Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

How to Understand Very Weak Cr-Cr Double Bond and Negative Spin Population in Trinuclear Cr Complexes：Theoretical Insight

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Table S1. DFT-optimized Cr-Cr bond distances (Å) of $[Cr_3(dpa)_4]Cl_2$ **1** and $[Cr_3(dpa)_4](N_3)_2$ **2** with various functional

functional	R(Cr^1-Cr^2) / R(Cr^2-Cr^3) [Å]	
	$[Cr_3(dpa)_4]Cl_2$ **1**	$[Cr_3(dpa)_4](N_3)_2$ **2**
B3PW91	2.464 / 2.464	2.461 / 2.461
BLYP	2.429 / 2.429	2.426 / 2.426
B3LYP	2.479 / 2.479	2.475 / 2.475
M06	2.449 / 2.449	2.444 / 2.444
M06L	2.394 / 2.394	2.384 / 2.384
PBE0	2.468 / 2.468	2.463 / 2.463
exp.	2.3647 / 2.3647[S1]	2.131 / 2.534[S2]

Table S2. DFT-optimized bond distance (Å) between metal and ligand of $[Cr_3(dpa)_4Cl_2]$ **1** at experimental Cr-Cr bond distance with various functional.

functional	r(Cr^2-N)	r(Cr^1-N)	r(Cr^1-Cl)	RMSE
B3PW91	2.048	2.141	2.525	0.022
BLYP	2.070	2.156	2.561	0.038
B3LYP	2.067	2.159	2.546	0.038
M06	2.035	2.137	2.492	0.027
M06L	2.035	2.141	2.459	0.041
PBE0	2.043	2.138	2.513	0.023
exp.[S1]	2.023	2.124	2.551	

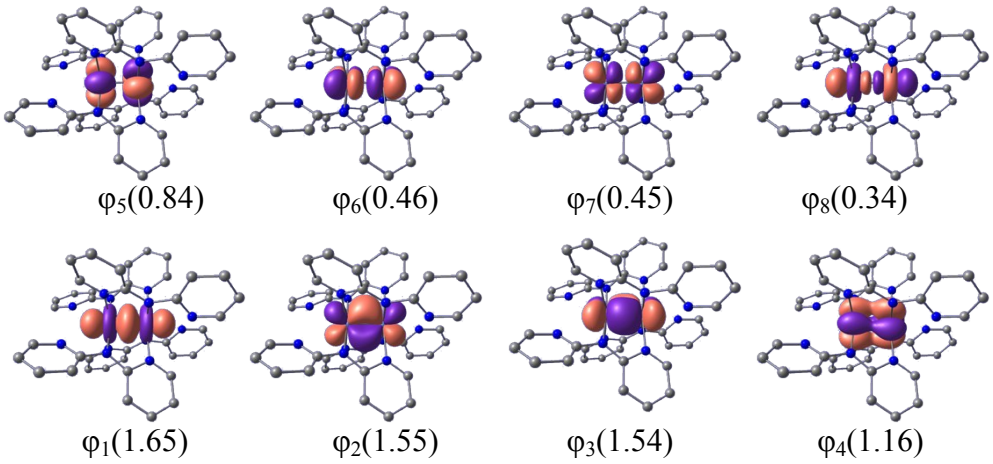


Figure S1. CASSCF natural orbitals of $Cr_2(dpa)_4$ with their occupation number.

Effective Bond Order (EBO) of trinuclear Cr complex $[Cr_3(dpa)_4Cl_2]$ with symmetrical structure 2sym

In this complex, the occupation numbers of natural orbitals are 1.48, 1.19, 1.19, and 1.04 for σ-type φ_1, one π-type φ_2, the other π-type φ_3, and δ-type φ_4, respectively, and 0.96, 0.81, 0.81, and 0.52 for δ*-type φ_9, π*-type φ_{10}, the other π*-type φ_{11}, and δ*-type φ_{12}, respectively, as shown in Figure 3, where the superscript * represents anti-bonding MO. Because non-bonding d orbital does not participate in Cr-Cr bonding and anti-bonding interactions at all (Figure 3), they are not counted in evaluation of EBO. The difference between the occupation numbers of bonding and antibonding MOs is 0.96, 0.38, 0.38, and 0.05 for σ-type, π-type, the other π-type, and δ-type interactions, respectively. The one-half of the sum of them is 0.89, which corresponds to the sum of EBOs of two Cr-Cr bonds. Hence, the EBO of one Cr-Cr bond is 0.44.

This value is much smaller than one, indicating that the Cr-Cr bonding interaction is even weaker than Cr-Cr single bond despite of the fact that this complex has two Cr-Cr double bonds.

This evaluation is the same as that employed for EBO of dinuclear Cr complex but this method cannot be employed for evaluation of EBO of trinuclear Cr complex with nonsymmetrical structure because one Cr-Cr bond is not equivalent to the other Cr-Cr bond.

Table S3. Main configurations of CASSCF and CASCI wavefunctions of (a) $[Cr_3(dpa)_4Cl_2]$ **1sym** and (b) $[Cr_3(dpa)_4(N_3)_2]$ **2asym**.

