

Supporting Information:

A Non-Perturbative Pairwise-Additive Analysis of Charge Transfer Contributions to Intermolecular Interaction Energies

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Working basis

In this section, we describe a method to construct an orthogonal working molecular orbital (MO) basis. We will work with the occupied and unoccupied space defined by the polarized wavefunction throughout this section. The polarized wavefunction (Φ_{POL}) gives a set of non-orthogonal occupied orbitals spanning the occupied space. In order to convert this set to an orthogonal basis, we symmetrically orthogonalize it as shown in Eq. (1) where the columns of the $\mathbf{T}^{\text{ortho}}$ and \mathbf{T} contain the orthogonal and non-orthogonal occupied orbitals. Symmetric orthogonalization is sufficient as there is no linear dependency in the occupied

space.

$$\mathbf{T}^{\text{ortho}} = \mathbf{T}\boldsymbol{\sigma}_{OO}^{-1/2} \quad (1)$$

$$\boldsymbol{\sigma}_{OO} = \mathbf{T}^T \mathbf{S} \mathbf{T} \quad (2)$$

Φ_{POL} also gives a set of non-orthogonal virtual orbitals defined by FERFs. As these orbitals might have some overlap with the occupied space, we will project them out first as shown in Eq. (3) where $\mathbf{P} = \mathbf{T}\boldsymbol{\sigma}_{OO}^{-1}\mathbf{T}^T$ is the projector onto the occupied space. These orbitals are orthogonalized using standard canonical orthogonalization in order to account for linear dependence in the virtual space. \mathbf{U} is matrix of eigenvectors with eigenvalues greater than threshold and \mathbf{s} is a diagonal matrix of eigenvalues greater than threshold.

$$\mathbf{V}^{\text{proj}} = (\mathbf{I} - \mathbf{P}\mathbf{S})\mathbf{V} \quad (3)$$

$$\mathbf{V}^{\text{ortho}} = \mathbf{V}^{\text{proj}}\mathbf{U}\mathbf{s}^{-1/2} \quad (4)$$

The space not spanned by these the occupied and the FERF virtual space is the void space. An orthogonal basis for this space is formed by the eigenvectors of the projector (\mathbf{R}_{POL}) for this space (Eq. (6)). and

$$\mathbf{P}_{\text{POL}} = \mathbf{C}_{\text{POL}}\boldsymbol{\sigma}\mathbf{C}_{\text{POL}}^T \quad (5)$$

$$\mathbf{R}_{\text{POL}} = \mathbf{I} - \mathbf{P}_{\text{POL}} \quad (6)$$

$$\mathbf{R}^{\text{ortho}} \leftarrow \text{eigenvectors}(\mathbf{R}_{\text{POL}}) \quad (7)$$

An orthogonal basis for the entire Hilbert space is formed by the columns of $\mathbf{T}^{\text{ortho}}$, $\mathbf{V}^{\text{ortho}}$, and $\mathbf{R}^{\text{ortho}}$.

Cost function and gradient

In this section, we describe the cost function to be minimized to solve for $\mathbf{X}_{OV}^{\text{CT}}$ and derive its corresponding gradient. Let \mathbf{U}_{XY} be the cumulative unitary transformation generated by $\boldsymbol{\theta}_X$ and $\boldsymbol{\theta}_Y$ respectively where \mathbf{U}_X (referred to as $\mathbf{U}_{\text{curr}}^{\text{CT}}$ in Eq. (26)) denotes the current step taken and \mathbf{U}_Y denotes the next step.

$$\mathbf{U}_X = e^{\boldsymbol{\theta}_X} \quad (8)$$

$$\mathbf{U}_Y = e^{\boldsymbol{\theta}_Y} \quad (9)$$

$$\mathbf{U}_{XY} = \mathbf{U}_X \mathbf{U}_Y \quad (10)$$

As we are trying to find the generator of unitary transformation that rotates the polarized density matrix (\mathbf{P}^{POL}) to the fully-relaxed density matrix (\mathbf{P}^{CT}), we are trying to find the $\boldsymbol{\theta}$ that satisfies Eq. (11)

$$\mathbf{P}^{\text{CT}} = e^{\boldsymbol{\theta}} \mathbf{P}^{\text{POL}} e^{-\boldsymbol{\theta}} \quad (11)$$

Hence, we define the cost function C as shown in Eq. (12)

$$C = \|\mathbf{P}^{\text{CT}} - \mathbf{U}_{XY} \mathbf{P}^{\text{POL}} \mathbf{U}_{XY}^\dagger\|_F^2 \quad (12)$$

Before minimizing the cost function C , let us form a working orthogonal basis. Let \mathbb{H} denote the Hilbert space of the whole complex. For the polarized wavefunction Φ_{POL} , \mathbb{H} can be partitioned into occupied space (\mathbb{T}), virtual space spanned by FERFs (\mathbb{Q}), and the void space which is the unoccupied space not spanned by FERFs (\mathbb{R}). \mathbb{Q} and \mathbb{R} can be clubbed together to form the unoccupied space \mathbb{V} . These spaces can also be made strongly orthogonal

to each other without loss of generality.

$$\begin{aligned}\mathbb{H} &= \mathbb{T} \oplus \mathbb{Q} \oplus \mathbb{R} \\ \mathbb{H} &= \mathbb{T} \oplus \mathbb{V} \quad \text{where } \mathbb{V} = \mathbb{Q} \oplus \mathbb{R}\end{aligned}\tag{13}$$

Let the columns of \mathbf{T} and \mathbf{V} form an orthonormal basis for the occupied and unoccupied subspaces respectively. Let N_T and N_V be the dimensions of these subspaces respectively. In this orthonormal projectors, the density matrix which is the projector on the occupied space can be written as

$$\mathbf{P}^{\text{POL}} = \begin{bmatrix} \mathbf{I}_{N_T \times N_T} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\tag{14}$$

