0.162	-0.127
CHCH_2^-	-0.194	-0.066	-0.004	0.133	-0.094	-0.040	-0.041
$\text{C}_6\text{H}_4\text{Cl}^-$	-0.185	-0.070	0.056	0.089	-0.105	0.098	-0.278
$\text{C}_6\text{H}_4\text{NO}_2^-$	-0.175	-0.079	0.062	0.089	-0.064	0.088	-0.338
$\text{C}_6\text{H}_4\text{OMe}^-$	-0.193	-0.066	0.052	0.079	-0.121	0.142	-0.270
H_2S	-0.034	-0.166	0.085	-0.112	0.040	-0.036	0.183
He	-0.002	-0.012	0.006	-0.005	0.025	-0.009	0.025
$\text{C}_3\text{H}_4\text{N}_2$	-0.062	-0.191	0.040	-0.177	-0.126	-0.031	-0.015
NH_2^-	-0.195	-0.005	-0.082	-0.093	-0.141	-0.129	0.069
NMe_3	-0.055	-0.236	0.044	-0.219	-0.226	-0.002	0.134
$\text{C}_4\text{H}_4\text{O}$	-0.036	-0.112	0.083	-0.200	-0.088	0.096	0.006
OMe	-0.184	0.078	-0.029	-0.244	-0.132	-0.051	-0.121
PF_3	-0.036	-0.218	0.119	-0.059	0.312	0.208	-0.097
PCl_3	-0.024	-0.210	0.072	-0.007	0.399	0.049	-0.058
PMe_3	-0.063	-0.294	0.098	-0.081	-0.022	0.120	0.066
SiH_3^-	-0.175	-0.035	0.175	0.214	-0.057	0.104	0.241
SiMe_3^-	-0.187	-0.092	0.158	0.231	-0.137	0.275	0.175
SMe^-	-0.171	0.062	0.135	-0.045	-0.032	0.019	0.124
$\text{C}_4\text{H}_4\text{S}$	-0.041	-0.152	0.150	-0.149	0.028	0.181	0.070
Xe	-0.018	-0.070	0.139	-0.121	0.051	0.040	0.144

Table S13: First seven hidden descriptors of the metal fragments for the Full Set of data. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

Metal Frag.	$\text{HD}_{M1=M_1}$	$\text{HD}_{M2=M_2}$	$\text{HD}_{M3=M_3}$	$\text{HD}_{M4=M_4}$	$\text{HD}_{M5=M_5}$	$\text{HD}_{M6=M_6}$	M_7
AlCl ₃	0.077	0.064	0.181	0.084	0.224	0.177	0.238
AuPH ₃ ⁺	0.146	0.074	-0.012	-0.164	-0.052	0.089	-0.187
Co(NH ₃) ₅ ³⁺	0.291	-0.230	-0.050	-0.246	0.006	-0.090	0.315
CrO ₃	0.092	0.199	0.072	0.074	0.098	0.197	0.060
Cu(NH ₃) ₃ ²⁺	0.206	-0.170	0.042	-0.171	0.097	-0.032	-0.036
FeCl ₂ ⁺	0.179	-0.033	0.063	0.137	0.101	0.009	-0.162
Fe(CO) ₄	0.064	0.162	0.069	-0.219	-0.090	0.045	-0.018
IrCO(PH ₃) ₂ ⁺	0.142	0.038	0.036	-0.119	-0.200	0.098	0.093
K ⁺	0.091	-0.123	0.130	-0.018	-0.069	0.162	-0.234
MnO ₃ ⁺	0.220	0.208	-0.123	0.066	0.111	-0.011	-0.293
Mo(SH) ₃ ⁺	0.171	-0.019	0.136	0.165	-0.163	-0.118	-0.067
Nb(NH ₂) ₄ ⁺	0.121	-0.146	0.291	0.007	-0.025	-0.187	-0.009
OsO ₃ ²⁺	0.368	0.266	-0.447	0.306	0.025	-0.386	0.030
PdH(PH ₃) ₂ ⁺	0.122	-0.021	0.062	-0.194	-0.084	0.009	-0.094
PdPH ₃	0.044	0.137	0.080	-0.032	-0.311	0.003	-0.072
PtF ₅ ⁻	0.017	0.414	0.036	-0.103	0.210	0.024	0.442
Rh(H ₂ O) ₅ ³⁺	0.329	-0.056	-0.223	-0.212	-0.100	-0.225	0.223
Ru(SH) ₄	0.065	0.114	0.160	-0.106	-0.173	-0.134	-0.042
TaMe ₄ ⁺	0.170	-0.058	0.145	0.252	0.015	0.131	0.057
TiCl ₃ ⁺	0.187	-0.017	0.114	0.303	0.052	0.030	-0.060
W(CO) ₅	0.068	0.153	0.074	-0.075	-0.212	0.073	0.031
ZnCH ₃ ⁺	0.159	-0.010	0.013	-0.039	0.170	0.279	-0.057
ZrCl ₅ ⁻	0.002	0.158	0.325	0.229	0.013	-0.232	0.044
Ag(NHC) ⁺	0.121	0.009	0.037	-0.119	-0.058	0.140	-0.193
AuCl ₃	0.093	0.191	0.065	-0.290	0.191	-0.105	-0.105
AuCN	0.078	0.173	0.014	-0.107	-0.073	0.190	0.050
Cr(H ₂ O) ₅ ²⁺	0.184	-0.229	0.149	-0.004	-0.205	-0.046	0.095
CuCH ₃	0.050	0.103	0.080	-0.015	-0.036	0.182	0.109
CuCN	0.072	0.132	0.033	0.020	-0.026	0.300	0.070
FeCl ₃ ⁻	-0.013	0.163	0.264	0.125	0.005	-0.259	-0.014
FeCl ₃	0.079	0.061	0.190	0.082	0.088	-0.076	-0.165
GaCl ₃	0.077	0.060	0.178	-0.070	0.254	-0.011	0.076
HgI ₂	0.058	0.018	0.187	-0.273	0.108	-0.265	-0.295
InCl ₂ ⁺	0.173	-0.031	0.054	-0.077	0.273	0.042	0.018
Ni(PF ₃) ₃	0.062	0.114	0.099	-0.142	-0.136	-0.067	-0.079
NiPH ₃	0.051	0.169	0.073	0.107	-0.364	0.126	0.079
PtPH ₃	0.056	0.198	0.053	-0.040	-0.326	0.018	0.094
SnMe ₃ ⁺	0.141	-0.061	0.121	-0.155	0.191	0.054	0.022
Y(H ₂ O) ₅ ³⁺	0.272	-0.339	0.076	0.151	-0.057	0.040	0.240
ZnCl ₃ ⁻	-0.015	0.190	0.177	0.017	0.121	-0.093	0.059
ZnNH ₃ ²⁺	0.282	0.100	-0.272	0.073	0.034	0.257	-0.257
Zr(Ome) ₃ ⁺	0.147	-0.060	0.159	0.202	0.005	0.125	-0.062

Table S14: First seven hidden descriptors of the ligands for the Full Set of data, ordered by their values in decreasing order. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum. Results are split in two separate tables, part A and part B.

Table S14, PART A			
$\text{HD}_{L1} = \mathbf{L}_1$	$\text{HD}_{L2} = \mathbf{L}_2$	$\text{HD}_{L3} = \mathbf{L}_3$	$\text{HD}_{L4} = \mathbf{L}_4$
He -0.002	S^{2-} 0.323	I^- 0.267	H^- 0.406
H_2 -0.008	Br^- 0.173	SCN^- 0.236	Bpin^- 0.347
Xe -0.018	I^- 0.171	Br^- 0.205	SiMe_3^- 0.231
PCl_3 -0.024	Cl^- 0.160	NCS^- 0.182	SiH_3^- 0.214
CO -0.025	SCN^- 0.142	SiH_3^- 0.175	CH_3^- 0.143
H_2O -0.034	NCS^- 0.126	SiMe_3^- 0.158	CHCH_2^- 0.133
H_2S -0.034	F^- 0.109	$\text{C}_4\text{H}_4\text{S}$ 0.150	CN^- 0.114
PF_3 -0.036	SH^- 0.089	Cl^- 0.150	C_6H_5^- 0.108
$\text{C}_4\text{H}_4\text{O}$ -0.036	OMe 0.078	SH^- 0.146	$\text{C}_6\text{H}_4\text{Cl}^-$ 0.089
NCH -0.039	SMe^- 0.062	Xe 0.139	$\text{C}_6\text{H}_4\text{NO}_2^-$ 0.089
PH_3 -0.041	OH^- 0.057	SMe^- 0.135	$\text{C}_6\text{H}_4\text{OMe}^-$ 0.079
$\text{C}_4\text{H}_4\text{S}$ -0.041	CN^- 0.045	PF_3 0.119	CCH^- 0.071
NH_3 -0.046	O^{2-} 0.042	PH_3 0.102	CO 0.030
NMe_3 -0.055	CCH^- 0.020	PMe_3 0.098	He -0.005
$\text{C}_5\text{H}_5\text{N}$ -0.059	NH_2^- -0.005	CN^- 0.085	PCl_3 -0.007
$\text{C}_3\text{H}_4\text{N}_2$ -0.062	He -0.012	H_2S 0.085	H_2 -0.019
PMe_3 -0.063	SiH_3^- -0.035	$\text{C}_4\text{H}_4\text{O}$ 0.083	SCN^- -0.023
NHC -0.076	C_6H_5^- -0.065	PCl_3 0.072	SH^- -0.023
SCN^- -0.142	H_2 -0.065	$\text{C}_6\text{H}_4\text{NO}_2^-$ 0.062	S^{2-} -0.029
I^- -0.146	CHCH_2^- -0.066	CCH^- 0.057	SMe^- -0.045
Br^- -0.149	$\text{C}_6\text{H}_4\text{OMe}^-$ -0.066	$\text{C}_6\text{H}_4\text{Cl}^-$ 0.056	I^- -0.048
NCS^- -0.150	Xe -0.070	Bpin^- 0.054	PF_3 -0.059
Cl^- -0.155	$\text{C}_6\text{H}_4\text{Cl}^-$ -0.070	$\text{C}_6\text{H}_4\text{OMe}^-$ 0.052	NHC -0.065
CN^- -0.158	Bpin^- -0.074	NCH 0.051	Br^- -0.066
SH^- -0.165	$\text{C}_6\text{H}_4\text{NO}_2^-$ -0.079	$\text{C}_5\text{H}_5\text{N}$ 0.051	PH_3 -0.072
SMe^- -0.171	CH_3^- -0.081	H_2 0.049	PMe_3 -0.081
SiH_3^- -0.175	SiMe_3^- -0.092	NMe_3 0.044	Cl^- -0.093
$\text{C}_6\text{H}_4\text{NO}_2^-$ -0.175	$\text{C}_4\text{H}_4\text{O}$ -0.112	$\text{C}_3\text{H}_4\text{N}_2$ 0.040	NH_2^- -0.093
F^- -0.176	H_2O -0.121	C_6H_5^- 0.040	H_2S -0.112
CCH^- -0.177	NCH -0.122	S^{2-} 0.014	NCH -0.112
OMe -0.184	$\text{C}_4\text{H}_4\text{S}$ -0.152	H_2O 0.006	Xe -0.121
$\text{C}_6\text{H}_4\text{Cl}^-$ -0.185	H_2S -0.166	He 0.006	NH_3 -0.125
SiMe_3^- -0.187	$\text{C}_3\text{H}_4\text{N}_2$ -0.191	CO 0.003	$\text{C}_4\text{H}_4\text{S}$ -0.149
OH^- -0.187	CO -0.197	CHCH_2^- -0.004	H_2O -0.157
C_6H_5^- -0.191	$\text{C}_5\text{H}_5\text{N}$ -0.199	NH_3 -0.006	$\text{C}_5\text{H}_5\text{N}$ -0.173
$\text{C}_6\text{H}_4\text{OMe}^-$ -0.193	NH_3 -0.204	NHC -0.016	$\text{C}_3\text{H}_4\text{N}_2$ -0.177
CHCH_2^- -0.194	PCl_3 -0.210	OMe -0.029	OH^- -0.178
NH_2^- -0.195	PH_3 -0.216	CH_3^- -0.039	F^- -0.179
Bpin^- -0.197	PF_3 -0.218	NH_2^- -0.082	NCS^- -0.194
CH_3^- -0.197	H^- -0.225	F^- -0.083	$\text{C}_4\text{H}_4\text{O}$ -0.200
H^- -0.220	NMe_3 -0.236	OH^- -0.094	NMe_3 -0.219
S^{2-} -0.307	PMe_3 -0.294	H^- -0.302	OMe -0.244
O^{2-} -0.379	NHC -0.320	O^{2-} -0.658	O^{2-} -0.254

Table S14, PART B

HD_{L5} = L₅	HD_{L6} = L₆	L₇
CO 0.495	O ²⁻ 0.319	SiH ₃ ⁻ 0.241
PCl ₃ 0.399	S ²⁻ 0.300	H ⁻ 0.218
PF ₃ 0.312	SiMe ₃ ⁻ 0.275	SH ⁻ 0.191
O ²⁻ 0.237	PF ₃ 0.208	I ⁻ 0.187
H ₂ 0.170	C ₄ H ₄ S 0.181	H ₂ S 0.183
CN ⁻ 0.161	C ₆ H ₄ OMe ⁻ 0.142	SiMe ₃ ⁻ 0.175
S ²⁻ 0.155	PMe ₃ 0.120	S ²⁻ 0.174
NCH 0.146	SiH ₃ ⁻ 0.104	PH ₃ 0.168
PH ₃ 0.131	C ₆ H ₄ Cl ⁻ 0.098	CH ₃ ⁻ 0.164
SCN ⁻ 0.127	C ₄ H ₄ O 0.096	Xe 0.144
I ⁻ 0.089	C ₆ H ₄ NO ₂ ⁻ 0.088	Br ⁻ 0.140
CCH ⁻ 0.083	C ₆ H ₅ ⁻ 0.082	NMe ₃ 0.134
Br ⁻ 0.076	Bpin ⁻ 0.076	SMe ⁻ 0.124
NCS ⁻ 0.071	PCl ₃ 0.049	NH ₃ 0.101
H ⁻ 0.062	Xe 0.040	O ²⁻ 0.099
Cl ⁻ 0.055	SMe ⁻ 0.019	Cl ⁻ 0.085
Xe 0.051	C ₅ H ₅ N 0.017	C ₄ H ₄ S 0.070
H ₂ S 0.040	SCN ⁻ 0.000	NH ₂ ⁻ 0.069
C ₄ H ₄ S 0.028	NMe ₃ -0.002	H ₂ 0.067
He 0.025	He -0.009	PMe ₃ 0.066
SH ⁻ 0.001	PH ₃ -0.013	H ₂ O 0.066
Bpin ⁻ -0.017	NCS ⁻ -0.016	NCH 0.026
PMe ₃ -0.022	NHC -0.016	He 0.025
SMe ⁻ -0.032	C ₃ H ₄ N ₂ -0.031	C ₄ H ₄ O 0.006
NHC -0.053	H ₂ S -0.036	C ₃ H ₄ N ₂ -0.015
SiH ₃ ⁻ -0.057	CHCH ₂ ⁻ -0.040	CHCH ₂ ⁻ -0.041
C ₆ H ₄ NO ₂ ⁻ -0.064	OMe -0.051	SCN ⁻ -0.051
F ⁻ -0.080	I ⁻ -0.053	PCl ₃ -0.058
C ₄ H ₄ O -0.088	H ₂ -0.073	OH ⁻ -0.069
NH ₃ -0.089	SH ⁻ -0.089	Bpin ⁻ -0.069
H ₂ O -0.093	CH ₃ ⁻ -0.099	NHC -0.072
CHCH ₂ ⁻ -0.094	H ₂ O -0.119	C ₅ H ₅ N -0.085
C ₆ H ₄ Cl ⁻ -0.105	NH ₂ ⁻ -0.129	PF ₃ -0.097
OH ⁻ -0.108	Br ⁻ -0.135	OMe -0.121
C ₆ H ₅ ⁻ -0.108	CCH ⁻ -0.162	CCH ⁻ -0.127
C ₅ H ₅ N -0.120	NH ₃ -0.168	CO -0.145
C ₆ H ₄ OMe ⁻ -0.121	NCH -0.171	F ⁻ -0.162
C ₃ H ₄ N ₂ -0.126	CO -0.196	CN ⁻ -0.162
OMe -0.132	Cl ⁻ -0.198	C ₆ H ₅ ⁻ -0.238
SiMe ₃ ⁻ -0.137	OH ⁻ -0.220	C ₆ H ₄ OMe ⁻ -0.270
NH ₂ ⁻ -0.141	CN ⁻ -0.239	C ₆ H ₄ Cl ⁻ -0.278
CH ₃ ⁻ -0.181	F ⁻ -0.306	NCS ⁻ -0.288
NMe ₃ -0.226	H ⁻ -0.354	C ₆ H ₄ NO ₂ ⁻ -0.338

Table S15: First seven hidden descriptors of the metal fragments for the Full Set of data, ordered by their values in decreasing order. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum. Results are split in two separate tables, part A and part B.

Table S15, PART A			
$\mathbf{HD}_{M1} = \mathbf{M}_1$	$\mathbf{HD}_{M2} = \mathbf{M}_2$	$\mathbf{HD}_{M3} = \mathbf{M}_3$	$\mathbf{HD}_{M4} = \mathbf{M}_4$
OsO ₃ ²⁺ 0.368	PtF ₅ ⁻ 0.414	ZrCl ₅ ⁻ 0.325	OsO ₃ ²⁺ 0.306
Rh(H ₂ O) ₅ ³⁺ 0.329	OsO ₃ ²⁺ 0.266	Nb(NH ₂) ₄ ⁺ 0.291	TiCl ₃ ⁺ 0.303
Co(NH ₃) ₅ ³⁺ 0.291	MnO ₃ ⁺ 0.208	FeCl ₃ ⁻ 0.264	TaMe ₄ ⁺ 0.252
ZnNH ₃ ²⁺ 0.282	CrO ₃ 0.199	FeCl ₃ 0.190	ZrCl ₅ ⁻ 0.229
Y(H ₂ O) ₅ ³⁺ 0.272	PtPH ₃ 0.198	HgI ₂ 0.187	Zr(Ome) ₃ ⁺ 0.202
MnO ₃ ⁺ 0.220	AuCl ₃ 0.191	AlCl ₃ 0.181	Mo(SH) ₃ ⁺ 0.165
Cu(NH ₃) ₃ ²⁺ 0.206	ZnCl ₃ ⁻ 0.190	GaCl ₃ 0.178	Y(H ₂ O) ₅ ³⁺ 0.151
TiCl ₃ ⁺ 0.187	AuCN 0.173	ZnCl ₃ ⁻ 0.177	FeCl ₂ ⁺ 0.137
Cr(H ₂ O) ₅ ²⁺ 0.184	NiPH ₃ 0.169	Ru(SH) ₄ 0.160	FeCl ₃ ⁻ 0.125
FeCl ₂ ⁺ 0.179	FeCl ₃ ⁻ 0.163	Zr(Ome) ₃ ⁺ 0.159	NiPH ₃ 0.107
InCl ₂ ⁺ 0.173	Fe(CO) ₄ 0.162	Cr(H ₂ O) ₅ ²⁺ 0.149	AlCl ₃ 0.084
Mo(SH) ₃ ⁺ 0.171	ZrCl ₅ ⁻ 0.158	TaMe ₄ ⁺ 0.145	FeCl ₃ 0.082
TaMe ₄ ⁺ 0.170	W(CO) ₅ 0.153	Mo(SH) ₃ ⁺ 0.136	CrO ₃ 0.074
ZnCH ₃ ⁺ 0.159	PdPH ₃ 0.137	K ⁺ 0.130	ZnNH ₃ ²⁺ 0.073
Zr(Ome) ₃ ⁺ 0.147	CuCN 0.132	SnMe ₃ ⁺ 0.121	MnO ₃ ⁺ 0.066
AuPH ₃ ⁺ 0.146	Ru(SH) ₄ 0.114	TiCl ₃ ⁺ 0.114	CuCN 0.020
IrCO(PH ₃) ₂ ⁺ 0.142	Ni(PF ₃) ₃ 0.114	Ni(PF ₃) ₃ 0.099	ZnCl ₃ ⁻ 0.017
SnMe ₃ ⁺ 0.141	CuCH ₃ 0.103	PdPH ₃ 0.080	Nb(NH ₂) ₄ ⁺ 0.007
PdH(PH ₃) ₂ ⁺ 0.122	ZnNH ₃ ²⁺ 0.100	CuCH ₃ 0.080	Cr(H ₂ O) ₅ ²⁺ -0.004
Nb(NH ₂) ₄ ⁺ 0.121	AuPH ₃ ⁺ 0.074	Y(H ₂ O) ₅ ³⁺ 0.076	CuCH ₃ -0.015
Ag(NHC) ⁺ 0.121	AlCl ₃ 0.064	W(CO) ₅ 0.074	K ⁺ -0.018
AuCl ₃ 0.093	FeCl ₃ 0.061	NiPH ₃ 0.073	PdPH ₃ -0.032
CrO ₃ 0.092	GaCl ₃ 0.060	CrO ₃ 0.072	ZnCH ₃ ⁺ -0.039
K ⁺ 0.091	IrCO(PH ₃) ₂ ⁺ 0.038	Fe(CO) ₄ 0.069	PtPH ₃ -0.040
FeCl ₃ 0.079	HgI ₂ 0.018	AuCl ₃ 0.065	GaCl ₃ -0.070
AuCN 0.078	Ag(NHC) ⁺ 0.009	FeCl ₂ ⁺ 0.063	W(CO) ₅ -0.075
AlCl ₃ 0.077	ZnCH ₃ ⁺ -0.010	PdH(PH ₃) ₂ ⁺ 0.062	InCl ₂ ⁺ -0.077
GaCl ₃ 0.077	TiCl ₃ ⁺ -0.017	InCl ₂ ⁺ 0.054	PtF ₅ ⁻ -0.103
CuCN 0.072	Mo(SH) ₃ ⁺ -0.019	PtPH ₃ 0.053	Ru(SH) ₄ -0.106
W(CO) ₅ 0.068	PdH(PH ₃) ₂ ⁺ -0.021	Cu(NH ₃) ₃ ²⁺ 0.042	AuCN -0.107
Ru(SH) ₄ 0.065	InCl ₂ ⁺ -0.031	Ag(NHC) ⁺ 0.037	IrCO(PH ₃) ₂ ⁺ -0.119
Fe(CO) ₄ 0.064	FeCl ₂ ⁺ -0.033	IrCO(PH ₃) ₂ ⁺ 0.036	Ag(NHC) ⁺ -0.119
Ni(PF ₃) ₃ 0.062	Rh(H ₂ O) ₅ ³⁺ -0.056	PtF ₅ ⁻ 0.036	Ni(PF ₃) ₃ -0.142
HgI ₂ 0.058	TaMe ₄ ⁺ -0.058	CuCN 0.033	SnMe ₃ ⁺ -0.155
PtPH ₃ 0.056	SnMe ₃ ⁺ -0.061	AuCN 0.014	AuPH ₃ ⁺ -0.164
NiPH ₃ 0.051	K ⁺ -0.123	ZnCH ₃ ⁺ 0.013	Cu(NH ₃) ₃ ²⁺ -0.171
CuCH ₃ 0.050	Nb(NH ₂) ₄ ⁺ -0.146	AuPH ₃ ⁺ -0.012	PdH(PH ₃) ₂ ⁺ -0.194
PdPH ₃ 0.044	Cu(NH ₃) ₃ ²⁺ -0.170	Co(NH ₃) ₅ ³⁺ -0.050	Rh(H ₂ O) ₅ ³⁺ -0.212
PtF ₅ ⁻ 0.017	Cr(H ₂ O) ₅ ²⁺ -0.229	MnO ₃ ⁺ -0.123	Fe(CO) ₄ -0.219
ZrCl ₅ ⁻ 0.002	Co(NH ₃) ₅ ³⁺ -0.230	Rh(H ₂ O) ₅ ³⁺ -0.223	Co(NH ₃) ₅ ³⁺ -0.246
FeCl ₃ ⁻ -0.013	Y(H ₂ O) ₅ ³⁺ -0.339	ZnNH ₃ ²⁺ -0.272	HgI ₂ -0.273
ZnCl ₃ ⁻ -0.015	Zr(Ome) ₃ ⁺ -0.060	OsO ₃ ²⁺ -0.447	AuCl ₃ -0.290

Table S15, PART B

$\mathbf{HD}_{M5} = \mathbf{M}_5$	$\mathbf{HD}_{M6} = \mathbf{M}_6$	$\mathbf{M}_7$
InCl ₂ ⁺ 0.273	CuCN 0.300	PtF ₅ ⁻ 0.442
GaCl ₃ 0.254	ZnCH ₃ ⁺ 0.279	Co(NH ₃) ₅ ³⁺ 0.315
AlCl ₃ 0.224	ZnNH ₃ ²⁺ 0.257	Y(H ₂ O) ₅ ³⁺ 0.240
PtF ₅ ⁻ 0.210	CrO ₃ 0.197	AlCl ₃ 0.238
SnMe ₃ ⁺ 0.191	AuCN 0.190	Rh(H ₂ O) ₅ ³⁺ 0.223
AuCl ₃ 0.191	CuCH ₃ 0.182	CuCH ₃ 0.109
ZnCH ₃ ⁺ 0.170	AlCl ₃ 0.177	Cr(H ₂ O) ₅ ²⁺ 0.095
ZnCl ₃ ⁻ 0.121	K ⁺ 0.162	PtPH ₃ 0.094
MnO ₃ ⁺ 0.111	Ag(NHC) ⁺ 0.140	IrCO(PH ₃) ₂ ⁺ 0.093
HgI ₂ 0.108	TaMe ₄ ⁺ 0.131	NiPH ₃ 0.079
FeCl ₂ ⁺ 0.101	NiPH ₃ 0.126	GaCl ₃ 0.076
CrO ₃ 0.098	Zr(Ome) ₃ ⁺ 0.125	CuCN 0.070
Cu(NH ₃) ₃ ²⁺ 0.097	IrCO(PH ₃) ₂ ⁺ 0.098	CrO ₃ 0.060
FeCl ₃ 0.088	AuPH ₃ ⁺ 0.089	ZnCl ₃ ⁻ 0.059
TiCl ₃ ⁺ 0.052	W(CO) ₅ 0.073	TaMe ₄ ⁺ 0.057
ZnNH ₃ ²⁺ 0.034	SnMe ₃ ⁺ 0.054	AuCN 0.050
OsO ₃ ²⁺ 0.025	Fe(CO) ₄ 0.045	ZrCl ₅ ⁻ 0.044
TaMe ₄ ⁺ 0.015	InCl ₂ ⁺ 0.042	W(CO) ₅ 0.031
ZrCl ₅ ⁻ 0.013	Y(H ₂ O) ₅ ³⁺ 0.040	OsO ₃ ²⁺ 0.030
Co(NH ₃) ₅ ³⁺ 0.006	TiCl ₃ ⁺ 0.030	SnMe ₃ ⁺ 0.022
FeCl ₃ ⁻ 0.005	PtF ₅ ⁻ 0.024	InCl ₂ ⁺ 0.018
Zr(Ome) ₃ ⁺ 0.005	PtPH ₃ 0.018	Nb(NH ₂) ₄ ⁺ -0.009
Nb(NH ₂) ₄ ⁺ -0.025	PdH(PH ₃) ₂ ⁺ 0.009	FeCl ₃ ⁻ -0.014
CuCN -0.026	FeCl ₂ ⁺ 0.009	Fe(CO) ₄ -0.018
CuCH ₃ -0.036	PdPH ₃ 0.003	Cu(NH ₃) ₃ ²⁺ -0.036
AuPH ₃ ⁺ -0.052	GaCl ₃ -0.011	Ru(SH) ₄ -0.042
Y(H ₂ O) ₅ ³⁺ -0.057	MnO ₃ ⁺ -0.011	ZnCH ₃ ⁺ -0.057
Ag(NHC) ⁺ -0.058	Cu(NH ₃) ₃ ²⁺ -0.032	TiCl ₃ ⁺ -0.060
K ⁺ -0.069	Cr(H ₂ O) ₅ ²⁺ -0.046	Zr(Ome) ₃ ⁺ -0.062
AuCN -0.073	Ni(PF ₃) ₃ -0.067	Mo(SH) ₃ ⁺ -0.067
PdH(PH ₃) ₂ ⁺ -0.084	FeCl ₃ -0.076	PdPH ₃ -0.072
Fe(CO) ₄ -0.090	Co(NH ₃) ₅ ³⁺ -0.090	Ni(PF ₃) ₃ -0.079
Rh(H ₂ O) ₅ ³⁺ -0.100	ZnCl ₃ ⁻ -0.093	PdH(PH ₃) ₂ ⁺ -0.094
Ni(PF ₃) ₃ -0.136	AuCl ₃ -0.105	AuCl ₃ -0.105
Mo(SH) ₃ ⁺ -0.163	Mo(SH) ₃ ⁺ -0.118	FeCl ₂ ⁺ -0.162
Ru(SH) ₄ -0.173	Ru(SH) ₄ -0.134	FeCl ₃ -0.165
IrCO(PH ₃) ₂ ⁺ -0.200	Nb(NH ₂) ₄ ⁺ -0.187	AuPH ₃ ⁺ -0.187
Cr(H ₂ O) ₅ ²⁺ -0.205	Rh(H ₂ O) ₅ ³⁺ -0.225	Ag(NHC) ⁺ -0.193
W(CO) ₅ -0.212	ZrCl ₅ ⁻ -0.232	K ⁺ -0.234
PdPH ₃ -0.311	FeCl ₃ ⁻ -0.259	ZnNH ₃ ²⁺ -0.257
PtPH ₃ -0.326	HgI ₂ -0.265	MnO ₃ ⁺ -0.293
NiPH ₃ -0.364	OsO ₃ ²⁺ -0.386	HgI ₂ -0.295

3.4 Errors by number of hidden descriptors (k) and weights $\mathbf{W}$ for the Full Set of data.

We present in Table S16 the maximum and average errors obtained when a given k (number of hidden descriptors) is used for the calculation of the estimated BDE. The errors are the subtraction between the computational BDEs and the BDEs estimated from the use of a given number of hidden descriptors (using the corresponding hidden descriptors HD_{Lk} , HD_{Mk} and diagonal matrix $\mathbf{W}$) for the Full Set of data. The matrix of weights $\mathbf{W}$ is diagonal, and only the elements of the diagonal are presented in the Table.

Please note that in this case we are not reporting estimated hidden descriptors or BDEs from few reference calculations for the new ligands and the new metal fragments in Full Set of data, we are just using the ones obtained from simply applying the SVD to the Full Set of BDEs.

Table S16: Maximum absolute and average error (in kcal/mol) of the estimated BDE with respect to the number of hidden descriptors (k) considered for the Full Set of data. The diagonal term in matrix $\mathbf{W}$ is also provided.

Full Set of data			
k	Max error	Aver error	Weight, $\mathbf{W}_{k,k}$
1	102.9	11.5	7261.8
2	105.3	7.3	492.8
3	31.6	4.4	412.9
4	23.7	2.8	189.5
5	15.3	2.1	107.9
6	10.0	1.4	91.9
7	7.6	1.1	47.1
8	7.6	0.9	34.0
9	5.7	0.8	30.4
10	5.4	0.7	22.9
11	5.1	0.6	19.4
12	4.8	0.6	16.7
13	4.8	0.5	14.8
14	4.6	0.4	13.4
15	3.6	0.4	11.1
16	3.5	0.4	10.1
17	2.1	0.3	9.6
18	1.9	0.3	7.8
19	1.7	0.3	6.9
20	1.6	0.2	6.6
21	1.5	0.2	5.8
22	1.5	0.2	5.0

4 Actual Training Set (B3LYP-D3 in vacuum)

4.1 Description of the procedure used to select the Actual Training Set

Along the study we noticed that hidden descriptors obtained for the Initial Training Set and the hidden descriptors for the Full Set of data are quite different, compare Tables S3 and S4 with Tables S12 and S13. If we compare them by performing a regression analysis between the vector of hidden descriptors for each k in one and the other Set we obtain r^2 of 0.9999 for the first PC and 0.942 for the fourth SV, indicating that both data sets capture the same chemistry for these two SVs. For the second, fifth and seventh we see a moderate correlation of 0.638, 0.637 and 0.743. And very minor correlation is found for the third and sixth 0.397 and 0.347, indicating that they do not describe the same properties of the ligands and metal fragments, or at least not with the same type of vectors. Please note that we can not compare all ligands in the Full Set of data with the Initial Training Set. We are only comparing the hidden descriptors of the ligands in the Initial Training Set but with the hidden descriptors obtained by processing all data in the Full Set.

Also looking at the necessary number of hidden descriptors (k), see Tables S7 and S16, we observed that the Initial Training Set needs of 5 hidden descriptors to get a maximum and an average error of below 10 and 2 kcal/mol respectively while the Full Set of data needs 6 to get to the same type of errors. Consequently we can only conclude that our Initial Training Set does not have ligands and metal fragments different enough in chemical nature to represent the broad space of the Full data set. This has different consequences, being the most important that this Initial Training Set would not be useful to extract general conclusions further away than from the second hidden descriptor. It is also worrying the fact that the Initial Training Set does not need of the sixth hidden descriptor, so that some attribute needed in the Full data set is not needed in the smaller subspace.

With this in mind we decided to make some changes in our training set, the basic idea was to exchange some ligands and metal fragments from the Extended Set to the Initial Training Set. These exchanges should allow us to capture a broader area of the chemical space but at the same time we want to keep the essence of the Initial Training Set and the variety in the Extended Set. We tried different ways of performing this exchanges but finally we decided to move three ligands and metal fragments out of the Initial Training Set and add three ligands and metal fragments from the Full data set. To choose which ligands and metal fragments were exchanged we looked for a set able to produce hidden descriptors similar to those of the Full Set of data.

The procedure used to select which ligands to remove from the Initial Training Set and which to add in is independent on the procedure to remove and add the metal fragments and viceversa. The method consists on:

- Compute the hidden descriptors for ligands and metal fragments of the Full data set.
- Select the three ligands to remove from the Initial Training Set. To do it, we will proceed in few steps:

1. Look for all possible combinations of sets of ligands of the Initial Training Set containing three species less (all combinations of 19 (22-3) ligands). These are the reduced sets of data.
 2. Perform a SVD analysis for all reduced sets. Obtain the hidden descriptors for ligands.
 3. Carry out a regression analysis between the hidden descriptors of the all reduced sets and the corresponding hidden descriptors for the Full Set of data. Do it from hidden descriptors one to seven.
 4. For each reduced set add-up the r^2 of the first seven hidden descriptors.
 5. Look among all reduced sets for the three with higher sum of r^2 . These three sets of 19 ligands of the Initial Training Set are the most representative of the chemical space in the Full Set of data. They will be used in the procedure to add three new ligands in.
- Select the three ligands to add in the new training set.
 1. We take one of the three best reduced sets of ligands according to the previous procedure. We look for all possible combinations resulting from adding three new ligands to that reduced set. The new ligands to add must be from the Full Set of data and different from the ones already in the reduced set. We will call all these combinations new sets.
 2. Perform a SVD analysis for all new sets. Obtain the hidden descriptors for the ligands in all new sets.
 3. Carry out a regression analysis between the hidden descriptors of all new sets and the corresponding hidden descriptors for the Full data set. Do it from hidden descriptors one to seven.
 4. For each new set add-up the r^2 of all seven hidden descriptors.
 5. Look among all new sets for the ones with higher sum of r^2 . This sets of 22 ligands, are the more representative of the chemical space in the Full Set of data for the given reduced set.
 6. We repeat the procedure for the other two best reduced sets.
 7. We choose among the three reduced sets the best new set, the one with higher sum of r^2 for k one to seven. The ligands in this new set will be the ones used in the Actual Training Set.
 - Select the three metal fragments to remove from the Initial Training Set. We repeat the procedure detailed for ligands, but for metal fragments instead.
 - Select the three metal fragments to add at the new training set. We repeat the procedure detailed for ligands, but for metal fragments instead. The new sets will have in this case 23 metal fragments and will be the ones used in the Actual Training Set.