(a) $[Cr_3(dpa)_4Cl_2]$ **1sym**

CASSCF with natural orbitals												
Configuration												Coefficient
φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9	φ_{10}	φ_{11}	φ_{12}	
σ	π	π	δ	NBδ	NBπ	NBπ	NBσ	δ*	π*	π*	σ*	
2	2	2	2	α	α	α	α	0	0	0	0	0.159
2	2	2	α	α	α	α	α	β	0	0	0	0.151
2	2	2	0	α	α	α	α	2	0	0	0	0.145
2	β	2	α	α	α	α	α	β	0	α	0	−0.122
2	2	β	α	α	α	α	α	β	α	0	0	0.122
2	β	2	2	α	α	α	α	0	α	0	0	−0.116
2	2	β	0	α	α	α	α	0	0	α	0	0.116

CAS-CI with localized orbitals												
Configuration												Coefficient
Cr^1				Cr^2				Cr^3				
σ	π	π	δ	σ	π	π	δ	σ	π	π	δ	
α	α	α	α	β	β	β	β	α	α	α	α	0.696
α	α	α	α	α	β	β	β	β	α	α	α	0.140
β	α	α	α	α	β	β	β	α	α	α	α	0.140
α	α	α	α	2	β	β	β	0	α	α	α	−0.121
0	α	α	α	2	β	β	β	α	α	α	α	0.121
α	α	α	α	0	β	β	β	2	α	α	α	−0.107
2	α	α	α	0	β	β	β	α	α	α	α	0.107

(b) $[Cr_3(dpa)_4(N_3)_2]$ **2asym**.

CASSCF with natural orbitals												
Configuration												Coefficient
φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9	φ_{10}	φ_{11}	φ_{12}	
σ	π	π	δ	NBδ	NBπ	NBπ	NBσ	δ*	π*	π*	σ*	
2	2	2	2	α	α	α	α	0	0	0	0	0.166

2	2	2	0	α	α	α	α	2	0	0	0	0.150
2	β	2	2	α	α	α	α	0	α	0	0	0.107
2	2	β	2	α	α	α	α	0	0	α	0	−0.106
2	2	2	α	α	α	α	α	β	0	0	0	0.103
2	0	2	2	α	α	α	α	0	2	0	0	−0.101
2	2	0	2	α	α	α	α	0	0	2	0	−0.101

CAS-CI with localized orbitals

Configuration												Coefficient
Cr^1				Cr^2				Cr^3				
1	2	3	4	1	2	3	4	1	2	3	4	
α	α	α	α	β	β	β	β	α	α	α	α	0.663
β	α	α	α	β	β	α	β	α	α	α	α	0.122
α	β	α	α	β	α	β	β	α	α	α	α	−0.122
α	α	β	α	α	β	β	β	α	α	α	α	−0.115
β	α	α	α	α	β	β	β	α	α	α	α	−0.112
α	β	α	α	β	β	β	α	α	α	α	α	0.109
β	α	α	α	β	α	β	β	α	α	α	α	0.107

Explanation of Spin Polarization based on CASSCF orbitals:

Spin polarization mechanism cannot be clearly understood on the basis of simple scheme. We wish to present its qualitative explanation based on CASSCF orbitals (Table S3 (a)), using ϕ_4, ϕ_5, and ϕ_9 because these MOs consist of d_{yz} orbitals of Cr^1, Cr^2, and Cr^3.

$$\phi_4 = a_1 \chi_1 + a_2 \chi_2 + a_3 \chi_3, \text{ where } a_1 = a_3 \quad \text{(S1)}$$

$$\phi_5 = b_1 \chi_1 - b_3 \chi_3, \text{ where } b_1 = b_3 \quad \text{(S2)}$$

$$\phi_9 = -c_1 \chi_1 + c_2 \chi_2 + -c_3 \chi_3, \text{ where } c_1 = c_3 \quad \text{(S3)}$$

In the above representations, a_i, b_i, c_i are LCAO coefficient (we defined they are positive; see Figure 3). The total wave function is represented approximately by eq. S4:

$$\psi = \Phi_1 + \lambda \Phi_2 + \bullet\bullet\bullet\bullet \quad \text{(S4)}$$

where λ is positive, as shown in Table S3. The main configuration Φ_1 and the second leading term Φ_2 are represented by eqs. (S5) and (S6), where the other terms are omitted for brevity:

$$\Phi_1 = |\phi_4 \bar{\phi}_4 \phi_5| \quad \text{(S5)}$$

$$\Phi_2 = |\phi_4 \bar{\phi}_9 \phi_5| \quad \text{(S6)}$$

In the main configuration, the α-spin is found on Cr^1 and Cr^3, where their spin densities (ρ_s) are approximately b_1^2 and b_3^2 (= b_1^2), respectively.

$$\rho_s (Cr^1) = \rho_s (Cr^3) = b_1^2 \quad \text{(S7)}$$

In the second leading term, the spin density is approximately represented, as follows:

$$\rho_s (Cr^1) = (1+\lambda)^2 a_1^2 - (a_1 - \lambda c_1)^2 + \lambda^2 b_1^2$$
$$= 2\lambda (a_1^2 + a_1 c_1) + \lambda^2 (a_1^2 - c_1^2 + b_1^2) \quad \text{(S8a)}$$

The LCAO coefficient b^1 is larger than a^1 and c^1 because ϕ_4 and ϕ_9 are three-center MOs and ϕ_5 is two-center MO. The LCAO coefficient c^1 is similar to a^1 but slightly larger than a^1, because a re-normalization factor is smaller in the anti-bonding MO than in the bonding MO; $a^1 \leq c^1$. Thus, eq. S8b is obtained, indicating that the α spin density increases on the Cr^1 and Cr^3, because λ is positive.

$$\rho_s (Cr^1) \sim 2\lambda (a_1^2 + a_1 c_1) + \lambda^2 b_1^2 > 0.0 \quad \text{(S8b)}$$

The same calculation was performed on the Cr^2:

$$\rho_s (Cr^2) = (1+\lambda)^2 a_2^2 - (a_2 + \lambda c_2)^2$$
$$= 2\lambda (a_2^2 - a_2 c_2) + \lambda^2 (a_2^2 - c_2^2) < 0.0. \quad \text{(S9)}$$

Thus, the negative spin density appears on the Cr^2 by the second leading term.

