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Trinuclear and tetranuclear cyclopentadienyl vanadium carbonyl clusters: unusual carbonyl groups in Herrmann's mysterious $(C_5H_5)_4V_4(CO)_4$ exhibiting low CO stretching frequencies

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Complete Gaussian 09 reference (Reference 19)

Table S1. The values of V-V bond (Å) for $Cp_2V_2(CO)_5$.

	V-V (Å)
BP86	2.452
PBE	2.447
Exp.[7]	2.459

Table S2. The ν(CO) vibrational frequencies (cm^{-1}) for $Cp_2V_2(CO)_5$.

	ν(CO)(cm^{-1})
BP86	1836,1865,1891,1926,1966
PBE	1846,1875,1900,1935,1976
Exp.[7]	1817,1858,1890,1944,1990

Table S3. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol) at the BP86/DZP and PBE/DZP levels of the theory for **4T-1, 4T-4** and **4Q-3** of $Cp_4V_4(CO)_4$.

		4T-1(C_1)	**4T-4(C_1)**	**4Q-3(C_2)**
BP86	E	-5004.565892	-5004.351694	-5004.339048
	ΔE	0	134.4	142.3
PBE	E	-5001.665012	-5001.452130	-5001.439427
	ΔE	0	133.6	141.6

Table S4. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol) at the BP86/ 6-311+ G(2d,2p) and PBE/6-311+ G(2d,2p) levels of the theory for **4T-1, 4T-4** and **4Q-3** of $Cp_4V_4(CO)_4$.

		4T-1(C_1)	**4T-4(C_1)**	**4Q-3(C_2)**
BP86	E	-5004.660285	-5004.440550	-5004.428948
	ΔE	0	137.9	145.2
PBE	E	-5001.755946	-5001.536529	-5001.524838
	ΔE	0	137.7	145.0

Table S5. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol) with the Grimme's dispersion corrections (IOP (3/124=3)) at BP86/DZP and PBE/DZP levels of the theory for **4T-1, 4T-4** and **4Q-3** of $Cp_4V_4(CO)_4$.

		4T-1(C_1)	**4T-4(C_1)**	**4Q-3(C_2)**
BP86	E	-5004.689729	-5004.513805	-5004.500926
	ΔE	0	110.4	118.5
PBE	E	-5001.753646	-5001.568092	-5001.555354
	ΔE	0	116.4	124.4

Table S6. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $\langle S^2 \rangle$, number of imaginary vibrational frequencies (Nimg) for the singlet stationary points of $Cp_4V_4(CO)_4$.

Singlet		**4S-1(S_4)**	**4S-2(C_1)**	**4S-3(C_1)**	**4S-4(D_{2d})**	**4S-5(C_2)**
BP86	E	-5004.564269	-5004.553768	-5004.551280	-5004.544045	-5004.542863
	ΔE	1.0	7.6	9.2	13.7	14.5
	$<S^2>$	0.0	0.0	0.0	0.0	0.0
	Nimg	0	0	0	0	0
PBE	E	-5001.664066	-5001.654313	-5001.650915	-5001.644531	-5001.643272
	ΔE	0.6	6.7	8.8	12.9	13.6
	$<S^2>$	0.0	0.0	0.0	0.0	0.0
	Nimg	0	0	0	0	0

Table S7. Total Energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $\langle S^2 \rangle$, number of imaginary vibrational frequencies (Nimg) for the triplet stationary points of $Cp_4V_4(CO)_4$.

Triplet		**4T-1(C_1)**	**4T-2(C_1)**	**4T-3(C_2)**
BP86	E	-5004.565892	-5004.548402	-5004.545326
	ΔE	0	11.0	12.9
	$<S^2>$	2.12	2.05	2.05
	Nimg	0	0	0
PBE	E	-5001.665012	-5001.648298	-5001.644947
	ΔE	0	10.5	12.6
	$<S^2>$	2.12	2.05	2.06
	Nimg	0	0	0

Table S8. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values ⟨S^2⟩, number of imaginary vibrational frequencies (Nimg) for the quintet stationary points of $Cp_4V_4(CO)_4$

Quintet		**4Q-1(C_1)**	**4Q-2(C_1)**
BP86	E	-5004.557093	-5004.544384
	ΔE	5.5	13.5
	<S^2>	6.09	6.07
	Nimg	0	0
PBE	E	-5001.647534	-5001.644291
	ΔE	11.0	13.0
	<S^2>	6.20	6.08
	Nimg	0	0

Table S9. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the ten lowest energy stationary points of $Cp_4V_4(CO)_4$ (infrared intensities in parentheses are in km/mol).

	PBE
4S-1(S_4)	1551(23), 1553(263), 1553(263), 1559(0)
4S-2(C_1)	1330(65), 1722(292), 1752(770), 1787(506)
4S-3(C_1)	1678(610), 1694(211), 1713(439), 1725(271)
4S-4(D_{2d})	1629(669), 1629(669), 1642(211), 1658(0)
4S-5(C_2)	1626(668), 1626(660), 1639(219), 1655(0)
4T-1(C_1)	1382(50), 1532(189), 1634(345), 1667(323)
4T-2(C_1)	1315(55), 1741(425), 1759(628), 1814(561)
4T-3(C_2)	1529(294), 1529(26), 1540(339), 1569(17)
4Q-1(C_1)	1476(117), 1503(226), 1657(373), 1672(243)
4Q-2(C_1)	1646(372), 1667(344), 1694(649), 1707(134)

Table S10. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), number of imaginary vibrational frequencies (Nimg) for the three singlet stationary points of $Cp_3V_3(CO)_9$.

		9S-1(C_3)	**9S-2(C_1)**	**9S-3(C_s)**
BP86	E	-4433.578680	-4433.568298	-4433.553551
	ΔE	0	6.5	15.8
	Nimg	0	0	0
PBE	E	-4430.676327	-4430.665704	-4430.651992
	ΔE	0	6.7	15.3
	Nimg	0	0	0

Table S11. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the three singlet stationary points of $Cp_3V_3(CO)_9$ (infrared intensities in parentheses are in km/mol).

	PBE
9S-1(C_3)	1840(40), 1840(40), 1880(1013), 1904(633), 1904(633), 1915(260), 1932(430), 1932(430), 1993(880)
9S-2(C_1)	1765(324), 1793(147), 1874(305), 1901(563), 1912(33), 1922(142), 1944(616), 1961(1464), 1999(641)
9S-3(C_s)	1723(337), 1804(251), 1868(410), 1870(314), 1879(140), 1930(17), 1949(1408), 1950(438), 1993(1356)

Table S12. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $\langle S^2 \rangle$, number of imaginary vibrational frequencies (Nimg) at BP86/TZP level of the theory for the singlet stationary points of $Cp_4V_4(CO)_4$.

		4S-1(S_4)	**4S-2(C_1)**	**4S-3(C_1)**	**4S-4(D_{2d})**	**4S-5(C_2)**
BP86	E	-5004.838821	-5004.832983	-5004.832489	-5004.821611	-5004.820511
	ΔE	2.0	5.7	6.0	12.8	13.5
	$\langle S^2 \rangle$	0.0	0.0	0.0	0.0	0.0
	Nimg	0	0	0	3(11*i*,7*i*,7*i*)[a]	0

[a]These imaginary frequencies were reduced to 0*i* by using the larger (120,974) integration.

Table S13. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values ⟨S^2⟩, number of imaginary vibrational frequencies (Nimg) at BP86/TZP level of the theory for the triplet stationary points of $Cp_4V_4(CO)_4$.

		4T-1(C_1)	**4T-2(C_1)**	**4T-3(C_2)**
BP86	E	-5004.842002	-5004.827879	-5004.819127
	ΔE	0	8.9	14.4
	<S^2>	2.1	2.1	2.1
	Nimg	0	0	0

Table S14. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values ⟨S^2⟩, number of imaginary vibrational frequencies (Nimg) at BP86/TZP level of the theory for the quintet stationary points of $Cp_4V_4(CO)_4$.

		4Q-1(C_1)	**4Q-2(C_2)**
BP86	E	-5004.831936	-5004.823626
	ΔE	6.3	11.5
	<S^2>	6.1	6.0
	Nimg	0	0

Table S15. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), number of imaginary vibrational frequencies (Nimg) at BP86/TZP level of the theory for the singlet stationary points of $Cp_3V_3(CO)_9$.

		9S-1(C_3)	**9S-2(C_1)**	**9S-3(C_s)**
BP86	E	-4433.929323	-4433.917701	-4433.901157
	ΔE	0	7.3	17.7
	Nimg	0	0	0

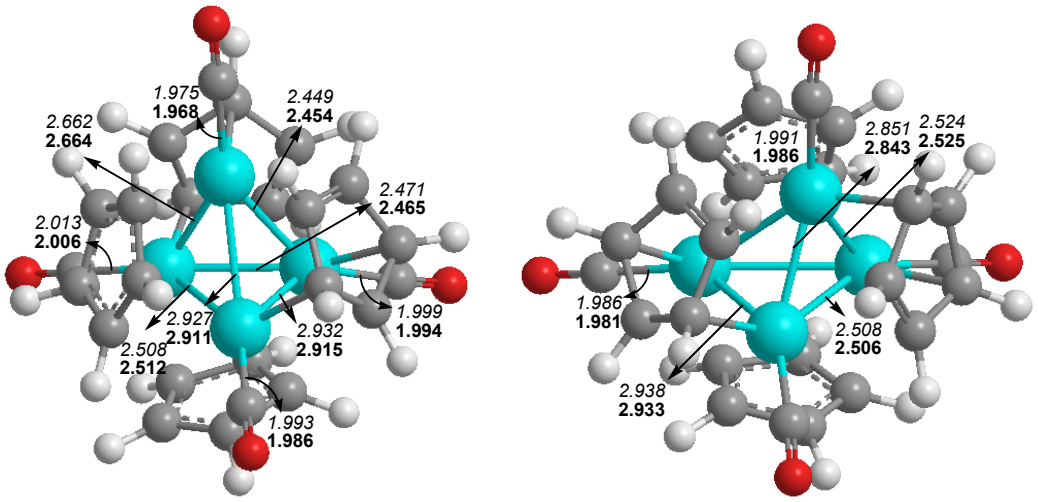
Table S16. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $\langle S^2 \rangle$, number of imaginary vibrational frequencies (Nimg) at PBE0/DZP level of the theory for the lowest energy structure and one quintet stationary point of $Cp_4V_4(CO)_4$.

		4T-1(C_1)	**4Q-1(C_1)**
PBE0	E	-5001.657687	-5001.652138
	ΔE	0	3.5
	$<S^2>$	3.5	7.3
	Nimg	0	0

Table S17. Total energies (E, in hartree), number of imaginary vibrational frequencies (Nimg) at BP86/DZP and PBE/DZP levels of the theory for the stationary points of $Cp_2V_2(CO)_n$(n=6, 5, 4, 3, 2, 1).

		$Cp_2V_2(CO)_6$(C_{2v})	$Cp_2V_2(CO)_5$(C_s)	$Cp_2V_2(CO)_4$(C_s)
BP86	E	–2955.732464	-2842.387986	-2729.007233
	Nimg	0	0	0
PBE	E	-2953.793219	-2840.569460	-2727.309052
	Nimg	0	0	0
		$Cp_2V_2(CO)_3$(C_s)	$Cp_2V_2(CO)_2$(C_s)	$Cp_2V_2(CO)$ (C_s)
BP86	E	-2615.630904	-2502.223405	-2388.804308
	Nimg	0	1(16*i*) [a]	1(3*i*)
PBE	E	-2614.054169	-2500.767570	-2387.470156
	Nimg	0	1(13*i*)[a]	1(7*i*)

[a]These imaginary frequencies were reduced to 0*i* by using the larger (120,974) integration.



4T-4(C_1) **4Q-3(C_2)**

Figure S1. The optimized structures for $Cp_4V_4(CO)_4$ by BP86 and PBE methods. The upper numbers (italics) were obtained by the BP86 method, while the lower numbers (bold face) were obtained by the PBE method. The data in all of the other figures in the present paper have the same arrangement. In all of the structure figures blue circles (●) represent vanadium atoms; red circles (●) represent oxygen atoms; and gray circles (●) represent carbon atoms.

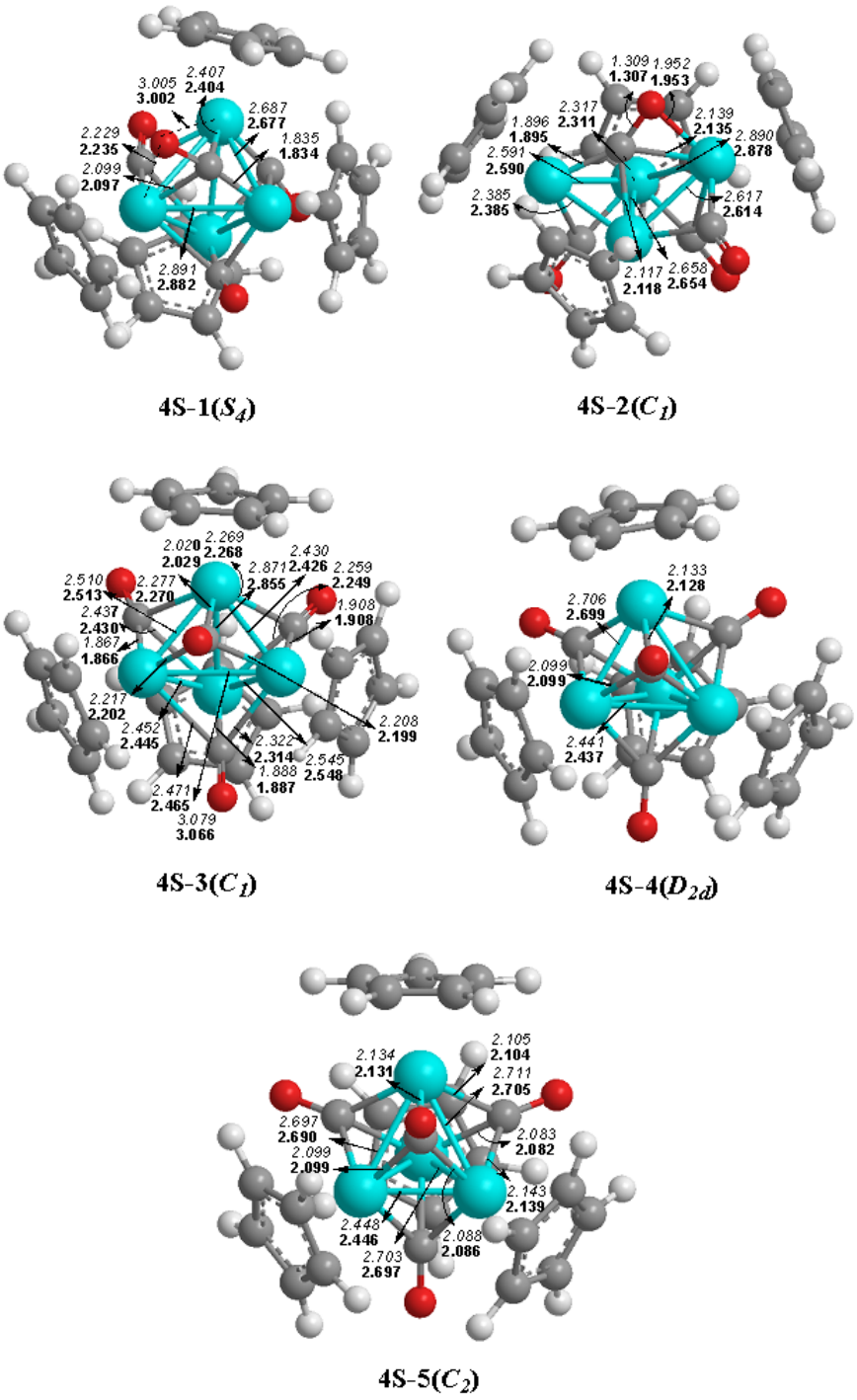


Figure S2. The five optimized singlet structures for $Cp_4V_4(CO)_4$ by BP86 and PBE methods.

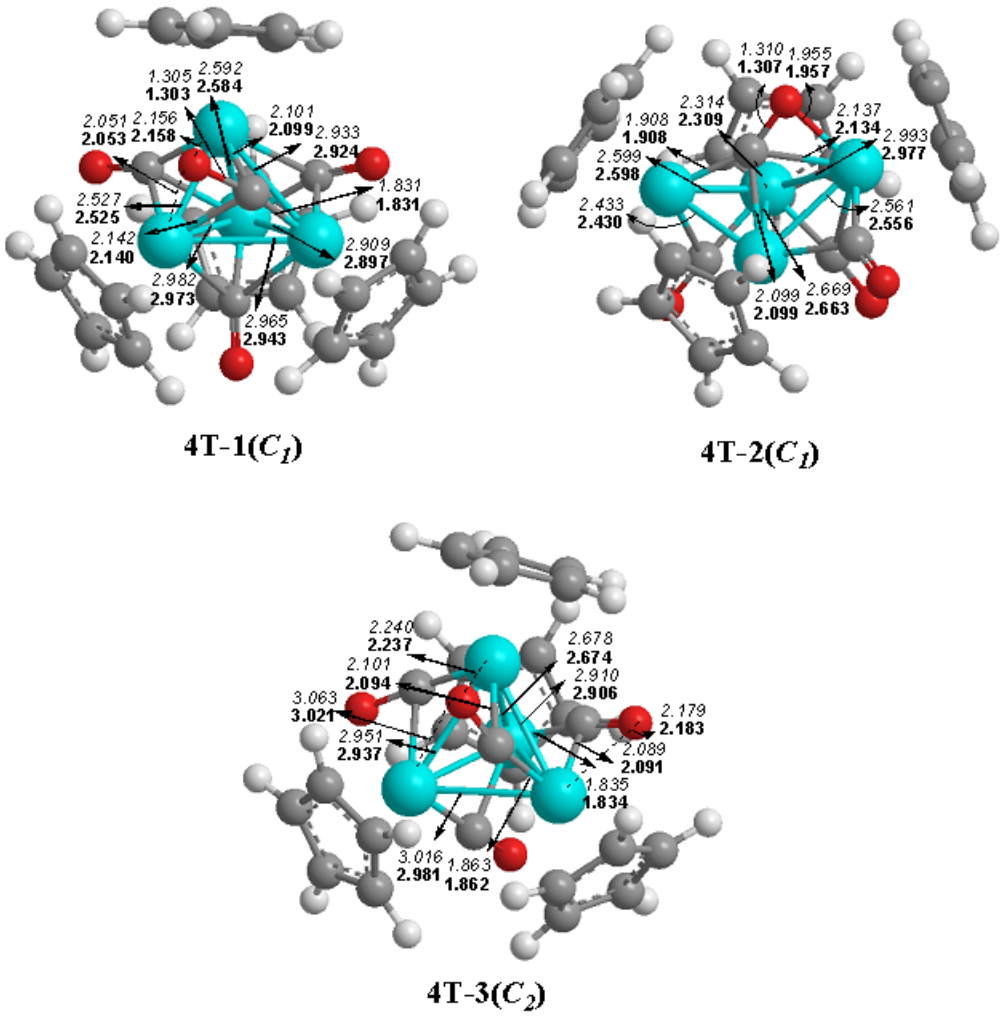


Figure S3. The three optimized triplet structures for $Cp_4V_4(CO)_4$ by BP86 and PBE methods.

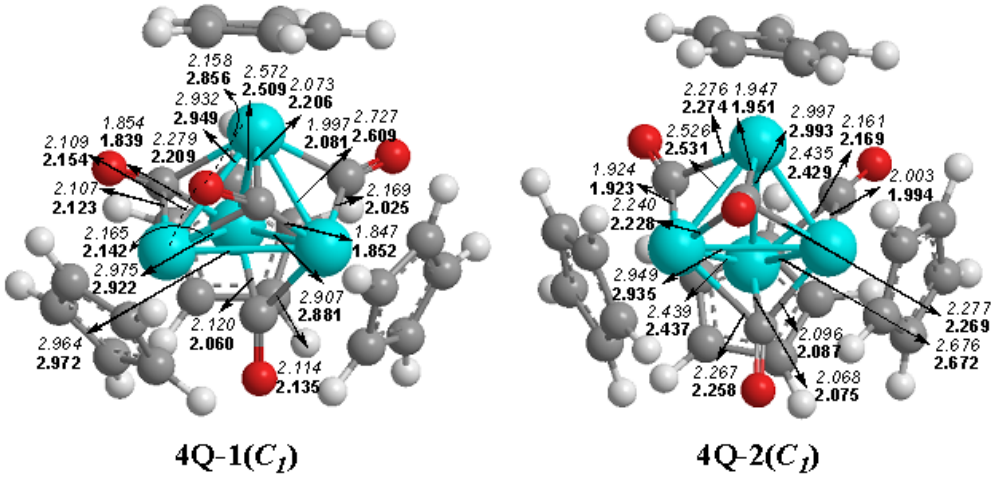


Figure S4. The two optimized quintet structures for $Cp_4V_4(CO)_4$ by BP86 and PBE methods.

