

Supporting Information

For

Normal-to-Abnormal Rearrangement of an N-Heterocyclic Carbene with a Silylene Transition Metal Complex

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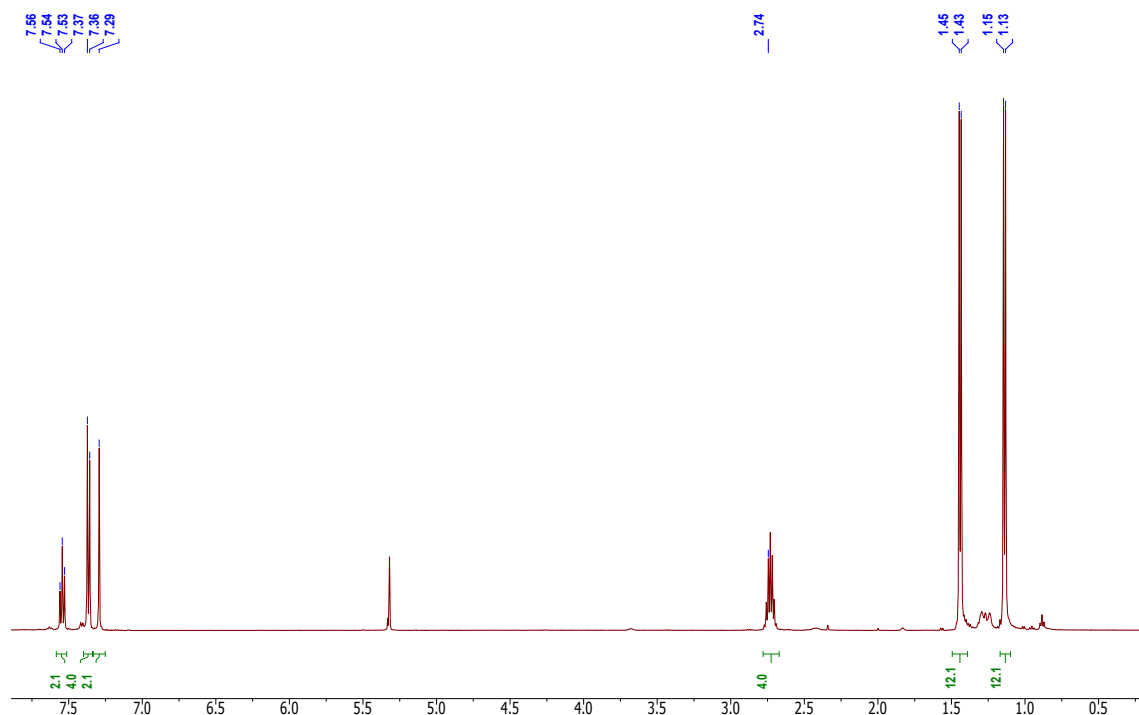
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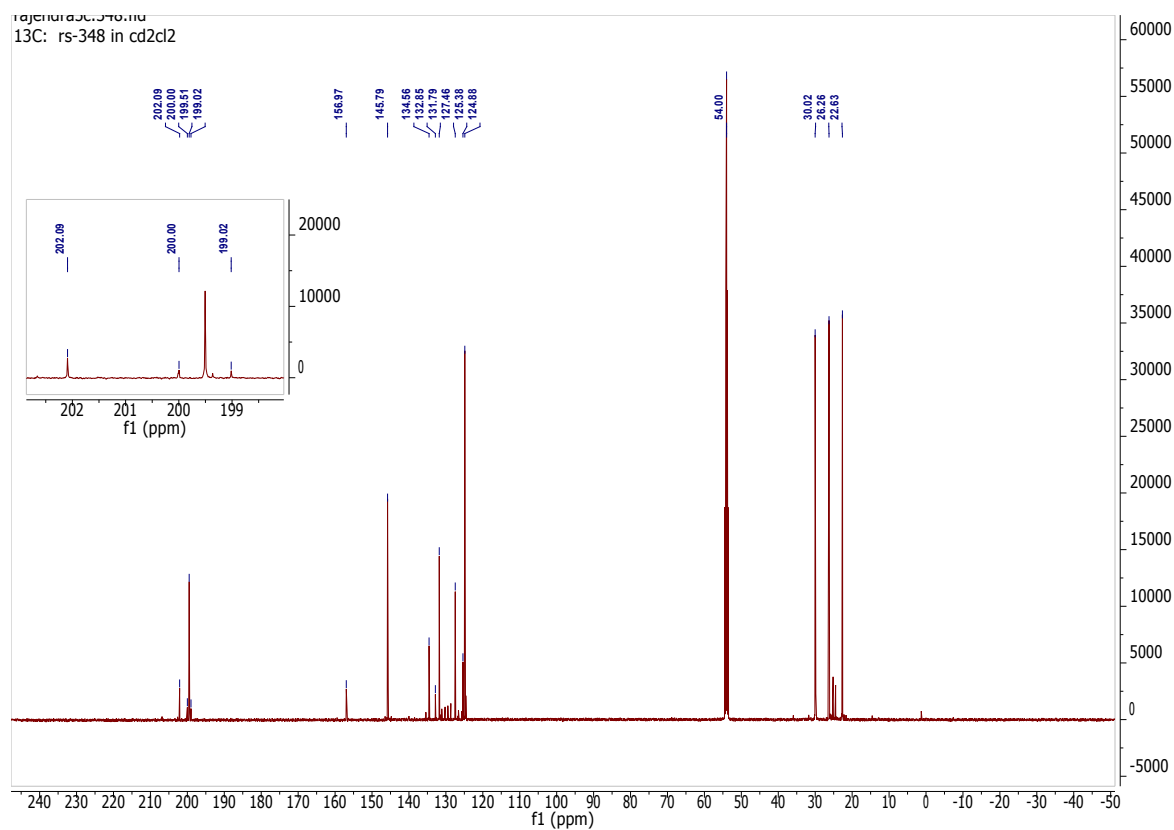
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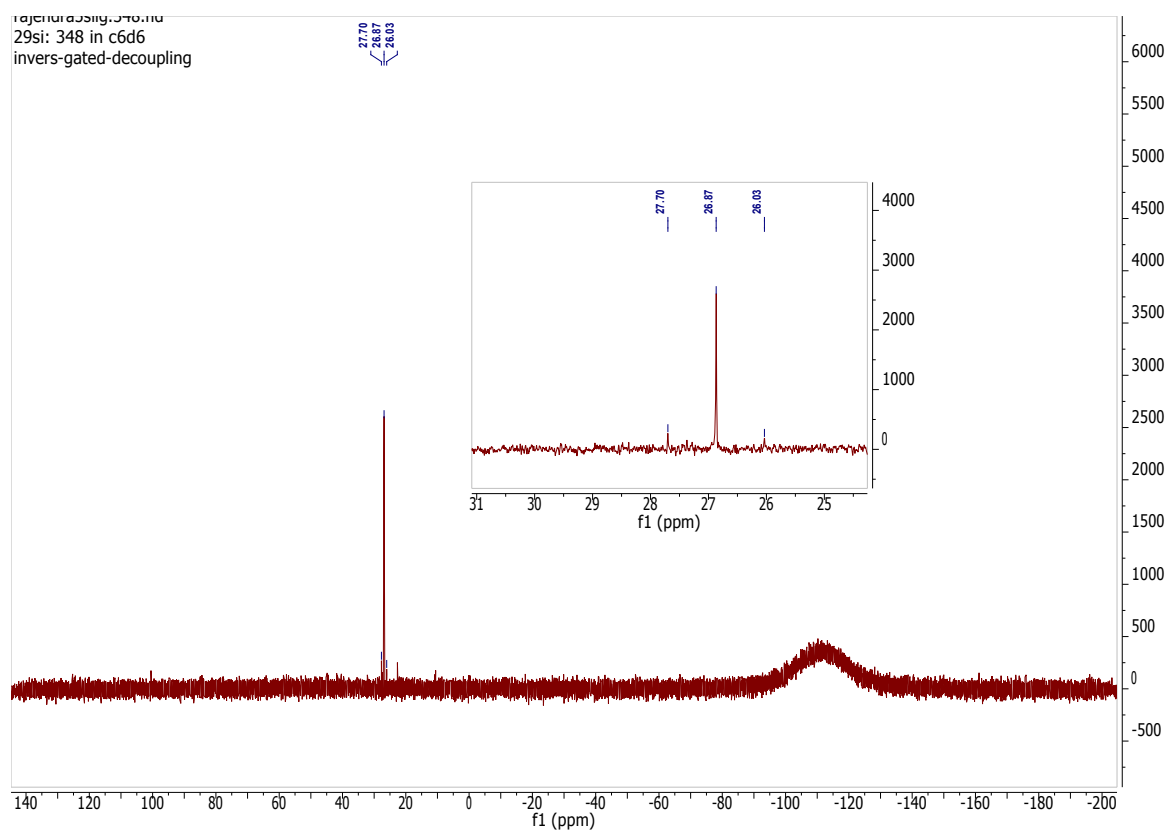
Plots of NMR Spectra