Table S4. Main configurations of CASSCF and CASCI wavefunction of (a) allene molecule and (b) allyl radical.

CASSCF with natural orbitals								
(a) allene molecule					(b) allyl radical			
Configuration				Coefficient	Configuration			coefficient
φ_1	φ_2	φ_3	φ_4		φ_1	φ_2	φ_3	
2	2	0	0	0.917	2	α	0	0.735
0	2	2	0	−0.265	α	α	β	0.552
2	0	0	2	−0.265	β	α	α	0.282
0	0	2	2	0.080	α	β	α	0.269
					0	α	2	−0.053
CASCI with localized orbitals								
(a) allene molecule					(b) allyl radical			
Configuration				Coefficient	Configuration			Coefficient
Lmo1	Lmo2	Lmo3	Lmo1		Lmo1	Lmo2	Lmo3	
α	β	β	α	0.401	α	β	α	0.708
β	α	α	β	0.401	β	α	α	−0.354
β	α	β	α	0.362	α	α	β	0.354
α	β	α	β	0.362				

Formal shortness ratio (FSR) and orbital shortness ratio (OSR)

The FSR for an A-B bond is defined by eq. S11

$$FSR_{AB} = R_{A\text{-}B} / (R_A + R_B) \qquad \text{(S11)}$$

where $R_{A\text{-}B}$ is the A-B bond length in a molecule and R_A and R_B are the atomic radii of A and B, respectively. For example, $FSR_{N\text{-}N}$ of dinitrogen molecule is evaluated to be 0.783 using $R_N = 0.70$. $FSR_{Cr\text{-}Cr}$ for several Cr quadruple bonds was evaluated previously to be 0.74 to 0.78, which is similar to that of dinitrogen molecule. Using R_{Cr} = 1.186 which was employed in the previous theoretical study of Cr dinuclear complex,[S3] the FSR is evaluated to be 1.012 for **1sym** and 0.957 and 1.059 for shorter and longer Cr-Cr bonds, respectively, for **2asym**.

Because the bond distance depends on the orbital expansion, the bond distance must be discussed on the basis of orbital overlap. For this reason, OSR was proposed by Kurokawa *et al*.[S3]

$$OSR = R_{M\text{-}M} / R^{\sigma}_{Smax} \qquad \text{(S12)}$$

where distance R^{σ}_{Smax} is providing the maximum overlap integral for σ-σ bond because the σ-bonding interaction is always more important than the π-bonding interaction. The OSR of dinitrogen molecule is 0.752, which is similar to the FSR value. R^{σ}_{Smax} was evaluated to be 1.520 Å for σ-σ interaction of Cr 3d orbitals.

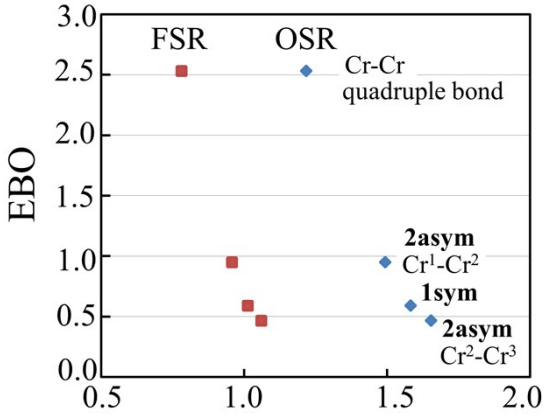
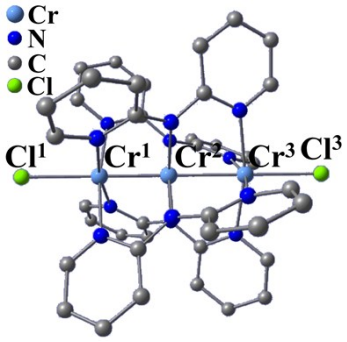


Figure S2. Relationships of EBO with FSR and OSR.



Cr^1-Cr^2 = 2.269 Å, Cr^2-Cr^3 = 2.512 Å
Cr^1-Cl^1 = 2.530 Å, Cr^3-Cl^3 = 2.510 Å

Figure S3. Optimized structure of (a) $[Cr_3(dpa)_4Cl_2]$ **1asym** with non-symmetrical structure. Two Cr-Cr bond distances are fixed to those of $[Cr_3(dpa)_4(N_3)_2]$ **2asym** with asymmetrical structures. The Cr^1-Cl^1 distance was 0.015 Å elongated but the Cr^3-Cl^3 one was shortened only 0.005 Å from symmetrical structure to asymmetrical one.

Complete reference 75

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr. J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT,

References.

S1. F. A. Cotton, L.M. Daniels, C.A. Murillo, I. Pascual, *J. Am. Chem. Soc.* 1997, **119***,* 10223.

S2. Y. Turov, J. F. Berry, *Dalton Trans*., 2012, **41**, 8153.

S3. Y. I. Kurokawa, Y. Nakao, and S. Sakaki, *J. Phys. Chem. A,* 2009, **113**, 3202.