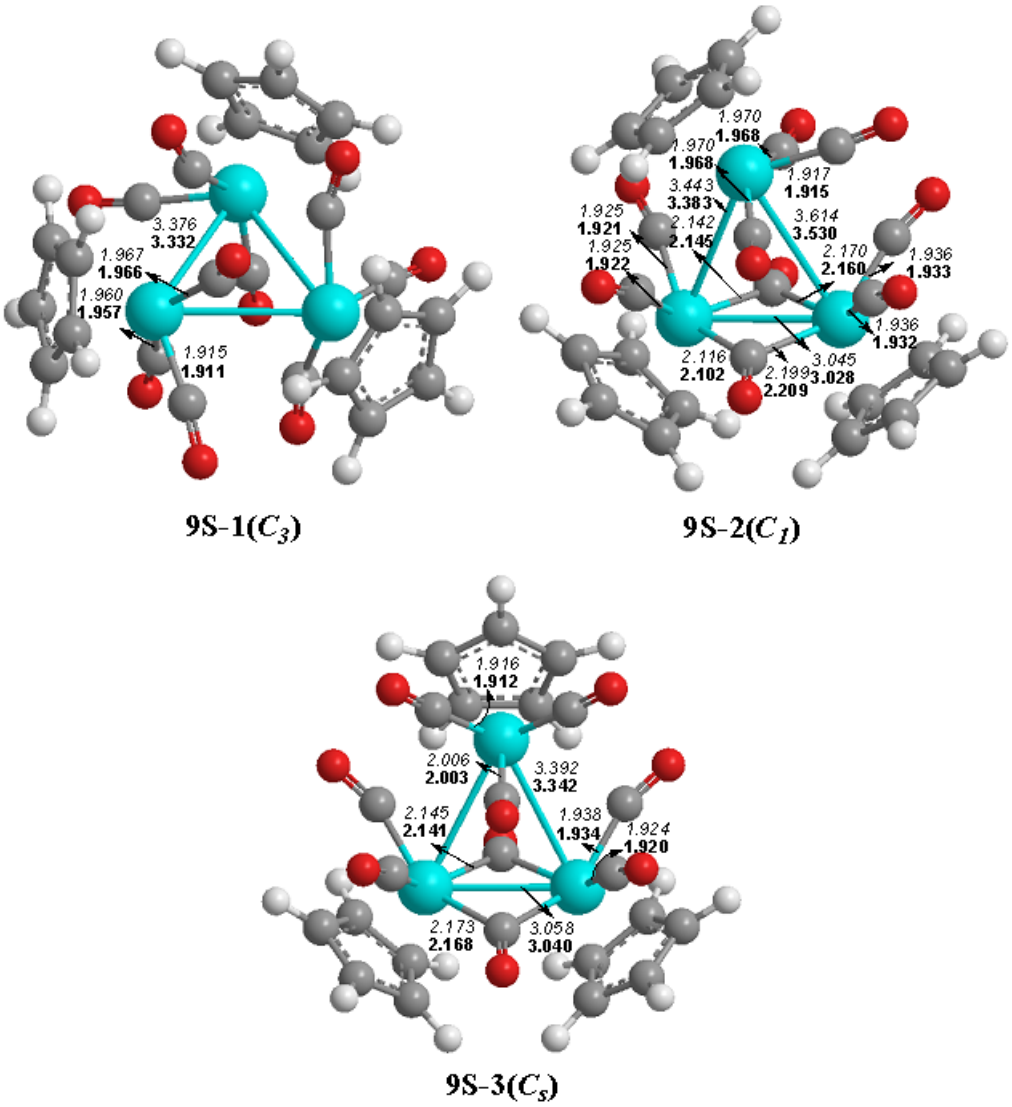
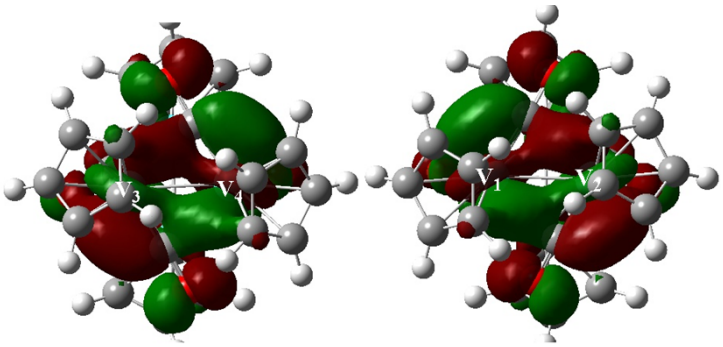


Figure S5. The three optimized singlet structures for $Cp_3V_3(CO)_9$ by BP86 and PBE methods.

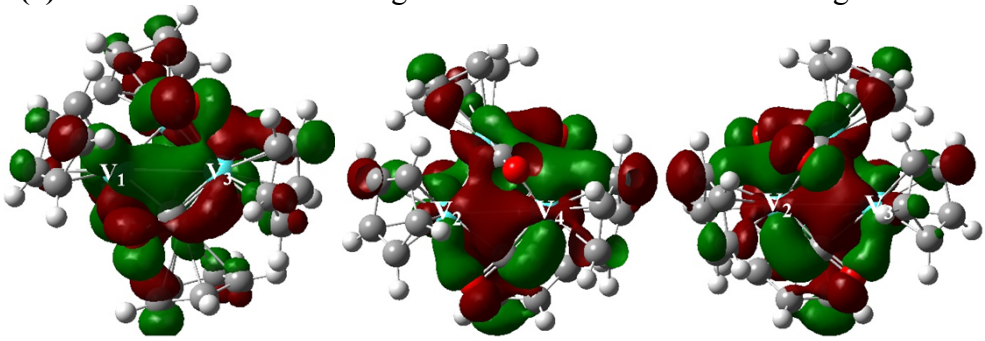
4S-1 has two short V-V double bonds, namely, 2.687 Å for V_1-V_2 and V_3-V_4. The other four V-V single bonds are relatively longer, namely, 2.891 Å for V_1-V_3, V_1-V_4, V_2-V_3 and V_2-V_4 bonds. This leads to give 16-electron configuration for each vanadium atom. The molecular orbital diagrams of **4S-1** are shown in Figure S6. The HOMO-2 and HOMO-7 orbitals can be assigned to the π-bonding orbital and σ-bonding orbital of V_1-V_2 double bond, respectively. HOMO-1 and HOMO-5 orbitals can be regarded as π-bonding orbital and σ-bonding orbital of V_3-V_4 double bond, respectively. The HOMO, HOMO-6, HOMO-4 and HOMO-3 orbitals are consistent with the σ-bonding orbitals of V_1-V_3, V_1-V_4, V_2-V_3 and V_2-V_4 single bonds, respectively.



HOMO-1 V_3-V_4 π-bonding

HOMO-2 V_1-V_2 π-bonding

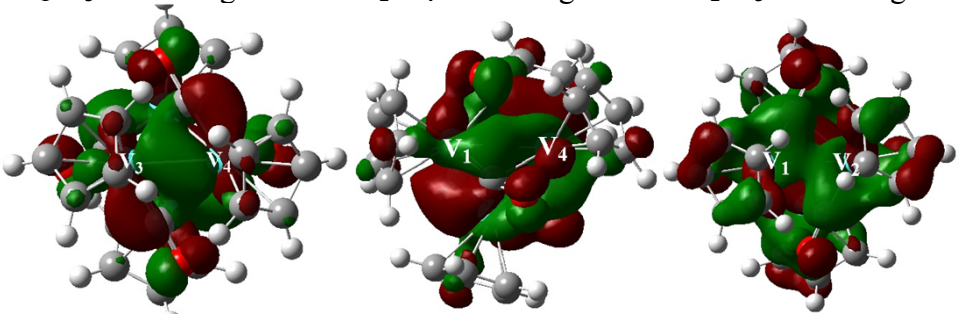
(a) The molecular orbital diagrams related to the V-V π-bonding of **4S-1**.



HOMO V_1-V_3 σ-bonding

HOMO-3 V_2-V_4 σ-bonding

HOMO-4 V_2-V_3 σ-bonding



HOMO-5 V_3-V_4 σ-bonding

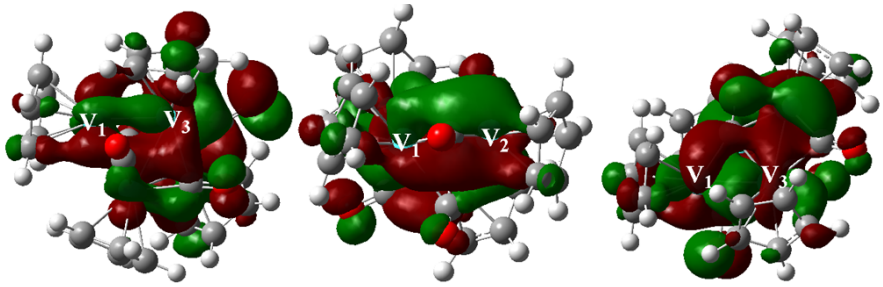
HOMO-6 V_1-V_4 σ-bonding

HOMO-7 V_1-V_2 σ-bonding

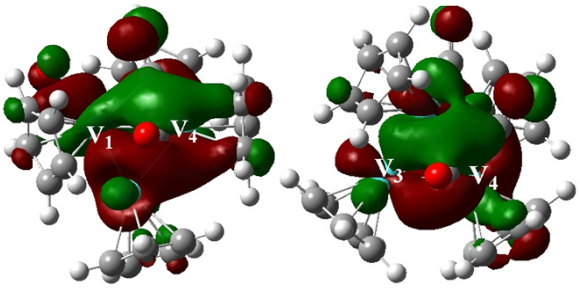
(b) The molecular orbital diagrams related to the V-V σ-bonding of **4S-1**.

Figure S6. The comments and molecular orbital diagrams related to the V-V π-bonding orbitals (a) and V-V σ-bonding orbitals (b) of **4S-1**.

4S-2 has one short V-V triple bond, i.e. 2.385 Å for V_1-V_3. The other three V-V double bonds are relatively longer, namely, 2.617 Å for V_1-V_2 bond, 2.591 Å for V_3-V_4 bond and 2.658 Å for V_1-V_4 bond. The distance for the last V_2-V_4 single bond is 2.890 Å. The distance for V_2···V_3 is 3.845 Å, indicating there was only a slight bonding interaction between these two vanadium atoms. The four-electron donor η^2-μ_4-CO group in **4S-2** accommodates the electron deficiency of this structure, thus to give 18-electron configurations for three vanadium atoms and 16-electron configuration for one vanadium atom. The molecular orbital diagrams of **4S-2** are shown in Figure S7. The HOMO, HOMO-2 and HOMO-6 orbitals are consistent with two π-bonding orbitals and σ-bonding orbital of V_1-V_3 triple bond, respectively. The HOMO-1 and HOMO-14 orbitals are corresponding to π-bonding orbital and σ-bonding orbital of V_1-V_2 double bond, respectively. The HOMO-5 and HOMO-3 orbitals can be regarded as π-bonding orbital and σ-bonding orbital of V_3-V_4 double bond, respectively. The HOMO-4 and HOMO-15 orbitals can be assigned as π-bonding orbital and σ-bonding orbital of V_1-V_4 double bond, respectively. The HOMO-7 orbital is corresponding to σ-bonding orbital of V_2-V_4 single bond.

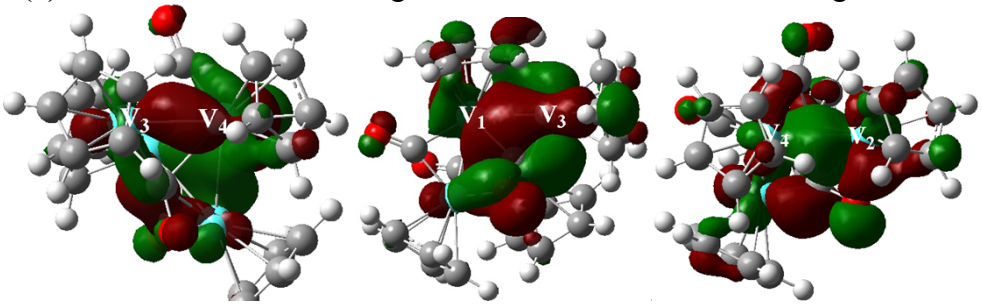


HOMO V_1-V_3 π-bonding | **HOMO-1** V_1-V_2 π-bonding | **HOMO-2** V_1-V_3 π-bonding

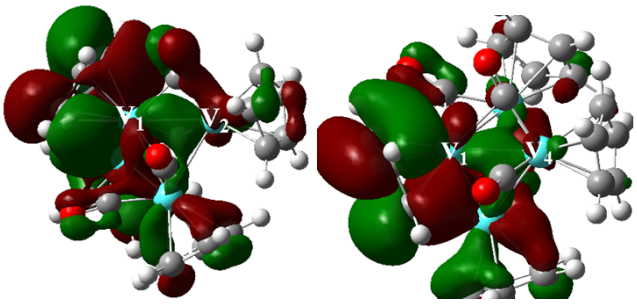


HOMO-4 V_1-V_4 π-bonding | **HOMO-5** V_3-V_4 π-bonding

(a) The molecular orbital diagrams related to the V-V π-bonding of **4S-2**.



HOMO-3 V_3-V_4 σ-bonding | **HOMO-6** V_1-V_3 σ-bonding | **HOMO-7** V_2-V_4 σ-bonding



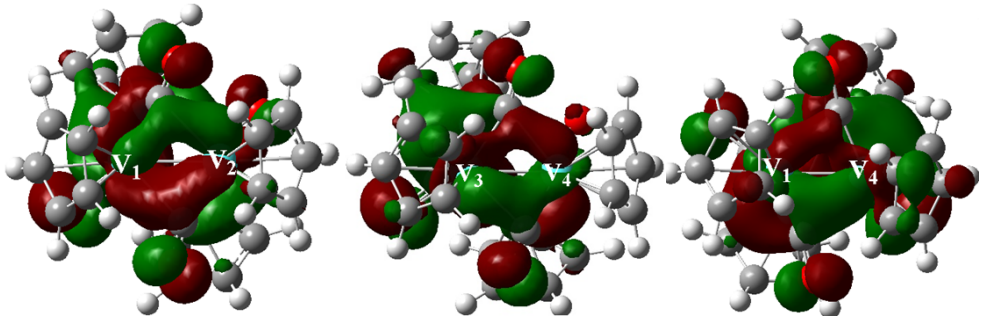
HOMO-14 **HOMO-15**

V_1-V_2 σ-bonding V_1-V_4 σ-bonding

(b) The molecular orbital diagrams related to the V-V σ-bonding of **4S-2.**

Figure S7. The comments and molecular orbital diagrams related to the V-V π-bonding orbitals (a) and V-V σ-bonding orbitals (b) of **4S-2**.

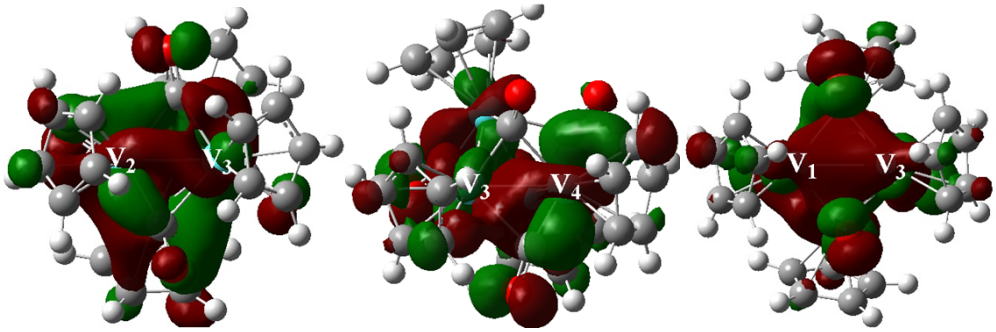
4S-3 has two short V-V triple bonds, namely, 2.452 Å for V_1-V_4 and 2.430 Å for V_2-V_3. The distances for the relatively longer V_1-V_2 and V_3-V_4 double bonds are 2.545 and 2.510 Å. The last two V-V single bonds, namely, V_1-V_3 and V_2-V_4 have distances of 2.871 and 3.079 Å, respectively. This leads to the favored 18-electron configuration for each vanadium atom. The molecular orbital diagrams of **4S-3** are shown in Figure S8. The HOMO-6, HOMO-13 and HOMO-4 orbitals are corresponding to two π-bonding orbitals and σ-bonding orbital of V_1-V_4 triple bonds, respectively. The HOMO-10, HOMO-15 and HOMO orbitals are consistent with two π-bonding orbitals and σ-bonding orbital of V_2-V_3 triple bond, respectively. The HOMO-2 and HOMO-12 orbitals are corresponding to π-bonding orbital and σ-bonding orbital of V_1-V_2 double bond, respectively. The HOMO-5 and HOMO-1 orbitals can be regarded as π-bonding orbital and σ-bonding orbital of V_3-V_4 double bond, respectively. The HOMO-3 and HOMO-7 orbitals can be assigned as σ-bonding orbitals of V_1-V_3 and V_2-V_4 single bonds, respectively.



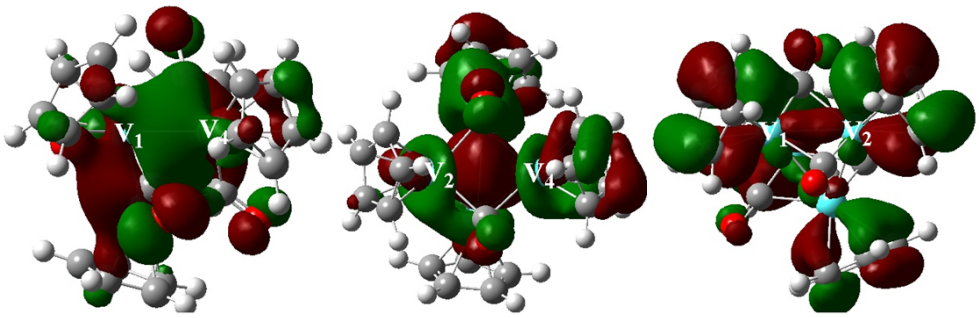
HOMO-2 V_1-V_2 π-bonding | **HOMO-5** V_3-V_4 π-bonding | **HOMO-6** V_1-V_4 π-bonding

HOMO-10 V_2-V_3 π-bonding | **HOMO-13** V_1-V_4 π-bonding | **HOMO-15** V_2-V_3 π-bonding

(a) The molecular orbital diagrams related to the V-V π-bonding of **4S-3.**



HOMO V_2-V_3 σ-bonding | **HOMO-1** V_3-V_4 σ-bonding | **HOMO-3** V_1-V_3 σ-bonding



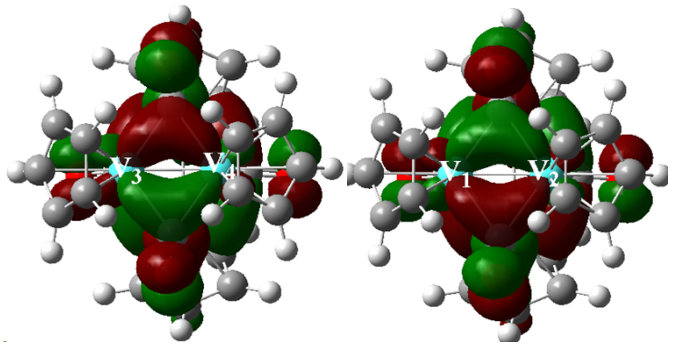
HOMO-4 **HOMO-7** **HOMO-12**

V_1-V_4 σ-bonding V_2-V_4 σ-bonding V_1-V_2 σ-bonding

(b) The molecular orbital diagrams related to the V-V σ-bonding of **4S-3.**

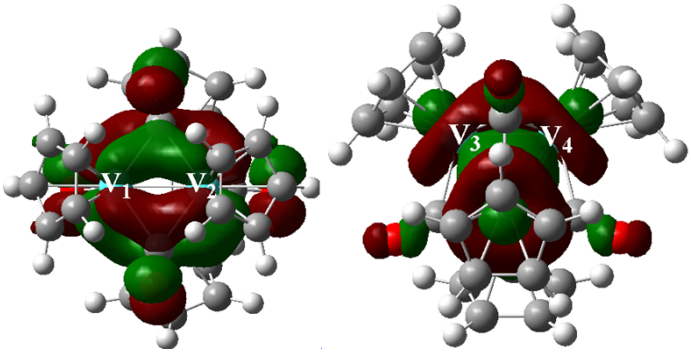
Figure S8. The comments and molecular orbital diagrams related to the V-V π-bonding orbitals (a) and V-V σ-bonding orbitals (b) of **4S-3**.

4S-4 has two short V-V triple bonds, namely, 2.441 Å for V_1-V_2 and V_3-V_4. The other four long V-V single bonds are relatively longer, i.e. 2.706 Å for V_1-V_3, V_1-V_4, V_2-V_3 and V_2-V_4 bonds. This leads to 18-electron configurations for two vanadium atoms and 16-electron configuration for another two vanadium atoms. The molecular orbital diagrams of **4S-4** are shown in Figure S9. The HOMO-1, HOMO-4 and HOMO-14 orbitals can be regarded as two π-bonding orbitals and σ-bonding orbital of V_1-V_2 triple bond, respectively. The HOMO, HOMO-7 and HOMO-6 orbitals are corresponding to two π-bonding orbitals and σ-bonding orbital of V_3-V_4 triple bond, respectively. The HOMO-11, HOMO-5, HOMO-3 and HOMO-2 orbitals can be considered as σ-bonding orbitals of V_1-V_3, V_1-V_4, V_2-V_3 and V_2-V_4 single bonds, respectively.



HOMO V_3-V_4 π-bonding

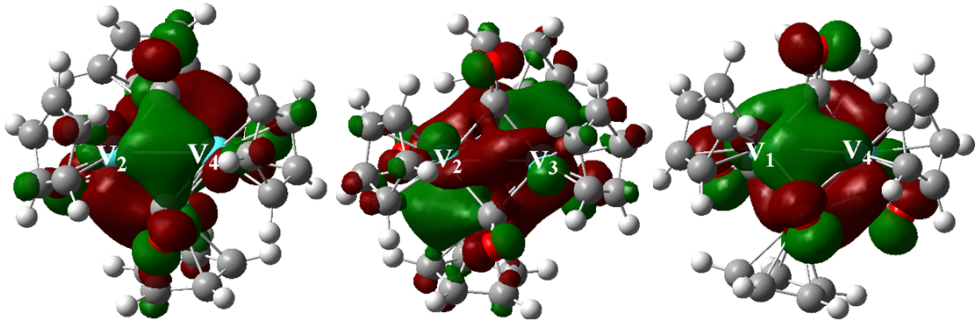
HOMO-1 V_1-V_2 π-bonding



HOMO-4 V_1-V_2 π-bonding

HOMO-7 V_3-V_4 π-bonding

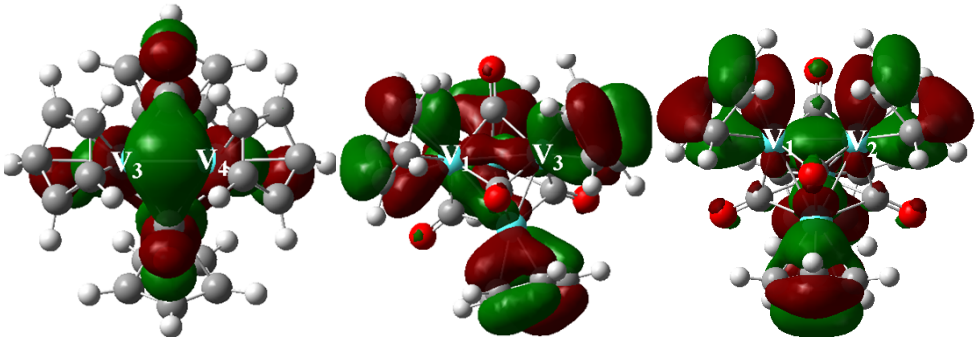
(a) The molecular orbital diagrams related to the V-V π-bonding of **4S-4.**



HOMO-2 V_2-V_4 σ-bonding

HOMO-3 V_2-V_3 σ-bonding

HOMO-5 V_1-V_4 σ-bonding



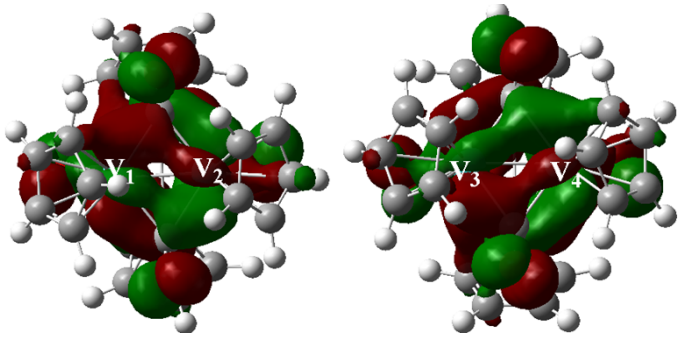
HOMO-6 **HOMO-11** **HOMO-14**

V_3-V_4 σ-bonding V_1-V_3 σ-bonding V_1-V_2 σ-bonding

(b) The molecular orbital diagrams related to the V-V σ-bonding of **4S-4.**

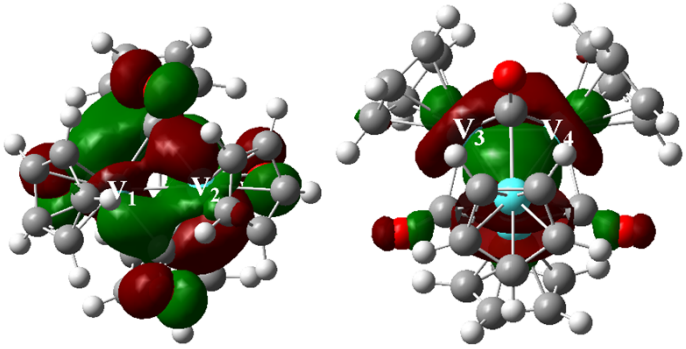
Figure S9. The comments and molecular orbital diagrams related to the V-V π-bonding orbitals (a) and V-V σ-bonding orbitals (b) of **4S-4**.