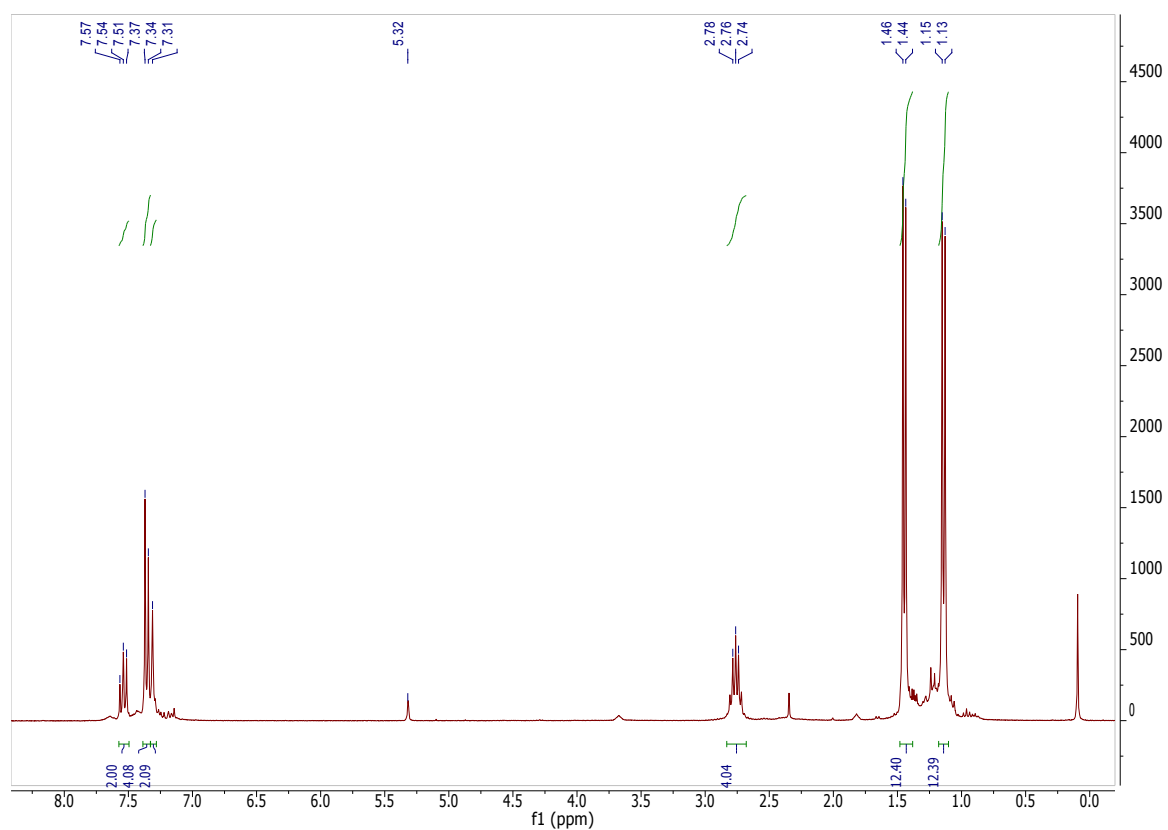
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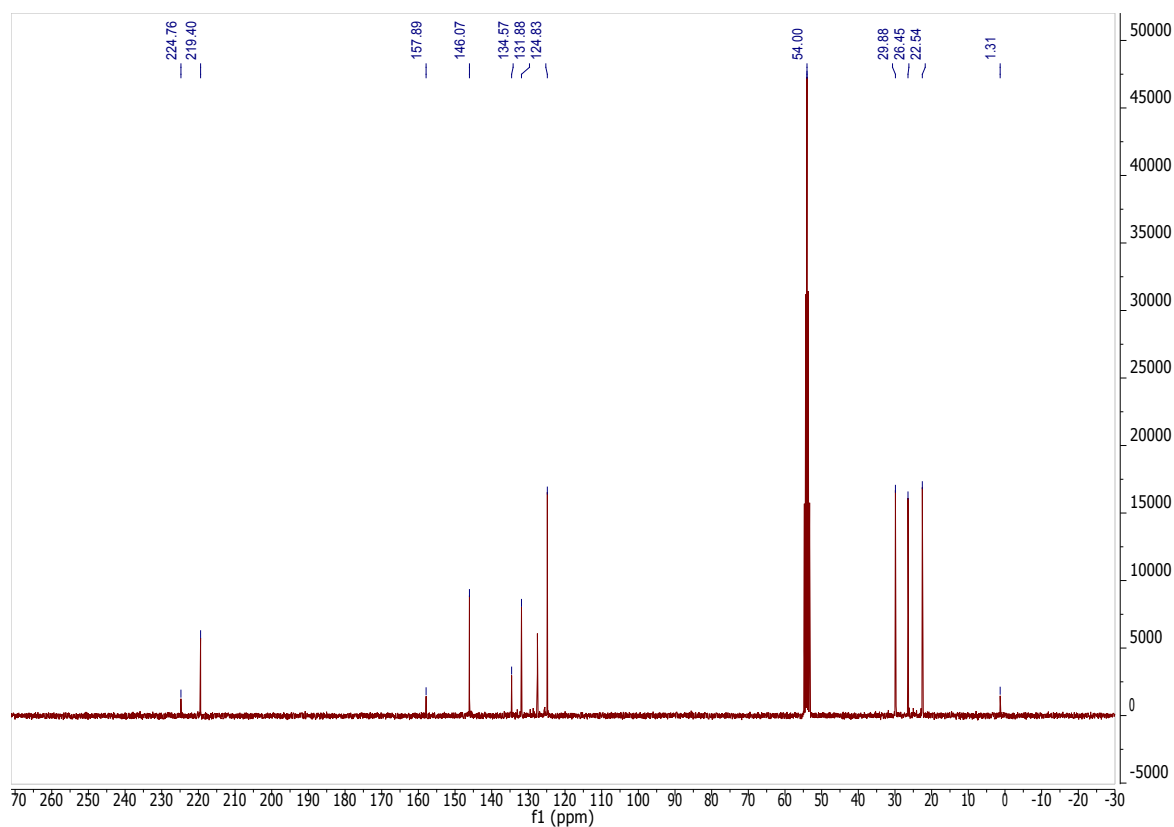
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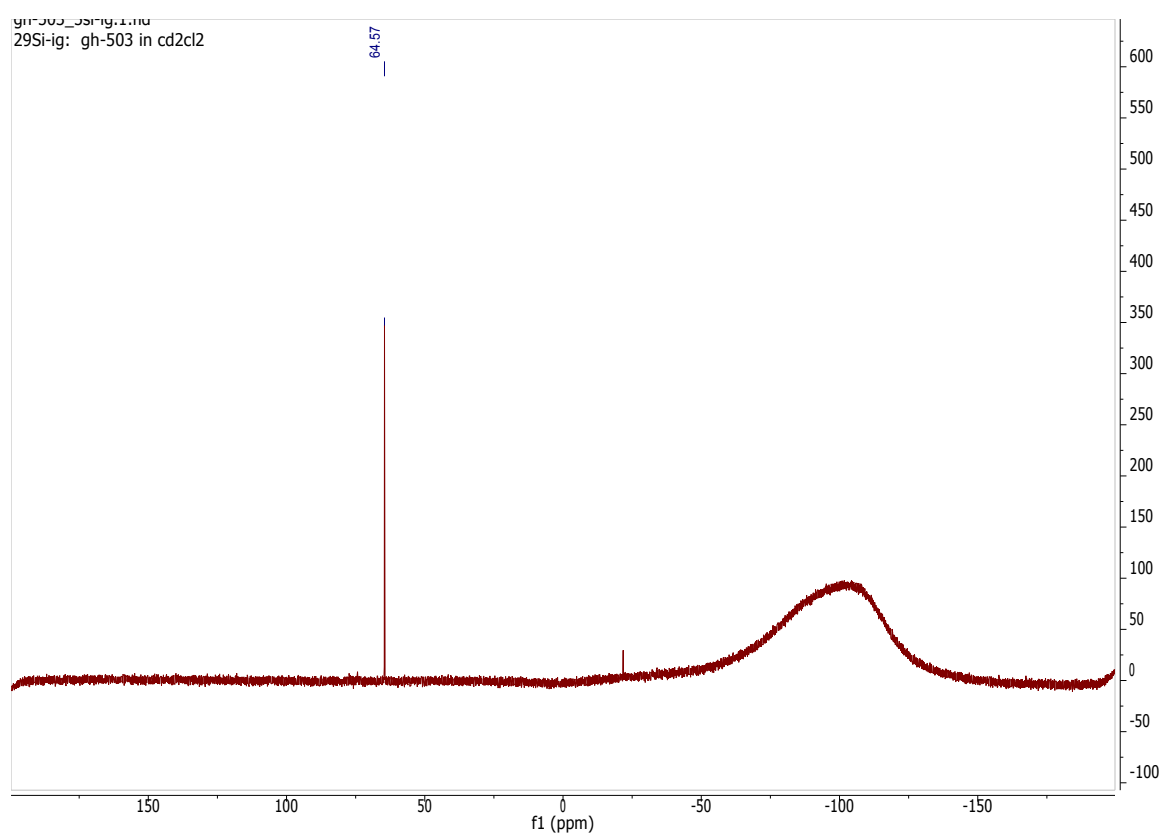
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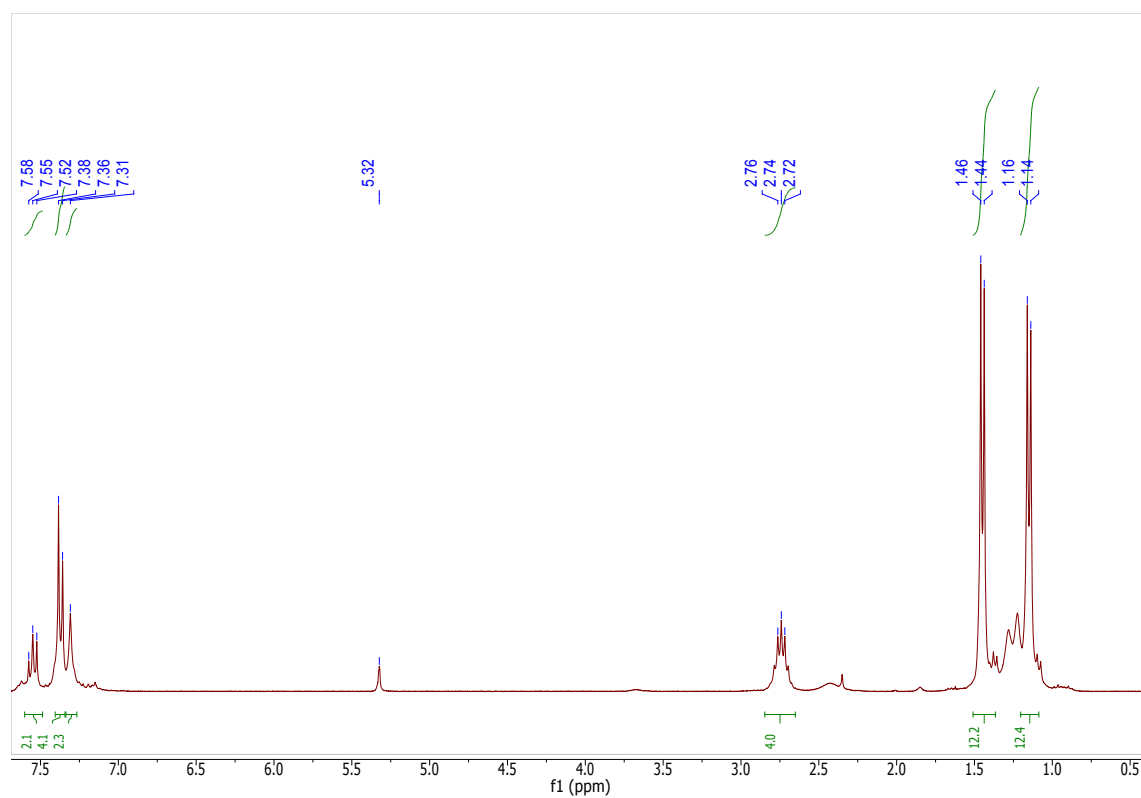
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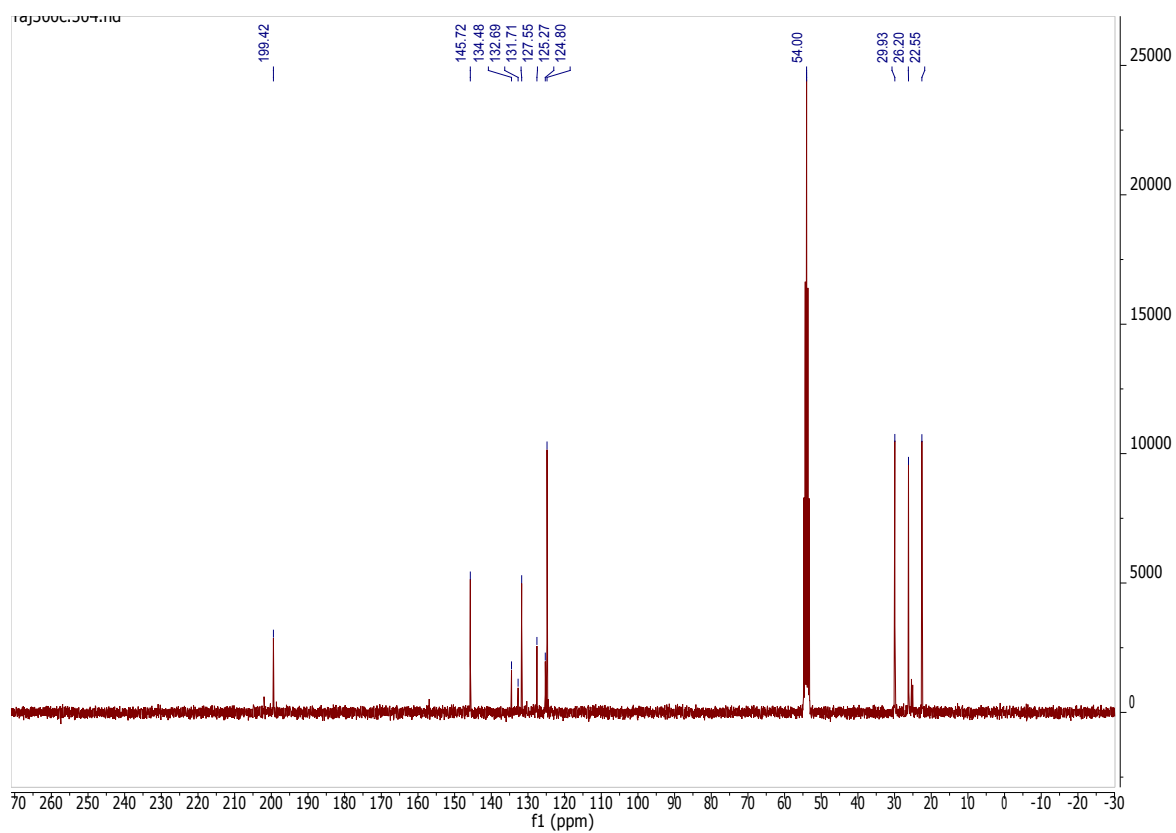
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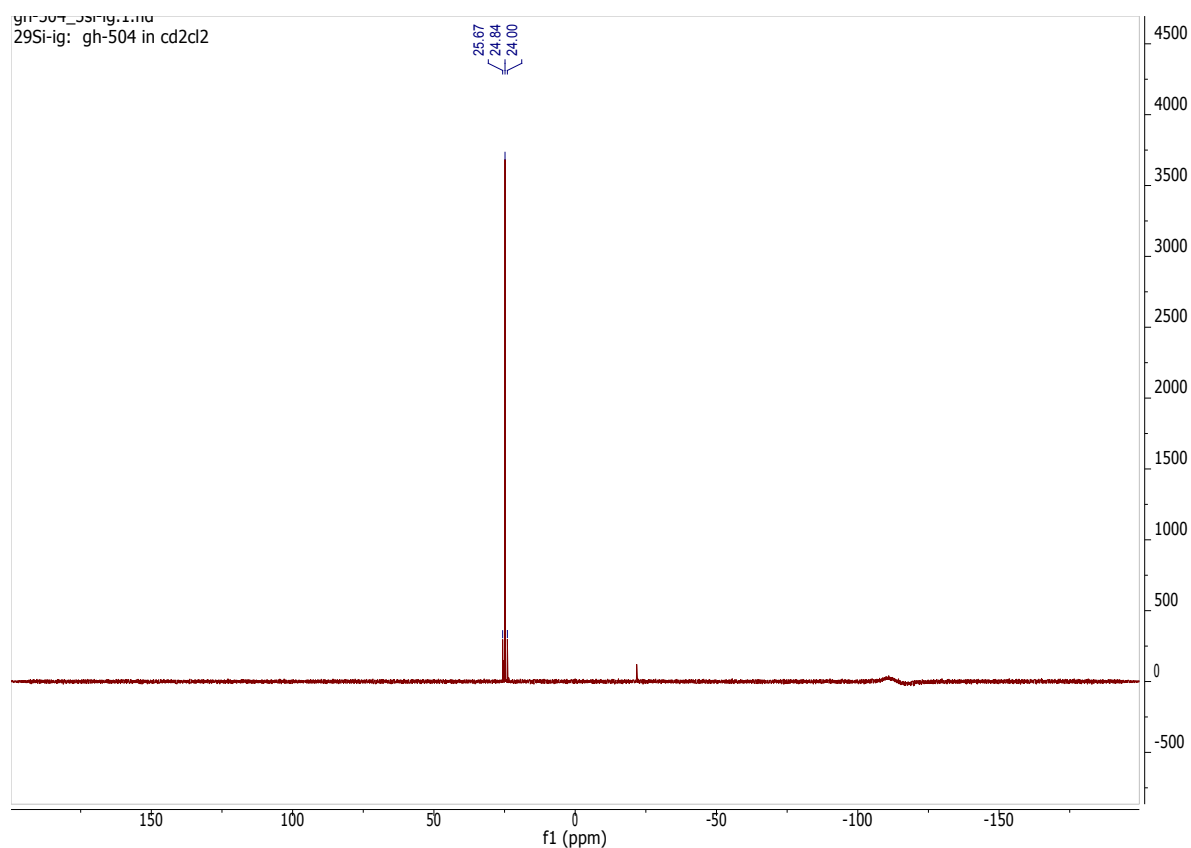
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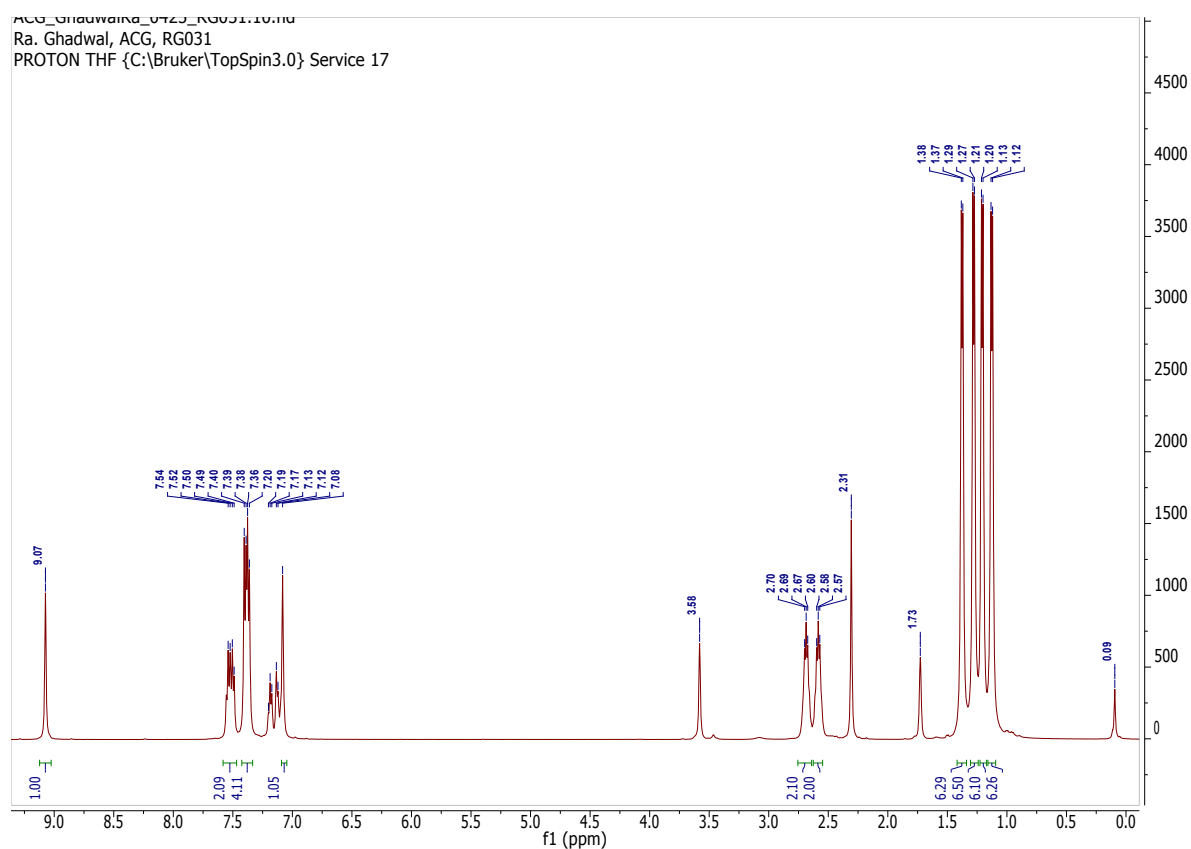
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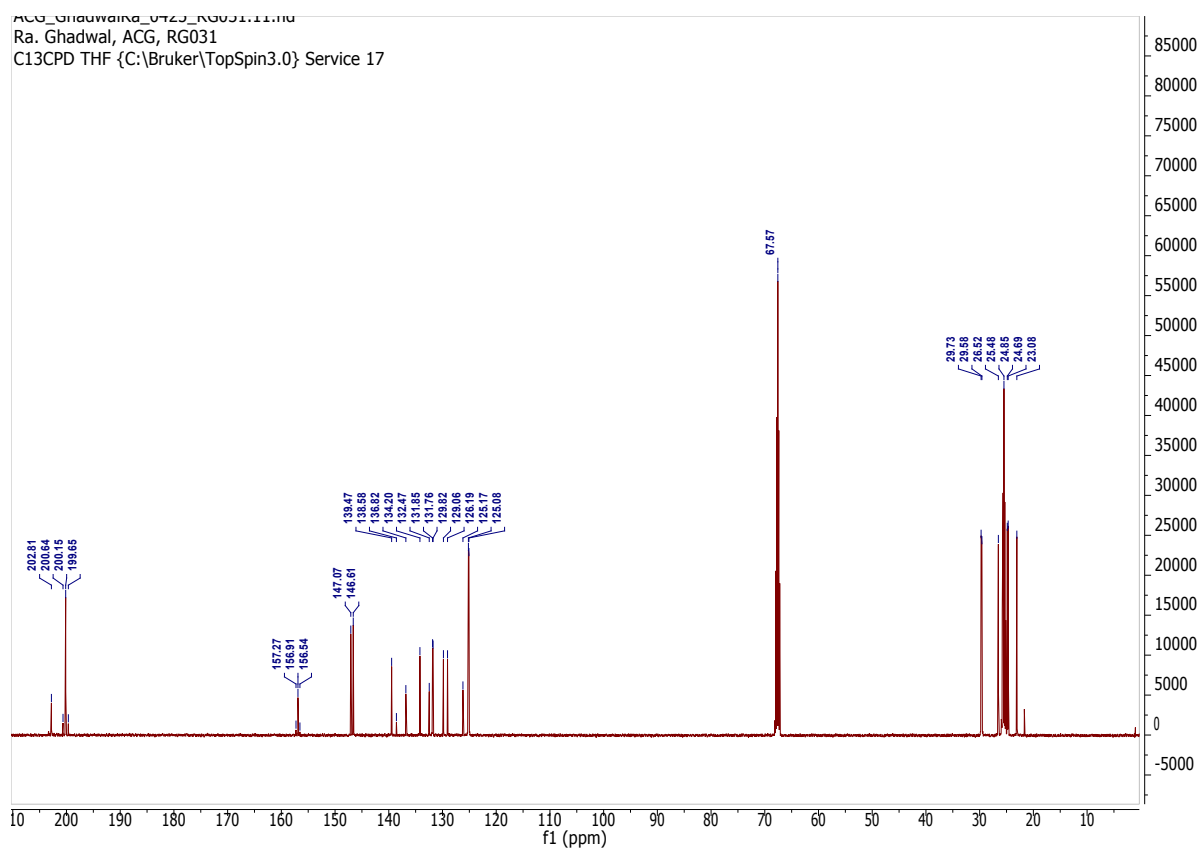
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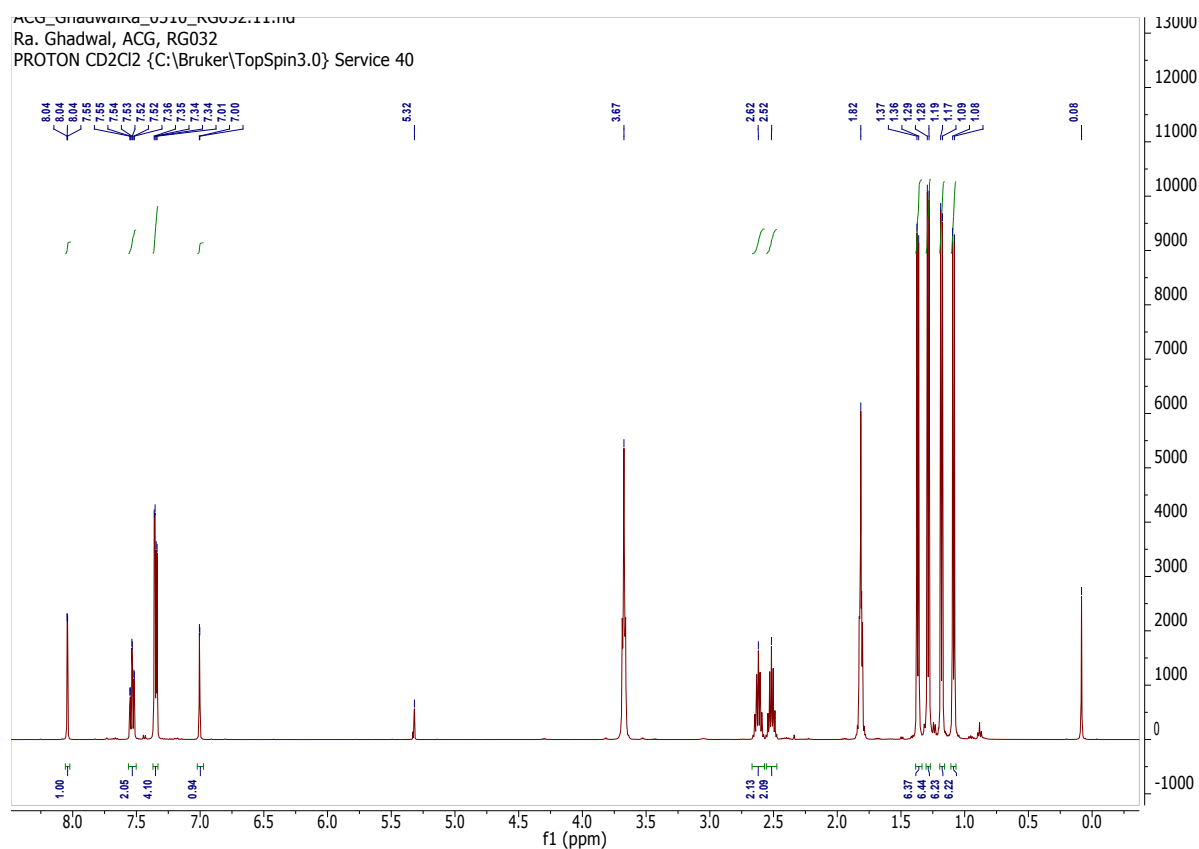
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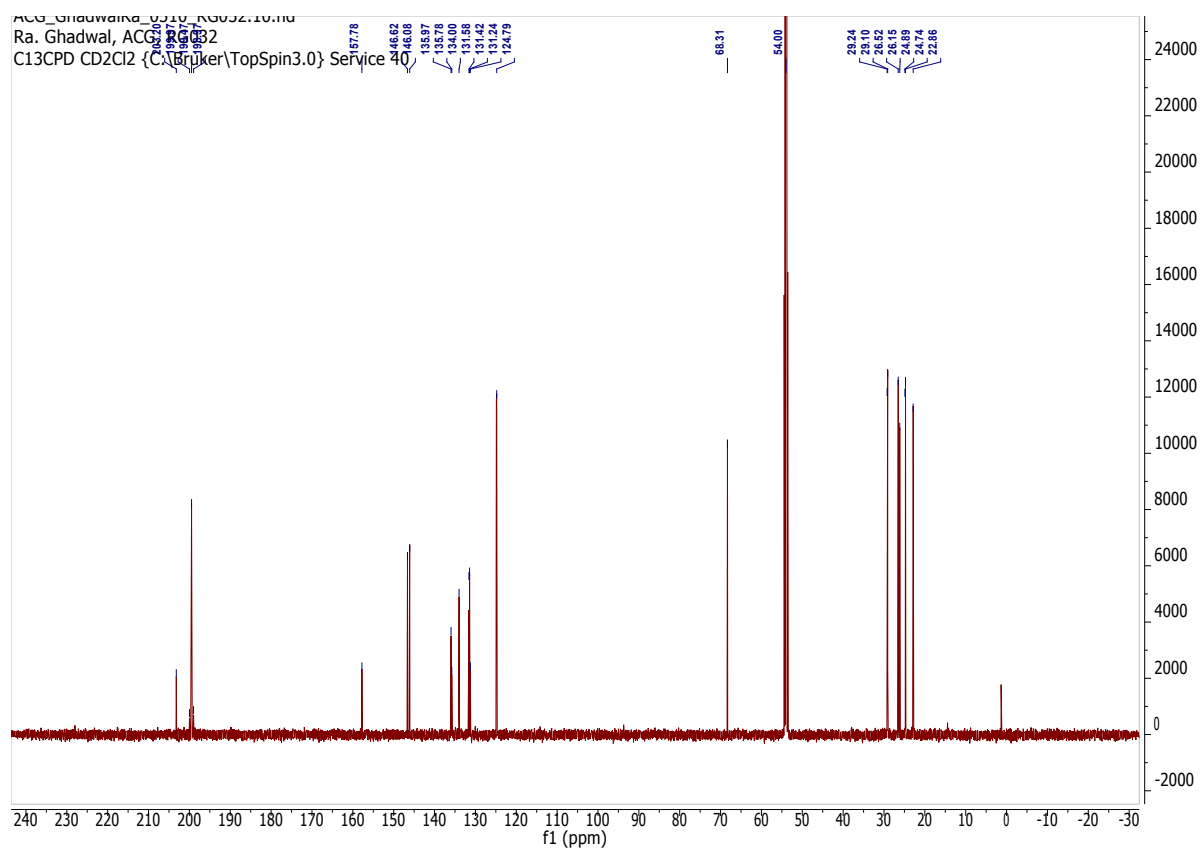
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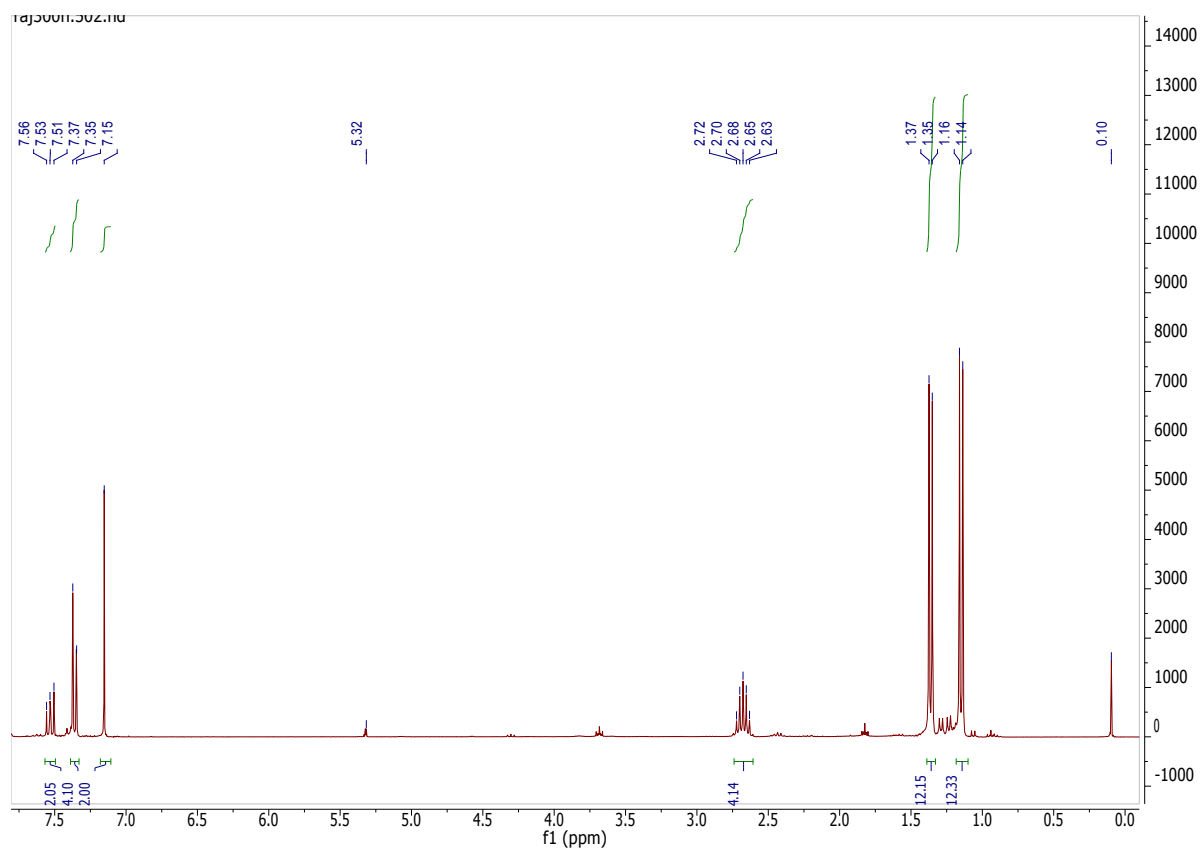
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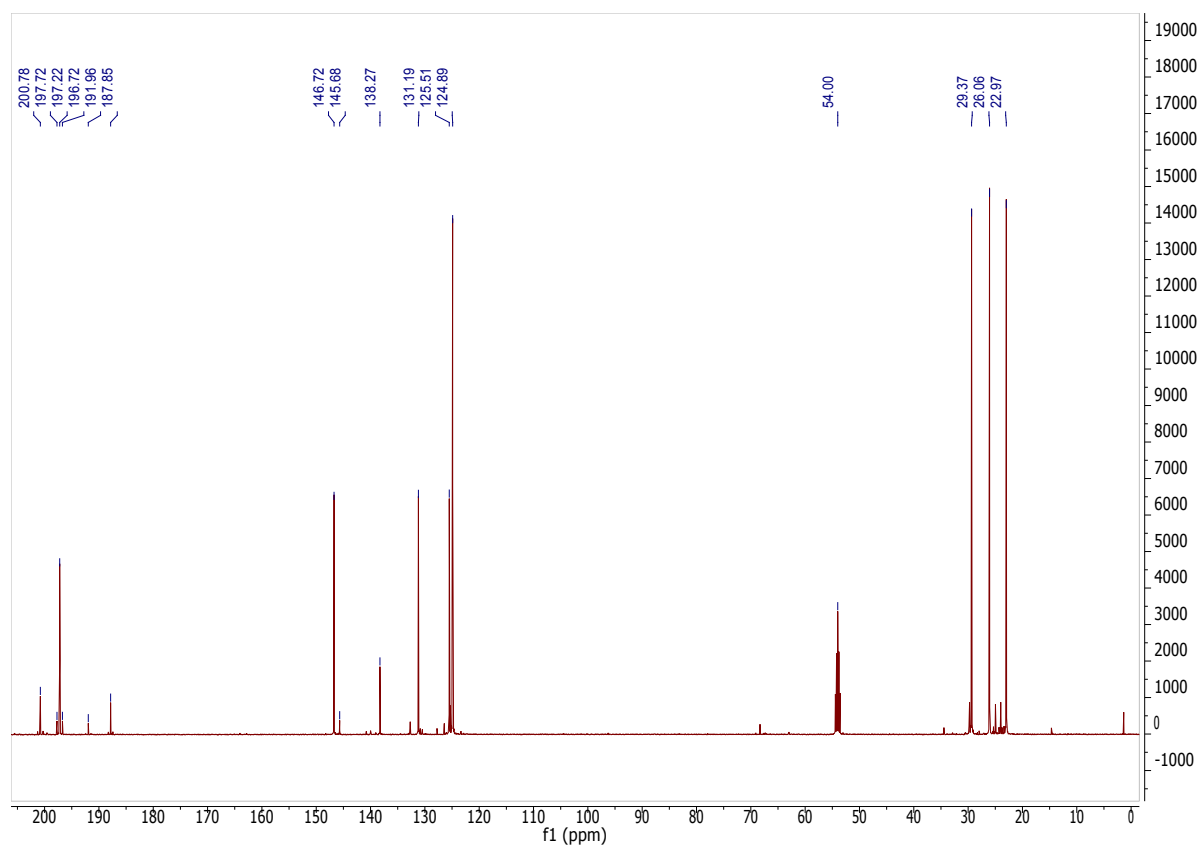
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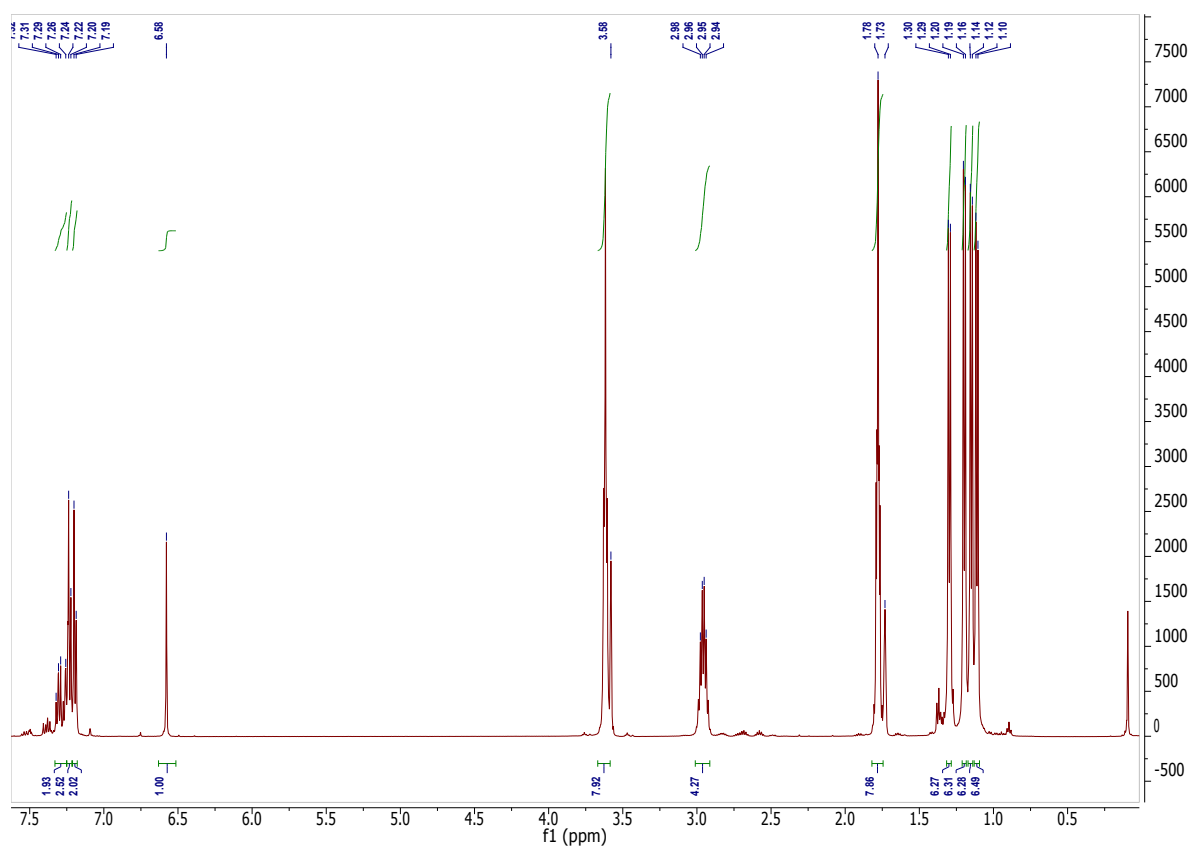
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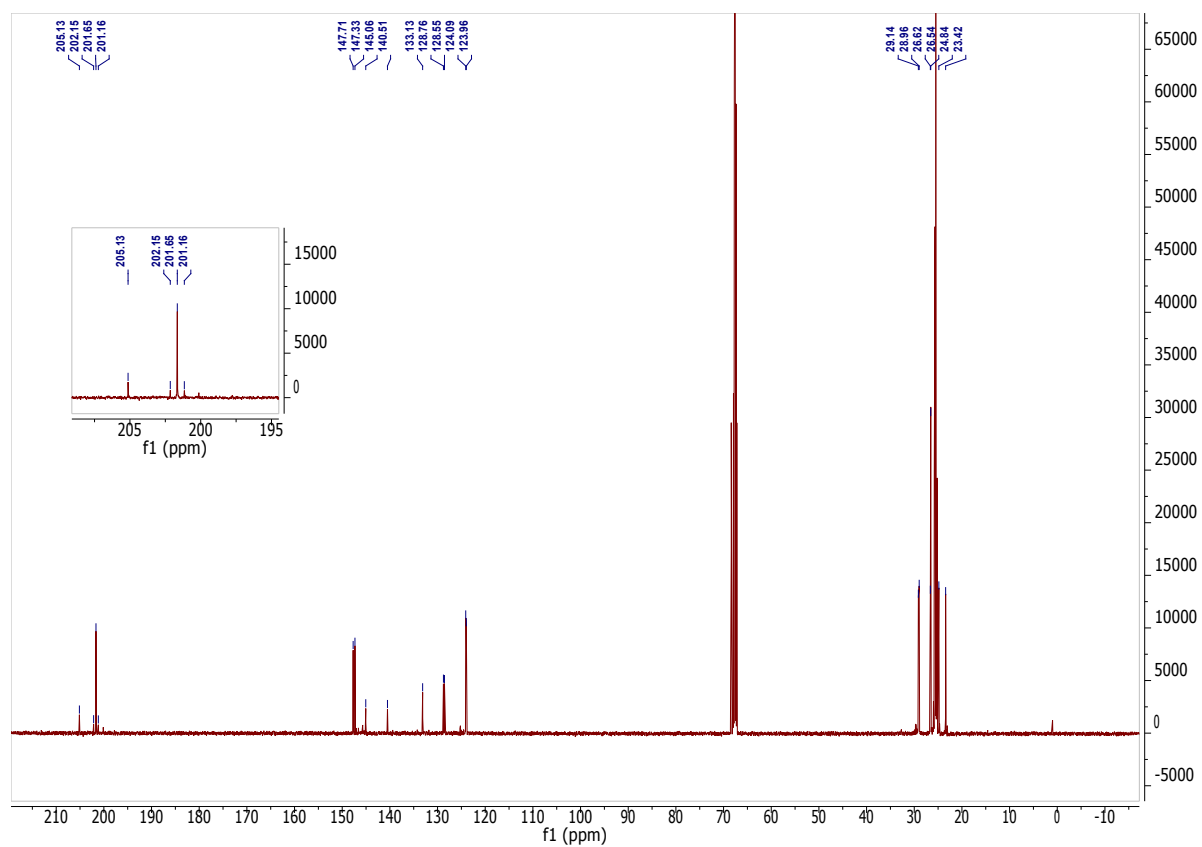
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Plot 15. ¹³C{¹H} NMR Spectrum of compound (IPr)W(CO)₅ (**8-W**).

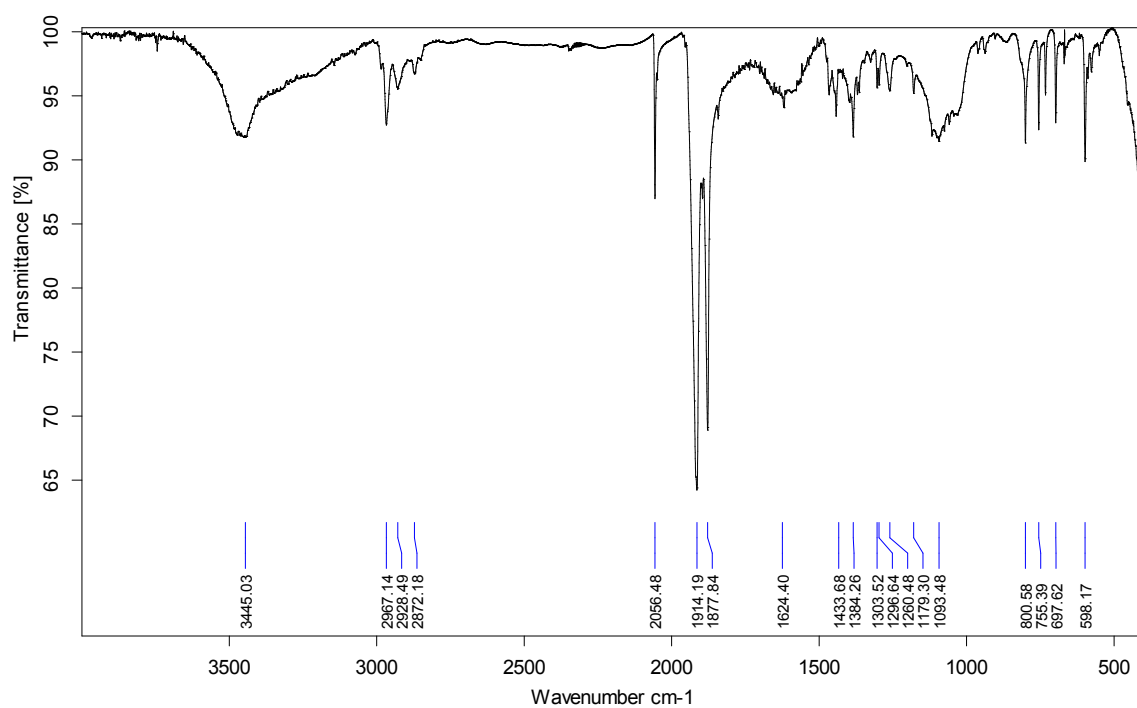


Plot 16. ¹H NMR Spectrum of compound {(CO)₅W}(IPr^H)Li(THF)₂ (**10-W**).

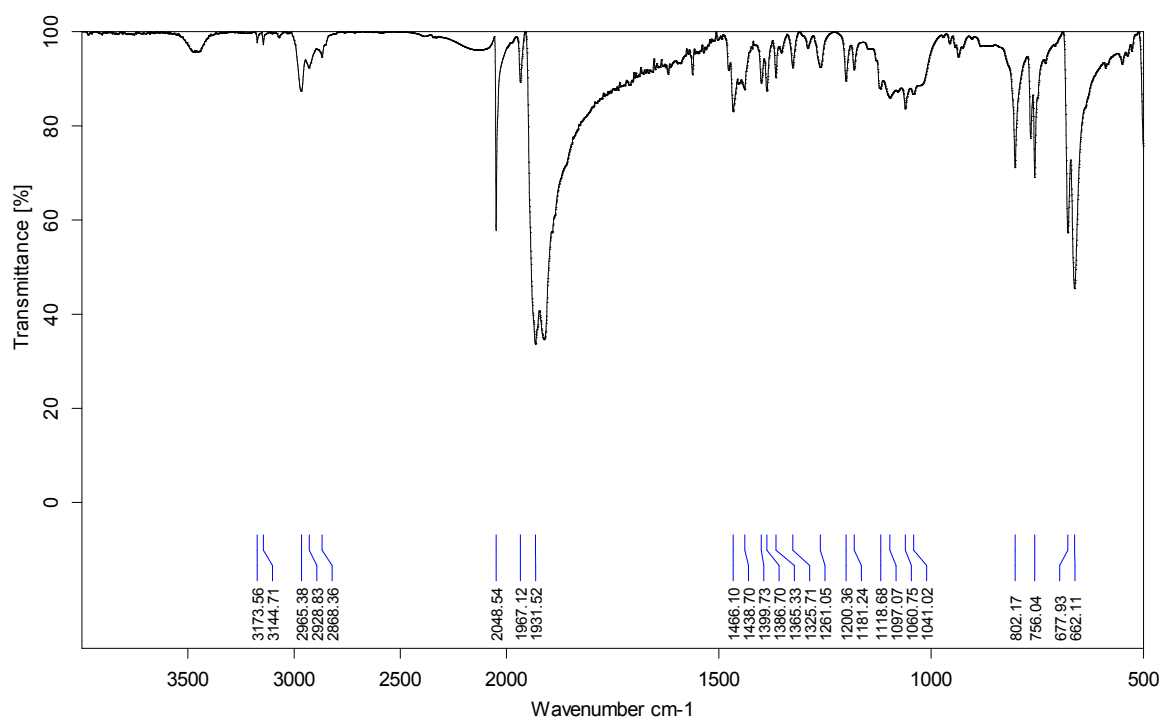


Plot 17. ^{13}C $\{^1\text{H}\}$ NMR Spectrum of compound $\{(\text{CO})_5\text{W}\}(\text{IPr}^{\text{H}})\text{Li}(\text{THF})_2$ (**10-W**).