 # Cartesian coordinate of optimized structures

DMRG-CASPT2 results

1

Cr	0.000000000	0.000000000	0.000187001
Cr	0.000000000	0.000000000	2.405187173
Cr	0.000000000	0.000000000	-2.404813172
N	0.000000000	-2.045487145	-0.000010001
N	0.000000000	2.045487145	-0.000010001
N	-0.757710054	-1.994112142	2.186973155
N	0.757710054	1.994112142	2.186973155
N	0.757481057	-1.994219141	-2.187083155
N	-0.757481057	1.994219141	-2.187083155
N	-2.045487145	0.000000000	-0.000010001
N	2.045487145	0.000000000	-0.000010001
N	-1.994112142	0.757710054	2.186973155
N	1.994112142	-0.757710054	2.186973155
N	-1.994219141	-0.757481057	-2.187083155
N	1.994219141	0.757481057	-2.187083155
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C	1.426496103	2.542309185	3.222379231
C	-2.003587145	-3.800116271	3.179941232
C	2.003587145	3.800116271	3.179941232
C	-1.907355135	-4.521589325	1.984060145
C	1.907355135	4.521589325	1.984060145
C	-1.231909087	-3.974907284	0.909167065
C	1.231909087	3.974907284	0.909167065
C	-0.634128047	-2.695569193	1.022782076
C	0.634128047	2.695569193	1.022782076
C	0.633969045	-2.695645193	-1.022860072
C	-0.633969045	2.695645193	-1.022860072
C	1.231702089	-3.975010288	-0.909259067
C	-1.231702089	3.975010288	-0.909259067
C	1.907086138	-4.521730324	-1.984177140
C	-1.907086138	4.521730324	-1.984177140
C	2.003245143	-3.800287274	-3.180078231
C	-2.003245143	3.800287274	-3.180078231

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C	3.974907284	-1.231909087	0.909167065
C	-2.695569193	0.634128047	1.022782076
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C	-2.542474183	-1.426146100	-3.222530232
C	2.542474183	1.426146100	-3.222530232
H	-1.462511107	-1.921055137	4.120763298
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H	2.521458183	4.193872304	4.054377292
H	-2.377274174	-5.503594399	1.886630136
H	2.377274174	5.503594399	1.886630136
H	-1.186935086	-4.500289326	-0.044163001
H	1.186935086	4.500289326	-0.044163001
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H	-1.186772083	4.500356326	0.044095001
H	2.377014173	-5.503731397	-1.886748137
H	-2.377014173	5.503731397	-1.886748137
H	2.521020183	-4.194085303	-4.054553291
H	-2.521020183	4.194085303	-4.054553291

H	1.462098106	-1.921241138	-4.120929295
H	-1.462098106	1.921241138	-4.120929295
H	-1.921055137	1.462511107	4.120763298
H	1.921055137	-1.462511107	4.120763298
H	-4.193872304	2.521458183	4.054377292
H	4.193872304	-2.521458183	4.054377292
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H	5.503594399	-2.377274174	1.886630136
H	-4.500289326	1.186935086	-0.044163001
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H	-4.500356326	-1.186772083	0.044095001
H	4.500356326	1.186772083	0.044095001
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H	1.921241138	1.462098106	-4.120929295
Cl	0.000000000	0.000000000	4.920432355
Cl	0.000000000	0.000000000	-4.920093353

#

2

Cr	0.000000000	0.000000000	2.271000163
Cr	0.000000000	0.000000000	0.000000000
Cr	0.000000000	0.000000000	-2.514000181
N	0.773522055	1.985442144	2.100082151
N	0.030335001	2.049213146	-0.083276005
N	-0.728059051	1.992087144	-2.273566165
N	1.988432144	-0.771970057	2.100142149
N	2.047921149	-0.030993001	-0.083684005
N	1.997981142	0.735390056	-2.272105164
N	-0.791329060	-1.981140145	2.102889150
N	-0.014953999	-2.048166148	-0.068151007
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N	-1.976035140	0.782278055	2.104949152
N	-2.049310149	0.016415999	-0.069143003

N	-2.001690145	-0.720689051	-2.268366162
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C	2.018670146	3.771363271	3.123222226
C	1.942866141	4.501865322	1.930833137
C	1.274757093	3.971049285	0.842854059
C	0.664645048	2.696522194	0.941243069
C	-0.589804044	2.699596195	-1.113990082
C	-1.163930084	3.991535287	-1.014079074
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C	-1.944289140	3.811392276	-3.282327235
C	-1.392932099	2.542547183	-3.309490236
C	2.525254183	-1.425701104	3.149214227
C	3.776744274	-2.017576147	3.119491225
C	4.501208322	-1.949393140	1.922999139
C	3.967537284	-1.282171094	0.835895061
C	2.695681193	-0.667299046	0.938938069
C	2.700730195	0.593722041	-1.110047082
C	3.992207289	1.166914082	-0.999082074
C	4.550252327	1.835833131	-2.071548151
C	3.825828273	1.955490140	-3.263578236
C	2.556999183	1.404098099	-3.301718236
C	-1.474756105	-2.515713181	3.134971225
C	-2.044470146	-3.776897269	3.105441225
C	-1.925346140	-4.517600323	1.922964139
C	-1.240055089	-3.984081286	0.848138063
C	-0.651986048	-2.698867195	0.950112070
C	0.610400046	-2.697920195	-1.098103081
C	1.210576085	-3.976191285	-0.984678070
C	1.863625134	-4.534603328	-2.067670150
C	1.934395140	-3.826007273	-3.272994236
C	1.360870096	-2.566475186	-3.312757238
C	-2.503443180	1.459216106	3.144112228
C	-3.765121271	2.027624148	3.126277224
C	-4.511372325	1.913953139	1.946463138
C	-3.984007286	1.235544091	0.863768065
C	-2.698150197	0.647233047	0.954260068