4S-5 has two short V-V triple bonds, namely, V_1-V_2 and V_3-V_4 with distance of 2.448 Å, and four longer V-V single bonds, i.e. 2.771 Å for V_1-V_3, 2.697 Å for V_1-V_4, 2.703 Å for V_2-V_3 and 2.711 Å for V_2-V_4. This leads to 18-electron configurations for two vanadium atoms and 16-electron configurations for another two vanadium atoms. The molecular orbital diagrams of **4S-5** are shown in Figure S10. The HOMO, HOMO-5 and HOMO-6 orbitals can be regarded as two π-bonding orbitals and σ-bonding orbital of V_1-V_2 triple bond, respectively. The HOMO-1, HOMO-7 and HOMO-14 orbitals are corresponding to two π-bonding orbitals and σ-bonding orbital of V_3-V_4 triple bond, respectively. The HOMO-3, HOMO-13, HOMO-2 and HOMO-4 orbitals can be regarded as σ-bonding orbitals of V_1-V_3, V_1-V_4, V_2-V_3 and V_2-V_4 single bonds, respectively.



HOMO V_1-V_2 π-bonding

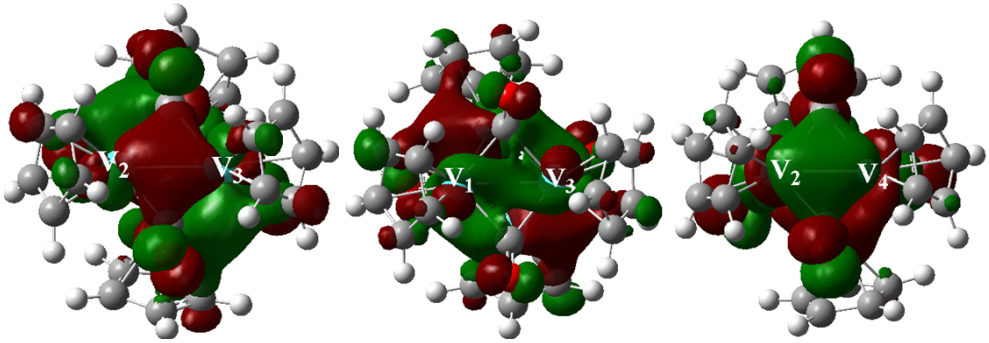
HOMO-1 V_3-V_4 π-bonding



HOMO-5 V_1-V_2 π-bonding

HOMO-7 V_3-V_4 π-bonding

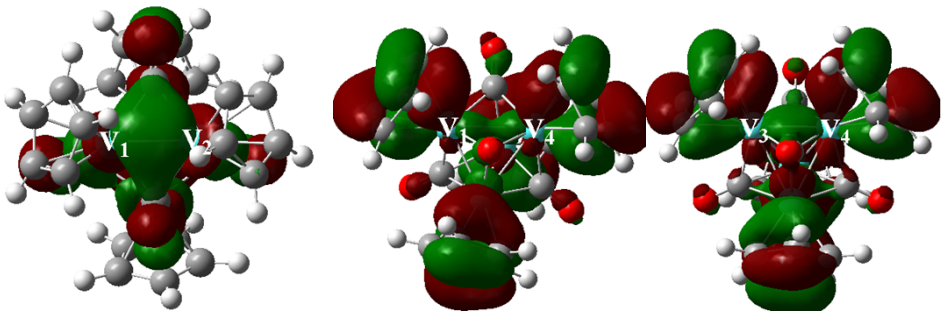
(a) The molecular orbital diagrams related to the V-V π-bonding of **4S-5.**



HOMO-2 V_2-V_3 σ-bonding

HOMO-3 V_1-V_3 σ-bonding

HOMO-4 V_2-V_4 σ-bonding



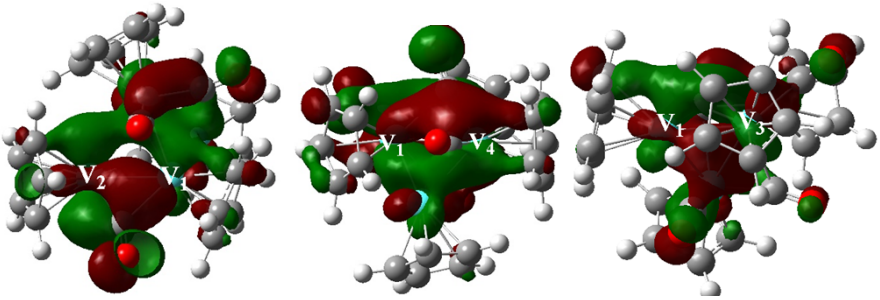
HOMO-6 **HOMO-13** **HOMO-14**

V_1-V_2 σ-bonding V_1-V_4 σ-bonding V_3-V_4 σ-bonding

(b) The molecular orbital diagrams related to the V-V σ-bonding of **4S-5.**

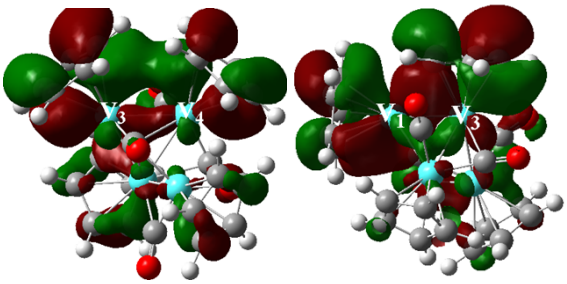
Figure S10. The comments and molecular orbital diagrams related to the V-V π-bonding orbitals (a) and V-V σ-bonding orbitals (b) of **4S-5**.

4T-2 has one short V_1-V_3 triple bond with distance of 2.443 Å. The relatively longer V-V double bonds are with distance of 2.561 Å for V_1-V_2, 2.669 Å for V_1-V_4 and 2.599 Å for V_3-V_4. The distance of V_2-V_4 single bond is 2.993 Å. The distance for $V_2 \cdots V_3$ is 3.874 Å, which is too long for any significant direct metal-metal interaction between these two vanadium atoms. The four-electron donor η^2-μ_4-CO group in **4T-2** accommodates the electron deficiency of this structure, leading to 17-electron configurations for two vanadium atoms and 18-electron configurations for another two vanadium atoms. The molecular orbital diagrams of **4T-2** are shown in Figure S11. The HOMO-7, HOMO-16 and HOMO-13 orbitals can be assigned as two π-bonding orbitals and σ-bonding orbital of V_1-V_3 triple bond, respectively. The HOMO-2 and HOMO-3 orbitals are corresponding to π-bonding orbital and σ-bonding orbital of V_1-V_2 double bond, respectively. The HOMO-5 and HOMO-8 orbitals can be regarded as π-bonding orbital and σ-bonding orbital of V_1-V_4 double bond, respectively. The HOMO-14 and HOMO-4 orbitals can be regarded as π-bonding orbital and σ-bonding orbital of V_3-V_4 double bond, respectively. The HOMO-6 orbital is consistent with σ-bonding orbital of V_2-V_4 single bond.



HOMO-2 **HOMO-5** **HOMO-7**

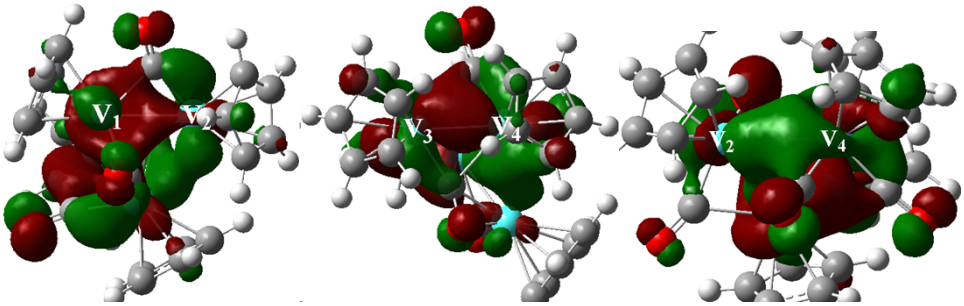
V_1-V_2 π-bonding V_1-V_4 π-bonding V_1-V_3 π-bonding



HOMO-14 **HOMO-16**

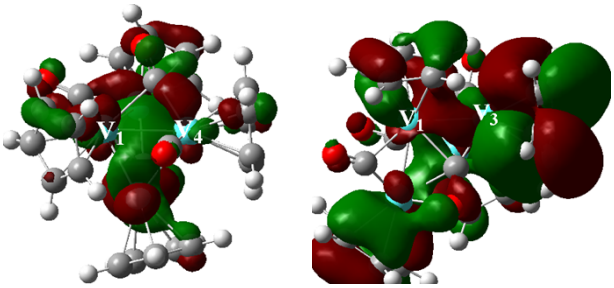
V_3-V_4 π-bonding V_1-V_3 π-bonding

(a) The molecular orbital diagrams related to the V-V π-bonding of **4T-2.**



HOMO-3 **HOMO-4** **HOMO-6**

V_1-V_2 σ-bonding V_3-V_4 σ-bonding V_2-V_4 σ-bonding



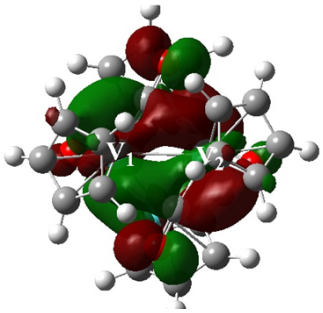
HOMO-8 **HOMO-13**

V_1-V_4 σ-bonding V_1-V_3 σ-bonding

(b) The molecular orbital diagrams related to the V-V σ-bonding of **4T-2.**

Figure S11. The comments and molecular orbital diagrams related to the V-V π-bonding orbitals (a) and V-V σ-bonding orbitals (b) of **4T-2**.

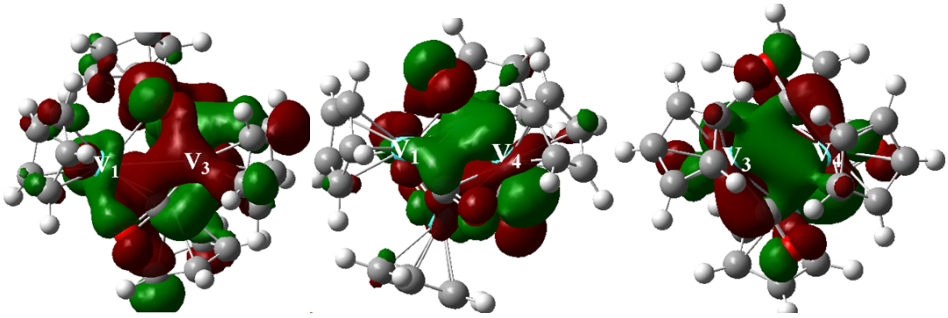
4T-3 has one short V_1-V_2 double bond with distance of 2.678 Å. The other five V-V single bonds are relatively long with distance of 2.910, 2.951, 2.951, 2.910 and 3.016 Å for V_1-V_3, V_1-V_4, V_2-V_3, V_2-V_4 and V_3-V_4, respectively. This leads to 16-electron configurations for two vanadium atoms and 15-electron configurations for another two vanadium atoms. The molecular orbital diagrams of **4T-3** are shown in Figure S12. The HOMO-3 and HOMO-8 orbitals can be assigned as π-bonding orbital and σ-bonding orbital of V_1-V_2 double bond, respectively. The HOMO-2, HOMO-4, HOMO-7, HOMO-6 and HOMO-5 orbitals are corresponding to σ-bonding orbitals of V_1-V_3, V_1-V_4, V_2-V_3, V_2-V_4 and V_3-V_4 single bonds, respectively.



HOMO-3

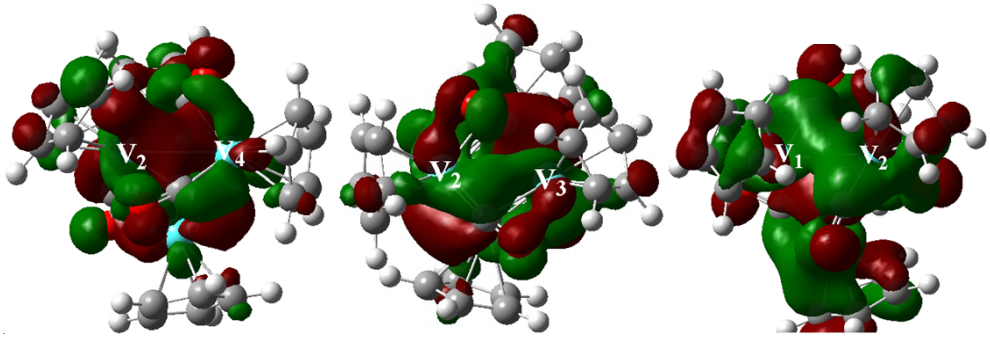
V_1-V_2 π-bonding

(a) The molecular orbital diagrams related to the V-V π-bonding of **4T-3.**



HOMO-2 **HOMO-4** **HOMO-5**

V_1-V_3 σ-bonding **V_1-V_4** σ-bonding **V_3-V_4** σ-bonding



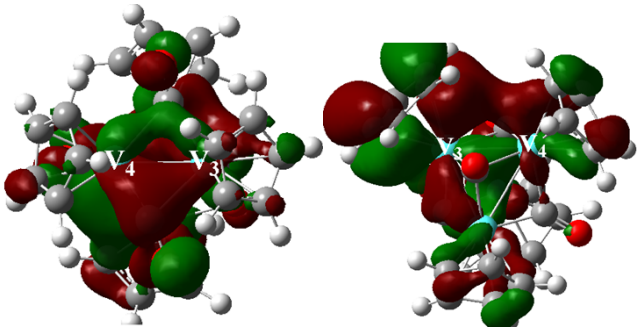
HOMO-6 **HOMO-7** **HOMO-8**

V_2-V_4 σ-bonding **V_2-V_3** σ-bonding **V_1-V_2** σ-bonding

(b) The molecular orbital diagrams related to the V-V σ-bonding of **4T-3**

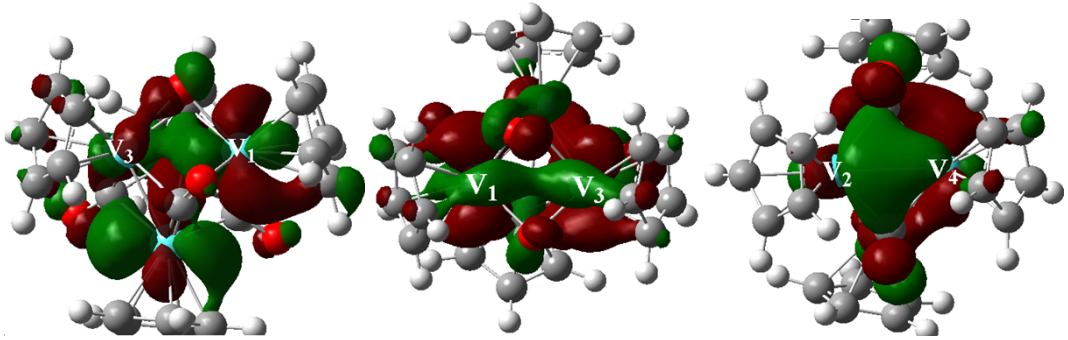
Figure S12. The comments and molecular orbital diagrams related to the V-V π-bonding orbitals (a) and V-V σ-bonding orbitals (b) of **4T-3**.

4Q-1 has one short V_3-V_4 triple bond with distance of 2.572 Å. The other five V-V single bonds of 4Q-1 are relatively longer, namely, 2.964 Å for V_1-V_2, 2.932 Å for V_1-V_3, 2.975 Å for V_1-V_4, 2.727 Å for V_2-V_3 and 2.907 Å for V_2-V_4. This leads to 17-electron configurations for two vanadium atoms and 15-electron configurations for another two vanadium atoms. The molecular orbital diagrams of **4Q-1** are shown in Figure S13. The HOMO-7, HOMO-17 and HOMO-6 orbitals can be assigned as two π-bonding orbitals and σ-bonding orbital of V_3-V_4 triple bond, respectively. The SOMO and SOMO-1 orbitals are consistent with two half-filled σ-bonding orbitals of V_1-V_3 single bond. The HOMO-8, HOMO-9, HOMO-13 and HOMO-5 orbitals are corresponding to the σ-bonding orbitals of V_1-V_2, V_1-V_4, V_2-V_3 and V_2-V_4 single bonds, respectively.

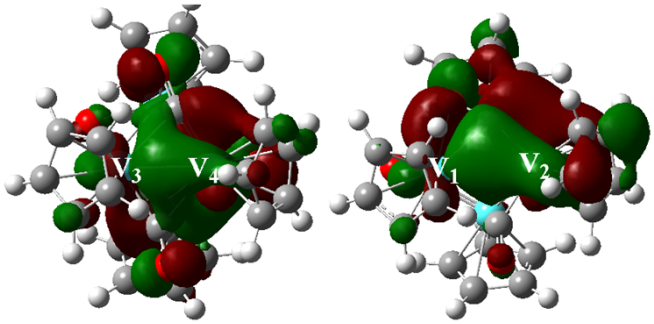


HOMO-7 **HOMO-17**
V_3-V_4 π-bonding V_3-V_4 π-bonding

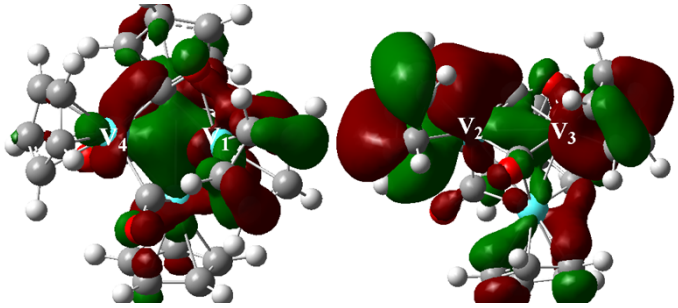
(a) The molecular orbital diagrams related to the V-V π-bonding of **4Q-1.**



SOMO **SOMO-1** **HOMO-5**
V_1-V_3 σ-bonding V_1-V_3 σ-bonding V_2-V_4 σ-bonding



HOMO-6 **HOMO-8**
V_3-V_4 σ-bonding V_1-V_2 σ-bonding



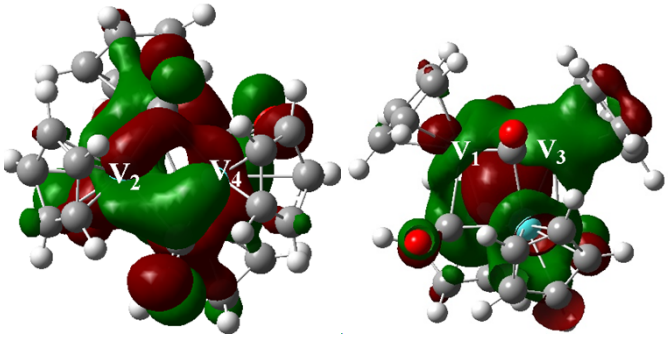
HOMO-9 **HOMO-13**

V_1-V_4 σ-bonding V_2-V_3 σ-bonding

(b) The molecular orbital diagrams related to the V-V σ-bonding of **4Q-1.**

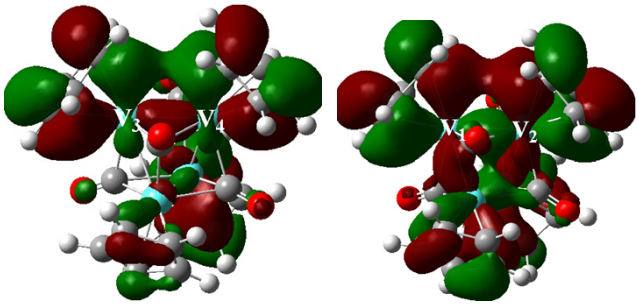
Figure S13. The comments and molecular orbital diagrams related to the V-V π-bonding orbitals (a) and V-V σ-bonding orbitals (b) of **4Q-1**.

4Q-2 has four short V-V double bonds, namely, 2.435 Å for V_1-V_2, 2.676 Å for V_1-V_3, 2.526 Å for V_2-V_4 and 2.439 Å for V_3-V_4. The distances for the other two V_1-V_4 and V_2-V_3 single bonds are 2.949 and 2.997 Å, respectively. This leads to 17-electron configuration for each vanadium atom. The molecular orbital diagrams of **4Q-2** are shown in Figure S14. The HOMO-17 and HOMO-7 orbitals are corresponding to π-bonding orbital and σ-bonding orbital of V_1-V_2 double bond, respectively. The HOMO-9, SOMO and SOMO-3 orbitals can be regarded as π-bonding orbital and two half-filled σ-bonding orbitals of V_1-V_3 double bond, respectively. The HOMO-4 and HOMO-5 orbitals can be assigned to π-bonding orbital and σ-bonding orbital of V_2-V_4 double bond, respectively. The HOMO-16 and HOMO-8 orbitals are corresponding to π-bonding orbital and σ-bonding orbital of V_3-V_4 double bond, respectively. The HOMO-6 and HOMO-13 orbitals can be considered as σ-bonding orbitals of V_1-V_4 and V_2-V_3 single bonds, respectively.