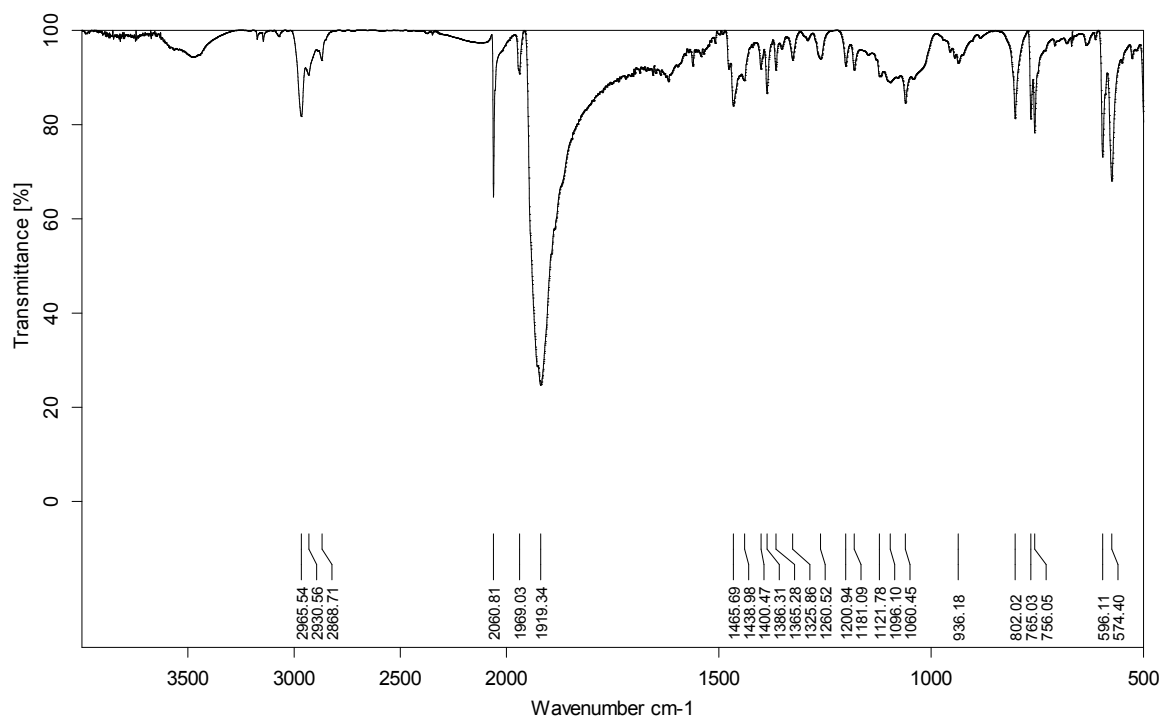
Plots of IR Spectra



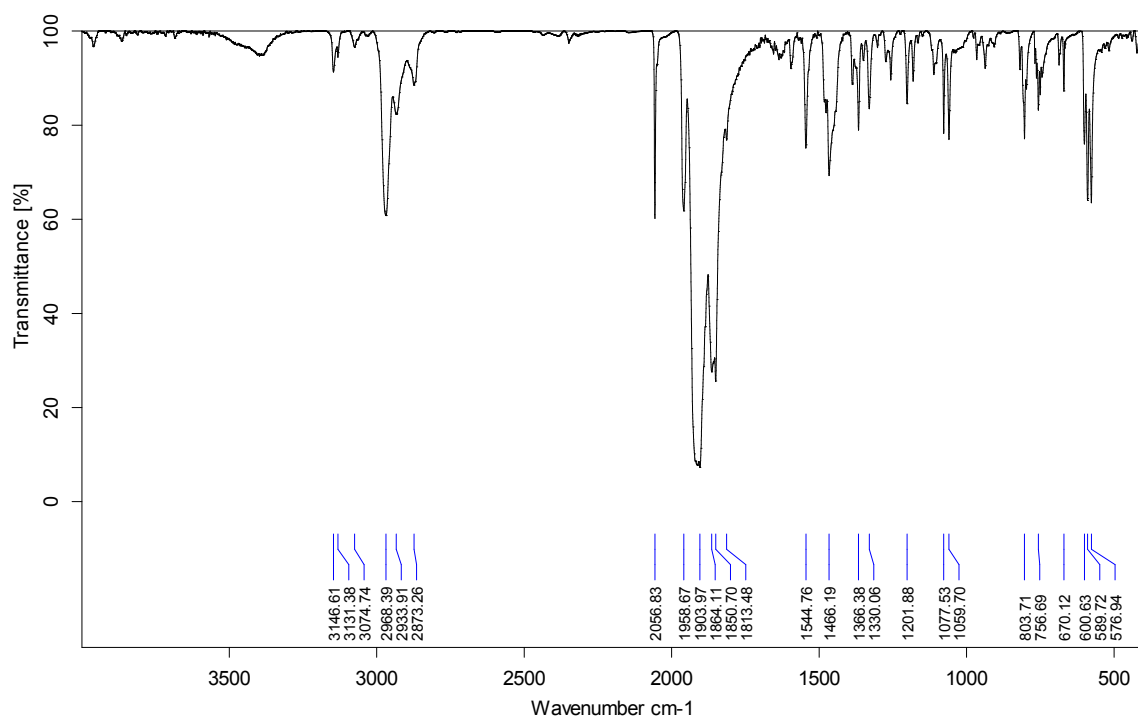
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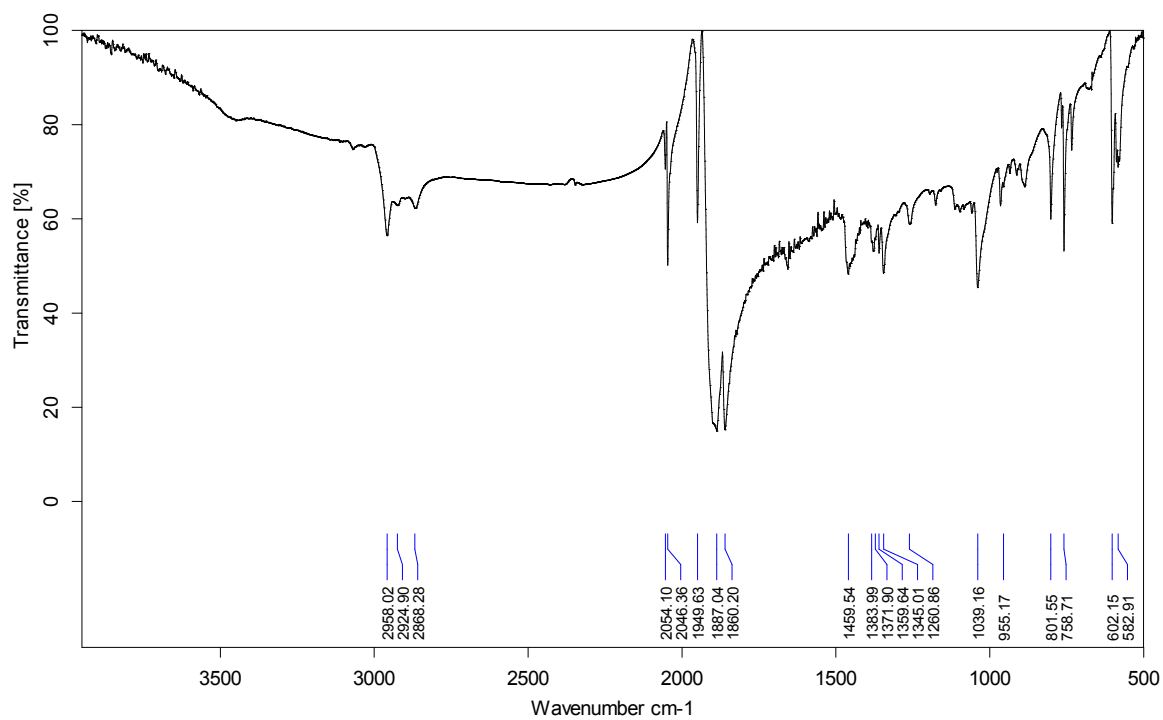
Plot 19. IR Spectrum of 4-Cr.



Plot 20. IR Spectrum of **4-W**.



Plot 21. IR Spectrum of **6-W**.



Plot 22. IR Spectrum of **10-W**.

Crystallographic details

Suitable single crystals were selected from the mother liquor under Schlenk conditions and covered with perfluorinated polyether oil on a microscope slide, which was cooled with a nitrogen gas flow using the X-Temp2 device.¹ All data were collected at 100 K. The diffraction data of compound **4-Cr** and **6-W** were collected on a Bruker D8 three circle diffractometer, equipped with a SMART APEX II CCD detector and an BRUKER SRA rotating anode source (Mo K α radiation) with MONTEL Graded multilayer optics. The diffraction data of compound **4-W** and **7-W** were collected on a Bruker D8 three circle diffractometer, equipped with a SMART APEX II CCD detector and an INCOATEC microfocus source (Mo K α radiation) with INCOATEC Quazar mirror optics. The diffraction data of compound **8-W** were collected on a Bruker D8 three circle diffractometer, equipped with a SMART APEX II CCD detector and an INCOATEC microfocus source (Ag K α radiation) with INCOATEC Quazar mirror optics. The diffraction data of **10-W** were collected on a Rigaku Oxford Supernova four circle diffractometer equipped with an EOS CCD detector and micro-focus sealed X-ray tube. Except of **10-W**, all data were integrated with SAINT.² A multi-scan absorption correction and a 3λ -correction³ for Mo K α sources with SADABS⁴ were applied. Data of **10-W** were collected, integrated and finalized using CrysAlisPro,⁵ a numerical absorption correction was applied based on gaussian integration over a multifaceted crystal model and a empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structure solution was performed with SHELXT⁶ and structure refinement was performed with SHELXL,⁷ using the graphical user interface SHELXLE⁸ resp. Olex2⁹ for **10-W**. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were assigned to ideal positions and refined using a riding model with U_{iso} constrained to 1.2 (1.5) times the U_{eq} value of the parent carbon atom. **10-W** reveals a disorder of three carbon atoms of a thf molecule attached to lithium (C37 to C40) with ratio 83:17. Within the disordered part the anisotropic displacement parameters were constrained to be same pairwise and equivalent bond length were restrained to be same. Crystal and refinement details, as well as CCDC numbers are provided in Table S1. Crystallographic data has been deposited with the Cambridge Crystallographic Centre. Copies of the data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. X-ray Crystallographic Data and Collection Parameters of Compounds **4-Cr**, **4-W**, **6-W**, **8-W**, and **10-W**.

Compound	4-Cr	4-W	6-W	7-W	8-W	10-W
CCDC Number	1514802	1514798	1514799	1514801	1514800	1515745
Empirical formula	C ₄₅ H ₅₇ Cl ₆ Cr _{0.75} N ₃ O ₃ Si _{1.50}	C ₆₄ H ₇₉ Cl ₆ N ₅ O ₄ Si ₂ W	C _{42.50} H ₄₈ N ₂ O ₅ W	C ₄₄ H ₄₉ ClN ₂ O ₅ W	C ₃₂ H ₃₆ N ₂ O ₅ W	C ₄₀ H ₅₁ LiN ₂ O ₇ W
Formula weight [g/mol]	981.77	1435.05	850.68	905.15	712.48	862.61
Temperature [K]	100(2)	100(2)	100(2)	100(2)	100(2)	100.0(1)
Wavelength [Å]	0.71073	0.71073	0.71073	0.71073	0.56086	0.71073
Crystal system, space group	Monoclinic, <i>P2₁/n</i>	Monoclinic, <i>Pn</i>	Triclinic, <i>P</i> -1	Monoclinic, <i>P2₁/n</i>	Orthorhombic, <i>Cmcm</i>	Monoclinic, <i>P2₁/n</i>
Unit cell dimensions [Å]	<i>a</i> = 12.434(2)	<i>a</i> = 12.696(2)	<i>a</i> = 12.193(2)	<i>a</i> = 10.587(2)	<i>a</i> = 11.250(2)	10.86235(11)
	<i>b</i> = 48.155(2)	<i>b</i> = 16.539(2)	<i>b</i> = 13.362(2)	<i>b</i> = 19.360(2)	<i>b</i> = 13.869(2)	18.91698(18)
	<i>c</i> = 16.728(2)	<i>c</i> = 16.499(3)	<i>c</i> = 14.396(3)	<i>c</i> = 21.345(3)	<i>c</i> = 19.759(3)	19.27237(18)
α [°]	90	90	105.95(2)	90	90	90
β [°]	105.65(3)	103.35(2)	105.03(2)	102.83(2)	90	90.4081(9)
γ [°]	90	90	110.55(2)	90	90	90
Volume [Å ³]	9645(2)	3370.8(11)	1939.8(7)	4265.7(11)	3082.9(8)	3960.04(7)
Z	8	2	2	4	4	4
Absorption coefficient [mm ⁻¹]	0.595	2.035	3.023	2.815	2.035	2.966
F(000)	4104	1468	862	1832	1424	1752.0
Crystal size [mm]	-	0.371 x 0.159 x 0.074	-	-	0.230 x 0.224 x 0.200	0.28 × 0.18 × 0.13

Table S1. X-ray Crystallographic Data and Collection Parameters of Compounds **4-Cr**, **4-W**, **6-W**, **8-W**, and **10-W** (continues..).

Theta range for data collection [°]	1.333 to 25.062	1.231 to 27.487	1.602 to 33.443	1.437 to 28.346	1.627 to 23.659	3.0 to 30.1
Reflections collected / unique	142790/ 16579	57844/ 15424	60979/ 13473	98396/ 10642	23603 / 2539	137501/11634
R_{int}	0.0555	0.0219	0.0244	0.0892	0.0290	0.0521
Completeness [%]	97.0	100.0	100.0	100.0	100.0	100.0
Max. and min. transmission	0.4286 and 0.4066	0.2616 and 0.2002	0.9092 and 0.7995	0.7457 and 0.6958	0.4275 and 0.3974	0.736 and 0.511
Data / restraints / parameters	16579 / 81 / 1121	15424 / 377 / 829	13473 / 636 / 562	10642 / 0 / 486	2539 / 0 / 112	11634/10/478
Goodness-of-fit on F^2	1.032	1.043	1.053	1.075	1.112	1.086
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0430$, $wR2 = 0.0887$	$R1 = 0.0185$, $wR2 = 0.0442$	$R1 = 0.0211$, $wR2 = 0.0486$	$R1 = 0.0370$, $wR2 = 0.0645$	$R1 = 0.0128$, $wR2 = 0.0305$	$R1 = 0.0212$, $wR_2 = 0.0465$
R indices (all data)	$R1 = 0.0675$, $wR2 = 0.0983$	$R1 = 0.0196$, $wR2 = 0.0447$	$R1 = 0.0240$, $wR2 = 0.0494$	$R1 = 0.0586$, $wR2 = 0.0690$	$R1 = 0.0137$, $wR2 = 0.0308$	$R1 = 0.0275$, $wR_2 = 0.0486$
Largest diff. peak and hole ($\text{e}\text{\AA}^{-3}$)	0.594 and -0.859	0.765 and -0.288	2.332 and -1.096	0.554 and -0.891	0.499 and -1.841	1.26/-0.67

Compound 4-Cr

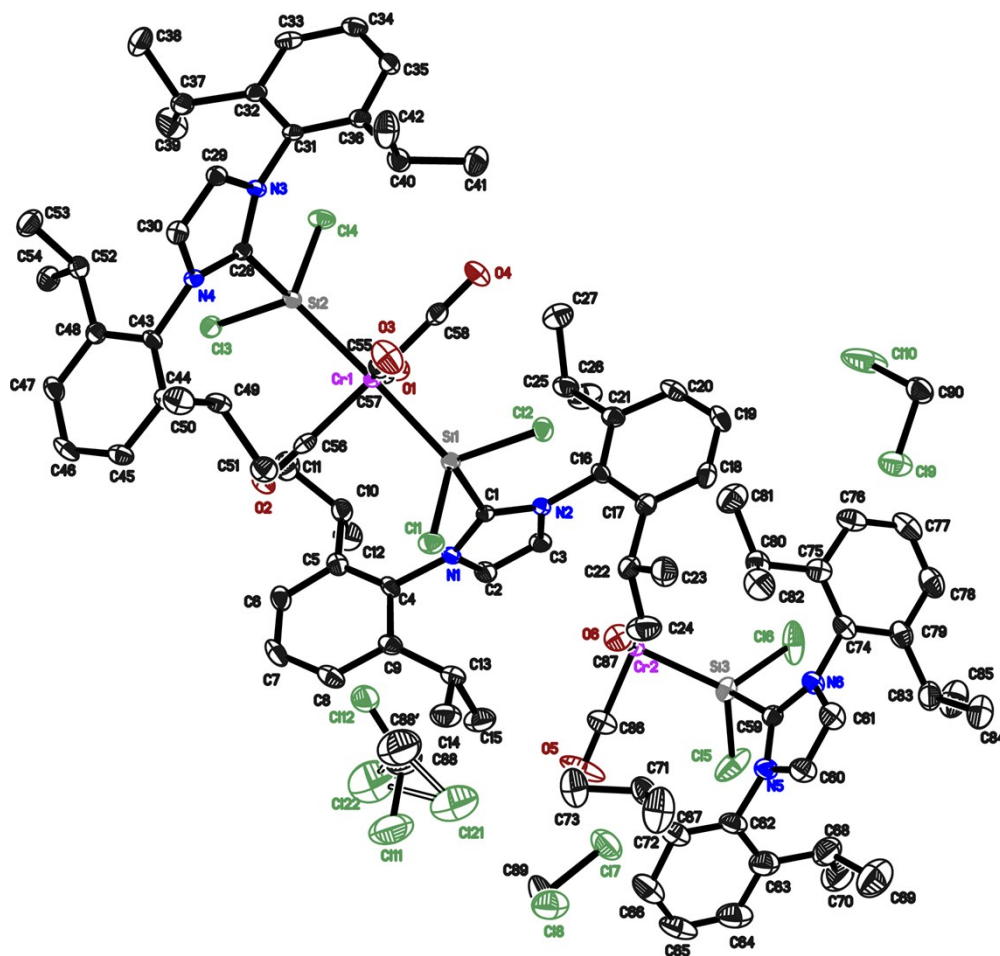


Figure S1. Molecular structure of compound 4-Cr. Anisotropic displacement parameters are depicted at the 50% probability level. Due to crystal symmetry 1.5 molecules are within the asymmetric unit. Cr2 lies on an inversion center. The second half of this molecule is defined by his inversion and is not depicted for clarity. Hydrogen atoms are omitted for clarity. Selected experimental and theoretical [BP86+D3(BJ)/def2-SVP] {M06/def2-SVP} bond lengths (Å) and bond angles (°): C1—Si1, 1.988(3) [1.992]{2.029}; Si1—C11, 2.1272(10) [2.148]{2.136}; Si1—C12, 2.1291(10) [2.146]{2.141}; Si1—Cr1, 2.3118(12) [2.279]{2.287}; Si2—Cr1, 2.3113(12) [2.279]{2.286}; C28—Si2, 1.989(3) [1.992]{2.029}; Cr1—C56, 1.892(3) [1.858]{1.868}; Cr1—C58, 1.852(3) [1.858]{1.868}; Si1—Cr—Si2, 177.76(3) [180.0]{177.8}; C1—Si1—Cr1, 125.41(8) [118.3]{119.8}; C11—Si1—C12, 97.54(5) [98.9]{98.3}; C56—Cr1—C58, 178.63(12) [180.0]{179.2}; C55—Cr1—C57, 166.73(12) [180.0]{178.0}; C56—Cr1—C57, 95.87(12) [94.2]{94.9}.

Table S2. Bond lengths [Å] and angles [°] of Compound **4-Cr**.

Cr(1)-C(58)	1.852(3)	O(5)-C(86)	1.149(4)	C(10)-C(11)	1.518(4)
Cr(1)-C(57)	1.876(3)	O(6)-C(87)	1.156(3)	C(10)-C(12)	1.533(4)
Cr(1)-C(55)	1.880(3)	N(1)-C(1)	1.366(3)	C(13)-C(14)	1.521(4)
Cr(1)-C(56)	1.892(3)	N(1)-C(2)	1.377(3)	C(13)-C(15)	1.527(4)
Cr(1)-Si(2)	2.3113(12)	N(1)-C(4)	1.463(3)	C(16)-C(21)	1.389(4)
Cr(1)-Si(1)	2.3118(12)	N(2)-C(1)	1.365(3)	C(16)-C(17)	1.404(4)
Cr(2)-C(86)#1	1.866(3)	N(2)-C(3)	1.383(4)	C(17)-C(18)	1.389(4)
Cr(2)-C(86)	1.866(3)	N(2)-C(16)	1.454(3)	C(17)-C(22)	1.528(4)
Cr(2)-C(87)#1	1.868(3)	N(3)-C(28)	1.365(3)	C(18)-C(19)	1.378(4)
Cr(2)-C(87)	1.868(3)	N(3)-C(29)	1.374(3)	C(19)-C(20)	1.370(4)
Cr(2)-Si(3)#1	2.3039(11)	N(3)-C(31)	1.462(3)	C(20)-C(21)	1.398(4)
Cr(2)-Si(3)	2.3039(11)	N(4)-C(28)	1.371(3)	C(21)-C(25)	1.517(4)
Cl(1)-Si(1)	2.1272(10)	N(4)-C(30)	1.380(3)	C(22)-C(23)	1.524(4)
Cl(2)-Si(1)	2.1291(10)	N(4)-C(43)	1.462(3)	C(22)-C(24)	1.531(4)
Cl(3)-Si(2)	2.1341(10)	N(5)-C(59)	1.362(4)	C(25)-C(27)	1.524(4)
Cl(4)-Si(2)	2.1105(10)	N(5)-C(60)	1.380(4)	C(25)-C(26)	1.542(5)
Cl(5)-Si(3)	2.1048(13)	N(5)-C(62)	1.460(4)	C(29)-C(30)	1.337(4)
Cl(6)-Si(3)	2.1157(13)	N(6)-C(59)	1.369(4)	C(31)-C(32)	1.396(4)
Cl(7)-C(89)	1.753(3)	N(6)-C(61)	1.385(4)	C(31)-C(36)	1.398(4)
Cl(8)-C(89)	1.751(4)	N(6)-C(74)	1.460(4)	C(32)-C(33)	1.386(4)
Cl(9)-C(90)	1.753(3)	C(2)-C(3)	1.330(4)	C(32)-C(37)	1.520(4)
Cl(10)-C(90)	1.738(3)	C(4)-C(5)	1.397(4)	C(33)-C(34)	1.379(4)
Si(1)-C(1)	1.988(3)	C(4)-C(9)	1.401(4)	C(34)-C(35)	1.379(4)
Si(2)-C(28)	1.989(3)	C(5)-C(6)	1.394(4)	C(35)-C(36)	1.388(4)
Si(3)-C(59)	1.977(3)	C(5)-C(10)	1.514(4)	C(36)-C(40)	1.525(4)
O(1)-C(55)	1.151(4)	C(6)-C(7)	1.375(4)	C(37)-C(38)	1.519(4)
O(2)-C(56)	1.150(3)	C(7)-C(8)	1.386(4)	C(37)-C(39)	1.530(4)
O(3)-C(57)	1.153(3)	C(8)-C(9)	1.390(4)	C(40)-C(41)	1.527(4)
O(4)-C(58)	1.159(3)	C(9)-C(13)	1.521(4)	C(40)-C(42)	1.529(4)

C(43)-C(44)	1.397(4)	C(77)-C(78)	1.371(5)	C(86)-Cr(2)-C(87)#1 89.62(13)
C(43)-C(48)	1.405(4)	C(78)-C(79)	1.395(5)	C(86)#1-Cr(2)-C(87) 89.62(13)
C(44)-C(45)	1.394(4)	C(79)-C(83)	1.521(5)	C(86)-Cr(2)-C(87) 90.38(13)
C(44)-C(49)	1.514(4)	C(80)-C(82)	1.526(5)	C(87)#1-Cr(2)-C(87) 180.00(17)
C(45)-C(46)	1.376(4)	C(80)-C(81)	1.534(5)	C(86)#1-Cr(2)-Si(3)#1 88.85(11)
C(46)-C(47)	1.378(4)	C(83)-C(85)	1.529(5)	C(86)-Cr(2)-Si(3)#1 91.15(11)
C(47)-C(48)	1.391(4)	C(83)-C(84)	1.534(5)	C(87)#1-Cr(2)-Si(3)#1 97.13(9)
C(48)-C(52)	1.521(4)	C(88)-Cl(11)	1.703(6)	C(87)-Cr(2)-Si(3)#1 82.87(9)
C(49)-C(51)	1.525(4)	C(88)-Cl(12)	1.772(4)	C(86)#1-Cr(2)-Si(3) 91.15(11)
C(49)-C(50)	1.544(4)	C(88')-Cl(21)	1.71(2)	C(86)-Cr(2)-Si(3) 88.85(11)
C(52)-C(54)	1.523(4)	C(88')-Cl(22)	1.80(2)	C(87)#1-Cr(2)-Si(3) 82.86(9)
C(52)-C(53)	1.535(4)	Cl(21)-Cl(22)	2.39(2)	C(87)-Cr(2)-Si(3) 97.13(9)
C(60)-C(61)	1.332(4)			Si(3)#1-Cr(2)-Si(3) 180.0
C(62)-C(67)	1.395(5)	C(58)-Cr(1)-C(57) 84.51(12)		C(1)-Si(1)-Cl(1) 97.87(8)
C(62)-C(63)	1.411(5)	C(58)-Cr(1)-C(55) 82.23(13)		C(1)-Si(1)-Cl(2) 98.94(8)
C(63)-C(64)	1.386(5)	C(57)-Cr(1)-C(55) 166.73(12)		Cl(1)-Si(1)-Cl(2) 97.54(5)
C(63)-C(68)	1.527(5)	C(58)-Cr(1)-C(56) 178.63(12)		C(1)-Si(1)-Cr(1) 125.41(8)
C(64)-C(65)	1.366(6)	C(57)-Cr(1)-C(56) 95.87(12)		Cl(1)-Si(1)-Cr(1) 118.20(4)
C(65)-C(66)	1.375(5)	C(55)-Cr(1)-C(56) 97.40(12)		Cl(2)-Si(1)-Cr(1) 113.87(4)
C(66)-C(67)	1.409(5)	C(58)-Cr(1)-Si(2) 90.33(9)		C(28)-Si(2)-Cl(4) 100.35(8)
C(67)-C(71)	1.505(5)	C(57)-Cr(1)-Si(2) 95.34(9)		C(28)-Si(2)-Cl(3) 98.81(8)
C(68)-C(69)	1.513(5)	C(55)-Cr(1)-Si(2) 85.21(9)		Cl(4)-Si(2)-Cl(3) 97.50(5)
C(68)-C(70)	1.534(5)	C(56)-Cr(1)-Si(2) 88.33(8)		C(28)-Si(2)-Cr(1) 123.38(8)
C(71)-C(73)	1.527(5)	C(58)-Cr(1)-Si(1) 91.77(9)		Cl(4)-Si(2)-Cr(1) 115.09(4)
C(71)-C(72)	1.532(5)	C(57)-Cr(1)-Si(1) 85.66(9)		Cl(3)-Si(2)-Cr(1) 117.28(4)
C(74)-C(79)	1.394(4)	C(55)-Cr(1)-Si(1) 94.28(9)		C(59)-Si(3)-Cl(5) 100.07(10)
C(74)-C(75)	1.398(4)	C(56)-Cr(1)-Si(1) 89.57(8)		C(59)-Si(3)-Cl(6) 97.78(9)
C(75)-C(76)	1.394(4)	Si(2)-Cr(1)-Si(1) 177.76(3)		Cl(5)-Si(3)-Cl(6) 96.72(6)
C(75)-C(80)	1.513(4)	C(86)#1-Cr(2)-C(86) 180.00(18)		C(59)-Si(3)-Cr(2) 124.88(9)
C(76)-C(77)	1.384(5)	C(86)#1-Cr(2)-C(87)#1 90.38(13)		Cl(5)-Si(3)-Cr(2) 114.78(5)