Expressing the cost function in this orthonormal basis and taking its derivative with respect to the elements of the generator $\boldsymbol{\theta}_Y$,

$$\begin{aligned}\frac{\partial C}{\partial(\boldsymbol{\theta}_Y)_{ia}} &= \frac{\partial}{\partial(\boldsymbol{\theta}_Y)_{ia}} \sum_{p,q} \left((\mathbf{P}^{\text{CT}} - \mathbf{U}_{XY} \mathbf{P}^{\text{POL}} \mathbf{U}_{XY}^\dagger)_{pq}^2 \right) \\ &= 2 \sum_{p,q} (\mathbf{P}^{\text{CT}} - \mathbf{U}_{XY} \mathbf{P}^{\text{POL}} \mathbf{U}_{XY}^\dagger)_{pq} \frac{\partial}{\partial(\boldsymbol{\theta}_Y)_{ia}} (\mathbf{P}^{\text{CT}} - \mathbf{U}_{XY} \mathbf{P}^{\text{POL}} \mathbf{U}_{XY}^\dagger)_{pq}\end{aligned}\tag{15}$$

Consider,

$$\begin{aligned}\frac{\partial}{\partial(\boldsymbol{\theta}_Y)_{ia}} (\mathbf{P}^{\text{CT}} - \mathbf{U}_{XY} \mathbf{P}^{\text{POL}} \mathbf{U}_{XY}^\dagger)_{pq} &= \frac{\partial}{\partial(\boldsymbol{\theta}_Y)_{ia}} (\mathbf{P}_{pq}^{\text{CT}} - \sum_{k,l,m,n} (\mathbf{U}_X)_{pk} (\mathbf{U}_Y)_{kl} P_{lm}^{\text{POL}} (\mathbf{U}_Y^\dagger)_{mn} (\mathbf{U}_X^\dagger)_{nq}) \\ &= - \sum_{k,l,m,n} (\mathbf{U}_X)_{pk} \frac{\partial (\mathbf{U}_Y)_{kl}}{\partial(\boldsymbol{\theta}_Y)_{ia}} P_{lm}^{\text{POL}} (\mathbf{U}_Y^\dagger)_{mn} (\mathbf{U}_X^\dagger)_{nq} \\ &\quad - \sum_{k,l,m,n} (\mathbf{U}_X)_{pk} (\mathbf{U}_Y)_{kl} P_{lm}^{\text{POL}} \frac{\partial (\mathbf{U}_Y^\dagger)_{mn}}{\partial(\boldsymbol{\theta}_Y)_{ia}} (\mathbf{U}_X^\dagger)_{nq}\end{aligned}\tag{16}$$

We know that $\frac{\partial(U_Y)_{kl}}{\partial(\theta_Y)_{ia}} = \delta_{ki}\delta_{la} - \delta_{ka}\delta_{li}$. Substituting this above,

$$\begin{aligned} \frac{\partial}{\partial(\theta_Y)_{ia}} (\mathbf{P}^{\text{CT}} - \mathbf{U}_{XY} \mathbf{P}^{\text{POL}} \mathbf{U}_{XY}^\dagger)_{pq} &= - \sum_{m,n} (\mathbf{U}_X)_{pi} P_{am}^{\text{POL}} (\mathbf{U}_Y^\dagger)_{mn} (\mathbf{U}_X^\dagger)_{nq} + \sum_{m,n} (\mathbf{U}_X)_{pa} P_{im}^{\text{POL}} (\mathbf{U}_Y^\dagger)_{mn} (\mathbf{U}_X^\dagger)_{nq} \\ &\quad - \sum_{k,l} (\mathbf{U}_X)_{pk} (\mathbf{U}_Y)_{kl} P_{la}^{\text{POL}} (\mathbf{U}_X^\dagger)_{iq} + \sum_{k,l} (\mathbf{U}_X)_{pk} (\mathbf{U}_Y)_{kl} P_{li}^{\text{POL}} (\mathbf{U}_X^\dagger)_{aq} \end{aligned}$$

Evaluating the above expression at $\theta_Y = \mathbf{0}$, we have $\mathbf{U}_Y = \mathbf{I}$ and $\mathbf{U}_{XY} = \mathbf{U}_X$.

$$\begin{aligned} \frac{\partial}{\partial(\theta_Y)_{ia}} (\mathbf{P}^{\text{CT}} - \mathbf{U}_{XY} \mathbf{P}^{\text{POL}} \mathbf{U}_{XY}^\dagger)_{pq} \Big|_{\theta_Y = \mathbf{0}} &= - \sum_m (\mathbf{U}_X)_{pi} P_{am}^{\text{POL}} (\mathbf{U}_X^\dagger)_{mq} + \sum_m (\mathbf{U}_X)_{pa} P_{im}^{\text{POL}} (\mathbf{U}_X^\dagger)_{mq} \\ &\quad - \sum_l (\mathbf{U}_X)_{pl} P_{la}^{\text{POL}} (\mathbf{U}_X^\dagger)_{iq} + \sum_l (\mathbf{U}_X)_{pl} P_{li}^{\text{POL}} (\mathbf{U}_X^\dagger)_{aq} \end{aligned}$$

From Eq. (14), we know that $P_{am}^{\text{POL}} = P_{la}^{\text{POL}} = 0$ as a is an index for the unoccupied space.

Thus we have,

$$\begin{aligned} \frac{\partial}{\partial(\theta_Y)_{ia}} (\mathbf{P}^{\text{CT}} - \mathbf{U}_{XY} \mathbf{P}^{\text{POL}} \mathbf{U}_{XY}^\dagger)_{pq} \Big|_{\theta_Y = \mathbf{0}} &= \sum_m (\mathbf{U}_X)_{pa} P_{im}^{\text{POL}} (\mathbf{U}_X^\dagger)_{mq} + \sum_l (\mathbf{U}_X)_{pl} P_{li}^{\text{POL}} (\mathbf{U}_X^\dagger)_{aq} \\ &= (\mathbf{U}_X)_{pa} (\mathbf{U}_X^\dagger)_{iq} + (\mathbf{U}_X)_{pi} (\mathbf{U}_X^\dagger)_{aq} \end{aligned} \quad (17)$$