HOMO-4 **HOMO-9**

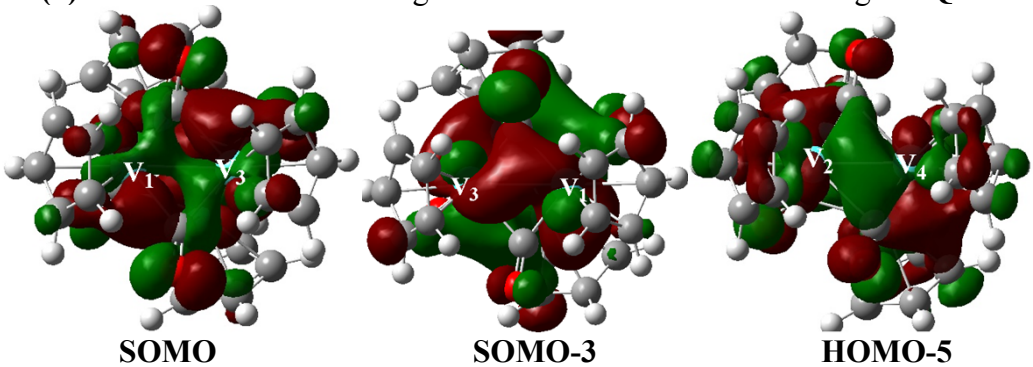
V_2-V_4 π-bonding V_1-V_3 π-bonding



HOMO-16 **HOMO-17**

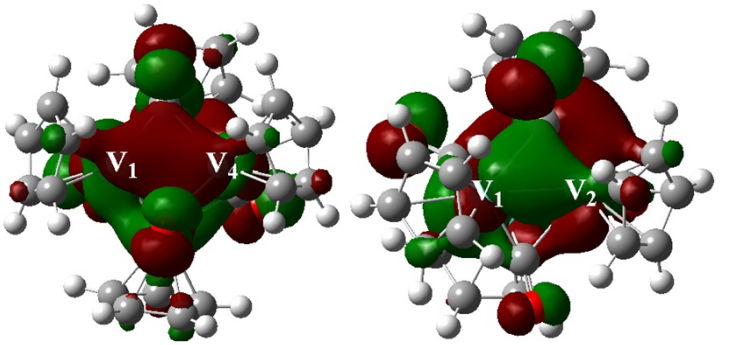
V_3-V_4 π-bonding V_1-V_2 π-bonding

(a) The molecular orbital diagrams related to the V-V π-bonding of **4Q-2.**



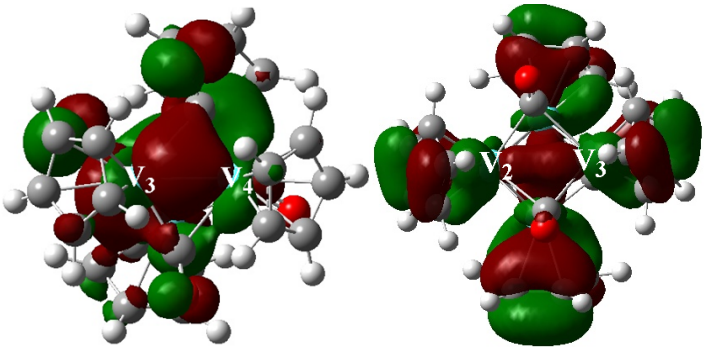
SOMO **SOMO-3** **HOMO-5**

V_1-V_3 σ-bonding V_1-V_3 σ-bonding V_2-V_4 σ-bonding



HOMO-6 **HOMO-7**

V_1-V_4 σ-bonding V_1-V_2 σ-bonding



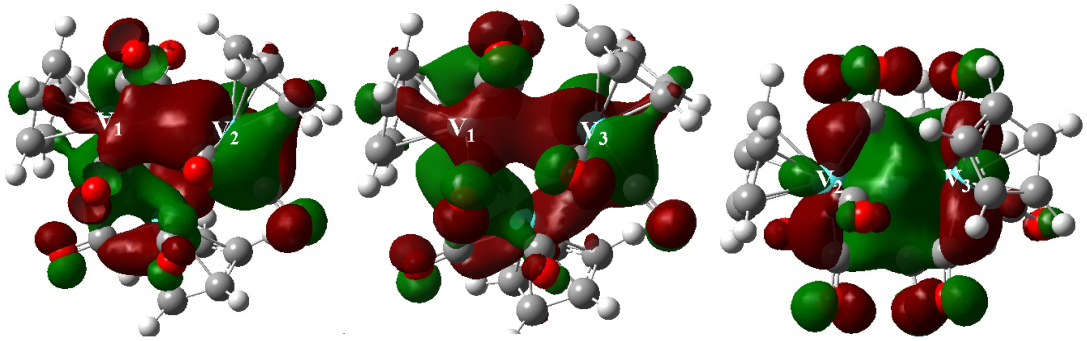
HOMO-8 **HOMO-13**

V_3-V_4 σ-bonding V_2-V_3 σ-bonding

(b) The molecular orbital diagrams related to the V-V σ-bonding of **4Q-2.**

Figure S14. The comments and molecular orbital diagrams related to the V-V π-bonding orbitals (a) and V-V σ-bonding orbitals (b) of **4Q-2**.

9S-1 has three equal V-V single bonds, namely V_1-V_2, V_1-V_3 and V_2-V_3 with distance of 3.376 Å. This leads to 18-electron configuration for each vanadium atom. The molecular orbital diagrams of **9S-1** are shown in Figure S15. HOMO-2, HOMO-3, and HOMO-5 orbitals are consistent with σ-bonding orbitals of V_1-V_2, V_1-V_3 and V_2-V_3 single bonds, respectively.



HOMO-2 **HOMO-3** **HOMO-5**

V_1-V_2 σ-bonding V_1-V_3 σ-bonding V_2-V_3 σ-bonding

Figure S15. The comments and molecular orbital diagrams related to the V-V σ-bonding orbitals of **9S-1**.

Table S18. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4S-1** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.715736	0.111456	3.385156
6	-2.849004	0.675497	2.707010
1	-3.172318	1.718527	2.750457
6	-3.472774	-0.376109	1.964922
1	-4.330381	-0.260827	1.298338
6	-1.639690	-1.277098	3.046026
1	-0.880963	-1.986058	3.385306
6	-2.726806	-1.583463	2.162719
1	-2.927810	-2.553498	1.701941
1	-1.032683	0.655504	4.040710
6	2.726806	1.583463	2.162719
6	1.639690	1.277098	3.046026
1	0.880963	1.986058	3.385306
6	1.715736	-0.111456	3.385156
1	1.032683	-0.655504	4.040710
6	3.472774	0.376109	1.964922
1	4.330381	0.260827	1.298338
6	2.849004	-0.675497	2.707010
1	3.172318	-1.718527	2.750457
1	2.927810	2.553498	1.701941
6	1.277098	-1.639690	-3.046026
6	1.583463	-2.726806	-2.162719
1	2.553498	-2.927810	-1.701941
6	0.376109	-3.472774	-1.964922

1	0.260827	-4.330381	-1.298338
6	-0.111456	-1.715736	-3.385156
1	-0.655504	-1.032683	-4.040710
6	-0.675497	-2.849004	-2.707010
1	-1.718527	-3.172318	-2.750457
1	1.986058	-0.880963	-3.385306
6	0.675497	2.849004	-2.707010
6	0.111456	1.715736	-3.385156
1	0.655504	1.032683	-4.040710
6	-1.277098	1.639690	-3.046026
1	-1.986058	0.880963	-3.385306
6	-0.376109	3.472774	-1.964922
1	-0.260827	4.330381	-1.298338
6	-1.583463	2.726806	-2.162719
1	-2.553498	2.927810	-1.701941
1	1.718527	3.172318	-2.750457
23	1.343007	0.037873	1.089662
23	-1.343007	-0.037873	1.089662
23	-0.037873	1.343007	-1.089662
23	0.037873	-1.343007	-1.089662
6	0.497026	-1.583463	0.944179
6	-0.497026	1.583463	0.944179
6	-1.583463	-0.497026	-0.944179
6	1.583463	0.497026	-0.944179
8	0.011803	2.700687	0.677740
8	-2.700687	0.011803	-0.677740
8	-0.011803	-2.700687	0.677740
8	2.700687	-0.011803	-0.677740

Table S19. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4S-2** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
23	0.061574	-1.351544	0.534845
23	-1.962869	-0.177205	-0.636812
23	1.880484	-0.232444	-0.527623
23	0.159146	1.301948	0.652984
6	-3.415241	1.408387	-1.568392
6	-3.703756	0.128819	-2.144342
1	-3.559462	-0.144412	-3.193470
6	-4.127263	-0.748864	-1.099664
1	-4.413953	-1.797743	-1.204644
6	-3.654126	1.324473	-0.160021
1	-3.538907	2.132994	0.564890
6	-4.097215	-0.008191	0.134104
1	-4.336187	-0.404866	1.123903
1	-3.044244	2.277993	-2.117725
6	1.602072	-2.767219	-0.431555
6	0.390172	-3.492045	-0.122029
1	-0.253751	-3.996307	-0.845105
6	0.229874	-3.502313	1.306012
1	-0.604731	-3.959417	1.842112
6	2.152056	-2.273259	0.815103
1	3.135687	-1.816353	0.976895
6	1.278406	-2.723131	1.877478
1	1.404442	-2.471283	2.934521
1	2.077263	-2.748839	-1.415843

6	0.594274	3.361340	-0.309115
6	-0.811014	3.270095	-0.051033
1	-1.600579	3.300080	-0.802635
6	-0.992560	3.164477	1.370676
1	-1.944518	3.074150	1.899455
6	1.276850	3.306497	0.948198
1	2.356476	3.346004	1.110122
6	0.295231	3.190159	1.988000
1	0.500887	3.105547	3.057944
1	1.054773	3.460079	-1.294499
6	2.909229	-0.226430	-2.609665
6	3.856438	-0.691447	-1.641622
1	4.303445	-1.690037	-1.605345
6	4.113549	0.374385	-0.715200
1	4.789974	0.336486	0.143814
6	2.580009	1.129327	-2.283682
1	1.870983	1.754977	-2.830995
6	3.327812	1.503704	-1.119759
1	3.328612	2.484289	-0.642545
1	2.489897	-0.801807	-3.440030
6	0.104809	-0.112670	-1.181492
8	-0.755476	0.061847	-2.152050
6	1.552293	0.570247	1.703181
8	2.408427	0.328489	2.517951
6	-1.983112	-1.972150	0.040453
8	-2.567109	-2.986244	0.356752
6	-1.101249	0.288867	1.689196
8	-1.768721	-0.141247	2.601365

Table S20. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4S-3** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
23	-0.893702	-1.159831	-0.642795
6	-1.660768	-1.870876	-2.684586
6	-1.142835	-2.998004	-1.951000
6	-1.958988	-3.190765	-0.792023
6	-2.983869	-2.178453	-0.802962
6	-2.803638	-1.380205	-1.975705
1	-1.246632	-1.457187	-3.607029
1	-0.252879	-3.574286	-2.216874
1	-1.824625	-3.957284	-0.024622
1	-3.764572	-2.053312	-0.048455
23	1.300347	-0.861283	0.611910
6	2.289216	-1.563069	2.561692
6	2.027967	-2.707976	1.725584
6	2.810337	-2.579483	0.535382
6	3.551811	-1.350182	0.625749
6	3.235109	-0.735550	1.880944
1	1.824872	-1.350911	3.527947
1	1.320134	-3.509332	1.951319
1	2.824335	-3.272786	-0.308975
1	4.231250	-0.958732	-0.135351
23	0.848371	1.121006	-0.719610
6	2.808661	2.350183	-0.647423
6	1.697751	3.269231	-0.582644
6	0.960131	3.156402	-1.796994

6	1.605225	2.164088	-2.616010
6	2.756914	1.684864	-1.911823
1	3.554548	2.196481	0.136108
1	1.453731	3.912227	0.266325
1	0.033913	3.679247	-2.045986
1	1.257762	1.814441	-3.592354
23	-1.233552	0.887384	0.662555
6	-3.497729	1.264138	0.926844
6	-2.814296	2.528852	0.932318
6	-1.934456	2.542656	2.062080
6	-2.069134	1.293280	2.760241
6	-3.042053	0.510512	2.055457
1	-4.227407	0.937737	0.181504
1	-2.934320	3.324664	0.192831
1	-1.239543	3.344453	2.327460
1	-1.522303	0.990908	3.656402
6	1.267180	-1.034916	-1.288343
8	1.636787	-1.381983	-2.398307
6	-0.851914	-1.491075	1.215006
8	-1.014955	-1.919491	2.337266
6	-1.381336	1.167333	-1.177832
8	-1.708232	1.528485	-2.295324
6	0.868064	1.191502	1.299182
8	1.249853	1.754853	2.307712
1	3.598676	0.232324	2.235854
1	-3.345920	-0.505185	2.319452
1	-3.398193	-0.509935	-2.262296
1	3.431754	0.899285	-2.260222

Table S21. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4S-4** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
23	0.000000	-1.220470	1.041788
6	1.161657	-2.918232	2.048221
6	0.715152	-2.017871	3.074966
6	-0.715152	-2.017871	3.074966
6	-1.161657	-2.918232	2.048221
6	0.000000	-3.478820	1.422139
1	2.202373	-3.114304	1.778439
1	1.365107	-1.413084	3.711562
1	-1.365107	-1.413084	3.711562
1	-2.202373	-3.114304	1.778439
23	0.000000	1.220470	1.041788
6	-1.161657	2.918232	2.048221
6	-0.715152	2.017871	3.074966
6	0.715152	2.017871	3.074966
6	1.161657	2.918232	2.048221
6	0.000000	3.478820	1.422139
1	-2.202373	3.114304	1.778439
1	-1.365107	1.413084	3.711562
1	1.365107	1.413084	3.711562
1	2.202373	3.114304	1.778439
23	1.220470	0.000000	-1.041788
6	2.918232	1.161657	-2.048221
6	2.017871	0.715152	-3.074966
6	2.017871	-0.715152	-3.074966

6	2.918232	-1.161657	-2.048221
6	3.478820	0.000000	-1.422139
1	3.114304	2.202373	-1.778439
1	1.413084	1.365107	-3.711562
1	1.413084	-1.365107	-3.711562
1	3.114304	-2.202373	-1.778439
23	-1.220470	0.000000	-1.041788
6	-2.918232	-1.161657	-2.048221
6	-2.017871	-0.715152	-3.074966
6	-2.017871	0.715152	-3.074966
6	-2.918232	1.161657	-2.048221
6	-3.478820	0.000000	-1.422139
1	-3.114304	-2.202373	-1.778439
1	-1.413084	-1.365107	-3.711562
1	-1.413084	1.365107	-3.711562
1	-3.114304	2.202373	-1.778439
6	1.707368	0.000000	1.034556
8	2.785119	0.000000	1.618808
6	-1.707368	0.000000	1.034556
8	-2.785119	0.000000	1.618808
6	0.000000	-1.707368	-1.034556
8	0.000000	-2.785119	-1.618808
6	0.000000	1.707368	-1.034556
8	0.000000	2.785119	-1.618808
1	0.000000	4.164049	0.571279
1	-4.164049	0.000000	-0.571279
1	0.000000	-4.164049	0.571279
1	4.164049	0.000000	-0.571279

Table S22. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4S-5** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
23	0.870439	1.029864	0.858725
6	2.897161	1.466593	1.874688
6	2.611402	2.525053	0.956879
6	1.411284	3.183696	1.394793
6	0.963567	2.527931	2.592770
6	1.877605	1.467606	2.886455
1	3.714471	0.745956	1.794712
1	3.178266	2.761420	0.053279
1	0.928961	4.035061	0.908200
1	0.056930	2.768650	3.152863
23	-0.851604	1.049206	-0.881655
6	-2.892985	1.953432	-1.418506
6	-2.063569	3.004499	-0.903103
6	-0.939949	3.155416	-1.776285
6	-1.073773	2.198281	-2.842049
6	-2.282878	1.463197	-2.621576
1	-3.810054	1.576078	-0.958738
1	-2.237725	3.549105	0.027902
1	-0.108442	3.853014	-1.649798
1	-0.358670	2.043731	-3.653612
23	0.851604	-1.049206	-0.881655
6	2.282878	-1.463197	-2.621576
6	1.073773	-2.198281	-2.842049
6	0.939949	-3.155416	-1.776285

6	2.063569	-3.004499	-0.903103
6	2.892985	-1.953432	-1.418506
1	2.646454	-0.628106	-3.225131
1	0.358670	-2.043731	-3.653612
1	0.108442	-3.853014	-1.649798
1	2.237725	-3.549105	0.027902
23	-0.870439	-1.029864	0.858725
6	-1.877605	-1.467606	2.886455
6	-0.963567	-2.527931	2.592770
6	-1.411284	-3.183696	1.394793
6	-2.611402	-2.525053	0.956879
6	-2.897161	-1.466593	1.874688
1	-1.789392	-0.747265	3.703376
1	-0.056930	-2.768650	3.152863
1	-0.928961	-4.035061	0.908200
1	-3.178266	-2.761420	0.053279
6	1.204196	1.037018	-1.219330
8	1.989575	1.603098	-1.971909
6	-1.204196	1.054250	1.176465
8	-1.971855	1.627039	1.942801
6	1.204196	-1.054250	1.176465
8	1.971855	-1.627039	1.942801
6	-1.204196	-1.037018	-1.219330
8	-1.989575	-1.603098	-1.971909
1	-2.646454	0.628106	-3.225131
1	-3.714471	-0.745956	1.794712
1	1.789392	0.747265	3.703376
1	3.810054	-1.576078	-0.958738

Table S23. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4T-1** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-2.168823	-2.313215	2.199218
6	-0.930432	-3.039384	2.075045
1	-0.777158	-3.951426	1.492686
6	0.059472	-2.352643	2.846015
1	1.115614	-2.619309	2.930353
6	-1.936114	-1.195861	3.068244
1	-2.664689	-0.421097	3.320135
6	-0.561566	-1.210018	3.457068
1	-0.057047	-0.473578	4.086533
1	-3.117127	-2.574768	1.721742
6	-2.104993	-0.682136	-3.059440
6	-2.809568	-1.322451	-1.980464
1	-2.761387	-2.384978	-1.732013
6	-3.560444	-0.327784	-1.281468
1	-4.185493	-0.487581	-0.399726
6	-2.443564	0.706873	-3.029752
1	-2.035461	1.477080	-3.689819
6	-3.324661	0.937725	-1.923531
1	-3.743010	1.899924	-1.617106
1	-1.431058	-1.172338	-3.766283
6	1.712714	3.502303	0.010441
6	0.355550	3.963294	0.154981
1	-0.223414	4.496514	-0.604721
6	-0.109657	3.568187	1.450657

1	-1.116395	3.723645	1.846969
6	2.072143	2.814657	1.208105
1	3.015786	2.304728	1.414054
6	0.942614	2.842496	2.094681
1	0.898011	2.374909	3.080643
1	2.338479	3.627593	-0.878012
6	3.015330	-1.683748	-2.286012
6	3.427010	-0.369726	-1.888065
1	3.524846	0.497279	-2.545919
6	3.622241	-0.379905	-0.468631
1	3.913568	0.467974	0.154039
6	3.013280	-2.517999	-1.113466
1	2.695190	-3.563296	-1.081658
6	3.376840	-1.717202	0.006363
1	3.421425	-2.032975	1.050766
1	2.742063	-1.996710	-3.297344
23	-1.318748	0.206240	-1.068920
23	-0.670828	-0.961983	1.152164
23	1.412329	-0.846324	-0.875458
23	0.298403	1.687479	0.186798
6	-1.761068	0.967398	0.643562
6	-0.390563	-1.859227	-0.428376
6	1.101518	-0.057775	1.382991
6	0.656328	0.634185	-1.644172
8	0.117784	-2.513379	-1.376505
8	2.051005	-0.015227	2.158125
8	-2.489816	1.465128	1.492485
8	-0.011577	1.737939	-1.839695

Table S24. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4T-2** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
23	-0.051158	-1.359104	0.444823
23	-2.007485	-0.150380	-0.682669
23	1.863761	-0.287665	-0.606387
23	0.240175	1.283989	0.677108
6	-3.467358	1.502724	-1.444123
6	-3.851371	0.255981	-2.035035
1	-3.815056	0.014535	-3.101061
6	-4.227106	-0.637951	-0.983574
1	-4.572122	-1.667521	-1.102068
6	-3.590202	1.378906	-0.021616
1	-3.384958	2.156516	0.716372
6	-4.066577	0.057674	0.266804
1	-4.239840	-0.360121	1.262012
1	-3.105841	2.375413	-1.994971
6	1.545192	-2.960373	-0.153946
6	0.358873	-3.623758	0.298184
1	-0.282612	-4.267481	-0.307101
6	0.146228	-3.294550	1.682524
1	-0.687364	-3.645710	2.296006
6	2.039290	-2.163020	0.945626
1	3.014281	-1.658519	1.006257
6	1.163873	-2.380078	2.082579
1	1.281403	-1.913907	3.063649
1	2.022525	-3.106646	-1.126403

6	0.610784	3.325157	-0.352205
6	-0.770115	3.243038	0.015780
1	-1.612390	3.268408	-0.675767
6	-0.845341	3.151952	1.448921
1	-1.754527	3.076895	2.050509
6	1.387048	3.286039	0.848826
1	2.476102	3.330770	0.924064
6	0.486648	3.184796	1.964353
1	0.773778	3.119696	3.016609
1	0.993717	3.400156	-1.372460
6	2.771287	-0.403420	-2.724783
6	3.742287	-0.881609	-1.787623
1	4.142611	-1.899222	-1.736183
6	4.100053	0.204828	-0.915330
1	4.821011	0.165000	-0.093660
6	2.524125	0.979115	-2.434406
1	1.815942	1.618409	-2.966760
6	3.348974	1.355856	-1.324887
1	3.407850	2.348949	-0.876332
1	2.277351	-0.988758	-3.505519
6	0.064422	-0.059623	-1.199226
8	-0.779776	0.273042	-2.143698
6	1.735197	0.637147	1.646026
8	2.638295	0.427833	2.410615
6	-2.043574	-2.017392	-0.237499
8	-2.568458	-3.094125	-0.070800
6	-0.904138	0.271478	1.841107
8	-1.560637	-0.111961	2.779863

Table S25. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4T-3** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-3.353992	0.408300	-1.699930
6	-2.655158	1.144897	-2.716408
1	-2.691157	2.226389	-2.868920
6	-1.908593	0.202229	-3.492587
1	-1.230819	0.449996	-4.312948
6	-3.021017	-0.975251	-1.844354
1	-3.379650	-1.796823	-1.220295
6	-2.120665	-1.107429	-2.953910
1	-1.663804	-2.036245	-3.303723
1	-4.015259	0.838740	-0.944888
6	-2.120666	1.107422	2.953913
6	-3.021019	0.975241	1.844357
1	-3.379655	1.796813	1.220300
6	-3.353988	-0.408310	1.699932
1	-4.015255	-0.838751	0.944890
6	-1.908588	-0.202236	3.492588
1	-1.230813	-0.450000	4.312949
6	-2.655151	-1.144906	2.716409
1	-2.691146	-2.226398	2.868920
1	-1.663808	2.036239	3.303725
6	3.035748	-1.837096	0.901981
6	2.164717	-2.937890	1.196340
1	1.733550	-3.170098	2.172873
6	1.913844	-3.630466	-0.030510