Cl(6)-Si(3)-Cr(2)	117.61(5)	C(7)-C(6)-C(5)	122.1(3)	N(3)-C(28)-N(4)	104.2(2)
C(1)-N(1)-C(2)	110.8(2)	C(6)-C(7)-C(8)	119.9(3)	N(3)-C(28)-Si(2)	128.03(19)
C(1)-N(1)-C(4)	129.1(2)	C(7)-C(8)-C(9)	121.4(3)	N(4)-C(28)-Si(2)	126.70(19)
C(2)-N(1)-C(4)	119.7(2)	C(8)-C(9)-C(4)	116.5(3)	C(30)-C(29)-N(3)	107.6(2)
C(1)-N(2)-C(3)	110.6(2)	C(8)-C(9)-C(13)	120.9(3)	C(29)-C(30)-N(4)	107.1(2)
C(1)-N(2)-C(16)	131.4(2)	C(4)-C(9)-C(13)	122.4(2)	C(32)-C(31)-C(36)	123.4(2)
C(3)-N(2)-C(16)	117.8(2)	C(5)-C(10)-C(11)	113.7(3)	C(32)-C(31)-N(3)	116.8(2)
C(28)-N(3)-C(29)	110.7(2)	C(5)-C(10)-C(12)	110.5(2)	C(36)-C(31)-N(3)	119.5(2)
C(28)-N(3)-C(31)	128.5(2)	C(11)-C(10)-C(12)	108.3(3)	C(33)-C(32)-C(31)	117.2(2)
C(29)-N(3)-C(31)	119.2(2)	C(14)-C(13)-C(9)	113.6(3)	C(33)-C(32)-C(37)	120.2(3)
C(28)-N(4)-C(30)	110.5(2)	C(14)-C(13)-C(15)	109.2(3)	C(31)-C(32)-C(37)	122.6(2)
C(28)-N(4)-C(43)	129.2(2)	C(9)-C(13)-C(15)	109.9(3)	C(34)-C(33)-C(32)	120.9(3)
C(30)-N(4)-C(43)	119.6(2)	C(21)-C(16)-C(17)	123.8(3)	C(33)-C(34)-C(35)	120.3(3)
C(59)-N(5)-C(60)	110.7(2)	C(21)-C(16)-N(2)	118.1(2)	C(34)-C(35)-C(36)	121.6(3)
C(59)-N(5)-C(62)	128.8(2)	C(17)-C(16)-N(2)	117.7(2)	C(35)-C(36)-C(31)	116.4(3)
C(60)-N(5)-C(62)	120.1(3)	C(18)-C(17)-C(16)	116.3(3)	C(35)-C(36)-C(40)	121.4(2)
C(59)-N(6)-C(61)	110.2(2)	C(18)-C(17)-C(22)	121.5(3)	C(31)-C(36)-C(40)	122.1(2)
C(59)-N(6)-C(74)	129.2(2)	C(16)-C(17)-C(22)	122.2(2)	C(38)-C(37)-C(32)	110.2(2)
C(61)-N(6)-C(74)	119.6(2)	C(19)-C(18)-C(17)	121.6(3)	C(38)-C(37)-C(39)	111.4(3)
N(2)-C(1)-N(1)	104.0(2)	C(20)-C(19)-C(18)	120.3(3)	C(32)-C(37)-C(39)	112.4(3)
N(2)-C(1)-Si(1)	129.1(2)	C(19)-C(20)-C(21)	121.3(3)	C(36)-C(40)-C(41)	112.6(2)
N(1)-C(1)-Si(1)	125.99(19)	C(16)-C(21)-C(20)	116.7(3)	C(36)-C(40)-C(42)	110.6(2)
C(3)-C(2)-N(1)	107.3(2)	C(16)-C(21)-C(25)	122.8(3)	C(41)-C(40)-C(42)	108.0(2)
C(2)-C(3)-N(2)	107.3(2)	C(20)-C(21)-C(25)	120.5(3)	C(44)-C(43)-C(48)	123.1(2)
C(5)-C(4)-C(9)	124.0(3)	C(23)-C(22)-C(17)	112.1(3)	C(44)-C(43)-N(4)	119.0(2)
C(5)-C(4)-N(1)	117.8(2)	C(23)-C(22)-C(24)	110.1(3)	C(48)-C(43)-N(4)	117.4(2)
C(9)-C(4)-N(1)	117.5(2)	C(17)-C(22)-C(24)	112.7(3)	C(45)-C(44)-C(43)	116.9(3)
C(6)-C(5)-C(4)	116.0(3)	C(21)-C(25)-C(27)	111.6(3)	C(45)-C(44)-C(49)	119.0(2)
C(6)-C(5)-C(10)	121.0(3)	C(21)-C(25)-C(26)	110.8(3)	C(43)-C(44)-C(49)	123.7(2)
C(4)-C(5)-C(10)	122.8(3)	C(27)-C(25)-C(26)	109.8(3)	C(46)-C(45)-C(44)	121.3(3)

C(45)-C(46)-C(47) 120.4(3)	C(62)-C(67)-C(71) 123.2(3)	C(88')-Cl(21)-Cl(22) 48.7(9)
C(46)-C(47)-C(48) 121.2(3)	C(66)-C(67)-C(71) 121.5(3)	C(88')-Cl(22)-Cl(21) 45.6(8)
C(47)-C(48)-C(43) 116.9(3)	C(69)-C(68)-C(63) 110.3(4)	Cl(8)-C(89)-Cl(7) 113.58(19)
C(47)-C(48)-C(52) 120.4(2)	C(69)-C(68)-C(70) 108.9(3)	
C(43)-C(48)-C(52) 122.5(2)	C(63)-C(68)-C(70) 114.7(3)	
C(44)-C(49)-C(51) 113.6(2)	C(67)-C(71)-C(73) 115.2(3)	
C(44)-C(49)-C(50) 108.5(2)	C(67)-C(71)-C(72) 110.5(3)	
C(51)-C(49)-C(50) 109.0(2)	C(73)-C(71)-C(72) 107.1(3)	
C(48)-C(52)-C(54) 113.2(2)	C(79)-C(74)-C(75) 123.7(3)	
C(48)-C(52)-C(53) 110.2(2)	C(79)-C(74)-N(6) 116.3(3)	
C(54)-C(52)-C(53) 109.7(2)	C(75)-C(74)-N(6) 119.9(3)	
O(1)-C(55)-Cr(1) 172.4(3)	C(76)-C(75)-C(74) 116.5(3)	
O(2)-C(56)-Cr(1) 179.2(3)	C(76)-C(75)-C(80) 121.4(3)	
O(3)-C(57)-Cr(1) 174.0(2)	C(74)-C(75)-C(80) 122.1(3)	
O(4)-C(58)-Cr(1) 178.7(3)	C(77)-C(76)-C(75) 121.3(3)	
N(5)-C(59)-N(6) 104.3(2)	C(78)-C(77)-C(76) 120.4(3)	
N(5)-C(59)-Si(3) 126.9(2)	C(77)-C(78)-C(79) 121.3(3)	
N(6)-C(59)-Si(3) 128.2(2)	C(74)-C(79)-C(78) 116.8(3)	
C(61)-C(60)-N(5) 107.4(3)	C(74)-C(79)-C(83) 123.2(3)	
C(60)-C(61)-N(6) 107.4(3)	C(78)-C(79)-C(83) 120.0(3)	
C(67)-C(62)-C(63) 124.7(3)	C(75)-C(80)-C(82) 112.8(3)	
C(67)-C(62)-N(5) 118.4(3)	C(75)-C(80)-C(81) 113.7(3)	
C(63)-C(62)-N(5) 116.6(3)	C(82)-C(80)-C(81) 107.7(3)	
C(64)-C(63)-C(62) 116.1(3)	C(79)-C(83)-C(85) 111.7(3)	
C(64)-C(63)-C(68) 120.7(3)	C(79)-C(83)-C(84) 111.4(3)	
C(62)-C(63)-C(68) 123.2(3)	C(85)-C(83)-C(84) 110.7(3)	
C(65)-C(64)-C(63) 121.2(4)	O(5)-C(86)-Cr(2) 179.5(4)	
C(64)-C(65)-C(66) 121.5(4)	O(6)-C(87)-Cr(2) 178.6(3)	
C(65)-C(66)-C(67) 121.2(4)	Cl(11)-C(88)-Cl(12) 111.9(3)	
C(62)-C(67)-C(66) 115.2(3)	Cl(21)-C(88')-Cl(22) 85.6(13)	

Compound 4-W

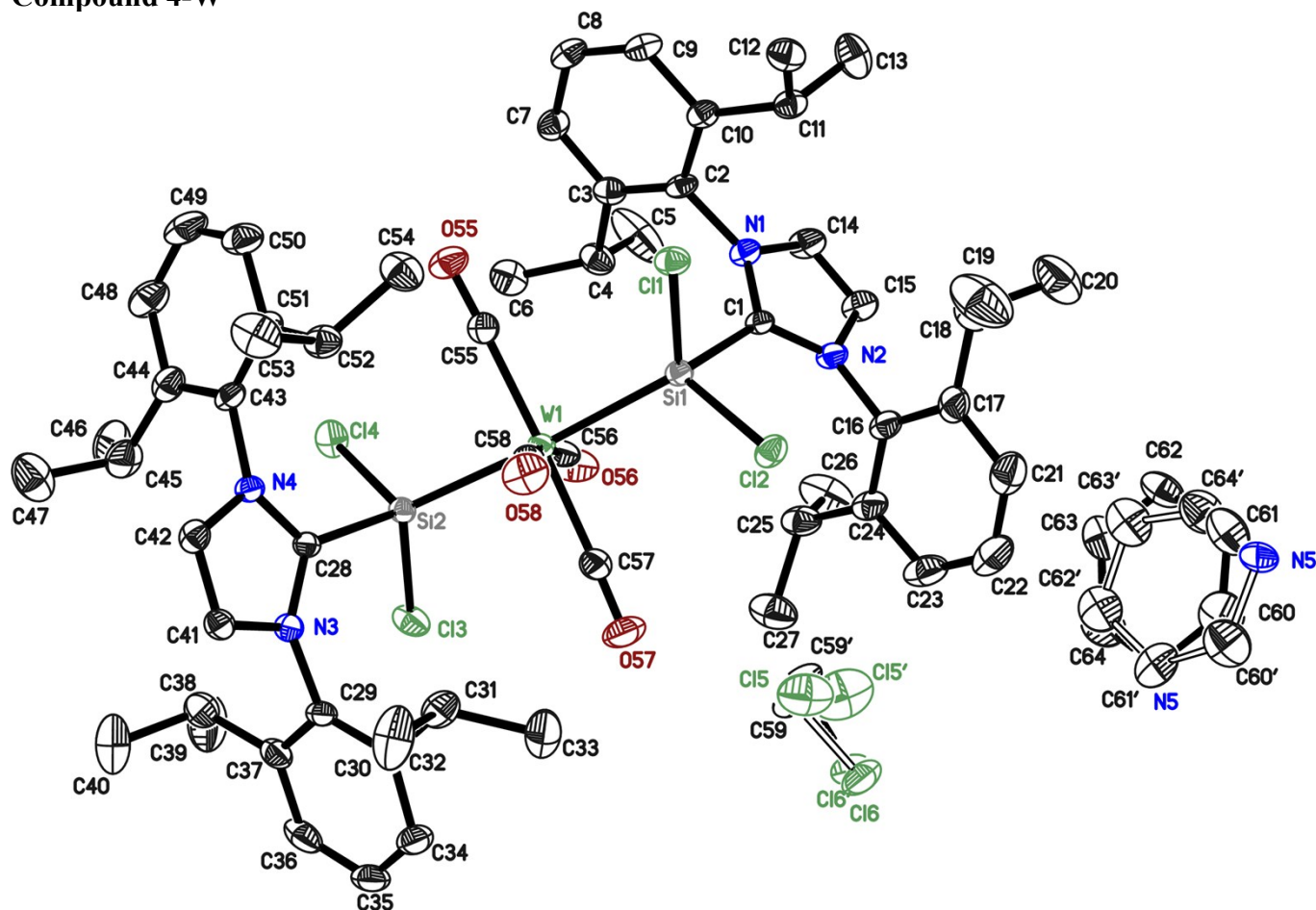


Figure S2. Molecular structure of compound **4-W**. Anisotropic displacement parameters are depicted at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected experimental and theoretical [BP86+D3(BJ)/def2-SVP] {M06/def2-SVP} bond lengths (Å) and bond angles (°): C1—Si1, 1.996(3) [1.984]{2.019}; Si1—Cl1, 2.1292(19) [2.141]{2.142}; Si1—Cl2, 2.134(2) [2.149]{2.139}; Si1—W1, 2.464(2) [2.474]{2.494}; Si2—W1, 2.4707(19) [2.481]{2.485}; C28—Si2, 1.983(3) [1.982]{2.017}; W1—C56, 2.017(4) [2.041]{2.055}; W1—C58, 2.031(3) [2.043]{2.056}; Si1—W1—Si2, 176.41(7) [174.6]{178.6}; C1—Si1—W1, 126.15(11) [120.8]{123.1}; Cl1—Si1—Cl2, 96.73(7) [99.3]{98.9}; C56—W1—C58, 169.94(16) [167.0]{175.1}; C55—W1—C57, 176.7(4) [176.1]{177.1}; C56—W1—C57, 82.92(17) [84.7]{85.8}.

Table S3. Bond lengths [Å] and angles [°] of Compound **4-W**.

W(1)-C(57)	2.013(8)	C(2)-C(10)	1.405(5)	C(31)-C(32)	1.551(6)
W(1)-C(56)	2.017(4)	C(3)-C(7)	1.395(5)	C(34)-C(35)	1.376(6)
W(1)-C(58)	2.031(3)	C(3)-C(4)	1.518(5)	C(35)-C(36)	1.378(6)
W(1)-C(55)	2.039(8)	C(4)-C(6)	1.534(5)	C(36)-C(37)	1.393(5)
W(1)-Si(1)	2.464(2)	C(4)-C(5)	1.543(5)	C(37)-C(38)	1.521(5)
W(1)-Si(2)	2.4707(19)	C(7)-C(8)	1.389(5)	C(38)-C(39)	1.525(6)
Cl(1)-Si(1)	2.1292(19)	C(8)-C(9)	1.381(5)	C(38)-C(40)	1.526(6)
Cl(2)-Si(1)	2.134(2)	C(9)-C(10)	1.395(4)	C(41)-C(42)	1.340(5)
Cl(3)-Si(2)	2.111(2)	C(10)-C(11)	1.524(5)	C(43)-C(51)	1.391(5)
Cl(4)-Si(2)	2.1226(19)	C(11)-C(12)	1.526(5)	C(43)-C(44)	1.414(5)
Si(1)-C(1)	1.996(3)	C(11)-C(13)	1.541(5)	C(44)-C(48)	1.391(5)
Si(2)-C(28)	1.983(3)	C(14)-C(15)	1.337(5)	C(44)-C(45)	1.506(5)
O(55)-C(55)	1.154(9)	C(16)-C(24)	1.390(5)	C(45)-C(47)	1.532(6)
O(56)-C(56)	1.158(4)	C(16)-C(17)	1.392(5)	C(45)-C(46)	1.533(5)
O(57)-C(57)	1.145(10)	C(17)-C(21)	1.397(6)	C(48)-C(49)	1.381(6)
O(58)-C(58)	1.154(4)	C(17)-C(18)	1.520(6)	C(49)-C(50)	1.377(6)
N(1)-C(1)	1.360(4)	C(18)-C(20)	1.523(6)	C(50)-C(51)	1.407(5)
N(1)-C(14)	1.377(4)	C(18)-C(19)	1.538(8)	C(51)-C(52)	1.520(5)
N(1)-C(2)	1.473(4)	C(21)-C(22)	1.363(7)	C(52)-C(54)	1.526(5)
N(2)-C(1)	1.361(4)	C(22)-C(23)	1.374(6)	C(52)-C(53)	1.535(5)
N(2)-C(15)	1.390(4)	C(23)-C(24)	1.415(5)	C(59)-Cl(5)	1.762(11)
N(2)-C(16)	1.467(4)	C(24)-C(25)	1.502(6)	C(59)-Cl(6)	1.769(10)
N(3)-C(28)	1.372(4)	C(25)-C(26)	1.540(6)	C(59')-Cl(6')	1.767(19)
N(3)-C(41)	1.385(4)	C(25)-C(27)	1.541(5)	C(59')-Cl(5')	1.768(19)
N(3)-C(29)	1.460(4)	C(29)-C(37)	1.398(5)	N(5)-C(64)	1.307(10)
N(4)-C(28)	1.365(4)	C(29)-C(30)	1.400(5)	N(5)-C(60)	1.450(9)
N(4)-C(42)	1.388(4)	C(30)-C(34)	1.395(5)	C(60)-C(61)	1.304(10)
N(4)-C(43)	1.459(4)	C(30)-C(31)	1.514(5)	C(61)-C(62)	1.473(9)
C(2)-C(3)	1.399(5)	C(31)-C(33)	1.533(5)	C(62)-C(63)	1.429(7)

C(63)-C(64)	1.435(10)	C(28)-Si(2)-Cl(4)	99.77(12)	C(9)-C(8)-C(7)	120.8(3)
N(5')-C(64')	1.406(18)	Cl(3)-Si(2)-Cl(4)	97.87(8)	C(8)-C(9)-C(10)	121.1(3)
N(5')-C(60')	1.462(19)	C(28)-Si(2)-W(1)	123.96(11)	C(9)-C(10)-C(2)	116.6(3)
C(60')-C(61')	1.417(18)	Cl(3)-Si(2)-W(1)	115.44(8)	C(9)-C(10)-C(11)	120.2(3)
C(61')-C(62')	1.42(2)	Cl(4)-Si(2)-W(1)	115.48(8)	C(2)-C(10)-C(11)	123.1(3)
C(62')-C(63')	1.48(2)	C(1)-N(1)-C(14)	110.5(3)	C(10)-C(11)-C(12)	113.5(3)
C(63')-C(64')	1.475(19)	C(1)-N(1)-C(2)	128.9(3)	C(10)-C(11)-C(13)	110.3(3)
		C(14)-N(1)-C(2)	120.1(3)	C(12)-C(11)-C(13)	109.1(3)
C(57)-W(1)-C(56)	82.92(17)	C(1)-N(2)-C(15)	110.4(3)	C(15)-C(14)-N(1)	107.7(3)
C(57)-W(1)-C(58)	87.03(18)	C(1)-N(2)-C(16)	129.0(3)	C(14)-C(15)-N(2)	106.7(3)
C(56)-W(1)-C(58)	169.94(16)	C(15)-N(2)-C(16)	119.7(3)	C(24)-C(16)-C(17)	124.4(3)
C(57)-W(1)-C(55)	176.7(4)	C(28)-N(3)-C(41)	110.8(3)	C(24)-C(16)-N(2)	118.4(3)
C(56)-W(1)-C(55)	94.64(14)	C(28)-N(3)-C(29)	129.9(3)	C(17)-C(16)-N(2)	117.1(3)
C(58)-W(1)-C(55)	95.40(15)	C(41)-N(3)-C(29)	118.9(3)	C(16)-C(17)-C(21)	117.0(4)
C(57)-W(1)-Si(1)	93.4(2)	C(28)-N(4)-C(42)	110.8(3)	C(16)-C(17)-C(18)	123.2(3)
C(56)-W(1)-Si(1)	98.56(11)	C(28)-N(4)-C(43)	127.9(3)	C(21)-C(17)-C(18)	119.8(4)
C(58)-W(1)-Si(1)	82.31(10)	C(42)-N(4)-C(43)	120.4(3)	C(17)-C(18)-C(20)	110.1(4)
C(55)-W(1)-Si(1)	89.2(2)	N(1)-C(1)-N(2)	104.7(3)	C(17)-C(18)-C(19)	112.2(4)
C(57)-W(1)-Si(2)	89.7(2)	N(1)-C(1)-Si(1)	126.0(2)	C(20)-C(18)-C(19)	109.5(4)
C(56)-W(1)-Si(2)	83.63(11)	N(2)-C(1)-Si(1)	128.8(2)	C(22)-C(21)-C(17)	120.7(4)
C(58)-W(1)-Si(2)	96.03(10)	C(3)-C(2)-C(10)	123.7(3)	C(21)-C(22)-C(23)	121.2(4)
C(55)-W(1)-Si(2)	87.8(2)	C(3)-C(2)-N(1)	119.2(3)	C(22)-C(23)-C(24)	121.2(4)
Si(1)-W(1)-Si(2)	176.41(7)	C(10)-C(2)-N(1)	116.7(3)	C(16)-C(24)-C(23)	115.4(4)
C(1)-Si(1)-Cl(1)	97.70(12)	C(7)-C(3)-C(2)	116.9(3)	C(16)-C(24)-C(25)	122.2(3)
C(1)-Si(1)-Cl(2)	99.55(13)	C(7)-C(3)-C(4)	120.6(3)	C(23)-C(24)-C(25)	122.3(3)
Cl(1)-Si(1)-Cl(2)	96.73(7)	C(2)-C(3)-C(4)	122.3(3)	C(24)-C(25)-C(26)	112.1(4)
C(1)-Si(1)-W(1)	126.15(11)	C(3)-C(4)-C(6)	114.5(3)	C(24)-C(25)-C(27)	112.9(3)
Cl(1)-Si(1)-W(1)	116.67(8)	C(3)-C(4)-C(5)	109.6(3)	C(26)-C(25)-C(27)	108.8(3)
Cl(2)-Si(1)-W(1)	114.80(8)	C(6)-C(4)-C(5)	107.5(3)	N(4)-C(28)-N(3)	104.1(3)
C(28)-Si(2)-Cl(3)	100.02(12)	C(8)-C(7)-C(3)	120.7(3)	N(4)-C(28)-Si(2)	126.6(2)

N(3)-C(28)-Si(2) 128.5(2)	C(41)-C(42)-N(4) 107.2(3)	O(56)-C(56)-W(1) 173.8(3)
C(37)-C(29)-C(30) 123.8(3)	C(51)-C(43)-C(44) 123.9(3)	O(57)-C(57)-W(1) 176.7(6)
C(37)-C(29)-N(3) 117.7(3)	C(51)-C(43)-N(4) 119.4(3)	O(58)-C(58)-W(1) 174.8(3)
C(30)-C(29)-N(3) 118.1(3)	C(44)-C(43)-N(4) 116.3(3)	Cl(5)-C(59)-Cl(6) 115.0(8)
C(34)-C(30)-C(29) 116.4(3)	C(48)-C(44)-C(43) 116.3(3)	Cl(6')-C(59')-Cl(5') 103.4(15)
C(34)-C(30)-C(31) 121.2(3)	C(48)-C(44)-C(45) 121.5(3)	C(64)-N(5)-C(60) 117.0(6)
C(29)-C(30)-C(31) 122.4(3)	C(43)-C(44)-C(45) 122.1(3)	C(61)-C(60)-N(5) 126.2(7)
C(30)-C(31)-C(33) 113.2(3)	C(44)-C(45)-C(47) 109.8(3)	C(60)-C(61)-C(62) 116.4(7)
C(30)-C(31)-C(32) 110.1(3)	C(44)-C(45)-C(46) 113.8(4)	C(63)-C(62)-C(61) 119.6(6)
C(33)-C(31)-C(32) 108.5(3)	C(47)-C(45)-C(46) 109.4(3)	C(62)-C(63)-C(64) 117.3(6)
C(35)-C(34)-C(30) 121.2(4)	C(49)-C(48)-C(44) 121.1(4)	N(5)-C(64)-C(63) 123.5(7)
C(34)-C(35)-C(36) 120.8(3)	C(50)-C(49)-C(48) 121.3(3)	C(64')-N(5')-C(60') 97.6(16)
C(35)-C(36)-C(37) 121.0(4)	C(49)-C(50)-C(51) 120.6(4)	C(61')-C(60')-N(5') 128.9(16)
C(36)-C(37)-C(29) 116.8(3)	C(43)-C(51)-C(50) 116.6(3)	C(60')-C(61')-C(62') 126.5(13)
C(36)-C(37)-C(38) 121.3(3)	C(43)-C(51)-C(52) 122.3(3)	C(61')-C(62')-C(63') 111.7(18)
C(29)-C(37)-C(38) 121.9(3)	C(50)-C(51)-C(52) 120.8(3)	C(64')-C(63')-C(62') 111.5(17)
C(37)-C(38)-C(39) 112.3(3)	C(51)-C(52)-C(54) 113.6(3)	N(5')-C(64')-C(63') 142.8(19)
C(37)-C(38)-C(40) 110.7(3)	C(51)-C(52)-C(53) 108.7(3)	
C(39)-C(38)-C(40) 109.2(4)	C(54)-C(52)-C(53) 108.6(3)	
C(42)-C(41)-N(3) 107.1(3)	O(55)-C(55)-W(1) 178.2(7)	

Compound 6-W

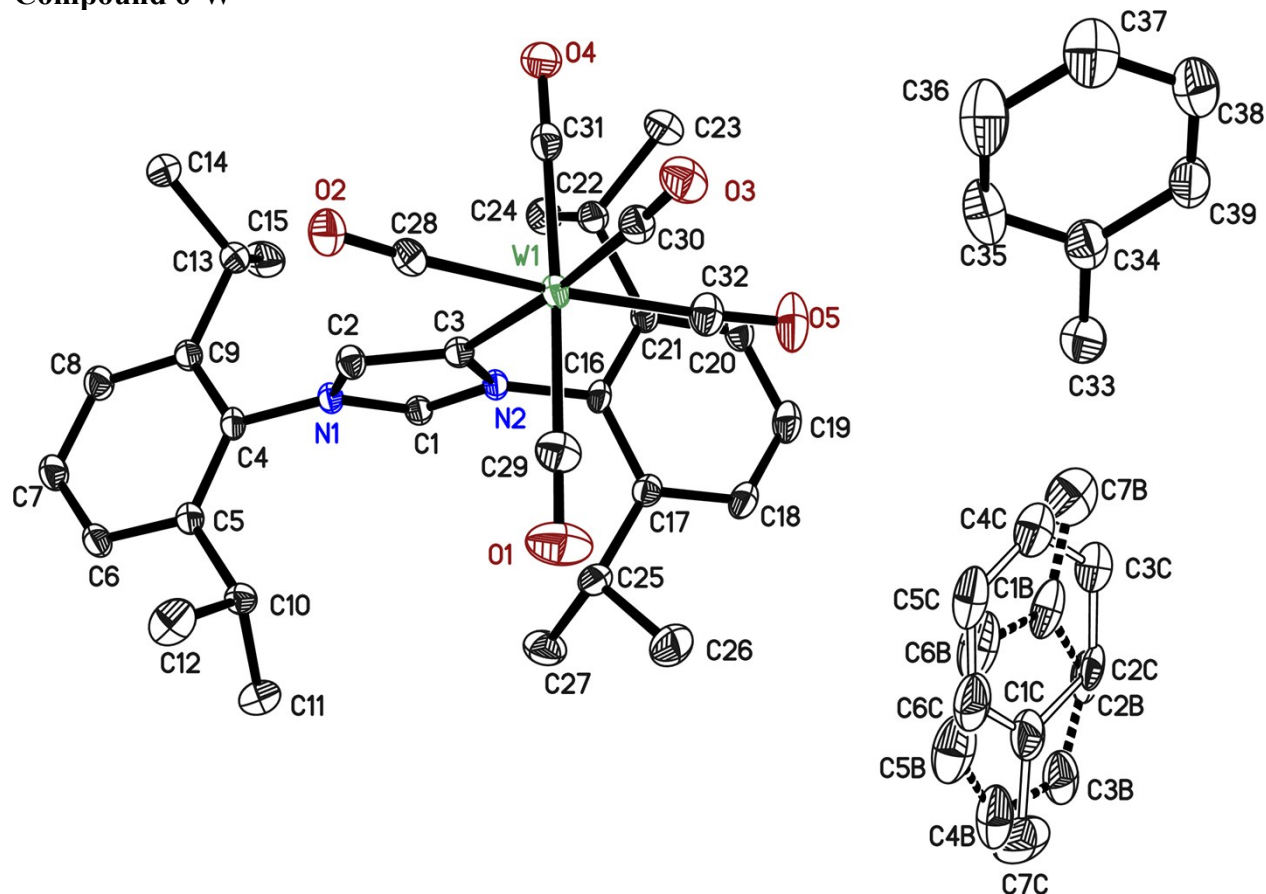


Figure S3. Molecular structure of compound **6-W**. Anisotropic displacement parameters are depicted at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected experimental and theoretical [BP86+D3(BJ)/def2-SVP] {M06/def2-SVP} bond lengths (Å) and bond angles (°): C3—W1, 2.2480(15) [2.245]{2.281}; C2—C3, 1.379(2) [1.394]{1.383}; W1—C30, 1.9964(16) [2.038]{2.036}; W1—C28, 2.0282(17) [2.065]{2.065}; W1—C32, 2.0543(17) [2.055]{2.076}; N1—C1, 1.3291(19) [1.346]{1.329}; N2—C1, 1.3291(19) [1.353]{1.341}; C3—W1—C30, 174.73(6) [176.8]{176.4}; C32—W1—C28, 172.70(6) [174.8]{176.4}; C31—W1—C29, 175.81(6) [174.3]{175.7}; C31—W1—C32, 90.23(7) [88.5]{90.4}; N2—C3—C2, 102.37(12) [102.6]{102.3}; N1—C1—N2, 108.34(13) [107.4]{108.1}.

Table S4. Bond lengths [Å] and angles [°] of Compound **6-W**.