Plugging Eq. (17) into Eq. (15),

$$\begin{aligned} \frac{\partial C}{\partial(\theta_Y)_{ia}} \Big|_{\theta_Y = \mathbf{0}} &= 2 \sum_{p,q} \left(P_{pq}^{\text{CT}} - \sum_{j,k} (\mathbf{U}_X)_{pj} P_{jk}^{\text{POL}} (\mathbf{U}_{kq}^\dagger) \right) \left((\mathbf{U}_X)_{pa} (\mathbf{U}_X^\dagger)_{iq} + (\mathbf{U}_X)_{pi} (\mathbf{U}_X^\dagger)_{aq} \right) \\ &= 2 \sum_{p,q} \left((\mathbf{U}_X^\dagger)_{iq} P_{qp}^{\text{CT}} (\mathbf{U}_X)_{pa} + (\mathbf{U}_X^\dagger)_{ip} P_{pq}^{\text{CT}} (\mathbf{U}_X)_{qa} \right. \\ &\quad \left. - \sum_k^{N_T} (\mathbf{U}_X^\dagger)_{jq} (\mathbf{U}_X^\dagger)_{jp} (\mathbf{U}_X)_{pa} (\mathbf{U}_X^\dagger)_{iq} - \sum_k^{N_T} (\mathbf{U}_X)_{pj} (\mathbf{U}_X)_{pi} (\mathbf{U}_X^\dagger)_{jq} (\mathbf{U}_X)_{qa} \right) \end{aligned} \quad (18)$$

From Eq. (18), we can see that the first two terms of the RHS are equal and the third and fourth terms are 0 as $\sum_p (\mathbf{U}_X^\dagger)_{jp} (\mathbf{U}_X)_{pa} = 0$ and $\sum_p (\mathbf{U}_X^\dagger)_{jq} (\mathbf{U}_X)_{qa} = 0$ as basis vectors

spanning \mathbb{T} and \mathbb{V} are orthonormal to each other. Finally, we have

$$\frac{\partial C}{\partial(\boldsymbol{\theta}_Y)_{ia}} \Big|_{\boldsymbol{\theta}_Y=\mathbf{0}} = 4 \sum_{p,q} (\mathbf{U}_X^\dagger)_{iq} P_{qp}^{\text{CT}} (\mathbf{U}_X)_{pa} \quad (19)$$

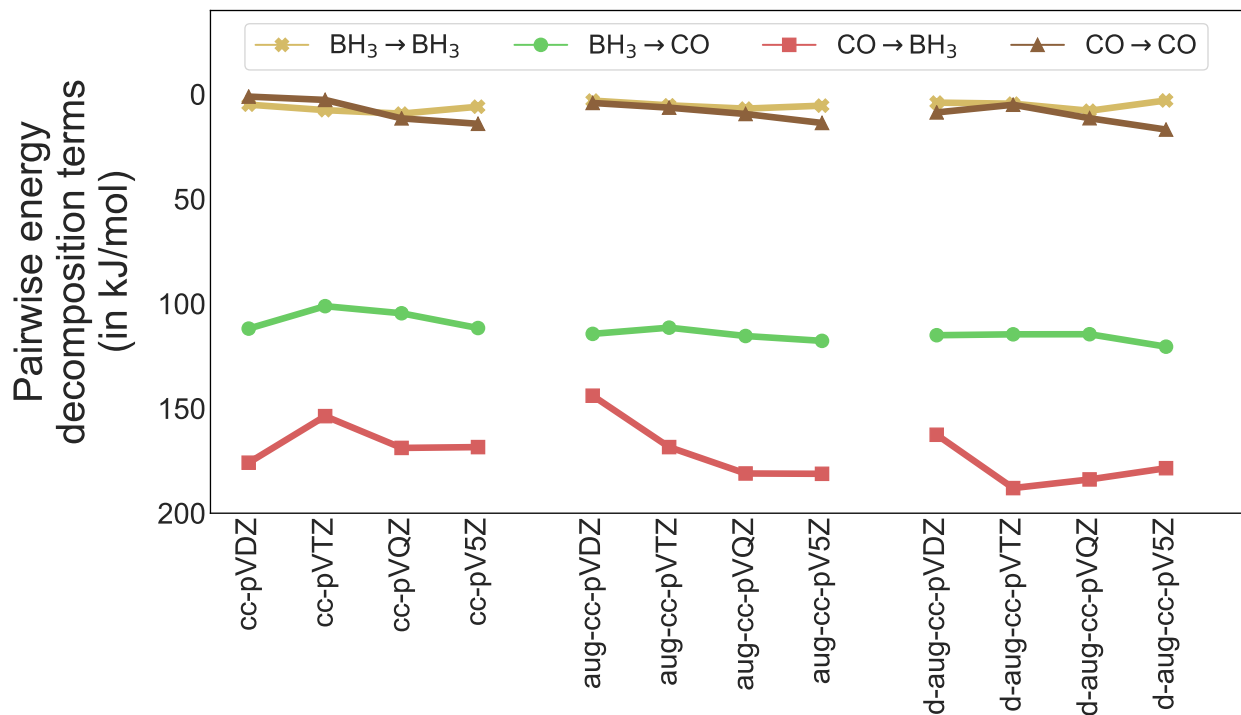


Figure S1: Convergence properties of the non-perturbative pairwise energy decomposition components of the total charge transfer energy with respect to increasing the highest angular momentum of the basis set for the Dunning basis set series: cc-pVXZ, aug-cc-pVXZ, and d-aug-cc-pVXZ (X=D, T, Q, and 5) for the BH₃-CO system at equilibrium geometry using ω B97X-D.