This was done through the use of the script presented in section 9.2. The first is to choose the ligands and the second the metal fragments.

The application of this procedure to our Initial Training Set selected signaled I^- , NCS^- and SCN^- as the ligands to be removed and $\text{C}_6\text{H}_4\text{OMe}^-$, PCl_3 and SiMe_3^- as new ligands to be added. As for the metal fragments AlCl_3 , K^+ and ZnCH_3^+ were removed and AuCl_3 , HgI_2 and InCl_2^+ were added.

So, finally the set of ligands and metal fragments we will use as training set contains Br^- , CH_3^- , Cl^- , CN^- , CO , F^- , C_6H_5^- , H_2 , H_2O , H^- , NCH , NH_3 , NHC , O^{2-} , OH^- , PH_3 , $\text{C}_5\text{H}_5\text{N}$, S^{2-} , SH^- , $\text{C}_6\text{H}_4\text{OMe}^-$, PCl_3 and SiMe_3 as ligands and AuPH_3^+ , $\text{Co}(\text{NH}_3)_5^{3+}$, CrO_3 , $\text{Cu}(\text{NH}_3)_3^{2+}$, FeCl_2^+ , $\text{Fe}(\text{CO})_4$, $\text{IrCO}(\text{PH}_3)_2^+$, MnO_3^+ , $\text{Mo}(\text{SH})_3^+$, $\text{Nb}(\text{NH}_2)_4^+$, OsO_3^{2+} , $\text{PdH}(\text{PH}_3)_2^+$, PdPH_3 , PtF_5^- , $\text{Rh}(\text{H}_2\text{O})_5^{3+}$, $\text{Ru}(\text{SH})_4$, TaMe_4^+ , TiCl_3^+ , $\text{W}(\text{CO})_5$, ZrCl_5^- AuCl_3 , HgI_2 and InCl_2^+ as metal fragments. We will call this set Actual Training Set.

We applied the SVD analysis to the Actual Training Set and we obtained the corresponding hidden descriptors $\mathbf{HD}_{Lk}$ and $\mathbf{HD}_{Mk}$. If we perform a regression analysis between the hidden descriptors of the Full Set of data and the hidden descriptors of the Actual Training Set we obtain good correlation for until the seventh hidden descriptor. 0.9998 k_1 , 0.998 k_2 , 0.982 k_3 , 0.972 k_4 , 0.953 k_5 , 0.941 k_6 , 0.898 k_7 , 0.314 k_8 , 0.882 k_9 , 0.302 k_{10} .

4.2 BDE matrix of the Actual Training Set

The matrix of bond dissociation energies in vacuum and B3LYP-D3 for the Actual Training Set is presented in Table S17. This is the matrix **BDE**, the starting point of the statistical analysis.

Table S17: Bond dissociation energies (kcal/mol) for the Actual Training Set. Calculations in vacuum with the B3LYP-D3 functional. Results are split in two separate tables, part A and part B.

Table S17, PART A											
	Br ⁻	CH ₃ ⁻	Cl ⁻	CN ⁻	CO	F ⁻	C ₆ H ₅ ⁻	H ₂	H ₂ O	H ⁻	NCH
AuPH ₃ ⁺	-154.0	-218.7	-159.6	-174.5	-37.8	-176.7	-205.5	-12.8	-35.9	-255.9	-43.5
Co(NH ₃) ₅ ³⁺	-333.75	-410.35	-341.65	-346.75	-31.45	-376.35	-405.05	-8.85	-49.25	-445.75	-63.05
CrO ₃	-80.0	-142.1	-88.2	-101.2	-34.1	-122.4	-131.3	-12.0	-39.2	-175.8	-39.5
Cu(NH ₃) ₃ ²⁺	-231.4	-295.0	-238.4	-240.5	-16.3	-268.1	-283.0	-3.4	-34.6	-327.5	-40.6
FeCl ₂ ⁺	-192.9	-254.8	-201.2	-197.4	-26.0	-233.7	-243.4	-8.2	-48.5	-280.9	-49.1
Fe(CO) ₄	-47.1	-102.1	-51.2	-72.2	-36.6	-70.6	-93.1	-10.0	-17.7	-148.2	-24.5
IrCO(PH ₃) ₂ ⁺	-148.3	-205.3	-154.8	-170.7	-44.8	-178.4	-198.6	-15.5	-33.0	-246.7	-42.7
MnO ₃ ⁺	-233.1	-325.2	-240.4	-247.7	-54.4	-271.8	-309.5	-23.8	-70.0	-352.0	-76.4
Mo(SH) ₃ ⁺	-174.9	-240.6	-185.3	-185.7	-41.4	-222.5	-228.6	-15.1	-42.8	-265.7	-48.0
Nb(NH ₂) ₄ ⁺	-116.5	-169.4	-126.6	-129.3	-4.8	-168.3	-157.8	6.6	-16.9	-205.5	-16.9
OsO ₃ ²⁺	-413.8	-517.8	-419.4	-418.3	-82.1	-439.7	-522.5	-35.5	-110.0	-529.8	-129.0
PdH(PH ₃) ₂ ⁺	-128.0	-179.0	-133.0	-144.2	-25.1	-151.6	-170.1	-6.3	-22.7	-219.4	-28.5
PdPH ₃	-32.4	-64.3	-35.9	-49.5	-36.1	-47.9	-60.3	-10.6	-13.9	-103.1	-21.1
PtF ₅ ⁻	25.9	-44.1	21.6	-10.8	-39.1	0.7	-45.2	-7.4	-29.9	-78.3	-23.7
Rh(H ₂ O) ₅ ³⁺	-375.0	-465.5	-381.6	-392.0	-58.7	-405.1	-466.3	-24.6	-67.7	-498.7	-86.2
Ru(SH) ₄	-47.3	-99.7	-52.2	-70.4	-28.3	-74.7	-89.5	-1.4	-18.2	-140.6	-23.0
TaMe ₄ ⁺	-180.8	-238.9	-193.0	-189.3	-27.6	-236.2	-225.9	-6.3	-46.4	-264.4	-49.6
TiCl ₃ ⁺	-197.7	-262.9	-210.5	-202.9	-31.6	-255.0	-249.5	-10.0	-55.2	-285.1	-56.2
W(CO) ₅	-55.6	-101.8	-60.2	-77.3	-41.7	-81.9	-95.7	-12.7	-21.2	-144.6	-30.5
ZrCl ₅ ⁻	38.5	-5.1	30.5	21.4	-6.5	-10.1	0.4	2.0	-13.6	-36.1	-3.9
AuCl ₃	-72.9	-154.2	-77.3	-101.2	-26.9	-97.1	-141.2	-2.2	-26.3	-191.9	-24.8
HgI ₂	-39.4	-96.8	-42.6	-52.2	-2.6	-58.5	-84.7	-0.5	-7.2	-133.5	-4.5
InCl ₂ ⁺	-182.6	-255.2	-192.0	-195.4	-18.3	-226.1	-242.7	-2.4	-42.1	-284.6	-42.1

Table S17, PART B

	NH ₃	NHC	O ²⁻	OH ⁻	PH ₃	C ₅ H ₅ N	S ²⁻	SH ⁻	C ₆ H ₄ OMe ⁻	PCl ₃	SiMe ₃ ⁻
AuPH ₃ ⁺	-55.7	-91.3	-391.2	-191.5	-53.8	-62.2	-315.1	-174.9	-206.2	-42.2	-206.3
Co(NH ₃) ₅ ³⁺	-64.85	-117.65	-783.75	-390.55	-56.15	-95.35	-678.15	-356.35	-408.95	-54.25	-399.65
CrO ₃	-56.4	-81.5	-267.8	-131.4	-44.4	-59.7	-159.0	-98.0	-131.4	-36.1	-126.2
Cu(NH ₃) ₃ ²⁺	-47.7	-85.0	-572.9	-279.8	-36.8	-65.9	-482.9	-251.0	-284.2	-29.1	-281.0
FeCl ₂ ⁺	-62.2	-98.5	-514.9	-251.6	-48.0	-77.4	-408.3	-217.5	-247.2	-35.2	-234.0
Fe(CO) ₄	-31.0	-56.8	-179.2	-79.4	-30.6	-32.0	-116.1	-62.5	-93.0	-30.5	-101.3
IrCO(PH ₃) ₂ ⁺	-47.7	-83.7	-396.0	-189.4	-45.2	-58.4	-313.2	-165.8	-199.0	-40.8	-189.4
MnO ₃ ⁺	-98.5	-149.1	-573.8	-293.8	-94.8	-117.6	-453.6	-263.3	-311.6	-81.7	-323.3
Mo(SH) ₃ ⁺	-54.8	-93.9	-521.4	-240.5	-47.6	-69.9	-392.5	-199.5	-231.2	-41.7	-215.9
Nb(NH ₂) ₄ ⁺	-23.9	-44.2	-422.2	-176.2	-9.9	-30.1	-294.1	-131.4	-158.5	-6.2	-143.3
OsO ₃ ²⁺	-147.2	-245.5	-912.0	-478.4	-159.3	-203.4	-795.0	-453.9	-536.5	-156.6	-535.4
PdH(PH ₃) ₂ ⁺	-34.0	-61.2	-346.1	-161.4	-30.5	-41.1	-278.8	-143.0	-170.3	-26.0	-166.6
PdPH ₃	-24.3	-43.5	-146.5	-54.5	-29.1	-24.7	-80.2	-43.0	-60.3	-33.2	-56.9
PtF ₅ ⁻	-46.3	-77.1	-32.7	-13.5	-39.6	-48.9	34.5	5.1	-45.3	-38.2	-42.4
Rh(H ₂ O) ₅ ³⁺	-94.2	-166.2	-846.9	-429.1	-97.1	-132.2	-749.0	-405.5	-470.9	-96.8	-470.1
Ru(SH) ₄	-28.5	-54.1	-226.1	-81.3	-28.7	-31.1	-130.8	-60.6	-89.4	-29.3	-92.1
TaMe ₄ ⁺	-58.5	-88.5	-515.0	-248.8	-41.7	-71.9	-385.1	-198.4	-228.0	-29.9	-201.8
TiCl ₃ ⁺	-69.7	-103.4	-557.7	-270.8	-52.5	-84.4	-418.8	-218.8	-252.4	-39.8	-234.6
W(CO) ₅	-33.2	-58.0	-202.4	-87.8	-34.0	-36.8	-125.8	-68.9	-95.6	-35.9	-95.3
ZrCl ₅ ⁻	-21.2	-32.8	-108.0	-15.5	-7.0	-18.3	14.9	25.9	-0.6	-9.5	14.8
AuCl ₃	-45.8	-84.3	-255.8	-116.9	-42.0	-48.2	-176.9	-100.0	-141.2	-31.9	-149.4
HgI ₂	-11.8	-27.3	-200.6	-71.1	-5.1	-15.1	-133.1	-56.6	-85.3	-4.6	-87.4
InCl ₂ ⁺	-54.3	-93.8	-480.0	-239.5	-40.8	-72.6	-388.4	-206.9	-244.8	-26.4	-236.2

4.3 Hidden descriptor tables for the Actual Training Set

We performed a SVD analysis as explained in the main text, also for the Actual Training Set. We obtained hidden descriptors $\mathbf{HD}_{Lk}$ for the ligands and hidden descriptors $\mathbf{HD}_{Mk}$ for the metal fragments. Tables S18 and S19 report the values for the first seven hidden descriptors for each ligand and metal fragment, respectively. In the Tables S20 and S21 the same values appear ordered in decreasing order and with the corresponding name of the ligand next to it. This arrangement allows for an easier visualization of the ligands having larger and lower values for a given hidden descriptor.

The SVD analysis was performed with the script presented in Section 9.1 of this Supporting Information.

Table S18: First seven hidden descriptors of the ligands for the Actual Training Set. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

Ligand	$\mathbf{HD}_{L1} = \mathbf{L}_1$	$\mathbf{HD}_{L2} = \mathbf{L}_2$	$\mathbf{HD}_{L3} = \mathbf{L}_3$	$\mathbf{HD}_{L4} = \mathbf{L}_4$	$\mathbf{HD}_{L5} = \mathbf{L}_5$	$\mathbf{HD}_{L6} = \mathbf{L}_6$	$\mathbf{L}_7$
Br ⁻	0.190	0.217	0.301	0.096	-0.124	-0.123	0.127
CH ₃ ⁻	0.252	-0.112	0.034	-0.188	0.234	-0.109	0.257
Cl ⁻	0.196	0.203	0.235	0.131	-0.096	-0.204	0.083
CN ⁻	0.201	0.053	0.170	-0.152	-0.223	-0.255	-0.324
CO	0.034	-0.252	0.013	-0.004	-0.585	-0.186	-0.111
F ⁻	0.222	0.124	-0.043	0.225	0.075	-0.420	-0.248
C ₆ H ₅ ⁻	0.245	-0.091	0.147	-0.137	0.161	0.075	-0.401
H ₂	0.011	-0.076	0.064	0.049	-0.249	-0.066	0.140
H ₂ O	0.043	-0.161	0.029	0.234	0.161	-0.111	0.095
H ⁻	0.278	-0.298	-0.264	-0.590	-0.104	-0.290	0.151
NCH	0.050	-0.155	0.082	0.188	-0.146	-0.122	0.060
NH ₃	0.059	-0.266	0.027	0.210	0.157	-0.146	0.196
NHC	0.099	-0.420	0.043	0.151	0.136	0.060	-0.034
O ²⁻	0.480	0.021	-0.683	0.264	-0.113	0.259	0.023
OH ⁻	0.237	0.049	-0.047	0.228	0.172	-0.277	-0.038
PH ₃	0.054	-0.279	0.157	0.164	-0.149	0.080	0.314
C ₅ H ₅ N	0.077	-0.258	0.116	0.281	0.202	0.062	-0.111
S ²⁻	0.391	0.395	0.104	-0.002	-0.160	0.357	0.129
SH ⁻	0.211	0.113	0.238	0.046	0.007	-0.067	0.299
C ₆ H ₄ OMe ⁻	0.248	-0.095	0.169	-0.092	0.179	0.165	-0.431
PCl ₃	0.049	-0.273	0.189	0.137	-0.375	0.348	-0.175
SiMe ₃ ⁻	0.243	-0.135	0.279	-0.285	0.175	0.276	0.204

Table S19: First seven hidden descriptors of the metal fragments for the Actual Training Set. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

Metal Frag.	$\text{HD}_{M1} = \text{M}_1$	$\text{HD}_{M2} = \text{M}_2$	$\text{HD}_{M3} = \text{M}_3$	$\text{HD}_{M4} = \text{M}_4$	$\text{HD}_{M5} = \text{M}_5$	$\text{HD}_{M6} = \text{M}_6$	M_7
AuPH_3^+	-0.178	0.091	-0.008	0.167	0.099	0.186	-0.275
$\text{Co}(\text{NH}_3)_5^{3+}$	-0.352	-0.324	-0.027	0.240	-0.038	0.059	0.396
CrO_3	-0.113	0.262	0.102	-0.085	-0.119	0.406	0.077
$\text{Cu}(\text{NH}_3)_3^{2+}$	-0.251	-0.235	0.074	0.197	-0.146	0.058	-0.049
FeCl_2^+	-0.219	-0.064	0.108	-0.142	-0.139	0.061	-0.232
$\text{Fe}(\text{CO})_4$	-0.078	0.227	0.081	0.253	0.170	0.094	-0.053
$\text{IrCO}(\text{PH}_3)_2^+$	-0.174	0.051	0.058	0.098	0.310	0.191	0.114
MnO_3^+	-0.264	0.230	-0.126	-0.083	-0.118	0.156	-0.429
$\text{Mo}(\text{SH})_3^+$	-0.211	-0.045	0.214	-0.220	0.234	-0.136	-0.079
$\text{Nb}(\text{NH}_2)_4^+$	-0.154	-0.189	0.409	-0.021	-0.033	-0.217	0.116
OsO_3^{2+}	-0.437	0.237	-0.499	-0.337	-0.007	-0.400	0.008
$\text{PdH}(\text{PH}_3)_2^+$	-0.150	-0.026	0.090	0.218	0.125	0.061	-0.082
PdPH_3	-0.055	0.189	0.119	0.028	0.449	-0.012	-0.046
PtF_5^-	-0.018	0.555	0.017	0.117	-0.271	0.069	0.499
$\text{Rh}(\text{H}_2\text{O})_5^{3+}$	-0.395	-0.124	-0.245	0.187	0.155	-0.156	0.250
$\text{Ru}(\text{SH})_4$	-0.083	0.167	0.218	0.083	0.208	-0.209	-0.068
TaMe_4^+	-0.210	-0.092	0.220	-0.294	-0.012	0.276	0.097
TiCl_3^+	-0.229	-0.052	0.188	-0.348	-0.077	0.158	-0.081
$\text{W}(\text{CO})_5$	-0.084	0.212	0.103	0.079	0.335	0.135	0.060
ZrCl_5^-	-0.009	0.214	0.439	-0.264	-0.101	-0.332	0.204
AuCl_3	-0.113	0.256	0.069	0.310	-0.282	-0.114	-0.172
HgI_2	-0.074	0.027	0.237	0.338	-0.176	-0.382	-0.265
InCl_2^+	-0.211	-0.055	0.074	0.091	-0.377	0.170	0.002

Table S20: First seven hidden descriptors of the ligands for the Actual Training Set, ordered by their values in decreasing order. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

HD _{L1} = L ₁	HD _{L2} = L ₂	HD _{L3} = L ₃	HD _{L4} = L ₄	HD _{L5} = L ₅	HD _{L6} = L ₆	L ₇
O ²⁻ 0.48	S ²⁻ 0.39	Br ⁻ 0.30	C ₅ H ₅ N 0.28	CH ₃ ⁻ 0.23	S ²⁻ 0.36	PH ₃ 0.31
S ²⁻ 0.39	Br ⁻ 0.22	SiMe ₃ ⁻ 0.28	O ²⁻ 0.26	C ₅ H ₅ N 0.20	PCl ₃ 0.35	SH ⁻ 0.30
H ⁻ 0.28	Cl ⁻ 0.20	SH ⁻ 0.24	H ₂ O 0.23	C ₆ H ₄ OMe ⁻ 0.18	SiMe ₃ ⁻ 0.28	CH ₃ ⁻ 0.26
CH ₃ ⁻ 0.25	F ⁻ 0.12	Cl ⁻ 0.24	OH ⁻ 0.23	SiMe ₃ ⁻ 0.17	O ²⁻ 0.26	SiMe ₃ ⁻ 0.20
C ₆ H ₄ OMe ⁻ 0.25	SH ⁻ 0.11	PCl ₃ 0.19	F ⁻ 0.23	OH ⁻ 0.17	C ₆ H ₄ OMe ⁻ 0.16	NH ₃ 0.20
C ₆ H ₅ ⁻ 0.25	CN ⁻ 0.05	CN ⁻ 0.17	NH ₃ 0.21	H ₂ O 0.16	PH ₃ 0.08	H ⁻ 0.15
SiMe ₃ ⁻ 0.24	OH ⁻ 0.05	C ₆ H ₄ OMe ⁻ 0.17	NCH 0.19	C ₆ H ₅ ⁻ 0.16	C ₆ H ₅ ⁻ 0.07	H ₂ 0.14
OH ⁻ 0.24	O ²⁻ 0.02	PH ₃ 0.16	PH ₃ 0.16	NH ₃ 0.16	C ₅ H ₅ N 0.06	S ²⁻ 0.13
F ⁻ 0.22	H ₂ -0.08	C ₆ H ₅ ⁻ 0.15	NHC 0.15	NHC 0.14	NHC 0.06	Br ⁻ 0.13
SH ⁻ 0.21	C ₆ H ₅ ⁻ -0.09	C ₅ H ₅ N 0.12	PCl ₃ 0.14	F ⁻ 0.08	H ₂ -0.07	H ₂ O 0.10
CN ⁻ 0.20	C ₆ H ₄ OMe ⁻ -0.09	S ²⁻ 0.10	Cl ⁻ 0.13	SH ⁻ 0.01	SH ⁻ -0.07	Cl ⁻ 0.08
Cl ⁻ 0.20	CH ₃ ⁻ -0.11	NCH 0.08	Br ⁻ 0.10	Cl ⁻ -0.10	CH ₃ ⁻ -0.11	NCH 0.06
Br ⁻ 0.19	SiMe ₃ ⁻ -0.13	H ₂ 0.06	H ₂ 0.05	H ⁻ -0.10	H ₂ O -0.11	O ²⁻ 0.02
NHC 0.10	NCH -0.15	NHC 0.04	SH ⁻ 0.05	O ²⁻ -0.11	NCH -0.12	NHC -0.03
C ₅ H ₅ N 0.08	H ₂ O -0.16	CH ₃ ⁻ 0.03	S ²⁻ 0.00	Br ⁻ -0.12	Br ⁻ -0.12	OH ⁻ -0.04
NH ₃ 0.06	CO -0.25	H ₂ O 0.03	CO 0.00	NCH -0.15	NH ₃ -0.15	C ₅ H ₅ N -0.11
PH ₃ 0.05	C ₅ H ₅ N -0.26	NH ₃ 0.03	C ₆ H ₄ OMe ⁻ -0.09	PH ₃ -0.15	CO -0.19	CO -0.11
NCH 0.05	NH ₃ -0.27	CO 0.01	C ₆ H ₅ ⁻ -0.14	S ²⁻ -0.16	Cl ⁻ -0.20	PCl ₃ -0.18
PCl ₃ 0.05	PCl ₃ -0.27	F ⁻ -0.04	CN ⁻ -0.15	CN ⁻ -0.22	CN ⁻ -0.25	F ⁻ -0.25
H ₂ O 0.04	PH ₃ -0.28	OH ⁻ -0.05	CH ₃ ⁻ -0.19	H ₂ -0.25	OH ⁻ -0.28	CN ⁻ -0.32
CO 0.03	H ⁻ -0.30	H ⁻ -0.26	SiMe ₃ ⁻ -0.28	PCl ₃ -0.38	H ⁻ -0.29	C ₆ H ₅ ⁻ -0.40
H ₂ 0.01	NHC -0.42	O ²⁻ -0.68	H ⁻ -0.59	CO -0.58	F ⁻ -0.42	C ₆ H ₄ OMe ⁻ -0.43

Table S21: First seven hidden descriptors of the metal fragments for the Actual Training Set, ordered by their values in decreasing order. Values derived from BDEs obtained with the B3LYP-D3 functional in vacuum.

$\mathbf{HD}_{M1} = \mathbf{M}_1$	$\mathbf{HD}_{M2} = \mathbf{M}_2$	$\mathbf{HD}_{M3} = \mathbf{M}_3$	$\mathbf{HD}_{M4} = \mathbf{M}_4$
ZrCl ₅ ⁻ -0.01	PtF ₅ ⁻ 0.55	ZrCl ₅ ⁻ 0.44	HgI ₂ 0.34
PtF ₅ ⁻ -0.02	CrO ₃ 0.26	Nb(NH ₂) ₄ ⁺ 0.41	AuCl ₃ 0.31
PdPH ₃ -0.06	AuCl ₃ 0.26	HgI ₂ 0.24	Fe(CO) ₄ 0.25
HgI ₂ -0.07	OsO ₃ ²⁺ 0.24	TaMe ₄ ⁺ 0.22	Co(NH ₃) ₅ ³⁺ 0.24
Fe(CO) ₄ -0.08	MnO ₃ ⁺ 0.23	Ru(SH) ₄ 0.22	PdH(PH ₃) ₂ ⁺ 0.22
Ru(SH) ₄ -0.08	Fe(CO) ₄ 0.23	Mo(SH) ₃ ⁺ 0.21	Cu(NH ₃) ₃ ²⁺ 0.20
W(CO) ₅ -0.08	ZrCl ₅ ⁻ 0.21	TiCl ₃ ⁺ 0.19	Rh(H ₂ O) ₅ ³⁺ 0.19
CrO ₃ -0.11	W(CO) ₅ 0.21	PdPH ₃ 0.12	AuPH ₃ ⁺ 0.17
AuCl ₃ -0.11	PdPH ₃ 0.19	FeCl ₂ ⁺ 0.11	PtF ₅ ⁻ 0.12
PdH(PH ₃) ₂ ⁺ -0.15	Ru(SH) ₄ 0.17	W(CO) ₅ 0.10	IrCO(PH ₃) ₂ ⁺ 0.10
Nb(NH ₂) ₄ ⁺ -0.15	AuPH ₃ ⁺ 0.09	CrO ₃ 0.10	InCl ₂ ⁺ 0.09
IrCO(PH ₃) ₂ ⁺ -0.17	IrCO(PH ₃) ₂ ⁺ 0.05	PdH(PH ₃) ₂ ⁺ 0.09	Ru(SH) ₄ 0.08
AuPH ₃ ⁺ -0.18	HgI ₂ 0.03	Fe(CO) ₄ 0.08	W(CO) ₅ 0.08
TaMe ₄ ⁺ -0.21	PdH(PH ₃) ₂ ⁺ -0.03	Cu(NH ₃) ₃ ²⁺ 0.07	PdPH ₃ 0.03
Mo(SH) ₃ ⁺ -0.21	Mo(SH) ₃ ⁺ -0.04	InCl ₂ ⁺ 0.07	Nb(NH ₂) ₄ ⁺ -0.02
InCl ₂ ⁺ -0.21	TiCl ₃ ⁺ -0.05	AuCl ₃ 0.07	MnO ₃ ⁺ -0.08
FeCl ₂ ⁺ -0.22	InCl ₂ ⁺ -0.06	IrCO(PH ₃) ₂ ⁺ 0.06	CrO ₃ -0.08
TiCl ₃ ⁺ -0.23	FeCl ₂ ⁺ -0.06	PtF ₅ ⁻ 0.02	FeCl ₂ ⁺ -0.14
Cu(NH ₃) ₃ ²⁺ -0.25	TaMe ₄ ⁺ -0.09	AuPH ₃ ⁺ -0.01	Mo(SH) ₃ ⁺ -0.22
MnO ₃ ⁺ -0.26	Rh(H ₂ O) ₅ ³⁺ -0.12	Co(NH ₃) ₅ ³⁺ -0.03	ZrCl ₅ ⁻ -0.26
Co(NH ₃) ₅ ³⁺ -0.35	Nb(NH ₂) ₄ ⁺ -0.19	MnO ₃ ⁺ -0.13	TaMe ₄ ⁺ -0.29
Rh(H ₂ O) ₅ ³⁺ -0.40	Cu(NH ₃) ₃ ²⁺ -0.23	Rh(H ₂ O) ₅ ³⁺ -0.24	OsO ₃ ²⁺ -0.34
OsO ₃ ²⁺ -0.44	Co(NH ₃) ₅ ³⁺ -0.32	OsO ₃ ²⁺ -0.50	TiCl ₃ ⁺ -0.35

$\mathbf{HD}_{M5} = \mathbf{M}_5$	$\mathbf{HD}_{M6} = \mathbf{M}_6$	$\mathbf{HD}_{M7} = \mathbf{M}_7$
PdPH ₃ 0.45	CrO ₃ 0.41	PtF ₅ ⁻ 0.50
W(CO) ₅ 0.34	TaMe ₄ ⁺ 0.28	Co(NH ₃) ₅ ³⁺ 0.40
IrCO(PH ₃) ₂ ⁺ 0.31	IrCO(PH ₃) ₂ ⁺ 0.19	Rh(H ₂ O) ₅ ³⁺ 0.25
Mo(SH) ₃ ⁺ 0.23	AuPH ₃ ⁺ 0.19	ZrCl ₅ ⁻ 0.20
Ru(SH) ₄ 0.21	InCl ₂ ⁺ 0.17	Nb(NH ₂) ₄ ⁺ 0.12
Fe(CO) ₄ 0.17	TiCl ₃ ⁺ 0.16	IrCO(PH ₃) ₂ ⁺ 0.11
Rh(H ₂ O) ₅ ³⁺ 0.16	MnO ₃ ⁺ 0.16	TaMe ₄ ⁺ 0.10
PdH(PH ₃) ₂ ⁺ 0.12	W(CO) ₅ 0.13	CrO ₃ 0.08
AuPH ₃ ⁺ 0.10	Fe(CO) ₄ 0.09	W(CO) ₅ 0.06
OsO ₃ ²⁺ -0.01	PtF ₅ ⁻ 0.07	OsO ₃ ²⁺ 0.01
TaMe ₄ ⁺ -0.01	FeCl ₂ ⁺ 0.06	InCl ₂ ⁺ 0.00
Nb(NH ₂) ₄ ⁺ -0.03	PdH(PH ₃) ₂ ⁺ 0.06	PdPH ₃ -0.05
Co(NH ₃) ₅ ³⁺ -0.04	Co(NH ₃) ₅ ³⁺ 0.06	Cu(NH ₃) ₃ ²⁺ -0.05
TiCl ₃ ⁺ -0.08	Cu(NH ₃) ₃ ²⁺ 0.06	Fe(CO) ₄ -0.05
ZrCl ₅ ⁻ -0.10	PdPH ₃ -0.01	Ru(SH) ₄ -0.07
MnO ₃ ⁺ -0.12	AuCl ₃ -0.11	Mo(SH) ₃ ⁺ -0.08
CrO ₃ -0.12	Mo(SH) ₃ ⁺ -0.14	TiCl ₃ ⁺ -0.08
FeCl ₂ ⁺ -0.14	Rh(H ₂ O) ₅ ³⁺ -0.16	PdH(PH ₃) ₂ ⁺ -0.08
Cu(NH ₃) ₃ ²⁺ -0.15	Ru(SH) ₄ -0.21	AuCl ₃ -0.17
HgI ₂ -0.18	Nb(NH ₂) ₄ ⁺ -0.22	FeCl ₂ ⁺ -0.23
PtF ₅ ⁻ -0.27	ZrCl ₅ ⁻ -0.33	HgI ₂ -0.27
AuCl ₃ -0.28	HgI ₂ -0.38	AuPH ₃ ⁺ -0.27
InCl ₂ ⁺ -0.38	OsO ₃ ²⁺ -0.40	MnO ₃ ⁺ -0.43

4.4 Errors by number of SVs and Diagonal matrix $\mathbf{W}$ for the Actual Training Set

We present in Table S22 the maximum and average errors obtained when a given number of hidden descriptors (k) is used for the calculation of the estimated BDE. The errors are the subtraction between the computational BDEs and the BDEs estimated from the use of a given number of hidden descriptors. They are obtained using the corresponding hidden descriptors $\mathbf{L}$, $\mathbf{M}$ and $\mathbf{W}$) for the Actual Training Set.

Table S22: Maximum absolute and average error (in kcal/mol) of the estimated BDE with respect to the number of hidden descriptors (k) considered for the Actual Training Set. The weight of the last included k , the diagonal term $\mathbf{W}_{k,k}$ is also provided.

Actual Training set			
k	Max error	Aver error	Weight, $\mathbf{W}_{k,k}$
1	86.7	13.4	4691.4
2	88.0	8.7	292.7
3	28.1	5.2	252.3
4	14.4	3.2	119.3
5	13.2	2.3	59.0
6	8.1	1.4	54.1
7	6.0	1.1	24.6
8	5.2	0.8	22.0
9	3.0	0.7	15.5
10	2.6	0.5	12.6
11	2.2	0.4	9.2
12	1.7	0.3	7.4
13	1.6	0.2	5.8
14	1.2	0.2	4.4
15	0.8	0.1	4.0
16	0.6	0.1	2.5
17	0.6	0.1	1.7
18	0.3	0.1	1.3
19	0.3	0.0	1.2
20	0.2	0.0	0.9
21	0.1	0.0	0.6
22	0.0	0.0	0.5

4.5 Errors associated to each metal fragment and ligand

Table S22 gives for the Actual Training Set the maximum and average error associated to the use of six hidden descriptors is 8.1 and 1.4 kcal/mol, respectively. These values are not uniformly distributed among the whole initial set of metal fragments and ligands, and here we are reporting the errors associated to each ligand and metal fragment, Table S23.

Table S23: Maximum absolute and average error (kcal/mol) of the estimated BDEs associated to each ligand (left) and each metal fragment (right) in the Actual Training Set (6 hidden descriptors).

Error associated to each Ligand			Error associated to each Metal Fragment		
Ligand	Max error	Ave error	Metal Fragment	Max error	Ave error
Br ⁻	2.6	0.9	AuPH ₃ ⁺	3.9	1.8
CH ₃ ⁻	3.8	1.5	Co(NH ₃) ₅ ³⁺	4.6	2.0
Cl ⁻	1.9	0.7	CrO ₃	5.4	1.4
CN ⁻	5.6	1.9	Cu(NH ₃) ₃ ²⁺	1.8	0.7
CO	5.6	1.5	FeCl ₂ ⁺	4.1	1.7
F ⁻	3.8	1.8	Fe(CO) ₄	3.5	1.2
C ₆ H ₅ ⁻	6.1	1.7	IrCO(PH ₃) ₂ ⁺	3.9	1.3
H ₂	5.7	1.7	MnO ₃ ⁺	8.1	2.5
H ₂ O	2.7	0.9	Mo(SH) ₃ ⁺	5.6	2.0
H ⁻	3.5	1.3	Nb(NH ₂) ₄ ⁺	2.9	1.1
NCH	2.5	1.0	OsO ₃ ²⁺	1.9	0.8
NH ₃	3.1	1.0	PdH(PH ₃) ₂ ⁺	2.7	1.0
NHC	5.0	1.6	PdPH ₃	2.1	0.9
O ²⁻	2.3	0.8	PtF ₅ ⁻	6.1	2.3
OH ⁻	3.1	0.7	Rh(H ₂ O) ₅ ³⁺	3.6	1.3
PH ₃	4.6	1.4	Ru(SH) ₄	5.1	1.5
C ₅ H ₅ N	3.2	1.0	TaMe ₄ ⁺	4.2	0.9
S ²⁻	5.4	2.1	TiCl ₃ ⁺	1.6	0.7
SH ⁻	4.1	1.5	W(CO) ₅	2.2	0.8
C ₆ H ₄ OMe ⁻	6.3	1.7	ZrCl ₅ ⁻	3.3	1.2
PCl ₃	4.4	1.5	AuCl ₃	3.9	1.6
SiMe ₃ ⁻	8.1	2.2	HgI ₂	5.7	1.8
			InCl ₂ ⁺	3.1	1.1

5 Estimation of bond dissociation energies of new metal fragments or ligands.

5.1 Procedure for the estimation of BDEs of new ligands or metal fragments.

The bond dissociation energies between the metal fragments and the ligands can be estimated satisfactorily with a set of six hidden descriptors for the ligand $\mathbf{HD}_L$, six for the metal fragment $\mathbf{HD}_M$ and using the diagonal matrix $\mathbf{HD}_W$, see main text. Achieving sensible hidden descriptors for a new metal fragment $\mathbf{i}'$ not present in the Actual Training Set matrix $\mathbf{BDE}$, could be used to estimate the bond dissociation energies of this metal fragment with all ligands in matrix $\mathbf{BDE}$ without need of computing them. Similarly for a new ligand $\mathbf{j}'$, we could estimate the bond dissociation energies of this ligand with all metal fragments in $\mathbf{BDE}$. To obtain these new hidden descriptors we have developed a new procedure. The procedure needs of explicit computation of the bond dissociation energies of the new ligand or metal fragment with a small reference set of metal fragments or ligands from the species in $\mathbf{BDE}$. The process needs of three steps: i) selection of the set of metal fragments/ligands of reference, ii) extraction of parameters from the initial data matrix, iii) calculation of new hidden descriptors from the parameters and reference bond dissociation energies.

i) selection of the set of metal fragments/ligands of reference: The reference bond dissociation energies are key in getting good hidden descriptors. By choosing an adequate reference set of metal fragments or ligands of diverse chemical nature, we are more likely to get accurate estimated bond dissociation energies. We have tested different ways of choosing them, and the best is based on finding the reference set with a higher determinant for the corresponding matrix of hidden descriptors. The more different the hidden descriptors of the ligand/metals in the set the higher the determinant. If the hidden descriptors are different the nature of the ligands/metals will be different too. The procedure used looks independently for the ligands and metal fragments of reference. To do so, we perform an SVD analysis to obtain the hidden descriptors for the Actual Training Set. Then, we look in the group of 22 ligands and 23 metal fragments for all different possible combinations of six ligands or metal fragments. Then we compute the determinant for each set of ligands or metal fragments, if it is higher than a given threshold we save it, if it is lower we discard it. The set with higher determinant will be our reference set. We repeat the same process for the metal fragments independently of the chosen ligands. The script used to perform such process is presented in section 9.3.