W(1)-C(30)	1.9964(16)	C(13)-C(15)	1.530(2)	C(1B)-C(2B)	1.385(11)
W(1)-C(28)	2.0282(17)	C(13)-C(14)	1.532(2)	C(1B)-C(6B)	1.398(11)
W(1)-C(31)	2.0345(19)	C(16)-C(21)	1.399(2)	C(1B)-C(7B)	1.506(12)
W(1)-C(29)	2.050(2)	C(16)-C(17)	1.404(2)	C(2B)-C(3B)	1.387(12)
W(1)-C(32)	2.0543(17)	C(17)-C(18)	1.397(2)	C(3B)-C(4B)	1.383(12)
W(1)-C(3)	2.2480(15)	C(17)-C(25)	1.516(2)	C(4B)-C(5B)	1.375(12)
O(1)-C(29)	1.139(2)	C(18)-C(19)	1.382(3)	C(5B)-C(6B)	1.364(12)
N(1)-C(1)	1.3291(19)	C(19)-C(20)	1.382(3)		
N(1)-C(2)	1.3884(19)	C(20)-C(21)	1.397(2)	C(30)-W(1)-C(28)	85.70(7)
N(1)-C(4)	1.4444(18)	C(21)-C(22)	1.517(2)	C(30)-W(1)-C(31)	91.02(7)
C(1)-N(2)	1.3398(18)	C(22)-C(24)	1.533(2)	C(28)-W(1)-C(31)	89.36(7)
O(2)-C(28)	1.143(2)	C(22)-C(23)	1.534(2)	C(30)-W(1)-C(29)	93.14(7)
N(2)-C(3)	1.4129(19)	C(25)-C(26)	1.528(2)	C(28)-W(1)-C(29)	90.47(7)
N(2)-C(16)	1.4414(18)	C(25)-C(27)	1.533(2)	C(31)-W(1)-C(29)	175.81(6)
C(2)-C(3)	1.379(2)	C(33)-C(34)	1.503(3)	C(30)-W(1)-C(32)	87.02(7)
O(3)-C(30)	1.153(2)	C(34)-C(39)	1.391(3)	C(28)-W(1)-C(32)	172.70(6)
O(4)-C(31)	1.142(2)	C(34)-C(35)	1.399(3)	C(31)-W(1)-C(32)	90.23(7)
C(4)-C(5)	1.400(2)	C(35)-C(36)	1.378(3)	C(29)-W(1)-C(32)	90.47(8)
C(4)-C(9)	1.402(2)	C(36)-C(37)	1.384(3)	C(30)-W(1)-C(3)	174.73(6)
O(5)-C(32)	1.142(2)	C(37)-C(38)	1.389(3)	C(28)-W(1)-C(3)	89.31(6)
C(5)-C(6)	1.395(2)	C(38)-C(39)	1.377(3)	C(31)-W(1)-C(3)	87.23(6)
C(5)-C(10)	1.520(2)	C(1C)-C(6C)	1.386(12)	C(29)-W(1)-C(3)	88.59(6)
C(6)-C(7)	1.389(2)	C(1C)-C(2C)	1.393(11)	C(32)-W(1)-C(3)	97.95(6)
C(7)-C(8)	1.383(2)	C(1C)-C(7C)	1.512(13)	C(1)-N(1)-C(2)	107.78(12)
C(8)-C(9)	1.396(2)	C(2C)-C(3C)	1.390(11)	C(1)-N(1)-C(4)	124.98(12)
C(9)-C(13)	1.517(2)	C(3C)-C(4C)	1.354(11)	C(2)-N(1)-C(4)	127.10(13)
C(10)-C(12)	1.532(2)	C(4C)-C(5C)	1.384(12)	N(1)-C(1)-N(2)	108.34(13)
C(10)-C(11)	1.533(2)	C(5C)-C(6C)	1.385(12)	C(1)-N(2)-C(3)	111.24(12)

C(1)-N(2)-C(16)	121.39(12)	C(19)-C(18)-C(17)	121.02(15)	C(3C)-C(4C)-C(5C)	119.4(11)
C(3)-N(2)-C(16)	127.23(12)	C(20)-C(19)-C(18)	120.58(15)	C(4C)-C(5C)-C(6C)	118.7(12)
C(3)-C(2)-N(1)	110.28(13)	C(19)-C(20)-C(21)	121.02(16)	C(5C)-C(6C)-C(1C)	122.0(13)
C(2)-C(3)-N(2)	102.37(12)	C(20)-C(21)-C(16)	117.16(15)	C(2B)-C(1B)-C(6B)	117.3(11)
C(2)-C(3)-W(1)	128.66(11)	C(20)-C(21)-C(22)	121.09(14)	C(2B)-C(1B)-C(7B)	123.6(11)
N(2)-C(3)-W(1)	128.96(10)	C(16)-C(21)-C(22)	121.75(13)	C(6B)-C(1B)-C(7B)	119.1(11)
C(5)-C(4)-C(9)	123.25(13)	C(21)-C(22)-C(24)	110.61(13)	C(1B)-C(2B)-C(3B)	122.1(12)
C(5)-C(4)-N(1)	117.86(13)	C(21)-C(22)-C(23)	112.34(14)	C(4B)-C(3B)-C(2B)	120.3(13)
C(9)-C(4)-N(1)	118.88(13)	C(24)-C(22)-C(23)	110.79(14)	C(5B)-C(4B)-C(3B)	116.9(12)
C(6)-C(5)-C(4)	117.18(14)	C(17)-C(25)-C(26)	112.44(14)	C(6B)-C(5B)-C(4B)	123.9(12)
C(6)-C(5)-C(10)	119.64(14)	C(17)-C(25)-C(27)	110.47(14)	C(5B)-C(6B)-C(1B)	119.5(12)
C(4)-C(5)-C(10)	123.18(13)	C(26)-C(25)-C(27)	109.63(15)		
C(7)-C(6)-C(5)	121.10(15)	O(2)-C(28)-W(1)	175.43(14)		
C(8)-C(7)-C(6)	120.14(14)	O(1)-C(29)-W(1)	179.7(2)		
C(7)-C(8)-C(9)	121.36(15)	O(3)-C(30)-W(1)	177.40(14)		
C(8)-C(9)-C(4)	116.96(14)	O(4)-C(31)-W(1)	179.51(15)		
C(8)-C(9)-C(13)	119.93(14)	O(5)-C(32)-W(1)	173.57(14)		
C(4)-C(9)-C(13)	123.11(13)	C(39)-C(34)-C(35)	117.4(2)		
C(5)-C(10)-C(12)	110.63(13)	C(39)-C(34)-C(33)	121.54(19)		
C(5)-C(10)-C(11)	111.34(13)	C(35)-C(34)-C(33)	121.05(19)		
C(12)-C(10)-C(11)	110.51(15)	C(36)-C(35)-C(34)	121.4(2)		
C(9)-C(13)-C(15)	111.16(14)	C(35)-C(36)-C(37)	120.1(2)		
C(9)-C(13)-C(14)	110.81(14)	C(36)-C(37)-C(38)	119.3(2)		
C(15)-C(13)-C(14)	110.79(15)	C(39)-C(38)-C(37)	120.1(2)		
C(21)-C(16)-C(17)	123.18(14)	C(38)-C(39)-C(34)	121.57(19)		
C(21)-C(16)-N(2)	118.86(13)	C(6C)-C(1C)-C(2C)	118.1(10)		
C(17)-C(16)-N(2)	117.95(14)	C(6C)-C(1C)-C(7C)	124.0(12)		
C(18)-C(17)-C(16)	117.01(15)	C(2C)-C(1C)-C(7C)	118.0(11)		
C(18)-C(17)-C(25)	121.34(14)	C(3C)-C(2C)-C(1C)	118.7(11)		
C(16)-C(17)-C(25)	121.65(14)	C(4C)-C(3C)-C(2C)	122.6(11)		

Compound 7-W

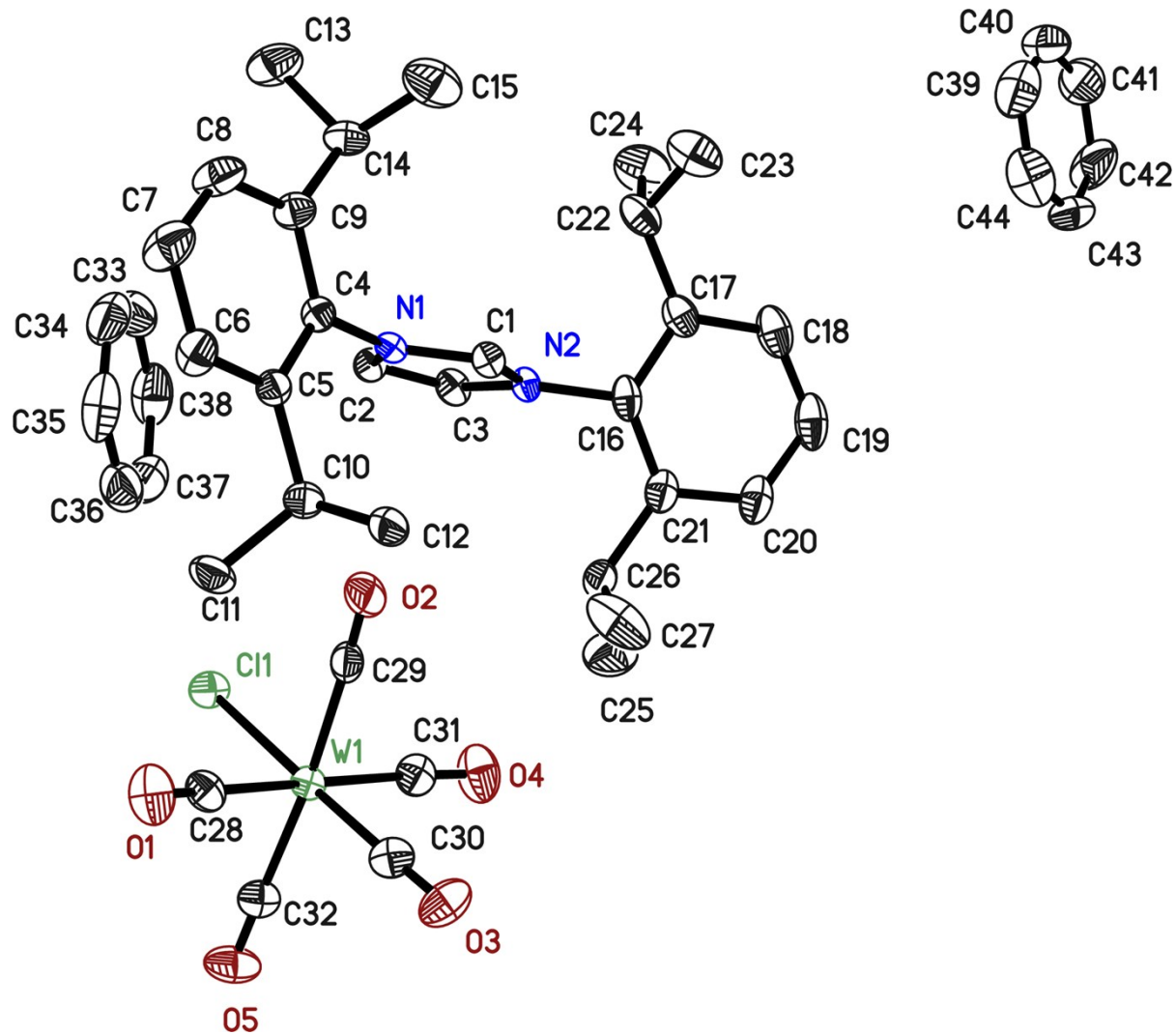


Figure S4. Molecular structure of compound 7-W. H-atoms have been omitted for clarity. Anisotropic displacement parameters are depicted at the 50% probability level.

Table S5. Bond lengths [Å] and angles [°] of Compound **7-W**.

W(1)-C(30)	1.952(4)	C(10)-C(11)	1.532(4)	
W(1)-C(29)	2.030(4)	C(13)-C(14)	1.518(5)	C(30)-W(1)-C(29) 90.50(15)
W(1)-C(31)	2.034(4)	C(14)-C(15)	1.527(5)	C(30)-W(1)-C(31) 85.97(15)
W(1)-C(28)	2.036(4)	C(16)-C(21)	1.393(5)	C(29)-W(1)-C(31) 92.44(14)
W(1)-C(32)	2.039(4)	C(16)-C(17)	1.399(5)	C(30)-W(1)-C(28) 88.39(15)
W(1)-Cl(1)	2.5585(9)	C(17)-C(18)	1.398(5)	C(29)-W(1)-C(28) 83.77(14)
O(1)-C(28)	1.145(4)	C(17)-C(23)	1.515(5)	C(31)-W(1)-C(28) 173.17(14)
O(2)-C(29)	1.143(4)	C(18)-C(19)	1.380(5)	C(30)-W(1)-C(32) 91.84(15)
O(3)-C(30)	1.165(4)	C(19)-C(20)	1.378(5)	C(29)-W(1)-C(32) 174.99(14)
O(4)-C(31)	1.149(4)	C(20)-C(21)	1.389(5)	C(31)-W(1)-C(32) 92.15(15)
O(5)-C(32)	1.145(4)	C(21)-C(26)	1.517(5)	C(28)-W(1)-C(32) 91.87(14)
N(1)-C(1)	1.341(4)	C(22)-C(23)	1.518(5)	C(30)-W(1)-Cl(1) 177.94(11)
N(1)-C(2)	1.377(4)	C(23)-C(24)	1.533(5)	C(29)-W(1)-Cl(1) 89.55(10)
N(1)-C(4)	1.457(4)	C(25)-C(26)	1.519(5)	C(31)-W(1)-Cl(1) 91.97(11)
N(2)-C(1)	1.335(4)	C(26)-C(27)	1.513(6)	C(28)-W(1)-Cl(1) 93.67(11)
N(2)-C(3)	1.380(4)	C(33)-C(34)	1.369(7)	C(32)-W(1)-Cl(1) 88.27(10)
N(2)-C(16)	1.455(4)	C(33)-C(38)	1.370(6)	C(1)-N(1)-C(2) 108.7(3)
C(2)-C(3)	1.343(4)	C(34)-C(35)	1.356(7)	C(1)-N(1)-C(4) 125.6(3)
C(4)-C(9)	1.394(4)	C(35)-C(36)	1.356(6)	C(2)-N(1)-C(4) 125.6(3)
C(4)-C(5)	1.398(4)	C(36)-C(37)	1.351(6)	C(1)-N(2)-C(3) 108.5(3)
C(5)-C(6)	1.389(4)	C(37)-C(38)	1.348(6)	C(1)-N(2)-C(16) 125.8(3)
C(5)-C(10)	1.513(4)	C(39)-C(40)	1.355(7)	C(3)-N(2)-C(16) 125.5(3)
C(6)-C(7)	1.390(5)	C(39)-C(44)	1.386(7)	N(2)-C(1)-N(1) 108.1(3)
C(7)-C(8)	1.383(5)	C(40)-C(41)	1.346(7)	C(3)-C(2)-N(1) 107.2(3)
C(8)-C(9)	1.392(5)	C(41)-C(42)	1.357(7)	C(2)-C(3)-N(2) 107.5(3)
C(9)-C(14)	1.520(5)	C(42)-C(43)	1.375(6)	C(9)-C(4)-C(5) 124.4(3)
C(10)-C(12)	1.528(4)	C(43)-C(44)	1.370(6)	C(9)-C(4)-N(1) 117.3(3)

C(5)-C(4)-N(1)	118.2(3)	C(17)-C(16)-N(2)	117.1(3)	O(2)-C(29)-W(1)	174.4(3)
C(6)-C(5)-C(4)	116.3(3)	C(18)-C(17)-C(16)	115.9(3)	O(3)-C(30)-W(1)	178.4(3)
C(6)-C(5)-C(10)	121.2(3)	C(18)-C(17)-C(23)	121.0(3)	O(4)-C(31)-W(1)	174.3(3)
C(4)-C(5)-C(10)	122.5(3)	C(16)-C(17)-C(23)	123.1(3)	O(5)-C(32)-W(1)	177.8(3)
C(5)-C(6)-C(7)	121.1(3)	C(19)-C(18)-C(17)	121.3(4)	C(34)-C(33)-C(38)	119.4(4)
C(8)-C(7)-C(6)	120.6(3)	C(20)-C(19)-C(18)	120.3(3)	C(35)-C(34)-C(33)	120.2(4)
C(7)-C(8)-C(9)	120.8(3)	C(19)-C(20)-C(21)	121.7(4)	C(34)-C(35)-C(36)	119.4(4)
C(8)-C(9)-C(4)	116.7(3)	C(20)-C(21)-C(16)	116.1(3)	C(37)-C(36)-C(35)	120.9(4)
C(8)-C(9)-C(14)	120.9(3)	C(20)-C(21)-C(26)	121.7(3)	C(38)-C(37)-C(36)	120.0(4)
C(4)-C(9)-C(14)	122.4(3)	C(16)-C(21)-C(26)	122.2(3)	C(37)-C(38)-C(33)	120.0(4)
C(5)-C(10)-C(12)	110.1(3)	C(17)-C(23)-C(22)	111.8(3)	C(40)-C(39)-C(44)	119.4(5)
C(5)-C(10)-C(11)	113.5(3)	C(17)-C(23)-C(24)	110.6(3)	C(41)-C(40)-C(39)	121.4(5)
C(12)-C(10)-C(11)	109.4(3)	C(22)-C(23)-C(24)	111.4(3)	C(40)-C(41)-C(42)	119.9(5)
C(13)-C(14)-C(15)	110.8(3)	C(27)-C(26)-C(21)	110.9(3)	C(41)-C(42)-C(43)	120.1(5)
C(9)-C(14)-C(15)	110.2(3)	C(27)-C(26)-C(25)	111.0(3)	C(44)-C(43)-C(42)	119.8(4)
C(21)-C(16)-C(17)	124.6(3)	C(21)-C(26)-C(25)	113.5(3)	C(43)-C(44)-C(39)	119.1(4)
C(21)-C(16)-N(2)	118.3(3)	O(1)-C(28)-W(1)	173.3(3)		

Compound 8-W

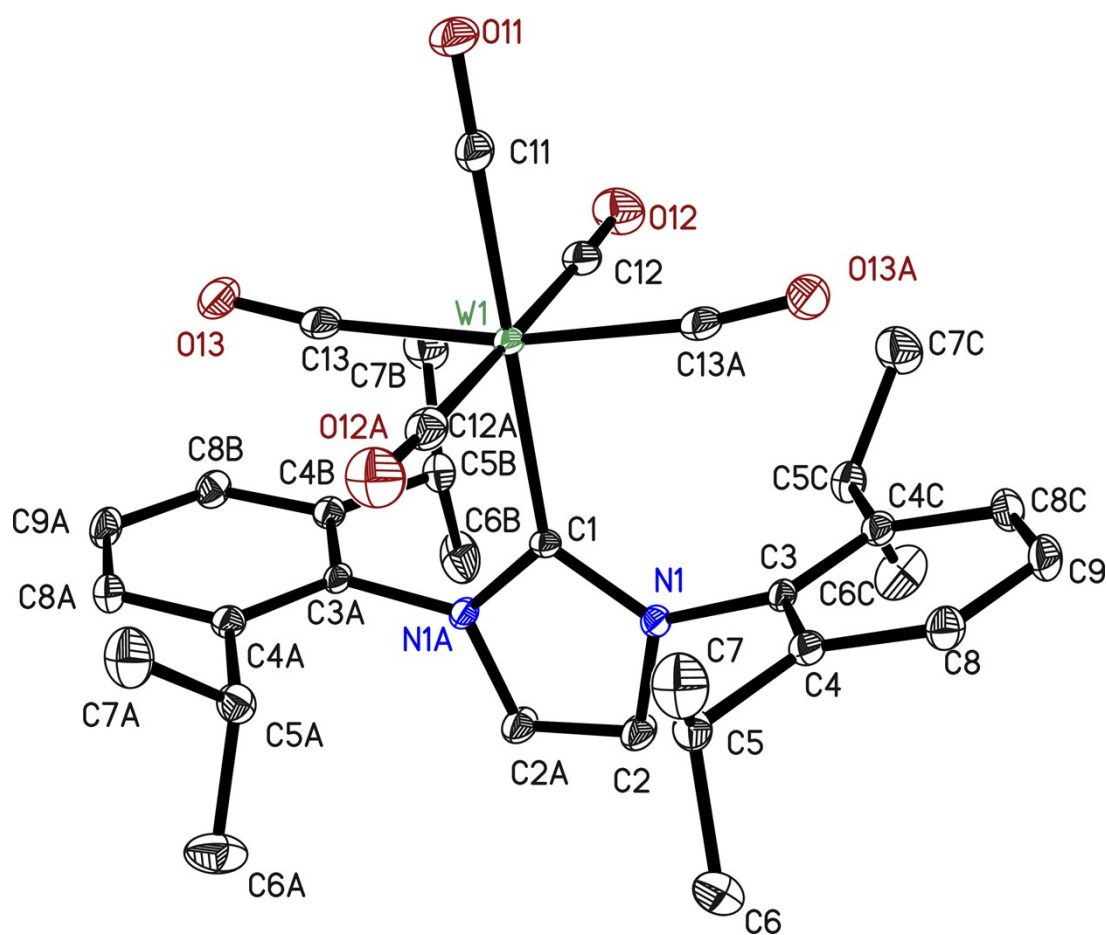


Figure S5: Molecular structure of compound **8-W**. Anisotropic displacement parameters are depicted at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected experimental and theoretical [BP86+D3(BJ)/def2-SVP] {M06/def2-SVP} bond lengths (Å) and bond angles (°): C1—W1, 2.260(2) [2.244]{2.294}; C2—C2A, 1.348(3) [1.367]{1.351}; W1—C11, 1.997(2) [2.034]{2.031}; W1—C13, 2.0560(18) [2.062]{2.074}; W1—C13A, 2.0560(18) [2.062]{2.074}; N1—C1, 1.3713(18) [1.379]{1.368}; N1A—C1, 1.3712(18) [1.379]{1.368}; C1—W1—C11, 180.0 [180.0]{179.4}; C13—W1—C13A, 169.46(9) [168.4]{168.7}; C12—W1—C12A, 178.85(9) [179.6]{177.6}; C11—W1—C12, 89.42(5) [84.2]{91.2}; N1A—C2A—C2A, 106.60(9) [106.5]{106.6}; N1—C1—N1A, 102.74(18) [102.8]{102.9}.

Table S6. Bond lengths [$\text{\AA}$] and angles [$^\circ$] of Compound **8-W**.

W(1)-C(11)	1.997(2)	C(12)-W(1)-C(13)	89.947(4)	O(12)-C(12)-W(1)	177.42(16)
W(1)-C(12)#1	2.049(2)	C(11)-W(1)-C(13)#2	84.73(4)	O(13)-C(13)-W(1)	171.34(14)
W(1)-C(12)	2.049(2)	C(12)#1-W(1)-C(13)#2	89.947(5)		
W(1)-C(13)	2.0560(18)	C(12)-W(1)-C(13)#2	89.947(4)		
W(1)-C(13)#2	2.0560(18)	C(13)-W(1)-C(13)#2	169.46(9)		
W(1)-C(1)	2.260(2)	C(11)-W(1)-C(1)	180.0		
N(1)-C(1)	1.3713(18)	C(12)#1-W(1)-C(1)	90.58(5)		
N(1)-C(2)	1.390(2)	C(12)-W(1)-C(1)	90.58(5)		
N(1)-C(3)	1.4462(19)	C(13)-W(1)-C(1)	95.27(4)		
C(1)-N(1)#2	1.3712(18)	C(13)#2-W(1)-C(1)	95.27(4)		
C(2)-C(2)#2	1.348(3)	C(1)-N(1)-C(2)	112.02(13)		
C(3)-C(4)#3	1.4026(14)	C(1)-N(1)-C(3)	126.96(13)		
C(3)-C(4)	1.4027(14)	C(2)-N(1)-C(3)	121.02(13)		
C(4)-C(8)	1.3992(16)	N(1)#2-C(1)-N(1)	102.74(18)		
C(4)-C(5)	1.5193(17)	N(1)#2-C(1)-W(1)	128.63(9)		
C(5)-C(7)	1.5330(19)	N(1)-C(1)-W(1)	128.63(9)		
C(5)-C(6)	1.5343(19)	C(2)#2-C(2)-N(1)	106.60(9)		
C(8)-C(9)	1.3878(15)	C(4)#3-C(3)-C(4)	123.14(14)		
C(9)-C(8)#3	1.3878(15)	C(4)#3-C(3)-N(1)	118.37(7)		
O(11)-C(11)	1.152(3)	C(4)-C(3)-N(1)	118.38(7)		
O(12)-C(12)	1.144(3)	C(8)-C(4)-C(3)	117.30(12)		
O(13)-C(13)	1.144(2)	C(8)-C(4)-C(5)	120.39(11)		
		C(3)-C(4)-C(5)	122.31(10)		
C(11)-W(1)-C(12)#1	89.42(5)	C(4)-C(5)-C(7)	112.46(10)		
C(11)-W(1)-C(12)	89.42(5)	C(4)-C(5)-C(6)	110.39(10)		
C(12)#1-W(1)-C(12)	178.85(9)	C(7)-C(5)-C(6)	110.01(12)		
C(11)-W(1)-C(13)	84.73(4)	C(9)-C(8)-C(4)	120.79(12)		
C(12)#1-W(1)-C(13)	89.947(4)	C(8)#3-C(9)-C(8)	120.67(15)		

Compound 10-W

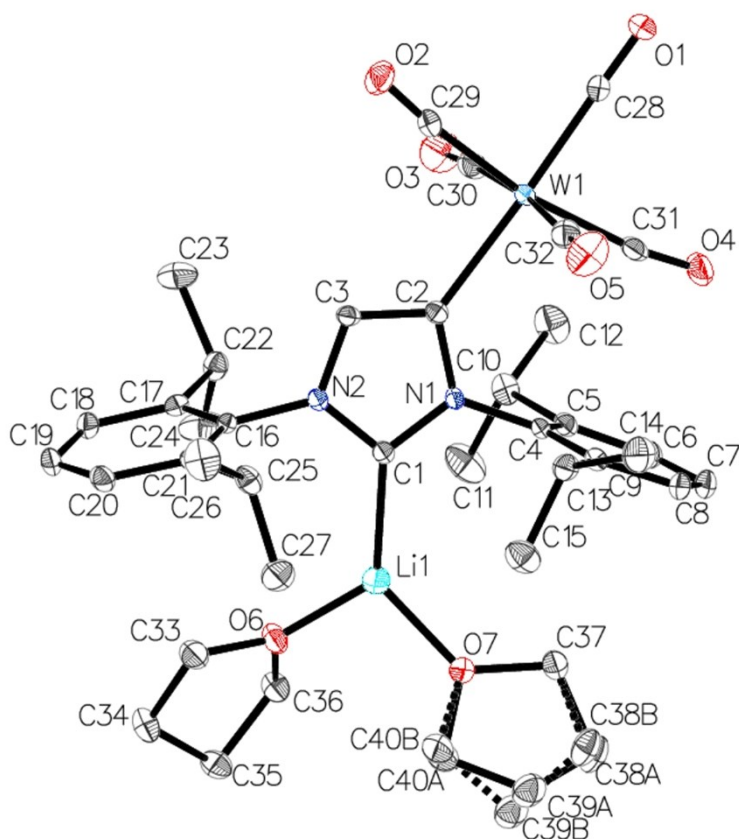
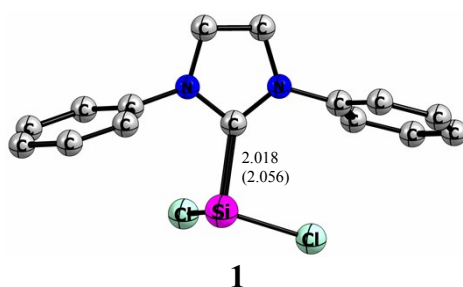


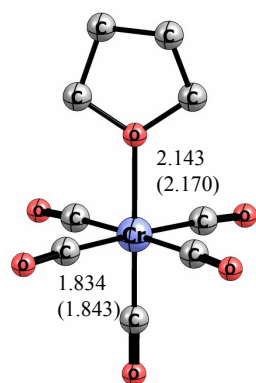
Figure S6: Molecular structure of compound **10-W**. Anisotropic displacement parameters are depicted at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected experimental and theoretical [BP86+D3(BJ)/def2-SVP] {M06/def2-SVP} bond lengths (Å) and bond angles (°): C2–W1, 2.2570(18) [2.259]{2.291}; C2–C3, 1.369(2) [1.384]{1.371}; C1–Li1, 2.106(4) [2.0455]{2.069}; N1–C1, 1.370(2) [1.378]{1.367}; N2–C1, 1.357(2) [1.368]{1.351}; N1–C2–C3, 101.60(15) [102.1]{101.9}; N1–C1–N2, 102.04(15) [102.1]{102.7}.

Computational Details

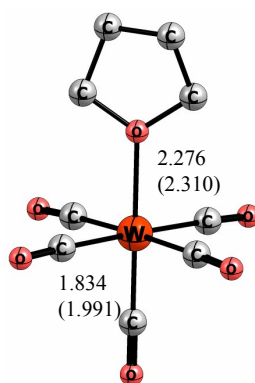
Geometry optimizations were performed using the Gaussian 09 optimizer¹⁰ together with TurboMole V7.0.¹¹ energies and gradients. All geometry optimizations were computed using the functional BP86¹² and M06¹³ functionals in combination with the def2-SVP basis set.¹⁴ In the case of BP86 the dispersion interactions were estimated using the D3 approximations of Grimme with Becke-Johnson (BJ) damping.¹⁵ The stationary points were located with the Berny algorithm¹⁶ using redundant internal coordinates. Analytical Hessians were computed to determine the nature of stationary points (one and zero imaginary frequencies for transition states and minima, respectively)¹⁷ and to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects using the standard statistical-mechanics relationships for an ideal gas.¹⁸ The energies were improved by single point calculations at the BP86+D3(BJ)/def2-TZVPP and M06def2-TZVPP level of theory. Unless otherwise stated, Gibbs energies have been computed at 298.15 K. For these calculations the tetrahydrofuran (THF) solvent was described with the Conductor-like Screening Model (COSMO) with a dielectricity constant $\epsilon = 7.426$.¹⁹

Figure S7. Optimized geometries of the calculated molecules at the BP86-D3(BJ)/def2-SVP level and at M06/def2-SVP (in parenthesis). Selected bond lengths are given in Å. Hydrogen atoms and isopropyl groups were omitted for clarity. Relative Gibbs energies at BP86-D3(BJ)/def2-TZVPP//BP86-D3(BJ)/def2-SVP and M06/def2-TZVPP//M06/def2-SVP (in parenthesis) in kcal/mol. The coordinates of all atoms are given in Table S9.