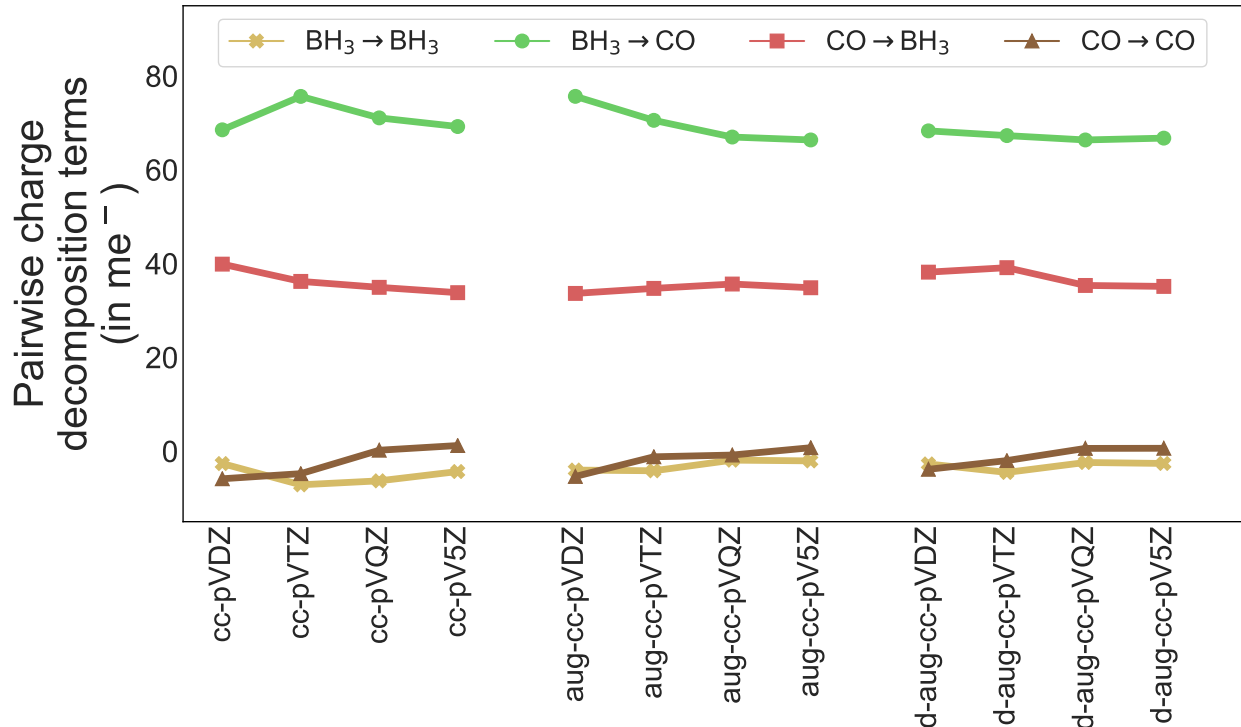


Figure S2: Convergence properties of the non-perturbative pairwise charge decomposition components of total charge transfer with respect to increasing the highest angular momentum of the basis set for the Dunning basis set series: cc-pVXZ, aug-cc-pVXZ, and d-aug-cc-pVXZ (X=D, T, Q, and 5) for the BH₃-CO system at equilibrium geometry using ω B97X-D.

Table S1: Adiabatic energy decomposition analysis for the DNA base pairs thymine(T)-adenine(A), guanine(G)-cytosine(C), and their corresponding metallated versions. All values are in kJ/mol.

System	ΔE_{INT}	ΔE_{FRZ}	ΔE_{POL}	ΔE_{CT}
T(1):A(2)	-69.4	-31.8	-11.5	-20.6
G(1):C(2)	-134.3	-64.8	-27.5	-28.5
Na ⁺ G(1):C(2)	-149.3	-77.1	-31.7	-29.4
Mg ²⁺ G(1):C(2)	-214.2	-120.9	-53.7	-21.2
Ca ²⁺ G(1):C(2)	-195.2	-114.1	-48.3	-16.5

Table S2: Energy decomposition analysis and non-perturbative charge decomposition analysis for the adduct BH₃-NCl_pH_q ($p + q = 3$). All values are in kJ/mol.

	Energy decomposition analysis					non-perturbative charge decomposition			
	ΔE_{INT}	ΔE_{GD}	ΔE_{FRZ}	ΔE_{POL}	ΔE_{CT}	BH ₃ →BH ₃	BH ₃ →NCl _m H _n	NCl _m H _n →BH ₃	NCl _m H _n →NCl _p H _q
BH ₃ -NH ₃	-133.1	56.3	116.5	-148.1	-157.7	-2.7	-16.4	-138.1	-0.5
BH ₃ -NCH ₂	-113.7	49.3	141.3	-156.5	-147.9	-2.6	-28.3	-117.9	0.9
BH ₃ -NCl ₂ H	-87.3	42.6	152.4	-138.7	-143.6	-2.3	-32.7	-109.2	0.6
BH ₃ -NCl ₃	-58.2	34.1	145.5	-111.1	-126.7	-1.7	-29.8	-95.6	0.5

Table S3: Adiabatic energy decomposition analysis for the adduct $\text{BX}_3\text{-NH}_3$ ($X = \text{F}, \text{Cl}, \text{or}, \text{Br}$). All values are in kJ/mol.

System	ΔE_{INT}	ΔE_{FRZ}	ΔE_{POL}	ΔE_{CT}
$\text{BF}_3\text{-NH}_3$	-90.8	-20.4	-6.6	-63.8
$\text{BCl}_3\text{-NH}_3$	-107.7	-10.6	-3.2	-93.8
$\text{BBr}_3\text{-NH}_3$	-119.2	-9.9	-3.0	-106.3

Table S4: Adiabatic energy decomposition analysis for the adduct $\text{BH}_3\text{-NMe}_p\text{H}_q$ ($p+q = 3$). All values are in kJ/mol.

System	ΔE_{INT}	ΔE_{FRZ}	ΔE_{POL}	ΔE_{CT}
$\text{BH}_3\text{-NH}_3$	-133.1	-16.7	-14.5	-101.9
$\text{BH}_3\text{-NMeH}_2$	-153.2	-18.3	-28.2	-106.8
$\text{BH}_3\text{-NMe}_2\text{H}$	-163.1	-19.7	-37.4	-106.0
$\text{BH}_3\text{-NMe}_3$	-163.8	-21.1	-40.4	-102.3