Following this procedure and for the Actual Training Set, the set of ligands of reference for matrix $\mathbf{BDE}$ is: Cl^- , H_2O , H^- , O^{2-} , $\text{C}_6\text{H}_4\text{OMe}^-$ and PCl_3 . And the set of metal fragments of reference is: AuPH_3^+ , $\text{Cu}(\text{NH}_3)_3^{2+}$, OsO_3^{2+} , PtF_5^- , $\text{Ru}(\text{SH})_4$ and TiCl_3^+ .

ii) extraction of parameters from the initial data matrix: To obtain new hidden descriptors we have tested several methods but the one achieving better estimated bond dissociation energies consists on expressing

the hidden descriptors, $\mathbf{HD}_L$ or $\mathbf{HD}_M$, in the basis of the bond dissociation energies of the Actual Training Set matrix $\mathbf{BDE}$, see equation 2 (derived from equation 1 of the main text). The parameters $\alpha_{k,ref}$ and the constant or term independent β_k are extracted by performing linear regressions for each descriptor, $\mathbf{HD}_{L(kj)}$, with the bond dissociation energies of all ligands and the metal fragments of the reference set included in the Actual Training Set matrix $\mathbf{BDE}_{ij}$ for $i=\text{ref}$, that is $\mathbf{BDE}_{ref,j}$. Similarly for metal fragments $\alpha_{k,ref}$ and β_k are obtained from $\mathbf{HD}_{M(ki)}$ and $\mathbf{BDE}_{i,ref}$.

$$HD_{L(kj)} = \sum_{ref=1}^6 \alpha_{k,ref} \cdot BDE_{ref,j} + \beta_k \quad (2)$$

$$HD_{M(ki)} = \sum_{ref=1}^6 \alpha_{k,ref} \cdot BDE_{i,ref} + \beta_k \quad (3)$$

Table S24: Values of the fitted equation based on the vacuum Actual training set

Estimation of descriptors for new ligands, $\mathbf{HD}_{L1-6}$							
	$\alpha_{k,ref1}$	$\alpha_{k,ref2}$	$\alpha_{k,ref3}$	$\alpha_{k,ref4}$	$\alpha_{k,ref5}$	$\alpha_{k,ref6}$	β_k
k	AuPH_3^+	$\text{Cu}(\text{NH}_3)_3^{2+}$	OsO_3^{2+}	PtF_5^-	$\text{Ru}(\text{SH})_4$	TiCl_3^+	
1	-0.0000772552	-0.0003868597	-0.0001395635	-0.0000383948	-0.0001392313	-0.0001187452	0.0021848302
2	0.0019317413	-0.0032147086	0.0004412619	0.0036048507	0.0019712987	0.0001596553	-0.0090176047
3	-0.0017217058	0.0005639329	-0.0032287924	0.0009461012	0.0055579601	0.0048752938	0.0253814256
4	0.0025846033	0.0123850745	-0.0021541268	0.0030005050	0.0032420026	-0.0130585729	-0.0517956187
5	0.0072391719	-0.0052298370	0.0003919718	-0.0139157970	0.0197389414	-0.0079242451	-0.3576429801
6	0.0220593816	-0.0028849310	-0.0085726989	0.0035188363	-0.0200861539	0.0086105080	-0.2078832521
Estimation of descriptors for new metal fragments, $\mathbf{HD}_{M1-6}$							
	$\alpha_{k,ref1}$	$\alpha_{k,ref2}$	$\alpha_{k,ref3}$	$\alpha_{k,ref4}$	$\alpha_{k,ref5}$	$\alpha_{k,ref6}$	β_k
k	Cl^-	H_2O	H^-	O^{2-}	$\text{C}_6\text{H}_4\text{OMe}^-$	PCl_3	
1	0.0002509238	0.0000491560	0.0001486995	0.0001429730	0.0002210716	0.0000181149	0.0046719629
2	0.0038089454	-0.0070359031	-0.0030741939	0.0007487861	0.0006880377	-0.0034813971	-0.0599381822
3	0.0031077329	0.0004437931	0.0003645779	-0.0028223532	0.0023786455	0.0020768228	0.0777534936
4	0.0039693626	0.0125666712	-0.0070594438	0.0028159090	-0.0037573136	0.0022057261	-0.1331844390
5	-0.0149363509	0.0151204168	-0.0015272163	-0.0007336813	0.0170585379	-0.0177574977	0.3482715799
6	-0.0163124692	-0.0207641867	-0.0096336878	0.0049838179	0.0165954339	0.0078198948	0.1282810294

Then we can use these $\alpha_{k,ref}$ values and the terms independent β_k to extrapolate the hidden descriptors of a new ligand or metal fragment.

iii) calculation of new hidden descriptors from the parameters and reference bond dissociation energies: Once we have $\alpha_{k,ref}$ and β_k , we can estimate the hidden descriptors of a new ligand j' $\mathbf{HD}_{L(kj')}$ or a new metal i' $\mathbf{HD}_{M(ki')}$, see equation 4. Where $\mathbf{BDE}_{ref,j'}$ and $\mathbf{BDE}_{ref,i'}$ are the computed bond dissociation energies of a new ligand or metal fragment with the metal fragments or ligands of the reference systems. For a new ligand “ j' ” the six hidden descriptors $\mathbf{HD}_{L(kj')}$ are estimated from the six bond dissociation energies computed with this new ligand and the metal fragment of reference $\mathbf{BDE}_{ref,j'}$ and the $\alpha_{k,ref}$ and β_k in Table S24 (top). For a new metal fragment “ i' ” the six hidden descriptors $\mathbf{HD}_{M(ki')}$ are estimated from the six bond dissociation energies

computed with this new metal fragment and the ligands of reference $\mathbf{BDE}_{i',ref}$ and the $\alpha_{k,ref}$ and β_k in Table S24 (bottom).

$$HD_{L(kj')} = \sum_{ref=1}^6 \alpha_{k,ref} \cdot BDE_{ref,j'} + \beta_k \quad (4)$$

$$HD_{M(ki')} = \sum_{ref=1}^6 \alpha_{k,ref} \cdot BDE_{i',ref} + \beta_k \quad (5)$$

Points ii) and iii) can be performed with the script presented in section 9.4.

Then, when we have descriptors $\mathbf{HD}_{L(kj')}$ or $\mathbf{HD}_{M(ki')}$, we can use them to estimate the unknown bond dissociation energies of a this new ligand “ j ’ ” or metal fragments “ i ’ ” with the other metal fragments “ i ” or ligands “ j ” from which we have descriptors $\mathbf{HD}_L$ and $\mathbf{HD}_M$ by using equation 6.

$$BDE_{i,j'} = HD_{M(i)} \cdot HD_W \cdot HD_{L(j')}^T \quad (6)$$

$$BDE_{i',j} = HD_{M(i')} \cdot HD_W \cdot HD_{L(j)}^T \quad (7)$$

5.2 Errors in the estimation of BDEs for the Full data set

As was done above with Table S23 for the Actual Training Set, Tables S25, S26 and S27 show the maximum and average errors in the estimation of the BDEs following the methodology described in Section 5.1 and for the rest of ligands and metal fragments in the Full data set. Tables S25 and S26 correspond to errors in the estimation of BDEs between one fragment in the Actual Training Set and one fragment in the Extended Set (Full Set of data without the Actual Training Set). Tables S27 correspond to the BDE when both fragments are in the Extended Set.

Table S25: Maximum (absolute) and average error (kcal/mol) associated to each ligand (left) and each metal fragment (right) of the estimated BDEs between ligands in the Extended Set and metal fragments in the Actual Training Set (6 hidden descriptors).

Error associated to each Ligand			Error associated to each Metal Fragment		
Ligand	Abs Max error	Ave error	Metal Fragment	Abs Max error	Ave error
I ⁻	3.9	0.2	AuPH ₃ ⁺	6.9	0.7
NCS ⁻	12.9	0.9	Co(NH ₃) ₅ ³⁺	11.1	0.0
SCN ⁻	8.6	0.6	CrO ₃	4.1	-0.9
Bpin ⁻	8.4	0.0	Cu(NH ₃) ₃ ²⁺	0.4	0.0
CCH ⁻	5.6	0.4	FeCl ₂ ⁺	6.6	0.2
CHCH ₂ ⁻	4.5	0.1	Fe(CO) ₄	10.3	0.0
C ₆ H ₄ Cl ⁻	6.8	-0.6	IrCO(PH ₃) ₂ ⁺	10.9	0.6
C ₆ H ₄ NO ₂ ⁻	8.3	0.7	MnO ₃ ⁺	11.0	-0.4
H ₂ S	12.2	-1.8	Mo(SH) ₃ ⁺	8.6	0.3
He	11.7	2.5	Nb(NH ₂) ₄ ⁺	7.9	-1.0
C ₃ H ₄ N ₂	4.0	-0.3	OsO ₃ ²⁺	1.5	0.1
NH ₂ ⁻	11.1	0.8	PdH(PH ₃) ₂ ⁺	6.2	0.1
NMe ₃	11.0	-0.5	PdPH ₃	11.7	0.0
C ₄ H ₄ O	7.7	0.7	PtF ₅ ⁻	2.4	-0.4
OMe	7.0	-0.5	Rh(H ₂ O) ₅ ³⁺	9.2	0.7
PF ₃	4.0	-0.8	Ru(SH) ₄	2.1	0.2
PMe ₃	5.1	-1.1	TaMe ₄ ⁺	4.1	0.2
SiH ₃ ⁻	11.0	0.0	TiCl ₃ ⁺	1.0	0.0
SMe ⁻	7.5	-2.1	W(CO) ₅	9.9	0.0
C ₄ H ₄ S	11.5	-1.3	ZrCl ₅ ⁻	11.5	-0.5
Xe	9.2	1.6	AuCl ₃	9.4	-0.1
			HgI ₂	12.9	-0.7
			InCl ₂ ⁺	5.8	0.5

Table S26: Maximum (absolute) and average error (kcal/mol) associated to each ligand (left) and each metal fragment (right) of the estimated BDEs between ligands in the Actual Training Set and metal fragments in the Extended Set (6 hidden descriptors).

Error associated to each Ligand			Error associated to each Metal Fragment		
Ligand	Abs Max error	Ave error	Metal Fragment	Abs Max error	Ave error
Br ⁻	3.9	-0.3	AlCl ₃	10.5	0.0
CH ₃ ⁻	5.7	0.1	K ⁺	16.5	1.1
Cl ⁻	0.9	-0.2	ZnCH ₃ ⁺	10.8	0.9
CN ⁻	6.1	0.6	Ag(NHC) ⁺	8.1	0.5
CO	16.5	4.1	AuCN	5.1	-0.4
F ⁻	10.5	0.6	Cr(H ₂ O) ₅ ²⁺	6.5	-0.8
C ₆ H ₅ ⁻	3.6	-0.5	CuCH ₃	5.3	0.0
H ₂	4.7	1.6	CuCN	5.2	-0.1
H ₂ O	1.3	-0.6	FeCl ₃ ⁻	8.0	1.2
H ⁻	3.8	-1.8	FeCl ₃	4.7	-0.3
NCH	6.1	0.6	GaCl ₃	5.0	-0.4
NH ₃	3.9	-0.6	Ni(PF ₃) ₃	3.9	-0.2
NHC	5.1	-0.9	NiPH ₃	4.6	-0.5
O ²⁻	2.0	0.9	PtPH ₃	7.6	-1.1
OH ⁻	6.7	-0.4	SnMe ₃ ⁺	3.4	0.2
PH ₃	7.7	0.7	Y(H ₂ O) ₅ ³⁺	5.7	0.3
C ₅ H ₅ N	4.2	-1.6	ZnCl ₃ ⁻	13.9	1.7
S ²⁻	11.7	0.6	ZnNH ₃ ²⁺	13.9	1.4
SH ⁻	3.4	-0.1	Zr(Ome) ₃ ⁺	3.6	0.6
C ₆ H ₄ OMe ⁻	4.5	-1.2			
PCl ₃	1.1	0.0			
SiMe ₃ ⁻	8.3	2.5			

Table S27: Maximum (absolute) and average error (kcal/mol) associated to each ligand (left) and each metal fragment (right) of the estimated BDEs between ligands in the Extended Set and metal fragments also in the Extended Set (6 hidden descriptors).

Error associated to each Ligand			Error associated to each Metal Fragment		
Ligand	Abs Max error	Ave error	Metal Fragment	Abs Max error	Ave error
I ⁻	6.1	-0.4	AlCl ₃	6.1	-0.3
NCS ⁻	10.9	-2.4	K ⁺	10.9	-0.1
SCN ⁻	6.9	0.0	ZnCH ₃ ⁺	5.9	0.7
Bpin ⁻	6.8	3.1	Ag(NHC) ⁺	8.6	0.0
CCH ⁻	7.7	-1.2	AuCN	7.9	-0.3
CHCH ₂ ⁻	3.6	0.6	Cr(H ₂ O) ₅ ²⁺	7.7	-0.6
C ₆ H ₄ Cl ⁻	6.3	-1.7	CuCH ₃	7.8	-0.7
C ₆ H ₄ NO ₂ ⁻	8.1	-0.9	CuCN	8.0	-0.2
H ₂ S	10.4	-0.9	FeCl ₃ ⁻	11.6	-1.4
He	11.6	4.6	FeCl ₃	9.6	-1.3
C ₃ H ₄ N ₂	5.8	-1.5	GaCl ₃	10.4	-1.0
NH ₂ ⁻	4.6	0.4	Ni(PF ₃) ₃	8.4	-0.8
NMe ₃	10.6	-2.7	NiPH ₃	11.6	1.0
C ₄ H ₄ O	6.6	-0.3	PtPH ₃	10.6	-0.2
OMe	11.6	0.5	SnMe ₃ ⁺	5.5	0.0
PF ₃	6.1	1.0	Y(H ₂ O) ₅ ³⁺	9.4	0.6
PMe ₃	6.9	-1.2	ZnCl ₃ ⁻	9.4	-0.3
SiH ₃ ⁻	9.4	2.7	ZnNH ₃ ²⁺	10.7	2.2
SMe ⁻	3.8	-1.1	Zr(Ome) ₃ ⁺	2.5	0.6
C ₄ H ₄ S	11.5	-2.3			
Xe	11.0	1.2			

6 Role of dispersion (B3LYP in vacuum)

6.1 Results of SVD-based matrix decomposition

The main analysis is carried out on calculations with the B3LYP-D3 functional, thus including dispersion. We evaluate the role of dispersion by repeating the analysis of the initial set of metal fragments with BDEs obtained with the B3LYP functional. The B3LYP calculations are single-point, carried out on the already available B3LYP-D3 structures. The average and maximum error relative to the number of hidden descriptors (k) considered is presented in Table S28. The product of the vectors associated to a given metal fragment and ligand by the diagonal matrix $\mathbf{W}$ produce the estimated BDE, see equation 1 in the main text. The elements of the diagonal matrix provide thus an estimation of the importance of each hidden descriptor. Table S28 shows the relative weights for the two sets of BDE in vacuum that have been analyzed in this work on the Actual Training Set. The correlation between the hidden descriptors obtained for B3LYP-D3 and B3LYP calculations (data in Tables S18 and S30 is very high 0.9998, 0.864, 0.887, 0.997, 0.960, 0.962 and 0.52 for $k = 1, 2, 3, 4, 5, 6$ and 7. Indicating that the effect of the Dispersion correction in these systems is very small.

Table S28: Maximum absolute and average error (in kcal/mol) of the estimated BDE with respect to the number of hidden descriptors (k) considered for the Actual Training Set. The weight of the last included k diagonal term in matrix $\mathbf{W}_{k,k}$ is also provided, for results in vacuum B3LYP-D3 in vacuum without Dispersion effects B3LYP.

k	Vacuum			Vacuum no-Dispersion		
	Max error	Aver error	Weight, $\mathbf{W}_{k,k}$	Max error	Aver error	Weight, $\mathbf{W}_{k,k}$
1	86.7	13.4	4691	92.8	13.4	4645
2	88.0	8.7	293	93.9	9.3	281
3	28.1	5.2	252	25.2	5.2	269
4	14.4	3.2	119	14.0	3.1	122
5	13.2	2.3	59	13.5	2.3	58
6	8.1	1.4	54	8.0	1.4	53
7	6.0	1.1	25	7.9	1.1	24
8	5.2	0.8	22	5.3	0.9	22
9	3.0	0.7	15	3.8	0.7	15
10	2.6	0.5	13	3.0	0.5	14
11	2.2	0.4	9	2.3	0.4	10
12	1.7	0.3	7	2.0	0.3	8
13	1.6	0.2	6	2.0	0.2	6
14	1.2	0.2	4	1.1	0.2	5
15	0.8	0.1	4	0.7	0.1	4
16	0.6	0.1	2	0.6	0.1	3
17	0.6	0.1	2	0.5	0.1	2
18	0.3	0.1	1	0.4	0.0	2
19	0.3	0.0	1	0.2	0.0	1
20	0.2	0.0	1	0.1	0.0	1
21	0.1	0.0	1	0.1	0.0	1
22	0.0	0.0	0	0.0	0.0	0

6.2 BDE matrix

The BDE between the ligands metal fragments in the Actual Training Set computed using B3LYP functional, with no dispersion correction, are presented in Table S29.

Table S29: Bond dissociation energies (kcal/mol) in the Actual Training Set. Calculations in vacuum with the B3LYP functional (no Dispersion). Results are split in two separate tables, part A and part B.

Table S29, PART A												
	Br ⁻	CH ₃ ⁻	Cl ⁻	CN ⁻	CO	F ⁻	C ₆ H ₅ ⁻	H ₂	H ₂ O	H ⁻	NCH	
AuPH ₃ ⁺	-153.5	-217.8	-159.2	-173.4	-36.5	-176.6	-202.8	-12.6	-34.8	-256.0	-42.6	
Co(NH ₃) ₅ ³⁺	-328.4	-403.7	-337.2	-342.4	-27.3	-374.8	-394.6	-5.7	-43.6	-444.3	-58.6	
CrO ₃	-78.4	-140.2	-86.8	-99.4	-32.1	-121.6	-127.3	-10.8	-37.7	-175.0	-37.9	
Cu(NH ₃) ₃ ²⁺	-228.0	-290.1	-235.4	-237.2	-13.5	-266.5	-276.5	-1.1	-30.5	-326.2	-37.5	
FeCl ₂ ⁺	-191.5	-251.7	-200.0	-195.6	-24.7	-233.2	-238.7	-7.1	-46.3	-280.4	-47.6	
Fe(CO) ₄	-44.3	-96.9	-48.9	-69.6	-34.5	-69.2	-86.5	-8.4	-13.6	-147.5	-21.8	
IrCO(PH ₃) ₂ ⁺	-145.6	-202.3	-152.7	-168.0	-42.4	-177.3	-191.8	-14.2	-30.5	-246.1	-40.1	
MnO ₃ ⁺	-231.5	-321.9	-239.1	-245.9	-52.9	-271.0	-304.2	-22.4	-67.7	-351.1	-74.7	
Mo(SH) ₃ ⁺	-172.9	-238.9	-184.1	-183.9	-40.5	-222.4	-224.1	-15.9	-42.3	-266.3	-46.7	
Nb(NH ₂) ₄ ⁺	-113.4	-166.6	-123.9	-126.7	-2.2	-166.7	-152.3	8.1	-14.2	-204.7	-14.3	
OsO ₃ ²⁺	-412.3	-514.9	-418.2	-416.4	-80.7	-439.0	-516.6	-34.6	-107.9	-529.0	-127.0	
PdH(PH ₃) ₂ ⁺	-125.4	-176.4	-131.0	-141.8	-22.8	-150.6	-164.3	-5.3	-20.6	-219.0	-26.3	
PdPH ₃	-31.9	-63.5	-35.6	-48.5	-35.1	-47.7	-58.0	-10.5	-13.3	-103.1	-20.5	
PtF ₅ ⁻	27.7	-41.3	23.0	-8.3	-36.5	1.5	-38.7	-5.8	-27.9	-77.5	-21.0	
Rh(H ₂ O) ₅ ³⁺	-371.1	-461.6	-378.3	-388.4	-55.2	-403.4	-458.2	-22.3	-64.8	-497.5	-82.8	
Ru(SH) ₄	-43.3	-94.8	-49.1	-66.6	-25.1	-72.6	-80.4	0.8	-14.5	-138.6	-19.2	
TaMe ₄ ⁺	-178.5	-236.2	-191.0	-187.4	-26.2	-235.3	-220.7	-5.5	-44.5	-263.8	-47.9	
TiCl ₃ ⁺	-195.5	-259.6	-208.7	-200.5	-29.6	-254.1	-243.5	-8.6	-52.7	-284.3	-54.0	
W(CO) ₅	-52.2	-97.4	-57.4	-74.6	-39.4	-80.5	-88.2	-10.8	-18.0	-143.6	-27.4	
ZrCl ₅ ⁻	42.0	-0.3	33.2	25.0	-3.3	-8.7	8.5	4.5	-9.6	-34.7	-0.2	
AuCl ₃	-71.0	-151.0	-75.8	-98.6	-24.3	-96.3	-135.0	-0.8	-23.9	-190.9	-22.4	
HgI ₂	-37.7	-92.7	-41.2	-49.7	-0.1	-57.7	-78.3	1.6	-4.3	-132.3	-2.1	
InCl ₂ ⁺	-181.5	-254.0	-191.0	-194.0	-16.8	-225.7	-239.4	-1.6	-40.9	-284.2	-40.7	

Table S29, PART B

	NH ₃	NHC	O ²⁻	OH ⁻	PH ₃	C ₅ H ₅ N	S ²⁻	SH ⁻	C ₆ H ₄ OMe ⁻	PCl ₃	SiMe ₃ ⁻
AuPH ₃ ⁺	-54.5	-88.0	-391.2	-191.2	-52.0	-59.4	-314.9	-174.2	-203.4	-37.1	-203.3
Co(NH ₃) ₅ ³⁺	-57.9	-108.4	-782.6	-386.9	-49.8	-84.9	-675.6	-350.8	-398.6	-43.1	-389.2
CrO ₃	-54.4	-77.5	-267.1	-130.3	-41.9	-55.7	-157.9	-96.5	-127.5	-29.7	-122.1
Cu(NH ₃) ₃ ²⁺	-42.5	-78.8	-572.5	-277.1	-32.5	-59.1	-480.7	-247.1	-277.4	-21.6	-274.2
FeCl ₂ ⁺	-58.8	-94.2	-514.3	-250.3	-45.1	-72.5	-407.1	-215.2	-242.5	-30.3	-229.3
Fe(CO) ₄	-25.7	-50.0	-177.8	-76.9	-26.0	-25.0	-114.2	-59.2	-86.3	-22.9	-93.0
IrCO(PH ₃) ₂ ⁺	-44.7	-77.7	-394.8	-187.6	-41.5	-52.1	-311.4	-163.0	-192.0	-31.4	-181.7
MnO ₃ ⁺	-95.1	-144.4	-573.0	-292.5	-91.1	-112.2	-452.6	-261.4	-306.3	-76.8	-317.6
Mo(SH) ₃ ⁺	-53.2	-89.6	-521.2	-240.3	-45.3	-65.9	-390.7	-197.9	-225.6	-32.9	-209.0
Nb(NH ₂) ₄ ⁺	-20.8	-38.8	-420.2	-174.0	-6.8	-24.4	-291.2	-128.3	-152.9	0.7	-137.5
OsO ₃ ²⁺	-144.3	-240.4	-911.2	-477.1	-155.5	-197.8	-793.9	-452.0	-530.6	-151.1	-528.5
PdH(PH ₃) ₂ ⁺	-31.5	-56.3	-345.1	-159.9	-27.6	-36.2	-276.9	-140.4	-164.3	-18.1	-160.0
PdPH ₃	-23.5	-40.8	-146.4	-54.2	-27.7	-22.4	-79.8	-42.3	-57.9	-28.7	-54.3
PtF ₅ ⁻	-43.3	-71.0	-31.8	-12.0	-36.0	-42.2	36.0	7.4	-38.7	-30.3	-35.2
Rh(H ₂ O) ₅ ³⁺	-90.3	-159.1	-845.8	-427.0	-92.3	-124.7	-747.1	-402.0	-462.7	-86.1	-466.6
Ru(SH) ₄	-23.7	-46.0	-224.1	-78.5	-23.8	-22.7	-127.9	-57.0	-80.4	-13.5	-82.3
TaMe ₄ ⁺	-56.0	-84.0	-513.5	-247.2	-38.7	-67.0	-382.6	-195.8	-222.7	-24.1	-196.6
TiCl ₃ ⁺	-66.2	-97.9	-556.8	-269.1	-48.4	-78.5	-416.8	-216.0	-246.4	-33.3	-227.9
W(CO) ₅	-28.8	-51.0	-200.3	-85.4	-29.2	-29.1	-123.1	-65.0	-88.0	-26.9	-86.9
ZrCl ₅ ⁻	-15.8	-25.1	-106.7	-13.0	-1.9	-9.5	17.8	29.9	7.7	-1.6	23.2
AuCl ₃	-42.6	-78.1	-254.6	-115.3	-38.2	-42.0	-175.0	-97.5	-134.9	-23.7	-141.8
HgI ₂	-7.8	-21.5	-199.2	-69.2	-1.8	-8.3	-131.1	-53.8	-78.7	0.8	-79.9
InCl ₂ ⁺	-52.8	-90.2	-479.3	-238.8	-38.6	-68.8	-387.4	-205.6	-241.5	-21.1	-232.7

6.3 Hidden descriptor tables

Tables S30 and S31 report the values for the first seven hidden descriptors for each ligand and metal fragment, respectively. Tables S32 and S33 report the same data but with the hidden descriptors for each k ordered in decreasing order.

Table S30: First seven hidden descriptors of the ligands. BDE between two fragments in the Actual Training Set. BDEs obtained from B3LYP (no Dispersion) in vacuum.

Ligand	$\text{HD}_{L1} = \mathbf{L}_1$	$\text{HD}_{L2} = \mathbf{L}_2$	$\text{HD}_{L3} = \mathbf{L}_3$	$\text{HD}_{L4} = \mathbf{L}_4$	$\text{HD}_{L5} = \mathbf{L}_5$	$\text{HD}_{L6} = \mathbf{L}_6$	$\mathbf{L}_7$
Br^-	0.190	0.091	0.356	0.082	-0.142	-0.105	0.027
CH_3^-	0.252	-0.120	-0.019	-0.186	0.210	-0.146	0.267
Cl^-	0.197	0.099	0.289	0.119	-0.130	-0.186	0.012
CN^-	0.201	-0.009	0.167	-0.161	-0.257	-0.221	-0.283
CO	0.032	-0.243	-0.084	-0.007	-0.621	-0.080	0.050
F^-	0.223	0.123	0.007	0.223	0.013	-0.431	-0.419
C_6H_5^-	0.242	-0.132	0.112	-0.134	0.179	0.029	-0.180
H_2	0.010	-0.097	0.033	0.051	-0.283	-0.019	0.147
H_2O	0.041	-0.172	-0.024	0.234	0.130	-0.141	0.178
H^-	0.280	-0.180	-0.386	-0.586	-0.150	-0.233	0.104
NCH	0.048	-0.180	0.022	0.177	-0.176	-0.098	0.026
NH_3	0.057	-0.269	-0.064	0.203	0.121	-0.167	0.164
NHC	0.095	-0.414	-0.102	0.141	0.146	0.038	0.168
O^{2-}	0.484	0.251	-0.610	0.301	-0.053	0.290	-0.107
OH^-	0.237	0.052	-0.023	0.229	0.120	-0.303	-0.028
PH_3	0.052	-0.321	0.041	0.138	-0.144	0.125	0.162
$\text{C}_5\text{H}_5\text{N}$	0.072	-0.288	0.038	0.277	0.195	0.013	0.007
S^{2-}	0.393	0.331	0.242	-0.003	-0.119	0.365	0.392
SH^-	0.210	0.015	0.258	0.033	-0.017	-0.067	0.304
$\text{C}_6\text{H}_4\text{OMe}^-$	0.245	-0.145	0.131	-0.094	0.211	0.112	-0.202
PCl_3	0.043	-0.318	0.109	0.144	-0.258	0.417	-0.385
SiMe_3^-	0.240	-0.212	0.215	-0.299	0.218	0.250	-0.206

Table S31: First seven hidden descriptors of the metal fragments. BDE between two fragments in the Actual Training Set. BDEs obtained from B3LYP (no Dispersion) in vacuum.

Metal Frag.	$\mathbf{HD}_{M1} = \mathbf{M}_1$	$\mathbf{HD}_{M2} = \mathbf{M}_2$	$\mathbf{HD}_{M3} = \mathbf{M}_3$	$\mathbf{HD}_{M4} = \mathbf{M}_4$	$\mathbf{HD}_{M5} = \mathbf{M}_5$	$\mathbf{HD}_{M6} = \mathbf{M}_6$	$\mathbf{M}_7$
AuPH ₃ ⁺	-0.178	0.097	0.028	0.164	0.121	0.153	-0.290
Co(NH ₃) ₅ ³⁺	-0.352	-0.322	-0.134	0.238	-0.019	0.080	0.439
CrO ₃	-0.112	0.214	0.194	-0.080	-0.080	0.406	0.274
Cu(NH ₃) ₃ ²⁺	-0.251	-0.260	-0.015	0.186	-0.133	0.066	0.051
FeCl ₂ ⁺	-0.220	-0.089	0.067	-0.151	-0.107	0.076	-0.347
Fe(CO) ₄	-0.076	0.156	0.178	0.264	0.211	0.040	0.089
IrCO(PH ₃) ₂ ⁺	-0.173	0.015	0.083	0.098	0.342	0.155	-0.132
MnO ₃ ⁺	-0.264	0.273	-0.029	-0.071	-0.076	0.139	0.013
Mo(SH) ₃ ⁺	-0.211	-0.104	0.172	-0.246	0.217	-0.132	-0.304
Nb(NH ₂) ₄ ⁺	-0.153	-0.323	0.292	-0.050	-0.095	-0.220	0.224
OsO ₃ ²⁺	-0.439	0.427	-0.372	-0.302	-0.054	-0.398	0.003
PdH(PH ₃) ₂ ⁺	-0.149	-0.067	0.083	0.207	0.129	0.053	-0.189
PdPH ₃	-0.055	0.137	0.180	0.022	0.427	-0.114	0.024
PtF ₅ ⁻	-0.016	0.490	0.245	0.138	-0.261	0.126	0.176
Rh(H ₂ O) ₅ ³⁺	-0.396	-0.030	-0.265	0.206	0.091	-0.186	0.198
Ru(SH) ₄	-0.080	0.040	0.278	0.088	0.146	-0.208	-0.023
TaMe ₄ ⁺	-0.210	-0.150	0.156	-0.307	0.037	0.282	-0.026
TiCl ₃ ⁺	-0.229	-0.107	0.142	-0.357	-0.042	0.171	-0.060
W(CO) ₅	-0.081	0.136	0.190	0.094	0.365	0.077	0.160
ZrCl ₅ ⁻	-0.006	0.015	0.483	-0.270	-0.158	-0.330	0.280
AuCl ₃	-0.112	0.198	0.173	0.308	-0.301	-0.058	-0.231
HgI ₂	-0.072	-0.084	0.233	0.312	-0.214	-0.358	-0.254
InCl ₂ ⁺	-0.212	-0.066	0.041	0.078	-0.358	0.245	-0.155

Table S32: First seven hidden descriptors of the ligands for the Actual Training Set, ordered by their values in decreasing order. Values derived from BDEs obtained from B3LYP (no Dispersion) in vacuum.

$\text{HD}_{L1} = L_1$	$\text{HD}_{L2} = L_2$	$\text{HD}_{L3} = L_3$	$\text{HD}_{L4} = L_4$	$\text{HD}_{L5} = L_5$	$\text{HD}_{L6} = L_6$	L_7
O^{2-} 0.48	S^{2-} 0.33	Br^- 0.36	O^{2-} 0.30	SiMe_3^- 0.22	PCl_3 0.42	S^{2-} 0.39
S^{2-} 0.39	O^{2-} 0.25	Cl^- 0.29	$\text{C}_5\text{H}_5\text{N}$ 0.28	$\text{C}_6\text{H}_4\text{OMe}^-$ 0.21	S^{2-} 0.37	SH^- 0.30
H^- 0.28	F^- 0.12	SH^- 0.26	H_2O 0.23	CH_3^- 0.21	O^{2-} 0.29	CH_3^- 0.27
CH_3^- 0.25	Cl^- 0.10	S^{2-} 0.24	OH^- 0.23	$\text{C}_5\text{H}_5\text{N}$ 0.19	SiMe_3^- 0.25	H_2O 0.18
$\text{C}_6\text{H}_4\text{OMe}^-$ 0.25	Br^- 0.09	SiMe_3^- 0.22	F^- 0.22	C_6H_5^- 0.18	PH_3 0.12	NHC 0.17
C_6H_5^- 0.24	OH^- 0.05	CN^- 0.17	NH_3 0.20	NHC 0.15	$\text{C}_6\text{H}_4\text{OMe}^-$ 0.11	NH_3 0.16
SiMe_3^- 0.24	SH^- 0.01	$\text{C}_6\text{H}_4\text{OMe}^-$ 0.13	NCH 0.18	H_2O 0.13	NHC 0.04	PH_3 0.16
OH^- 0.24	CN^- -0.01	C_6H_5^- 0.11	PCl_3 0.14	NH_3 0.12	C_6H_5^- 0.03	H_2 0.15
F^- 0.22	H_2 -0.10	PCl_3 0.11	NHC 0.14	OH^- 0.12	$\text{C}_5\text{H}_5\text{N}$ 0.01	H^- 0.10
SH^- 0.21	CH_3^- -0.12	PH_3 0.04	PH_3 0.14	F^- 0.01	H_2 -0.02	CO 0.05
CN^- 0.20	C_6H_5^- -0.13	$\text{C}_5\text{H}_5\text{N}$ 0.04	Cl^- 0.12	SH^- -0.02	SH^- -0.07	Br^- 0.03
Cl^- 0.20	$\text{C}_6\text{H}_4\text{OMe}^-$ -0.14	H_2 0.03	Br^- 0.08	O^{2-} -0.05	CO -0.08	NCH 0.03
Br^- 0.19	H_2O -0.17	NCH 0.02	H_2 0.05	S^{2-} -0.12	NCH -0.10	Cl^- 0.01
NHC 0.09	NCH -0.18	F^- 0.01	SH^- 0.03	Cl^- -0.13	Br^- -0.10	$\text{C}_5\text{H}_5\text{N}$ 0.01
$\text{C}_5\text{H}_5\text{N}$ 0.07	H^- -0.18	CH_3^- -0.02	S^{2-} 0.00	Br^- -0.14	H_2O -0.14	OH^- -0.03
NH_3 0.06	SiMe_3^- -0.21	OH^- -0.02	CO -0.01	PH_3 -0.14	CH_3^- -0.15	O^{2-} -0.11
PH_3 0.05	CO -0.24	H_2O -0.02	$\text{C}_6\text{H}_4\text{OMe}^-$ -0.09	H^- -0.15	NH_3 -0.17	C_6H_5^- -0.18
NCH 0.05	NH_3 -0.27	NH_3 -0.06	C_6H_5^- -0.13	NCH -0.18	Cl^- -0.19	$\text{C}_6\text{H}_4\text{OMe}^-$ -0.20
PCl_3 0.04	$\text{C}_5\text{H}_5\text{N}$ -0.29	CO -0.08	CN^- -0.16	CN^- -0.26	CN^- -0.22	SiMe_3^- -0.21
H_2O 0.04	PCl_3 -0.32	NHC -0.10	CH_3^- -0.19	PCl_3 -0.26	H^- -0.23	CN^- -0.28
CO 0.03	PH_3 -0.32	H^- -0.39	SiMe_3^- -0.30	H_2 -0.28	OH^- -0.30	PCl_3 -0.39
H_2 0.01	NHC -0.41	O^{2-} -0.61	H^- -0.59	CO -0.62	F^- -0.43	F^- -0.42

Table S33: First seven hidden descriptors of the metal fragments for the Actual Training Set, ordered by their values in decreasing order. Values derived from BDEs obtained from B3LYP (no Dispersion) in vacuum.