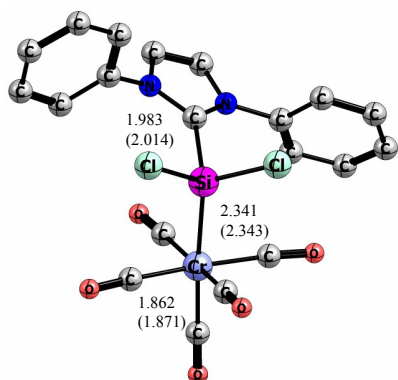




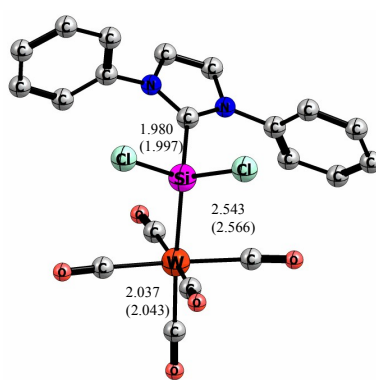
2-Cr



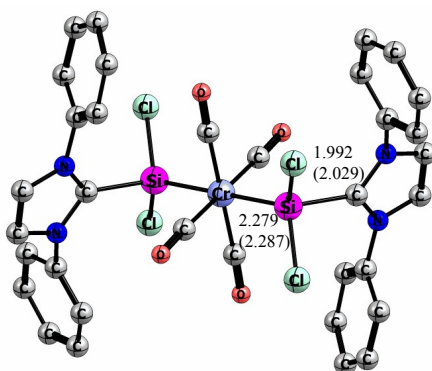
2-W



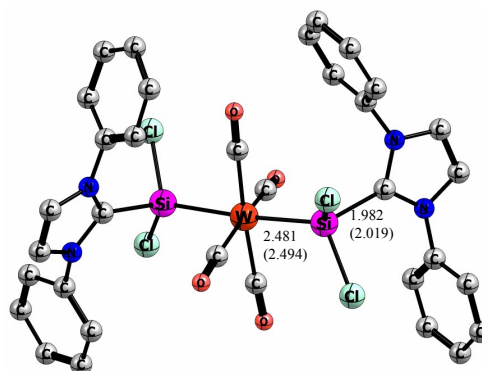
3-Cr



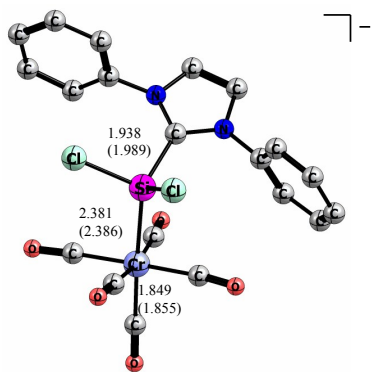
3-W



4-Cr

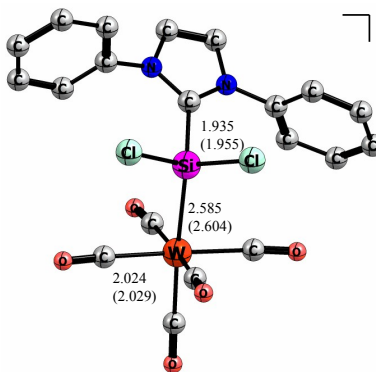


4-W



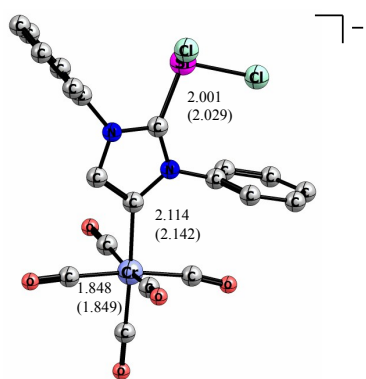
5a-Cr

$\Delta G_{\text{rel}} = 0.0$ kcal/mol



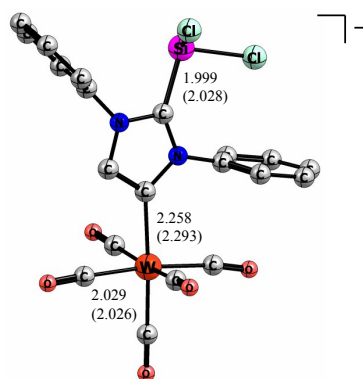
5a-W

$\Delta G_{\text{rel}} = 0.0$ kcal/mol



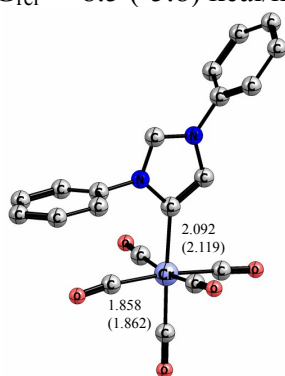
5b-Cr

$\Delta G_{\text{rel}} = -8.5$ (-5.8) kcal/mol



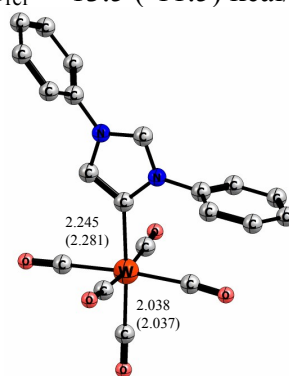
5b-W

$\Delta G_{\text{rel}} = -13.5$ (-11.5) kcal/mol



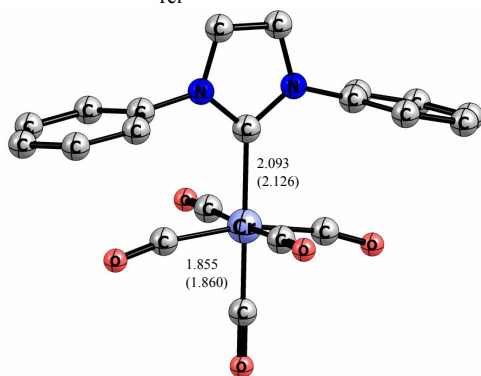
6-Cr

$\Delta G_{\text{rel}} = 0.0$ kcal/mol



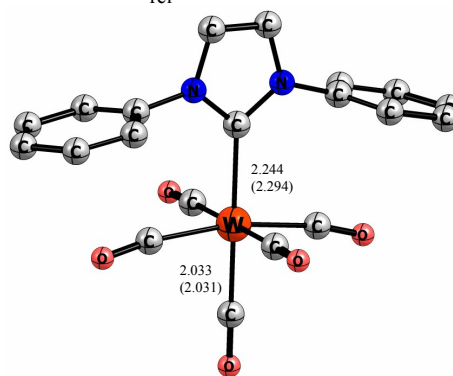
6-W

$\Delta G_{\text{rel}} = 0.0$ kcal/mol



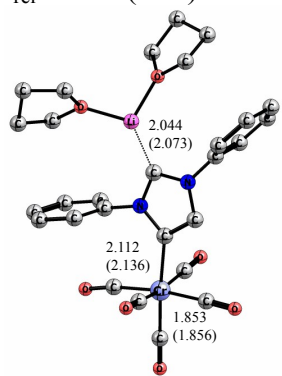
8-Cr

$\Delta G_{\text{rel}} = -9.9$ (-5.1) kcal/mol

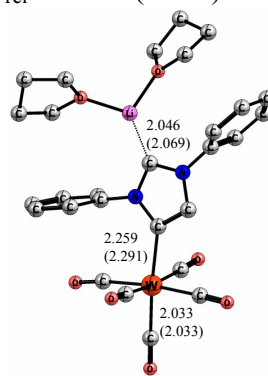


8-W

$\Delta\Delta G_{\text{rel}} = -12.1$ (-13.5) kcal/mol



10-Cr



10-W

Table S7. Bond dissociation energies (in kcal/mol) at the BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP and PCM(THF)- BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP (in parenthesis) level of theory.

	$D_e(\text{CO}_{\text{trans}})$	$D_e(\text{L-M}(\text{CO})_5 \rightarrow \text{L} + \text{M}(\text{CO})_5)$ (L = THF, NHC, aNHC)	$D_e(\text{L-SiCl}_2\text{-M}(\text{CO})_5 \rightarrow \text{L-SiCl}_2 + \text{M}(\text{CO})_5)$ (L = NHC, aNHC)
$\text{Cr}(\text{CO})_6$	44.8 (43.0)	---	
$\text{W}(\text{CO})_6$	47.0 (43.5)	---	
2-Cr	58.9 (58.7)	26.3 (25.2)	
2-W	69.2 (67.8)	30.5 (28.7)	
3-Cr	52.1 (51.5)		61.5 (58.2)
3-W	51.7 (50.6)		62.1 (57.2)
6-Cr		69.2 (65.2)	
6-W		74.7 (69.2)	
8-Cr		67.0 (65.0)	
8-W		74.4 (71.0)	

Table S8. Bond dissociation energies (in kcal/mol) at the M06/def2-TZVPP//M06/def2-SVP and PCM(THF)- M06/def2-TZVPP//M06/def2-SVP (in parenthesis) level of theory.

	$D_e(\text{CO}_{\text{trans}})$	$D_e(\text{L-M}(\text{CO})_5 \rightarrow \text{L} + \text{M}(\text{CO})_5)$ (L = THF, NHC, aNHC)	$D_e(\text{L-SiCl}_2\text{-M}(\text{CO})_5 \rightarrow \text{L-SiCl}_2 + \text{M}(\text{CO})_5)$ (L = NHC, aNHC)
$\text{Cr}(\text{CO})_6$	41.6 (33.2)	---	
$\text{W}(\text{CO})_6$	44.2 (31.4)	---	
2-Cr	54.4 (44.5)	25.8 (14.2)	
2-W	63.5 (58.9)	26.3 (19.5)	
3-Cr	45.6 (43.6)		47.2 (42.0)
3-W	45.7 (40.6)		48.1 (38.4)
6-Cr		55.0 (51.4)	
6-W		61.8 (50.0)	
8-Cr		50.5 (46.6)	
8-W		58.7 (50.4)	

Table S9. Cartesian coordinates at the BP86/def2-SVP and M06-2X/def2-SVP level of theory.
Energies at the different levels in Hartrees.

CO (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -113.2305809913

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -113.3658964973

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -113.3666362218

O 0.000000 0.000000 1.145590

C 0.000000 0.000000 0.003677

CO (M06/def2-SVP)

E (M06/def2-SVP) = -113.1642657

E (M06/def2-TZVPP//M06/def2-SVP) = -113.301306

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -113.3018683

O 0.000000000000 0.000000000000 0.484375000000

C 0.000000000000 0.000000000000 -0.645834000000

THF (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -232.2993959119

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) =

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -232.5680426544

C -0.013340 -0.000460 1.415750

O -0.022343 0.004247 -0.015127

C 1.426530 0.324445 1.837807

H 1.586346 1.423257 1.859419

C 1.319331 0.000503 -0.513721

C 2.225605 -0.307849 0.687151

H 3.248763 0.102390 0.575999

H -0.754809 0.739747 1.786764

H 1.564909 0.998612 -0.951999

H 1.404757 -0.751559 -1.327864

H 2.312768 -1.404836 0.836857

H 1.688398 -0.077330 2.836590

H -0.321797 -1.004774 1.796953

THF (M06/def2-SVP)

E (M06/def2-SVP) = -232.1131708

E (M06/def2-TZVPP//M06/def2-SVP) = -232.3775213

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -232.3801365

C -1.149890000000 -0.429512000000 0.138477000000

O 0.002267000000 -1.232467000000 -0.003894000000

C -0.725457000000 0.980133000000 -0.238311000000

H -0.766770000000 1.113977000000 -1.333910000000

C 1.152979000000 -0.424799000000 -0.133594000000

C 0.719901000000 0.984731000000 0.236045000000

H 1.342229000000 1.767011000000 -0.224748000000

H -1.958408000000 -0.828209000000 -0.498777000000

H 1.527293000000 -0.460854000000 -1.178268000000

H 1.956283000000 -0.818223000000 0.513725000000

H 0.760023000000 1.124846000000 1.330899000000

H -1.351480000000 1.761547000000 0.218950000000

H -1.512500000000 -0.463671000000 1.187580000000

NHC (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -1159.377119071

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1160.624268748

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1160.634510325

N	5.630891000000	13.196520000000	6.004489000000
C	5.622819000000	12.320301000000	4.940620000000
C	5.643710000000	14.541861000000	5.616503000000
H	5.658464000000	15.363358000000	6.339101000000
C	5.604440000000	12.787277000000	7.382889000000
C	6.804129000000	12.350850000000	7.990569000000
C	8.093628000000	12.212213000000	7.192611000000
H	7.984348000000	12.826583000000	6.275525000000
C	9.329771000000	12.722352000000	7.949707000000
H	10.221703000000	12.691931000000	7.291300000000
H	9.561418000000	12.097927000000	8.837348000000
H	9.194321000000	13.766701000000	8.296819000000
C	8.260473000000	10.747317000000	6.741736000000
H	7.389907000000	10.434947000000	6.131685000000
H	8.334654000000	10.072182000000	7.619820000000
H	9.179923000000	10.623486000000	6.133824000000
C	6.750114000000	11.980640000000	9.349299000000
H	7.665048000000	11.631400000000	9.850207000000
C	5.551553000000	12.052895000000	10.069249000000
H	5.531398000000	11.764997000000	11.131487000000
N	5.629863000000	13.188681000000	3.870357000000
C	5.640464000000	14.536870000000	4.248437000000
H	5.640003000000	15.353169000000	3.519821000000
C	5.649539000000	12.768877000000	2.495011000000
C	4.442412000000	12.349970000000	1.889745000000
C	3.150221000000	12.240985000000	2.687886000000
H	3.270044000000	12.860724000000	3.600020000000
C	1.923820000000	12.767012000000	1.925856000000
H	1.031192000000	12.758179000000	2.583958000000
H	1.681355000000	12.139489000000	1.043298000000
H	2.078244000000	13.805812000000	1.570130000000
C	2.956868000000	10.783009000000	3.150474000000
H	3.821400000000	10.459931000000	3.763525000000
H	2.870987000000	10.102284000000	2.277784000000
H	2.035026000000	10.680563000000	3.758778000000
C	4.490435000000	11.968633000000	0.533880000000
H	3.569556000000	11.632488000000	0.034911000000
C	5.690567000000	12.013443000000	-0.185700000000
H	5.706085000000	11.717150000000	-1.245705000000
C	6.880749000000	12.812130000000	1.793895000000
C	8.173758000000	13.169445000000	2.519095000000
H	7.921702000000	13.916676000000	3.300673000000
C	9.240723000000	13.797500000000	1.612271000000
H	10.104715000000	14.137359000000	2.218273000000
H	9.633539000000	13.071491000000	0.870564000000
H	8.846458000000	14.671924000000	1.055846000000
C	8.713278000000	11.919539000000	3.245027000000
H	7.946822000000	11.496363000000	3.923544000000
H	8.992625000000	11.134869000000	2.511658000000
H	9.613756000000	12.168850000000	3.843794000000
C	6.874834000000	12.429180000000	0.439834000000
H	7.812322000000	12.449259000000	-0.133793000000
C	4.374695000000	12.858248000000	8.084383000000

C	3.087940000000	13.233709000000	7.357209000000
H	3.352787000000	13.971951000000	6.571337000000
C	2.032098000000	13.885316000000	8.260398000000
H	1.174065000000	14.236544000000	7.652426000000
H	1.626842000000	13.170490000000	9.006288000000
H	2.441436000000	14.755991000000	8.811787000000
C	2.526633000000	11.989206000000	6.638499000000
H	3.285448000000	11.548705000000	5.962401000000
H	2.233738000000	11.213786000000	7.376401000000
H	1.630581000000	12.250746000000	6.038312000000
C	4.374624000000	12.485507000000	9.441289000000
H	3.438106000000	12.527097000000	10.015326000000

NHC (M06/def2-SVP)

E (M06/def2-SVP) = 158.2958443

E (M06/def2-TZVPP//M06/def2-SVP) = -1159.5588299

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -1159.5650638

N	1.065070000000	0.004126000000	0.573151000000
C	0.001948000000	-0.029155000000	-0.284696000000
C	0.684924000000	-0.031624000000	1.911796000000
H	1.410043000000	-0.005790000000	2.723925000000
C	2.431932000000	0.113866000000	0.165200000000
C	2.925305000000	1.370552000000	-0.221574000000
C	2.030805000000	2.587753000000	-0.311930000000
H	1.135860000000	2.395303000000	0.309468000000
C	2.689427000000	3.857247000000	0.210561000000
H	1.958928000000	4.682619000000	0.234963000000
H	3.519925000000	4.187117000000	-0.437212000000
H	3.090183000000	3.726903000000	1.229000000000
C	1.564446000000	2.766347000000	-1.755053000000
H	1.022329000000	1.871426000000	-2.102004000000
H	2.429555000000	2.925887000000	-2.422747000000
H	0.897110000000	3.639328000000	-1.851741000000
C	4.271098000000	1.453917000000	-0.592795000000
H	4.683509000000	2.417916000000	-0.907033000000
C	5.090646000000	0.333318000000	-0.567903000000
H	6.142180000000	0.419641000000	-0.857334000000
N	-1.054033000000	-0.095429000000	0.578051000000
C	-0.666400000000	-0.103670000000	1.915089000000
H	-1.387042000000	-0.152845000000	2.730073000000
C	-2.425921000000	-0.133864000000	0.175114000000
C	-2.990460000000	-1.361028000000	-0.208596000000
C	-2.161106000000	-2.623564000000	-0.301119000000
H	-1.264327000000	-2.487216000000	0.332218000000
C	-2.893269000000	-3.861292000000	0.199039000000
H	-2.206729000000	-4.722979000000	0.232972000000
H	-3.725839000000	-4.146156000000	-0.467147000000
H	-3.307649000000	-3.716559000000	1.210119000000
C	-1.683281000000	-2.809887000000	-1.739548000000
H	-1.072262000000	-1.950087000000	-2.061272000000
H	-2.545944000000	-2.894268000000	-2.423923000000
H	-1.081229000000	-3.728629000000	-1.842114000000
C	-4.338986000000	-1.367602000000	-0.578281000000
H	-4.806069000000	-2.306952000000	-0.890549000000
C	-5.093149000000	-0.201040000000	-0.557699000000
H	-6.147683000000	-0.228121000000	-0.847800000000
C	-3.165951000000	1.061530000000	0.198316000000
C	-2.504707000000	2.385955000000	0.517685000000
H	-1.636516000000	2.181821000000	1.170865000000

C	-3.411708000000	3.361658000000	1.253252000000
H	-2.837227000000	4.244695000000	1.577154000000
H	-4.225748000000	3.735343000000	0.608601000000
H	-3.871395000000	2.908553000000	2.146746000000
C	-1.967532000000	3.005689000000	-0.770637000000
H	-1.261923000000	2.326507000000	-1.277752000000
H	-2.795822000000	3.217912000000	-1.469494000000
H	-1.446915000000	3.957015000000	-0.563036000000
C	-4.510765000000	1.002317000000	-0.174198000000
H	-5.113149000000	1.915604000000	-0.173335000000
C	3.239940000000	-1.037781000000	0.192236000000
C	2.649165000000	-2.394473000000	0.515986000000
H	1.843029000000	-2.244564000000	1.257894000000
C	3.647604000000	-3.370831000000	1.118502000000
H	3.131943000000	-4.286799000000	1.449169000000
H	4.409427000000	-3.683639000000	0.383856000000
H	4.173480000000	-2.943597000000	1.987956000000
C	2.009551000000	-2.980630000000	-0.741823000000
H	1.242548000000	-2.305833000000	-1.157763000000
H	2.776645000000	-3.138887000000	-1.520356000000
H	1.537043000000	-3.954743000000	-0.527858000000
C	4.579243000000	-0.900600000000	-0.178804000000
H	5.235672000000	-1.775451000000	-0.171640000000

aNHC (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -1159.352295780

E (BP86+D3(BJ)/def2-TZVPP/BP86+D3(BJ)/def2-SVP) = -1160.600082063

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP/BP86+D3(BJ)/def2-SVP) = -1160.616259645

N	0.612643000000	0.036882000000	4.506681000000
C	-0.731147000000	-0.021077000000	4.547347000000
H	-1.333585000000	-0.152488000000	5.451986000000
N	-1.165489000000	0.114344000000	3.266959000000
C	0.995043000000	0.216820000000	3.159022000000
H	2.065176000000	0.282606000000	2.931182000000
C	-0.120929000000	0.273156000000	2.325318000000
C	1.481654000000	-0.126245000000	5.637332000000
C	1.915235000000	-1.434430000000	5.964169000000
C	2.781771000000	-1.572472000000	7.064704000000
H	3.134326000000	-2.573800000000	7.353277000000
C	3.202501000000	-0.452014000000	7.795501000000
H	3.881336000000	-0.581081000000	8.652105000000
C	2.767012000000	0.831964000000	7.438778000000
H	3.107456000000	1.702444000000	8.019130000000
C	1.899529000000	1.024596000000	6.346680000000
C	1.417126000000	-2.645674000000	5.184146000000
H	1.004554000000	-2.274315000000	4.223530000000
C	0.269745000000	-3.339485000000	5.945172000000
H	-0.145698000000	-4.179181000000	5.351591000000
H	-0.557036000000	-2.634127000000	6.161567000000
H	0.624046000000	-3.746557000000	6.915043000000
C	2.542210000000	-3.635600000000	4.842186000000
H	2.965365000000	-4.114162000000	5.749607000000
H	3.370761000000	-3.133762000000	4.304221000000
H	2.154987000000	-4.447511000000	4.194085000000
C	1.381333000000	2.408421000000	5.975369000000
H	0.949152000000	2.337150000000	4.956106000000
C	2.496358000000	3.465430000000	5.926681000000
H	3.314198000000	3.157743000000	5.245173000000
H	2.938496000000	3.649011000000	6.927809000000

H	2.093598000000	4.432742000000	5.564234000000
C	0.247344000000	2.827463000000	6.931876000000
H	-0.572992000000	2.082254000000	6.935937000000
H	-0.182134000000	3.804526000000	6.630802000000
H	0.619599000000	2.920911000000	7.973402000000
C	-2.562466000000	0.056234000000	2.923689000000
C	-3.210510000000	-1.202756000000	2.948447000000
C	-4.584840000000	-1.229847000000	2.641493000000
H	-5.124417000000	-2.187286000000	2.652146000000
C	-5.270569000000	-0.054162000000	2.307580000000
H	-6.344815000000	-0.096158000000	2.071092000000
C	-4.593147000000	1.172088000000	2.255941000000
H	-5.140266000000	2.081536000000	1.970658000000
C	-3.221149000000	1.254853000000	2.560582000000
C	-2.449700000000	2.568790000000	2.510124000000
H	-1.444561000000	2.307343000000	2.111261000000
C	-3.071811000000	3.606450000000	1.567134000000
H	-3.235086000000	3.189139000000	0.553474000000
H	-2.398823000000	4.482052000000	1.469500000000
H	-4.045336000000	3.985796000000	1.943583000000
C	-2.262269000000	3.155194000000	3.924147000000
H	-1.651148000000	4.080514000000	3.886776000000
H	-1.749920000000	2.443016000000	4.599837000000
H	-3.241584000000	3.409493000000	4.381309000000
C	-2.415072000000	-2.482077000000	3.192532000000
H	-1.641177000000	-2.256222000000	3.955386000000
C	-1.668912000000	-2.877570000000	1.900006000000
H	-1.035703000000	-2.043044000000	1.535130000000
H	-2.393727000000	-3.136179000000	1.100317000000
H	-1.021040000000	-3.761247000000	2.077143000000
C	-3.255580000000	-3.643790000000	3.737131000000
H	-3.984260000000	-4.014764000000	2.986953000000
H	-3.820211000000	-3.355598000000	4.647099000000
H	-2.599539000000	-4.498716000000	3.997978000000

aNHC (M06/def2-SVP)

E (M06/def2-SVP) = -1158.2670942

E (M06/def2-TZVPP//M06/def2-SVP) = -1159.5308386

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -1159.5425778

N	-1.059504000000	0.140006000000	0.539894000000
C	0.018456000000	0.063984000000	-0.234731000000
H	0.011823000000	-0.011555000000	-1.324092000000
N	1.093301000000	0.087377000000	0.571886000000
C	-0.615595000000	0.217183000000	1.867868000000
H	-1.370917000000	0.283710000000	2.653590000000
C	0.764367000000	0.183774000000	1.938236000000
C	-2.411114000000	0.069087000000	0.085241000000
C	-3.009697000000	-1.199259000000	-0.018116000000
C	-4.330548000000	-1.251216000000	-0.468838000000
H	-4.826438000000	-2.221473000000	-0.572572000000
C	-5.023245000000	-0.088006000000	-0.788396000000
H	-6.056743000000	-0.150137000000	-1.141399000000
C	-4.411201000000	1.153372000000	-0.657187000000
H	-4.970758000000	2.059847000000	-0.910477000000
C	-3.091624000000	1.261301000000	-0.209514000000
C	-2.242611000000	-2.467119000000	0.296464000000
H	-1.353531000000	-2.187046000000	0.891785000000
C	-1.748160000000	-3.127042000000	-0.988369000000
H	-1.147713000000	-4.024284000000	-0.760852000000

H	-1.120940000000	-2.444449000000	-1.586560000000
H	-2.595945000000	-3.438740000000	-1.623410000000
C	-3.053154000000	-3.449841000000	1.131293000000
H	-3.912194000000	-3.855670000000	0.569817000000
H	-3.441561000000	-2.981311000000	2.049530000000
H	-2.427570000000	-4.307462000000	1.427465000000
C	-2.421424000000	2.613698000000	-0.089759000000
H	-1.472948000000	2.473633000000	0.460546000000
C	-3.262529000000	3.604776000000	0.705179000000
H	-3.544047000000	3.199488000000	1.690194000000
H	-4.190861000000	3.876165000000	0.173819000000
H	-2.701824000000	4.538885000000	0.871056000000
C	-2.079124000000	3.167401000000	-1.470059000000
H	-1.414960000000	2.487559000000	-2.030015000000
H	-1.571670000000	4.143042000000	-1.388153000000
H	-2.990247000000	3.314200000000	-2.076098000000
C	2.428056000000	-0.024257000000	0.063723000000
C	2.889581000000	-1.290423000000	-0.336761000000
C	4.183559000000	-1.368739000000	-0.859529000000
H	4.578173000000	-2.334751000000	-1.186863000000
C	4.982688000000	-0.235524000000	-0.961282000000
H	5.992948000000	-0.318313000000	-1.373200000000
C	4.510181000000	0.999359000000	-0.531157000000
H	5.157468000000	1.878440000000	-0.601841000000
C	3.222231000000	1.132226000000	-0.006329000000
C	2.678636000000	2.472546000000	0.441349000000
H	2.006586000000	2.268744000000	1.295351000000
C	3.757229000000	3.431220000000	0.920077000000
H	4.406253000000	2.970778000000	1.681758000000
H	3.298170000000	4.328412000000	1.365607000000
H	4.398932000000	3.778900000000	0.091335000000
C	1.857462000000	3.119339000000	-0.673167000000
H	1.429841000000	4.080257000000	-0.339638000000
H	1.021901000000	2.480731000000	-1.005410000000
H	2.491347000000	3.320685000000	-1.555345000000
C	2.048340000000	-2.533224000000	-0.123730000000
H	0.989797000000	-2.258405000000	-0.291845000000
C	2.168042000000	-2.997413000000	1.327753000000
H	1.892196000000	-2.196151000000	2.033708000000
H	3.207601000000	-3.300230000000	1.545405000000
H	1.514492000000	-3.867433000000	1.514387000000
C	2.375093000000	-3.666092000000	-1.083838000000
H	3.373272000000	-4.094673000000	-0.888193000000
H	2.349054000000	-3.341450000000	-2.137281000000
H	1.651072000000	-4.488281000000	-0.963093000000

1 (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -2369.185934937

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2370.847273602

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2370.863298205

N	5.452099	12.918347	6.019231
C	5.492435	12.103263	4.919260
C	5.432454	14.257919	5.652016
H	5.412064	15.058738	6.395004
C	5.549441	12.441373	7.378838
C	6.836970	12.100370	7.861671
C	8.085294	12.239902	6.997997
H	7.761826	12.270201	5.938062
C	8.801539	13.571049	7.298684

H	9.682558	13.700210	6.637085
H	9.155018	13.603333	8.350081
H	8.128219	14.438457	7.144614
C	9.027904	11.034528	7.128016
H	8.481736	10.095041	6.910406
H	9.475213	10.960320	8.140593
H	9.863527	11.124276	6.405068
C	6.924495	11.659082	9.194089
H	7.905004	11.381240	9.606550
C	5.779694	11.558932	9.996310
H	5.869851	11.206701	11.035038
N	5.502634	12.958618	3.856105
C	5.458047	14.284681	4.281699
H	5.458046	15.112197	3.567322
C	5.614662	12.599767	2.462213
C	4.453452	12.189124	1.773429
C	3.111673	12.071712	2.482550
H	3.314857	11.929944	3.562704
C	2.296680	13.369246	2.319702
H	1.337014	13.300894	2.871880
H	2.064661	13.562339	1.251424
H	2.849388	14.249700	2.706719
C	2.320102	10.832273	2.041556
H	2.941593	9.922376	2.147160
H	1.968625	10.907906	0.991288
H	1.426216	10.708944	2.684627
C	4.599378	11.882765	0.408529
H	3.722050	11.552182	-0.165261
C	5.848859	11.966727	-0.220418
H	5.941242	11.712789	-1.287297
C	6.893930	12.679199	1.868464
C	8.138186	13.001255	2.689791
H	7.809861	13.508951	3.620488
C	9.099297	13.960904	1.970842
H	9.939513	14.237224	2.639573
H	9.543267	13.497952	1.065871
H	8.587165	14.892792	1.656779
C	8.847574	11.698542	3.111623
H	8.157035	11.010065	3.635799
H	9.228769	11.154218	2.223273
H	9.706852	11.918060	3.777920
C	6.985333	12.352336	0.502720
H	7.963541	12.388468	0.001609
C	4.372672	12.340774	8.155604
C	3.009068	12.730653	7.599945
H	3.074223	12.654203	6.495253
C	2.668945	14.188578	7.970659
H	1.693724	14.486146	7.533985
H	2.601384	14.308999	9.071850
H	3.434336	14.901995	7.606080
C	1.892203	11.775783	8.049028
H	2.156502	10.727489	7.813900
H	1.686470	11.859957	9.136243
H	0.950017	12.019201	7.518129
C	4.520511	11.893858	9.482763
H	3.630030	11.797571	10.119911
Si	5.665462	10.113303	5.207910
Cl	5.797201	9.510702	3.109968
Cl	3.471591	9.960494	5.484005