1	1.235121	-4.477410	-0.157578
6	3.328795	-1.860438	-0.501778
1	3.968729	-1.157133	-1.039742
6	2.625026	-2.967175	-1.083573
1	2.618857	-3.242048	-2.141917
1	3.414102	-1.114826	1.628152
6	2.625014	2.967186	1.083571
6	3.328786	1.860452	0.501776
1	3.968724	1.157151	1.039740
6	3.035740	1.837109	-0.901983
1	3.414097	1.114841	-1.628155
6	1.913828	3.630473	0.030508
1	1.235101	4.477414	0.157576
6	2.164703	2.937898	-1.196342
1	1.733535	3.170105	-2.172875
1	2.618844	3.242060	2.141914
23	-1.065283	-0.190747	1.325538
23	-1.065286	0.190744	-1.325537
23	1.060947	1.485708	0.258858
23	1.060955	-1.485705	-0.258859
6	-0.965731	-1.653310	0.220998
6	-0.965741	1.653305	-0.220997
6	0.974556	-0.218458	-1.621346
6	0.974556	0.218460	1.621345
8	-0.737027	2.702926	0.439824
8	0.737644	0.491551	-2.620650
8	-0.737012	-2.702930	-0.439822
8	0.737649	-0.491550	2.620650

Table S26. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4T-4** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
23	0.181742	-0.871792	1.251134
23	1.678973	0.340750	-0.354366
23	-1.070855	1.205020	0.153597
23	-0.875197	-0.956518	-0.980862
6	-1.439636	-2.162226	-2.472398
6	0.141937	-1.632110	3.114555
6	-2.334777	2.721421	0.105629
6	3.567895	0.839313	-0.747450
8	-1.836688	-2.838921	-3.352957
8	0.120601	-2.117787	4.187018
8	4.687982	1.118826	-0.982938
8	-3.088497	3.628014	0.108283
6	1.293301	-2.127471	-1.318451
6	2.536977	-1.573567	-0.790123
1	3.479058	-1.624633	-1.349022
6	2.440753	-1.733705	0.666674
1	3.283051	-1.559395	1.345265
6	0.546671	-2.745438	-0.224971
1	-0.192020	-3.540123	-0.375484
6	1.345541	-2.636296	0.996917
1	1.355503	-3.382731	1.797165
1	1.177209	-2.395451	-2.371342
6	0.087157	1.255364	2.330797
6	-0.146520	2.577042	1.743946

1	-0.894862	3.292020	2.096229
6	1.029874	2.937264	1.029861
1	1.167079	3.890995	0.508863
6	1.483291	0.864470	2.021675
1	2.106346	0.331213	2.750557
6	2.057077	1.944678	1.199135
1	3.116232	2.220593	1.217133
1	-0.428590	0.974887	3.253260
6	-3.016438	-0.105712	-0.247261
6	-2.758878	-1.554560	-0.260072
1	-3.355598	-2.291877	-0.806896
6	-2.073617	-1.825580	0.998565
1	-1.881764	-2.835680	1.376140
6	-2.825898	0.420007	1.119952
1	-3.539127	1.095559	1.608165
6	-2.153884	-0.655150	1.853594
1	-2.158200	-0.707149	2.946010
1	-3.706129	0.359148	-0.959986
6	1.231116	0.860824	-2.625372
6	1.000729	2.058064	-1.906897
1	1.740797	2.851751	-1.766298
6	-0.444508	2.233940	-1.680010
1	-0.888632	3.228459	-1.816219
6	-0.046570	0.199968	-2.863131
1	-0.206601	-0.439516	-3.736748
6	-1.079455	1.024076	-2.252371
1	-2.103384	1.026670	-2.640839
1	2.172387	0.574949	-3.106535

Table S27. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4Q-1** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
23	-1.523915	-1.142916	-0.272777
23	-0.430379	1.604586	-0.476246
23	1.190850	-0.479020	-1.157761
23	0.794489	-0.272767	1.375385
6	0.085274	3.829600	-0.014225
6	-0.009816	3.634073	-1.433539
1	0.807178	3.742030	-2.152049
6	-1.361158	3.255022	-1.738691
1	-1.756792	3.030208	-2.732277
6	-1.194043	3.555318	0.557322
1	-1.443095	3.573256	1.620789
6	-2.090783	3.192578	-0.504434
1	-3.142519	2.916411	-0.392156
1	0.996810	4.087033	0.529948
6	2.567843	-0.879142	2.685686
6	2.345914	0.519051	2.902547
1	3.022810	1.326382	2.612883
6	1.044374	0.678207	3.473100
1	0.560945	1.625364	3.724624
6	1.403784	-1.592023	3.146379
1	1.263208	-2.675614	3.127549
6	0.464440	-0.628007	3.630178
1	-0.535796	-0.840900	4.015224
1	3.462770	-1.329312	2.246594

6	-3.639944	-0.944428	-1.159930
6	-3.674843	-0.442888	0.178663
1	-3.886854	0.584186	0.481285
6	-3.362512	-1.525517	1.073877
1	-3.291875	-1.452502	2.161632
6	-3.288601	-2.335629	-1.101221
1	-3.134089	-2.999208	-1.956411
6	-3.138844	-2.692093	0.280718
1	-2.819741	-3.668982	0.653440
1	-3.800546	-0.360776	-2.070666
6	2.102810	-2.064405	-2.561628
6	2.302990	-0.746281	-3.108510
1	1.850646	-0.359628	-4.026029
6	3.151402	-0.021180	-2.212709
1	3.483839	1.013947	-2.320160
6	2.832365	-2.150975	-1.337925
1	2.846847	-3.010661	-0.663139
6	3.467024	-0.888711	-1.107210
1	4.077048	-0.616224	-0.243523
1	1.464343	-2.844024	-2.984854
6	-0.674045	0.243673	-1.701544
8	-0.644917	-0.968055	-2.181716
6	-1.115473	0.642857	1.277541
8	-1.886663	0.984503	2.159353
6	1.662412	1.159994	-0.118965
8	2.556586	1.962176	0.131709
6	0.327628	-1.821028	0.468760
8	-0.273550	-2.845710	0.033658

Table S28. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4Q-2** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
23	1.048811	1.049647	-0.686028
6	1.233107	3.021874	-1.865223
6	2.010271	3.130660	-0.666672
6	3.055864	2.144329	-0.724813
6	2.917019	1.432308	-1.960890
6	1.790371	1.969734	-2.664814
1	0.340563	3.600943	-2.113275
1	1.833058	3.823733	0.159335
1	3.815832	1.972252	0.041511
1	3.526744	0.588213	-2.293733
23	1.154644	-0.952017	0.696693
6	2.482592	-2.821424	0.868196
6	3.344183	-1.670714	0.787006
6	3.098453	-0.854329	1.935116
6	2.083109	-1.490604	2.726638
6	1.713589	-2.710941	2.070177
1	2.418638	-3.624886	0.130215
1	4.043839	-1.455283	-0.024114
1	3.559917	0.111001	2.157214
1	1.649577	-1.099634	3.650957
23	-1.226673	0.868164	0.711386
6	-1.789412	2.848897	1.787763
6	-2.076753	1.761386	2.676023
6	-3.080405	0.944190	2.060081

6	-3.413629	1.522887	0.790159
6	-2.609781	2.702475	0.622293
1	-1.037742	3.624323	1.955208
1	-1.586750	1.567584	3.633763
1	-3.480613	0.013900	2.472256
1	-4.140122	1.135781	0.070983
23	-0.954840	-1.114359	-0.683474
6	-1.724392	-1.758224	-2.743660
6	-2.845002	-1.248693	-2.004399
6	-3.044530	-2.084688	-0.862778
6	-2.046305	-3.121969	-0.892209
6	-1.240145	-2.922304	-2.058571
1	-1.303542	-1.323627	-3.653727
1	-3.405894	-0.345048	-2.255161
1	-3.806419	-1.957301	-0.089428
1	-1.922862	-3.912119	-0.147220
6	0.817709	1.257282	1.292324
8	1.221798	1.771872	2.322721
6	1.215322	-1.152981	-1.238975
8	1.670552	-1.573778	-2.286817
6	-0.946396	1.058716	-1.328237
8	-1.519238	1.551986	-2.290636
6	-1.018098	-1.384489	1.220286
8	-1.363493	-1.849526	2.291520
1	0.931704	-3.398392	2.402677
1	-0.368176	-3.513279	-2.350486
1	1.397356	1.612799	-3.620318
1	-2.607200	3.351305	-0.257161

Table S29. Theoretical cartesian coordinates (in Å) for the structure of $Cp_4V_4(CO)_4$ **4Q-3** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
23	-0.513917	1.152721	-0.996990
23	-1.448045	-0.247453	0.862547
23	1.448045	0.247453	0.862547
23	0.513917	-1.152721	-0.996990
6	0.697227	-2.793829	-2.109920
6	-0.697227	2.793829	-2.109920
6	3.074660	0.452788	1.983687
6	-3.074660	-0.452788	1.983687
8	0.872840	-3.750870	-2.777467
8	-0.872840	3.750870	-2.777467
8	-4.058184	-0.596633	2.618149
8	4.058184	0.596633	2.618149
6	-1.880896	-1.567841	-1.340937
6	-2.909952	-0.909914	-0.542325
1	-3.827388	-1.421327	-0.226563
6	-2.852069	0.504059	-0.954771
1	-3.615627	1.231039	-0.655629
6	-1.388072	-0.632201	-2.358581
1	-0.950994	-0.953530	-3.310464
6	-2.126605	0.623572	-2.225333
1	-2.434017	1.250375	-3.069006
1	-1.837957	-2.655496	-1.440315
6	-0.113978	2.852271	0.658254
6	0.872840	2.407319	1.630692

1	1.874208	2.836121	1.738829
6	0.215083	1.597137	2.595974
1	0.659661	1.241236	3.530597
6	-1.379437	2.277140	1.043043
1	-2.344637	2.661282	0.699309
6	-1.204852	1.528276	2.282256
1	-1.966391	1.464309	3.065638
1	0.005049	3.760782	0.062114
6	2.852069	-0.504059	-0.954771
6	2.126605	-0.623572	-2.225333
1	2.434017	-1.250375	-3.069006
6	1.388072	0.632201	-2.358581
1	0.950994	0.953530	-3.310464
6	2.909952	0.909914	-0.542325
1	3.827388	1.421327	-0.226563
6	1.880896	1.567841	-1.340937
1	1.837957	2.655496	-1.440315
1	3.615627	-1.231039	-0.655629
6	-0.872840	-2.407319	1.630692
6	-0.215083	-1.597137	2.595974
1	-0.659661	-1.241236	3.530597
6	1.204852	-1.528276	2.282256
1	1.966391	-1.464309	3.065638
6	0.113978	-2.852271	0.658254
1	-0.005049	-3.760782	0.062114
6	1.379437	-2.277140	1.043043
1	2.344637	-2.661282	0.699309
1	-1.874208	-2.836121	1.738829

Table S30. Theoretical cartesian coordinates (in Å) for the structure of $Cp_3V_3(CO)_9$ **9S-1** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.324891	1.579705	1.873078
8	-0.492148	1.649100	3.034528
6	0.960278	1.234687	-1.584981
8	1.462848	1.252817	-2.660697
6	1.530510	-0.508489	1.873078
8	1.674237	-0.398337	3.034528
6	0.589131	-1.448969	-1.584981
8	0.353547	-1.893272	-2.660697
6	-1.549409	0.214282	-1.584981
8	-1.816395	0.640455	-2.660697
6	-1.205619	-1.071216	1.873078
8	-1.182089	-1.250763	3.034528
6	-2.858246	0.383801	0.647958
8	-3.676289	1.123675	1.075523
6	1.761505	2.283413	0.647958
8	2.811276	2.621922	1.075523
6	1.096741	-2.667214	0.647958
8	0.865013	-3.745597	1.075523
6	-3.614830	-1.776737	-0.889429
6	-2.541931	-2.340812	-1.661862
6	-3.486100	-2.259283	0.460580
1	-4.396447	-1.112587	-1.266331
6	-1.768249	-3.177037	-0.799171
1	-2.349717	-2.170536	-2.723423

6	-2.334426	-3.120943	0.511598
1	-4.153704	-2.032358	1.295588
1	-0.883278	-3.746970	-1.086676
1	-1.967188	-3.660745	1.387583
6	3.346114	-2.242166	-0.889429
6	3.298168	-1.030971	-1.661862
6	3.699646	-1.889410	0.460580
1	3.161752	-3.251141	-1.266331
6	3.635519	0.057170	-0.799171
1	3.054598	-0.949647	-2.723423
6	3.870029	-0.461201	0.511598
1	3.836926	-2.581034	1.295588
1	3.686610	1.108544	-1.086676
1	4.153892	0.126738	1.387583
6	0.268716	4.018903	-0.889429
6	-0.756237	3.371783	-1.661862
6	-0.213546	4.148693	0.460580
1	1.234695	4.363728	-1.266331
6	-1.867270	3.119867	-0.799171
1	-0.704881	3.120183	-2.723423
6	-1.535603	3.582144	0.511598
1	0.316778	4.613392	1.295588
1	-2.803332	2.638426	-1.086676
1	-2.186704	3.534007	1.387583
23	0.000000	1.949093	-0.023835
23	1.687964	-0.974547	-0.023835
23	-1.687964	-0.974547	-0.023835

Table S31. Theoretical cartesian coordinates (in Å) for the structure of $Cp_3V_3(CO)_9$ **9S-2** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.159920	0.272073	-1.523628
6	-1.152607	0.301389	1.526681
6	2.213617	-2.240500	0.012458
6	-0.547929	-2.323735	1.332632
6	-0.546185	-2.358373	-1.310526
6	1.503931	-0.628077	-1.871578
6	1.515585	-0.602307	1.876253
6	0.592336	2.053257	-1.353338
6	0.602154	2.081977	1.347210
8	-1.434637	0.322954	-2.689822
8	-1.429829	0.322353	2.693131
8	2.428857	-3.398125	0.021591
8	-0.193163	-3.114998	2.130016
8	-0.181528	-3.167699	-2.084955
8	1.432409	-0.809160	-3.028540
8	1.448113	-0.769156	3.035440
8	1.236171	2.495411	-2.244621
8	1.263425	2.528621	2.223045
6	3.675300	0.825691	1.144287
6	4.187929	-0.448875	0.709579
6	3.370142	1.600951	-0.016149
1	3.560248	1.159947	2.177975
6	4.181839	-0.456068	-0.728178
1	4.536974	-1.255607	1.358803

6	3.665279	0.814014	-1.171337
1	2.965913	2.614212	-0.019368
1	4.525189	-1.269497	-1.372046
1	3.541059	1.137831	-2.207273
6	-1.634483	3.512362	1.106405
6	-1.054839	3.954350	-0.133024
6	-2.713513	2.627091	0.799697
1	-1.315007	3.804672	2.109433
6	-1.786324	3.333269	-1.206113
1	-0.221371	4.652581	-0.240646
6	-2.806635	2.516197	-0.625447
1	-3.350463	2.133687	1.536563
1	-1.599136	3.458036	-2.275161
1	-3.538386	1.928718	-1.182325
6	-3.176943	-2.160782	1.188639
6	-3.642408	-0.914896	0.668421
6	-2.868787	-3.018128	0.070012
1	-3.082897	-2.415681	2.246467
6	-3.630616	-0.992562	-0.763605
1	-3.955026	-0.058850	1.268248
6	-3.157454	-2.285643	-1.137519
1	-2.512276	-4.049092	0.127031
1	-3.928874	-0.209041	-1.461870
1	-3.048839	-2.653205	-2.160237
23	2.047698	-0.330284	-0.001273
23	-1.447418	-1.249708	-0.003776
23	-0.726909	1.708845	0.005098

Table S32. Theoretical cartesian coordinates (in Å) for the structure of $Cp_3V_3(CO)_9$ **9S-3** using the BP86 method.

Standard orientation:

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.481823	-0.639706	0.000000
6	-1.368846	-1.698665	0.000000
6	-1.006131	2.755818	1.371235
6	-1.662685	-0.500659	2.221793
6	0.629592	0.519490	2.469702
6	-1.006131	2.755818	-1.371235
6	-1.705624	1.024175	0.000000
6	0.629592	0.519490	-2.469702
6	-1.662685	-0.500659	-2.221793
8	2.688727	-0.583328	0.000000
8	-2.369668	-2.352526	0.000000
8	-1.669716	3.294185	2.179869
8	-2.672500	-0.255595	2.774033
8	0.988347	1.246122	3.337203
8	-1.669716	3.294185	-2.179869
8	-2.879532	0.885293	0.000000
8	0.988347	1.246122	-3.337203
8	-2.672500	-0.255595	-2.774033
6	-0.519479	-2.824388	-2.899746
6	0.361793	-1.933994	-3.606098
6	0.206014	-3.371797	-1.797576
1	-1.555959	-3.051948	-3.159803
6	1.633847	-1.939032	-2.928430
1	0.114724	-1.365848	-4.505919

6	1.532877	-2.829856	-1.817084
1	-0.190354	-4.091610	-1.079492
1	2.524244	-1.377749	-3.220266
1	2.337234	-3.055924	-1.115861
6	-0.519479	-2.824388	2.899746
6	0.206014	-3.371797	1.797576
6	0.361793	-1.933994	3.606098
1	-1.555959	-3.051948	3.159803
6	1.532877	-2.829856	1.817084
1	-0.190354	-4.091610	1.079492
6	1.633847	-1.939032	2.928430
1	0.114724	-1.365848	4.505919
1	2.337234	-3.055924	1.115861
1	2.524244	-1.377749	3.220266
6	2.282235	2.264672	-0.714282
6	1.483088	3.362989	-1.163360
6	2.282235	2.264672	0.714282
1	2.809735	1.549399	-1.345403
6	0.982782	4.055232	0.000000
1	1.310285	3.639195	-2.205585
6	1.483088	3.362989	1.163360
1	2.809735	1.549399	1.345403
1	0.368634	4.958932	0.000000
1	1.310285	3.639195	2.205585
23	0.040333	-1.068569	-1.528849
23	0.040333	-1.068569	1.528849
23	0.069013	1.959486	0.000000

Table S33. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the five singlet structures of $Cp_4V_4(CO)_4$ by the BP86 method (infrared intensities in parentheses are in km/mol).

4S-1	4S-2	4S-3	4S-4	4S-5
51.1 (e, 0.0)	39.8 (a, 0.1)	26.6 (a, 0.1)	9.0 (b_1, 0.0)	41.7 (a, 0.0)
51.1 (e, 0.0)	44.2 (a, 0.1)	36.2 (a, 0.5)	16.0 (e, 0.0)	48.6 (b, 0.0)
54.8 (b, 0.1)	56.4 (a, 0.8)	42.8 (a, 0.3)	16.0 (e, 0.0)	52.0 (a, 0.0)
75.3 (a, 0.0)	58.3 (a, 0.4)	45.9 (a, 0.1)	16.8 (a_2, 0.0)	56.7 (a, 0.0)
83.8 (b, 0.0)	69.7 (a, 0.4)	56.2 (a, 0.4)	47.2 (b_1, 0.0)	61.7 (b, 0.0)
84.7 (e, 1.0)	74.4 (a, 0.1)	61.4 (a, 0.4)	59.5 (a_1, 0.0)	62.4 (a, 0.0)
84.7 (e, 1.0)	85.2 (a, 0.5)	66.1 (a, 0.0)	76.9 (e, 1.5)	75.4 (a, 1.1)
89.5 (a, 0.0)	95.3 (a, 0.5)	74.2 (a, 2.2)	76.9 (e, 1.5)	79.3 (b, 0.5)
116.4 (a, 0.0)	107.1 (a, 0.1)	80.1 (a, 0.2)	84.9 (b_2, 0.1)	85.8 (b, 0.1)
119.1 (b, 0.2)	112.2 (a, 0.2)	89.0 (a, 1.3)	105.2 (a_2, 0.0)	118.8 (a, 0.4)
147.4 (e, 1.0)	112.5 (a, 0.4)	111.6 (a, 3.7)	110.8 (e, 1.9)	123.8 (b, 1.2)
147.4 (e, 1.0)	121.7 (a, 0.5)	121.4 (a, 1.2)	110.8 (e, 1.9)	132.1 (b, 0.2)
157.1 (e, 0.1)	127.0 (a, 0.2)	125.1 (a, 0.3)	129.6 (b_1, 0.0)	133.1 (a, 2.6)
157.1 (e, 0.1)	135.3 (a, 0.1)	127.7 (a, 1.3)	141.6 (e, 1.0)	140.0 (b, 1.3)
163.3 (b, 0.0)	147.5 (a, 0.6)	131.3 (a, 1.5)	141.6 (e, 1.0)	149.0 (a, 0.0)
168.0 (a, 0.0)	149.2 (a, 0.2)	149.9 (a, 1.1)	171.0 (a_1, 0.0)	171.5 (a, 0.3)
180.1 (b, 0.3)	159.2 (a, 0.2)	154.7 (a, 0.6)	187.7 (e, 3.0)	190.3 (a, 0.1)
198.0 (a, 0.0)	169.0 (a, 0.2)	157.2 (a, 0.0)	187.7 (e, 3.0)	194.0 (b, 4.6)
199.5 (e, 3.1)	174.7 (a, 0.5)	164.7 (a, 1.6)	190.5 (a_2, 0.0)	196.4 (b, 2.4)
199.5 (e, 3.1)	184.3 (a, 2.5)	171.2 (a, 5.4)	192.2 (a_1, 0.0)	198.2 (a, 3.1)
218.7 (a, 0.0)	194.5 (a, 1.0)	185.4 (a, 0.8)	195.7 (b_2, 7.2)	201.0 (b, 2.0)
219.4 (b, 2.5)	202.2 (a, 1.1)	189.6 (a, 0.9)	209.8 (b_2, 0.7)	205.3 (b, 0.6)
241.5 (a, 0.0)	217.1 (a, 2.9)	196.7 (a, 2.8)	220.5 (e, 0.2)	221.2 (b, 0.1)
247.4 (e, 1.2)	229.4 (a, 0.2)	216.4 (a, 4.0)	220.5 (e, 0.2)	224.5 (a, 0.1)
247.4 (e, 1.2)	249.2 (a, 0.4)	218.9 (a, 3.1)	225.9 (b_1, 0.0)	231.9 (a, 0.2)
250.1 (b, 10.2)	288.9 (a, 2.4)	228.8 (a, 1.4)	247.3 (a_1, 0.0)	237.1 (a, 0.0)
288.2 (e, 2.9)	291.1 (a, 3.8)	282.6 (a, 1.0)	273.7 (a_2, 0.0)	270.0 (b, 1.0)
288.2 (e, 2.9)	293.4 (a, 4.5)	295.2 (a, 3.5)	275.7 (e, 0.8)	275.3 (b, 0.2)
293.1 (a, 0.0)	303.5 (a, 1.1)	298.1 (a, 1.7)	275.7 (e, 0.8)	276.1 (a, 0.4)
296.5 (b, 2.2)	305.8 (a, 0.9)	303.9 (a, 2.8)	296.3 (b_2, 2.8)	298.8 (a, 11.9)
308.7 (e, 1.2)	316.7 (a, 0.5)	308.2 (a, 6.6)	302.6 (e, 4.0)	299.4 (b, 7.0)
308.7 (e, 1.2)	326.8 (a, 7.7)	312.5 (a, 2.2)	302.6 (e, 4.0)	303.9 (b, 4.7)
319.8 (b, 5.3)	343.3 (a, 1.5)	316.6 (a, 1.2)	316.4 (a_1, 0.0)	318.9 (a, 0.0)
323.7 (a, 0.0)	347.2 (a, 1.7)	321.5 (a, 0.4)	325.6 (e, 1.6)	324.0 (b, 0.0)
348.4 (b, 12.6)	370.3 (a, 2.1)	335.8 (a, 0.2)	325.6 (e, 1.6)	329.4 (a, 0.0)
376.7 (e, 3.0)	386.9 (a, 0.2)	356.2 (a, 2.2)	348.8 (b_1, 0.0)	336.9 (b, 0.1)
376.7 (e, 3.0)	401.3 (a, 11.6)	386.3 (a, 2.2)	350.0 (a_2, 0.0)	337.9 (a, 0.0)
398.2 (a, 0.0)	406.4 (a, 17.9)	391.0 (a, 2.9)	371.2 (a_1, 0.0)	372.9 (a, 0.0)
432.0 (e, 2.4)	433.0 (a, 4.3)	398.6 (a, 2.2)	379.2 (b_2, 7.1)	376.3 (b, 5.7)
432.0 (e, 2.4)	445.2 (a, 2.8)	417.6 (a, 2.1)	393.1 (e, 0.1)	398.1 (b, 0.2)
444.4 (a, 0.0)	454.6 (a, 6.0)	443.2 (a, 10.1)	393.1 (e, 0.1)	400.2 (a, 0.0)
450.4 (b, 0.0)	478.7 (a, 6.3)	455.2 (a, 0.6)	421.7 (a_1, 0.0)	429.8 (a, 0.1)
557.1 (a, 0.0)	484.2 (a, 22.3)	470.1 (a, 13.1)	450.1 (e, 0.7)	443.4 (b, 1.4)
564.1 (b, 0.8)	492.6 (a, 32.6)	477.6 (a, 12.7)	450.1 (e, 0.7)	444.9 (a, 0.6)
564.9 (e, 15.5)	505.7 (a, 1.3)	483.1 (a, 0.8)	458.4 (e, 1.2)	456.2 (b, 0.4)
564.9 (e, 15.5)	511.4 (a, 11.4)	494.8 (a, 17.9)	458.4 (e, 1.2)	457.6 (a, 1.2)