$\text{HD}_{M1} = \mathbf{M}_1$	$\text{HD}_{M2} = \mathbf{M}_2$	$\text{HD}_{M3} = \mathbf{M}_3$	$\text{HD}_{M4} = \mathbf{M}_4$	$\text{HD}_{M5} = \mathbf{M}_5$	$\text{HD}_{M6} = \mathbf{M}_6$	$\text{HD}_{M7} = \mathbf{M}_7$
$\text{ZrCl}_5^- -0.01$	$\text{PtF}_5^- -0.49$	$\text{ZrCl}_5^- -0.48$	$\text{HgI}_2 -0.31$	$\text{PdPH}_3 -0.43$	$\text{CrO}_3 -0.41$	$\text{Co}(\text{NH}_3)_5^{3+} -0.44$
$\text{PtF}_5^- -0.02$	$\text{OsO}_3^{2+} -0.43$	$\text{Nb}(\text{NH}_2)_4^+ -0.29$	$\text{AuCl}_3 -0.31$	$\text{W}(\text{CO})_5 -0.36$	$\text{TaMe}_4^+ -0.28$	$\text{ZrCl}_5^- -0.28$
$\text{PdPH}_3 -0.06$	$\text{MnO}_3^+ -0.27$	$\text{Ru}(\text{SH})_4 -0.28$	$\text{Fe}(\text{CO})_4 -0.26$	$\text{IrCO}(\text{PH}_3)_2^+ -0.34$	$\text{InCl}_2^+ -0.25$	$\text{CrO}_3 -0.27$
$\text{HgI}_2 -0.07$	$\text{CrO}_3 -0.21$	$\text{PtF}_5^- -0.24$	$\text{Co}(\text{NH}_3)_5^{3+} -0.24$	$\text{Mo}(\text{SH})_3^+ -0.22$	$\text{TiCl}_3^+ -0.17$	$\text{Nb}(\text{NH}_2)_4^+ -0.22$
$\text{Fe}(\text{CO})_4 -0.08$	$\text{AuCl}_3 -0.20$	$\text{HgI}_2 -0.23$	$\text{PdH}(\text{PH}_3)_2^+ -0.21$	$\text{Fe}(\text{CO})_4 -0.21$	$\text{IrCO}(\text{PH}_3)_2^+ -0.15$	$\text{Rh}(\text{H}_2\text{O})_5^{3+} -0.20$
$\text{Ru}(\text{SH})_4 -0.08$	$\text{Fe}(\text{CO})_4 -0.16$	$\text{CrO}_3 -0.19$	$\text{Rh}(\text{H}_2\text{O})_5^{3+} -0.21$	$\text{Ru}(\text{SH})_4 -0.15$	$\text{AuPH}_3^+ -0.15$	$\text{PtF}_5^- -0.18$
$\text{W}(\text{CO})_5 -0.08$	$\text{PdPH}_3 -0.14$	$\text{W}(\text{CO})_5 -0.19$	$\text{Cu}(\text{NH}_3)_3^{2+} -0.19$	$\text{PdH}(\text{PH}_3)_2^+ -0.13$	$\text{MnO}_3^+ -0.14$	$\text{W}(\text{CO})_5 -0.16$
$\text{AuCl}_3 -0.11$	$\text{W}(\text{CO})_5 -0.14$	$\text{PdPH}_3 -0.18$	$\text{AuPH}_3^+ -0.16$	$\text{AuPH}_3^+ -0.12$	$\text{PtF}_5^- -0.13$	$\text{Fe}(\text{CO})_4 -0.09$
$\text{CrO}_3 -0.11$	$\text{AuPH}_3^+ -0.10$	$\text{Fe}(\text{CO})_4 -0.18$	$\text{PtF}_5^- -0.14$	$\text{Rh}(\text{H}_2\text{O})_5^{3+} -0.09$	$\text{Co}(\text{NH}_3)_5^{3+} -0.08$	$\text{Cu}(\text{NH}_3)_3^{2+} -0.05$
$\text{PdH}(\text{PH}_3)_2^+ -0.15$	$\text{Ru}(\text{SH})_4 -0.04$	$\text{AuCl}_3 -0.17$	$\text{IrCO}(\text{PH}_3)_2^+ -0.10$	$\text{TaMe}_4^+ -0.04$	$\text{W}(\text{CO})_5 -0.08$	$\text{PdPH}_3 -0.02$
$\text{Nb}(\text{NH}_2)_4^+ -0.15$	$\text{ZrCl}_5^- -0.02$	$\text{Mo}(\text{SH})_3^+ -0.17$	$\text{W}(\text{CO})_5 -0.09$	$\text{Co}(\text{NH}_3)_5^{3+} -0.02$	$\text{FeCl}_2^+ -0.08$	$\text{MnO}_3^+ -0.01$
$\text{IrCO}(\text{PH}_3)_2^+ -0.17$	$\text{IrCO}(\text{PH}_3)_2^+ -0.01$	$\text{TaMe}_4^+ -0.16$	$\text{Ru}(\text{SH})_4 -0.09$	$\text{TiCl}_3^+ -0.04$	$\text{Cu}(\text{NH}_3)_3^{2+} -0.07$	$\text{OsO}_3^{2+} -0.00$
$\text{AuPH}_3^+ -0.18$	$\text{Rh}(\text{H}_2\text{O})_5^{3+} -0.03$	$\text{TiCl}_3^+ -0.14$	$\text{InCl}_2^+ -0.08$	$\text{OsO}_3^{2+} -0.05$	$\text{PdH}(\text{PH}_3)_2^+ -0.05$	$\text{Ru}(\text{SH})_4 -0.02$
$\text{TaMe}_4^+ -0.21$	$\text{InCl}_2^+ -0.07$	$\text{IrCO}(\text{PH}_3)_2^+ -0.08$	$\text{PdPH}_3 -0.02$	$\text{MnO}_3^+ -0.08$	$\text{Fe}(\text{CO})_4 -0.04$	$\text{TaMe}_4^+ -0.03$
$\text{Mo}(\text{SH})_3^+ -0.21$	$\text{PdH}(\text{PH}_3)_2^+ -0.07$	$\text{PdH}(\text{PH}_3)_2^+ -0.08$	$\text{Nb}(\text{NH}_2)_4^+ -0.05$	$\text{CrO}_3 -0.08$	$\text{AuCl}_3 -0.06$	$\text{TiCl}_3^+ -0.06$
$\text{InCl}_2^+ -0.21$	$\text{HgI}_2 -0.08$	$\text{FeCl}_2^+ -0.07$	$\text{MnO}_3^+ -0.07$	$\text{Nb}(\text{NH}_2)_4^+ -0.10$	$\text{PdPH}_3 -0.11$	$\text{IrCO}(\text{PH}_3)_2^+ -0.13$
$\text{FeCl}_2^+ -0.22$	$\text{FeCl}_2^+ -0.09$	$\text{InCl}_2^+ -0.04$	$\text{CrO}_3 -0.08$	$\text{FeCl}_2^+ -0.11$	$\text{Mo}(\text{SH})_3^+ -0.13$	$\text{InCl}_2^+ -0.15$
$\text{TiCl}_3^+ -0.23$	$\text{Mo}(\text{SH})_3^+ -0.10$	$\text{AuPH}_3^+ -0.03$	$\text{FeCl}_2^+ -0.15$	$\text{Cu}(\text{NH}_3)_3^{2+} -0.13$	$\text{Rh}(\text{H}_2\text{O})_5^{3+} -0.19$	$\text{PdH}(\text{PH}_3)_2^+ -0.19$
$\text{Cu}(\text{NH}_3)_3^{2+} -0.25$	$\text{TiCl}_3^+ -0.11$	$\text{Cu}(\text{NH}_3)_3^{2+} -0.01$	$\text{Mo}(\text{SH})_3^+ -0.25$	$\text{ZrCl}_5^- -0.16$	$\text{Ru}(\text{SH})_4 -0.21$	$\text{AuCl}_3 -0.23$
$\text{MnO}_3^+ -0.26$	$\text{TaMe}_4^+ -0.15$	$\text{MnO}_3^+ -0.03$	$\text{ZrCl}_5^- -0.27$	$\text{HgI}_2 -0.21$	$\text{Nb}(\text{NH}_2)_4^+ -0.22$	$\text{HgI}_2 -0.25$
$\text{Co}(\text{NH}_3)_5^{3+} -0.35$	$\text{Cu}(\text{NH}_3)_3^{2+} -0.26$	$\text{Co}(\text{NH}_3)_5^{3+} -0.13$	$\text{OsO}_3^{2+} -0.30$	$\text{PtF}_5^- -0.26$	$\text{ZrCl}_5^- -0.33$	$\text{AuPH}_3^+ -0.29$
$\text{Rh}(\text{H}_2\text{O})_5^{3+} -0.40$	$\text{Co}(\text{NH}_3)_5^{3+} -0.32$	$\text{Rh}(\text{H}_2\text{O})_5^{3+} -0.27$	$\text{TaMe}_4^+ -0.31$	$\text{AuCl}_3 -0.30$	$\text{HgI}_2 -0.36$	$\text{Mo}(\text{SH})_3^+ -0.30$
$\text{OsO}_3^{2+} -0.44$	$\text{Nb}(\text{NH}_2)_4^+ -0.32$	$\text{OsO}_3^{2+} -0.37$	$\text{TiCl}_3^+ -0.36$	$\text{InCl}_2^+ -0.36$	$\text{OsO}_3^{2+} -0.40$	$\text{FeCl}_2^+ -0.35$

7 Role of solvation (B3LYP-D3 in water)

7.1 Results of SVD-based matrix decomposition

The main analysis is carried out on calculations with the B3LYP-D3 functional in vacuum. We evaluate the role of solvation by repeating the analysis of the Actual Training Set of metal fragments with BDEs obtained with the B3LYP-D3 functional in a solvent continuum model (PCM) for water. The solvent calculations are single-point, carried out on the already available structures in vacuum. The average and maximum error relative to the number of hidden descriptors considered is presented in Table S34. The analysis of the results obtained in vacuum and in water continuum have some similitudes and some divergences. If we look at the differences in the weights of each hidden descriptor in Table S34 we observe important discrepancies. The weight of the first hidden descriptor in water is about one third of the weight of the same hidden descriptor in vacuum. The weight of the second is also reduced but more slightly, it's about a 70% of the value in gas phase. The third hidden descriptor behaves similarly to first being reduced by one third (it is a 34% of the gas phase value). The rest of the hidden descriptors are about a 75% of the gas phase value. This differences also affect the hidden descriptors, if we compute the correlation between the hidden descriptors in vacuum and water continuum we obtain Table S35. There is some correlation for the first descriptor $r^2 = 0.81$ then the correlation is very minor, 0.35, 0.48, 0.52 0.43 0.04 and 0.18 for **HD**_{L2} to **HD**_{L7}.

Table S34: Maximum absolute and average error (in kcal/mol) of the estimated BDE with respect to the number of considered hidden descriptors (k) for the Actual Training Set. The weight of the last included k, diagonal term in matrix $\mathbf{W}$, is also provided, for results B3LYP-D3 in vacuum and in water.

k	Vacuum			Water		
	Max error	Aver error	Weight, $\mathbf{W}_{k,k}$	Max error	Aver error	Weight, $\mathbf{W}_{k,k}$
1	86.7	13.4	4691	49.3	8.0	1529
2	88.0	8.7	293	24.9	4.0	204
3	28.1	5.2	252	21.5	2.9	85
4	14.4	3.2	119	11.8	2.0	69
5	13.2	2.3	59	6.5	1.3	47
6	8.1	1.4	54	5.6	1.0	25
7	6.0	1.1	25	3.4	0.8	22
8	5.2	0.8	22	2.8	0.6	12
9	3.0	0.7	15	2.8	0.5	10
10	2.6	0.5	13	2.2	0.4	9
11	2.2	0.4	9	2.1	0.3	7
12	1.7	0.3	7	2.1	0.2	6
13	1.6	0.2	6	1.0	0.2	5
14	1.2	0.2	4	1.0	0.2	4
15	0.8	0.1	4	0.9	0.1	3
16	0.6	0.1	2	0.9	0.1	3
17	0.6	0.1	2	0.4	0.1	2
18	0.3	0.1	1	0.2	0.0	2
19	0.3	0.0	1	0.2	0.0	1
20	0.2	0.0	1	0.1	0.0	1
21	0.1	0.0	1	0.1	0.0	0
22	0.0	0.0	0	0.0	0.0	0

Table S35: Correlation r^2 between the hidden descriptors obtained from BDEs in vacuum and in solution.

	vac. $\mathbf{HD}_{L1}$	vac. $\mathbf{HD}_{L2}$	vac. $\mathbf{HD}_{L3}$	vac. $\mathbf{HD}_{L4}$	vac. $\mathbf{HD}_{L5}$	vac. $\mathbf{HD}_{L6}$	vac. $\mathbf{L}_7$
water $\mathbf{HD}_{L1}$	0.81	0.05	0.17	0.21	0.18	0.09	0.01
water $\mathbf{HD}_{L2}$	0.49	0.35	0.38	0.16	0.02	0.01	0.00
water $\mathbf{HD}_{L3}$	0.00	0.33	0.48	0.07	0.00	0.05	0.10
water $\mathbf{HD}_{L4}$	0.24	0.00	0.02	0.52	0.12	0.26	0.01
water $\mathbf{HD}_{L5}$	0.00	0.03	0.02	0.01	0.43	0.47	0.00
water $\mathbf{HD}_{L6}$	0.01	0.19	0.00	0.11	0.24	0.04	0.00
water $\mathbf{L}_7$	0.03	0.01	0.01	0.01	0.01	0.00	0.18

7.2 BDE matrix

The BDE between the ligands metal fragments in the Actual Training Set computed using B3LYP-D3 functional in water solvent (PCM) are presented in Table S36.

Table S36: Bond dissociation energies (kcal/mol) in the Actual Training Set. Calculations in water with the B3LYP-D3 functional. Results are split in two separate tables, part A and part B.

Table S36, PART A												
	Br ⁻	CH ₃ ⁻	Cl ⁻	CN ⁻	CO	F ⁻	C ₆ H ₅ ⁻	H ₂	H ₂ O	H ⁻	NCH	
AuPH ₃ ⁺	-33.8	-87.4	-35.2	-56.8	-26.4	-38.8	-85.6	-4.7	-18.6	-95.9	-22.8	
Co(NH ₃) ₅ ³⁺	-36.3	-101.0	-40.0	-56.4	-10.6	-58.5	-97.4	4.4	-21.0	-106.5	-21.9	
CrO ₃	-40.2	-104.9	-44.9	-59.3	-16.8	-66.0	-100.6	3.1	-24.8	-107.3	-25.3	
Cu(NH ₃) ₃ ²⁺	-24.9	-73.5	-27.2	-38.7	-5.6	-40.1	-70.5	1.7	-15.2	-77.3	-14.0	
FeCl ₂ ⁺	-32.4	-90.7	-36.2	-40.3	4.6	-55.9	-86.8	11.5	-13.2	-88.5	-8.4	
Fe(CO) ₄	-22.3	-72.5	-23.2	-47.7	-35.5	-29.9	-71.5	-9.9	-17.4	-89.2	-23.2	
IrCO(PH ₃) ₂ ⁺	-23.2	-73.0	-25.4	-47.5	-25.0	-34.6	-75.3	3.3	-11.6	-83.8	-17.3	
MnO ₃ ⁺	-72.4	-163.1	-75.0	-88.1	-19.8	-91.2	-156.5	3.6	-35.1	-158.6	-34.1	
Mo(SH) ₃ ⁺	-30.9	-92.5	-37.3	-45.1	-19.2	-60.9	-89.6	5.0	-16.1	-90.5	-15.6	
Nb(NH ₂) ₄ ⁺	-5.0	-49.8	-9.7	-20.0	2.3	-34.4	-48.0	12.1	-5.2	-57.0	-2.8	
OsO ₃ ²⁺	-86.2	-187.1	-89.0	-94.6	4.5	-102.2	-187.8	20.3	-26.3	-180.1	-23.5	
PdH(PH ₃) ₂ ⁺	-16.7	-58.4	-17.5	-34.5	-16.9	-21.6	-59.4	1.0	-8.8	-69.6	-12.4	
PdPH ₃	-15.9	-44.7	-16.9	-34.6	-33.1	-18.3	-46.1	-6.4	-9.3	-58.1	-16.7	
PtF ₅ ⁻	-30.9	-109.3	-33.4	-63.7	-26.9	-44.5	-108.6	2.3	-16.3	-115.5	-23.6	
Rh(H ₂ O) ₅ ³⁺	-59.5	-140.2	-62.5	-84.6	-27.1	-72.7	-140.1	-2.4	-27.6	-145.8	-33.5	
Ru(SH) ₄	-16.0	-64.8	-17.9	-40.1	-23.5	-26.4	-64.7	1.8	-10.6	-77.7	-15.4	
TaMe ₄ ⁺	-19.6	-71.2	-24.8	-29.3	12.1	-54.7	-67.6	16.2	-7.1	-71.8	-2.8	
TiCl ₃ ⁺	-43.8	-106.5	-52.4	-51.6	-1.0	-82.2	-102.5	13.8	-23.3	-99.8	-17.3	
W(CO) ₅	-18.1	-58.3	-19.3	-40.3	-30.7	-27.6	-60.6	-3.0	-12.3	-72.7	-19.3	
ZrCl ₅ ⁻	-5.9	-48.5	-11.5	-20.3	1.4	-39.3	-46.5	9.3	-5.4	-52.2	-3.3	
AuCl ₃	-43.6	-126.0	-44.0	-70.6	-26.3	-50.3	-121.8	-2.2	-23.7	-131.8	-25.2	
HgI ₂	-2.1	-52.3	-2.1	-11.3	0.0	-5.1	-49.7	-0.2	1.9	-60.8	1.9	
InCl ₂ ⁺	-56.4	-125.9	-61.1	-71.1	-13.6	-80.9	-121.6	0.4	-33.6	-124.0	-30.5	

Table S36, PART B

	NH ₃	NHC	O ²⁻	OH ⁻	PH ₃	C ₅ H ₅ N	S ²⁻	SH ⁻	C ₆ H ₄ OMe ⁻	PCl ₃	SiMe ₃ ⁻
AuPH ₃ ⁺	-36.8	-62.0	-90.6	-52.7	-36.2	-36.1	-73.6	-50.3	-86.4	-24.6	-91.2
Co(NH ₃) ₅ ³⁺	-36.5	-57.8	-114.5	-70.4	-23.6	-34.1	-81.7	-53.7	-97.9	-6.9	-97.3
CrO ₃	-44.6	-67.2	-150.0	-80.2	-33.0	-44.9	-91.1	-58.7	-101.4	-18.4	-104.0
Cu(NH ₃) ₃ ²⁺	-28.3	-44.1	-83.6	-50.7	-16.2	-28.7	-59.6	-37.8	-70.9	-4.3	-71.0
FeCl ₂ ⁺	-27.9	-47.4	-152.7	-73.2	-14.1	-28.8	-105.4	-53.2	-89.7	0.7	-89.6
Fe(CO) ₄	-32.2	-54.4	-55.5	-39.7	-31.8	-31.1	-45.8	-35.4	-71.7	-28.2	-86.5
IrCO(PH ₃) ₂ ⁺	-26.8	-52.5	-84.8	-47.1	-23.8	-29.9	-58.4	-38.9	-75.8	-16.4	-73.3
MnO ₃ ⁺	-64.4	-100.3	-222.1	-117.1	-61.2	-67.5	-163.1	-102.0	-159.2	-36.5	-180.7
Mo(SH) ₃ ⁺	-29.6	-52.8	-176.1	-79.9	-19.8	-31.8	-107.6	-54.0	-91.8	-10.6	-81.8
Nb(NH ₂) ₄ ⁺	-12.8	-25.0	-115.2	-43.6	-0.2	-13.0	-48.9	-15.9	-48.9	3.0	-40.9
OsO ₃ ²⁺	-59.8	-112.2	-280.1	-138.1	-60.8	-67.9	-225.2	-125.6	-197.8	-32.2	-210.2
PdH(PH ₃) ₂ ⁺	-20.8	-39.8	-55.5	-31.7	-19.0	-22.5	-39.8	-28.9	-59.8	-14.7	-62.9
PdPH ₃	-20.0	-38.2	-47.6	-26.1	-24.7	-20.4	-36.5	-25.3	-46.4	-29.7	-46.8
PtF ₅ ⁻	-44.4	-77.9	-100.0	-62.0	-41.0	-47.9	-73.5	-53.9	-108.5	-28.3	-116.2
Rh(H ₂ O) ₅ ³⁺	-53.1	-91.0	-161.2	-94.1	-48.8	-56.7	-129.1	-84.8	-140.6	-31.3	-153.6
Ru(SH) ₄	-24.3	-47.5	-79.0	-36.2	-22.8	-24.7	-44.1	-28.4	-65.2	-17.7	-71.6
TaMe ₄ ⁺	-20.9	-32.7	-150.7	-67.9	-2.9	-17.5	-82.9	-34.3	-70.0	13.1	-51.6
TiCl ₃ ⁺	-37.6	-58.3	-204.1	-100.5	-19.8	-39.2	-126.8	-64.3	-105.2	-1.7	-96.3
W(CO) ₅	-25.4	-45.4	-55.0	-34.9	-25.0	-26.6	-37.8	-29.1	-60.8	-24.0	-66.4
ZrCl ₅ ⁻	-16.2	-29.0	-116.1	-48.1	-2.5	-15.0	-50.3	-17.7	-47.5	1.1	-35.5
AuCl ₃	-48.4	-82.8	-122.8	-72.0	-48.2	-48.5	-99.5	-69.3	-122.1	-31.5	-140.5
HgI ₂	-1.9	-18.0	-47.2	-16.2	0.6	-4.1	-33.8	-14.7	-50.4	-4.8	-62.6
InCl ₂ ⁺	-49.4	-75.7	-158.4	-96.0	-36.4	-54.0	-124.9	-78.3	-123.7	-14.8	-125.4

7.3 Hidden descriptor tables

Tables S37 and S38 report the values resulting from the B3LYP-D3 calculations in water for the first seven hidden descriptors for each ligand and metal fragment, respectively. Tables S39 and S40 report the same data but with the hidden descriptors ordered in decreasing order.

Table S37: First seven hidden descriptors of the ligands. BDE between two fragments in the Actual Training Set. BDEs obtained from B3LYP-D3 in water.

Ligand	$\text{HD}_{L1} = \mathbf{L}_1$	$\text{HD}_{L2} = \mathbf{L}_2$	$\text{HD}_{L3} = \mathbf{L}_3$	$\text{HD}_{L4} = \mathbf{L}_4$	$\text{HD}_{L5} = \mathbf{L}_5$	$\text{HD}_{L6} = \mathbf{L}_6$	$\mathbf{L}_7$
Br^-	0.117	-0.028	0.391	0.130	0.062	-0.066	0.011
CH_3^-	0.309	-0.102	-0.098	-0.150	0.215	-0.017	0.133
Cl^-	0.127	0.008	0.326	0.188	0.098	-0.098	0.005
CN^-	0.168	-0.184	-0.031	0.206	0.067	0.020	-0.321
CO	0.041	-0.295	-0.294	0.371	-0.357	-0.444	-0.025
F^-	0.170	0.163	-0.007	0.340	0.331	-0.008	0.106
C_6H_5^-	0.302	-0.120	-0.083	-0.161	0.117	-0.028	-0.169
H_2	-0.013	-0.143	0.013	0.118	-0.021	-0.355	0.373
H_2O	0.057	-0.048	0.053	0.240	0.182	-0.074	0.322
H^-	0.317	-0.219	-0.399	-0.175	0.137	-0.221	-0.061
NCH	0.059	-0.134	-0.013	0.274	0.071	-0.099	0.106
NH_3	0.113	-0.104	-0.002	0.235	0.129	0.296	0.063
NHC	0.191	-0.195	-0.083	0.116	-0.075	0.300	-0.301
O^{2-}	0.418	0.633	-0.306	0.123	-0.376	0.156	0.191
OH^-	0.221	0.172	-0.018	0.231	0.208	-0.017	0.014
PH_3	0.094	-0.210	0.198	0.152	-0.261	0.356	-0.035
$\text{C}_5\text{H}_5\text{N}$	0.118	-0.108	0.057	0.200	0.064	0.281	0.011
S^{2-}	0.298	0.250	0.426	-0.122	-0.233	-0.387	-0.248
SH^-	0.178	-0.031	0.340	0.042	-0.005	-0.105	-0.094
$\text{C}_6\text{H}_4\text{OMe}^-$	0.308	-0.098	-0.038	-0.199	0.063	-0.030	-0.254
PCl_3	0.052	-0.248	0.061	0.094	-0.533	0.092	0.098
SiMe_3^-	0.321	-0.261	0.170	-0.401	-0.080	0.140	0.552

Table S38: First seven hidden descriptors of the metal fragments. BDE between two fragments in the Actual Training Set. BDEs obtained from B3LYP-D3 in water.

Metal Frag.	$\text{HD}_{M1} = \mathbf{M}_1$	$\text{HD}_{M2} = \mathbf{M}_2$	$\text{HD}_{M3} = \mathbf{M}_3$	$\text{HD}_{M4} = \mathbf{M}_4$	$\text{HD}_{M5} = \mathbf{M}_5$	$\text{HD}_{M6} = \mathbf{M}_6$	$\mathbf{M}_7$
AuPH_3^+	-0.178	0.195	0.010	-0.101	0.062	0.103	0.182
$\text{Co}(\text{NH}_3)_5^{3+}$	-0.201	0.051	0.071	0.010	-0.474	0.148	0.089
CrO_3	-0.224	-0.011	0.090	-0.247	-0.088	-0.251	-0.249
$\text{Cu}(\text{NH}_3)_3^{2+}$	-0.145	0.035	0.063	0.035	-0.344	-0.010	0.030
FeCl_2^+	-0.198	-0.230	-0.004	0.161	-0.073	0.119	0.015
$\text{Fe}(\text{CO})_4$	-0.143	0.313	0.150	-0.069	0.049	0.156	-0.230
$\text{IrCO}(\text{PH}_3)_2^+$	-0.151	0.122	0.170	-0.043	0.032	0.078	0.395
MnO_3^+	-0.350	0.021	-0.249	-0.113	0.164	-0.238	-0.505
$\text{Mo}(\text{SH})_3^+$	-0.210	-0.243	0.166	-0.194	0.341	0.397	-0.017
$\text{Nb}(\text{NH}_2)_4^+$	-0.112	-0.245	0.388	0.087	0.075	-0.178	-0.105
OsO_3^{2+}	-0.417	-0.193	-0.501	0.368	0.299	-0.120	0.311
$\text{PdH}(\text{PH}_3)_2^+$	-0.114	0.152	0.140	0.105	-0.024	0.006	0.149
PdPH_3	-0.097	0.186	0.122	-0.210	0.393	0.259	0.174
PtF_5^-	-0.210	0.279	0.154	0.083	-0.084	-0.453	0.240
$\text{Rh}(\text{H}_2\text{O})_5^{3+}$	-0.293	0.174	-0.126	-0.049	-0.064	0.185	0.016
$\text{Ru}(\text{SH})_4$	-0.132	0.129	0.264	0.032	0.161	-0.141	-0.020
TaMe_4^+	-0.158	-0.371	0.229	0.055	-0.187	-0.014	0.260
TiCl_3^+	-0.245	-0.357	0.011	-0.233	-0.055	0.076	-0.099
$\text{W}(\text{CO})_5$	-0.120	0.218	0.175	-0.114	0.098	0.052	0.017
ZrCl_5^-	-0.112	-0.256	0.350	-0.058	0.081	-0.250	-0.022
AuCl_3	-0.247	0.268	-0.006	0.152	0.001	-0.140	-0.096
HgI_2	-0.085	0.056	0.238	0.700	-0.006	0.348	-0.350
InCl_2^+	-0.266	0.008	-0.185	-0.223	-0.390	0.248	-0.060

Table S39: First seven hidden descriptors of the ligands for the Actual Training Set, ordered by their values in decreasing order. Values derived from BDEs obtained from B3LYP-D3 in water.

$\text{HD}_{L_1} = L_1$	$\text{HD}_{L_2} = L_2$	$\text{HD}_{L_3} = L_3$	$\text{HD}_{L_4} = L_4$	$\text{HD}_{L_5} = L_5$	$\text{HD}_{L_6} = L_6$	L_7
O^{2-} 0.42	O^{2-} 0.63	S^{2-} 0.43	CO 0.37	F^- 0.33	PH_3 0.36	SiMe_3^- 0.55
SiMe_3^- 0.32	S^{2-} 0.25	Br^- 0.39	F^- 0.34	CH_3^- 0.21	NHC 0.30	H_2 0.37
H^- 0.32	OH^- 0.17	SH^- 0.34	NCH 0.27	OH^- 0.21	NH_3 0.30	H_2O 0.32
CH_3^- 0.31	F^- 0.16	Cl^- 0.33	H_2O 0.24	H_2O 0.18	$\text{C}_5\text{H}_5\text{N}$ 0.28	O^{2-} 0.19
$\text{C}_6\text{H}_4\text{OMe}^-$ 0.31	Cl^- 0.01	PH_3 0.20	NH_3 0.24	H^- 0.14	O^{2-} 0.16	CH_3^- 0.13
C_6H_5^- 0.30	Br^- -0.03	SiMe_3^- 0.17	OH^- 0.23	NH_3 0.13	SiMe_3^- 0.14	NCH 0.11
S^{2-} 0.30	SH^- -0.03	PCl_3 0.06	CN^- 0.21	C_6H_5^- 0.12	PCl_3 0.09	F^- 0.11
OH^- 0.22	H_2O -0.05	$\text{C}_5\text{H}_5\text{N}$ 0.06	$\text{C}_5\text{H}_5\text{N}$ 0.20	Cl^- 0.10	CN^- 0.02	PCl_3 0.10
NHC 0.19	$\text{C}_6\text{H}_4\text{OMe}^-$ -0.10	H_2O 0.05	Cl^- 0.19	NCH 0.07	F^- -0.01	NH_3 0.06
SH^- 0.18	CH_3^- -0.10	H_2 0.01	PH_3 0.15	CN^- 0.07	OH^- -0.02	OH^- 0.01
F^- 0.17	NH_3 -0.10	NH_3 0.00	Br^- 0.13	$\text{C}_5\text{H}_5\text{N}$ 0.06	CH_3^- -0.02	Br^- 0.01
CN^- 0.17	$\text{C}_5\text{H}_5\text{N}$ -0.11	F^- -0.01	O^{2-} 0.12	$\text{C}_6\text{H}_4\text{OMe}^-$ 0.06	C_6H_5^- -0.03	$\text{C}_5\text{H}_5\text{N}$ 0.01
Cl^- 0.13	C_6H_5^- -0.12	NCH -0.01	H_2 0.12	Br^- 0.06	$\text{C}_6\text{H}_4\text{OMe}^-$ -0.03	Cl^- 0.00
$\text{C}_5\text{H}_5\text{N}$ 0.12	NCH -0.13	OH^- -0.02	NHC 0.12	SH^- 0.00	Br^- -0.07	CO -0.02
Br^- 0.12	H_2 -0.14	CN^- -0.03	PCl_3 0.09	H_2 -0.02	H_2O -0.07	PH_3 -0.03
NH_3 0.11	CN^- -0.18	$\text{C}_6\text{H}_4\text{OMe}^-$ -0.04	SH^- 0.04	NHC -0.07	Cl^- -0.10	H^- -0.06
PH_3 0.09	NHC -0.20	NHC -0.08	S^{2-} -0.12	SiMe_3^- -0.08	NCH -0.10	SH^- -0.09
NCH 0.06	PH_3 -0.21	C_6H_5^- -0.08	CH_3^- -0.15	S^{2-} -0.23	SH^- -0.10	C_6H_5^- -0.17
H_2O 0.06	H^- -0.22	CH_3^- -0.10	C_6H_5^- -0.16	PH_3 -0.26	H^- -0.22	S^{2-} -0.25
PCl_3 0.05	PCl_3 -0.25	CO -0.29	H^- -0.18	CO -0.36	H_2 -0.35	$\text{C}_6\text{H}_4\text{OMe}^-$ -0.25
CO 0.04	SiMe_3^- -0.26	O^{2-} -0.31	$\text{C}_6\text{H}_4\text{OMe}^-$ -0.20	O^{2-} -0.38	S^{2-} -0.39	NHC -0.30
H_2 -0.01	CO -0.30	H^- -0.40	SiMe_3^- -0.40	PCl_3 -0.53	CO -0.44	CN^- -0.32

Table S40: First seven hidden descriptors of the metal fragments for the Actual Training Set, ordered by their values in decreasing order. Values derived from BDEs obtained from B3LYP-D3 in water.