C	-2.698185197	-0.607853042	-1.100637077
C	-3.978623288	-1.204113084	-0.991551072
C	-4.533507328	-1.859181135	-2.075186150
C	-3.818813272	-1.937740138	-3.276445239
C	-2.557414185	-1.367897099	-3.313009237
H	1.449860104	1.881793133	4.038511288
H	2.530065182	4.155859301	4.005585287
H	2.422686176	5.480290396	1.846993135
H	1.245342088	4.505477322	-0.106022006
H	-1.110855082	4.525096325	-0.065764005
H	-2.277441166	5.534668401	-2.004966144
H	-2.457032176	4.205596300	-4.159283300
H	-1.468757103	1.910181137	-4.196094304
H	1.896504139	-1.432402102	4.042813293
H	4.164225297	-2.525586184	4.002481287
H	5.477363395	-2.433265175	1.835845133
H	4.497568323	-1.255915092	-0.115572010
H	4.519092328	1.108917083	-0.047314002
H	5.541660398	2.285433166	-1.974855143
H	4.222155304	2.473549179	-4.136405296
H	1.946599142	1.492241105	-4.201375302
H	-1.561205114	-1.893161135	4.026054292
H	-2.576020184	-4.155824301	3.977871285
H	-2.388040174	-5.503875397	1.835781134
H	-1.180741087	-4.524168328	-0.096061006
H	1.184051086	-4.492827324	-0.025821003
H	2.334585170	-5.516046399	-1.970099142
H	2.431079175	-4.230533302	-4.154800301
H	1.374669097	-1.950019141	-4.215075304
H	-1.860838132	1.530897112	4.022978290
H	-4.142997299	2.550987184	4.004093288
H	-5.498989398	2.375277170	1.867823134
H	-4.530163324	1.182268086	-0.077295005
H	-4.499752323	-1.174327083	-0.035258001
H	-5.516769398	-2.326920170	-1.980631145
H	-4.219989302	-2.438687178	-4.157393301

H	-1.934149141	-1.392830100	-4.211120302
N	0.139226010	0.034835003	4.425304318
N	-0.578739043	-0.214682013	5.357648388
N	-1.265378093	-0.454698033	6.261136448
N	-0.046031002	-0.140022009	-4.651500334
N	0.264425019	0.551303039	-5.586505402
N	0.562018042	1.209361088	-6.493312469

DFT (B3PW91) results

1

Cr	0.000000000	0.000000000	2.464161000
Cr	0.000000000	0.000000000	0.000000000
Cr	0.000000000	0.000000000	-2.464161000
N	0.736795000	2.003540000	2.201233000
N	0.000000000	2.043123000	0.000000000
N	-0.736795000	2.003540000	-2.201233000
N	2.003540000	-0.736795000	2.201233000
N	2.043123000	0.000000000	0.000000000
N	2.003540000	0.736795000	-2.201233000
N	-0.736795000	-2.003540000	2.201233000
N	0.000000000	-2.043123000	0.000000000
N	0.736795000	-2.003540000	-2.201233000
N	-2.003540000	0.736795000	2.201233000
N	-2.043123000	0.000000000	0.000000000
N	-2.003540000	-0.736795000	-2.201233000
C	1.396289000	2.562966000	3.237276000
C	1.974747000	3.819717000	3.189531000
C	1.892190000	4.529312000	1.985606000
C	1.227098000	3.972094000	0.910005000
C	0.624930000	2.694861000	1.028523000
C	-0.624930000	2.694861000	-1.028523000
C	-1.227098000	3.972094000	-0.910005000
C	-1.892190000	4.529312000	-1.985606000
C	-1.974747000	3.819717000	-3.189531000
C	-1.396289000	2.562966000	-3.237276000
C	2.562966000	-1.396289000	3.237276000
C	3.819717000	-1.974747000	3.189531000

C	4.529312000	-1.892190000	1.985606000
C	3.972094000	-1.227098000	0.910005000
C	2.694861000	-0.624930000	1.028523000
C	2.694861000	0.624930000	-1.028523000
C	3.972094000	1.227098000	-0.910005000
C	4.529312000	1.892190000	-1.985606000
C	3.819717000	1.974747000	-3.189531000
C	2.562966000	1.396289000	-3.237276000
C	-1.396289000	-2.562966000	3.237276000
C	-1.974747000	-3.819717000	3.189531000
C	-1.892190000	-4.529312000	1.985606000
C	-1.227098000	-3.972094000	0.910005000
C	-0.624930000	-2.694861000	1.028523000
C	0.624930000	-2.694861000	-1.028523000
C	1.227098000	-3.972094000	-0.910005000
C	1.892190000	-4.529312000	-1.985606000
C	1.974747000	-3.819717000	-3.189531000
C	1.396289000	-2.562966000	-3.237276000
C	-2.562966000	1.396289000	3.237276000
C	-3.819717000	1.974747000	3.189531000
C	-4.529312000	1.892190000	1.985606000
C	-3.972094000	1.227098000	0.910005000
C	-2.694861000	0.624930000	1.028523000
C	-2.694861000	-0.624930000	-1.028523000
C	-3.972094000	-1.227098000	-0.910005000
C	-4.529312000	-1.892190000	-1.985606000
C	-3.819717000	-1.974747000	-3.189531000
C	-2.562966000	-1.396289000	-3.237276000
H	1.425579000	1.950701000	4.142233000
H	2.483949000	4.220964000	4.065651000
H	2.364686000	5.509513000	1.882744000
H	1.192638000	4.487863000	-0.049045000
H	-1.192638000	4.487863000	0.049045000
H	-2.364686000	5.509513000	-1.882744000
H	-2.483949000	4.220964000	-4.065651000
H	-1.425579000	1.950701000	-4.142233000