1 (M06/def2-SVP)

E (M06/def2-SVP) = -2367.9095146

E (M06/def2-TZVPP/M06/def2-SVP) = -2369.5727004

E (PCM(THF)-M06/def2-TZVPP/M06/def2-SVP) = -2369.5845676

N	-1.162943000000	0.119219000000	-0.820819000000
C	-0.059568000000	-0.000649000000	-0.041881000000
C	-0.819598000000	0.165192000000	-2.158634000000
H	-1.572711000000	0.265870000000	-2.937581000000
C	-2.508609000000	0.273254000000	-0.333953000000
C	-2.899976000000	1.544252000000	0.127651000000
C	-1.956685000000	2.729370000000	0.124444000000
H	-0.922536000000	2.340535000000	0.142698000000
C	-2.117365000000	3.539603000000	-1.159464000000
H	-1.400647000000	4.378214000000	-1.187959000000
H	-3.135025000000	3.962541000000	-1.228962000000
H	-1.951946000000	2.923884000000	-2.059503000000
C	-2.110932000000	3.610137000000	1.356179000000
H	-2.038324000000	3.014560000000	2.280642000000
H	-3.074922000000	4.147179000000	1.363481000000
H	-1.318486000000	4.375612000000	1.379659000000
C	-4.216821000000	1.686811000000	0.565229000000
H	-4.559547000000	2.658476000000	0.932539000000
C	-5.097804000000	0.610575000000	0.547683000000
H	-6.125266000000	0.743707000000	0.898414000000
N	0.978989000000	-0.016697000000	-0.906109000000
C	0.532409000000	0.076375000000	-2.213599000000
H	1.228840000000	0.087497000000	-3.050149000000
C	2.381165000000	0.022952000000	-0.583738000000
C	3.074479000000	-1.180993000000	-0.406838000000
C	2.391042000000	-2.527180000000	-0.498592000000
H	1.299330000000	-2.358116000000	-0.484996000000
C	2.746133000000	-3.218558000000	-1.811377000000
H	2.226280000000	-4.186922000000	-1.898733000000
H	3.831089000000	-3.414426000000	-1.873124000000
H	2.471503000000	-2.604927000000	-2.686081000000
C	2.705579000000	-3.410865000000	0.701759000000
H	2.494293000000	-2.883001000000	1.645192000000
H	3.760981000000	-3.734486000000	0.709257000000
H	2.082710000000	-4.319836000000	0.677980000000
C	4.441368000000	-1.091768000000	-0.135293000000
H	5.020112000000	-2.009027000000	0.011187000000
C	5.071961000000	0.142449000000	-0.030805000000
H	6.141738000000	0.188875000000	0.192571000000
C	2.984473000000	1.286012000000	-0.486834000000
C	2.200269000000	2.576478000000	-0.617298000000
H	1.168577000000	2.327782000000	-0.929233000000
C	2.777645000000	3.491385000000	-1.690324000000
H	2.151940000000	4.391386000000	-1.809837000000
H	3.794243000000	3.833015000000	-1.431205000000
H	2.836188000000	2.985032000000	-2.668320000000
C	2.094929000000	3.285959000000	0.730183000000
H	1.677940000000	2.619013000000	1.502939000000
H	3.084831000000	3.620088000000	1.086182000000
H	1.454016000000	4.180843000000	0.650848000000
C	4.351099000000	1.318622000000	-0.202566000000
H	4.859351000000	2.283510000000	-0.105585000000
C	-3.370620000000	-0.834602000000	-0.355565000000
C	-2.947247000000	-2.186200000000	-0.890552000000
H	-1.842336000000	-2.220324000000	-0.882851000000

C	-3.430449000000	-2.360798000000	-2.328955000000
H	-3.105255000000	-3.332362000000	-2.736184000000
H	-4.533087000000	-2.329847000000	-2.373932000000
H	-3.054573000000	-1.571362000000	-3.000346000000
C	-3.435157000000	-3.338761000000	-0.022350000000
H	-3.140883000000	-3.197817000000	1.028636000000
H	-4.531426000000	-3.456363000000	-0.070611000000
H	-2.994884000000	-4.286864000000	-0.371629000000
C	-4.678648000000	-0.633016000000	0.094384000000
H	-5.379983000000	-1.472678000000	0.091724000000
Si	-0.310118000000	-0.107850000000	1.996027000000
Cl	1.795255000000	-0.108944000000	2.532616000000
Cl	-0.612387000000	-2.280069000000	1.800539000000

2-Cr (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -1843.265670028

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1844.330852747

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1844.339706106

Cr	5.642492	9.695084	4.920484
C	5.188000	12.652034	6.031776
O	5.683066	11.838039	4.943548
C	5.142332	14.071455	5.467958
H	4.182453	14.246509	4.939605
O	5.584972	6.694442	4.889202
C	5.607294	7.861699	4.901276
O	2.700458	9.631480	5.735503
C	3.820396	9.692640	5.428761
O	4.797477	9.619718	1.986898
C	5.122027	9.688523	3.101162
C	6.212460	12.655846	3.874404
C	6.312387	14.059773	4.469299
H	6.240342	14.851700	3.699200
O	8.579875	9.536195	4.101956
C	7.463132	9.633611	4.411013
O	6.484244	9.525990	7.851104
C	6.162224	9.630252	6.738856
H	4.199035	12.257635	6.337963
H	5.512649	12.608460	3.010773
H	7.186050	12.230001	3.561094
H	7.277988	14.186139	5.001079
H	5.244613	14.842961	6.255198
H	5.886737	12.558517	6.892534

2-Cr (M06/def2-SVP)

E (M06/def2-SVP) = -1842.4290343

E (M06/def2-TZVPP//M06/def2-SVP) = -1843.5042222

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -1843.4973248

Cr	0.739872000000	0.000034000000	-0.000017000000
C	-2.237581000000	-1.171348000000	0.135943000000
O	-1.430331000000	-0.000050000000	-0.000903000000
C	-3.636858000000	-0.724216000000	-0.234017000000
H	-3.777332000000	-0.774159000000	-1.327402000000
O	3.736112000000	0.000307000000	0.000225000000
C	2.582810000000	0.000243000000	0.000173000000
O	0.812047000000	-2.348774000000	-1.948184000000
C	0.760200000000	-1.466122000000	-1.216142000000
O	0.765561000000	1.939387000000	-2.358739000000
C	0.736314000000	1.211505000000	-1.472082000000

C	-2.237681000000	1.171444000000	-0.135815000000
C	-3.636831000000	0.724030000000	0.234434000000
H	-4.418208000000	1.341234000000	-0.232434000000
O	0.811708000000	2.348552000000	1.948479000000
C	0.759937000000	1.466048000000	1.216243000000
O	0.765819000000	-1.939588000000	2.358400000000
C	0.736378000000	-1.211525000000	1.471882000000
H	-1.832300000000	-1.959041000000	-0.520280000000
H	-2.174876000000	1.531646000000	-1.181089000000
H	-1.832148000000	1.958433000000	0.521110000000
H	-3.777079000000	0.773872000000	1.327852000000
H	-4.418050000000	-1.341452000000	0.233117000000
H	-2.174392000000	-1.530374000000	1.181618000000

2-Cr-CO (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -1729.930036878

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1730.866582986

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1730.875048534

Cr	5.631285	9.741984	4.920029
C	5.105720	12.647777	5.997626
O	5.755729	11.840866	4.985216
C	5.027439	14.055525	5.399363
H	4.068001	14.191958	4.859417
O	2.689122	9.662873	5.710378
C	3.818316	9.723060	5.416898
O	4.740848	9.666028	2.006478
C	5.089852	9.725662	3.119423
C	6.156702	12.644508	3.855579
C	6.202626	14.066861	4.405790
H	6.097951	14.832724	3.613201
O	8.550528	9.529600	4.053580
C	7.436918	9.629417	4.387201
O	6.461371	9.536050	7.850933
C	6.145821	9.634766	6.732184
H	4.113824	12.206118	6.219441
H	5.408453	12.530742	3.038843
H	7.131025	12.259165	3.497601
H	7.162411	14.245243	4.933219
H	5.097206	14.846215	6.171042
H	5.725293	12.600868	6.918915

2-Cr-CO (M06/def2-SVP)

E (M06/def2-SVP) = -1729.1734629

E (M06/def2-TZVPP//M06/def2-SVP) = -1730.1115698

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -1730.1199385

Cr	-1.109974000000	0.000158000000	0.000157000000
C	1.851446000000	-1.170044000000	-0.142070000000
O	1.047520000000	-0.000255000000	0.001234000000
C	3.251838000000	-0.726030000000	0.229459000000
H	3.392715000000	-0.781644000000	1.322617000000
O	-1.241000000000	-2.460044000000	1.799519000000
C	-1.175634000000	-1.532197000000	1.120731000000
O	-1.072115000000	1.786600000000	2.473058000000
C	-1.097548000000	1.114187000000	1.539082000000
C	1.851762000000	1.169717000000	0.141727000000
C	3.251818000000	0.725169000000	-0.230624000000
H	4.033507000000	1.339814000000	0.239405000000
O	-1.240680000000	2.459818000000	-1.799840000000

C	-1.175296000000	1.532199000000	-1.120718000000
O	-1.073770000000	-1.785943000000	-2.472876000000
C	-1.098235000000	-1.113538000000	-1.538840000000
H	1.445547000000	-1.960558000000	0.510565000000
H	1.788879000000	1.526794000000	1.188372000000
H	1.445411000000	1.959350000000	-0.511708000000
H	3.392052000000	0.780624000000	-1.323873000000
H	4.033061000000	-1.340807000000	-0.241170000000
H	1.787657000000	-1.525557000000	-1.189219000000

2-W (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -865.9862723639

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -866.9231868046

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -866.9330734577

W	5.641681	9.634622	4.920150
C	5.155836	12.728331	6.021035
O	5.686783	11.910395	4.945682
C	5.128678	14.145240	5.451335
H	4.184416	14.320214	4.895959
O	5.579768	6.476027	4.885910
C	5.602710	7.644540	4.898429
O	2.553546	9.561764	5.857117
C	3.665997	9.620416	5.519138
O	4.709052	9.600016	1.829489
C	5.044980	9.640409	2.943051
C	6.248125	12.730309	3.887419
C	6.327829	14.132997	4.486573
H	6.276079	14.924265	3.714353
O	8.724540	9.462427	3.979071
C	7.615297	9.556480	4.319579
O	6.572609	9.495677	8.008404
C	6.238066	9.573497	6.896422
H	4.159861	12.327300	6.292975
H	5.570056	12.676147	3.008017
H	7.228556	12.298224	3.606680
H	7.277738	14.261072	5.045109
H	5.209503	14.917761	6.239891
H	5.831008	12.630592	6.898868

2-W (M06/def2-SVP)

E (M06/def2-SVP) = -865.2563948

E (M06/def2-TZVPP//M06/def2-SVP) = -866.1952447

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -866.2032004

W	0.544184000000	-0.000057000000	0.000218000000
C	-2.575793000000	-1.181568000000	0.168816000000
O	-1.765044000000	-0.003471000000	0.071553000000
C	-3.962910000000	-0.728500000000	-0.236344000000
H	-4.072374000000	-0.766609000000	-1.333585000000
O	3.686651000000	0.011804000000	-0.107393000000
C	2.531614000000	0.007432000000	-0.066684000000
O	0.618822000000	-2.560881000000	-1.956295000000
C	0.562371000000	-1.647839000000	-1.260679000000
O	0.526620000000	1.962363000000	-2.558697000000
C	0.510204000000	1.262566000000	-1.647643000000
C	-2.572350000000	1.170942000000	-0.080242000000
C	-3.978644000000	0.715115000000	0.247955000000
H	-4.748061000000	1.335051000000	-0.234609000000
O	0.725178000000	2.565265000000	1.945966000000

C	0.630717000000	1.650111000000	1.257773000000
O	0.723730000000	-1.957926000000	2.558121000000
C	0.633118000000	-1.261959000000	1.648958000000
H	-2.143946000000	-1.956130000000	-0.485638000000
H	-2.477015000000	1.532201000000	-1.122100000000
H	-2.179923000000	1.951652000000	0.591547000000
H	-4.149064000000	0.754148000000	1.337358000000
H	-4.756518000000	-1.351009000000	0.201684000000
H	-2.540327000000	-1.550107000000	1.211673000000

2-W-CO (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -752.6394012929

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -753.4434703714

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -753.4547912391

W	5.624331	9.727752	4.914347
C	5.068324	12.705669	5.984646
O	5.732348	11.895650	4.972337
C	4.987106	14.103766	5.370507
H	4.034788	14.225175	4.815159
O	2.536859	9.582882	5.803776
C	3.659828	9.676595	5.485984
O	4.675008	9.673237	1.841041
C	5.024209	9.721314	2.957052
C	6.162379	12.701294	3.844095
C	6.179442	14.121959	4.396215
H	6.078291	14.883657	3.599432
O	8.686298	9.443621	3.967303
C	7.578076	9.581757	4.315677
O	6.531808	9.522878	7.995784
C	6.205235	9.619078	6.876947
H	4.082843	12.246074	6.195073
H	5.433097	12.566558	3.015337
H	7.147826	12.314280	3.521777
H	7.128251	14.313821	4.937984
H	5.037812	14.901009	6.136663
H	5.688870	12.660401	6.904093

2-W-CO (M06/def2-SVP)

E (M06/def2-SVP) = -751.9854192

E (M06/def2-TZVPP//M06/def2-SVP) = -752.7895675

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -752.8042998

W	-0.790908000000	-0.000167000000	-0.000354000000
C	2.233118000000	-1.178534000000	-0.126879000000
O	1.428016000000	0.000390000000	0.001753000000
C	3.629624000000	-0.722602000000	0.239435000000
H	3.771168000000	-0.767642000000	1.332665000000
O	-0.940717000000	-2.570486000000	1.918838000000
C	-0.864990000000	-1.645944000000	1.231575000000
O	-0.792098000000	1.918586000000	2.576108000000
C	-0.794748000000	1.229016000000	1.650650000000
C	2.232597000000	1.179889000000	0.128671000000
C	3.629493000000	0.724235000000	-0.236697000000
H	4.410888000000	1.342114000000	0.229116000000
O	-0.939985000000	2.569778000000	-1.920081000000
C	-0.864419000000	1.645413000000	-1.232555000000
O	-0.786303000000	-1.919173000000	-2.576514000000
C	-0.791189000000	-1.229310000000	-1.651259000000
H	1.818253000000	-1.952600000000	0.538597000000

H	2.158324000000	1.543658000000	1.171054000000
H	1.817633000000	1.952838000000	-0.538073000000
H	3.771741000000	0.769219000000	-1.329837000000
H	4.411494000000	-1.340184000000	-0.225976000000
H	2.159503000000	-1.540808000000	-1.169852000000

3-Cr (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -3980.210792437

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3982.672127634

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3982.689286414

N	5.925240	12.504739	5.943339
C	5.780278	11.732393	4.815589
C	6.168869	13.828736	5.601137
H	6.302269	14.596661	6.366202
C	5.692570	12.116738	7.322121
C	6.786505	12.083500	8.218536
C	8.198160	12.494549	7.820832
H	8.249850	12.535918	6.716886
C	8.499490	13.910379	8.357698
H	9.498218	14.251211	8.017075
H	8.494223	13.922710	9.467111
H	7.750965	14.656402	8.021683
C	9.278281	11.506649	8.291890
H	9.086594	10.483276	7.921701
H	9.343225	11.465026	9.398110
H	10.269464	11.822536	7.911182
C	6.511889	11.735211	9.554949
H	7.341854	11.676654	10.273173
C	5.210576	11.449369	9.973920
H	5.021961	11.154749	11.017005
N	5.926507	12.607962	3.769636
C	6.171742	13.894049	4.235590
H	6.286932	14.733300	3.545656
C	5.608759	12.404190	2.368076
C	4.269718	12.630012	1.979814
C	3.168860	12.948566	2.984080
H	3.645293	13.173092	3.959344
C	2.364034	14.197583	2.586992
H	1.624825	14.446246	3.375292
H	1.799901	14.041043	1.644991
H	3.022903	15.077558	2.443148
C	2.258114	11.724317	3.198095
H	2.833890	10.841855	3.536142
H	1.740364	11.445759	2.257414
H	1.483135	11.946517	3.959606
C	3.968815	12.486662	0.611792
H	2.934569	12.637552	0.268895
C	4.964015	12.145766	-0.311155
H	4.708424	12.036174	-1.375817
C	6.637245	12.046138	1.468502
C	8.046134	11.755580	1.963416
H	7.937266	11.290880	2.963335
C	8.870279	13.045728	2.143333
H	9.872405	12.804184	2.549063
H	9.000675	13.565634	1.171674
H	8.393666	13.754336	2.847830
C	8.798184	10.753160	1.079235
H	8.201439	9.837879	0.908044
H	9.066920	11.192245	0.096072

H	9.742122	10.451017	1.573123
C	6.282295	11.927133	0.113444
H	7.046900	11.636341	-0.619503
C	4.346668	11.921699	7.734805
C	3.164304	12.217395	6.815344
H	3.436370	11.876811	5.797249
C	2.899890	13.737482	6.758337
H	2.063092	13.956956	6.064170
H	2.623785	14.125500	7.760278
H	3.781412	14.307294	6.406941
C	1.878826	11.475733	7.202758
H	2.053822	10.388511	7.306338
H	1.451413	11.857884	8.152715
H	1.110022	11.622997	6.418512
C	4.139791	11.558446	9.076539
H	3.117151	11.371440	9.429970
Si	5.824873	9.751715	4.741396
Cl	5.193623	9.391644	2.741569
Cl	4.043678	9.244645	5.794613
Cr	7.777311	8.667572	5.442185
C	9.278782	7.790596	6.107214
O	10.221181	7.256906	6.535957
C	6.719203	7.110294	5.382259
O	6.071972	6.147298	5.317737
C	8.696434	10.272671	5.246206
O	9.279927	11.269005	5.042451
C	8.245581	8.229987	3.680523
O	8.533656	7.907078	2.600176
C	7.154639	8.904140	7.200187
O	6.755835	8.935145	8.293414

3-Cr (M06/def2-SVP)

E (M06/def2-SVP) = -3978.2708457

E (M06/def2-TZVPP//M06/def2-SVP) = -3980.7362653

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -3980.7488157

N	-0.259186000000	1.495392000000	1.024020000000
C	0.523398000000	0.606879000000	0.350103000000
C	0.388024000000	1.939329000000	2.160920000000
H	-0.074783000000	2.666318000000	2.824260000000
C	-1.525435000000	2.082009000000	0.634212000000
C	-2.675842000000	1.763761000000	1.377186000000
C	-2.653803000000	0.875348000000	2.604027000000
H	-1.682893000000	0.352299000000	2.637491000000
C	-2.768819000000	1.729888000000	3.866889000000
H	-2.691858000000	1.101606000000	4.769326000000
H	-3.742845000000	2.247475000000	3.903965000000
H	-1.989858000000	2.507728000000	3.929129000000
C	-3.745044000000	-0.189254000000	2.609357000000
H	-3.720545000000	-0.819093000000	1.707993000000
H	-4.752311000000	0.253862000000	2.684332000000
H	-3.616575000000	-0.853377000000	3.479170000000
C	-3.871057000000	2.384503000000	1.004103000000
H	-4.789479000000	2.145205000000	1.548273000000
C	-3.911214000000	3.292530000000	-0.041454000000
H	-4.860430000000	3.753915000000	-0.327762000000
N	1.665906000000	0.517374000000	1.080563000000
C	1.591991000000	1.325364000000	2.198147000000
H	2.427771000000	1.406297000000	2.890115000000
C	2.945536000000	-0.046728000000	0.709681000000

C	3.816581000000	0.781822000000	-0.013096000000
C	3.438300000000	2.177286000000	-0.468849000000
H	2.466386000000	2.442848000000	-0.015679000000
C	4.442175000000	3.217967000000	0.014389000000
H	4.108673000000	4.233828000000	-0.254845000000
H	5.435755000000	3.072314000000	-0.442212000000
H	4.570078000000	3.181479000000	1.109248000000
C	3.246437000000	2.241497000000	-1.981851000000
H	2.500123000000	1.509643000000	-2.333781000000
H	4.190245000000	2.039136000000	-2.516816000000
H	2.905058000000	3.248579000000	-2.280406000000
C	5.068849000000	0.253591000000	-0.338017000000
H	5.775856000000	0.858011000000	-0.915206000000
C	5.425507000000	-1.030106000000	0.053969000000
H	6.409440000000	-1.425677000000	-0.213665000000
C	3.271259000000	-1.348078000000	1.120625000000
C	2.276599000000	-2.207715000000	1.867473000000
H	1.272496000000	-1.915782000000	1.514622000000
C	2.320174000000	-1.945893000000	3.370862000000
H	1.563870000000	-2.558526000000	3.888292000000
H	3.312106000000	-2.206660000000	3.780236000000
H	2.117063000000	-0.892988000000	3.624261000000
C	2.434144000000	-3.694588000000	1.589820000000
H	2.476034000000	-3.911868000000	0.511244000000
H	3.340504000000	-4.107568000000	2.066074000000
H	1.573313000000	-4.243913000000	2.005760000000
C	4.538537000000	-1.819869000000	0.778736000000
H	4.830243000000	-2.833404000000	1.066697000000
C	-1.516673000000	3.069000000000	-0.375311000000
C	-0.233379000000	3.595157000000	-0.988091000000
H	0.479905000000	2.757355000000	-1.058673000000
C	0.388329000000	4.660146000000	-0.083886000000
H	1.348667000000	5.005661000000	-0.504783000000
H	-0.278484000000	5.535857000000	0.000818000000
H	0.585451000000	4.293363000000	0.936538000000
C	-0.401056000000	4.153355000000	-2.393536000000
H	-0.943905000000	3.457398000000	-3.050429000000
H	-0.934893000000	5.119382000000	-2.391375000000
H	0.588528000000	4.337328000000	-2.843125000000
C	-2.743674000000	3.641492000000	-0.711869000000
H	-2.786893000000	4.392500000000	-1.504447000000
Si	-0.055094000000	-0.617307000000	-1.140632000000
Cl	1.814945000000	-1.327278000000	-1.842350000000
Cl	-0.499327000000	0.778430000000	-2.675179000000
Cr	-1.700301000000	-2.226046000000	-0.700744000000
C	-3.075458000000	-3.460966000000	-0.410266000000
O	-3.925715000000	-4.211633000000	-0.218613000000
C	-1.790332000000	-2.384830000000	-2.586996000000
O	-1.820847000000	-2.483924000000	-3.730001000000
C	-1.354876000000	-2.035690000000	1.126783000000
O	-1.064201000000	-1.941866000000	2.244316000000
C	-0.397469000000	-3.586415000000	-0.758692000000
O	0.395332000000	-4.416266000000	-0.823691000000
C	-2.948385000000	-0.814120000000	-0.834468000000
O	-3.717787000000	0.028426000000	-0.981690000000

3-Cr-CO (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -3866.885247259

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3869.218594107

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3869.235990013

N	5.955078	12.535142	5.971759
C	5.807100	11.755079	4.848232
C	6.208135	13.855595	5.622098
H	6.346940	14.626731	6.383119
C	5.715385	12.163256	7.353625
C	6.801050	12.158281	8.261327
C	8.214900	12.570821	7.872287
H	8.271939	12.621703	6.769497
C	8.520953	13.978924	8.424929
H	9.522274	14.319253	8.091101
H	8.511741	13.982615	9.534447
H	7.776431	14.730599	8.092023
C	9.285825	11.568414	8.333935
H	9.085868	10.554947	7.938897
H	9.340829	11.503417	9.439732
H	10.282628	11.884467	7.967145
C	6.518624	11.833825	9.602059
H	7.343115	11.799705	10.328451
C	5.217531	11.540494	10.016143
H	5.023188	11.263039	11.062908
N	5.951405	12.628072	3.799214
C	6.208385	13.914235	4.256202
H	6.336142	14.746984	3.560652
C	5.641719	12.409630	2.399803
C	4.285671	12.505881	2.013319
C	3.163131	12.762913	3.009903
H	3.620010	12.935877	4.004313
C	2.374833	14.036155	2.654801
H	1.604753	14.242553	3.425818
H	1.851608	13.934221	1.681968
H	3.040387	14.920441	2.587682
C	2.243138	11.536040	3.145677
H	2.811717	10.637131	3.449318
H	1.733166	11.310247	2.186700
H	1.460289	11.723719	3.908538
C	3.997570	12.327222	0.647725
H	2.952216	12.375765	0.307943
C	5.018378	12.082676	-0.279710
H	4.769635	11.940536	-1.342194
C	6.696838	12.175584	1.493380
C	8.140168	12.085118	1.958511
H	8.131560	11.959636	3.057459
C	8.899084	13.391683	1.656317
H	9.938725	13.333258	2.037498
H	8.943249	13.584242	0.564009
H	8.413335	14.268691	2.130318
C	8.861835	10.863630	1.369019
H	8.270227	9.941538	1.517592
H	9.052515	10.981093	0.282032
H	9.843253	10.724294	1.864348
C	6.353626	12.014825	0.138709
H	7.147025	11.815997	-0.596189
C	4.368094	11.965322	7.761596
C	3.188340	12.248488	6.835145
H	3.462423	11.891130	5.823746
C	2.927162	13.767868	6.754668
H	2.089909	13.977541	6.058091
H	2.653650	14.173006	7.750625
H	3.809200	14.329517	6.391503

C	1.901376	11.513469	7.229588
H	2.076708	10.427918	7.349832
H	1.470257	11.910093	8.172043
H	1.135933	11.648688	6.439898
C	4.154075	11.621872	9.107692
H	3.130097	11.432426	9.455898
Si	5.858388	9.763361	4.791058
Cl	5.340316	9.396796	2.753901
Cl	3.993711	9.298388	5.730783
Cr	7.692594	8.702791	5.584026
C	6.582368	7.191690	5.487015
O	5.867028	6.278538	5.367693
C	8.577242	10.307396	5.330345
O	9.079606	11.336122	5.049997
C	8.294777	8.179889	3.888476
O	8.654198	7.824219	2.837431
C	7.070441	8.957271	7.340762
O	6.658038	9.000185	8.431303

3-Cr-CO (M06/def2-SVP)

E (M06/def2-SVP) = -3865.0217947

E (M06/def2-TZVPP//M06/def2-SVP) = -3867.3581748

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -3867.3733843

N	-0.896384000000	1.011952000000	1.040999000000
C	0.171278000000	0.513211000000	0.355444000000
C	-0.474954000000	1.620548000000	2.208007000000
H	-1.185138000000	2.085898000000	2.887920000000
C	-2.285600000000	1.096082000000	0.636103000000
C	-3.250654000000	0.360978000000	1.348130000000
C	-2.930895000000	-0.477647000000	2.569315000000
H	-1.838426000000	-0.599569000000	2.637854000000
C	-3.399582000000	0.244416000000	3.832891000000
H	-3.121100000000	-0.327800000000	4.733170000000
H	-4.496727000000	0.363572000000	3.839935000000
H	-2.966363000000	1.254619000000	3.927641000000
C	-3.529453000000	-1.878665000000	2.519688000000
H	-3.243525000000	-2.422087000000	1.605826000000
H	-4.631237000000	-1.858989000000	2.569682000000
H	-3.174535000000	-2.468313000000	3.380795000000
C	-4.583391000000	0.494794000000	0.949213000000
H	-5.356052000000	-0.078293000000	1.470251000000
C	-4.941065000000	1.335961000000	-0.091736000000
H	-5.987737000000	1.410590000000	-0.399475000000
N	1.258048000000	0.837275000000	1.105908000000
C	0.871728000000	1.509836000000	2.250278000000
H	1.608254000000	1.872550000000	2.964508000000
C	2.661647000000	0.847927000000	0.741455000000
C	3.134233000000	1.990809000000	0.077788000000
C	2.234279000000	3.130185000000	-0.354683000000
H	1.232697000000	2.971465000000	0.083085000000
C	2.733010000000	4.473013000000	0.167596000000
H	2.019261000000	5.276163000000	-0.079140000000
H	3.700784000000	4.753002000000	-0.281556000000
H	2.864737000000	4.459537000000	1.262498000000
C	2.056304000000	3.147560000000	-1.870492000000
H	1.657155000000	2.191301000000	-2.248128000000
H	3.015079000000	3.334062000000	-2.384187000000
H	1.360568000000	3.952216000000	-2.166325000000
C	4.498930000000	2.035696000000	-0.221475000000