$\text{HD}_{M1} = \mathbf{M}_1$	$\text{HD}_{M2} = \mathbf{M}_2$	$\text{HD}_{M3} = \mathbf{M}_3$	$\text{HD}_{M4} = \mathbf{M}_4$	$\text{HD}_{M5} = \mathbf{M}_5$	$\text{HD}_{M6} = \mathbf{M}_6$	$\text{HD}_{M7} = \mathbf{M}_7$
HgI ₂ -0.08	Fe(CO) ₄ 0.31	Nb(NH ₂) ₄ ⁺ 0.39	HgI ₂ 0.70	PdPH ₃ 0.39	Mo(SH) ₃ ⁺ 0.40	IrCO(PH ₃) ₂ ⁺ 0.39
PdPH ₃ -0.10	PtF ₅ ⁻ 0.28	ZrCl ₅ ⁻ 0.35	OsO ₃ ²⁺ 0.37	Mo(SH) ₃ ⁺ 0.34	HgI ₂ 0.35	OsO ₃ ²⁺ 0.31
Nb(NH ₂) ₄ ⁺ -0.11	AuCl ₃ 0.27	Ru(SH) ₄ 0.26	FeCl ₂ ⁺ 0.16	OsO ₃ ²⁺ 0.30	PdPH ₃ 0.26	TaMe ₄ ⁺ 0.26
ZrCl ₅ ⁻ -0.11	W(CO) ₅ 0.22	HgI ₂ 0.24	AuCl ₃ 0.15	MnO ₃ ⁺ 0.16	InCl ₂ ⁺ 0.25	PtF ₅ ⁻ 0.24
PdH(PH ₃) ₂ ⁺ -0.11	AuPH ₃ ⁺ 0.20	TaMe ₄ ⁺ 0.23	PdH(PH ₃) ₂ ⁺ 0.11	Ru(SH) ₄ 0.16	Rh(H ₂ O) ₅ ³⁺ 0.18	AuPH ₃ ⁺ 0.18
W(CO) ₅ -0.12	PdPH ₃ 0.19	W(CO) ₅ 0.18	Nb(NH ₂) ₄ ⁺ 0.09	W(CO) ₅ 0.10	Fe(CO) ₄ 0.16	PdPH ₃ 0.17
Ru(SH) ₄ -0.13	Rh(H ₂ O) ₅ ³⁺ 0.17	IrCO(PH ₃) ₂ ⁺ 0.17	PtF ₅ ⁻ 0.08	ZrCl ₅ ⁻ 0.08	Co(NH ₃) ₅ ³⁺ 0.15	PdH(PH ₃) ₂ ⁺ 0.15
Fe(CO) ₄ -0.14	PdH(PH ₃) ₂ ⁺ 0.15	Mo(SH) ₃ ⁺ 0.17	TaMe ₄ ⁺ 0.05	Nb(NH ₂) ₄ ⁺ 0.07	FeCl ₂ ⁺ 0.12	Co(NH ₃) ₅ ³⁺ 0.09
Cu(NH ₃) ₃ ²⁺ -0.15	Ru(SH) ₄ 0.13	PtF ₅ ⁻ 0.15	Cu(NH ₃) ₃ ²⁺ 0.04	AuPH ₃ ⁺ 0.06	AuPH ₃ ⁺ 0.10	Cu(NH ₃) ₃ ²⁺ 0.03
IrCO(PH ₃) ₂ ⁺ -0.15	IrCO(PH ₃) ₂ ⁺ 0.12	Fe(CO) ₄ 0.15	Ru(SH) ₄ 0.03	Fe(CO) ₄ 0.05	IrCO(PH ₃) ₂ ⁺ 0.08	W(CO) ₅ 0.02
TaMe ₄ ⁺ -0.16	HgI ₂ 0.06	PdH(PH ₃) ₂ ⁺ 0.14	Co(NH ₃) ₅ ³⁺ 0.01	IrCO(PH ₃) ₂ ⁺ 0.03	TiCl ₃ ⁺ 0.08	Rh(H ₂ O) ₅ ³⁺ 0.02
AuPH ₃ ⁺ -0.18	Co(NH ₃) ₅ ³⁺ 0.05	PdPH ₃ 0.12	IrCO(PH ₃) ₂ ⁺ -0.04	AuCl ₃ 0.00	W(CO) ₅ 0.05	FeCl ₂ ⁺ 0.02
FeCl ₂ ⁺ -0.20	Cu(NH ₃) ₃ ²⁺ 0.04	CrO ₃ 0.09	Rh(H ₂ O) ₅ ³⁺ -0.05	HgI ₂ -0.01	PdH(PH ₃) ₂ ⁺ 0.01	Mo(SH) ₃ ⁺ -0.02
Co(NH ₃) ₅ ³⁺ -0.20	MnO ₃ ⁺ 0.02	Co(NH ₃) ₅ ³⁺ 0.07	ZrCl ₅ ⁻ -0.06	PdH(PH ₃) ₂ ⁺ -0.02	Cu(NH ₃) ₃ ²⁺ -0.01	Ru(SH) ₄ -0.02
Mo(SH) ₃ ⁺ -0.21	InCl ₂ ⁺ 0.01	Cu(NH ₃) ₃ ²⁺ 0.06	Fe(CO) ₄ -0.07	TiCl ₃ ⁺ -0.05	TaMe ₄ ⁺ -0.01	ZrCl ₅ ⁻ -0.02
PtF ₅ ⁻ -0.21	CrO ₃ -0.01	TiCl ₃ ⁺ 0.01	AuPH ₃ ⁺ -0.10	Rh(H ₂ O) ₅ ³⁺ -0.06	OsO ₃ ²⁺ -0.12	InCl ₂ ⁺ -0.06
CrO ₃ -0.22	OsO ₃ ²⁺ -0.19	AuPH ₃ ⁺ 0.01	MnO ₃ ⁺ -0.11	FeCl ₂ ⁺ -0.07	AuCl ₃ -0.14	AuCl ₃ -0.10
TiCl ₃ ⁺ -0.24	FeCl ₂ ⁺ -0.23	FeCl ₂ ⁺ 0.00	W(CO) ₅ -0.11	PtF ₅ ⁻ -0.08	Ru(SH) ₄ -0.14	TiCl ₃ ⁺ -0.10
AuCl ₃ -0.25	Mo(SH) ₃ ⁺ -0.24	AuCl ₃ -0.01	Mo(SH) ₃ ⁺ -0.19	CrO ₃ -0.09	Nb(NH ₂) ₄ ⁺ -0.18	Nb(NH ₂) ₄ ⁺ -0.11
InCl ₂ ⁺ -0.27	Nb(NH ₂) ₄ ⁺ -0.25	Rh(H ₂ O) ₅ ³⁺ -0.13	PdPH ₃ -0.21	TaMe ₄ ⁺ -0.19	MnO ₃ ⁺ -0.24	Fe(CO) ₄ -0.23
Rh(H ₂ O) ₅ ³⁺ -0.29	ZrCl ₅ ⁻ -0.26	InCl ₂ ⁺ -0.18	InCl ₂ ⁺ -0.22	Cu(NH ₃) ₃ ²⁺ -0.34	ZrCl ₅ ⁻ -0.25	CrO ₃ -0.25
MnO ₃ ⁺ -0.35	TiCl ₃ ⁺ -0.36	MnO ₃ ⁺ -0.25	TiCl ₃ ⁺ -0.23	InCl ₂ ⁺ -0.39	CrO ₃ -0.25	HgI ₂ -0.35
OsO ₃ ²⁺ -0.42	TaMe ₄ ⁺ -0.37	OsO ₃ ²⁺ -0.50	CrO ₃ -0.25	Co(NH ₃) ₅ ³⁺ -0.47	PtF ₅ ⁻ -0.45	MnO ₃ ⁺ -0.50

8 Chemical meaning of the hidden descriptors

8.1 List of best conventional descriptors for each hidden descriptor of the ligands, $\mathbf{HD}_{Lk}$. Actual Training Set B3LYP-D3 in vacuum.

Please note that in the regression analysis performed we have not taken into account the H_2 ligand. This ligand coordinates to metal fragments in η^2 coordination mode and some conventional descriptors are difficult to be defined (i. e. Metal-ligand distance, charge of the central atom ...).

Table S41: First 15 conventional descriptors with best correlation with the first hidden descriptor $\mathbf{HD}_{L1}$ the ligands for the Actual Training Set B3LYP-D3 in vacuum.

Molec. Desc.	Definition	r^2
602	Energy of the first Lone Pair of Ti from NBO analysis of L-TiCl_3^+ , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.976
594	Energy of the Lone Pair of Ta from NBO analysis of L-TaMe_4^+ , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.973
604	Energy of the second Lone Pair of Ti from NBO analysis of L-TiCl_3^+ , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.973
557	Energy of the third Lone Pair of Pt from NBO analysis of L-PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.971
556	Energy of the second Lone Pair of Pt from NBO analysis of L-PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.967
555	Energy of the first Lone Pair of Pt from NBO analysis of L-PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.964
136	Ionization potential, IP, computed as Energy of the cation- Energy of the ligand.	0.963
3	Energy of the HOMO orbital of the free ligand.	0.956
13	Total charge of the free ligand.	0.946
554	Energy of the L-Pt bond from NBO analysis of L-PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.928
148	LUMO β of the cation.	0.925
4	Energy of the HOMO-1 orbital of the free ligand.	0.894
14	Mulliken charge on the central atom with hydrogens added into it of the free ligand.	0.891
572	Energy of the L-Pt bond from NBO analysis of L-PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.880
527	Frequency of the CO trans to L in L-Fe(CO)_4 .	0.852

Table S42: First 15 conventional descriptors with best correlation with the second hidden descriptor $\mathbf{HD}_{L2}$ of the ligands for the Actual Training Set B3LYP-D3 in vacuum.

Molec. Desc.	Definition	r^2
57	APT total charge of the ligand in $L\text{-Fe(CO)}_4$.	0.831
56	Mulliken total charge of the ligand in $L\text{-Fe(CO)}_4$.	0.803
104	Mulliken total charge of the ligand in PtF_5^- .	0.793
129	Average APT total charge of the ligand in $L\text{-K}^+$, $L\text{-AlCl}_3$, $L\text{-TiCl}_3^+$, $L\text{-Fe(CO)}_4$, $L\text{-OsO}_3^{2+}$, $L\text{-TaMe}_4^+$, PtF_5^- and AuPH_3^+ .	0.783
68	Average of Mulliken total charge of the ligand in $L\text{-K}^+$, $L\text{-AlCl}_3$, $L\text{-TiCl}_3^+$ and $L\text{-Fe(CO)}_4$.	0.777
117	APT total charge of the ligand in AuPH_3^+ .	0.763
69	Average of APT total charge of the ligand in $L\text{-K}^+$, $L\text{-AlCl}_3$, $L\text{-TiCl}_3^+$ and $L\text{-Fe(CO)}_4$.	0.756
660	Donation of the higher π orbitals according to CDA analysis (SDD basis set).	0.742
33	APT total charge of the ligand in $L\text{-AlCl}_3$.	0.721
128	Average Mulliken total charge of the ligand in $L\text{-K}^+$, $L\text{-AlCl}_3$, $L\text{-TiCl}_3^+$, $L\text{-Fe(CO)}_4$, $L\text{-OsO}_3^{2+}$, $L\text{-TaMe}_4^+$, PtF_5^- and AuPH_3^+ .	0.696
157	Number of lone pairs of the central atom of the ligand.	0.692
20	Mulliken total charge of the ligand in $L\text{-K}^+$.	0.692
638	Fe-CO distance in the different $L\text{-Fe(CO)}_4$ complexes for the CO <i>trans</i> to the ligand L.	0.688
45	APT total charge of the ligand in $L\text{-TiCl}_3^+$.	0.685
21	APT total charge of the ligand in $L\text{-K}^+$.	0.684

Table S43: First 15 conventional descriptors with best correlation with the third hidden descriptor $\mathbf{HD}_{L3}$ of the ligands for the Actual Training Set B3LYP-D3 in vacuum.

Molec. Desc.	Definition	r^2
489	(Mulliken charge on the central atom of the free ligand) ² /(Cavity volume of the ligand in water with SMD according to Gaussian defaults).	0.840
410	(Mulliken charge on the central atom of the free ligand) ² /(Box Volume).	0.839
491	(NPA charge on the central atom of the free ligand) ² /(Cavity volume of the ligand in water with SMD according to Gaussian defaults).	0.836
412	(NPA charge on the central atom of the free ligand) ² /(Box Volume).	0.836
490	(APT charge on the central atom of the free ligand) ² /(Cavity volume of the ligand in water with SMD according to Gaussian defaults).	0.823
411	(APT charge on the central atom of the free ligand) ² /(Box Volume).	0.822
494	(APT charge on the central atom of the free ligand with hydrogens added into it) ² /(Cavity volume of the ligand in water with SMD according to Gaussian defaults).	0.804
493	(Mulliken charge on the central atom of the free ligand with hydrogens added into it) ² /(Cavity volume of the ligand in water with SMD according to Gaussian defaults).	0.803
415	(APT charge on the central atom of the free ligand with hydrogens added into it) ² /(Box Volume).	0.799
414	(Mulliken charge on the central atom of the free ligand with hydrogens added into it) ² /(Box Volume).	0.798
492	(Total charge of the free ligand) ² /(Cavity volume of the ligand in water with SMD according to Gaussian defaults).	0.790
413	(Total charge of the free ligand) ² /(Box Volume).	0.786
632	Electrophilicity index, ω , computed according to Koopmans' theorem as $\mu^2/(2\eta) = ((\epsilon_{HOMO} + \epsilon_{LUMO})/2)^2/(-\epsilon_{HOMO} + \epsilon_{LUMO})$ with energies from NBO analysis.	0.771
499	(Mulliken charge on the central atom of the free ligand) ² /(Cavity surface of the ligand in water with SMD according to Gaussian defaults).	0.759
501	(NPA charge on the central atom of the free ligand) ² /(Cavity surface of the ligand in water with SMD according to Gaussian defaults).	0.753

Table S44: First 15 conventional descriptors with best correlation with the fourth hidden descriptor $\mathbf{HD}_{L4}$ of the ligands for the Actual Training Set B3LYP-D3 in vacuum.

Molec. Desc.	Definition	r^2
613	L/Ta ionic - L/Ta covalent Natural Bond Order from NBO analysis of L-TaMe_4^+ , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.775
612	L/Ta ionic - L/Ta covalent Natural Bond Order from NBO analysis of L-TaMe_4^+ , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.774
600	% covalent Natural Bond Order from NBO analysis of L-TaMe_4^+ , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.756
592	% covalent Natural Bond Order from NBO analysis of L-TaMe_4^+ , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.754
611	L/Ti ionic - L/Ti covalent Natural Bond Order from NBO analysis of L-TiCl_3^+ , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.751
656	Interaction energy $-\text{BDE}_{\pi\text{-backdonation}}$ (TZVP basis sets).	0.748
610	% covalent Natural Bond Order from NBO analysis of L-TiCl_3^+ , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.746
657	BDE $-\text{BDE}_{\pi\text{-backdonation}}$ (SDD/TZVP basis sets).	0.731
547	% Pt of the L-Pt bond from NBO analysis of L-PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.662
643	Distortion energy, energy to bring the ligand and the metal complex at the geometry of the complex. It is computed as $\text{BDE} - \text{Interaction energy}$. The interaction energy is $E_{M-L} - E_{M^*} - E_{L^*}$. M^* and L^* denote the fragments at the geometry of the complex. BDE corresponds to the energy obtained with SDD/lanl2dz basis set while Interaction energy corresponds to single points at TZVP basis set.	0.653
614	L/Pt ionic - L/Pt covalent Natural Bond Order from NBO analysis of L-PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.637
548	Coefficient of Pt of the L-Pt bond from NBO analysis of L-PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.632
563	% covalent Natural Bond Order from NBO analysis of L-PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.618
645	Distortion energy, energy to bring the ligand and the metal complex at the geometry of the complex. It is computed as $\text{BDE} - \text{Interaction energy}$. The interaction energy is $E_{M-L} - E_{M^*} - E_{L^*}$. M^* and L^* denote the fragments at the geometry of the complex. All energies computed at SDD/lanl2dz level.	0.597
565	% Pt of the L-Pt bond from NBO analysis of L-PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.548

Table S45: First 15 conventional descriptors with best correlation with the fifth hidden descriptor $\mathbf{HD}_{L5}$ of the ligands for the Actual Training Set B3LYP-D3 in vacuum.

Molec. Desc.	Definition	r^2
652	Back-donation of the higher π orbitals according to CDA analysis (TZVP basis set).	0.656
659	Back-donation of the higher σ orbital according to CDA analysis (SDD basis set).	0.641
584	Distance between the central atom and PtF_5^- in L-PtF_5^- / Distance between the central atom and $\text{Fe}(\text{CO})_4$ in $\text{L-Fe}(\text{CO})_4$.	0.561
583	Distance between the central atom and $\text{Fe}(\text{CO})_4$ in $\text{L-Fe}(\text{CO})_4$ / Distance between the central atom and PtF_5^- in L-PtF_5^- .	0.555
197	APT charge on central atom / (Crystal ionic radius of the central atom of the ligand) ² .	0.398
173	APT charge on central atom / Effective ionic radius of the central atom of the ligand.	0.397
577	Distance between the central atom and K^+ in L-K^+ / Distance between the central atom and TiCl_3^+ in L-TiCl_3^+ .	0.366
203	APT charge on central atom / (Effective ionic radius of the central atom of the ligand) ² .	0.364
167	APT charge on central atom / Crystal ionic radius of the central atom of the ligand.	0.355
537	q backdonation of Charge Decomposition Analysis of $\text{L-Fe}(\text{CO})_4$, with TZVP basis set.	0.348
171	NPA charge on central atom / Effective ionic radius of the central atom of the ligand.	0.347
195	NPA charge on central atom / (Crystal ionic radius of the central atom of the ligand) ² .	0.344
165	NPA charge on central atom / Crystal ionic radius of the central atom of the ligand.	0.340
580	Distance between the central atom and TiCl_3^+ in L-TiCl_3^+ / Distance between the central atom and K^+ in L-K^+ .	0.333
201	NPA charge on central atom / (Effective ionic radius of the central atom of the ligand) ² .	0.332

Table S46: First 15 conventional descriptors with best correlation with the sixth hidden descriptor $\mathbf{HD}_{L6}$ of the ligands for the Actual Training Set B3LYP-D3 in vacuum.

Molec. Desc.	Definition	r^2
316	(APT charge on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex) / $L-K^+$ distance.	0.586
317	(APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex) / $L-K^+$ distance.	0.575
50	(Mulliken total charge of the ligand in $L-TiCl_3^+$) - (Total charge of the free ligand).	0.571
308	APT charge on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex.	0.547
309	APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex.	0.525
387	(APT charge on the central atom of the free ligand with hydrogens added into it) ² /(Effective ionic radius of the central atom of the ligand) ³ .	0.484
312	(APT charge on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex) x $L-K^+$ distance.	0.471
162	Molar Volume computed according to Gaussian's keyword Volume.	0.471
87	(APT total charge of the ligand in $L-OsO_3^{2+}$) - (Total charge of the free ligand).	0.467
313	(APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex) x $L-K^+$ distance.	0.437
257	Cavity volume of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).	0.425
86	(Mulliken total charge of the ligand in $L-OsO_3^{2+}$) - (Total charge of the free ligand).	0.420
258	Surface area of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).	0.414
161	Box Volume computed according to Gaussian's keyword Volume.	0.404
140	Softness, S, computed as $1/(IP-EA) = 1/(\text{Energy of the anion} + \text{Energy of the cation} - 2 \times \text{Energy of the ligand})$.	0.403

8.2 Correlation between the hidden descriptors and the BDEs, in vacuum

We have considered if some of the BDEs of the metal fragments can be a good descriptor for some of the hidden descriptors $\mathbf{HD}_{Lk}$. We have look for the correlation between them. The BDEs of the metal fragments are used as conventional descriptors for the ligands and viceversa. Results are presented in Tables S55 and S56.

Table S47: Correlation (r^2) between the BDEs of the metal fragments and $\mathbf{HD}_{L1} = \mathbf{L}_1$ to $\mathbf{L}_7$ the of the ligands for the Actual Training Set B3LYP-D3 in vacuum.

$\mathbf{HD}_{L1} = \mathbf{L}_1$	$\mathbf{HD}_{L2} = \mathbf{L}_2$	$\mathbf{HD}_{L3} = \mathbf{L}_3$	$\mathbf{HD}_{L4} = \mathbf{L}_4$	$\mathbf{HD}_{L5} = \mathbf{L}_5$	$\mathbf{HD}_{L6} = \mathbf{L}_6$	$\mathbf{L}_7$
AuPH ₃ ⁺	0.994	0.304	0.227	0.141	0.021	0.041 0.000
Co(NH ₃) ₅ ³⁺	0.994	0.418	0.171	0.102	0.019	0.038 0.001
CrO ₃	0.921	0.139	0.416	0.109	0.044	0.028 0.002
Cu(NH ₃) ₃ ²⁺	0.997	0.400	0.193	0.099	0.021	0.035 0.000
FeCl ₂ ⁺	0.997	0.362	0.242	0.074	0.025	0.041 0.000
Fe(CO) ₄	0.856	0.073	0.377	0.255	0.014	0.044 0.001
IrCO(PH ₃) ₂ ⁺	0.995	0.315	0.252	0.120	0.013	0.039 0.001
MnO ₃ ⁺	0.996	0.303	0.219	0.116	0.035	0.054 0.000
Mo(SH) ₃ ⁺	0.989	0.338	0.286	0.062	0.014	0.048 0.000
Nb(NH ₂) ₄ ⁺	0.978	0.326	0.332	0.054	0.012	0.035 0.000
OsO ₃ ²⁺	0.992	0.363	0.158	0.103	0.031	0.073 0.001
PdH(PH ₃) ₂ ⁺	0.995	0.325	0.239	0.129	0.015	0.038 0.000
PdPH ₃	0.780	0.046	0.547	0.139	0.000	0.061 0.001
PtF ₅ ⁻	0.070	0.851	0.092	0.083	0.048	0.010 0.012
Rh(H ₂ O) ₅ ³⁺	0.994	0.397	0.158	0.115	0.020	0.051 0.001
Ru(SH) ₄	0.882	0.102	0.478	0.117	0.007	0.065 0.000
TaMe ₄ ⁺	0.986	0.363	0.285	0.053	0.020	0.031 0.001
TiCl ₃ ⁺	0.989	0.355	0.278	0.054	0.023	0.038 0.000
W(CO) ₅	0.894	0.109	0.433	0.164	0.006	0.044 0.002
ZrCl ₅ ⁻	0.062	0.165	0.838	0.036	0.004	0.027 0.001
AuCl ₃	0.909	0.111	0.300	0.216	0.047	0.062 0.000
HgI ₂	0.935	0.154	0.361	0.163	0.023	0.061 0.000
InCl ₂ ⁺	0.998	0.348	0.222	0.101	0.033	0.035 0.000

Table S48: Correlation (r^2) between the BDEs of the ligands and the $\mathbf{HD}_{M1} = \mathbf{M}_1$ to $\mathbf{M}_7$ of the metal fragments for the Actual Training Set B3LYP-D3 in vacuum.

$\mathbf{HD}_{M1} = \mathbf{M}_1$	$\mathbf{HD}_{M2} = \mathbf{M}_2$	$\mathbf{HD}_{M3} = \mathbf{M}_3$	$\mathbf{HD}_{M4} = \mathbf{M}_4$	$\mathbf{HD}_{M5} = \mathbf{M}_5$	$\mathbf{HD}_{M6} = \mathbf{M}_6$	$\mathbf{M}_7$	
Br^-	0.997	0.292	0.489	0.034	0.001	0.000	0.000
CH_3^-	0.996	0.239	0.533	0.030	0.008	0.001	0.000
Cl^-	0.998	0.301	0.473	0.039	0.002	0.000	0.000
CN^-	0.994	0.267	0.524	0.024	0.001	0.000	0.000
CO	0.305	0.094	0.733	0.055	0.114	0.005	0.001
F^-	0.993	0.328	0.413	0.059	0.005	0.000	0.000
C_6H_5^-	0.994	0.224	0.554	0.030	0.006	0.002	0.000
H_2O	0.403	0.036	0.740	0.073	0.087	0.003	0.006
H^-	0.750	0.008	0.625	0.222	0.023	0.000	0.000
NCH	0.992	0.249	0.540	0.018	0.005	0.001	0.000
NH_3	0.820	0.022	0.713	0.138	0.000	0.000	0.000
NHC	0.708	0.000	0.705	0.170	0.019	0.000	0.001
O^{2-}	0.759	0.003	0.767	0.105	0.012	0.004	0.000
OH^-	0.986	0.357	0.367	0.066	0.004	0.003	0.000
PH_3	0.996	0.299	0.438	0.061	0.006	0.000	0.000
$\text{C}_5\text{H}_5\text{N}$	0.641	0.006	0.828	0.099	0.000	0.004	0.002
S^{2-}	0.807	0.014	0.709	0.138	0.015	0.003	0.000
SH^-	0.994	0.349	0.423	0.034	0.002	0.003	0.000
$\text{C}_6\text{H}_4\text{OMe}^-$	0.998	0.269	0.509	0.035	0.003	0.001	0.000
PCl_3	0.993	0.218	0.557	0.033	0.006	0.003	0.000
SiMe_3^-	0.576	0.014	0.835	0.077	0.009	0.025	0.001

8.3 List of best conventional descriptors for each hidden descriptor (k) of the ligands, $\mathbf{HD}_{L1}$. Actual Training Set B3LYP-D3 in water.

Please note that we use here the same conventional descriptors as in the previous section. They were derived from vacuum calculations. As stated before, in the regression analysis performed we have not taken into account the H_2 ligand. This ligand coordinates to metal fragments in η^2 coordination mode and some conventional descriptors are difficult to be defined (i. e. Metal-ligand distance, charge of the central atom ...).

Table S49: First 15 conventional descriptors with best correlation with the first hidden descriptor $\mathbf{HD}_{L1}$ of the ligands for the Actual Training Set B3LYP-D3 in water.

Molec. Desc.	Definition	r^2
535	Bonding energy from Charge Decomposition Analysis of L-Fe(CO)_4 .	0.9014240748
542	Bonding energy from Charge Decomposition Analysis of L-Fe(CO)_4 , with TZVP basis set.	0.9008381505
62	(Mulliken total charge of the ligand in L-Fe(CO)_4) - (Total charge of the free ligand).	0.8934158281
63	(APT total charge of the ligand in L-Fe(CO)_4) - (Total charge of the free ligand).	0.8586436061
148	LUMO β of the cation.	0.8404607095
136	Ionization potential, IP, computed as Energy of the cation- Energy of the ligand.	0.8135881416
39	(APT total charge of the ligand in L-AlCl_3) - (Total charge of the free ligand).	0.8117486775
3	Energy of the HOMO orbital of the free ligand.	0.7827748021
23	(APT charge on the central atom of the ligand in L-K^+) - (APT charge central atom of the free ligand).	0.780568149
560	L/Pt covalent Natural Bond Order from NBO analysis of L-PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.7767415439
74	Average of (Mulliken total charge of the ligand in complex) - (Total charge of the free ligand) in L-K^+ , L-AlCl_3 , L-TiCl_3^+ and L-Fe(CO)_4 .	0.77639018
110	(Mulliken total charge of the ligand in PtF_5^-) - (Total charge of the free ligand).	0.7725937974
604	Energy of the second Lone Pair of Ti from NBO analysis of L-TiCl_3^+ , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.7623898731
123	(APT total charge of the ligand in AuPH_3^+) - (Total charge of the free ligand).	0.7578710709
602	Energy of the first Lone Pair of Ti from NBO analysis of L-TiCl_3^+ , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.757394553

Table S50: First 15 conventional descriptors with best correlation with the second hidden descriptor $\mathbf{HD}_{L2}$ of the ligands for the Actual Training Set B3LYP-D3 in water.

Molec. Desc.	Definition	r^2
664	π /total contribution according to Second order perturbation theory analysis of the Fock matrix in NBO basis of $L-TiCl_3^+$.	0.8841913644
663	Ligand π donor contributions in the Second order perturbation theory analysis of the Fock matrix in NBO basis of $L-TiCl_3^+$.	0.8727735589
576	Distance between the central atom and PtF_5^- in $L-PtF_5^-$ / Distance between the central atom and $TiCl_3^+$ in $L-TiCl_3^+$.	0.8623964849
366	(Mulliken charge on the central atom of the free ligand) $^2/(L-K^+$ distance) 3 .	0.8328745045
367	(APT charge on the central atom of the free ligand) $^2/(L-K^+$ distance) 3 .	0.814770195
368	(NPA charge on the central atom of the free ligand) $^2/(L-K^+$ distance) 3 .	0.8130236028
479	(Mulliken charge on the central atom of the free ligand) 2 /(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).	0.8067019695
512	Bader $g(x)$, kinetic energy density, for the $L-TiCl_3^+$.	0.8005399225
608	L/Ti ionic Natural Bond Order from NBO analysis of $L-TiCl_3^+$, considering a single bond for $L = O^{2-}$ and S^{2-} .	0.7973403855
582	Distance between the central atom and $TiCl_3^+$ in $L-TiCl_3^+$ / Distance between the central atom and PtF_5^- in $L-PtF_5^-$.	0.7928264234
371	(APT charge on the central atom of the free ligand with hydrogens added into it) $^2/(L-K^+$ distance) 3 .	0.7890535093
370	(Mulliken charge on the central atom of the free ligand with hydrogens added into it) $^2/(L-K^+$ distance) 3 .	0.7890262429
440	(Mulliken charge on the central atom of the free ligand) 2 /(Cavity surface of the ligand in water with PCM according to Gaussian defaults).	0.7865233388
481	(NPA charge on the central atom of the free ligand) 2 /(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).	0.7754737336
369	(Total charge of the free ligand) $^2/(L-K^+$ distance) 3 .	0.766250223

Table S51: First 15 conventional descriptors with best correlation with the third hidden descriptor $\mathbf{HD}_{L3}$ of the ligands for the Actual Training Set B3LYP-D3 in water.

Molec. Desc.	Definition	r^2
573	Distance between the central atom and $\text{Fe}(\text{CO})_4$ in $\text{L}-\text{Fe}(\text{CO})_4$.	0.8917171269
574	Distance between the central atom and PtF_5^- in $\text{L}-\text{PtF}_5^-$.	0.838852011
160	Slater covalent atomic radius.	0.6679791182
161	Box Volume computed according to Gaussian's keyword Volume.	0.3640715571
345	Distance between the central atom and OsO_3^{2+} in $\text{L}-\text{OsO}_3^{2+}$ distance.	0.350877319
642	Solid angle of the ligand.	0.3429003849
236	Covalent radii from analysis of the Cambridge Structural Database.	0.3130800211
322	Distance between the central atom and TiCl_3^+ in $\text{L}-\text{TiCl}_3^+$ distance.	0.3121480418
390	$(\text{Mulliken charge on the central atom of the free ligand})^2 / (\text{Slater covalent atomic radius of the central atom of the ligand})^3$.	0.2929653717
638	$\text{Fe}-\text{CO}$ distance in the different $\text{L}-\text{Fe}(\text{CO})_4$ complexes for the CO <i>trans</i> to the ligand L.	0.2901336565
558	L/L Natural Bond Order from NBO analysis of $\text{L}-\text{PtF}_5^-$, considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .	0.2891739786
184	Total charge of the free ligand/ Box volume	0.2868540333
211	Mulliken charge on central atom / $(\text{Box volume})^2$.	0.2864878768
392	$(\text{NPA charge on the central atom of the free ligand})^2 / (\text{Slater covalent atomic radius of the central atom of the ligand})^3$.	0.2856265185
214	Total charge of the free ligand/ $(\text{Box volume})^2$.	0.2828927377

Table S52: First 15 conventional descriptors with best correlation with the fourth hidden descriptor $\mathbf{HD}_{L4}$ of the ligands for the Actual Training Set B3LYP-D3 in water.

Molec. Desc.	Definition	r^2
610	% covalent Natural Bond Order from NBO analysis of $L-TiCl_3^+$, considering a single bond for $L = O^{2-}$ and S^{2-} .	0.8441484237
611	L/Ti ionic - L/Ti covalent Natural Bond Order from NBO analysis of $L-TiCl_3^+$, considering a single bond for $L = O^{2-}$ and S^{2-} .	0.8047597833
563	% covalent Natural Bond Order from NBO analysis of $L-PtF_5^-$, considering a single bond for $L = O^{2-}$ and S^{2-} .	0.7874378484
614	L/Pt ionic - L/Pt covalent Natural Bond Order from NBO analysis of $L-PtF_5^-$, considering a single bond for $L = O^{2-}$ and S^{2-} .	0.7863843731
565	% Pt of the L-Pt bond from NBO analysis of $L-PtF_5^-$, considering a double bond for $L = O^{2-}$ and S^{2-} .	0.768948322
600	% covalent Natural Bond Order from NBO analysis of $L-TaMe_4^+$, considering a single bond for $L = O^{2-}$ and S^{2-} .	0.7545659751
592	% covalent Natural Bond Order from NBO analysis of $L-TaMe_4^+$, considering a double bond for $L = O^{2-}$ and S^{2-} .	0.75246917
645	Distortion energy, energy to bring the ligand and the metal complex at the geometry of the complex, in $L-Fe(CO)_4$. It is computed as BDE - Interaction energy. The interaction energy is $E_{M-L} - E_{M*} - E_{L*}$. M^* and L^* denote the fragments at the geometry of the complex. All energies computed at SDD/lanl2dz level.	0.7393948126
566	Coefficient of Pt of the L-Pt bond from NBO analysis of $L-PtF_5^-$, considering a double bond for $L = O^{2-}$ and S^{2-} .	0.7232224792
547	% Pt of the L-Pt bond from NBO analysis of $L-PtF_5^-$, considering a single bond for $L = O^{2-}$ and S^{2-} .	0.7181425558
646	Distortion energy, energy to bring the ligand and the metal complex at the geometry of the complex, in $L-Fe(CO)_4$. It is computed as BDE - Interaction energy, but here the zero-point energy correction is not performed. The interaction energy is $E_{M-L} - E_{M*} - E_{L*}$. M^* and L^* denote the fragments at the geometry of the complex. All energies computed at SDD/lanl2dz level.	0.7160330885
87	(APT total charge of the ligand in $L-OsO_3^{2+}$) - (Total charge of the free ligand).	0.6937832882
643	Distortion energy, energy to bring the ligand and the metal complex at the geometry of the complex, in $L-Fe(CO)_4$. It is computed as BDE - Interaction energy. The interaction energy is $E_{M-L} - E_{M*} - E_{L*}$. M^* and L^* denote the fragments at the geometry of the complex. BDE corresponds to the energy obtained with SDD/lanl2dz basis set while Interaction energy corresponds to single points at TZVP basis set.	0.6897384443
612	L/Ta ionic - L/Ta covalent Natural Bond Order from NBO analysis of $L-TaMe_4^+$, considering a single bond for $L = O^{2-}$ and S^{2-} .	0.6822514015
656	Interaction energy -BDE $_{\pi-backdonation}$ (TZVP basis sets), in $L-Fe(CO)_4$.	0.6717775445

Table S53: First 15 conventional descriptors with best correlation with the fifth hidden descriptor $\mathbf{HD}_{L5}$ of the ligands for the Actual Training Set B3LYP-D3 in water.

Molec. Desc.	Definition	r^2
577	Distance between the central atom and K^+ in $L-K^+$ / Distance between the central atom and $TiCl_3^+$ in $L-TiCl_3^+$.	0.5207152735
102	APT charge on the central atom of the ligand in PtF_5^- .	0.5116840833
316	(APT charge on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex) / $L-K^+$ distance.	0.498674647
12	Distance between the central atom and K^+ in $L-K^+$.	0.4964108068
580	Distance between the central atom and $TiCl_3^+$ in $L-TiCl_3^+$ / Distance between the central atom and K^+ in $L-K^+$.	0.4942331198
652	Back-donation of the higher π orbitals according to CDA analysis (TZVP basis set), in $L-Fe(CO)_4$.	0.4755929073
659	Back-donation of the higher σ orbital according to CDA analysis (SDD basis set), in $L-Fe(CO)_4$.	0.4738279658
317	(APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex) / $L-K^+$ distance.	0.4676426987
103	APT charge on the central atom with hydrogens added into it in PtF_5^- .	0.4492658681
308	APT charge on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex.	0.4442007138
584	Distance between the central atom and PtF_5^- in $L-PtF_5^-$ / Distance between the central atom and $Fe(CO)_4$ in $L-Fe(CO)_4$.	0.4234315167
314	(Mulliken charge on the central atom of the ligand in $L-K^+$ - Mulliken charge on the central atom of the complex) / $L-K^+$ distance.	0.4231102322
583	Distance between the central atom and $Fe(CO)_4$ in $L-Fe(CO)_4$ / Distance between the central atom and PtF_5^- in $L-PtF_5^-$.	0.4181557068
309	APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ - APT charge on the central atom of the complex.	0.4016131124
167	APT charge on central atom / Crystal ionic radius of the central atom of the ligand.	0.3783426575

Table S54: First 15 conventional descriptors with best correlation with the sixth hidden descriptor $\mathbf{HD}_{L6}$ of the ligands for the Actual Training Set B3LYP-D3 in water.

Molec. Desc.	Definition	r^2
528	Infrared frequency of the CO trans to L in $L-\text{Fe}(\text{CO})_4$.	0.6913756372
105	APT total charge of the ligand in PtF_5^- .	0.2463497914
104	Mulliken total charge of the ligand in PtF_5^- .	0.2393330676
621	Occupancy of the HOMO alpha orbital of the corresponding anion of the ligand according to an NBO analysis.	0.20749989
95	(APT charge on the central atom of the ligand in $L-\text{TaMe}_4^+$) - (APT charge central atom of the ligand).	0.2071549748
81	APT total charge of the ligand in $L-\text{OsO}_3^{2+}$.	0.206453023
128	Average Mulliken total charge of the ligand in $L-\text{K}^+$, $L-\text{AlCl}_3$, $L-\text{TiCl}_3^+$, $L-\text{Fe}(\text{CO})_4$, $L-\text{OsO}_3^{2+}$, $L-\text{TaMe}_4^+$, PtF_5^- and AuPH_3^+ .	0.2056655841
11	% of s character of the Lone Pair of the central atom of the free ligand, NBO.	0.1994166929
158	Crystal ionic radius of the central atom of the ligand.	0.1954484001
129	Average APT total charge of the ligand in $L-\text{K}^+$, $L-\text{AlCl}_3$, $L-\text{TiCl}_3^+$, $L-\text{Fe}(\text{CO})_4$, $L-\text{OsO}_3^{2+}$, $L-\text{TaMe}_4^+$, PtF_5^- and AuPH_3^+ .	0.1939187812
159	Effective Ionic radius of the central atom of the ligand.	0.192078827
68	Average of Mulliken total charge of the ligand in $L-\text{K}^+$, $L-\text{AlCl}_3$, $L-\text{TiCl}_3^+$ and $L-\text{Fe}(\text{CO})_4$.	0.1896753173
56	Mulliken total charge of the ligand in $L-\text{Fe}(\text{CO})_4$.	0.1794519679
116	Mulliken total charge of the ligand in AuPH_3^+ .	0.1788466282
92	Mulliken total charge of the ligand in $L-\text{TaMe}_4^+$.	0.1765849206

8.4 Correlation between the hidden descriptors and the BDEs, in water

We have considered if some of the BDEs for metal fragments can be a good descriptor of some of the hidden descriptor $\mathbf{HD}_{Lk}$. We have look for the correlation between them. The BDEs of the metal complexes in water are used as conventional descriptors for the ligands and viceversa. Results are presented in Tables S55 and S56.