H	1.950701000	-1.425579000	4.142233000
H	4.220964000	-2.483949000	4.065651000
H	5.509513000	-2.364686000	1.882744000
H	4.487863000	-1.192638000	-0.049045000
H	4.487863000	1.192638000	0.049045000
H	5.509513000	2.364686000	-1.882744000
H	4.220964000	2.483949000	-4.065651000
H	1.950701000	1.425579000	-4.142233000
H	-1.425579000	-1.950701000	4.142233000
H	-2.483949000	-4.220964000	4.065651000
H	-2.364686000	-5.509513000	1.882744000
H	-1.192638000	-4.487863000	-0.049045000
H	1.192638000	-4.487863000	0.049045000
H	2.364686000	-5.509513000	-1.882744000
H	2.483949000	-4.220964000	-4.065651000
H	1.425579000	-1.950701000	-4.142233000
H	-1.950701000	1.425579000	4.142233000
H	-4.220964000	2.483949000	4.065651000
H	-5.509513000	2.364686000	1.882744000
H	-4.487863000	1.192638000	-0.049045000
H	-4.487863000	-1.192638000	0.049045000
H	-5.509513000	-2.364686000	-1.882744000
H	-4.220964000	-2.483949000	-4.065651000
H	-1.950701000	-1.425579000	-4.142233000
Cl	0.000000000	0.000000000	4.965980000
Cl	0.000000000	0.000000000	-4.965980000

#

2

Cr	0.000000000	-2.461436000	-0.012535000
Cr	0.000000000	0.000000000	-0.021801000
Cr	0.000000000	2.461436000	-0.012535000
N	1.926416000	-2.204474000	0.894368000
N	1.452275000	0.005144000	1.423829000
N	0.896334000	2.204082000	1.910408000
N	0.913794000	-2.204305000	-1.942135000
N	1.441647000	0.005875000	-1.471428000

N	1.934993000	2.202512000	-0.910641000
N	-1.934993000	-2.202512000	-0.910641000
N	-1.441647000	-0.005875000	-1.471428000
N	-0.913794000	2.204305000	-1.942135000
N	-0.896334000	-2.204082000	1.910408000
N	-1.452275000	-0.005144000	1.423829000
N	-1.926416000	2.204474000	0.894368000
C	2.772865000	-3.253527000	0.839443000
C	4.071161000	-3.215841000	1.318553000
C	4.530362000	-2.008201000	1.858041000
C	3.679580000	-0.920648000	1.920674000
C	2.348128000	-1.030091000	1.448643000
C	1.476919000	1.037057000	2.320585000
C	1.968510000	0.933370000	3.646221000
C	1.891984000	2.014338000	4.503372000
C	1.314883000	3.210967000	4.060102000
C	0.821239000	3.242355000	2.768095000
C	0.864859000	-3.254702000	-2.786809000
C	1.341869000	-3.217952000	-4.085867000
C	1.875436000	-2.008944000	-4.548089000
C	1.935549000	-0.920270000	-3.698564000
C	1.465662000	-1.029817000	-2.366384000
C	2.341548000	1.035037000	-1.493300000
C	3.666035000	0.923871000	-1.986284000
C	4.529565000	1.999397000	-1.909929000
C	4.091593000	3.197008000	-1.331748000
C	2.799776000	3.235674000	-0.837278000
C	-2.799776000	-3.235674000	-0.837278000
C	-4.091593000	-3.197008000	-1.331748000
C	-4.529565000	-1.999397000	-1.909929000
C	-3.666035000	-0.923871000	-1.986284000
C	-2.341548000	-1.035037000	-1.493300000
C	-1.465662000	1.029817000	-2.366384000
C	-1.935549000	0.920270000	-3.698564000
C	-1.875436000	2.008944000	-4.548089000
C	-1.341869000	3.217952000	-4.085867000

C	-0.864859000	3.254702000	-2.786809000
C	-0.821239000	-3.242355000	2.768095000
C	-1.314883000	-3.210967000	4.060102000
C	-1.891984000	-2.014338000	4.503372000
C	-1.968510000	-0.933370000	3.646221000
C	-1.476919000	-1.037057000	2.320585000
C	-2.348128000	1.030091000	1.448643000
C	-3.679580000	0.920648000	1.920674000
C	-4.530362000	2.008201000	1.858041000
C	-4.071161000	3.215841000	1.318553000
C	-2.772865000	3.253527000	0.839443000
H	2.344115000	-4.156457000	0.396015000
H	4.704744000	-4.100479000	1.255853000
H	5.559564000	-1.912496000	2.213110000
H	4.032757000	0.039262000	2.296157000
H	2.368488000	-0.019639000	3.990785000
H	2.262946000	1.921746000	5.527164000
H	1.235832000	4.089991000	4.699175000
H	0.335780000	4.134943000	2.368849000
H	0.431540000	-4.159760000	-2.353595000
H	1.283099000	-4.104641000	-4.716926000
H	2.228795000	-1.913486000	-5.577916000
H	2.308305000	0.040376000	-4.052634000
H	4.004053000	-0.031138000	-2.386995000
H	5.552909000	1.901510000	-2.280788000
H	4.734082000	4.073154000	-1.249030000
H	2.423382000	4.139565000	-0.356673000
H	-2.423382000	-4.139565000	-0.356673000
H	-4.734082000	-4.073154000	-1.249030000
H	-5.552909000	-1.901510000	-2.280788000
H	-4.004053000	0.031138000	-2.386995000
H	-2.308305000	-0.040376000	-4.052634000
H	-2.228795000	1.913486000	-5.577916000
H	-1.283099000	4.104641000	-4.716926000
H	-0.431540000	4.159760000	-2.353595000
H	-0.335780000	-4.134943000	2.368849000