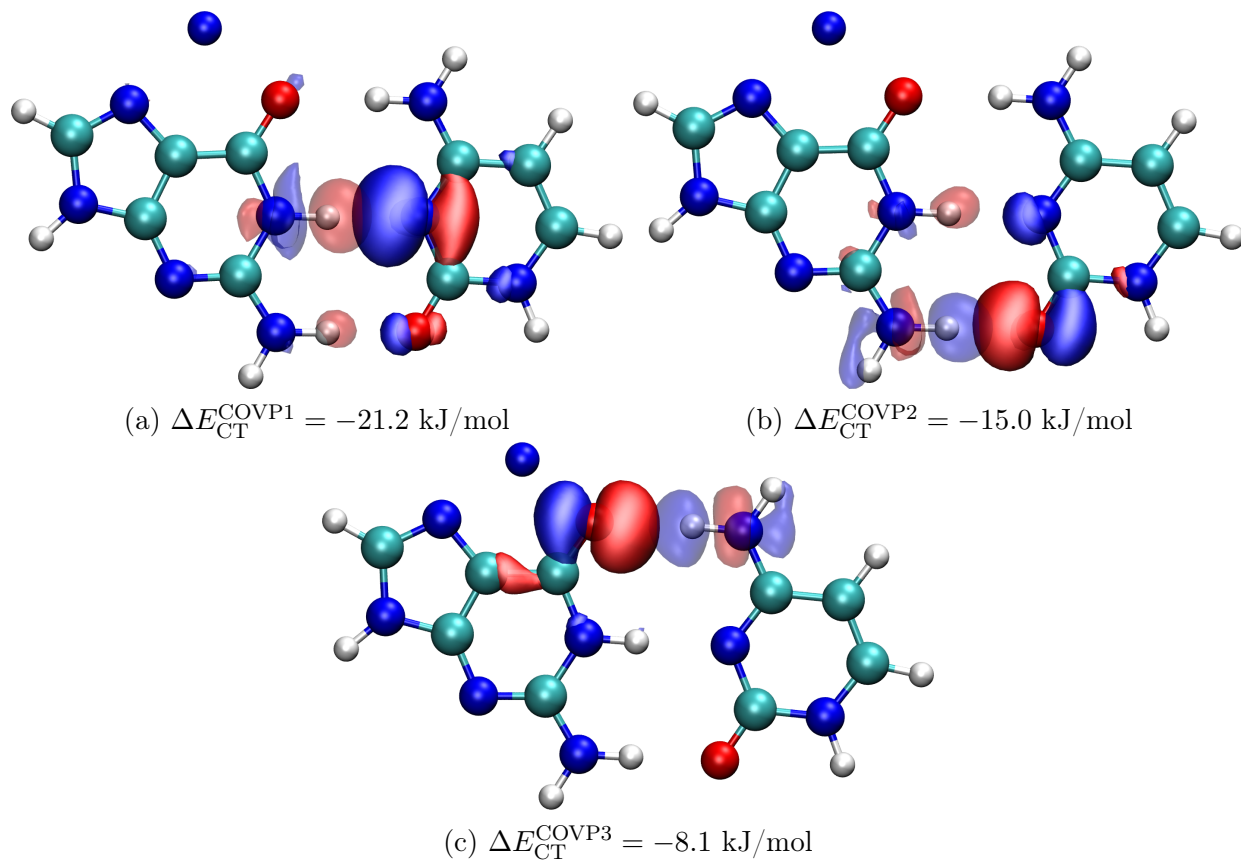


Figure S3: (a) Most significant COVP for Na^+ guanine:cytosine complex (b) Second most significant COVP (c) Third most significant COVP

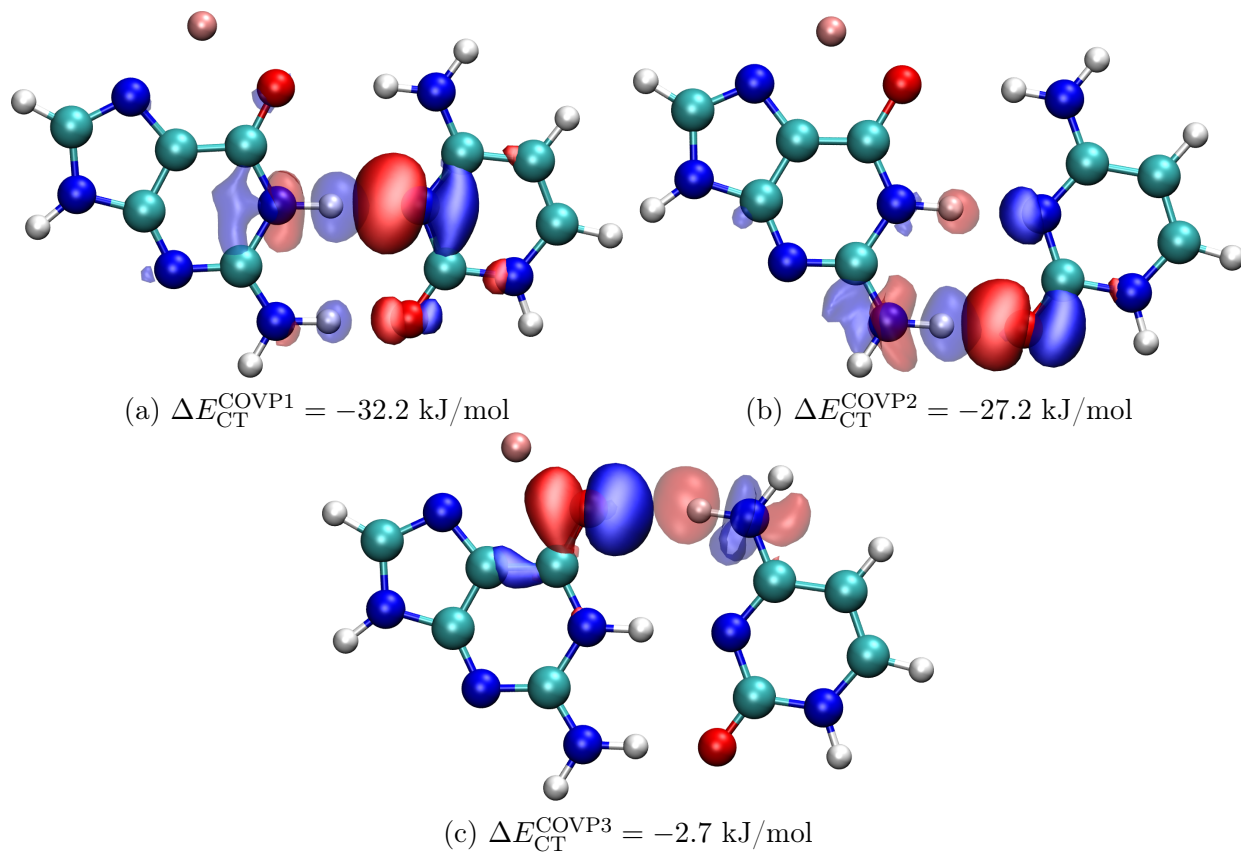


Figure S4: (a) Most significant COVP for Mg^{2+} guanine:cytosine complex (b) Second most significant COVP (c) Third most significant COVP.