576.2 (e, 5.3)	523.4 (a, 3.4)	509.8 (a, 9.2)	459.7 (b_1, 0.0)	458.9 (b, 1.5)
576.2 (e, 5.3)	530.8 (a, 4.9)	523.5 (a, 10.7)	460.6 (b_2, 0.1)	461.2 (a, 0.8)
577.0 (a, 0.0)	562.9 (a, 0.6)	543.4 (a, 15.2)	474.0 (a_1, 0.0)	469.4 (a, 0.0)
577.7 (b, 7.5)	567.0 (a, 0.8)	570.7 (a, 0.5)	478.2 (b_2, 48.6)	482.0 (b, 54.4)
580.4 (b, 3.7)	567.3 (a, 0.5)	572.9 (a, 0.4)	573.4 (b_2, 1.6)	568.9 (b, 0.2)
582.5 (a, 0.0)	571.0 (a, 0.2)	573.4 (a, 0.8)	573.6 (a_1, 0.0)	569.8 (a, 0.1)
584.2 (e, 9.3)	572.5 (a, 0.3)	576.1 (a, 0.8)	574.5 (e, 0.1)	574.7 (b, 2.0)
584.2 (e, 9.3)	575.5 (a, 0.3)	576.6 (a, 1.5)	574.5 (e, 0.1)	574.8 (a, 0.7)
623.3 (a, 0.0)	576.6 (a, 0.5)	577.4 (a, 0.3)	574.8 (e, 2.0)	575.8 (a, 0.0)
637.4 (e, 3.8)	580.8 (a, 3.8)	579.3 (a, 1.7)	574.8 (e, 2.0)	576.7 (b, 0.3)
637.4 (e, 3.8)	586.4 (a, 3.6)	580.1 (a, 2.7)	575.0 (a_2, 0.0)	577.7 (a, 0.5)
654.9 (b, 17.0)	616.3 (a, 3.8)	581.6 (a, 1.0)	576.2 (b_1, 0.0)	577.9 (b, 0.2)
768.1 (a, 0.0)	719.8 (a, 37.8)	768.7 (a, 74.9)	777.4 (a_2, 0.0)	773.4 (a, 8.2)
768.4 (e, 73.1)	740.7 (a, 25.8)	772.1 (a, 65.1)	778.4 (e, 84.4)	773.4 (b, 79.4)
768.4 (e, 73.1)	749.5 (a, 19.4)	776.5 (a, 86.0)	778.4 (e, 84.4)	774.3 (b, 40.8)
768.7 (b, 25.1)	753.5 (a, 13.0)	783.0 (a, 22.8)	778.7 (b_2, 120.1)	777.5 (a, 124.7)
772.8 (e, 39.9)	768.2 (a, 15.1)	784.4 (a, 13.7)	783.3 (e, 87.2)	778.6 (b, 122.8)
772.8 (e, 39.9)	777.8 (a, 29.9)	787.2 (a, 44.1)	783.3 (e, 87.2)	781.9 (a, 9.6)
781.1 (b,273.6)	780.1 (a, 136.0)	792.2 (a, 68.6)	783.6 (b_1, 0.0)	792.9 (a, 35.5)
783.6 (a, 0.0)	782.9 (a, 25.5)	792.5 (a, 21.8)	785.4 (a_1, 0.0)	793.7 (b, 108.4)
795.3 (e, 23.5)	788.9 (a, 58.3)	793.5 (a, 14.1)	801.5 (e, 1.2)	795.2 (b, 31.4)
795.3 (e, 23.5)	791.2 (a, 11.0)	794.8 (a, 45.9)	801.5 (e, 1.2)	797.5 (a, 7.0)
804.3 (a, 0.0)	794.9 (a, 38.7)	804.8 (a, 72.6)	811.1 (b_2, 96.6)	801.3 (a, 9.9)
804.5 (b, 28.3)	795.4 (a, 16.8)	814.0 (a, 14.2)	811.5 (a_1, 0.0)	801.4 (b, 22.8)
818.1 (b, 3.2)	803.2 (a, 50.4)	815.6 (a, 3.6)	815.0 (a_2, 0.0)	818.0 (b, 1.9)
818.2 (e, 0.1)	806.9 (a, 2.0)	816.4 (a, 0.4)	816.5 (b_1, 0.0)	818.0 (a, 0.2)
818.2 (e, 0.1)	811.6 (a, 2.0)	817.5 (a, 0.8)	818.2 (e, 4.5)	818.3 (b, 1.9)
818.2 (a, 0.0)	814.4 (a, 1.6)	818.4 (a, 27.9)	818.2 (e, 4.5)	818.7 (a, 0.6)
819.3 (e, 1.6)	815.2 (a, 0.1)	818.6 (a, 4.1)	819.3 (e, 0.2)	819.4 (a, 2.7)
819.3 (e, 1.6)	816.0 (a, 0.1)	819.0 (a, 8.0)	819.3 (e, 0.2)	820.0 (b, 7.7)
819.3 (a, 0.0)	816.9 (a, 1.5)	819.8 (a, 5.1)	819.4 (b_2, 23.8)	820.1 (b, 5.3)
819.6 (b, 6.2)	818.1 (a, 0.4)	820.3 (a, 15.7)	820.4 (a_1, 0.0)	820.9 (a, 0.0)
855.6 (a, 0.0)	830.7 (a, 4.0)	851.0 (a, 0.4)	862.1 (e, 13.5)	862.0 (b, 0.5)
855.9 (b, 4.5)	835.8 (a, 0.5)	855.7 (a, 0.4)	862.1 (e, 13.5)	862.2 (a, 1.3)
867.7 (e, 2.1)	848.1 (a, 0.7)	861.5 (a, 3.3)	863.3 (b_2, 9.7)	863.7 (a, 1.9)
867.7 (e, 2.1)	859.7 (a, 2.3)	862.9 (a, 0.3)	864.4 (a_1, 0.0)	864.6 (b, 4.3)
869.5 (e, 7.5)	860.7 (a, 0.6)	869.9 (a, 1.9)	870.1 (a_2, 0.0)	866.0 (a, 1.6)
869.5 (e, 7.5)	866.3 (a, 0.7)	870.7 (a, 4.7)	870.6 (b_1, 0.0)	866.3 (b, 8.9)
870.9 (a, 0.0)	867.7 (a, 2.9)	878.9 (a, 1.1)	878.1 (e, 2.4)	871.4 (a, 0.3)
870.9 (b, 4.2)	876.1 (a, 0.5)	879.9 (a, 0.2)	878.1 (e, 2.4)	871.6 (b, 5.6)
998.7 (e, 10.8)	968.4 (a, 7.0)	991.0 (a, 6.6)	994.7 (e, 8.4)	995.4 (a, 3.0)
998.7 (e, 10.8)	980.8 (a, 11.6)	991.9 (a, 4.9)	994.7 (e, 8.4)	996.1 (b, 11.9)
999.8 (a, 0.0)	989.7 (a, 8.8)	992.2 (a, 8.0)	995.6 (b_2, 7.5)	996.9 (a, 11.6)
999.9 (b, 4.3)	993.8 (a, 12.0)	994.2 (a, 5.1)	996.2 (a_1, 0.0)	997.6 (b, 5.3)
1003.4 (e, 17.8)	997.1 (a, 4.6)	996.0 (a, 5.6)	997.6 (a_2, 0.0)	998.1 (b, 6.4)
1003.4 (e, 17.8)	1004.0 (a, 5.5)	997.9 (a, 8.9)	998.3 (b_1, 0.0)	998.3 (a, 5.4)
1008.2 (a, 0.0)	1004.8 (a, 3.3)	999.3 (a, 8.0)	999.0 (e, 10.0)	1002.0 (a, 0.3)
1008.2 (b, 0.1)	1009.7 (a, 8.5)	1003.4 (a, 2.4)	999.0 (e, 10.0)	1002.3 (b, 5.7)
1045.6 (e, 0.3)	1027.2 (a, 3.1)	1037.9 (a, 0.7)	1043.2 (e, 0.6)	1043.6 (a, 1.4)
1045.6 (e, 0.3)	1040.0 (a, 2.4)	1039.3 (a, 0.8)	1043.2 (e, 0.6)	1043.8 (b, 0.8)
1047.9 (a, 0.0)	1041.8 (a, 5.9)	1040.8 (a, 1.3)	1043.9 (a_2, 0.0)	1044.9 (b, 0.3)
1048.4 (b, 0.2)	1043.5 (a, 1.2)	1041.2 (a, 0.7)	1045.1 (b_1, 0.0)	1045.3 (a, 2.0)
1049.3 (e, 1.9)	1045.7 (a, 0.3)	1044.0 (a, 0.4)	1045.6 (e, 2.5)	1046.4 (a, 0.6)

1049.3 (e, 1.9)	1047.4 (a, 1.2)	1045.8 (a, 1.2)	1045.6 (e, 2.5)	1046.7 (b, 2.9)
1053.7 (a, 0.0)	1051.5 (a, 2.9)	1047.2 (a, 0.6)	1049.3 (b_2, 0.3)	1050.5 (a, 0.0)
1054.4 (b, 6.8)	1055.6 (a, 2.1)	1050.3 (a, 0.6)	1049.5 (a_1, 0.0)	1050.9 (b, 1.0)
1116.9 (e, 0.6)	1088.9 (a, 9.4)	1110.8 (a, 1.8)	1113.1 (e, 1.6)	1113.6 (b, 1.6)
1116.9 (e, 0.6)	1114.5 (a, 2.9)	1111.9 (a, 2.6)	1113.1 (e, 1.6)	1113.6 (a, 1.7)
1118.4 (a, 0.0)	1116.1 (a, 3.9)	1112.7 (a, 1.8)	1113.5 (b_2, 4.4)	1113.8 (b, 3.5)
1118.4 (b, 4.6)	1119.0 (a, 4.9)	1114.2 (a, 1.1)	1113.7 (a_1, 0.0)	1113.9 (a, 0.0)
1228.0 (e, 0.0)	1212.5 (a, 0.1)	1219.8 (a, 0.0)	1223.7 (a_2, 0.0)	1224.2 (a, 0.0)
1228.0 (e, 0.0)	1225.8 (a, 0.1)	1222.1 (a, 0.0)	1224.2 (b_1, 0.0)	1224.3 (b, 0.0)
1231.4 (a, 0.0)	1226.1 (a, 0.1)	1222.7 (a, 0.0)	1225.6 (e, 0.0)	1227.9 (a, 0.0)
1231.6 (b, 0.0)	1228.9 (a, 0.1)	1225.9 (a, 0.0)	1225.6 (e, 0.0)	1228.3 (b, 0.1)
1365.7 (a, 0.0)	1318.3 (a, 64.6)	1358.6 (a, 0.7)	1364.4 (a_2, 0.0)	1364.3 (a, 0.1)
1365.8 (e, 3.4)	1336.4 (a, 2.8)	1362.4 (a, 1.4)	1364.4 (b_1, 0.0)	1364.3 (b, 0.1)
1365.8 (e, 3.4)	1342.5 (a, 1.0)	1363.5 (a, 1.1)	1367.6 (b_2, 1.4)	1366.5 (a, 0.1)
1366.5 (b, 0.0)	1366.7 (a, 0.6)	1364.1 (a, 0.7)	1367.9 (e, 0.3)	1367.1 (b, 0.3)
1372.6 (b, 0.4)	1370.8 (a, 0.6)	1369.0 (a, 0.3)	1367.9 (e, 0.3)	1368.2 (a, 0.4)
1372.7 (a, 0.0)	1371.0 (a, 0.1)	1370.3 (a, 1.1)	1368.3 (e, 1.0)	1368.5 (b, 1.8)
1373.4 (e, 3.0)	1374.5 (a, 0.7)	1370.8 (a, 0.7)	1368.3 (e, 1.0)	1371.4 (a, 0.2)
1373.4 (e, 3.0)	1375.4 (a, 0.2)	1371.8 (a, 1.3)	1368.8 (a_1, 0.0)	1371.6 (b, 0.9)
1417.6 (e, 2.7)	1379.7 (a, 0.2)	1409.8 (a, 2.6)	1412.5 (a_2, 0.0)	1413.8 (a, 0.8)
1417.6 (e, 2.7)	1389.0 (a, 1.1)	1411.3 (a, 1.9)	1412.9 (b_1, 0.0)	1413.9 (b, 4.2)
1418.5 (a, 0.0)	1403.5 (a, 2.7)	1411.7 (a, 1.9)	1413.9 (e, 5.7)	1414.7 (b, 1.6)
1418.6 (b, 3.6)	1411.8 (a, 1.4)	1413.3 (a, 1.6)	1413.9 (e, 5.7)	1414.9 (a, 2.2)
1420.8 (e, 3.1)	1413.0 (a, 2.1)	1414.5 (a, 1.8)	1415.8 (e, 0.6)	1418.4 (a, 1.0)
1420.8 (e, 3.1)	1414.3 (a, 1.7)	1418.6 (a, 1.6)	1415.8 (e, 0.6)	1418.5 (b, 2.8)
1423.1 (a, 0.0)	1419.2 (a, 1.2)	1419.4 (a, 1.9)	1417.2 (b_2, 6.8)	1419.5 (b, 0.8)
1423.2 (b, 0.8)	1422.7 (a, 1.7)	1427.0 (a, 2.8)	1417.7 (a_1, 0.0)	1419.9 (a, 0.4)
1538.0 (b,24.1)	1423.7 (a, 2.9)	1669.8(a,607.4)	1617.7 (e,670.9)	1615.0(b,671.6)
1539.7(e,260.8)	1711.5(a,305.3)	1686.9(a,229.1)	1617.7 (e,670.9)	1615.2(a,662.4)
1539.7(e,260.8)	1742.4(a,774.8)	1705.1(a,464.7)	1630.6(b_2,212.2)	1628.0(b,219.1)
1545.9 (a, 0.0)	1779.8(a,513.7)	1716.5(a,243.8)	1647.0 (a_1, 0.0)	1644.7 (a, 0.3)
3170.9 (e, 0.1)	3134.3 (a, 4.2)	3161.5 (a, 0.1)	3170.3 (a_2, 0.0)	3169.7 (b, 1.2)
3170.9 (e, 0.1)	3149.1 (a, 0.4)	3166.5 (a, 0.4)	3170.6 (b_1, 0.0)	3169.7 (a, 0.5)
3171.1 (a, 0.0)	3160.3 (a, 0.7)	3167.4 (a, 0.5)	3171.2 (e, 0.0)	3171.1 (b, 0.5)
3171.1 (b, 0.1)	3163.8 (a, 0.1)	3168.1 (a, 0.4)	3171.2 (e, 0.0)	3171.1 (a, 0.1)
3173.2 (e, 0.2)	3167.3 (a, 0.1)	3168.3 (a, 0.5)	3171.7 (e, 0.1)	3171.6 (b, 0.2)
3173.2 (e, 0.2)	3168.6 (a, 0.7)	3170.0 (a, 0.1)	3171.7 (e, 0.1)	3171.8 (a, 0.2)
3173.8 (a, 0.0)	3169.8 (a, 0.5)	3170.7 (a, 0.1)	3171.9 (b_2, 2.9)	3172.3 (b, 0.7)
3173.8 (b, 0.1)	3170.2 (a, 0.8)	3172.5 (a, 0.4)	3172.2 (a_1, 0.0)	3172.4 (a, 0.2)
3184.4 (e, 0.7)	3170.4 (a, 0.6)	3179.6 (a, 0.3)	3182.0 (a_2, 0.0)	3182.1 (b, 0.5)
3184.4 (e, 0.7)	3171.2 (a, 2.1)	3180.9 (a, 0.5)	3182.3 (b_1, 0.0)	3182.2 (a, 0.1)
3184.8 (a, 0.0)	3177.7 (a, 0.5)	3181.9 (a, 0.8)	3182.5 (e, 0.0)	3183.1 (b, 0.0)
3184.8 (b, 1.5)	3179.8 (a, 2.5)	3182.0 (a, 0.4)	3182.5 (e, 0.0)	3183.1 (a, 0.0)
3187.1 (a, 0.0)	3182.0 (a, 0.1)	3182.3 (a, 0.6)	3185.7 (e, 0.1)	3185.7 (b, 0.1)
3187.2 (b, 2.6)	3183.9 (a, 0.8)	3182.4 (a, 1.0)	3185.7 (e, 0.1)	3185.8 (a, 0.0)
3187.5 (e, 0.5)	3185.0 (a, 1.1)	3182.7 (a, 0.3)	3186.4 (a_1, 0.0)	3186.0 (b, 0.0)
3187.5 (e, 0.5)	3187.1 (a, 0.7)	3186.6 (a, 0.0)	3186.4 (b_2, 0.1)	3186.1 (a, 0.2)
3196.6 (a, 0.0)	3193.9 (a, 1.3)	3192.4 (a, 0.5)	3194.6 (e, 0.0)	3194.2 (b, 0.3)
3196.7 (b, 2.5)	3195.4 (a, 0.8)	3192.6 (a, 0.3)	3194.6 (e, 0.0)	3194.3 (a, 0.0)
3197.5 (e, 0.4)	3202.0 (a, 1.5)	3194.0 (a, 0.5)	3194.8 (b_2, 1.1)	3195.1 (b, 0.2)
3197.5 (e, 0.4)	3202.8 (a, 1.2)	3195.1 (a, 0.3)	3194.9 (a_1, 0.0)	3195.1 (a, 0.0)

Table S34. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the four triplet structures of $Cp_4V_4(CO)_4$ by the BP86 method (infrared intensities in parentheses are in km/mol).