H	-1.235832000	-4.089991000	4.699175000
H	-2.262946000	-1.921746000	5.527164000
H	-2.368488000	0.019639000	3.990785000
H	-4.032757000	-0.039262000	2.296157000
H	-5.559564000	1.912496000	2.213110000
H	-4.704744000	4.100479000	1.255853000
H	-2.344115000	4.156457000	0.396015000
N	0.126826000	-4.594533000	-0.079066000
N	-0.578519000	-5.535602000	0.177253000
N	-1.250457000	-6.448417000	0.419274000
N	-0.126826000	4.594533000	-0.079066000
N	0.578519000	5.535602000	0.177253000
N	1.250457000	6.448417000	0.419274000

DFT (M06L) results

1

Cr	0.000000000	0.000000000	-0.000004000
Cr	0.000000000	0.000000000	2.364586000
Cr	0.000000000	0.000000000	-2.364594000
N	0.000000000	2.034925000	-0.000004000
N	2.034925000	0.000000000	-0.000004000
N	0.000000000	-2.034925000	-0.000004000
N	-2.034925000	0.000000000	-0.000004000
N	0.869604000	1.943131000	2.134100000
N	1.943131000	-0.869604000	2.134100000
N	-0.869604000	-1.943131000	2.134100000
N	-1.943131000	0.869604000	2.134100000
N	-0.869607000	1.943129000	-2.134103000
N	1.943129000	0.869607000	-2.134103000
N	0.869607000	-1.943129000	-2.134103000
N	-1.943129000	-0.869607000	-2.134103000
C	1.656563000	2.441928000	3.110209000
C	0.689958000	2.673006000	0.989607000
C	2.284787000	3.673249000	3.028405000
C	1.305873000	3.936541000	0.848764000
C	2.100940000	4.429810000	1.865155000
C	-1.656562000	2.441928000	-3.110213000

C	-0.689958000	2.673004000	-0.989611000
C	-2.284803000	3.673240000	-3.028394000
C	-1.305889000	3.936531000	-0.848765000
C	-2.100962000	4.429794000	-1.865139000
C	2.441928000	-1.656563000	3.110209000
C	2.673006000	-0.689958000	0.989607000
C	3.673249000	-2.284787000	3.028405000
C	3.936541000	-1.305873000	0.848764000
C	4.429810000	-2.100940000	1.865155000
C	2.441928000	1.656562000	-3.110213000
C	2.673004000	0.689958000	-0.989611000
C	3.673240000	2.284803000	-3.028394000
C	3.936531000	1.305889000	-0.848765000
C	4.429794000	2.100962000	-1.865139000
C	-1.656563000	-2.441928000	3.110209000
C	-0.689958000	-2.673006000	0.989607000
C	-2.284787000	-3.673249000	3.028405000
C	-1.305873000	-3.936541000	0.848764000
C	-2.100940000	-4.429810000	1.865155000
C	1.656562000	-2.441928000	-3.110213000
C	0.689958000	-2.673004000	-0.989611000
C	2.284803000	-3.673240000	-3.028394000
C	1.305889000	-3.936531000	-0.848765000
C	2.100962000	-4.429794000	-1.865139000
C	-2.441928000	1.656563000	3.110209000
C	-2.673006000	0.689958000	0.989607000
C	-3.673249000	2.284787000	3.028405000
C	-3.936541000	1.305873000	0.848764000
C	-4.429810000	2.100940000	1.865155000
C	-2.441928000	-1.656562000	-3.110213000
C	-2.673004000	-0.689958000	-0.989611000
C	-3.673240000	-2.284803000	-3.028394000
C	-3.936531000	-1.305889000	-0.848765000
C	-4.429794000	-2.100962000	-1.865139000
H	1.748502000	1.802782000	3.992468000
H	2.905139000	4.024656000	3.851905000

H	2.598871000	5.394798000	1.745978000
H	1.192936000	4.478675000	-0.090967000
H	-1.748493000	1.802789000	-3.992477000
H	-2.905161000	4.024648000	-3.851888000
H	-2.598903000	5.394775000	-1.745951000
H	-1.192954000	4.478660000	0.090967000
H	1.802782000	-1.748502000	3.992468000
H	4.024656000	-2.905139000	3.851905000
H	5.394798000	-2.598871000	1.745978000
H	4.478675000	-1.192936000	-0.090967000
H	1.802789000	1.748493000	-3.992477000
H	4.024648000	2.905161000	-3.851888000
H	5.394775000	2.598903000	-1.745951000
H	4.478660000	1.192954000	0.090967000
H	-1.748502000	-1.802782000	3.992468000
H	-2.905139000	-4.024656000	3.851905000
H	-2.598871000	-5.394798000	1.745978000
H	-1.192936000	-4.478675000	-0.090967000
H	1.748493000	-1.802789000	-3.992477000
H	2.905161000	-4.024648000	-3.851888000
H	2.598903000	-5.394775000	-1.745951000
H	1.192954000	-4.478660000	0.090967000
H	-1.802782000	1.748502000	3.992468000
H	-4.024656000	2.905139000	3.851905000
H	-5.394798000	2.598871000	1.745978000
H	-4.478675000	1.192936000	-0.090967000
H	-1.802789000	-1.748493000	-3.992477000
H	-4.024648000	-2.905161000	-3.851888000
H	-5.394775000	-2.598903000	-1.745951000
H	-4.478660000	-1.192954000	0.090967000
Cl	0.000000000	0.000000000	4.823698000
Cl	0.000000000	0.000000000	-4.823703000