Table S55: Correlation (r^2) between the BDEs of the metal fragments and $\mathbf{HD}_{L1} = \mathbf{L}_1$ to $\mathbf{HD}_{L7}$ of the ligands for the Actual Training Set B3LYP-D3 in water.

	$\mathbf{HD}_{L1} = \mathbf{L}_1$	$\mathbf{HD}_{L2} = \mathbf{L}_2$	$\mathbf{HD}_{L3} = \mathbf{L}_3$	$\mathbf{HD}_{L4} = \mathbf{L}_4$	$\mathbf{HD}_{L5} = \mathbf{L}_5$	$\mathbf{HD}_{L6} = \mathbf{L}_6$	$\mathbf{L}_7$
AuPH ₃ ⁺	0.94	0.05	0.08	0.59	0.00	0.01	0.05
Co(NH ₃) ₅ ³⁺	0.98	0.15	0.07	0.47	0.04	0.01	0.03
CrO ₃	0.99	0.25	0.08	0.38	0.01	0.02	0.02
Cu(NH ₃) ₃ ²⁺	0.98	0.15	0.07	0.48	0.04	0.01	0.03
FeCl ₂ ⁺	0.97	0.37	0.03	0.35	0.00	0.00	0.02
Fe(CO) ₄	0.71	0.01	0.16	0.63	0.00	0.01	0.02
IrCO(PH ₃) ₂ ⁺	0.94	0.07	0.13	0.49	0.00	0.01	0.06
MnO ₃ ⁺	0.99	0.22	0.03	0.48	0.00	0.02	0.02
Mo(SH) ₃ ⁺	0.92	0.44	0.07	0.26	0.00	0.00	0.02
Nb(NH ₂) ₄ ⁺	0.88	0.44	0.15	0.20	0.00	0.01	0.01
OsO ₃ ²⁺	0.97	0.27	0.01	0.47	0.00	0.01	0.03
PdH(PH ₃) ₂ ⁺	0.87	0.01	0.13	0.61	0.01	0.01	0.04
PdPH ₃	0.69	0.00	0.22	0.48	0.04	0.00	0.08
PtF ₅ ⁻	0.88	0.02	0.10	0.60	0.01	0.03	0.04
Rh(H ₂ O) ₅ ³⁺	0.98	0.12	0.04	0.56	0.01	0.01	0.03
Ru(SH) ₄	0.89	0.04	0.19	0.50	0.00	0.02	0.03
TaMe ₄ ⁺	0.88	0.52	0.06	0.20	0.01	0.00	0.02
TiCl ₃ ⁺	0.91	0.49	0.04	0.23	0.00	0.01	0.02
W(CO) ₅	0.78	0.00	0.20	0.54	0.00	0.01	0.04
ZrCl ₅ ⁻	0.84	0.50	0.14	0.15	0.00	0.01	0.01
AuCl ₃	0.93	0.04	0.06	0.65	0.01	0.02	0.03
HgI ₂	0.83	0.02	0.10	0.75	0.00	0.00	0.00
InCl ₂ ⁺	0.99	0.24	0.03	0.44	0.03	0.01	0.03

Table S56: Correlation (r^2) between the BDEs of the ligands and the $\mathbf{HD}_{M1} = \mathbf{M}_1$ to $\mathbf{HD}_{M7}$ for metal fragments for the Actual Training Set B3LYP-D3 in water.

	$\mathbf{HD}_{M1} = \mathbf{M}_1$	$\mathbf{HD}_{M2} = \mathbf{M}_2$	$\mathbf{HD}_{M3} = \mathbf{M}_3$	$\mathbf{HD}_{M4} = \mathbf{M}_4$	$\mathbf{HD}_{M5} = \mathbf{M}_5$	$\mathbf{HD}_{M6} = \mathbf{M}_6$	$\mathbf{M}_7$
Br^-	0.96	0.00	0.90	0.02	0.00	0.01	0.00
CH_3^-	0.98	0.00	0.81	0.00	0.00	0.04	0.01
Cl^-	0.97	0.01	0.86	0.03	0.00	0.01	0.00
CN^-	0.84	0.05	0.75	0.04	0.00	0.04	0.00
CO	0.01	0.72	0.00	0.17	0.07	0.01	0.00
F^-	0.86	0.17	0.60	0.07	0.01	0.03	0.01
C_6H_5^-	0.98	0.00	0.82	0.00	0.00	0.04	0.00
H_2	0.11	0.75	0.02	0.05	0.00	0.08	0.05
H_2O	0.73	0.01	0.65	0.18	0.03	0.01	0.04
H^-	0.93	0.01	0.80	0.00	0.00	0.04	0.00
NCH	0.47	0.23	0.47	0.21	0.00	0.01	0.01
NH_3	0.84	0.02	0.70	0.08	0.00	0.08	0.01
NHC	0.87	0.04	0.75	0.02	0.00	0.07	0.00
O^{2-}	0.78	0.34	0.49	0.01	0.01	0.03	0.00
OH^-	0.92	0.14	0.66	0.03	0.00	0.03	0.00
PH_3	0.66	0.18	0.66	0.03	0.02	0.05	0.00
$\text{C}_5\text{H}_5\text{N}$	0.87	0.02	0.75	0.05	0.00	0.06	0.00
S^{2-}	0.94	0.12	0.77	0.00	0.00	0.01	0.00
SH^-	0.98	0.00	0.88	0.01	0.00	0.02	0.00
$\text{C}_6\text{H}_4\text{OMe}^-$	0.98	0.00	0.83	0.00	0.00	0.04	0.00
PCl_3	0.21	0.51	0.28	0.02	0.15	0.02	0.00
SiMe_3^-	0.91	0.02	0.82	0.01	0.00	0.04	0.01

8.5 List of conventional descriptors

Unless otherwise stated the conventional descriptors presented are computed at the same level of theory and programs as detailed in the computational details.

1. Mulliken charge on the central atom of the free ligand.
2. APT charge on the central atom of the free ligand.
3. Energy of the HOMO orbital of the free ligand.
4. Energy of the HOMO-1 orbital of the free ligand.
5. Energy of the LUMO orbital of the free ligand.
6. Energy of the LUMO+1 orbital of the free ligand.
7. NPA charge on the central atom of the free ligand, NBO.
8. Lowest Lone Pair energy of the free ligand, NBO.
9. Highest Lone Pair energy of the free ligand, NBO.
10. First Rydberg orbital energy of the free ligand, NBO.
11. % of s character of the Lone Pair of the central atom of the free ligand, NBO.
12. Distance between the central atom and K^+ in $L-K^+$.
13. Total charge of the free ligand.
14. Mulliken charge on the central atom with hydrogens added into it of the free ligand.
15. APT charge on the central atom with hydrogens added into it of the free ligand.
16. Mulliken charge on the central atom of the ligand in $L-K^+$.
17. Mulliken charge on the central atom with hydrogens added into it in $L-K^+$.
18. APT charge on the central atom of the ligand in $L-K^+$.
19. APT charge on the central atom with hydrogens added into it in $L-K^+$.
20. Mulliken total charge of the ligand in $L-K^+$.
21. APT total charge of the ligand in $L-K^+$.

22. (Mulliken charge on the central atom of the ligand in $L-K^+$) - (Mulliken charge on the central atom of the free ligand).
23. (APT charge on the central atom of the ligand in $L-K^+$) - (APT charge central atom of the free ligand).
24. (Mulliken charge on the central atom with hydrogens added into it in $L-K^+$) - (Mulliken charge on the central atom with hydrogens added into it of the free ligand).
25. (APT charge on the central atom with hydrogens added into it in $L-K^+$) - (APT charge on the central atom with hydrogens added into it of the free ligand).
26. (Mulliken total charge of the ligand in $L-K^+$) - (Total charge of the free ligand).
27. (APT total charge of the ligand in $L-K^+$) - (Total charge of the free ligand).
28. Mulliken charge on the central atom of the ligand in $L-AlCl_3$.
29. Mulliken charge on the central atom with hydrogens added into it in $L-AlCl_3$.
30. APT charge on the central atom of the ligand in $L-AlCl_3$.
31. APT charge on the central atom with hydrogens added into it in $L-AlCl_3$.
32. Mulliken total charge of the ligand in $L-AlCl_3$.
33. APT total charge of the ligand in $L-AlCl_3$.
34. (Mulliken charge on the central atom of the ligand in $L-AlCl_3$) - (Mulliken charge on the central atom of the free ligand).
35. (APT charge on the central atom of the ligand in $L-AlCl_3$) - (APT charge on the central atom of the free ligand).
36. (Mulliken charge on the central atom with hydrogens added into it in $L-AlCl_3$) - (Mulliken charge on the central atom with hydrogens added into it of the free ligand).
37. (APT charge on the central atom with hydrogens added into it in $L-AlCl_3$) - (APT charge on the central atom with hydrogens added into it of the free ligand).
38. (Mulliken total charge of the ligand in $L-AlCl_3$) - (Total charge of the free ligand).
39. (APT total charge of the ligand in $L-AlCl_3$) - (Total charge of the free ligand).
40. Mulliken charge on the central atom of the ligand in $L-TiCl_3^+$.
41. Mulliken charge on the central atom with hydrogens added into it in $L-TiCl_3^+$.

42. APT charge on the central atom of the ligand in $L-TiCl_3^+$.
43. APT charge on the central atom with hydrogens added into it in $L-TiCl_3^+$.
44. Mulliken total charge of the ligand in $L-TiCl_3^+$.
45. APT total charge of the ligand in $L-TiCl_3^+$.
46. (Mulliken charge on the central atom of the ligand in $L-TiCl_3^+$) - (Mulliken charge on the central atom of the free ligand).
47. (APT charge on the central atom of the ligand in $L-TiCl_3^+$) - (APT charge on the central atom of the free ligand).
48. (Mulliken charge on the central atom with hydrogens added into it in $L-TiCl_3^+$) - (Mulliken charge on the central atom with hydrogens added into it of the free ligand).
49. (APT charge on the central atom with hydrogens added into it in $L-TiCl_3^+$) - (APT charge on the central atom with hydrogens added into it of the free ligand).
50. (Mulliken total charge of the ligand in $L-TiCl_3^+$) - (Total charge of the free ligand).
51. (APT total charge of the ligand in $L-TiCl_3^+$) - (Total charge of the free ligand).
52. Mulliken charge on the central atom of the ligand in $L-Fe(CO)_4$.
53. Mulliken charge on the central atom of the ligand with hydrogens added into it in $L-Fe(CO)_4$.
54. APT charge on the central atom of the ligand in $L-Fe(CO)_4$.
55. APT charge on the central atom with hydrogens added into it in $L-Fe(CO)_4$.
56. Mulliken total charge of the ligand in $L-Fe(CO)_4$.
57. APT total charge of the ligand in $L-Fe(CO)_4$.
58. (Mulliken charge on the central atom of the ligand in $L-Fe(CO)_4$) - (Mulliken charge central atom of the ligand).
59. (APT charge on the central atom of the ligand in $L-Fe(CO)_4$) - (APT charge central atom of the ligand).
60. (Mulliken charge on the central atom with hydrogens added into it in $L-Fe(CO)_4$) - (Mulliken charge central atom with hydrogens added into it).
61. (APT charge on the central atom with hydrogens added into it in $L-Fe(CO)_4$) - (APT charge central atom with hydrogens added into it).

62. (Mulliken total charge of the ligand in $L\text{--Fe(CO)}_4$) - (Total charge of the free ligand).
63. (APT total charge of the ligand in $L\text{--Fe(CO)}_4$) - (Total charge of the free ligand).
64. Average of Mulliken charge on the central atom of the ligand in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
65. Average of Mulliken charge on the central atom with hydrogens added into it in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
66. Average of APT charge on the central atom of the ligand in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
67. Average of APT charge on the central atom with hydrogens added into it in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
68. Average of Mulliken total charge of the ligand in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
69. Average of APT total charge of the ligand in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
70. Average of (Mulliken charge on the central atom of the ligand) - (Mulliken charge central atom of the ligand) in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
71. Average of (APT charge on the central atom of the ligand in complex) - (APT charge central atom of the ligand) in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
72. Average of (Mulliken charge on the central atom with hydrogens added into it in complex) - (Mulliken charge central atom with hydrogens added into it) in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
73. Average of (APT charge on the central atom with hydrogens added into it in complex) - (APT charge central atom with hydrogens added into it) in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
74. Average of (Mulliken total charge of the ligand in complex) - (Total charge of the free ligand) in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
75. Average of (APT total charge of the ligand in complex) - (Total charge of the free ligand) in $L\text{--K}^+$, $L\text{--AlCl}_3$, $L\text{--TiCl}_3^+$ and $L\text{--Fe(CO)}_4$.
76. Mulliken charge on the central atom of the ligand in $L\text{--OsO}_3^{2+}$.
77. Mulliken charge on the central atom with hydrogens added into it in $L\text{--OsO}_3^{2+}$.
78. APT charge on the central atom of the ligand in $L\text{--OsO}_3^{2+}$.
79. APT charge on the central atom with hydrogens added into it in $L\text{--OsO}_3^{2+}$.

80. Mulliken total charge of the ligand in $L-OsO_3^{2+}$.
81. APT total charge of the ligand in $L-OsO_3^{2+}$.
82. (Mulliken charge on the central atom of the ligand in $L-OsO_3^{2+}$) - (Mulliken charge central atom of the ligand).
83. (APT charge on the central atom of the ligand in $L-OsO_3^{2+}$) - (APT charge central atom of the ligand).
84. (Mulliken charge on the central atom with hydrogens added into it in $L-OsO_3^{2+}$) - (Mulliken charge central atom with hydrogens added into it).
85. (APT charge on the central atom with hydrogens added into it in $L-OsO_3^{2+}$) - (APT charge central atom with hydrogens added into it).
86. (Mulliken total charge of the ligand in $L-OsO_3^{2+}$) - (Total charge of the free ligand).
87. (APT total charge of the ligand in $L-OsO_3^{2+}$) - (Total charge of the free ligand).
88. Mulliken charge on the central atom of the ligand in $L-TaMe_4^+$.
89. Mulliken charge on the central atom with hydrogens added into it in $L-TaMe_4^+$.
90. APT charge on the central atom of the ligand in $L-TaMe_4^+$.
91. APT charge on the central atom with hydrogens added into it in $L-TaMe_4^+$.
92. Mulliken total charge of the ligand in $L-TaMe_4^+$.
93. APT total charge of the ligand in $L-TaMe_4^+$.
94. (Mulliken charge on the central atom of the ligand in $L-TaMe_4^+$) - (Mulliken charge central atom of the ligand).
95. (APT charge on the central atom of the ligand in $L-TaMe_4^+$) - (APT charge central atom of the ligand).
96. (Mulliken charge on the central atom with hydrogens added into it in $L-TaMe_4^+$) - (Mulliken charge central atom with hydrogens added into it).
97. (APT charge on the central atom with hydrogens added into it in $L-TaMe_4^+$) - (APT charge central atom with hydrogens added into it).
98. (Mulliken total charge of the ligand in $L-TaMe_4^+$) - (Total charge of the free ligand).
99. (APT total charge of the ligand in $L-TaMe_4^+$) - (Total charge of the free ligand).
100. Mulliken charge on the central atom of the ligand in PtF_5^- .

101. Mulliken charge on the central atom with hydrogens added into it in PtF_5^- .
102. APT charge on the central atom of the ligand in PtF_5^- .
103. APT charge on the central atom with hydrogens added into it in PtF_5^- .
104. Mulliken total charge of the ligand in PtF_5^- .
105. APT total charge of the ligand in PtF_5^- .
106. (Mulliken charge on the central atom of the ligand in PtF_5^-) - (Mulliken charge central atom of the ligand).
107. (APT charge on the central atom of the ligand in PtF_5^-) - (APT charge central atom of the ligand).
108. (Mulliken charge on the central atom with hydrogens added into it in PtF_5^-) - (Mulliken charge central atom with hydrogens added into it).
109. (APT charge on the central atom with hydrogens added into it in PtF_5^-) - (APT charge central atom with hydrogens added into it).
110. (Mulliken total charge of the ligand in PtF_5^-) - (Total charge of the free ligand).
111. (APT total charge of the ligand in PtF_5^-) - (Total charge of the free ligand).
112. Mulliken charge on the central atom of the ligand in AuPH_3^+ .
113. Mulliken charge on the central atom with hydrogens added into it in AuPH_3^+ .
114. APT charge on the central atom of the ligand in AuPH_3^+ .
115. APT charge on the central atom with hydrogens added into it in AuPH_3^+ .
116. Mulliken total charge of the ligand in AuPH_3^+ .
117. APT total charge of the ligand in AuPH_3^+ .
118. (Mulliken charge on the central atom of the ligand in AuPH_3^+) - (Mulliken charge central atom of the ligand).
119. (APT charge on the central atom of the ligand in AuPH_3^+) - (APT charge central atom of the ligand).
120. (Mulliken charge on the central atom with hydrogens added into it in AuPH_3^+) - (Mulliken charge central atom with hydrogens added into it).
121. (APT charge on the central atom with hydrogens added into it in AuPH_3^+) - (APT charge central atom with hydrogens added into it).
122. (Mulliken total charge of the ligand in AuPH_3^+) - (Total charge of the free ligand).

123. (APT total charge of the ligand in AuPH_3^+) - (Total charge of the free ligand).
124. Average Mulliken charge on the central atom of the ligand in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
125. Average Mulliken charge on the central atom with hydrogens added into it in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
126. Average APT charge on the central atom of the ligand in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
127. Average APT charge on the central atom with hydrogens added into it in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
128. Average Mulliken total charge of the ligand in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
129. Average APT total charge of the ligand in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
130. Average of (Mulliken charge on the central atom of the ligand in complex) - (Mulliken charge central atom of the ligand) in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
131. Average of (APT charge on the central atom of the ligand in complex) - (APT charge central atom of the ligand) in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
132. Average of (Mulliken charge on the central atom with hydrogens added into it in complex) - (Mulliken charge central atom with hydrogens added into it) in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
133. Average of (APT charge on the central atom with hydrogens added into it in complex) - (APT charge central atom with hydrogens added into it) in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
134. Average of (Mulliken total charge of the ligand in complex) - (Total charge of the free ligand) in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
135. Average of (APT total charge of the ligand in complex) - (Total charge of the free ligand) in L-K^+ , L-AlCl_3 , L-TiCl_3^+ , L-Fe(CO)_4 , L-OsO_3^{2+} , L-TaMe_4^+ , PtF_5^- and AuPH_3^+ .
136. Ionization potential, IP, computed as Energy of the cation- Energy of the ligand.
137. Electron affinity, EA, computed as Energy of the ligand - Energy of the anion.

138. Chemical potential, μ , computed as $-(IP+EA)/2 = (\text{Energy of the anion}-\text{Energy of the cation})/2$. The Chemical potential $\mu = -\chi$; where χ = electronegativity.
139. Hardness, η , computed as $(IP-EA)/2 = (\text{Energy of the anion}+\text{Energy of the cation}-2\times\text{Energy of the ligand})/2$.
140. Softness, S , computed as $1/(IP-EA) = 1/(\text{Energy of the anion}+\text{Energy of the cation}-2\times\text{Energy of the ligand})$.
141. Electrophilicity index, ω , computed as $\mu^2/(2\eta) = (\text{Energy of the anion}-\text{Energy of the cation})^2/4(\text{Energy of the anion}+\text{Energy of the cation}-2\times\text{Energy of the ligand})$.
142. Chemical potential, μ , computed according to Koopmans' theorem as $-(IP+EA)/2 = -((- \varepsilon_{HOMO}) + (- \varepsilon_{LUMO}))/2$.
143. Hardness, η , computed according to Koopmans' theorem as $(IP-EA)/2 = (- \varepsilon_{HOMO} + \varepsilon_{LUMO})/2$.
144. Softness, S , computed according to Koopmans' theorem as $1/(IP-EA) = 1/(- \varepsilon_{HOMO} + \varepsilon_{LUMO})$.
145. Electrophilicity index, ω , computed according to Koopmans' theorem as $\mu^2/(2\eta) = ((\varepsilon_{HOMO} + \varepsilon_{LUMO})/2)^2/(- \varepsilon_{HOMO} + \varepsilon_{LUMO})$.
146. HOMO α of the cation.
147. LUMO α of the cation.
148. LUMO β of the cation.
149. HOMO α of the anion.
150. LUMO α of the anion.
151. LUMO β of the anion.
152. Mulliken charge of Osmium in $L-OsO_3^{2+}$.
153. APT charge of Osmium in $L-OsO_3^{2+}$.
154. Mulliken charge of Iron in $L-FeCl_2^+$.
155. Electronegativity of the central atom by Pauling Scale.
156. Electronegativity of the central atom by Mulliken-Jaffe.
157. Number of lone pairs of the central atom of the ligand.
158. Crystal ionic radius of the central atom of the ligand.
159. Effective Ionic radius of the central atom of the ligand.
160. Slater covalent atomic radius.

161. Box Volume computed according to Gaussian's keyword Volume.
162. Molar Volume computed according to Gaussian's keyword Volume.
163. Mulliken charge on central atom / Crystal ionic radius of the central atom of the ligand.
164. Mulliken charge with hydrogens added on the central atom / Crystal ionic radius of the central atom of the ligand.
165. NPA charge on central atom / Crystal ionic radius of the central atom of the ligand.
166. Total charge of the free ligand/ Crystal ionic radius of the central atom of the ligand.
167. APT charge on central atom / Crystal ionic radius of the central atom of the ligand.
168. APT charge with hydrogens added on the central atom / Crystal ionic radius of the central atom of the ligand.
169. Mulliken charge on central atom / Effective ionic radius of the central atom of the ligand.
170. Mulliken charge with hydrogens added on the central atom / Effective ionic radius of the central atom of the ligand.
171. NPA charge on central atom / Effective ionic radius of the central atom of the ligand.
172. Total charge of the free ligand/ Effective ionic radius of the central atom of the ligand.
173. APT charge on central atom / Effective ionic radius of the central atom of the ligand.
174. APT charge with hydrogens added on the central atom / Effective ionic atomic radius of the central atom of the ligand.
175. Mulliken charge on central atom / Slater covalent atomic radius of the central atom of the ligand.
176. Mulliken charge with hydrogens added on the central atom / Slater covalent atomic radius of the central atom of the ligand.
177. NPA charge on central atom / Slater covalent atomic radius of the central atom of the ligand.
178. Total charge of the free ligand/ Slater covalent atomic radius of the central atom of the ligand.
179. APT charge on central atom / Slater covalent atomic radius of the central atom of the ligand.
180. APT charge with hydrogens added on the central atom / Slater covalent atomic radius of the central atom of the ligand.
181. Mulliken charge on central atom / Box volume

182. Mulliken charge with hydrogens added on the central atom / Box Volume
183. NPA charge on central atom / Box volume
184. Total charge of the free ligand/ Box volume
185. APT charge on central atom / Box volume
186. APT charge with hydrogens added on the central atom / Box volume.
187. Mulliken charge on central atom / Molar volume.
188. Mulliken charge with hydrogens added on the central atom / Molar Volume.
189. NPA charge on central atom / Molar volume.
190. Total charge of the free ligand / Molar volume.
191. APT charge on central atom / Molar volume.
192. APT charge with hydrogens added on the central atom / Molar volume.
193. Mulliken charge on central atom / (Crystal ionic radius of the central atom of the ligand)².
194. Mulliken charge with hydrogens added on the central atom / (Crystal ionic radius of the central atom of the ligand)².
195. NPA charge on central atom / (Crystal ionic radius of the central atom of the ligand)².
196. Total charge of the free ligand/ (Crystal ionic radius of the central atom of the ligand)².
197. APT charge on central atom / (Crystal ionic radius of the central atom of the ligand)².
198. APT charge with hydrogens added on the central atom / (Crystal ionic radius of the central atom of the ligand)².
199. Mulliken charge on central atom / (Effective ionic radius of the central atom of the ligand)².
200. Mulliken charge with hydrogens added on the central atom / (Effective ionic radius of the central atom of the ligand)².
201. NPA charge on central atom / (Effective ionic radius of the central atom of the ligand)².
202. Total charge of the free ligand/ (Effective ionic radius of the central atom of the ligand)².
203. APT charge on central atom / (Effective ionic radius of the central atom of the ligand)².

204. APT charge with hydrogens added on the central atom / (Effective ionic atomic radius of the central atom of the ligand)².
205. Mulliken charge on central atom / (Slater covalent atomic radius of the central atom of the ligand)².
206. Mulliken charge with hydrogens added on the central atom / (Slater covalent atomic radius of the central atom of the ligand)².
207. NPA charge on central atom / (Slater covalent atomic radius of the central atom of the ligand)².
208. Total charge of the free ligand/ (Slater covalent atomic radius of the central atom of the ligand)².
209. APT charge on central atom / (Slater covalent atomic radius of the central atom of the ligand)².
210. APT charge with hydrogens added on the central atom / (Slater covalent atomic radius of the central atom of the ligand)².
211. Mulliken charge on central atom / (Box volume)².
212. Mulliken charge with hydrogens added on the central atom / (Box Volume)².
213. NPA charge on central atom / (Box volume)².
214. Total charge of the free ligand/ (Box volume)².
215. APT charge on central atom / (Box volume)².
216. APT charge with hydrogens added on the central atom / (Box Volume)².
217. Mulliken charge on central atom / (Molar volume)².
218. Mulliken charge with hydrogens added on the central atom / (Molar Volume)².
219. NPA charge on central atom / (Molar volume)².
220. Total charge of the free ligand / (Molar volume)².
221. APT charge on central atom / (Molar volume)².
222. Cavity volume of the ligand in water computed with PCM according to Gaussian defaults.
223. Mulliken charge on central atom / Cavity volume of the ligand in water computed with PCM according to Gaussian defaults.
224. Mulliken charge with hydrogens added on the central atom / Cavity volume of the ligand in water computed with PCM according to Gaussian defaults.

225. NPA charge on central atom / Cavity volume of the ligand in water computed with PCM according to Gaussian defaults.
226. Total charge of the free ligand/ Cavity volume of the ligand in water computed with PCM according to Gaussian defaults.
227. APT charge on central atom / Cavity volume of the ligand in water computed with PCM according to Gaussian defaults.
228. APT charge with hydrogens added on the central atom / Cavity volume of the ligand in water computed with PCM according to Gaussian defaults.
229. Surface area of the ligand in water computed with PCM according to Gaussian defaults.
230. Mulliken charge on central atom / Surface area of the ligand in water computed with PCM according to Gaussian defaults.
231. Mulliken charge with hydrogens added on the central atom / Surface area of the ligand in water computed with PCM according to Gaussian defaults.
232. NPA charge on central atom / Surface area of the ligand in water computed with PCM according to Gaussian defaults.
233. Total charge of the free ligand/ Surface area of the ligand in water computed with PCM according to Gaussian defaults.
234. APT charge on central atom / Surface area of the ligand in water computed with PCM according to Gaussian defaults.
235. APT charge with hydrogens added on the central atom / Surface area of the ligand in water computed with PCM according to Gaussian defaults.
236. Covalent radii from analysis of the Cambridge Structural Database.
237. Mulliken charge on central atom / Covalent radii from analysis of the Cambridge Structural Database.
238. Mulliken charge with hydrogens added on the central atom / Covalent radii from analysis of the Cambridge Structural Database.
239. NPA charge on central atom / Covalent radii from analysis of the Cambridge Structural Database.
240. Total charge of the free ligand/ Covalent radii from analysis of the Cambridge Structural Database.
241. APT charge on central atom / Covalent radii from analysis of the Cambridge Structural Database.

242. APT charge with hydrogens added on the central atom / Covalent radii from analysis of the Cambridge Structural Database.
243. Mulliken charge on central atom / (Covalent radii from analysis of the Cambridge Structural Database)².
244. Mulliken charge with hydrogens added on the central atom / (Covalent radii from analysis of the Cambridge Structural Database)².
245. NPA charge on central atom / (Covalent radii from analysis of the Cambridge Structural Database)².
246. Total charge of the free ligand / (Covalent radii from analysis of the Cambridge Structural Database)².
247. APT charge on central atom / (Covalent radii from analysis of the Cambridge Structural Database)².
248. APT charge with hydrogens added on the central atom / (Covalent radii from analysis of the Cambridge Structural Database)².
249. Mulliken charge on central atom / (Covalent radii from analysis of the Cambridge Structural Database)³.
250. Mulliken charge with hydrogens added on the central atom / (Covalent radii from analysis of the Cambridge Structural Database)³.
251. NPA charge on central atom / (Covalent radii from analysis of the Cambridge Structural Database)³.
252. Total charge of the free ligand / (Covalent radii from analysis of the Cambridge Structural Database)³.
253. APT charge on central atom / (Covalent radii from analysis of the Cambridge Structural Database)³.
254. APT charge with hydrogens added on the central atom / (Covalent radii from analysis of the Cambridge Structural Database)³.
255. Cavity volume of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
256. Surface area of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
257. Cavity volume of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
258. Surface area of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
259. Cavity volume of the ligand in water computed with SMD according to Gaussian defaults.
260. Surface area of the ligand in water computed with SMD according to Gaussian defaults.
261. Mulliken charge on central atom / Cavity volume of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).

262. Mulliken charge with hydrogens added on the central atom / Cavity volume of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
263. NPA charge on central atom / Cavity volume of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
264. Total charge of the free ligand / Cavity volume of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
265. APT charge on central atom / Cavity volume of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
266. APT charge with hydrogens added on the central atom / Cavity volume of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
267. Mulliken charge on central atom / Surface area of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
268. Mulliken charge with hydrogens added on the central atom / Surface area of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
269. NPA charge on central atom / Surface area of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
270. Total charge of the free ligand / Surface area of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
271. APT charge on central atom / Surface area of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
272. APT charge with hydrogens added on the central atom / Surface area of the ligand in water computed with PCM and the radii UA0 (United Atom Topological Model).
273. Mulliken charge on central atom / Cavity volume of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
274. Mulliken charge with hydrogens added on the central atom / Cavity volume of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
275. NPA charge on central atom / Cavity volume of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).

276. Total charge of the free ligand / Cavity volume of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
277. APT charge on central atom / Cavity volume of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
278. APT charge with hydrogens added on the central atom / Cavity volume of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
279. Mulliken charge on central atom / Surface area of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
280. Mulliken charge with hydrogens added on the central atom / Surface area of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
281. NPA charge on central atom / Surface area of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
282. Total charge of the free ligand / Surface area of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
283. APT charge on central atom / Surface area of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
284. APT charge with hydrogens added on the central atom / Surface area of the ligand in water computed with PCM and the radii Pauling (Merz-Kollman).
285. Mulliken charge on central atom / Cavity volume of the ligand in water computed with SMD according to Gaussian defaults.
286. Mulliken charge with hydrogens added on the central atom / Cavity volume of the ligand in water computed with SMD according to Gaussian defaults.
287. NPA charge on central atom / Cavity volume of the ligand in water computed with SMD according to Gaussian defaults.
288. Total charge of the free ligand / Cavity volume of the ligand in water computed with SMD according to Gaussian defaults.
289. APT charge on central atom / Cavity volume of the ligand in water computed with SMD according to Gaussian defaults.

290. APT charge with hydrogens added on the central atom / Cavity volume of the ligand in water computed with SMD according to Gaussian defaults.
291. Mulliken charge on central atom / Surface area of the ligand in water computed with SMD according to Gaussian defaults.
292. Mulliken charge with hydrogens added on the central atom / Surface area of the ligand in water computed with SMD according to Gaussian defaults.
293. NPA charge on central atom / Surface area of the ligand in water computed with SMD according to Gaussian defaults.
294. Total charge of the free ligand / Surface area of the ligand in water computed with SMD according to Gaussian defaults.
295. APT charge on central atom / Surface area of the ligand in water computed with SMD according to Gaussian defaults.
296. APT charge with hydrogens added on the central atom / Surface area of the ligand in water computed with SMD according to Gaussian defaults.
297. Total mass.
298. Mulliken charge on central atom / Total mass.
299. Mulliken charge with hydrogens added on the central atom / Total mass.
300. NPA charge on central atom / Total mass.
301. Total charge of the free ligand / Total mass.
302. APT charge on central atom / Total mass.
303. APT charge with hydrogens added on the central atom / Total mass.
304. Nucleophilicity computed as $1/\text{electrophilicity} = (2\eta)/\mu^2 = 4(\text{Energy of the anion} + \text{Energy of the cation} - 2 \times \text{Energy of the ligand}) / (\text{Energy of the anion} - \text{Energy of the cation})^2$.
305. Nucleophilicity computed as $1/\text{electrophilicity} = (2\eta)/\mu^2 = (-\varepsilon_{HOMO} + \varepsilon_{LUMO}) / ((\varepsilon_{HOMO} + \varepsilon_{LUMO})/2)^2$.
306. Mulliken charge on the central atom of the ligand in $L-K^+$ – Mulliken charge on the central atom of the complex.
307. Mulliken charge with hydrogens added on the central atom of the ligand in $L-K^+$ – Mulliken charge on the central atom of the complex.

308. APT charge on the central atom of the ligand in $L-K^+$ – APT charge on the central atom of the complex.
309. APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ – APT charge on the central atom of the complex.
310. (Mulliken charge on the central atom of the ligand in $L-K^+$ – Mulliken charge on the central atom of the complex) x $L-K^+$ distance.
311. (Mulliken charge with hydrogens added on the central atom of the ligand in $L-K^+$ – Mulliken charge on the central atom of the complex) x $L-K^+$ distance.
312. (APT charge on the central atom of the ligand in $L-K^+$ – APT charge on the central atom of the complex) x $L-K^+$ distance.
313. (APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ – APT charge on the central atom of the complex) x $L-K^+$ distance.
314. (Mulliken charge on the central atom of the ligand in $L-K^+$ – Mulliken charge on the central atom of the complex) / $L-K^+$ distance.
315. (Mulliken charge with hydrogens added on the central atom of the ligand in $L-K^+$ – Mulliken charge on the central atom of the complex) / $L-K^+$ distance.
316. (APT charge on the central atom of the ligand in $L-K^+$ – APT charge on the central atom of the complex) / $L-K^+$ distance.
317. (APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ – APT charge on the central atom of the complex) / $L-K^+$ distance.
318. (Mulliken charge on the central atom of the ligand in $L-K^+$ + Mulliken charge on the central atom of the complex) x $L-K^+$ distance.
319. (Mulliken charge with hydrogens added on the central atom of the ligand in $L-K^+$ + Mulliken charge on the central atom of the complex) x $L-K^+$ distance.
320. (APT charge on the central atom of the ligand in $L-K^+$ + APT charge on the central atom of the complex) x $L-K^+$ distance.
321. (APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ + APT charge on the central atom of the complex) x $L-K^+$ distance.
322. $L-TiCl_3^+$ distance.
323. Mulliken charge on Ti in $L-TiCl_3^+$.