4T-1	4T-2	4T-3	4T-4
19.6 (a, 0.0)	36.2 (a, 0.1)	27.9 (a, 0.0)	47.6 (a, 0.3)
29.1 (a, 0.1)	49.4 (a, 0.2)	35.1 (a, 0.0)	50.2 (a, 0.6)
32.3 (a, 0.0)	50.3 (a, 0.5)	49.0 (a, 0.0)	58.1 (a, 1.0)
45.8 (a, 0.0)	62.9 (a, 0.6)	54.2 (a, 0.0)	59.0 (a, 0.6)
49.1 (a, 0.0)	66.3 (a, 0.2)	64.8 (a, 0.0)	63.2 (a, 0.5)
55.1 (a, 0.1)	71.8 (a, 0.3)	72.1 (a, 0.0)	71.2 (a, 0.4)
82.1 (a, 0.1)	75.0 (a, 0.0)	81.1 (a, 0.9)	74.0 (a, 0.1)
89.8 (a, 0.6)	87.3 (a, 0.5)	82.8 (a, 0.4)	76.6 (a, 0.1)
93.9 (a, 0.3)	98.3 (a, 0.1)	95.4 (a, 0.7)	77.4 (a, 0.0)
120.1 (a, 0.1)	105.2 (a, 0.5)	107.0 (a, 0.0)	90.6 (a, 0.2)
132.0 (a, 1.2)	108.4 (a, 0.2)	114.0 (a, 0.2)	112.4 (a, 1.0)
133.6 (a, 0.7)	114.4 (a, 1.8)	129.4 (a, 0.9)	121.1 (a, 1.8)
143.6 (a, 0.0)	118.9 (a, 0.6)	140.4 (a, 0.5)	137.0 (a, 0.8)
161.4 (a, 1.0)	122.9 (a, 0.6)	149.2 (a, 0.3)	147.9 (a, 0.4)
162.7 (a, 1.1)	127.8 (a, 0.3)	153.5 (a, 0.0)	158.4 (a, 0.1)
170.2 (a, 0.5)	147.6 (a, 0.6)	159.9 (a, 0.1)	170.7 (a, 0.0)
172.0 (a, 0.8)	151.6 (a, 0.6)	165.7 (a, 0.0)	174.0 (a, 0.2)
183.3 (a, 0.4)	159.0 (a, 1.6)	181.6 (a, 0.4)	177.9 (a, 0.9)
187.5 (a, 1.6)	172.8 (a, 0.7)	194.2 (a, 1.6)	196.2 (a, 2.0)
191.8 (a, 2.2)	181.7 (a, 2.2)	202.3 (a, 2.5)	199.5 (a, 3.1)
207.0 (a, 2.2)	190.8 (a, 0.6)	206.3 (a, 0.5)	206.2 (a, 0.9)
214.5 (a, 0.6)	204.9 (a, 0.2)	212.6 (a, 2.0)	212.4 (a, 0.9)
234.5 (a, 1.2)	207.9 (a, 1.4)	234.1 (a, 3.0)	213.6 (a, 1.3)
260.0 (a, 1.9)	227.3 (a, 0.2)	235.7 (a, 0.4)	228.2 (a, 0.8)
269.5 (a, 0.8)	239.8 (a, 0.9)	252.0 (a, 0.9)	234.1 (a, 2.0)
290.5 (a, 1.9)	289.8 (a, 2.9)	255.9 (a, 6.9)	238.9 (a, 1.2)
294.7 (a, 2.3)	293.0 (a, 4.5)	283.7 (a, 2.8)	251.3 (a, 4.4)
297.2 (a, 8.7)	295.6 (a, 7.2)	286.1 (a, 2.8)	258.3 (a, 1.7)
299.8 (a, 4.2)	301.5 (a, 1.3)	288.4 (a, 2.9)	259.9 (a, 1.3)
306.4 (a, 3.6)	308.9 (a, 0.4)	294.0 (a, 0.7)	276.7 (a, 2.0)
310.8 (a, 0.8)	311.6 (a, 1.2)	305.1 (a, 2.2)	277.8 (a, 1.4)
326.1 (a, 2.3)	320.0 (a, 0.1)	315.0 (a, 2.5)	285.9 (a, 2.2)
333.0 (a, 1.3)	338.4 (a, 1.2)	319.2 (a, 0.4)	290.5 (a, 0.2)
354.2 (a, 5.5)	350.6 (a, 1.5)	324.7 (a, 0.1)	314.8 (a, 2.1)
361.9 (a, 3.1)	372.9 (a, 0.7)	345.7 (a, 13.8)	331.6 (a, 1.2)
377.4 (a, 4.3)	378.8 (a, 2.6)	354.4 (a, 3.6)	339.8 (a, 3.4)
390.3 (a, 6.7)	393.5 (a, 6.3)	375.8 (a, 2.8)	354.9 (a, 2.5)
399.5 (a, 8.1)	411.1 (a, 10.7)	383.1 (a, 1.0)	362.8 (a, 5.6)
421.8 (a, 3.8)	411.4 (a, 1.5)	395.6 (a, 0.0)	371.6 (a, 11.9)
434.4 (a, 1.9)	442.1 (a, 1.9)	404.3 (a, 30.1)	383.7 (a, 44.0)
438.9 (a, 3.2)	457.3 (a, 1.7)	432.4 (a, 3.5)	405.1 (a, 42.9)
477.1 (a, 0.3)	465.8 (a, 9.2)	443.6 (a, 0.2)	411.0 (a, 35.4)
478.5 (a, 4.4)	479.5 (a, 4.1)	518.2 (a, 5.3)	419.0 (a, 38.5)
493.3 (a, 2.1)	483.1 (a, 15.9)	532.0 (a, 0.7)	426.1 (a, 6.6)
505.7 (a, 6.1)	496.0 (a, 10.2)	564.2 (a, 0.2)	436.9 (a, 6.9)
511.5 (a, 9.9)	498.5 (a, 26.4)	567.9 (a, 3.9)	438.9 (a, 8.2)
552.4 (a, 2.8)	506.5 (a, 6.9)	570.6 (a, 0.0)	454.7 (a, 8.5)

571.1 (a, 3.9)	516.4 (a, 8.9)	570.9 (a, 0.4)	457.6 (a, 1.1)
573.1 (a, 0.1)	565.8 (a, 0.4)	575.3 (a, 0.3)	465.3 (a, 3.2)
573.7 (a, 0.2)	568.8 (a, 0.5)	575.6 (a, 1.4)	477.3 (a, 9.4)
577.2 (a, 1.1)	570.3 (a, 0.6)	576.4 (a, 5.1)	555.5 (a, 1.0)
578.0 (a, 0.5)	570.9 (a, 0.3)	576.8 (a, 4.7)	567.0 (a, 0.4)
578.7 (a, 1.0)	573.7 (a, 1.3)	579.9 (a, 1.1)	578.8 (a, 7.5)
579.8 (a, 2.6)	575.3 (a, 1.7)	583.3 (a, 8.7)	590.9 (a, 2.7)
583.4 (a, 1.7)	576.4 (a, 1.9)	610.7 (a, 6.2)	592.6 (a, 1.9)
593.4 (a, 3.3)	578.8 (a, 3.0)	612.9 (a, 1.1)	598.0 (a, 0.3)
616.0 (a, 5.0)	583.0 (a, 0.3)	634.3 (a, 7.6)	620.9 (a, 1.7)
622.2 (a, 9.3)	604.1 (a, 2.2)	640.5 (a, 29.6)	623.4 (a, 1.3)
770.3 (a, 49.6)	737.2 (a, 16.9)	746.6 (a, 74.9)	702.6 (a, 21.2)
774.7 (a, 96.5)	747.0 (a, 56.0)	750.3 (a, 32.4)	714.8 (a, 5.9)
775.2 (a, 53.9)	756.1 (a, 65.2)	757.7 (a, 54.5)	715.9 (a, 1.0)
778.4 (a, 146.5)	761.3 (a, 10.7)	758.4 (a, 21.7)	727.0 (a, 2.3)
780.9 (a, 36.0)	764.7 (a, 5.8)	769.8 (a, 12.4)	737.0 (a, 1.2)
782.0 (a, 11.2)	775.2 (a, 0.9)	775.3 (a, 71.9)	739.5 (a, 3.1)
785.9 (a, 36.6)	781.6 (a, 54.0)	777.3 (a, 159.8)	743.4 (a, 11.8)
789.8 (a, 34.8)	782.1 (a, 38.6)	780.0 (a, 46.8)	746.1 (a, 3.8)
793.9 (a, 30.2)	784.5 (a, 38.5)	781.5 (a, 36.1)	750.3 (a, 6.6)
795.8 (a, 32.0)	786.7 (a, 98.5)	792.5 (a, 39.4)	752.0 (a, 10.8)
797.8 (a, 21.4)	796.4 (a, 57.2)	796.6 (a, 9.9)	760.8 (a, 21.2)
803.1 (a, 38.8)	803.0 (a, 31.4)	802.1 (a, 13.3)	764.7 (a, 6.8)
815.3 (a, 1.2)	809.3 (a, 0.7)	814.9 (a, 0.1)	772.1 (a, 2.4)
816.2 (a, 0.2)	811.5 (a, 9.9)	816.3 (a, 0.5)	773.5 (a, 6.6)
816.9 (a, 0.9)	812.1 (a, 0.2)	816.5 (a, 0.4)	780.6 (a, 3.5)
817.6 (a, 5.3)	814.2 (a, 1.4)	816.8 (a, 0.7)	785.5 (a, 4.0)
818.6 (a, 4.6)	815.6 (a, 0.9)	817.8 (a, 2.2)	788.9 (a, 3.1)
819.2 (a, 5.8)	816.4 (a, 1.3)	818.2 (a, 3.0)	794.7 (a, 11.5)
819.4 (a, 0.8)	817.2 (a, 0.2)	818.7 (a, 0.1)	800.6 (a, 9.2)
820.2 (a, 2.8)	819.1 (a, 2.0)	819.2 (a, 1.6)	805.5 (a, 2.5)
857.6 (a, 1.2)	838.7 (a, 4.3)	837.7 (a, 0.1)	836.1 (a, 1.9)
859.8 (a, 6.2)	844.1 (a, 2.6)	854.4 (a, 1.7)	842.5 (a, 0.2)
860.9 (a, 1.4)	848.2 (a, 0.7)	859.4 (a, 4.3)	853.8 (a, 0.9)
863.3 (a, 0.8)	854.3 (a, 5.4)	863.0 (a, 3.0)	862.6 (a, 1.5)
864.7 (a, 2.6)	857.7 (a, 0.3)	863.3 (a, 8.4)	868.1 (a, 1.5)
867.0 (a, 5.0)	863.9 (a, 1.0)	867.2 (a, 2.9)	870.2 (a, 1.7)
867.8 (a, 1.2)	868.4 (a, 5.8)	868.3 (a, 11.2)	873.4 (a, 0.7)
870.6 (a, 1.4)	879.4 (a, 3.2)	869.4 (a, 2.8)	903.1 (a, 3.0)
992.1 (a, 7.0)	976.5 (a, 6.9)	994.8 (a, 13.9)	922.3 (a, 1.2)
994.8 (a, 6.8)	980.0 (a, 7.6)	996.2 (a, 1.8)	928.6 (a, 1.4)
995.3 (a, 9.4)	991.6 (a, 12.4)	996.5 (a, 11.0)	936.1 (a, 9.6)
995.5 (a, 10.5)	994.7 (a, 11.6)	998.0 (a, 2.5)	944.6 (a, 8.6)
997.6 (a, 3.1)	998.7 (a, 1.9)	998.3 (a, 1.0)	959.9 (a, 5.5)
999.2 (a, 10.4)	1000.5 (a, 7.0)	999.8 (a, 15.5)	961.6 (a, 5.2)
1000.7 (a, 12.6)	1007.0 (a, 0.8)	1002.4 (a, 20.7)	963.4 (a, 4.6)
1000.7 (a, 0.4)	1009.0 (a, 13.6)	1003.9 (a, 0.0)	966.3 (a, 1.4)
1038.5 (a, 0.5)	1031.3 (a, 4.5)	1037.0 (a, 0.3)	1006.9 (a, 13.5)
1041.8 (a, 0.7)	1040.0 (a, 1.5)	1040.7 (a, 0.4)	1012.1 (a, 13.0)
1043.7 (a, 0.3)	1042.4 (a, 1.6)	1044.4 (a, 2.2)	1017.3 (a, 0.7)
1044.4 (a, 1.2)	1044.3 (a, 4.8)	1045.4 (a, 0.0)	1019.1 (a, 0.5)
1045.2 (a, 0.2)	1046.5 (a, 0.1)	1045.7 (a, 0.6)	1026.2 (a, 1.7)
1045.8 (a, 0.3)	1048.3 (a, 0.8)	1045.7 (a, 1.8)	1030.0 (a, 2.2)

1046.4 (a, 0.6)	1053.7 (a, 1.3)	1047.1 (a, 1.4)	1033.3 (a, 0.1)
1048.5 (a, 0.9)	1055.4 (a, 3.6)	1049.9 (a, 2.8)	1034.3 (a, 6.0)
1113.3 (a, 2.3)	1095.6 (a, 5.5)	1114.8 (a, 2.0)	1036.4 (a, 1.3)
1114.2 (a, 1.2)	1111.5 (a, 4.4)	1115.3 (a, 0.8)	1040.9 (a, 0.7)
1114.7 (a, 1.8)	1114.0 (a, 3.2)	1115.8 (a, 4.1)	1052.9 (a, 1.8)
1115.7 (a, 2.1)	1117.7 (a, 5.4)	1116.8 (a, 2.0)	1054.8 (a, 4.3)
1222.3 (a, 0.0)	1210.7 (a, 0.3)	1224.0 (a, 0.0)	1204.3 (a, 0.1)
1223.6 (a, 0.0)	1226.4 (a, 0.0)	1225.7 (a, 0.0)	1207.0 (a, 0.1)
1224.4 (a, 0.0)	1228.2 (a, 0.1)	1226.0 (a, 0.0)	1211.8 (a, 0.1)
1226.6 (a, 0.0)	1230.2 (a, 0.0)	1229.8 (a, 0.0)	1213.2 (a, 0.2)
1365.3 (a, 8.5)	1302.8 (a, 54.0)	1365.4 (a, 0.0)	1259.6 (a, 1.6)
1365.7 (a, 0.2)	1337.2 (a, 0.3)	1366.0 (a, 2.5)	1266.1 (a, 2.5)
1366.1 (a, 2.7)	1356.0 (a, 0.8)	1366.5 (a, 3.4)	1267.1 (a, 0.6)
1366.3 (a, 1.2)	1363.7 (a, 0.3)	1366.7 (a, 0.1)	1276.1 (a, 2.3)
1367.2 (a, 0.9)	1370.6 (a, 0.7)	1370.6 (a, 0.7)	1281.0 (a, 1.4)
1368.7 (a, 0.2)	1371.4 (a, 0.2)	1370.6 (a, 3.1)	1284.4 (a, 5.4)
1369.6 (a, 2.7)	1372.3 (a, 0.4)	1371.6 (a, 0.2)	1297.5 (a, 2.4)
1371.1 (a, 38.8)	1373.1 (a, 0.3)	1372.1 (a, 3.3)	1316.4 (a, 3.6)
1372.4 (a, 3.6)	1378.5 (a, 0.3)	1412.5 (a, 4.0)	1325.6 (a, 2.1)
1410.7 (a, 1.6)	1392.0 (a, 1.7)	1413.9 (a, 1.1)	1336.4 (a, 1.4)
1411.8 (a, 1.3)	1409.2 (a, 1.8)	1416.9 (a, 2.4)	1337.0 (a, 0.2)
1414.1 (a, 1.0)	1410.8 (a, 3.5)	1417.8 (a, 2.0)	1342.5 (a, 0.9)
1415.5 (a, 2.9)	1412.6 (a, 1.6)	1418.6 (a, 0.4)	1347.2 (a, 1.3)
1418.1 (a, 1.1)	1414.8 (a, 1.8)	1418.9 (a, 3.3)	1358.9 (a, 3.8)
1419.8 (a, 1.8)	1418.0 (a, 1.7)	1419.8 (a, 1.2)	1394.1 (a, 2.3)
1421.6 (a, 1.6)	1421.6 (a, 3.0)	1421.2 (a, 0.4)	1412.2 (a, 1.4)
1422.7 (a, 2.7)	1422.1 (a, 0.5)	1516.7 (a, 25.4)	1893.2 (a,1786.4)
1517.7 (a, 188.3)	1730.9 (a, 430.9)	1516.7 (a, 282.3)	1898.1 (a,1934.7)
1625.8 (a, 357.9)	1748.6 (a, 635.8)	1540.0 (a, 358.4)	1898.8 (a,1887.7)
1655.8 (a, 314.0)	1802.8 (a, 567.1)	1568.5 (a, 18.7)	1920.4 (a, 22.4)
3157.4 (a, 0.5)	3099.8 (a, 5.3)	3164.8 (a, 0.1)	3091.4 (a, 4.2)
3160.6 (a, 0.7)	3149.5 (a, 0.5)	3164.8 (a, 0.1)	3101.8 (a, 4.0)
3165.7 (a, 0.1)	3160.7 (a, 0.6)	3170.6 (a, 0.1)	3102.8 (a, 1.5)
3165.8 (a, 0.1)	3164.8 (a, 0.2)	3170.7 (a, 0.1)	3106.1 (a, 3.7)
3167.4 (a, 0.3)	3167.0 (a, 0.0)	3172.0 (a, 0.4)	3124.3 (a, 2.6)
3170.0 (a, 0.2)	3170.5 (a, 1.2)	3172.1 (a, 0.1)	3125.8 (a, 0.5)
3171.2 (a, 0.1)	3170.7 (a, 0.2)	3172.2 (a, 0.0)	3128.6 (a, 1.1)
3174.3 (a, 0.1)	3171.2 (a, 0.5)	3172.6 (a, 0.0)	3130.2 (a, 0.8)
3177.8 (a, 0.6)	3171.4 (a, 0.3)	3181.2 (a, 1.1)	3132.7 (a, 6.3)
3178.7 (a, 0.6)	3174.1 (a, 0.6)	3181.2 (a, 0.4)	3133.6 (a, 0.2)
3182.0 (a, 0.5)	3175.9 (a, 0.3)	3183.7 (a, 1.0)	3135.0 (a, 0.9)
3182.3 (a, 0.3)	3181.3 (a, 0.6)	3183.9 (a, 0.2)	3139.7 (a, 2.5)
3182.5 (a, 0.7)	3182.1 (a, 1.2)	3184.3 (a, 0.6)	3143.0 (a, 2.4)
3182.6 (a, 0.1)	3186.9 (a, 1.3)	3184.7 (a, 1.4)	3145.2 (a, 2.7)
3183.2 (a, 0.3)	3187.0 (a, 1.2)	3185.8 (a, 1.7)	3145.4 (a, 1.7)
3188.7 (a, 0.5)	3187.3 (a, 0.5)	3186.0 (a, 0.2)	3146.0 (a, 0.3)
3192.9 (a, 0.6)	3194.0 (a, 0.5)	3195.2 (a, 0.6)	3151.9 (a, 1.1)
3194.3 (a, 0.4)	3196.8 (a, 0.8)	3195.4 (a, 0.6)	3157.3 (a, 0.7)
3194.4 (a, 0.2)	3196.9 (a, 1.5)	3195.7 (a, 1.5)	3163.0 (a, 1.9)
3200.6 (a, 0.2)	3207.1 (a, 1.1)	3196.6 (a, 0.4)	3166.5 (a, 0.3)

Table S35. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the three quintet structures of $Cp_4V_4(CO)_4$ by the BP86 method (infrared intensities in parentheses are in km/mol).

4Q-1	4Q-2	4Q-3
32.2 (a, 0.0)	45.2 (a, 0.8)	48.2 (a, 0.0)
36.3 (a, 0.0)	51.1 (a, 0.3)	49.8 (b, 0.5)
42.2 (a, 0.0)	53.9 (a, 0.2)	56.1 (a, 0.2)
49.5 (a, 0.1)	55.5 (a, 0.6)	59.6 (b, 1.4)
52.0 (a, 0.1)	57.4 (a, 1.0)	60.8 (a, 0.2)
62.1 (a, 0.0)	59.1 (a, 1.2)	61.0 (b, 0.3)
78.6 (a, 0.4)	61.9 (a, 0.0)	72.1 (a, 0.0)
92.1 (a, 0.3)	75.6 (a, 0.2)	73.0 (b, 0.1)
94.6 (a, 0.4)	77.2 (a, 0.4)	80.0 (b, 0.5)
114.1 (a, 1.5)	107.1 (a, 1.2)	85.2 (a, 0.1)
132.5 (a, 0.3)	117.7 (a, 0.2)	116.0 (a, 0.1)
135.0 (a, 0.3)	122.4 (a, 0.1)	117.9 (b, 0.0)
142.2 (a, 0.4)	125.5 (a, 0.1)	130.7 (a, 0.1)
145.6 (a, 0.3)	139.0 (a, 0.2)	142.7 (b, 0.1)
162.9 (a, 0.2)	147.4 (a, 1.0)	150.0 (a, 0.4)
172.3 (a, 1.2)	151.3 (a, 3.2)	158.5 (a, 0.1)
178.2 (a, 0.2)	159.3 (a, 2.9)	163.7 (b, 2.0)
179.0 (a, 0.6)	167.9 (a, 1.4)	180.1 (b, 3.7)
191.4 (a, 0.3)	173.5 (a, 1.8)	184.2 (a, 0.0)
195.2 (a, 1.1)	176.6 (a, 1.8)	192.3 (b, 3.3)
215.5 (a, 2.5)	179.6 (a, 2.8)	194.0 (a, 1.6)
226.5 (a, 0.3)	198.0 (a, 1.8)	207.5 (b, 1.3)
230.8 (a, 1.0)	204.1 (a, 1.6)	209.8 (a, 0.2)
264.2 (a, 3.9)	217.2 (a, 4.9)	219.1 (b, 1.9)
268.6 (a, 0.6)	222.1 (a, 1.3)	221.3 (a, 0.5)
282.9 (a, 1.4)	242.8 (a, 0.4)	234.0 (b, 0.5)
290.0 (a, 0.6)	247.3 (a, 10.7)	234.9 (a, 0.0)
297.5 (a, 4.7)	290.0 (a, 1.5)	237.4 (a, 0.0)
302.8 (a, 3.1)	292.9 (a, 3.1)	249.8 (b, 2.1)
311.7 (a, 4.5)	300.5 (a, 2.5)	252.1 (a, 0.1)
317.5 (a, 6.9)	305.2 (a, 4.3)	255.7 (b, 1.3)
324.8 (a, 5.6)	306.9 (a, 2.3)	270.5 (a, 0.7)
337.2 (a, 2.4)	317.3 (a, 0.3)	271.9 (b, 1.7)
341.7 (a, 7.2)	318.1 (a, 0.9)	283.7 (a, 0.4)
351.3 (a, 6.1)	324.9 (a, 4.0)	294.3 (b, 3.2)
359.9 (a, 6.6)	342.7 (a, 0.1)	311.1 (a, 0.0)
371.3 (a, 7.8)	354.0 (a, 1.3)	336.1 (b, 5.2)
376.1 (a, 11.8)	376.7 (a, 4.9)	365.7 (a, 0.7)
381.6 (a, 3.4)	383.8 (a, 4.4)	366.7 (b, 3.4)
396.3 (a, 10.4)	403.8 (a, 2.0)	394.0 (a, 29.9)
412.2 (a, 7.0)	417.3 (a, 6.4)	395.7 (b, 40.8)
420.4 (a, 0.9)	422.3 (a, 3.6)	405.6 (b, 43.9)
433.5 (a, 1.5)	435.2 (a, 0.3)	417.2 (b, 31.8)
449.9 (a, 2.2)	454.3 (a, 3.7)	418.2 (a, 15.4)
471.5 (a, 1.1)	460.7 (a, 7.4)	428.5 (a, 17.1)
494.6 (a, 11.2)	471.9 (a, 4.5)	441.5 (a, 7.9)
541.5 (a, 2.8)	479.6 (a, 0.3)	447.2 (b, 2.0)