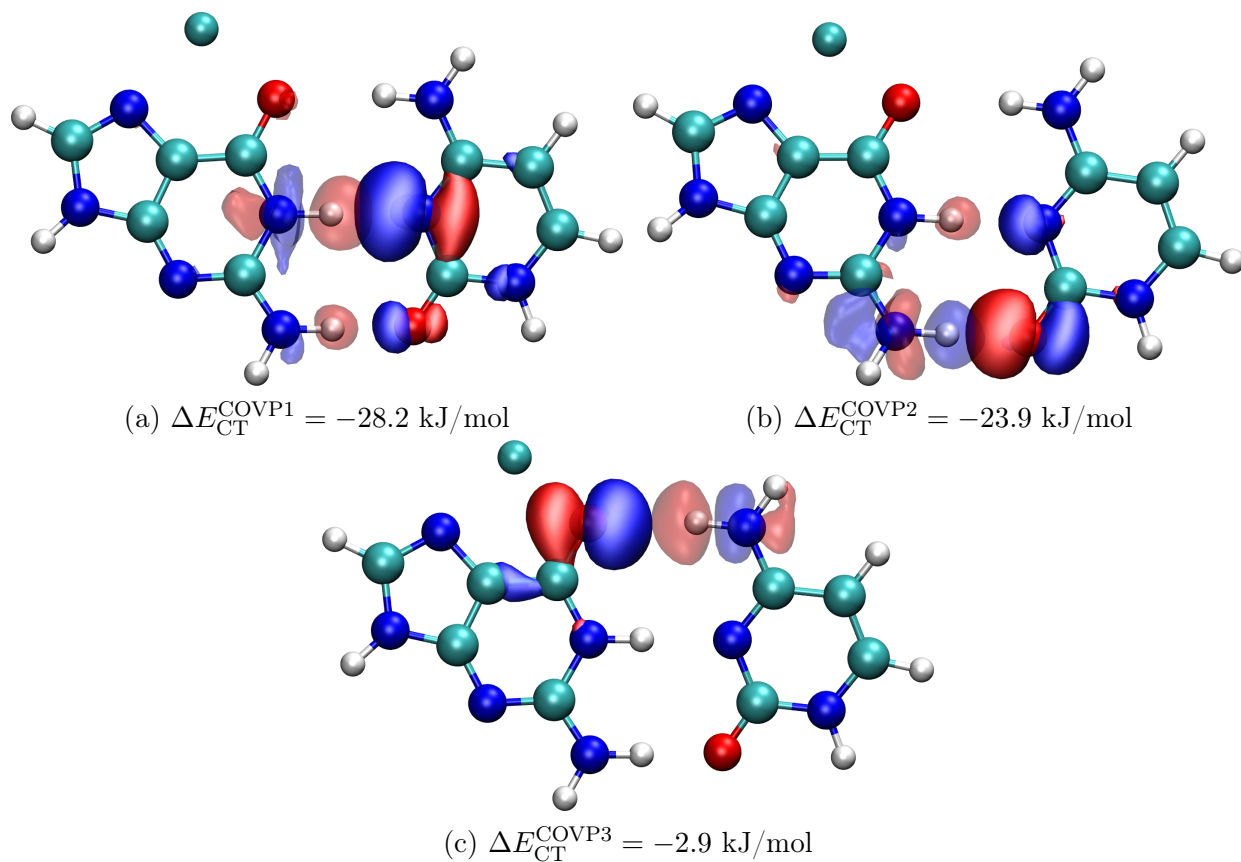


Figure S5: (a) Most significant COVP for Ca^{2+} guanine:cytosine complex (b) Second most significant COVP (c) Third most significant COVP.

Table S5: Variational forward-backward charge transfer analysis for a series of 3d transition metal hexacarbonyls. All values are in kJ/mol.

System	$\text{M}(\text{CO})_5 \rightarrow \text{CO}$	$\text{CO} \rightarrow \text{M}(\text{CO})_5$
$\text{V}(\text{CO})_6^-$	-76.2	-18.1
$\text{Cr}(\text{CO})_6$	-45.9	-28.2
$\text{Mn}(\text{CO})_6^+$	-22.6	-39.7

Table S6: Residual energy not decomposed into pairwise additive terms using the non-perturbative CT analysis for some representative systems considered in this work using ω B97X-D density functional and def2-TZVPD basis set. Residual energy is shown in both kJ/mol and as a percentage of total variational CT energy.

System	Residual CT energy (kJ/mol)	Residual CT energy
BF_3-NH_3	6.86E-04	4.40E-04%
BH_3-NH_3	9.03E-04	5.78E-04%
BH_3-CO	7.95E-04	2.70E-04%
Mg^{2+} guanine : cytosine	7.95E-04	1.18E-03%
$\text{Cr}(\text{CO})_6$	1.13E-06	5.33E-07%

Geometries

BH_3-CO

Charge=0, Multiplicity=1

B	-1.39961	0.70844	0.18735
H	-0.23322	0.93106	-0.03460
H	-1.99575	0.22613	-0.74595
H	-1.98125	1.61908	0.72730
C	-1.37842	-0.39863	1.23375
O	-1.36206	-1.21576	2.00602

Adenine – thymine

Charge = 0, Multiplicity=1

N	0.93525	0.00327	-0.37856
C	1.67122	0.00447	0.74242
C	3.06945	0.00430	0.59464
C	3.55409	0.00299	-0.70204
N	2.83563	0.00192	-1.82718
C	1.54067	0.00208	-1.57294
N	4.09798	0.00504	1.51249
C	5.17274	0.00449	0.78245
N	4.91459	0.00351	-0.56354
N	1.06445	0.00576	1.93073
H	0.86880	0.00126	-2.42521
H	6.18223	0.00493	1.16396
H	5.58348	0.00302	-1.31239
H	0.04879	0.00524	1.99236
H	1.62641	0.00609	2.76146
N	-3.90108	0.00699	-1.51169
C	-4.59567	0.00885	-0.33183
C	-3.98779	0.00849	0.86365
C	-2.52733	0.00612	0.87694
N	-1.90988	0.00427	-0.35524
C	-2.52226	0.00443	-1.58215
C	-4.71384	0.01056	2.16875
O	-1.86472	0.00574	1.90468
O	-1.92589	0.00347	-2.63504
H	-4.37932	0.00746	-2.39553
H	-0.86725	0.00300	-0.36549
H	-5.67377	0.01071	-0.42975
H	-4.44606	-0.86505	2.76243
H	-4.44328	0.88616	2.76118
H	-5.79328	0.01219	2.01585