#

2

Cr	0.000000000	-2.383710000	-0.024672000
Cr	0.000000000	0.000000000	-0.017913000

Cr	0.000000000	2.383710000	-0.024672000
N	1.978340000	-2.138780000	0.747062000
N	1.454909000	0.011238000	1.407533000
N	0.786456000	2.155219000	1.943449000
N	0.779769000	-2.148087000	-1.998819000
N	1.432578000	0.003462000	-1.471506000
N	1.981975000	2.141445000	-0.795892000
N	-1.981975000	-2.141445000	-0.795892000
N	-1.432578000	-0.003462000	-1.471506000
N	-0.779769000	2.148087000	-1.998819000
N	-0.786456000	-2.155219000	1.943449000
N	-1.454909000	-0.011238000	1.407533000
N	-1.978340000	2.138780000	0.747062000
C	2.871007000	-3.130615000	0.550075000
C	4.196324000	-3.053768000	0.942337000
C	4.630681000	-1.873542000	1.557394000
C	3.735499000	-0.841896000	1.766612000
C	2.390586000	-0.982642000	1.356439000
C	1.459489000	1.022873000	2.324398000
C	1.987789000	0.922029000	3.630872000
C	1.816068000	1.960744000	4.525584000
C	1.114339000	3.106115000	4.131859000
C	0.616477000	3.147423000	2.841739000
C	0.600706000	-3.143482000	-2.891069000
C	1.022305000	-3.073099000	-4.207702000
C	1.650250000	-1.896368000	-4.633248000
C	1.841066000	-0.861053000	-3.738286000
C	1.399647000	-0.994812000	-2.402702000
C	2.365845000	0.999341000	-1.449643000
C	3.687668000	0.869653000	-1.932363000
C	4.594925000	1.893043000	-1.738429000
C	4.196172000	3.051627000	-1.061387000
C	2.890891000	3.120551000	-0.606081000
C	-2.890891000	-3.120551000	-0.606081000
C	-4.196172000	-3.051627000	-1.061387000
C	-4.594925000	-1.893043000	-1.738429000

C	-3.687668000	-0.869653000	-1.932363000
C	-2.365845000	-0.999341000	-1.449643000
C	-1.399647000	0.994812000	-2.402702000
C	-1.841066000	0.861053000	-3.738286000
C	-1.650250000	1.896368000	-4.633248000
C	-1.022305000	3.073099000	-4.207702000
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C	-0.616477000	-3.147423000	2.841739000
C	-1.114339000	-3.106115000	4.131859000
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C	-1.987789000	-0.922029000	3.630872000
C	-1.459489000	-1.022873000	2.324398000
C	-2.390586000	0.982642000	1.356439000
C	-3.735499000	0.841896000	1.766612000
C	-4.630681000	1.873542000	1.557394000
C	-4.196324000	3.053768000	0.942337000
C	-2.871007000	3.130615000	0.550075000
H	2.461587000	-4.019133000	0.061082000
H	4.870490000	-3.889920000	0.761178000
H	5.675526000	-1.754233000	1.853010000
H	4.062821000	0.107734000	2.191619000
H	2.480825000	-0.003056000	3.931680000
H	2.206819000	1.872385000	5.541723000
H	0.953103000	3.945063000	4.807003000
H	0.048687000	4.008390000	2.481374000
H	0.104083000	-4.030041000	-2.486951000
H	0.854709000	-3.911906000	-4.882090000
H	1.970243000	-1.782895000	-5.671563000
H	2.275555000	0.086656000	-4.058926000
H	3.988317000	-0.068848000	-2.399991000
H	5.623171000	1.782250000	-2.090149000
H	4.880516000	3.879001000	-0.879771000
H	2.540734000	3.998773000	-0.058070000
H	-2.540734000	-3.998773000	-0.058070000
H	-4.880516000	-3.879001000	-0.879771000
H	-5.623171000	-1.782250000	-2.090149000

H	-3.988317000	0.068848000	-2.399991000
H	-2.275555000	-0.086656000	-4.058926000
H	-1.970243000	1.782895000	-5.671563000
H	-0.854709000	3.911906000	-4.882090000
H	-0.104083000	4.030041000	-2.486951000
H	-0.048687000	-4.008390000	2.481374000
H	-0.953103000	-3.945063000	4.807003000
H	-2.206819000	-1.872385000	5.541723000
H	-2.480825000	0.003056000	3.931680000
H	-4.062821000	-0.107734000	2.191619000
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H	-4.870490000	3.889920000	0.761178000
H	-2.461587000	4.019133000	0.061082000
N	0.090929000	-4.497796000	-0.086477000
N	-0.632621000	-5.309278000	0.438299000
N	-1.333288000	-6.093286000	0.945999000
N	-0.090929000	4.497796000	-0.086477000
N	0.632621000	5.309278000	0.438299000
N	1.333288000	6.093286000	0.945999000