555.0 (a, 2.7)	487.0 (a, 17.5)	459.9 (a, 0.3)
572.8 (a, 0.2)	496.6 (a, 3.2)	464.0 (b, 16.0)
575.7 (a, 0.2)	514.7 (a, 10.4)	468.8 (a, 9.6)
576.5 (a, 1.0)	574.4 (a, 0.8)	550.7 (a, 0.8)
579.8 (a, 1.4)	574.7 (a, 0.2)	551.6 (b, 0.4)
581.2 (a, 0.1)	575.2 (a, 0.4)	569.5 (b, 2.3)
581.9 (a, 1.0)	575.8 (a, 0.0)	572.4 (a, 2.9)
582.2 (a, 1.6)	576.3 (a, 0.5)	597.9 (b, 0.2)
583.1 (a, 0.2)	577.1 (a, 0.5)	602.4 (a, 0.2)
612.7 (a, 8.2)	579.6 (a, 0.1)	628.9 (a, 0.8)
632.8 (a, 2.8)	580.2 (a, 1.0)	630.1 (b, 2.7)
773.1 (a, 60.7)	779.8 (a, 87.1)	691.4 (b, 22.3)
774.9 (a, 73.6)	780.1 (a, 122.8)	698.7 (a, 16.7)
776.3 (a, 105.8)	783.7 (a, 90.4)	706.2 (b, 2.5)
777.9 (a, 50.8)	785.6 (a, 41.6)	708.5 (a, 2.3)
779.2 (a, 9.9)	788.6 (a, 22.1)	712.5 (b, 37.0)
785.6 (a, 36.4)	789.7 (a, 37.9)	719.7 (a, 3.6)
788.3 (a, 68.8)	789.9 (a, 36.5)	721.0 (b, 1.9)
788.8 (a, 63.1)	792.1 (a, 10.4)	737.0 (b, 5.4)
793.3 (a, 32.9)	798.2 (a, 26.8)	742.3 (a, 0.3)
796.9 (a, 30.7)	799.9 (a, 14.5)	745.0 (a, 3.8)
798.9 (a, 26.9)	803.8 (a, 92.1)	756.2 (b, 2.0)
800.7 (a, 8.2)	804.9 (a, 20.2)	768.1 (b, 18.5)
815.9 (a, 0.6)	816.8 (a, 1.5)	768.4 (a, 0.1)
816.5 (a, 1.7)	817.8 (a, 2.0)	771.2 (b, 1.1)
817.3 (a, 1.6)	818.5 (a, 1.9)	772.2 (a, 6.4)
818.0 (a, 4.5)	818.7 (a, 4.7)	778.7 (a, 19.9)
818.5 (a, 1.1)	819.2 (a, 0.2)	779.6 (b, 15.8)
818.7 (a, 4.3)	819.6 (a, 4.2)	789.8 (a, 0.0)
820.3 (a, 0.8)	820.1 (a, 1.9)	801.1 (b, 8.3)
821.0 (a, 6.7)	820.6 (a, 8.8)	801.3 (a, 2.7)
855.8 (a, 1.4)	856.1 (a, 0.7)	829.4 (a, 1.1)
857.0 (a, 0.8)	860.3 (a, 1.0)	834.1 (b, 1.6)
859.6 (a, 1.8)	861.9 (a, 2.0)	848.9 (b, 0.2)
862.2 (a, 0.3)	865.3 (a, 1.6)	851.5 (a, 0.1)
863.9 (a, 1.6)	866.3 (a, 1.0)	859.2 (b, 0.9)
866.9 (a, 1.0)	869.2 (a, 1.1)	860.3 (a, 2.3)
872.2 (a, 6.4)	871.6 (a, 2.0)	894.0 (b, 4.2)
875.3 (a, 0.3)	875.2 (a, 1.0)	894.9 (a, 0.2)
992.3 (a, 8.1)	993.3 (a, 6.6)	914.4 (b, 8.0)
993.8 (a, 8.0)	994.3 (a, 8.4)	919.5 (a, 4.4)
994.8 (a, 7.6)	995.2 (a, 9.5)	962.6 (b, 3.0)
995.9 (a, 6.8)	996.4 (a, 3.1)	965.2 (b, 8.6)
997.6 (a, 7.8)	997.1 (a, 2.3)	967.6 (a, 1.2)
999.9 (a, 3.9)	997.6 (a, 3.6)	970.8 (a, 1.0)
1000.5 (a, 17.6)	998.3 (a, 7.3)	976.3 (b, 5.9)
1002.7 (a, 3.6)	1000.4 (a, 7.0)	976.7 (a, 3.3)
1038.4 (a, 0.3)	1038.2 (a, 0.4)	998.7 (b, 23.4)
1041.2 (a, 1.0)	1041.0 (a, 0.3)	1002.7 (a, 4.7)
1042.6 (a, 0.3)	1041.5 (a, 0.4)	1015.6 (b, 0.5)
1043.6 (a, 0.0)	1042.5 (a, 0.4)	1016.8 (a, 0.1)
1045.1 (a, 1.0)	1043.3 (a, 0.1)	1033.3 (b, 0.0)
1045.9 (a, 0.6)	1044.9 (a, 0.6)	1034.5 (a, 0.7)

1047.0 (a, 0.2)	1045.7 (a, 0.2)	1035.4 (b, 2.9)
1049.2 (a, 0.5)	1049.4 (a, 0.0)	1038.7 (a, 1.6)
1113.0 (a, 2.5)	1112.9 (a, 1.6)	1039.8 (b, 2.3)
1113.3 (a, 2.4)	1113.0 (a, 1.8)	1041.9 (a, 0.0)
1113.5 (a, 2.3)	1113.4 (a, 3.2)	1056.5 (b, 4.8)
1115.6 (a, 2.4)	1113.5 (a, 0.2)	1059.0 (a, 4.4)
1223.0 (a, 0.0)	1219.3 (a, 0.0)	1204.0 (b, 0.2)
1223.9 (a, 0.0)	1221.9 (a, 0.0)	1204.3 (a, 0.1)
1224.0 (a, 0.0)	1223.3 (a, 0.0)	1215.3 (b, 0.0)
1226.1 (a, 0.0)	1223.6 (a, 0.0)	1216.8 (a, 0.0)
1359.9 (a, 51.6)	1365.2 (a, 0.6)	1265.5 (b, 0.5)
1365.8 (a, 0.1)	1366.2 (a, 1.0)	1266.2 (a, 0.3)
1367.1 (a, 1.5)	1366.5 (a, 0.7)	1271.7 (a, 0.7)
1368.3 (a, 2.6)	1366.7 (a, 0.3)	1272.0 (b, 2.8)
1368.5 (a, 1.4)	1367.2 (a, 0.3)	1307.8 (a, 6.4)
1368.7 (a, 1.9)	1367.2 (a, 0.2)	1309.9 (b, 1.6)
1369.0 (a, 1.1)	1369.0 (a, 0.1)	1314.3 (b, 2.7)
1369.6 (a, 2.7)	1370.2 (a, 0.3)	1314.8 (a, 0.2)
1370.2 (a, 0.6)	1411.6 (a, 3.0)	1332.6 (b, 0.9)
1410.8 (a, 1.6)	1412.4 (a, 2.1)	1335.3 (a, 0.0)
1412.7 (a, 1.1)	1413.6 (a, 2.4)	1336.5 (b, 6.5)
1413.3 (a, 0.5)	1415.1 (a, 1.1)	1337.6 (a, 1.0)
1413.6 (a, 2.2)	1416.1 (a, 0.9)	1369.0 (b, 0.2)
1418.3 (a, 2.2)	1416.6 (a, 2.6)	1371.4 (a, 1.2)
1420.1 (a, 1.9)	1419.1 (a, 1.8)	1401.8 (b, 0.8)
1421.7 (a, 2.4)	1419.7 (a, 1.6)	1401.8 (a, 0.3)
1421.8 (a, 1.6)	1637.7 (a, 373.2)	1887.8 (b, 1860.7)
1498.1 (a, 191.6)	1655.6 (a, 333.6)	1889.2 (a, 1888.4)
1616.0 (a, 360.5)	1685.3 (a, 667.1)	1892.7 (b, 2001.5)
1638.7 (a, 194.7)	1699.0 (a, 135.6)	1915.0 (a, 16.7)
3162.0 (a, 0.1)	3163.7 (a, 0.4)	3101.9 (b, 8.0)
3164.5 (a, 0.9)	3165.1 (a, 0.2)	3102.1 (a, 0.9)
3164.6 (a, 0.1)	3165.5 (a, 0.4)	3120.7 (a, 0.1)
3165.2 (a, 0.2)	3168.4 (a, 0.3)	3120.8 (b, 3.0)
3168.9 (a, 0.9)	3168.6 (a, 0.0)	3128.5 (a, 0.1)
3169.0 (a, 0.1)	3168.8 (a, 0.3)	3128.7 (b, 7.5)
3169.2 (a, 0.3)	3169.1 (a, 0.1)	3134.1 (b, 0.5)
3170.0 (a, 0.1)	3169.7 (a, 0.1)	3134.3 (a, 0.0)
3178.0 (a, 0.3)	3178.8 (a, 0.2)	3136.4 (b, 2.9)
3179.0 (a, 1.3)	3179.6 (a, 0.1)	3136.5 (a, 3.4)
3181.5 (a, 0.2)	3180.0 (a, 0.4)	3140.9 (b, 1.4)
3181.5 (a, 0.3)	3180.5 (a, 0.4)	3141.3 (a, 1.5)
3182.8 (a, 0.0)	3180.6 (a, 0.1)	3149.3 (b, 1.0)
3183.0 (a, 0.3)	3180.7 (a, 0.4)	3149.6 (a, 0.8)
3183.1 (a, 0.4)	3180.9 (a, 0.3)	3156.5 (b, 0.1)
3184.4 (a, 0.4)	3183.2 (a, 0.0)	3157.3 (a, 0.1)
3192.4 (a, 0.5)	3191.1 (a, 0.5)	3160.2 (b, 0.6)
3194.1 (a, 0.2)	3191.4 (a, 0.3)	3160.4 (a, 0.0)
3194.4 (a, 0.3)	3191.5 (a, 0.1)	3166.8 (a, 0.4)
3196.7 (a, 0.3)	3192.8 (a, 0.3)	3166.8 (b, 0.4)

Table S36. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the three singlet structures of $Cp_3V_3(CO)_9$ by the BP86 method (infrared intensities in parentheses are in km/mol).

9S-1	9S-2	9S-3
46.5 (e, 0.1)	25.2 (a, 0.0)	25.3 (a", 0.2)
46.5 (e, 0.1)	40.9 (a, 0.4)	33.2 (a", 0.0)
50.9 (a, 0.0)	47.8 (a, 1.0)	43.1 (a', 0.5)
60.1 (e, 0.0)	57.6 (a, 0.2)	58.2 (a", 0.0)
60.1 (e, 0.0)	70.1 (a, 0.1)	63.7 (a", 0.3)
73.2 (e, 0.0)	71.3 (a, 0.3)	75.3 (a', 0.1)
73.2 (e, 0.0)	73.7 (a, 0.0)	80.5 (a', 0.3)
76.4 (a, 0.0)	77.9 (a, 0.0)	81.4 (a", 0.2)
89.1 (e, 0.1)	82.1 (a, 0.0)	83.9 (a', 0.0)
89.1 (e, 0.1)	83.5 (a, 0.1)	93.6 (a", 0.0)
89.6 (a, 1.2)	88.4 (a, 0.0)	97.4 (a', 0.1)
94.2 (e, 0.2)	92.8 (a, 0.7)	105.2 (a', 0.4)
94.2 (e, 0.2)	95.0 (a, 0.7)	106.9 (a", 0.0)
104.5 (a, 0.7)	102.2 (a, 0.0)	110.9 (a', 0.1)
112.8 (e, 1.0)	108.9 (a, 0.0)	117.3 (a", 0.0)
112.8 (e, 1.0)	117.0 (a, 0.1)	120.4 (a', 0.1)
114.4 (a, 0.2)	118.7 (a, 0.1)	122.6 (a", 0.0)
124.2 (a, 0.0)	125.4 (a, 2.2)	132.1 (a', 0.3)
125.0 (e, 0.9)	139.4 (a, 0.3)	137.8 (a', 0.5)
125.0 (e, 0.9)	142.9 (a, 0.3)	145.1 (a", 0.0)
134.2 (a, 0.1)	146.7 (a, 1.1)	153.8 (a', 1.3)
143.2 (e, 1.3)	149.1 (a, 0.0)	155.9 (a', 0.3)
143.2 (e, 1.3)	152.1 (a, 0.4)	158.6 (a", 0.1)
156.7 (e, 2.2)	163.1 (a, 0.2)	171.0 (a', 2.4)
156.7 (e, 2.2)	166.8 (a, 0.1)	174.8 (a", 0.0)
160.6 (a, 0.1)	169.9 (a, 0.1)	185.6 (a", 0.1)
176.1 (a, 0.1)	174.3 (a, 0.1)	197.9 (a', 0.2)
180.5 (a, 0.1)	191.8 (a, 0.1)	210.2 (a", 0.1)
191.9 (e, 0.8)	212.0 (a, 0.0)	211.4 (a', 0.2)
191.9 (e, 0.8)	232.1 (a, 0.3)	233.7 (a", 0.8)
311.9 (e, 20.5)	285.9 (a, 2.4)	282.2 (a", 0.8)
311.9 (e, 20.5)	294.7 (a, 4.9)	286.1 (a', 0.2)
318.1 (a, 1.5)	310.6 (a, 2.3)	293.9 (a', 5.4)
319.9 (a, 7.4)	311.8 (a, 9.3)	304.4 (a", 5.4)
320.0 (e, 3.1)	315.5 (a, 3.0)	307.4 (a", 3.0)
320.0 (e, 3.1)	316.6 (a, 1.3)	310.9 (a', 2.0)
327.9 (a, 3.8)	318.3 (a, 6.7)	320.8 (a', 11.2)
329.8 (e, 14.8)	325.3 (a, 18.6)	323.4 (a', 4.7)
329.8 (e, 14.8)	334.2 (a, 4.8)	329.8 (a', 3.3)
366.0 (a, 2.2)	342.0 (a, 0.2)	337.2 (a", 1.6)
366.8 (e, 1.9)	360.5 (a, 3.6)	357.2 (a", 9.6)
366.8 (e, 1.9)	365.6 (a, 2.0)	367.4 (a', 5.0)
409.1 (e, 4.9)	368.7 (a, 5.8)	381.6 (a", 0.5)
409.1 (e, 4.9)	397.5 (a, 0.1)	397.2 (a', 1.2)
421.8 (a, 0.2)	413.1 (a, 0.0)	397.3 (a", 0.2)
427.9 (a, 10.6)	421.7 (a, 0.5)	419.3 (a', 6.3)
438.7 (e, 9.1)	428.7 (a, 7.6)	431.5 (a", 7.8)

438.7 (e, 9.1)	436.1 (a, 8.8)	435.8 (a', 9.7)
452.3 (e, 12.7)	436.6 (a, 8.4)	442.6 (a", 1.4)
452.3 (e, 12.7)	438.3 (a, 0.7)	448.8 (a', 4.7)
452.8 (a, 1.1)	449.8 (a, 29.0)	453.1 (a", 14.3)
476.9 (e, 24.2)	452.8 (a, 3.0)	462.9 (a', 5.5)
476.9 (e, 24.2)	465.1 (a, 23.7)	470.5 (a', 7.7)
477.1 (a, 0.1)	469.8 (a, 0.1)	483.5 (a', 67.7)
501.2 (e, 10.5)	477.0 (a, 25.4)	490.1 (a", 76.7)
501.2 (e, 10.5)	493.6 (a, 9.3)	493.5 (a", 87.9)
506.6 (a, 16.0)	498.6 (a, 171.8)	503.1 (a', 0.7)
543.4 (a, 0.1)	526.2 (a, 81.5)	519.9 (a', 28.1)
546.2 (e, 169.1)	533.3 (a, 143.9)	531.3 (a", 25.1)
546.2 (e, 169.1)	551.6 (a, 33.4)	541.5 (a", 246.2)
559.9 (a, 0.7)	554.2 (a, 37.8)	552.8 (a', 82.5)
568.4 (e, 38.0)	566.5 (a, 40.4)	556.4 (a', 15.3)
568.4 (e, 38.0)	567.5 (a, 15.6)	561.2 (a", 0.0)
569.7 (a, 41.3)	570.5 (a, 111.5)	571.7 (a', 0.3)
576.1 (e, 6.0)	572.1 (a, 4.8)	571.7 (a", 80.0)
576.1 (e, 6.0)	574.2 (a, 4.0)	576.6 (a', 62.0)
577.7 (a, 6.9)	575.7 (a, 1.1)	577.2 (a", 7.1)
582.6 (e, 17.4)	577.4 (a, 18.5)	577.7 (a", 1.1)
582.6 (e, 17.4)	578.9 (a, 2.1)	581.3 (a', 15.7)
586.7 (a, 2.7)	580.1 (a, 4.9)	582.4 (a", 7.8)
587.8 (e, 10.2)	581.8 (a, 5.7)	583.9 (a', 13.9)
587.8 (e, 10.2)	593.9 (a, 73.3)	600.2 (a', 19.7)
812.6 (a, 1.6)	782.0 (a, 30.4)	791.3 (a", 32.3)
812.9 (e, 9.1)	803.8 (a, 6.0)	806.3 (a', 77.9)
812.9 (e, 9.1)	807.9 (a, 28.7)	809.5 (a", 1.9)
817.4 (e, 83.9)	811.7 (a, 6.6)	812.8 (a", 0.7)
817.4 (e, 83.9)	812.3 (a, 1.5)	813.0 (a', 12.0)
818.0 (a, 7.2)	812.9 (a, 26.6)	815.8 (a', 11.7)
818.7 (e, 26.4)	813.4 (a, 49.1)	816.2 (a", 4.5)
818.7 (e, 26.4)	814.0 (a, 1.6)	816.8 (a', 50.6)
819.4 (a, 6.7)	814.8 (a, 83.0)	818.3 (a', 8.3)
825.7 (e, 31.3)	817.8 (a, 38.7)	818.6 (a", 0.2)
825.7 (e, 31.3)	818.3 (a, 2.9)	821.1 (a', 76.8)
827.1 (a, 5.1)	821.0 (a, 15.4)	822.6 (a", 49.0)
833.4 (e, 2.2)	821.6 (a, 30.8)	828.4 (a', 10.8)
833.4 (e, 2.2)	828.9 (a, 11.2)	830.4 (a', 25.1)
833.6 (a, 22.5)	838.5 (a, 6.6)	832.8 (a", 12.1)
883.7 (a, 2.3)	872.1 (a, 0.3)	877.6 (a", 0.0)
883.8 (e, 0.1)	877.2 (a, 1.6)	882.7 (a", 0.0)
883.8 (e, 0.1)	881.8 (a, 0.6)	885.8 (a', 2.9)
902.6 (a, 0.3)	887.1 (a, 0.9)	889.3 (a', 7.3)
902.9 (e, 0.5)	893.4 (a, 0.3)	891.4 (a", 1.0)
902.9 (e, 0.5)	903.0 (a, 1.6)	900.8 (a', 0.5)
995.0 (e, 0.9)	988.4 (a, 7.6)	989.4 (a", 7.9)
995.0 (e, 0.9)	993.7 (a, 3.6)	994.0 (a', 2.5)
995.4 (a, 10.7)	993.9 (a, 2.7)	994.4 (a", 2.6)
998.2 (e, 5.0)	997.9 (a, 1.1)	995.1 (a', 2.8)
998.2 (e, 5.0)	999.1 (a, 3.7)	998.0 (a", 0.0)
998.6 (a, 0.6)	1007.0 (a, 13.6)	1009.3 (a', 14.6)
1044.5 (e, 0.5)	1038.4 (a, 0.6)	1036.6 (a", 0.0)

1044.5 (e, 0.6)	1045.9 (a, 0.1)	1041.8 (a', 1.5)
1044.6 (a, 0.8)	1046.9 (a, 0.3)	1047.4 (a", 0.3)
1047.7 (a, 0.0)	1047.8 (a, 0.4)	1047.8 (a", 0.1)
1047.8 (e, 0.8)	1048.3 (a, 0.6)	1049.4 (a', 0.3)
1047.8 (e, 0.8)	1055.9 (a, 5.3)	1057.2 (a', 3.8)
1114.1 (e, 0.0)	1111.8 (a, 0.1)	1111.6 (a', 0.1)
1114.1 (e, 0.0)	1113.3 (a, 0.3)	1115.0 (a", 0.0)
1114.1 (a, 0.0)	1116.6 (a, 1.2)	1117.6 (a', 1.4)
1225.1 (a, 0.0)	1222.7 (a, 0.0)	1222.0 (a", 0.0)
1225.2 (e, 0.0)	1227.2 (a, 0.0)	1222.5 (a", 0.0)
1225.2 (e, 0.0)	1229.1 (a, 0.0)	1229.9 (a', 0.0)
1373.2 (e, 0.5)	1366.9 (a, 0.7)	1365.3 (a", 2.6)
1373.2 (e, 0.5)	1371.0 (a, 0.9)	1369.4 (a', 1.8)
1373.4 (a, 0.0)	1372.0 (a, 3.0)	1371.2 (a", 0.0)
1375.5 (e, 0.3)	1372.9 (a, 1.4)	1373.2 (a', 1.4)
1375.5 (e, 0.3)	1378.9 (a, 0.2)	1379.5 (a", 0.0)
1375.6 (a, 6.9)	1382.4 (a, 0.2)	1382.8 (a', 0.4)
1413.5 (e, 0.4)	1409.2 (a, 3.2)	1409.7 (a', 3.8)
1413.5 (e, 0.4)	1410.2 (a, 1.7)	1410.7 (a", 1.0)
1413.6 (a, 5.0)	1414.8 (a, 1.4)	1411.8 (a", 5.4)
1416.7 (a, 0.1)	1416.4 (a, 4.8)	1415.4 (a', 0.6)
1416.7 (e, 6.0)	1416.9 (a, 0.6)	1417.4 (a", 0.1)
1416.7 (e, 6.0)	1421.9 (a, 3.0)	1422.2 (a', 3.2)
1833.3 (e, 36.6)	1754.9 (a, 326.6)	1714.3 (a', 337.7)
1833.3 (e, 36.6)	1783.5 (a, 146.3)	1793.9 (a', 246.9)
1873.0 (a, 995.6)	1864.6 (a, 307.6)	1858.4 (a", 405.6)
1894.7 (e, 646.2)	1891.6 (a, 559.9)	1861.2 (a', 352.5)
1894.7 (e, 646.3)	1902.6 (a, 28.5)	1871.3 (a', 109.4)
1906.0 (a, 304.0)	1911.8 (a, 168.0)	1919.4 (a", 27.3)
1922.3 (e, 450.6)	1932.9 (a, 637.3)	1938.5 (a", 1436.9)
1922.3 (e, 450.5)	1950.9 (a, 1487.2)	1940.4 (a', 457.1)
1983.7 (a, 876.5)	1989.0 (a, 650.6)	1983.2 (a', 1391.9)
3171.2 (a, 0.4)	3173.3 (a, 0.1)	3175.0 (a", 0.1)
3171.2 (e, 0.1)	3173.7 (a, 0.0)	3175.3 (a', 0.2)
3171.2 (e, 0.1)	3177.8 (a, 0.4)	3178.0 (a', 0.1)
3178.7 (a, 0.0)	3178.5 (a, 0.0)	3180.5 (a", 0.0)
3178.7 (e, 0.1)	3179.8 (a, 0.2)	3181.0 (a', 0.4)
3178.7 (e, 0.1)	3183.7 (a, 0.8)	3188.5 (a", 1.7)
3187.3 (e, 0.1)	3187.4 (a, 0.2)	3189.4 (a", 0.0)
3187.3 (e, 0.1)	3188.1 (a, 1.3)	3190.0 (a', 0.1)
3187.3 (a, 1.5)	3189.2 (a, 0.1)	3192.4 (a", 0.1)
3189.4 (a, 0.4)	3190.0 (a, 0.1)	3193.2 (a', 0.1)
3189.4 (e, 0.8)	3192.4 (a, 0.2)	3194.4 (a', 0.5)
3189.4 (e, 0.8)	3196.0 (a, 0.1)	3206.1 (a", 0.4)
3203.4 (e, 0.0)	3201.3 (a, 1.5)	3206.5 (a", 0.2)
3203.4 (e, 0.0)	3204.6 (a, 0.1)	3206.9 (a', 2.3)
3203.4 (a, 0.1)	3208.1 (a, 0.9)	3216.8 (a', 0.6)

Complete Gaussian 09 reference (Reference 19)

Gaussian 09, Revision B.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.