guanine – cytosine

Charge=0, Multiplicity=1

N	-2.71342	-0.03847	0.00000
O	1.20960	2.30520	0.00000
N	-0.79313	1.23201	0.00000
C	-2.15789	1.18326	0.00000
N	-2.91822	2.25468	0.00000
C	-2.20356	3.39259	0.00000
C	-0.82822	3.56058	0.00000
C	-0.01516	2.39072	0.00000
N	-2.71003	4.65671	0.00000
C	-1.63428	5.51622	0.00000
N	-0.49613	4.89892	0.00000
H	-2.16332	-0.89459	0.00000
H	-3.71436	-0.08261	0.00000
H	-0.26632	0.34822	0.00000
H	-3.68517	4.89551	0.00000
H	-1.76809	6.58698	0.00000
O	-1.11321	-2.47931	0.00000
N	2.72139	-0.02967	0.00000
N	0.78997	-1.23187	0.00000
C	2.89188	-2.42337	0.00000
C	0.10811	-2.39792	0.00000
N	0.85582	-3.57753	0.00000
C	2.20860	-3.58117	0.00000
C	2.11745	-1.21115	0.00000
H	3.97064	-2.40651	0.00000
H	0.32769	-4.43351	0.00000
H	2.69059	-4.54922	0.00000
H	2.16866	0.84189	0.00000
H	3.72260	0.02130	0.00000

Na⁺ guanine – cytosine

Charge=+1, Multiplicity=1

N	-2.65427	-0.03416	0.03627
O	1.23315	2.41597	-0.06545
N	-0.73630	1.24166	-0.01668
C	-2.11519	1.17712	0.00788
N	-2.89187	2.24861	0.00465
C	-2.21123	3.38907	-0.02376
C	-0.84074	3.55313	-0.04865
C	-0.01845	2.40865	-0.04524
N	-2.70715	4.66311	-0.03474
C	-1.64204	5.51877	-0.06468
N	-0.49939	4.89434	-0.07407
H	-2.09506	-0.89372	0.03818
H	-3.65671	-0.08599	0.05442
H	-0.18946	0.35722	-0.01308
H	-3.68093	4.91639	-0.02263
H	-1.77192	6.58931	-0.07877
Na	1.84056	4.62888	-0.10276
O	-1.11024	-2.36217	0.03702
N	2.82195	-0.07269	-0.05055
N	0.84004	-1.19096	-0.00644
C	2.88894	-2.46889	-0.02441
C	0.11296	-2.33555	0.01748
N	0.80910	-3.53840	0.01934
C	2.15829	-3.59976	-0.00106
C	2.16524	-1.23419	-0.02692
H	3.96712	-2.49681	-0.04085
H	0.24667	-4.37374	0.03659
H	2.60010	-4.58655	0.00255
H	2.30412	0.80227	-0.05347
H	3.82405	-0.05981	-0.06808

Mg²⁺ guanine – cytosine

Charge=+2, Multiplicity=1

N	-2.61052	-0.03711	0.02913
O	1.23629	2.56983	-0.07040
N	-0.68532	1.23801	-0.02048
C	-2.08767	1.15804	0.00365
N	-2.88581	2.23779	0.00206
C	-2.24699	3.37849	-0.02531
C	-0.88101	3.52903	-0.05089
C	-0.05249	2.41972	-0.04797
N	-2.71709	4.67819	-0.03546
C	-1.66054	5.52027	-0.06499
N	-0.51309	4.87276	-0.07549
H	-2.03211	-0.90577	0.02630
H	-3.61605	-0.09801	0.04688
H	-0.10135	0.34587	-0.01622
H	-3.68792	4.95986	-0.02287
H	-1.77273	6.59371	-0.07830
Mg	1.45076	4.48589	-0.10116
O	-1.10289	-2.22319	0.01710
N	2.94599	-0.12510	-0.03382
N	0.89565	-1.13327	-0.00904
C	2.88131	-2.51154	-0.01200
C	0.12312	-2.25302	0.00700
N	0.75563	-3.48006	0.01205
C	2.09895	-3.60922	0.00302
C	2.22167	-1.24973	-0.01835
H	3.95711	-2.58991	-0.01938
H	0.15265	-4.28890	0.02365
H	2.49260	-4.61628	0.00852
H	2.48475	0.76840	-0.04205
H	3.94843	-0.16363	-0.04308

Ca²⁺ guanine–cytosine

Charge=+2, Multiplicity=1

N	-2.58298	-0.02635	0.12588
O	1.24827	2.53708	-0.29794
N	-0.67352	1.25761	-0.06985
C	-2.06212	1.17282	0.06706
N	-2.85085	2.24999	0.14043
C	-2.21180	3.39024	0.04367
C	-0.85156	3.55722	-0.11985
C	-0.02982	2.43714	-0.16788
N	-2.70333	4.67550	0.07637
C	-1.66509	5.53215	-0.06648
N	-0.51361	4.91001	-0.18933
H	-2.01933	-0.89045	0.00183
H	-3.58350	-0.08686	0.22211
H	-0.09705	0.37090	-0.08356
Ca	1.76233	4.63674	-0.55969
H	-3.67270	4.93583	0.18876
H	-1.79983	6.60293	-0.07610
O	-1.09576	-2.22619	-0.24098
N	2.93860	-0.14267	0.13480
N	0.89972	-1.14774	-0.05726
C	2.87318	-2.53252	0.10355
C	0.12503	-2.26268	-0.14235
N	0.75440	-3.49334	-0.11493
C	2.09120	-3.62701	0.00868
C	2.21776	-1.26905	0.05960
H	3.94410	-2.61578	0.20225
H	0.15213	-4.29975	-0.18306
H	2.48143	-4.63531	0.02510
H	2.47403	0.74792	0.07500
H	3.93527	-0.18024	0.24002

BF₃-NH₃

Charge=0, Multiplicity=1

B	-1.59518	0.54532	0.32606
F	-0.23695	0.73407	0.37665
F	-2.04606	0.02288	-0.85972
F	-2.32812	1.61046	0.78543
N	-1.88362	-0.66855	1.44789
H	-1.37027	-1.50567	1.19306
H	-1.58449	-0.36790	2.36960
H	-2.87397	-0.88713	1.47898

BCl₃-NH₃

Charge=0, Multiplicity=1

B	-1.59730	0.47668	0.37371
Cl	0.21507	0.75918	0.43351
Cl	-2.17485	-0.19770	-1.23203
Cl	-2.57784	1.91478	0.95444
N	-1.87918	-0.69508	1.45460
H	-1.36490	-1.53304	1.19591
H	-1.57836	-0.39161	2.37738
H	-2.87293	-0.90943	1.48346