324. APT charge on Ti in $L-TiCl_3^+$.
325. Mulliken charge on the central atom of the ligand in $L-TiCl_3^+$ – Mulliken charge on the central atom of the complex.
326. Mulliken charge with hydrogens added on the central atom of the ligand in $L-TiCl_3^+$ – Mulliken charge on the central atom of the complex.
327. APT charge on the central atom of the ligand in $L-TiCl_3^+$ – APT charge on the central atom of the complex.
328. APT charge with hydrogens added on the central atom of the ligand in $L-K^+$ – APT charge on the central atom of the complex.
329. (Mulliken charge on the central atom of the ligand in $L-TiCl_3^+$ – Mulliken charge on the central atom complex) x $L-TiCl_3^+$ distance.
330. (Mulliken charge with hydrogens added on the central atom of the ligand in $L-TiCl_3^+$ – Mulliken charge on the central atom of the complex) x $L-TiCl_3^+$ distance.
331. (APT charge on the central atom of the ligand in $L-TiCl_3^+$ – APT charge on the central atom complex) x $L-TiCl_3^+$ distance.
332. (APT charge with hydrogens added on the central atom of the ligand in $L-TiCl_3^+$ – APT charge on the central atom of the complex) x $L-TiCl_3^+$ distance.
333. (Mulliken charge on the central atom of the ligand in $L-TiCl_3^+$ – Mulliken charge on the central atom complex) / $L-TiCl_3^+$ distance.
334. (Mulliken charge with hydrogens added on the central atom of the ligand in $L-TiCl_3^+$ – Mulliken charge on the central atom of the complex) / $L-TiCl_3^+$ distance.
335. (APT charge on the central atom of the ligand in $L-TiCl_3^+$ – APT charge on the central atom complex) / $L-TiCl_3^+$ distance.
336. (APT charge with hydrogens added on the central atom of the ligand in $L-TiCl_3^+$ – APT charge on the central atom of the complex) / $L-TiCl_3^+$ distance.
337. Mulliken charge on the central atom of the ligand in $L-TiCl_3^+$ + Mulliken charge on the central atom of the complex.
338. Mulliken charge with hydrogens added on the central atom of the ligand in $L-TiCl_3^+$ + Mulliken charge on the central atom of the complex.
339. APT charge on the central atom of the ligand in $L-TiCl_3^+$ + APT charge on the central atom of the complex.

340. APT charge with hydrogens added on the central atom of the ligand in L-TiCl_3^+ + APT charge on the central atom of the complex.
341. (Mulliken charge on the central atom of the ligand in L-TiCl_3^+ + Mulliken charge on the central atom of the complex) x L-TiCl_3^+ distance.
342. (Mulliken charge with hydrogens added on the central atom of the ligand in L-TiCl_3^+ + Mulliken charge on the central atom of the complex) x L-TiCl_3^+ distance.
343. (APT charge on the central atom of the ligand in L-TiCl_3^+ + APT charge on the central atom of the complex) x L-TiCl_3^+ distance.
344. (APT charge with hydrogens added on the central atom of the ligand in L-TiCl_3^+ + APT charge on the central atom of the complex) x L-TiCl_3^+ distance.
345. L-OsO_3^{2+} distance.
346. Mulliken charge on the central atom of the ligand in L-OsO_3^{2+} - Mulliken charge on the central atom of the complex.
347. Mulliken charge with hydrogens added on the central atom of the ligand in L-OsO_3^{2+} - Mulliken charge on the central atom of the complex.
348. APT charge on the central atom of the ligand in L-OsO_3^{2+} - APT charge on the central atom of the complex.
349. APT charge with hydrogens added on the central atom of the ligand L-OsO_3^{2+} - APT charge on the central atom of the complex.
350. (Mulliken charge on the central atom of the ligand in L-OsO_3^{2+} - Mulliken charge on the central atom complex) x L-OsO_3^{2+} distance.
351. (Mulliken charge with hydrogens added on the central atom of the ligand in L-OsO_3^{2+} - Mulliken charge on the central atom of the complex) x L-OsO_3^{2+} distance.
352. (APT charge on the central atom of the ligand in L-OsO_3^{2+} - APT charge on the central atom complex) x L-OsO_3^{2+} distance.
353. (APT charge with hydrogens added on the central atom of the ligand in L-OsO_3^{2+} - APT charge on the central atom of the complex) x L-OsO_3^{2+} distance.
354. (Mulliken charge on the central atom of the ligand in L-OsO_3^{2+} - Mulliken charge on the central atom complex) / L-OsO_3^{2+} distance.

355. (Mulliken charge with hydrogens added on the central atom of the ligand in L-OsO_3^{2+} – Mulliken charge on the central atom of the complex) / L-OsO_3^{2+} distance.
356. (APT charge on the central atom of the ligand in L-OsO_3^{2+} – APT charge on the central atom complex) / L-OsO_3^{2+} distance.
357. (APT charge with hydrogens added on the central atom of the ligand in L-OsO_3^{2+} – APT charge on the central atom of the complex) / L-OsO_3^{2+} distance.
358. Mulliken charge on the central atom of the ligand in L-OsO_3^{2+} + Mulliken charge on the central atom of the complex.
359. Mulliken charge with hydrogens added on the central atom of the ligand in L-OsO_3^{2+} + Mulliken charge on the central atom of the complex.
360. APT charge on the central atom of the ligand in L-OsO_3^{2+} + APT charge on the central atom of the complex.
361. APT charge with hydrogens added on the central atom of the ligand in L-OsO_3^{2+} + APT charge on the central atom of the complex.
362. (Mulliken charge on the central atom of the ligand in L-OsO_3^{2+} + Mulliken charge on the central atom of the complex) x L-OsO_3^{2+} distance.
363. (Mulliken charge with hydrogens added on the central atom of the ligand in L-OsO_3^{2+} + Mulliken charge on the central atom of the complex) x L-OsO_3^{2+} distance.
364. (APT charge on the central atom of the ligand in L-OsO_3^{2+} + APT charge on the central atom of the complex) x L-OsO_3^{2+} distance.
365. (APT charge with hydrogens added on the central atom of the ligand in L-OsO_3^{2+} + APT charge on the central atom of the complex) x L-OsO_3^{2+} distance.
366. (Mulliken charge on the central atom of the free ligand)²/(L-K^+ distance)³.
367. (APT charge on the central atom of the free ligand)²/(L-K^+ distance)³.
368. (NPA charge on the central atom of the free ligand)²/(L-K^+ distance)³.
369. (Total charge of the free ligand)²/(L-K^+ distance)³.
370. (Mulliken charge on the central atom of the free ligand with hydrogens added into it)²/(L-K^+ distance)³.
371. (APT charge on the central atom of the free ligand with hydrogens added into it)²/(L-K^+ distance)³.

372. $(\text{Average of Mulliken charge of the central atom in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (L-K^+ \text{ distance})^3$.
373. $(\text{Average of Mulliken charge of the central atom with hydrogens added into it in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (L-K^+ \text{ distance})^3$.
374. $(\text{Average of APT charge of the central atom in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (L-K^+ \text{ distance})^3$.
375. $(\text{Average of APT charge of the central atom with hydrogens added into it in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (L-K^+ \text{ distance})^3$.
376. $(\text{Mulliken charge on the central atom of the free ligand})^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
377. $(\text{APT charge on the central atom of the free ligand})^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
378. $(\text{NPA charge on the central atom of the free ligand})^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
379. $(\text{Total charge of the free ligand})^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
380. $(\text{Mulliken charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
381. $(\text{APT charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
382. $(\text{Average of Mulliken charge of the central atom in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
383. $(\text{Average of Mulliken charge of the central atom with hydrogens added into it in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
384. $(\text{Average of APT charge of the central atom in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
385. $(\text{Average of APT charge of the central atom with hydrogens added into it in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Crystal ionic radius of the central atom of the ligand})^3$.
386. $(\text{APT charge on the central atom of the free ligand})^2 / (\text{Effective ionic radius of the central atom of the ligand})^3$.
387. $(\text{APT charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Effective ionic radius of the central atom of the ligand})^3$.

388. (Average of APT charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Effective ionic radius of the central atom of the ligand)³.
389. (Average of APT charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Effective ionic radius of the central atom of the ligand)³.
390. (Mulliken charge on the central atom of the free ligand)²/(Slater covalent atomic radius of the central atom of the ligand)³.
391. (APT charge on the central atom of the free ligand)²/(Slater covalent atomic radius of the central atom of the ligand)³.
392. (NPA charge on the central atom of the free ligand)²/(Slater covalent atomic radius of the central atom of the ligand)³.
393. (Total charge of the free ligand)²/(Slater covalent atomic radius of the central atom of the ligand)³.
394. (Mulliken charge on the central atom of the free ligand with hydrogens added into it)²/(Slater covalent atomic radius of the central atom of the ligand)³.
395. (APT charge on the central atom of the free ligand with hydrogens added into it)²/(Slater covalent atomic radius of the central atom of the ligand)³.
396. (Average of Mulliken charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Slater covalent atomic radius of the central atom of the ligand)³.
397. (Average of Mulliken charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Slater covalent atomic radius of the central atom of the ligand)³.
398. (Average of APT charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Slater covalent atomic radius of the central atom of the ligand)³.
399. (Average of APT charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Slater covalent atomic radius of the central atom of the ligand)³.
400. (Mulliken charge on the central atom of the free ligand)²/(Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand)³.
401. (APT charge on the central atom of the free ligand)²/(Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand)³.
402. (NPA charge on the central atom of the free ligand)²/(Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand)³.

403. $(\text{Total charge of the free ligand})^2 / (\text{Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand})^3$.
404. $(\text{Mulliken charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand})^3$.
405. $(\text{APT charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand})^3$.
406. $(\text{Average of Mulliken charge of the central atom in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand})^3$.
407. $(\text{Average of Mulliken charge of the central atom with hydrogens added into it in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand})^3$.
408. $(\text{Average of APT charge of the central atom in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand})^3$.
409. $(\text{Average of APT charge of the central atom with hydrogens added into it in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Covalent radii from analysis of the Cambridge Structural Database of the central atom of the ligand})^3$.
410. $(\text{Mulliken charge on the central atom of the free ligand})^2 / (\text{Box Volume})$.
411. $(\text{APT charge on the central atom of the free ligand})^2 / (\text{Box Volume})$.
412. $(\text{NPA charge on the central atom of the free ligand})^2 / (\text{Box Volume})$.
413. $(\text{Total charge of the free ligand})^2 / (\text{Box Volume})$.
414. $(\text{Mulliken charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Box Volume})$.
415. $(\text{APT charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Box Volume})$.
416. $(\text{Average of Mulliken charge of the central atom in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Box Volume})$.
417. $(\text{Average of Mulliken charge of the central atom with hydrogens added into it in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Box Volume})$.
418. $(\text{Average of APT charge of the central atom in } L-K^+, L-AlCl_3, L-TiCl_3^+ \text{ and } L-Fe(CO)_4)^2 / (\text{Box Volume})$.

419. (Average of APT charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Box Volume).
420. (Mulliken charge on the central atom of the free ligand)²/(Molar Volume).
421. (APT charge on the central atom of the free ligand)²/(Molar Volume).
422. (NPA charge on the central atom of the free ligand)²/(Molar Volume).
423. (Total charge of the free ligand)²/(Molar Volume).
424. (Mulliken charge on the central atom of the free ligand with hydrogens added into it)²/(Molar Volume).
425. (APT charge on the central atom of the free ligand with hydrogens added into it)²/(Molar Volume).
426. (Average of Mulliken charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Molar Volume).
427. (Average of Mulliken charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Molar Volume).
428. (Average of APT charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Molar Volume).
429. (Average of APT charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Molar Volume).
430. (Mulliken charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).
431. (APT charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).
432. (NPA charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).
433. (Total charge of the free ligand)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).
434. (Mulliken charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).
435. (APT charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).

436. (Average of Mulliken charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).
437. (Average of Mulliken charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).
438. (Average of APT charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).
439. (Average of APT charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity volume of the ligand in water with PCM according to Gaussian defaults).
440. (Mulliken charge on the central atom of the free ligand)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).
441. (APT charge on the central atom of the free ligand)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).
442. (NPA charge on the central atom of the free ligand)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).
443. (Total charge of the free ligand)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).
444. (Mulliken charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).
445. (APT charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).
446. (Average of Mulliken charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).
447. (Average of Mulliken charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).
448. (Average of APT charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).
449. (Average of APT charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with PCM according to Gaussian defaults).

450. (Mulliken charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
451. (APT charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
452. (NPA charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
453. (Total charge of the free ligand)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
454. (Mulliken charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
455. (APT charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
456. (Average of Mulliken charge of the central atom in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
457. (Average of Mulliken charge of the central atom with hydrogens added into it in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
458. (Average of APT charge of the central atom in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
459. (Average of APT charge of the central atom with hydrogens added into it in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity volume of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
460. (Mulliken charge on the central atom of the free ligand)²/(Cavity surface of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
461. (APT charge on the central atom of the free ligand)²/(Cavity surface of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
462. (NPA charge on the central atom of the free ligand)²/(Cavity surface of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
463. (Total charge of the free ligand)²/(Cavity surface of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).

464. (Mulliken charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity surface of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
465. (APT charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity surface of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
466. (Average of Mulliken charge of the central atom in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity surface of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
467. (Average of Mulliken charge of the central atom with hydrogens added into it in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity surface of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
468. (Average of APT charge of the central atom in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity surface of the ligand in water with PCM and the radii UA0 (United Atom Topological Model)).
469. (Mulliken charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
470. (APT charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
471. (NPA charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
472. (Total charge of the free ligand)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
473. (Mulliken charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
474. (APT charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
475. (Average of Mulliken charge of the central atom in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
476. (Average of Mulliken charge of the central atom with hydrogens added into it in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
477. (Average of APT charge of the central atom in L-K⁺, L-AlCl₃, L-TiCl₃⁺ and L-Fe(CO)₄)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).

478. (Average of APT charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity volume of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
479. (Mulliken charge on the central atom of the free ligand)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
480. (APT charge on the central atom of the free ligand)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
481. (NPA charge on the central atom of the free ligand)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
482. (Total charge of the free ligand)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
483. (Mulliken charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
484. (APT charge on the central atom of the free ligand with hydrogens added into it)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
485. (Average of Mulliken charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
486. (Average of Mulliken charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
487. (Average of APT charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
488. (Average of APT charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with PCM and the radii Pauling (Merz-Kollman)).
489. (Mulliken charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with SMD according to Gaussian defaults).
490. (APT charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with SMD according to Gaussian defaults).
491. (NPA charge on the central atom of the free ligand)²/(Cavity volume of the ligand in water with SMD according to Gaussian defaults).

492. $(\text{Total charge of the free ligand})^2 / (\text{Cavity volume of the ligand in water with SMD according to Gaussian defaults})$.
493. $(\text{Mulliken charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Cavity volume of the ligand in water with SMD according to Gaussian defaults})$.
494. $(\text{APT charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Cavity volume of the ligand in water with SMD according to Gaussian defaults})$.
495. $(\text{Average of Mulliken charge of the central atom in } \text{L-K}^+, \text{L-AlCl}_3, \text{L-TiCl}_3^+ \text{ and } \text{L-Fe(CO)}_4)^2 / (\text{Cavity volume of the ligand in water with SMD according to Gaussian defaults})$.
496. $(\text{Average of Mulliken charge of the central atom with hydrogens added into it in } \text{L-K}^+, \text{L-AlCl}_3, \text{L-TiCl}_3^+ \text{ and } \text{L-Fe(CO)}_4)^2 / (\text{Cavity volume of the ligand in water with SMD according to Gaussian defaults})$.
497. $(\text{Average of APT charge of the central atom in } \text{L-K}^+, \text{L-AlCl}_3, \text{L-TiCl}_3^+ \text{ and } \text{L-Fe(CO)}_4)^2 / (\text{Cavity volume of the ligand in water with SMD according to Gaussian defaults})$.
498. $(\text{Average of APT charge of the central atom with hydrogens added into it in } \text{L-K}^+, \text{L-AlCl}_3, \text{L-TiCl}_3^+ \text{ and } \text{L-Fe(CO)}_4)^2 / (\text{Cavity volume of the ligand in water with SMD according to Gaussian defaults})$.
499. $(\text{Mulliken charge on the central atom of the free ligand})^2 / (\text{Cavity surface of the ligand in water with SMD according to Gaussian defaults})$.
500. $(\text{APT charge on the central atom of the free ligand})^2 / (\text{Cavity surface of the ligand in water with SMD according to Gaussian defaults})$.
501. $(\text{NPA charge on the central atom of the free ligand})^2 / (\text{Cavity surface of the ligand in water with SMD according to Gaussian defaults})$.
502. $(\text{Total charge of the free ligand})^2 / (\text{Cavity surface of the ligand in water with SMD according to Gaussian defaults})$.
503. $(\text{Mulliken charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Cavity surface of the ligand in water with SMD according to Gaussian defaults})$.
504. $(\text{APT charge on the central atom of the free ligand with hydrogens added into it})^2 / (\text{Cavity surface of the ligand in water with SMD according to Gaussian defaults})$.
505. $(\text{Average of Mulliken charge of the central atom in } \text{L-K}^+, \text{L-AlCl}_3, \text{L-TiCl}_3^+ \text{ and } \text{L-Fe(CO)}_4)^2 / (\text{Cavity surface of the ligand in water with SMD according to Gaussian defaults})$.

506. (Average of Mulliken charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with SMD according to Gaussian defaults).
507. (Average of APT charge of the central atom in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with SMD according to Gaussian defaults).
508. (Average of APT charge of the central atom with hydrogens added into it in $L-K^+$, $L-AlCl_3$, $L-TiCl_3^+$ and $L-Fe(CO)_4$)²/(Cavity surface of the ligand in water with SMD according to Gaussian defaults).
509. Bader rho for the $L-TiCl_3^+$.
510. Bader gradient the $L-TiCl_3^+$.
511. Bader del2 for the $L-TiCl_3^+$.
512. Bader g(x), kinetic energy density, for the $L-TiCl_3^+$.
513. Bader k(x) for the $L-TiCl_3^+$.
514. Bader ellipticity for the $L-TiCl_3^+$.
515. Bader first eigenvalue for the $L-TiCl_3^+$.
516. Bader second eigenvalue for the $L-TiCl_3^+$.
517. Bader third eigenvalue for the $L-TiCl_3^+$.
518. Bader rho for the $L-K^+$.
519. Bader gradient the $L-K^+$.
520. Bader del2 for the $L-K^+$.
521. Bader g(x), kinetic energy density, for the $L-K^+$.
522. Bader k(x) for the $L-K^+$.
523. Bader ellipticity for the $L-K^+$.
524. Bader first eigenvalue for the $L-K^+$.
525. Bader second eigenvalue for the $L-K^+$.
526. Bader third eigenvalue for the $L-K^+$.
527. Frequency of the CO trans to L in $L-Fe(CO)_4$.
528. Infrared frequency of the CO trans to L in $L-Fe(CO)_4$.

529. q donation of Charge Decomposition Analysis of L–Fe(CO)₄.
530. q backdonation of Charge Decomposition Analysis of L–Fe(CO)₄.
531. Repulsive polarization of Charge Decomposition Analysis of L–Fe(CO)₄.
532. Residual of Charge Decomposition Analysis of L–Fe(CO)₄.
533. Chemical potential from Charge Decomposition Analysis of L–Fe(CO)₄.
534. Hardness from Charge Decomposition Analysis of L–Fe(CO)₄.
535. Bonding energy from Charge Decomposition Analysis of L–Fe(CO)₄.
536. q donation of Charge Decomposition Analysis of L–Fe(CO)₄, with TZVP basis set.
537. q backdonation of Charge Decomposition Analysis of L–Fe(CO)₄, with TZVP basis set.
538. Repulsive polarization of Charge Decomposition Analysis of L–Fe(CO)₄, with TZVP basis set.
539. Residual of Charge Decomposition Analysis of L–Fe(CO)₄, with TZVP basis set.
540. Chemical potential from Charge Decomposition Analysis of L–Fe(CO)₄, with TZVP basis set.
541. Hardness from Charge Decomposition Analysis of L–Fe(CO)₄, with TZVP basis set.
542. Bonding energy from Charge Decomposition Analysis of L–Fe(CO)₄, with TZVP basis set.
543. NPA charge on central atom of ligand from NBO analysis of L–PtF₅[–].
544. NPA charge on Pt from NBO analysis of L–PtF₅[–].
545. Total non-lewis from NBO analysis of L–PtF₅[–].
546. Occupancy of the L–Pt bond from NBO analysis of L–PtF₅[–], considering a single bond for L = O^{2–} and S^{2–}.
547. % Pt of the L–Pt bond from NBO analysis of L–PtF₅[–], considering a single bond for L = O^{2–} and S^{2–}.
548. Coefficient of Pt of the L–Pt bond from NBO analysis of L–PtF₅[–], considering a single bond for L = O^{2–} and S^{2–}.
549. % s of Pt on the L–Pt bond from NBO analysis of L–PtF₅[–], considering a single bond for L = O^{2–} and S^{2–}.
550. % p of Pt on the L–Pt bond from NBO analysis of L–PtF₅[–], considering a single bond for L = O^{2–} and S^{2–}.

551. % d of Pt on the L–Pt bond from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
552. Coefficient of the d orbital of the L–Pt bond from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
553. $E(2)$ on the L–Pt bond from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
554. Energy of the L–Pt bond from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
555. Energy of the first Lone Pair of Pt from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
556. Energy of the second Lone Pair of Pt from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
557. Energy of the third Lone Pair of Pt from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
558. L/L Natural Bond Order from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
559. L/Pt total Natural Bond Order from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
560. L/Pt covalent Natural Bond Order from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
561. L/Pt ionic Natural Bond Order from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
562. Pt/Pt Natural Bond Order from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
563. % covalent Natural Bond Order from NBO analysis of L–PtF_5^- , considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
564. Occupancy of the L–Pt bond from NBO analysis of L–PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
565. % Pt of the L–Pt bond from NBO analysis of L–PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
566. Coefficient of Pt of the L–Pt bond from NBO analysis of L–PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .

567. % s of Pt on the L–Pt bond from NBO analysis of L–PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
568. % p of Pt on the L–Pt bond from NBO analysis of L–PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
569. % d of Pt on the L–Pt bond from NBO analysis of L–PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
570. Coefficient of the d orbital of the L–Pt bond from NBO analysis of L–PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
571. E(2) on the L–Pt bond from NBO analysis of L–PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
572. Energy of the L–Pt bond from NBO analysis of L–PtF_5^- , considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
573. Distance between the central atom and $\text{Fe}(\text{CO})_4$ in $\text{L–Fe}(\text{CO})_4$.
574. Distance between the central atom and PtF_5^- in L–PtF_5^- .
575. Distance between the central atom and $\text{Fe}(\text{CO})_4$ in $\text{L–Fe}(\text{CO})_4$ / Distance between the central atom and TiCl_3^+ in L–TiCl_3^+ .
576. Distance between the central atom and PtF_5^- in L–PtF_5^- / Distance between the central atom and TiCl_3^+ in L–TiCl_3^+ .
577. Distance between the central atom and K^+ in L–K^+ / Distance between the central atom and TiCl_3^+ in L–TiCl_3^+ .
578. Distance between the central atom and $\text{Fe}(\text{CO})_4$ in $\text{L–Fe}(\text{CO})_4$ / Distance between the central atom and K^+ in L–K^+ .
579. Distance between the central atom and PtF_5^- in L–PtF_5^- / Distance between the central atom and K^+ in L–K^+ .
580. Distance between the central atom and TiCl_3^+ in L–TiCl_3^+ / Distance between the central atom and K^+ in L–K^+ .
581. Distance between the central atom and TiCl_3^+ in L–TiCl_3^+ / Distance between the central atom and $\text{Fe}(\text{CO})_4$ in $\text{L–Fe}(\text{CO})_4$.
582. Distance between the central atom and TiCl_3^+ in L–TiCl_3^+ / Distance between the central atom and PtF_5^- in L–PtF_5^- .

583. Distance between the central atom and $\text{Fe}(\text{CO})_4$ in $\text{L}-\text{Fe}(\text{CO})_4$ / Distance between the central atom and PtF_5^- in $\text{L}-\text{PtF}_5^-$.
584. Distance between the central atom and PtF_5^- in $\text{L}-\text{PtF}_5^-$ / Distance between the central atom and $\text{Fe}(\text{CO})_4$ in $\text{L}-\text{Fe}(\text{CO})_4$.
585. Occupancy of the Lone Pair of Ta from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
586. Energy of the Lone Pair of Ta from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
587. L/L Natural Bond Order from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
588. L/Ta total Natural Bond Order from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
589. L/Ta covalent Natural Bond Order from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
590. L/Ta ionic Natural Bond Order from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
591. Ta/Ta Natural Bond Order from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
592. % covalent Natural Bond Order from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a double bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
593. Occupancy of the Lone Pair of Ta from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
594. Energy of the Lone Pair of Ta from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
595. L/L Natural Bond Order from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
596. L/Ta total Natural Bond Order from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .
597. L/Ta covalent Natural Bond Order from NBO analysis of $\text{L}-\text{TaMe}_4^+$, considering a single bond for $\text{L} = \text{O}^{2-}$ and S^{2-} .

598. L/Ta ionic Natural Bond Order from NBO analysis of $L\text{--TaMe}_4^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
599. Ta/Ta Natural Bond Order from NBO analysis of $L\text{--TaMe}_4^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
600. % covalent Natural Bond Order from NBO analysis of $L\text{--TaMe}_4^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
601. Occupancy of the first Lone Pair of Ti from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
602. Energy of the first Lone Pair of Ti from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
603. Occupancy of the second Lone Pair of Ti from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
604. Energy of the second Lone Pair of Ti from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
605. L/L Natural Bond Order from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
606. L/Ti total Natural Bond Order from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
607. L/Ti covalent Natural Bond Order from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
608. L/Ti ionic Natural Bond Order from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
609. Ti/Ti Natural Bond Order from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
610. % covalent Natural Bond Order from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
611. L/Ti ionic – L/Ti covalent Natural Bond Order from NBO analysis of $L\text{--TiCl}_3^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .
612. L/Ta ionic – L/Ta covalent Natural Bond Order from NBO analysis of $L\text{--TaMe}_4^+$, considering a single bond for $L = \text{O}^{2-}$ and S^{2-} .

613. L/Ta ionic – L/Ta covalent Natural Bond Order from NBO analysis of $L-TaMe_4^+$, considering a double bond for $L = O^{2-}$ and S^{2-} .
614. L/Pt ionic – L/Pt covalent Natural Bond Order from NBO analysis of $L-PtF_5^-$, considering a single bond for $L = O^{2-}$ and S^{2-} .
615. Occupancy of the HOMO alpha orbital of the corresponding cation of the ligand according to an NBO analysis.
616. Energy of the HOMO alpha orbital of the corresponding cation of the ligand according to an NBO analysis.
617. Occupancy of the LUMO alpha orbital of the corresponding cation of the ligand according to an NBO analysis.
618. Energy of the LUMO alpha orbital of the corresponding cation of the ligand according to an NBO analysis.
619. Occupancy of the LUMO beta orbital of the corresponding cation of the ligand according to an NBO analysis.
620. Energy of the LUMO beta orbital of the corresponding cation of the ligand according to an NBO analysis.
621. Occupancy of the HOMO alpha orbital of the corresponding anion of the ligand according to an NBO analysis.
622. Energy of the HOMO alpha orbital of the corresponding anion of the ligand according to an NBO analysis.
623. Occupancy of the LUMO beta orbital of the corresponding anion of the ligand according to an NBO analysis.
624. Energy of the LUMO beta orbital of the corresponding anion of the ligand according to an NBO analysis.
625. Occupancy of the HOMO orbital of the ligand according to an NBO analysis.
626. Energy of the HOMO orbital of the ligand according to an NBO analysis.
627. Occupancy of the LUMO orbital of the ligand according to an NBO analysis.
628. Energy of the LUMO orbital of the ligand according to an NBO analysis.
629. Chemical potential, μ , computed according to Koopmans' theorem as $-(IP+EA)/2 = -((- \varepsilon_{HOMO}) + (- \varepsilon_{LUMO}))/2$ with energies from NBO analysis.
630. Hardness, η , computed according to Koopmans' theorem as $(IP-EA)/2 = (- \varepsilon_{HOMO} + \varepsilon_{LUMO})/2$ with energies from NBO analysis.
631. Softness, S , computed according to Koopmans' theorem as $1/(IP-EA) = 1/(- \varepsilon_{HOMO} + \varepsilon_{LUMO})$ with energies from NBO analysis.
632. Electrophilicity index, ω , computed according to Koopmans' theorem as $\mu^2/(2\eta) = ((\varepsilon_{HOMO} + \varepsilon_{LUMO})/2)^2/(- \varepsilon_{HOMO} + \varepsilon_{LUMO})$ with energies from NBO analysis.

633. Nucleophilicity computed as $1/\text{electrophilicity} = (2\eta)/\mu^2 = (-\varepsilon_{HOMO} + \varepsilon_{LUMO}) / ((\varepsilon_{HOMO} + \varepsilon_{LUMO})/2)^2$ with energies from NBO analysis.
634. Mulliken charge on K in $L-K^+$.
635. APT charge on K in $L-K^+$.
636. Valence Lewis electrons from NBO analysis of $L-TiCl_3^+$, considering a single bond for $L = O^{2-}$ and S^{2-} . Lewis structure selected with CHOOSE.
637. Total Lewis electrons from NBO analysis of $L-TiCl_3^+$, considering a single bond for $L = O^{2-}$ and S^{2-} . Lewis structure selected with CHOOSE.
638. Fe–CO distance in in the different $L-Fe(CO)_4$ complexes for the CO *trans* to the ligand L.
639. Electronegativity according to Mulliken scale considering the central atom and taking into account hybridization.
640. Electronegativity according to Allen scale.
641. Cone angle of the ligand.
642. Solid angle of the ligand.
643. Distortion energy, energy to bring the ligand and the metal complex at the geometry of the complex, in $L-Fe(CO)_4$. It is computed as BDE - Interaction energy. The interaction energy is $E_{M-L} - E_{M^*} - E_{L^*}$. M^* and L^* denote the fragments at the geometry of the complex. BDE corresponds to the energy obtained with SDD/lanl2dz basis set while Interaction energy corresponds to single points at TZVP basis set.
644. Distortion energy, energy to bring the ligand and the metal complex at the geometry of the complex, in $L-Fe(CO)_4$. It is computed as BDE - Interaction energy, but here the zero-point energy correction is not performed. The interaction energy is $E_{M-L} - E_{M^*} - E_{L^*}$. M^* and L^* denote the fragments at the geometry of the complex. BDE corresponds to the energy obtained with SDD/lanl2dz basis set while Interaction energy corresponds to single points at TZVP basis set.
645. Distortion energy, energy to bring the ligand and the metal complex at the geometry of the complex, in $L-Fe(CO)_4$. It is computed as BDE - Interaction energy. The interaction energy is $E_{M-L} - E_{M^*} - E_{L^*}$. M^* and L^* denote the fragments at the geometry of the complex. All energies computed at SDD/lanl2dz level.
646. Distortion energy, energy to bring the ligand and the metal complex at the geometry of the complex, in $L-Fe(CO)_4$. It is computed as BDE - Interaction energy, but here the zero-point energy correction is not performed. The interaction energy is $E_{M-L} - E_{M^*} - E_{L^*}$. M^* and L^* denote the fragments at the geometry of the complex. All energies computed at SDD/lanl2dz level.

647. Distortion energy corresponding only to the ligand, in L-Fe(CO)_4 .
648. Distortion energy corresponding only to the metal fragment, in L-Fe(CO)_4 .
649. Donation of the higher σ orbital according to CDA analysis (TZVP basis set), in L-Fe(CO)_4 .
650. Back-donation of the higher σ orbital according to CDA analysis (TZVP basis set), in L-Fe(CO)_4 .
651. Donation of the higher π orbitals according to CDA analysis (TZVP basis set), in L-Fe(CO)_4 .
652. Back-donation of the higher π orbitals according to CDA analysis (TZVP basis set), in L-Fe(CO)_4 .
653. Repulsive polarization of the higher π orbitals according to CDA analysis (TZVP basis set), in L-Fe(CO)_4 .
654. Residual of the higher π orbitals according to CDA analysis (TZVP basis set), in L-Fe(CO)_4 .
655. $\text{BDE}_{\pi\text{-backdonation}}$, BDE corresponding to the π orbitals according to CDA analysis (TZVP basis set), in L-Fe(CO)_4 .
656. Interaction energy $-\text{BDE}_{\pi\text{-backdonation}}$ (TZVP basis sets), in L-Fe(CO)_4 .
657. $\text{BDE} - \text{BDE}_{\pi\text{-backdonation}}$ (SDD/TZVP basis sets), in L-Fe(CO)_4 .
658. Donation of the higher σ orbital according to CDA analysis (SDD basis set), in L-Fe(CO)_4 .
659. Back-donation of the higher σ orbital according to CDA analysis (SDD basis set), in L-Fe(CO)_4 .
660. Donation of the higher π orbitals according to CDA analysis (SDD basis set), in L-Fe(CO)_4 .
661. Back-donation of the higher π orbitals according to CDA analysis (SDD basis set), in L-Fe(CO)_4 .
662. Sum of σ contributions in the Second order perturbation theory analysis of the Fock matrix in NBO basis of L-TiCl_3^+ .
663. Ligand π donor contributions in the Second order perturbation theory analysis of the Fock matrix in NBO basis of L-TiCl_3^+ .
664. π/total contribution according to Second order perturbation theory analysis of the Fock matrix in NBO basis of L-TiCl_3^+ .
665. Sum of σ and π contributions in the Second order perturbation theory analysis of the Fock matrix in NBO basis of L-TiCl_3^+ .
666. Substraction of σ and π contributions in the Second order perturbation theory analysis of the Fock matrix in NBO basis of L-TiCl_3^+ .