BBr₃-NH₃

Charge=0, Multiplicity=1

B	-1.62062	0.49314	0.42622
Br	0.36052	0.77141	0.45700
Br	-2.28711	-0.20549	-1.32786
Br	-2.65735	2.06939	1.09335
N	-1.90097	-0.68153	1.48934
H	-1.41915	-1.53020	1.20189
H	-1.56429	-0.40332	2.40867
H	-2.89964	-0.86928	1.54658

BH₃-NH₃

Charge=0, Multiplicity=1

B	-1.58381	0.55528	0.34974
H	-0.38328	0.72225	0.38092
H	-1.98319	0.12157	-0.70965
H	-2.21409	1.51121	0.74819
N	-1.87902	-0.64048	1.44259
H	-1.38608	-1.48859	1.18744
H	-1.57317	-0.36299	2.36835
H	-2.86964	-0.85142	1.48661

BH₃-NMeH₂

Charge=0, Multiplicity=1

B	-1.59029	0.54147	0.39945
H	-0.39079	0.72711	0.43604
H	-1.97430	0.09320	-0.66147
H	-2.23445	1.49911	0.77674
N	-1.87937	-0.63349	1.49587
H	-1.38938	-1.46918	1.19558
C	-1.48404	-0.28508	2.87007
H	-2.86906	-0.85414	1.46563
H	-0.42001	-0.05929	2.87101
H	-1.69613	-1.09524	3.56844
H	-2.02592	0.61129	3.16307

BH₃-NMe₂H

Charge=0, Multiplicity=1

B	-1.65861	0.49965	0.45298
H	-0.45988	0.69270	0.47355
H	-2.05038	0.05252	-0.60590
H	-2.30362	1.45632	0.83556
N	-1.93468	-0.67196	1.55441
H	-1.39656	-1.47217	1.23838
C	-1.44483	-0.29306	2.88935
C	-3.35278	-1.06310	1.59141
H	-0.38434	-0.06317	2.82100
H	-1.61396	-1.09433	3.61145
H	-1.97644	0.60373	3.20305
H	-3.65413	-1.38649	0.59816
H	-3.93824	-0.18679	1.86471
H	-3.52118	-1.86102	2.31737

BH₃-NMe₃

Charge=0, Multiplicity=1

B	-1.64959	0.48063	0.45236
H	-0.45143	0.67820	0.46539
H	-2.05248	0.07545	-0.61921
H	-2.29029	1.42127	0.87602
N	-1.90758	-0.74278	1.51306
C	-1.16084	-1.93826	1.07956
C	-1.44677	-0.33716	2.85395
C	-3.34795	-1.05555	1.56332
H	-0.38655	-0.10000	2.80202
H	-1.61644	-1.14081	3.57503
H	-1.99170	0.55415	3.15628
H	-3.67753	-1.34798	0.56899
H	-3.88925	-0.16164	1.86463
H	-3.53785	-1.86403	2.27386
H	-1.49956	-2.22155	0.08562
H	-1.32323	-2.76194	1.77935
H	-0.10253	-1.69175	1.03217

BH₃-NClH₂

Charge=0, Multiplicity=1

B	-1.53814	0.56757	0.34596
H	-0.32860	0.71229	0.34544
H	-1.97360	0.10722	-0.68119
H	-2.14127	1.51869	0.77989
N	-1.68261	-0.60847	1.46811
H	-1.16707	-1.43357	1.17646
H	-1.29749	-0.29016	2.35227
Cl	-3.29323	-1.16311	1.82886

BH₃-NCl₂H

Charge=0, Multiplicity=1

B	-1.61591	0.60936	0.30585
H	-0.43193	0.81038	0.22872
H	-2.12018	0.10704	-0.67266
H	-2.26226	1.50726	0.79531
N	-1.80504	-0.58507	1.42578
Cl	-1.07122	-2.10160	0.98489
Cl	-1.31931	-0.13703	3.03652
H	-2.79617	-0.79988	1.51139

BH₃-NCl₃

Charge=0, Multiplicity=1

B	-1.57622	0.64506	0.27283
H	-0.38144	0.79375	0.24696
H	-2.06443	0.13474	-0.70278
H	-2.20824	1.54234	0.76857
N	-1.75093	-0.58737	1.43594
Cl	-0.89748	-2.03312	0.95071
Cl	-1.11081	-0.08456	2.98367
Cl	-3.43245	-1.00039	1.65990

V(CO)₅-CO

Charge=-1, Multiplicity=1

V	-1.05210	1.59272	-0.03670
C	0.90067	1.57110	-0.03405
C	-3.00482	1.61663	-0.04089
C	-1.06987	-0.36021	-0.05396
C	-1.05834	1.58186	1.91658
C	-1.04625	1.60436	-1.98915
O	-1.06337	1.57707	3.06784
O	-1.04170	1.61032	-3.14041
O	2.05187	1.55644	-0.03428
O	-4.15598	1.63404	-0.04307
O	-1.07863	-1.51140	-0.06736
C	-1.03419	3.54531	-0.02414
O	-1.02535	4.69655	-0.01610

Cr(CO)₅-CO

Charge=0, Multiplicity=1

Cr	-1.05211	1.59284	-0.03692
C	0.85796	1.57173	-0.03412
C	-2.96212	1.61590	-0.04103
C	-1.06970	-0.31747	-0.05341
C	-1.05809	1.58204	1.87381
C	-1.04646	1.60430	-1.94662
O	-1.06308	1.57722	3.00875
O	-1.04195	1.61002	-3.08156
O	1.99283	1.55718	-0.03416
O	-4.09695	1.63306	-0.04290
O	-1.07824	-1.45232	-0.06656
C	-1.03442	3.50269	-0.02454
O	-1.02574	4.63759	-0.01643

Mn(CO)₅-CO

Charge=+1, Multiplicity=1

Mn	-1.05217	1.59359	-0.03842
C	0.85778	1.57339	-0.03352
C	-2.96213	1.61388	-0.04247
C	-1.07189	-0.31631	-0.05159
C	-1.05710	1.58062	1.87154
C	-1.04733	1.60611	-1.94849
O	-1.05998	1.57267	2.99262
O	-1.04449	1.61318	-3.06958
O	1.97881	1.56117	-0.02988
O	-4.08317	1.62573	-0.04420
O	-1.08351	-1.43732	-0.05906
C	-1.03233	3.50355	-0.02536
O	-1.02056	4.62455	-0.01727