9 Scripts

9.1 Script used to perform the SVD analysis on the BDE matrix for all possible number of hidden descriptors.

The script reads in the computational BDEs in a file called "Results.txt" (metal fragments in rows, ligands in columns). It performs the SVD analysis on the BDE matrix to obtain the ligand hidden descriptors, and prints them in a file called "descrip_ligands.txt". It also works out the hidden descriptors of the metal fragments, the diagonal matrix $\mathbf{W}$ for all of Singular Values, and it prints out both matrices in "descrip_metals.txt" and "matrixD.txt". It also computes and gives as output the errors for each number of hidden descriptors in different files: "total_errors_lig.txt", "maximum_errors_lig.txt", "average_errors_lig.txt", "maximum_errors_comp.txt" and "average_errors_comp.txt".

```
clear
data=load("Results.txt");

[coef_comp,relweights,coef_lig]=svd(data);

for num=1:22
for i=1:length(data(1,:));
for j=1:length(data(:,1));
BDE_lig(j,i)=coef_comp(j,1:num)*relweights(1:num,1:num)*coef_lig(i,1:num)';
end
end

errors_lig=data-BDE_lig;

[maxima(num,:),a]=max(abs(errors_lig));
average(num,:)=mean(abs(errors_lig));
maximac(num,:)=max(abs(errors_lig'));
averagec(num,:)=mean(abs(errors_lig'));

[total_errors(num,1),b]=max(maxima(num,:));
total_errors(num,2)=mean(average(num,:));
total_errors(num,3)=mean(relweights(num,num));
total_errors(num,4)=b
total_errors(num,5)=a(b)

end

dlmwrite('maximum_errors_lig.txt',maxima," ")
dlmwrite('total_errors_lig.txt',total_errors," ")
dlmwrite('average_errors_lig.txt',average," ")
dlmwrite('maximum_errors_comp.txt',maximac," ")
```

```
dlmwrite('average_errors_comp.txt',averagec," ")
```

```
dlmwrite('descrip_ligands.txt',coef_lig," ")
```

```
dlmwrite('descrip_metals.txt',coef_comp," ")
```

```
dlmwrite('matrixD.txt',relweights," ")
```

9.2 Script used to choose the ligands and metal fragments for the Actual Training Set.

The script reads in the computational BDEs of the Full Set of data in a file called "ResultsFull.txt" (metal fragments in rows, ligands in columns). It performs the SVD analysis on the BDE matrix of the Full Set to obtain the ligand hidden descriptors, the hidden descriptors of the metal fragments and the diagonal matrix $\mathbf{W}$ for all number of hidden descriptors (k) for this large set. It removes three metal fragments of the Initial Training Set (ligands 1 to 22 and metal fragments 1 to 23). In a file called "resumtrets_comp.txt" it prints out the removed metal fragments and the resulting corresponding correlation (between the hidden descriptors of the Full Set of data and the hidden descriptors of the reduced sets). It adds three ligands in and prints the correlation between the new sets of ligands and the Full Set of data in three files called "resumafegits1_lig.txt", "resumafegits2_lig.txt" and "resumafegits3_lig.txt". The same operation is done for the metal fragments and generates the files "resumafegits1_comp.txt", "resumafegits2_comp.txt" and "resumafegits3_comp.txt". Finally it prints out the nine best sets of hidden descriptors under the imposed restrictions in the file called "escollits_lig.txt" for the set of ligands and "escollits_comp.txt" for the set of metal fragments.

```
clear
data=load("ResultsFull.txt");
N_PC=7;

[coef_comp,relweights,coef_lig]=svd(data);

for i=1:length(data(1,:));
for j=1:length(data(:,1));
BDE_lig(j,i)=coef_comp(j,1:N_PC)*relweights(1:N_PC,1:N_PC)*coef_lig(i,1:N_PC)';
end
end

%We will look for the ligand in the training set (22 first ligands) that are less necessary to get good correlation between the PCs with a
%reduced set of ligands and the PCs with all ligands.
%Then we will remove these ligands
repe=zeros
item=zeros
it=zeros

for i=1:22
for k=i+1:22
for j=k+1:22

ll=zeros
l1l=zeros
tt=zeros
t1t=zeros
```

```

for l=1:22
if ((l ~= i )&&(l ~= k)&&(l ~= j))

l1=l1l+1
l1l=l1

reduit(l1,1:N_PC)=coef_lig(l,1:N_PC)
reduit_num(l1)=1
datared(:,l1)=data(:,l)

else

tt=ttt+1
ttt=tt

trets(tt,1:N_PC)=coef_lig(l,1:N_PC)
trets_num(tt)=1

endif
end

[coef_compred,relweightsred,coef_ligred]=svd(datared);

correlred=zeros
cred=zeros

for o=1:N_PC

des=[ones(19,1),coef_ligred(:,o)]
[b, bint, r, rint, stats] = regress (reduit(:,o), des)

correlred=stats(1)+cred
cred=correlred

end

item=it+1
it=item

resum(item,1)=i
resum(item,2)=k
resum(item,3)=j
resum(item,4)=correlred

end
end
end

dlmwrite('resumtrets_lig.txt',resum," ")

```

```

[rligsum,numligsum]=max(resum(:,4))

resum2=resum
resum2(numligsum,4)=zeros

[rligsum2,numligsum2]=max(resum2(:,4))

resum3=resum2
resum3(numligsum2,4)=zeros

[rligsum3,numligsum3]=max(resum3(:,4))

repe(1)=resum(numligsum,1)
repe(2)=resum(numligsum,2)
repe(3)=resum(numligsum,3)

repe2(1)=resum2(numligsum2,1)
repe2(2)=resum2(numligsum2,2)
repe2(3)=resum2(numligsum2,3)

repe3(1)=resum3(numligsum3,1)
repe3(2)=resum3(numligsum3,2)
repe3(3)=resum3(numligsum3,3)

item=zeros
a=zeros

for i=1:22
if (i ~= repe(1:end))
item=a+1
a=item
escollits(item)=i
escollit_mat(item,1:N_PC)=coef_lig(i,1:N_PC)
escollit_data(:,item)=data(:,i)
endif
end

item=zeros
a=zeros

for i=1:22
if (i ~= repe2(1:end))
item=a+1
a=item
escollits2(item)=i
escollit_mat2(item,1:N_PC)=coef_lig(i,1:N_PC)
escollit_data2(:,item)=data(:,i)
endif
end

item=zeros

```

```

a=zeros

for i=1:22
if (i != repe3(1:end))
item=a+1
a=item
escollits3(item)=i
escollit_mat3(item,1:N_PC)=coef_lig(i,1:N_PC)
escollit_data3(:,item)=data(:,i)
endif
end

%Now let's look at the complexes
repe_com=zeros
item=zeros
it=zeros

for i=1:23
for k=i+1:23
for j=k+1:23

l1=zeros
l11=zeros
tt=zeros
ttt=zeros

for l=1:23
if ((l != i )&&(l != k)&&(l !=j))

l1=l11+1
l11=l1

reduitcom(l1,1:N_PC)=coef_comp(l,1:N_PC)
reduitcom_num(l1)=1
datacomred(l1,:)=data(l,:)

else

tt=ttt+1
ttt=tt

trets(tt,1:N_PC)=coef_comp(l,1:N_PC)
trets_num(tt)=1

endif
end

[coef_compcomred,relweightscomred,coef_ligcomred]=svd(datacomred);

correlcomred=zeros

```

```

ccomred=zeros

for o=1:N_PC

des=[ones(20,1),coef_compcomred(:,o)]
[b, bint, r, rint, stats] = regress (reduitcom(:,o), des)

correlcomred=stats(1)+ccomred
ccomred=correlcomred

end

item=it+1
it=item

resumcom(item,1)=i
resumcom(item,2)=k
resumcom(item,3)=j
resumcom(item,4)=correlcomred

end
end
end

dlmwrite('resumtrets_comp.txt',resumcom," ")

[rcomsum,numcomsum]=max(resumcom(:,4))

resumcom2=resumcom
resumcom2(numcomsum,4)=zeros

[rcomsum2,numcomsum2]=max(resumcom2(:,4))

resumcom3=resumcom2
resumcom3(numcomsum2,4)=zeros

[rcomsum3,numcomsum3]=max(resumcom3(:,4))

repe_com(1)=resumcom(numcomsum,1)
repe_com(2)=resumcom(numcomsum,2)
repe_com(3)=resumcom(numcomsum,3)

repe_com2(1)=resumcom2(numcomsum2,1)
repe_com2(2)=resumcom2(numcomsum2,2)
repe_com2(3)=resumcom2(numcomsum2,3)

repe_com3(1)=resumcom3(numcomsum3,1)
repe_com3(2)=resumcom3(numcomsum3,2)
repe_com3(3)=resumcom3(numcomsum3,3)

item=zeros

```

```

a=zeros

for i=1:23
if (i != repe_com(1:end))
item=a+1
a=item
escollitscom(item)=i
escollitcom_mat(item,1:N_PC)=coef_comp(i,1:N_PC)
escollitcom_data(item,:)=data(i,:)
endif
end

item=zeros
a=zeros

for i=1:23
if (i != repe_com2(1:end))
item=a+1
a=item
escollitscom2(item)=i
escollitcom_mat2(item,1:N_PC)=coef_comp(i,1:N_PC)
escollitcom_data2(item,:)=data(i,:)
endif
end

item=zeros
a=zeros

for i=1:23
if (i != repe_com3(1:end))
item=a+1
a=item
escollitscom3(item)=i
escollitcom_mat3(item,1:N_PC)=coef_comp(i,1:N_PC)
escollitcom_data3(item,:)=data(i,:)
endif
end

%Now we will look in the total set of ligands for the ones with higher correlation with the PCs with all ligands
%expanding it back to 22 ligands and 25 complexes.

ru=zeros
ruru=zeros
item=zeros
it=zeros

for i=1:43
for k=i+1:43
for j=k+1:43

```

```

if ((escollits(1:end) != i )&&(escollits(1:end) != k)&&(escollits(1:end) != j))

datas1=[escollit_data(:,1:end),data(:,i),data(:,k),data(:,j)]
coef_ligalguns=[escollit_mat(:,1:N_PC);coef_lig(i,1:N_PC);coef_lig(k,1:N_PC);coef_lig(j,1:N_PC)]

[coef_comps1,relweightssl,coef_ligs1]=svd(datas1);

correltot=zeros
ctot=zeros

for o=1:N_PC

des=[ones(22,1),coef_ligs1(:,o)]
[b, bint, r, rint, stats] = regress (coef_ligalguns(:,o), des)

correltot=stats(1)+ctot
ctot=correltot
end

item=item+1
it=item

resumaf(item,1)=i
resumaf(item,2)=k
resumaf(item,3)=j
resumaf(item,4)=correltot

endif

end
end
end

dlmwrite('resumafegits1_lig.txt',resumaf," ")

[rligsum,numligsum]=max(resumaf(:,4))

afegit(1)=resumaf(numligsum,1)
afegit(2)=resumaf(numligsum,2)
afegit(3)=resumaf(numligsum,3)

resumaf_2=resumaf
resumaf_2(numligsum,4)=zeros

[rligsum_2,numligsum_2]=max(resumaf_2(:,4))

afegit_2(1)=resumaf_2(numligsum_2,1)
afegit_2(2)=resumaf_2(numligsum_2,2)
afegit_2(3)=resumaf_2(numligsum_2,3)

```

```

resumaf_3=resumaf_2
resumaf_3(numligsum_2,4)=zeros

[rligsum_3,numligsum_3]=max(resumaf_3(:,4))

afegit_3(1)=resumaf_3(numligsum_3,1)
afegit_3(2)=resumaf_3(numligsum_3,2)
afegit_3(3)=resumaf_3(numligsum_3,3)

collits(1,:)=[escollits(1:end),afegit(1:3),rligsum]
collits(2,:)=[escollits(1:end),afegit_2(1:3),rligsum_2]
collits(3,:)=[escollits(1:end),afegit_3(1:3),rligsum_3]


ru=zeros
ruru=zeros
item=zeros
it=zeros

for i=1:43
for k=i+1:43
for j=k+1:43
if ((escollits2(1:end) != i )&&(escollits2(1:end) != k)&&(escollits2(1:end) != j))

datasl2=[escollit_data2(:,1:end),data(:,i),data(:,k),data(:,j)]
coef_ligalgun2=[escollit_mat2(:,1:N_PC);coef_lig(i,1:N_PC);coef_lig(k,1:N_PC);coef_lig(j,1:N_PC)]

[coef_compsl2,relweightssl2,coef_ligsl2]=svd(datasl2);

correltot=zeros
ctot=zeros

for o=1:N_PC

des=[ones(22,1),coef_ligsl2(:,o)]
[b, bint, r, rint, stats] = regress (coef_ligalgun2(:,o), des)

correltot=stats(1)+ctot
ctot=correltot
end

item=it+1
it=item

resumaf2(item,1)=i
resumaf2(item,2)=k
resumaf2(item,3)=j
resumaf2(item,4)=correltot

endif

```

```

end
end
end

dlmwrite('resumafegits2_lig.txt',resumaf2," ")

[rligsum2,numligsum2]=max(resumaf2(:,4))

afegit2(1)=resumaf2(numligsum2,1)
afegit2(2)=resumaf2(numligsum2,2)
afegit2(3)=resumaf2(numligsum2,3)

resumaf2_2=resumaf2
resumaf2_2(numligsum2,4)=zeros

[rligsum2_2,numligsum2_2]=max(resumaf2_2(:,4))

afegit2_2(1)=resumaf2_2(numligsum2_2,1)
afegit2_2(2)=resumaf2_2(numligsum2_2,2)
afegit2_2(3)=resumaf2_2(numligsum2_2,3)

resumaf2_3=resumaf2_2
resumaf2_3(numligsum2_2,4)=zeros

[rligsum2_3,numligsum2_3]=max(resumaf2_3(:,4))

afegit2_3(1)=resumaf2_3(numligsum2_3,1)
afegit2_3(2)=resumaf2_3(numligsum2_3,2)
afegit2_3(3)=resumaf2_3(numligsum2_3,3)

collits(4,:)=[escollits2(1:end),afegit2(1:3),rligsum2]
collits(5,:)=[escollits2(1:end),afegit2_2(1:3),rligsum2_2]
collits(6,:)=[escollits2(1:end),afegit2_3(1:3),rligsum2_3]

ru=zeros
ruru=zeros
item=zeros
it=zeros

for i=1:43
for k=i+1:43
for j=k+1:43
if ((escollits3(1:end) != i )&&(escollits3(1:end) != k)&&(escollits3(1:end) != j))

datasl3=[escollit_data3(:,1:end),data(:,i),data(:,k),data(:,j)]
coef_ligalguns3=[escollit_mat3(:,1:N_PC);coef_lig(i,1:N_PC);coef_lig(k,1:N_PC);coef_lig(j,1:N_PC)]

[coef_compsl3,relweightssl3,coef_ligsl3]=svd(datasl3);

```

```

correltot=zeros
ctot=zeros

for o=1:N_PC

des=[ones(22,1),coef_ligs13(:,o)]
[b, bint, r, rint, stats] = regress (coef_ligalguns3(:,o), des)

correltot=stats(1)+ctot
ctot=correltot
end

item=it+1
it=item

resumaf3(item,1)=i
resumaf3(item,2)=k
resumaf3(item,3)=j
resumaf3(item,4)=correltot

endif

end
end
end

dlmwrite('resumafegits3_lig.txt',resumaf3," ")

[rligsum3,numligsum3]=max(resumaf3(:,4))

afegit3(1)=resumaf3(numligsum3,1)
afegit3(2)=resumaf3(numligsum3,2)
afegit3(3)=resumaf3(numligsum3,3)

resumaf3_2=resumaf3
resumaf3_2(numligsum3,4)=zeros

[rligsum3_2,numligsum3_2]=max(resumaf3_2(:,4))

afegit3_2(1)=resumaf3_2(numligsum3_2,1)
afegit3_2(2)=resumaf3_2(numligsum3_2,2)
afegit3_2(3)=resumaf3_2(numligsum3_2,3)

resumaf3_3=resumaf3_2
resumaf3_3(numligsum3_2,4)=zeros

[rligsum3_3,numligsum3_3]=max(resumaf3_3(:,4))

afegit3_3(1)=resumaf3_3(numligsum3_3,1)
afegit3_3(2)=resumaf3_3(numligsum3_3,2)

```

```

afegit3_3(3)=resumaf3_3(numligsum3_3,3)

collits(7,:)=[escollits3(1:end),afegit3(1:3),rligsum3]
collits(8,:)=[escollits3(1:end),afegit3_2(1:3),rligsum3_2]
collits(9,:)=[escollits3(1:end),afegit3_3(1:3),rligsum3_3]

dlmwrite('escollits_lig.txt',collits," ")

%Now we will look in the total set of ligands for the ones with lower correlation with the previous set of ligands
%expanding it back to 22 ligands and 25 complexes.

ru=zeros
ruru=zeros
item=zeros
it=zeros

for i=1:42
for k=i+1:42
for j=k+1:42
if ((escollitscom(1:end) != i )&&(escollitscom(1:end) != k)&&(escollitscom(1:end) != j))

dataslcom=[escollitcom_data(1:end,:);data(i,:);data(k,:);data(j,:)]
coef_compalguns=[escollitcom_mat(:,1:N_PC);coef_comp(i,1:N_PC);coef_comp(k,1:N_PC);coef_comp(j,1:N_PC)]

[coef_compslcom,relweightsslcom,coef_ligslcom]=svd(dataslcom);

correlcomtot=zeros
ccomtot=zeros

for o=1:N_PC

des=[ones(23,1),coef_compslcom(:,o)]
[b, bint, r, rint, stats] = regress (coef_compalguns(:,o), des)

correlcomtot=stats(1)+ccomtot
ccomtot=correlcomtot

end

item=it+1
it=item

resumafcom(item,1)=i
resumafcom(item,2)=k
resumafcom(item,3)=j
resumafcom(item,4)=correlcomtot

endif

end

```

```

end
end

dlmwrite('resumafegits1_comp.txt',resumafcom," ")

[rcomsum,numcomsum]=max(resumafcom(:,4))

afegitcom(1)=resumafcom(numcomsum,1)
afegitcom(2)=resumafcom(numcomsum,2)
afegitcom(3)=resumafcom(numcomsum,3)

resumafcom_2=resumafcom
resumafcom_2(numcomsum,4)=zeros

[rcomsum_2,numcomsum_2]=max(resumafcom_2(:,4))

afegitcom_2(1)=resumafcom_2(numcomsum_2,1)
afegitcom_2(2)=resumafcom_2(numcomsum_2,2)
afegitcom_2(3)=resumafcom_2(numcomsum_2,3)

resumafcom_3=resumafcom_2
resumafcom_3(numcomsum_2,4)=zeros

[rcomsum_3,numcomsum_3]=max(resumafcom_3(:,4))

afegitcom_3(1)=resumafcom_3(numcomsum_3,1)
afegitcom_3(2)=resumafcom_3(numcomsum_3,2)
afegitcom_3(3)=resumafcom_3(numcomsum_3,3)

collitscom(1,:)=[escollitscom(1:end),afegitcom(1:3),rcomsum]
collitscom(2,:)=[escollitscom(1:end),afegitcom_2(1:3),rcomsum_2]
collitscom(3,:)=[escollitscom(1:end),afegitcom_3(1:3),rcomsum_3]

ru=zeros
ruru=zeros
item=zeros
it=zeros

for i=1:42
for k=i+1:42
for j=k+1:42
if ((escollitscom2(1:end) ~= i )&&(escollitscom2(1:end) ~= k)&&(escollitscom2(1:end) ~= j))

dataslcom2=[escollitcom_data2(1:end,:);data(i,:);data(k,:);data(j,:)]
coef_compalguns2=[escollitcom_mat2(:,1:N_PC);coef_comp(i,1:N_PC);coef_comp(k,1:N_PC);coef_comp(j,1:N_PC)]

[coef_compslcom2,relweightsslcom2,coef_ligslcom2]=svd(dataslcom2);

correlcomtot=zeros
ccomtot=zeros

```

```

for o=1:N_PC

des=[ones(23,1),coef_compslcom2(:,o)]
[b, bint, r, rint, stats] = regress (coef_compalguns2(:,o), des)

correlcomtot=stats(1)+ccomtot
ccomtot=correlcomtot

end

item=it+1
it=item

resumafcom2(item,1)=i
resumafcom2(item,2)=k
resumafcom2(item,3)=j
resumafcom2(item,4)=correlcomtot

endif

end

end

end

dlmwrite('resumafegits2_comp.txt',resumafcom2," ")

[rcomsum2,numcomsum2]=max(resumafcom2(:,4))

afegitcom2(1)=resumafcom2(numcomsum2,1)
afegitcom2(2)=resumafcom2(numcomsum2,2)
afegitcom2(3)=resumafcom2(numcomsum2,3)

resumafcom2_2=resumafcom2
resumafcom2_2(numcomsum,4)=zeros

[rcomsum2_2,numcomsum2_2]=max(resumafcom2_2(:,4))

afegitcom2_2(1)=resumafcom2_2(numcomsum2_2,1)
afegitcom2_2(2)=resumafcom2_2(numcomsum2_2,2)
afegitcom2_2(3)=resumafcom2_2(numcomsum2_2,3)

resumafcom2_3=resumafcom2_2
resumafcom2_3(numcomsum2_2,4)=zeros

[rcomsum2_3,numcomsum2_3]=max(resumafcom2_3(:,4))

afegitcom2_3(1)=resumafcom2_3(numcomsum2_3,1)
afegitcom2_3(2)=resumafcom2_3(numcomsum2_3,2)
afegitcom2_3(3)=resumafcom2_3(numcomsum2_3,3)

collitscom(4,:)=[escollitscom2(1:end),afegitcom2(1:3),rcomsum2]

```

```

collitscom(5,:)=[escollitscom2(1:end),afegitcom2_2(1:3),rcomsum2_2]
collitscom(6,:)=[escollitscom2(1:end),afegitcom2_3(1:3),rcomsum2_3]

ru=zeros
ruru=zeros
item=zeros
it=zeros

for i=1:42
for k=i+1:42
for j=k+1:42
if ((escollitscom3(1:end) != i )&&(escollitscom3(1:end) != k)&&(escollitscom3(1:end) != j))

dataslcom3=[escollitcom_data3(1:end,:);data(i,:);data(k,:);data(j,:)]
coef_compalguns3=[escollitcom_mat3(:,1:N_PC);coef_comp(i,1:N_PC);coef_comp(k,1:N_PC);coef_comp(j,1:N_PC)]

[coef_compslcom3,relweightsslcom3,coef_ligslcom3]=svd(dataslcom3);

correlcomtot=zeros
ccomtot=zeros

for o=1:N_PC

des=[ones(23,1),coef_compslcom3(:,o)]
[b, bint, r, rint, stats] = regress (coef_compalguns3(:,o), des)

correlcomtot=stats(1)+ccomtot
ccomtot=correlcomtot

end

item=item+1
it=item

resumafcom3(item,1)=i
resumafcom3(item,2)=k
resumafcom3(item,3)=j
resumafcom3(item,4)=correlcomtot

endif

end
end
end

dlmwrite('resumafegits3_comp.txt',resumafcom3," ")

[rcomsum3,numcomsum3]=max(resumafcom3(:,4))

afegitcom3(1)=resumafcom3(numcomsum3,1)
afegitcom3(2)=resumafcom3(numcomsum3,2)

```

```

afegitcom3(3)=resumafcom3(numcomsum3,3)

resumafcom3_2=resumafcom3
resumafcom3_2(numcomsum3,4)=zeros

[rcomsum3_2,numcomsum3_2]=max(resumafcom3_2(:,4))

afegitcom3_2(1)=resumafcom3_2(numcomsum3_2,1)
afegitcom3_2(2)=resumafcom3_2(numcomsum3_2,2)
afegitcom3_2(3)=resumafcom3_2(numcomsum3_2,3)

resumafcom3_3=resumafcom3_2
resumafcom3_3(numcomsum3_2,4)=zeros

[rcomsum3_3,numcomsum3_3]=max(resumafcom3_3(:,4))

afegitcom3_3(1)=resumafcom3_3(numcomsum3_3,1)
afegitcom3_3(2)=resumafcom3_3(numcomsum3_3,2)
afegitcom3_3(3)=resumafcom3_3(numcomsum3_3,3)

collitscom(7,:)=[escollitscom3(1:end),afegitcom3(1:3),rcomsum3]
collitscom(8,:)=[escollitscom3(1:end),afegitcom3_2(1:3),rcomsum3_2]
collitscom(9,:)=[escollitscom3(1:end),afegitcom3_3(1:3),rcomsum3_3]

dlmwrite('escollits_comp.txt',collitscom," ")

```

9.3 Scripts used for the selection of the ligands and metal fragments of reference.

The script reads in the computational BDEs of the Actual Training Set in a file called "Results.txt" (metal fragments in rows, ligands in columns). It performs the SVD analysis on the BDE matrix of the Actual Training Set to obtain the ligand hidden descriptors, the hidden descriptors of the metal fragments, and the diagonal matrix **W**. The script asks for the number of hidden descriptors to consider (1 to 10) and a threshold value, both must be input in the prompt. It searches for all possible groups of the given number of ligands and computes the determinant of the matrix formed with the corresponding hidden descriptors. It stores the results of the determinants with a value higher than the given threshold. At the end searches for the set with higher determinant and prints the reference set in the file "vector_lig.txt" as output for the script corresponding to ligands of reference and "vector_comp.txt" as output for the script corresponding to the metal fragments of reference.

Script for ligands of reference:

```
zenbat=input("Number of ligands and metal fragments to take into account");
liston=input("Threshold of the determinant");

data=load("Results.txt");
```

```
[coef_comp,relweights,coef_lig]=svd(data);
```

```
berria=coef_lig(:,1:zenbat);
```

```
fila=0;
for i=1:length(berria(:,1))
berria(i,:)=berria(i,:)/(sum((berria(i,:)).^2))^(1/2);
end
a=0;
b=0;
c=0;
d=0;
e=0;
f=0;
g=0;
h=0;
i=0;
j=0;
```

```
if (zenbat >= 1)
for a=1:length(berria(:,1))-(zenbat-1)
matrize(1,:)=berria(a,:);
```

```
if (zenbat >= 2)
for b=(a+1):length(berria(:,1))-(zenbat-2)
matrize(2,:)=berria(b,:);
```

```

if (zenbat >= 3)
for c=(b+1):length(berria(:,1))-(zenbat-3)
matrize(3,:)=berria(c,:);

if (zenbat >= 4)
for d=(c+1):length(berria(:,1))-(zenbat-4)
matrize(4,:)=berria(d,:);

if (zenbat >= 5)
for e=(d+1):length(berria(:,1))-(zenbat-5)
matrize(5,:)=berria(e,:);

if (zenbat >= 6)
for f=(e+1):length(berria(:,1))-(zenbat-6)
matrize(6,:)=berria(f,:);

if (zenbat >= 7)
for g=(f+1):length(berria(:,1))-(zenbat-7)
matrize(7,:)=berria(g,:);

if (zenbat >= 8)
for h=(g+1):length(berria(:,1))-(zenbat-8)
matrize(8,:)=berria(h,:);

if (zenbat >= 9)
for i=(h+1):length(berria(:,1))-(zenbat-9)
matrize(9,:)=berria(i,:);

if (zenbat >= 10)
for j=(i+1):length(berria(:,1))
matrize(10,:)=berria(j,:);

deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f,g,h,i,j];
registro(fila,1)=deter;
end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f,g,h,i];
registro(fila,1)=deter;
end

end

```

```

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f,g,h];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f,g];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d];

```

```

registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,:)=[deter,a,b,c];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,:)=[deter,a,b];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a];
registro(fila,1)=deter;
end

end

end

end

[maximo, donde]=max(registro(:,1))
vector_lig=registro(donde,2:zenbat+1)

dlmwrite('vector_lig.txt',vector_lig," ");

```

Script for the metal fragments of reference:

```

zenbat=input("Number of ligands and metal fragments to take into account");
liston=input("Threshold of the determinant");

```

```

data=load("Results.txt");

[coef_comp,relweights,coe_lig]=svd(data);

mat_berria=coef_comp(:,1:zenbat);

fila=0;
for i=1:length(mat_berria(:,1))
mat_berria(i,:)=mat_berria(i,:)/(sum((mat_berria(i,:)).^2))^(1/2);
end
a=0;
b=0;
c=0;
d=0;
e=0;
f=0;
g=0;
h=0;
i=0;
j=0;

if (zenbat >= 1)
for a=1:length(mat_berria(:,1))-(zenbat-1)
matrize(1,:)=mat_berria(a,:);

if (zenbat >= 2)
for b=(a+1):length(mat_berria(:,1))-(zenbat-2)
matrize(2,:)=mat_berria(b,:);

if (zenbat >= 3)
for c=(b+1):length(mat_berria(:,1))-(zenbat-3)
matrize(3,:)=mat_berria(c,:);

if (zenbat >= 4)
for d=(c+1):length(mat_berria(:,1))-(zenbat-4)
matrize(4,:)=mat_berria(d,:);

if (zenbat >= 5)
for e=(d+1):length(mat_berria(:,1))-(zenbat-5)
matrize(5,:)=mat_berria(e,:);

if (zenbat >= 6)
for f=(e+1):length(mat_berria(:,1))-(zenbat-6)
matrize(6,:)=mat_berria(f,:);

if (zenbat >= 7)
for g=(f+1):length(mat_berria(:,1))-(zenbat-7)
matrize(7,:)=mat_berria(g,:);

if (zenbat >= 8)
for h=(g+1):length(mat_berria(:,1))-(zenbat-8)

```

```

matrize(8,:)=mat_berria(h,:);

if (zenbat >= 9)
for i=(h+1):length(mat_berria(:,1))-(zenbat-9)
matrize(9,:)=mat_berria(i,:);

if (zenbat >= 10)
for j=(i+1):length(mat_berria(:,1))
matrize(10,:)=mat_berria(j,:);

deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f,g,h,i,j];
registro(fila,1)=deter;
end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f,g,h,i];
registro(fila,1)=deter;
end
end
end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f,g,h];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f,g];
registro(fila,1)=deter;
end

end
end

```

```

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e,f];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d,e];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a,b,c,d];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,:)=[deter,a,b,c];
registro(fila,1)=deter;
end

end

end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,:)=[deter,a,b];
registro(fila,1)=deter;
end

```

```

end
end

else
deter=det(matrize);
if (deter>liston)
fila=fila+1;
registro(fila,2:zenbat+1)=[a];
registro(fila,1)=deter;
end

end
end
end

[maximo, donde]=max(registro(:,1))
vector_comp=registro(donde,2:zenbat+1)

dlmwrite("vector_comp.txt",vector_comp," ");

```

9.4 Script used to compute the estimated BDEs

The script reads in the computational BDEs of the Actual Training Set in a file called “Results.txt” (metal fragments in rows, ligands in columns), it also reads in two files “refnewlig.txt” and “refnewcomp.txt”, one containing the BDEs of the new ligands and the metal fragments of reference and the other containing the BDEs of the new metal fragments with the ligands of reference. It also needs of the BDEs of the Full Set of data to compute the errors in a file called “ResultsFull.txt”. The script must be edited if the ligand/metal fragments of reference change. Namely the lines `ligands_ref=[3 9 10 14 20 21]` and `complex_ref=[1 4 11 14 16 18]` must be changed accordingly. It performs the SVD analysis on the BDE matrix of the Actual Training Set to obtain the ligand hidden descriptors, the ones of the metal fragments, and the diagonal matrix **W**. Then it asks on the screen the number of new ligands and new complexes that should be considered. Then it performs a regression to find out the hidden descriptors of the new ligands and of the new metal fragments. The new BDEs are estimated and printed out in files called “BDE_newlig.txt”, “BDE_newcomp.txt” and “BDE_newcompnewlig.txt”. Then the errors (BDE computed -BDE estimated) are printed in files “Error_newlig.txt”, “Error_newcomp.txt” and “Error_newcompnewlig.txt”. A summary of the errors and the maximum errors are printed in separate files “ResumErrors.txt” and “MaxErrors.txt”.

```
clear

%The basis matrix {\bf BDE} is loaded from the file Results.txt.

data=load("Results.txt");
ligands=data;

[descr_comp,relweights,descr_lig]=svd(data);

% The errors for the basis matrix elements when 6 PCs
%are considered is computed.

for i=1:length(data(1,:));
for j=1:length(data(:,1));
errors_basis(j,i)=ligands(j,i)-(descr_comp(j,1:6)*relweights(1:6,1:6)*descr_lig(i,1:6)')
end
end

%The number of new ligands and new metal fragments is requested.
N_newlig= input("Write the number of new ligands that you want to consider:");
N_newcomp= input("Write the number of metal fragments that you want to consider:");

% The BDEs of reference for each new ligand and each new metal
%fragments are loaded from the files refnewlig.txt and refnewcomp.txt.
% Note that in both cases, each row must contain the BDEs of a
% metal fragment, and each columns the BDEs of a ligand.
```

```

if (N_newlig>0)
refnewlig=load("refnewlig.txt");
end

if (N_newcomp>0)
refnewcomp=load("refnewcomp.txt");
end

%The descriptors of the new ligands and new metal fragments
%are calculated, expressing them as a linear combination of the
%BDEs of reference and making a regression considering all the
%basis fragments.

ligands_ref=[3 9 10 14 20 21]
complex_ref=[1 4 11 14 16 18]

for m=1:N_newlig
for i=1:6
a_lig(i,:)=regress(descr_lig(:,i),[ones(22,1),ligands(complex_ref,:)']');
end
descr_newlig(m,:)=a_lig(:,2:7)*refnewlig(:,m)+a_lig(:,1);
end

for m=1:N_newcomp
for i=1:6
a_comp(i,:)=regress(descr_comp(:,i),[ones(23,1),ligands(:,ligands_ref)]);
end
descr_newcomp(m,:)=a_comp(:,2:7)*refnewcomp(m,:)+a_comp(:,1);
end

%The estimated BDE for the new ligand - basis metal fragment,
%basis ligand - new metal fragment and new ligand - new metal
%fragment structures are computed.

if (N_newlig > 0)
for i=1:N_newlig
for j=1:length(ligands(:,1))
BDE_newlig(j,i) = descr_comp(j,1:6)*relweights(1:6,1:6)*descr_newlig(i,1:6)';
end
end
dlmwrite('BDE_newlig.txt',BDE_newlig," ");
endif

if (N_newcomp > 0)
for i=1:length(ligands(1,:))
for j=1:N_newcomp
BDE_newcomp(j,i)= descr_newcomp(j,1:6)*relweights(1:6,1:6)*descr_lig(i,1:6)';
end

```

```

end
dlmwrite('BDE_newcomp.txt',BDE_newcomp," ");
endif

if ((N_newcomp > 0) && (N_newlig > 0))
for i=1:N_newlig
for j=1:N_newcomp
BDE_newcompnewlig(j,i)= descr_newcomp(j,1:6)*relweights(1:6,1:6)*descr_newlig(i,1:6)'
end
end
dlmwrite('BDE_newcompnewlig.txt',BDE_newcompnewlig," ");
endif

datatot=load("ResultsFull.txt")
k=length(ligands(:,1))

for i=1:N_newlig
for j=1:length(ligands(:,1))

k=i+length(ligands(1,:))

error_newlig(j,i)=datatot(j,k)-BDE_newlig(j,i)
end
end

for i=1:length(ligands(1,:))
for j=1:N_newcomp
l=j+length(ligands(:,1))
error_newcomp(j,i)=datatot(l,i)-BDE_newcomp(j,i)
end
end

for i=1:N_newlig
for j=1:N_newcomp
k=i+length(ligands(1,:))
l=j+length(ligands(:,1))
error_newcompnewlig(j,i)=datatot(l,k)-BDE_newcompnewlig(j,i)
end
end

dlmwrite('Error_newlig.txt',error_newlig," ");
dlmwrite('Error_newcomp.txt',error_newcomp," ");
dlmwrite('Error_newcompnewlig.txt',error_newcompnewlig," ");

maxerrors(1,1:21)=max(abs(error_newlig))
maxerrors(2,1:19)=max(abs(error_newcomp))
maxerrors(3,1:21)=max(abs(error_newcompnewlig))
maxerrors(4,1)=max(max(abs(error_newlig)))
maxerrors(5,1)=max(max(abs(error_newcomp)))
maxerrors(6,1)=max(max(abs(error_newcompnewlig)))
maxerrors(4,2)=mean(mean(abs(error_newlig)))

```

```
maxerrors(5,2)=mean(mean(abs(error_newcomp)))  
maxerrors(6,2)=mean(mean(abs(error_newcompnewlig)))  
  
dlmwrite('MaxErrors.txt',maxerrors," ");
```

9.5 Script used to study the meaning of the hidden descriptors.

The script reads in the computational BDEs of the Actual Training Set in a file called “Results.txt”(metal fragments in rows, ligands in columns), it also reads in a file with the conventional descriptors called “descriptorsconventional.txt” (ligands in rows, conventional descriptors in columns). It performs a SVD analysis of the BDEs obtaining the ligand hidden descriptors $\mathbf{HD}_{Lk}$. It writes them out in two files, “descriptors_lig.txt” for all ligands and “descriptors_lig_noH2.txt” where the row corresponding to the ligand H₂ has been removed. The reason for removing it is that several conventional descriptors are not unique for this ligand as two atoms are coordinated to the metal center (i. e. Metal-ligand distance, charge of the central atom ...). Then the regression of each $\mathbf{HD}_{L1} = \mathbf{L}_1$ to $\mathbf{L}_7$ is performed and the results saved in a file called “correl_7PCs.txt”.

```
clear
data=load("Results.txt");
N_PC=7;

[coef_comp,relweights,coef_lig]=svd(data);

coef_lig(:,1:N_PC);
coef_comp(:,1:N_PC);
relweights(1:N_PC,1:N_PC);

for i=1:length(data(1,:));
for j=1:length(data(:,1));
BDE_lig(j,i)=coef_comp(j,1:N_PC)*relweights(1:N_PC,1:N_PC)*coef_lig(i,1:N_PC)';
end
end

errors_lig=data-BDE_lig;

maxima=max(abs(errors_lig));
average=mean(abs(errors_lig));
maximacomp=max(abs(errors_lig'))
averagecomp=mean(abs(errors_lig'))

total_maximum=max(maxima);
total_average=mean(average);

dlmwrite('descriptors_lig.txt',coef_lig(:,1:N_PC)," ", 'precision', '%8.2f')
item=zeros
it=zeros

for i=1:length(data(1,:));
if(i != 7)

item=it+1
it=item
```

```

coef(item,1:N_PC)=coef_lig(i,1:N_PC)

endif
end

dlmwrite('descriptors_lig_noH2.txt',coef," ", 'precision', '%8.2f')

%We read the BDEs in
N_PC=7;

descrip=load("descriptorsconventional.txt");

m=length(coef(1,:));
p=length(descrip(1,:));
n=length(coef(:,1));

for i=1:p
for k=1:m

des=[ones(n,1),descrip(:,i)]

[b, bint, r, rint, stats] = regress (coef(:,k),des)

correlacio(i,k) = stats(1)
end
suma=zeros;
end

dlmwrite('correl_7PCs.txt',correlacio," ")

```