H	4.905618000000	2.899532000000	-0.756586000000
C	5.345148000000	0.999370000000	0.146377000000
H	6.410687000000	1.054385000000	-0.094091000000
C	3.486757000000	-0.224570000000	1.113484000000
C	2.919916000000	-1.465335000000	1.764837000000
H	1.911524000000	-1.603051000000	1.339709000000
C	2.767540000000	-1.303576000000	3.274750000000
H	2.340252000000	-2.218592000000	3.716538000000
H	3.750539000000	-1.123355000000	3.745029000000
H	2.100764000000	-0.471038000000	3.549422000000
C	3.716099000000	-2.722072000000	1.450469000000
H	3.893149000000	-2.834105000000	0.369063000000
H	4.690064000000	-2.731114000000	1.970174000000
H	3.160872000000	-3.611746000000	1.788697000000
C	4.843703000000	-0.116358000000	0.808435000000
H	5.521596000000	-0.931718000000	1.072834000000
C	-2.631363000000	2.034431000000	-0.361005000000
C	-1.638233000000	3.032607000000	-0.924370000000
H	-0.656841000000	2.534666000000	-1.008830000000
C	-1.490328000000	4.215245000000	0.033786000000
H	-0.755311000000	4.938176000000	-0.359957000000
H	-2.452863000000	4.743669000000	0.148945000000
H	-1.155281000000	3.912437000000	1.039397000000
C	-1.996657000000	3.543774000000	-2.312363000000
H	-2.225664000000	2.722232000000	-3.007924000000
H	-2.860134000000	4.230874000000	-2.286387000000
H	-1.151297000000	4.113064000000	-2.731885000000
C	-3.975877000000	2.109623000000	-0.725839000000
H	-4.278840000000	2.805431000000	-1.512113000000
Si	0.103680000000	-0.805671000000	-1.173292000000
Cl	2.121501000000	-0.735231000000	-1.839684000000
Cl	-0.796908000000	0.397717000000	-2.680222000000
Cr	-0.800841000000	-2.861563000000	-0.805409000000
C	-0.711252000000	-2.965223000000	-2.690815000000
O	-0.595370000000	-2.970817000000	-3.835718000000
C	-0.578375000000	-2.505226000000	1.004930000000
O	-0.317931000000	-2.204578000000	2.098414000000
C	0.893429000000	-3.689675000000	-0.780790000000
O	1.934402000000	-4.181155000000	-0.784563000000
C	-2.518057000000	-2.082473000000	-0.957615000000
O	-3.555750000000	-1.603589000000	-1.102034000000

3-W (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -3002.922847732

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3005.258291483

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3005.275121472

N	5.855295	12.550133	5.951022
C	5.725811	11.786990	4.816015
C	6.064112	13.883584	5.622957
H	6.175532	14.647249	6.395205
C	5.647526	12.137052	7.325305
C	6.765084	12.053709	8.188920
C	8.172660	12.435137	7.746871
H	8.203579	12.397272	6.640478
C	8.485300	13.883364	8.183956
H	9.479437	14.197054	7.806222
H	8.498189	13.962298	9.290557
H	7.736306	14.611541	7.815267
C	9.266810	11.492674	8.273487

H	9.082598	10.442789	7.982884
H	9.350357	11.536748	9.378310
H	10.248338	11.788916	7.854783
C	6.514213	11.693365	9.526666
H	7.358840	11.597200	10.222921
C	5.214387	11.441861	9.974454
H	5.044047	11.140092	11.018651
N	5.855349	12.675645	3.781064
C	6.067744	13.963220	4.258199
H	6.167553	14.810778	3.575961
C	5.590032	12.458224	2.373854
C	4.266950	12.678346	1.932781
C	3.134455	13.018598	2.895497
H	3.584022	13.317820	3.864349
C	2.294250	14.211729	2.410253
H	1.539098	14.485976	3.174448
H	1.744180	13.975464	1.476522
H	2.925104	15.102055	2.214019
C	2.259568	11.779575	3.168834
H	2.854199	10.938075	3.571927
H	1.773803	11.424737	2.236769
H	1.460996	12.023582	3.898807
C	4.018062	12.500486	0.558461
H	2.998602	12.643777	0.171263
C	5.047562	12.132023	-0.315801
H	4.831692	11.994270	-1.385997
C	6.652762	12.075121	1.526246
C	8.040059	11.797360	2.088399
H	7.889251	11.312551	3.076062
C	8.838395	13.095346	2.323207
H	9.820722	12.859813	2.777443
H	9.011661	13.625347	1.363853
H	8.318987	13.793054	3.008019
C	8.852014	10.818496	1.232119
H	8.277153	9.901512	1.005896
H	9.173538	11.279495	0.275167
H	9.768828	10.517065	1.775465
C	6.349139	11.921616	0.162250
H	7.138963	11.610651	-0.534727
C	4.308332	11.960012	7.762925
C	3.114440	12.263418	6.860426
H	3.381017	11.941921	5.834090
C	2.832675	13.781057	6.828581
H	1.989758	14.001448	6.141993
H	2.557423	14.150542	7.837803
H	3.705688	14.366368	6.481662
C	1.840321	11.501485	7.247232
H	2.028450	10.414810	7.331209
H	1.417737	11.863229	8.207353
H	1.062721	11.653163	6.472438
C	4.124390	11.586964	9.105595
H	3.106650	11.415352	9.480814
Si	5.781985	9.810293	4.724079
Cl	5.096876	9.444972	2.741166
Cl	4.042211	9.286228	5.841901
W	7.897907	8.576413	5.406891
C	9.502725	7.497623	6.045809
O	10.418423	6.886466	6.428711
C	6.676083	6.905978	5.368572
O	5.983608	5.976560	5.303493

C	9.041962	10.261347	5.215990
O	9.697615	11.212861	5.027581
C	8.304031	8.103893	3.445485
O	8.488738	7.767041	2.347304
C	7.267615	8.815977	7.354715
O	6.865844	8.837610	8.446730

3-W (M06/def2-SVP)

E (M06/def2-SVP) = -3001.090227

E (M06/def2-TZVPP//M06/def2-SVP) = -3003.4293152

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -3003.4419776

N	1.845182000000	1.264248000000	0.896932000000
C	1.375512000000	0.119209000000	0.337449000000
C	2.887306000000	0.986020000000	1.758977000000
H	3.397632000000	1.777805000000	2.302405000000
C	1.433529000000	2.627882000000	0.648844000000
C	0.347958000000	3.151133000000	1.375510000000
C	-0.381415000000	2.345289000000	2.436558000000
H	-0.519018000000	1.318261000000	2.041530000000
C	0.433929000000	2.251634000000	3.727222000000
H	-0.121240000000	1.672086000000	4.483363000000
H	0.611374000000	3.260184000000	4.140174000000
H	1.412162000000	1.765194000000	3.596356000000
C	-1.759669000000	2.890545000000	2.784029000000
H	-2.391250000000	3.057044000000	1.900019000000
H	-1.684957000000	3.846124000000	3.331349000000
H	-2.281365000000	2.181262000000	3.444557000000
C	-0.002293000000	4.477906000000	1.109953000000
H	-0.852229000000	4.926792000000	1.628692000000
C	0.705767000000	5.238337000000	0.187714000000
H	0.404855000000	6.271724000000	-0.005933000000
N	2.111331000000	-0.876803000000	0.891424000000
C	3.054157000000	-0.356236000000	1.756129000000
H	3.739956000000	-1.005571000000	2.296162000000
C	2.069197000000	-2.301082000000	0.652041000000
C	3.054768000000	-2.836340000000	-0.192045000000
C	4.081466000000	-1.979059000000	-0.906800000000
H	3.754972000000	-0.923440000000	-0.844319000000
C	5.444246000000	-2.093592000000	-0.227861000000
H	6.187541000000	-1.448783000000	-0.724964000000
H	5.817125000000	-3.131360000000	-0.276738000000
H	5.408257000000	-1.808746000000	0.836495000000
C	4.193261000000	-2.317817000000	-2.389212000000
H	3.215907000000	-2.250036000000	-2.891275000000
H	4.595581000000	-3.332706000000	-2.547619000000
H	4.883156000000	-1.616927000000	-2.886799000000
C	3.060957000000	-4.221567000000	-0.365553000000
H	3.810885000000	-4.676058000000	-1.020166000000
C	2.118780000000	-5.021797000000	0.265513000000
H	2.131768000000	-6.104191000000	0.110357000000
C	1.101259000000	-3.079133000000	1.313748000000
C	0.047016000000	-2.465229000000	2.219294000000
H	-0.396686000000	-1.616515000000	1.660371000000
C	0.624358000000	-1.909368000000	3.521242000000
H	-0.190653000000	-1.500847000000	4.141035000000
H	1.118835000000	-2.710081000000	4.099062000000
H	1.354098000000	-1.098180000000	3.374017000000
C	-1.087387000000	-3.419744000000	2.565328000000
H	-1.544944000000	-3.884159000000	1.678766000000

H	-0.738650000000	-4.226482000000	3.233863000000
H	-1.875878000000	-2.872936000000	3.105240000000
C	1.150219000000	-4.457381000000	1.088138000000
H	0.411575000000	-5.106688000000	1.562242000000
C	2.184650000000	3.376039000000	-0.274131000000
C	3.394320000000	2.812903000000	-0.995209000000
H	3.317483000000	1.708672000000	-0.978882000000
C	4.677929000000	3.220620000000	-0.272439000000
H	5.563148000000	2.796759000000	-0.774727000000
H	4.785554000000	4.319092000000	-0.274172000000
H	4.699043000000	2.893665000000	0.779273000000
C	3.474349000000	3.234543000000	-2.457231000000
H	2.544299000000	3.009361000000	-2.998813000000
H	3.684895000000	4.312235000000	-2.562115000000
H	4.297577000000	2.700424000000	-2.958737000000
C	1.792233000000	4.698013000000	-0.487863000000
H	2.342209000000	5.311872000000	-1.207087000000
Si	-0.121246000000	-0.057247000000	-0.972670000000
Cl	0.635986000000	-1.677810000000	-2.120878000000
Cl	0.352829000000	1.577283000000	-2.244518000000
W	-2.633011000000	-0.241894000000	-0.479640000000
C	-4.670311000000	-0.366969000000	-0.395672000000
O	-5.819282000000	-0.434527000000	-0.362178000000
C	-2.724930000000	-0.250671000000	-2.561439000000
O	-2.769005000000	-0.265618000000	-3.706813000000
C	-2.556730000000	-0.281690000000	1.576260000000
O	-2.519239000000	-0.326051000000	2.730854000000
C	-2.358247000000	-2.291267000000	-0.550561000000
O	-2.137053000000	-3.417735000000	-0.622076000000
C	-2.612932000000	1.827194000000	-0.525867000000
O	-2.527631000000	2.973140000000	-0.579958000000

3-W-CO (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -2889.603730029

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2891.806484248

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2891.824309520

N	5.885436	12.550239	5.958934
C	5.774629	11.768907	4.833301
C	6.092818	13.879717	5.613508
H	6.195814	14.654393	6.376042
C	5.657041	12.161893	7.337491
C	6.755684	12.125470	8.227843
C	8.160575	12.545591	7.815546
H	8.211749	12.531801	6.710336
C	8.432149	13.991350	8.285818
H	9.423332	14.337141	7.928556
H	8.426897	14.051166	9.393766
H	7.669304	14.706939	7.919328
C	9.264585	11.612937	8.338591
H	9.098270	10.566859	8.023106
H	9.330661	11.633371	9.445441
H	10.246874	11.934236	7.939981
C	6.486545	11.780252	9.565964
H	7.318887	11.719996	10.281094
C	5.185185	11.500608	9.991050
H	5.000362	11.209516	11.035842
N	5.906132	12.645154	3.786059
C	6.108541	13.940084	4.248123
H	6.208163	14.779168	3.555588

C	5.618770	12.421134	2.382837
C	4.285399	12.627566	1.965722
C	3.164564	12.955790	2.945338
H	3.623556	13.217250	3.920097
C	2.344611	14.178731	2.500768
H	1.592405	14.439233	3.272808
H	1.793815	13.984130	1.557876
H	2.990830	15.064633	2.336865
C	2.270350	11.724032	3.185122
H	2.854719	10.862837	3.560864
H	1.773456	11.405577	2.245792
H	1.479347	11.958964	3.926185
C	4.012020	12.452283	0.595729
H	2.983324	12.585623	0.229562
C	5.028014	12.099472	-0.300023
H	4.793440	11.963346	-1.366512
C	6.668349	12.055096	1.511783
C	8.070572	11.796336	2.042701
H	7.947163	11.321028	3.037433
C	8.858529	13.105697	2.245843
H	9.855052	12.886795	2.676942
H	9.000330	13.630571	1.278349
H	8.348188	13.801410	2.939369
C	8.871417	10.817736	1.175601
H	8.302249	9.890487	0.977927
H	9.160797	11.270316	0.204341
H	9.806555	10.534269	1.697024
C	6.340471	11.903270	0.153186
H	7.121166	11.604901	-0.559473
C	4.313224	11.966900	7.753950
C	3.129523	12.248078	6.831391
H	3.410895	11.912618	5.813925
C	2.840909	13.763704	6.774529
H	2.004120	13.970095	6.076184
H	2.553534	14.146601	7.775358
H	3.714754	14.347877	6.427719
C	1.854448	11.485636	7.213205
H	2.046965	10.401144	7.313997
H	1.418370	11.858488	8.163036
H	1.085732	11.622942	6.426971
C	4.110652	11.609339	9.098193
H	3.089206	11.423150	9.455837
Si	5.835517	9.791788	4.761715
Cl	5.156897	9.417314	2.775804
Cl	4.072827	9.277777	5.852742
W	7.845401	8.688062	5.449414
C	6.690677	6.980708	5.424122
O	6.012032	6.036858	5.354300
C	8.939157	10.394352	5.256119
O	9.545926	11.381321	5.056652
C	8.328930	8.179684	3.522547
O	8.563183	7.825879	2.435352
C	7.265375	8.905234	7.404185
O	6.896605	8.918868	8.512390

3-W-CO (M06/def2-SVP)

E (M06/def2-SVP) = -2887.844475

E (M06/def2-TZVPP//M06/def2-SVP) = -2890.0499325

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -2890.0702833

N	-0.363867000000	1.953727000000	0.922406000000
C	0.440721000000	1.013233000000	0.358537000000
C	0.348093000000	2.719513000000	1.824401000000
H	-0.126014000000	3.528535000000	2.375348000000
C	-1.754726000000	2.248567000000	0.656825000000
C	-2.739885000000	1.567487000000	1.393185000000
C	-2.389697000000	0.560510000000	2.471849000000
H	-1.492007000000	0.007385000000	2.135494000000
C	-2.047118000000	1.261872000000	3.786680000000
H	-1.794276000000	0.517927000000	4.560208000000
H	-2.914154000000	1.842927000000	4.146901000000
H	-1.194659000000	1.952840000000	3.701534000000
C	-3.486500000000	-0.461372000000	2.735213000000
H	-3.849483000000	-0.939244000000	1.813448000000
H	-4.352676000000	0.000032000000	3.240445000000
H	-3.106892000000	-1.249264000000	3.403784000000
C	-4.070370000000	1.908265000000	1.136528000000
H	-4.870234000000	1.388009000000	1.669027000000
C	-4.392965000000	2.890246000000	0.209004000000
H	-5.442419000000	3.132285000000	0.018926000000
N	1.655246000000	1.192783000000	0.938965000000
C	1.613197000000	2.242923000000	1.834904000000
H	2.494154000000	2.532142000000	2.403850000000
C	2.916844000000	0.535862000000	0.680049000000
C	3.833770000000	1.212875000000	-0.139288000000
C	3.518503000000	2.534452000000	-0.812459000000
H	2.430146000000	2.712431000000	-0.728112000000
C	4.240709000000	3.681596000000	-0.110059000000
H	3.981975000000	4.650114000000	-0.569082000000
H	5.334996000000	3.559213000000	-0.186913000000
H	3.992843000000	3.737805000000	0.962464000000
C	3.846015000000	2.527498000000	-2.301542000000
H	3.342793000000	1.695920000000	-2.817899000000
H	4.930857000000	2.445809000000	-2.482869000000
H	3.513276000000	3.470296000000	-2.765841000000
C	5.081139000000	0.614485000000	-0.328075000000
H	5.823772000000	1.107446000000	-0.962687000000
C	5.383626000000	-0.603594000000	0.264604000000
H	6.361836000000	-1.063154000000	0.096415000000
C	3.190826000000	-0.692798000000	1.305680000000
C	2.170653000000	-1.389334000000	2.187733000000
H	1.214547000000	-1.377444000000	1.628115000000
C	1.943514000000	-0.670648000000	3.518067000000
H	1.236587000000	-1.246733000000	4.136820000000
H	2.890709000000	-0.586029000000	4.079826000000
H	1.520458000000	0.340015000000	3.410322000000
C	2.507454000000	-2.845620000000	2.472713000000
H	2.739447000000	-3.414503000000	1.560128000000
H	3.369075000000	-2.929636000000	3.158633000000
H	1.651256000000	-3.331350000000	2.967253000000
C	4.449519000000	-1.250053000000	1.066455000000
H	4.706459000000	-2.212267000000	1.514097000000
C	-2.045571000000	3.272849000000	-0.261836000000
C	-0.968363000000	4.079646000000	-0.960943000000
H	-0.035342000000	3.486010000000	-0.952083000000
C	-0.709139000000	5.380959000000	-0.202027000000
H	0.089148000000	5.965375000000	-0.688929000000
H	-1.619103000000	6.005584000000	-0.184883000000
H	-0.409294000000	5.210732000000	0.844242000000
C	-1.292508000000	4.390096000000	-2.416728000000

H	-1.547783000000	3.481529000000	-2.981667000000
H	-2.129696000000	5.102862000000	-2.507358000000
H	-0.423099000000	4.860365000000	-2.904003000000
C	-3.392234000000	3.571192000000	-0.473353000000
H	-3.662076000000	4.351917000000	-1.190228000000
Si	-0.074066000000	-0.374007000000	-0.990844000000
Cl	1.761570000000	-0.441350000000	-2.070250000000
Cl	-1.203013000000	0.878065000000	-2.289969000000
W	-1.081330000000	-2.519894000000	-0.565242000000
C	-1.123354000000	-2.613812000000	-2.635156000000
O	-1.120378000000	-2.639342000000	-3.784257000000
C	-1.002457000000	-2.516161000000	1.485576000000
O	-0.928077000000	-2.543684000000	2.641801000000
C	0.819855000000	-3.309058000000	-0.632447000000
O	1.912300000000	-3.672662000000	-0.698760000000
C	-2.894282000000	-1.543599000000	-0.612694000000
O	-3.877158000000	-0.942539000000	-0.673687000000

4-Cr (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -6236.190101412

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -6240.172709466

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -6240.197494377

N	5.944102	11.914692	5.893474
C	5.621857	11.208061	4.757928
C	6.215572	13.242812	5.586675
H	6.481736	13.960806	6.365047
C	5.878131	11.475401	7.273823
C	7.081266	11.346914	8.006624
C	8.446270	11.689053	7.422958
H	8.348780	11.738086	6.322118
C	8.891221	13.081506	7.921033
H	9.851792	13.373232	7.449840
H	9.037664	13.077060	9.020991
H	8.147112	13.872055	7.696086
C	9.534410	10.650135	7.739064
H	9.255369	9.631507	7.420236
H	9.762552	10.612311	8.824075
H	10.470908	10.916420	7.211163
C	6.972467	10.962725	9.356980
H	7.889374	10.826146	9.947368
C	5.726182	10.733271	9.944075
H	5.665483	10.409837	10.994164
N	5.697696	12.131271	3.744784
C	6.062027	13.379986	4.236726
H	6.142352	14.246857	3.576924
C	5.211586	12.023033	2.383786
C	3.852499	12.345241	2.172432
C	2.903929	12.677967	3.318714
H	3.507541	12.814303	4.237844
C	2.155349	14.000713	3.081598
H	1.534896	14.256098	3.964640
H	1.474548	13.937515	2.208005
H	2.858215	14.839019	2.900862
C	1.934074	11.511884	3.588986
H	2.477964	10.575770	3.817021
H	1.288825	11.318685	2.707250
H	1.273959	11.750602	4.447891
C	3.381125	12.294570	0.847050
H	2.324272	12.519872	0.640940

C	4.238011	11.952722	-0.204987
H	3.852259	11.916315	-1.235136
C	6.106562	11.666527	1.349471
C	7.548187	11.272168	1.648050
H	7.515691	10.641942	2.561323
C	8.442829	12.489988	1.955844
H	9.472192	12.150938	2.184066
H	8.483202	13.175563	1.083872
H	8.092661	13.066479	2.832246
C	8.183471	10.429986	0.534946
H	7.549810	9.564793	0.267158
H	8.372535	11.035834	-0.376258
H	9.156671	10.030448	0.879374
C	5.582957	11.644018	0.044163
H	6.235307	11.359158	-0.791765
C	4.592704	11.336095	7.862467
C	3.316645	11.728654	7.121494
H	3.433988	11.417941	6.065007
C	3.127644	13.260423	7.153906
H	2.219172	13.548556	6.586023
H	3.007702	13.620100	8.196726
H	3.983972	13.800507	6.706615
C	2.056166	11.032701	7.650142
H	2.187586	9.935010	7.686518
H	1.779205	11.391635	8.663106
H	1.199301	11.250528	6.981888
C	4.549980	10.933095	9.208122
H	3.575996	10.787555	9.694443
Si	5.536345	9.225750	4.579366
Cl	4.540428	9.057892	2.683925
Cl	3.877594	8.779901	5.865087
Cr	7.449216	8.028578	4.897025
C	6.361188	6.533028	5.071207
O	5.681501	5.592724	5.252257
C	8.537769	9.523824	4.723265
O	9.217939	10.463925	4.542998
C	7.683146	7.812525	3.066388
O	7.855213	7.734014	1.912289
C	7.214623	8.244721	6.727571
O	7.041960	8.323137	7.881591
Si	9.362207	6.831528	5.214368
Cl	11.020651	7.277480	3.928288
Cl	10.358436	6.999601	7.109626
C	9.276831	4.849189	5.035960
N	8.954092	4.142458	3.900607
C	8.682765	2.814363	4.207646
H	8.416226	2.096304	3.429462
C	8.836982	2.677290	5.557530
N	9.201511	3.926049	6.049212
C	9.688310	4.034380	7.409968
C	8.793823	4.390779	8.444744
C	7.352011	4.785003	8.146915
H	7.383923	5.415065	7.233511
C	6.717351	5.627363	9.260239
H	5.743871	6.026701	8.916380
H	6.528984	5.021715	10.171720
C	6.457296	3.567054	7.839873
H	5.427776	3.905959	7.612139
H	6.807049	2.990415	6.963402
H	6.417463	2.881657	8.712010

C	9.318069	4.413313	9.749794
H	8.666101	4.698099	10.586046
C	10.663169	4.104751	9.998279
C	11.519570	3.763046	8.945804
H	12.576555	3.537873	9.151379
H	11.049428	4.141183	11.028237
C	11.047545	3.712359	7.620654
C	11.995636	3.379875	6.473913
H	11.391628	3.243509	5.555051
C	12.965146	4.546174	6.203328
H	13.610778	4.739369	7.084786
H	12.420969	5.482217	5.975682
H	13.624901	4.307713	5.344077
H	12.041950	1.218786	6.891516
C	12.744572	2.057249	6.710564
H	13.364688	1.802080	5.827222
H	13.425746	2.120488	7.583863
H	7.351092	6.492700	9.527385
H	8.756991	1.810464	6.217432
H	6.549296	4.317923	3.472783
C	6.451313	4.367356	2.372010
H	4.426658	5.139603	2.585008
C	5.362879	5.406227	2.056784
H	5.641923	6.424782	2.375840
C	6.006363	2.975019	1.873607
H	5.859432	2.979859	0.773715
H	6.750702	2.184501	2.097913
H	5.046048	2.682956	2.345113
C	9.019456	4.581645	2.520188
C	7.816006	4.709913	1.787866
C	7.924170	5.094245	0.437499
H	7.006990	5.230689	-0.152497
C	9.170162	5.323999	-0.150091
H	9.230363	5.647535	-1.200176
C	10.346703	5.124291	0.585352
H	11.320458	5.269997	0.098626
C	10.304617	4.721160	1.930987
C	11.581071	4.328635	2.671295
H	11.464195	4.639133	3.727893
C	12.841207	5.024848	2.142177
H	13.117733	4.666143	1.129013
H	12.709636	6.122530	2.106074
H	13.698417	4.807001	2.809981
C	11.770268	2.796897	2.638475
H	11.889751	2.437457	1.595521
H	12.679058	2.508770	3.205850
H	10.914237	2.256597	3.086070
H	5.134232	5.444410	0.971890

4-Cr (M06/def2-SVP)

E (M06/def2-SVP) = -6233.0255076

E (M06/def2-TZVPP//M06/def2-SVP) = -6237.0129852

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -6237.033087

N	4.042037000000	-1.379446000000	-0.949607000000
C	3.715068000000	-0.182564000000	-0.384944000000
C	4.996410000000	-1.205649000000	-1.934023000000
H	5.388264000000	-2.051422000000	-2.494144000000
C	3.610403000000	-2.714883000000	-0.595753000000
C	2.763747000000	-3.405535000000	-1.481256000000

C	2.297172000000	-2.834721000000	-2.805476000000
H	2.452454000000	-1.741997000000	-2.792954000000
C	3.130726000000	-3.420373000000	-3.945949000000
H	2.828004000000	-2.983098000000	-4.911564000000
H	2.985495000000	-4.512622000000	-4.012790000000
H	4.211823000000	-3.246815000000	-3.821183000000
C	0.818139000000	-3.071599000000	-3.091047000000
H	0.166199000000	-2.753130000000	-2.265117000000
H	0.604958000000	-4.135021000000	-3.293846000000
H	0.517887000000	-2.500213000000	-3.984077000000
C	2.411190000000	-4.713493000000	-1.139437000000
H	1.737197000000	-5.269897000000	-1.797124000000
C	2.885944000000	-5.304297000000	0.020558000000
H	2.580250000000	-6.321996000000	0.279807000000
N	4.486117000000	0.729932000000	-1.033587000000
C	5.273369000000	0.115269000000	-1.989013000000
H	5.974470000000	0.688291000000	-2.592394000000
C	4.774306000000	2.104150000000	-0.690398000000
C	5.841143000000	2.320787000000	0.193002000000
C	6.592251000000	1.188117000000	0.865364000000
H	6.275259000000	0.234961000000	0.403979000000
C	8.096958000000	1.302616000000	0.649909000000
H	8.618405000000	0.427729000000	1.071507000000
H	8.514819000000	2.195736000000	1.144585000000
H	8.350553000000	1.366192000000	-0.421673000000
C	6.240214000000	1.089932000000	2.347330000000
H	5.156929000000	0.954489000000	2.500801000000
H	6.544899000000	1.999855000000	2.892929000000
H	6.761370000000	0.233438000000	2.809697000000
C	6.169212000000	3.649156000000	0.478347000000
H	6.982185000000	3.866357000000	1.178520000000
C	5.472379000000	4.696405000000	-0.109701000000
H	5.745209000000	5.729796000000	0.123766000000
C	4.037739000000	3.136330000000	-1.291035000000
C	2.854086000000	2.837083000000	-2.185071000000
H	2.334687000000	1.971228000000	-1.735374000000
C	3.277729000000	2.438052000000	-3.596621000000
H	2.388360000000	2.211595000000	-4.206461000000
H	3.830246000000	3.261626000000	-4.082847000000
H	3.916181000000	1.540671000000	-3.614792000000
C	1.845155000000	3.971957000000	-2.253220000000
H	1.557401000000	4.328063000000	-1.252134000000
H	2.229863000000	4.825574000000	-2.839184000000
H	0.926220000000	3.619915000000	-2.750372000000
C	4.419907000000	4.442870000000	-0.983989000000
H	3.869464000000	5.279850000000	-1.421106000000
C	4.181248000000	-3.318296000000	0.544783000000
C	5.299340000000	-2.671530000000	1.342151000000
H	5.133878000000	-1.579531000000	1.361146000000
C	6.642035000000	-2.941745000000	0.661177000000
H	7.466386000000	-2.481452000000	1.232617000000
H	6.836660000000	-4.027344000000	0.609453000000
H	6.686335000000	-2.546744000000	-0.366680000000
C	5.365052000000	-3.133804000000	2.790864000000
H	4.384042000000	-3.078125000000	3.284777000000
H	5.737280000000	-4.169877000000	2.873740000000
H	6.064723000000	-2.497948000000	3.357420000000
C	3.771224000000	-4.617861000000	0.845111000000
H	4.170425000000	-5.112430000000	1.734357000000
Si	2.149734000000	0.191752000000	0.851352000000

Cl	2.724578000000	2.120184000000	1.583060000000
Cl	2.747375000000	-0.971377000000	2.540456000000
Cr	0.010224000000	-0.041798000000	0.078031000000
C	-0.532008000000	-0.135815000000	1.865556000000
O	-0.873311000000	-0.282823000000	2.964005000000
C	0.595902000000	0.008759000000	-1.687873000000
O	0.989923000000	0.101207000000	-2.776130000000
C	-0.178871000000	1.812236000000	-0.049819000000
O	-0.270049000000	2.957056000000	-0.181243000000
C	0.177846000000	-1.898609000000	0.190008000000
O	0.256345000000	-3.047253000000	0.295120000000
Si	-2.109652000000	-0.217323000000	-0.760082000000
Cl	-2.585619000000	1.004219000000	-2.449795000000
Cl	-2.693082000000	-2.116120000000	-1.557399000000
C	-3.738726000000	0.192199000000	0.377498000000
N	-4.063002000000	1.391839000000	0.936568000000
C	-5.093500000000	1.241021000000	1.844755000000
H	-5.495008000000	2.094854000000	2.385283000000
C	-5.421738000000	-0.069402000000	1.858370000000
N	-4.589293000000	-0.698740000000	0.952645000000
C	-4.885153000000	-2.061701000000	0.578004000000
C	-4.194918000000	-3.109125000000	1.204304000000
C	-3.053360000000	-2.831567000000	2.157937000000
H	-2.518542000000	-1.947268000000	1.762366000000
C	-2.040664000000	-3.962962000000	2.221949000000
H	-1.141339000000	-3.628369000000	2.764832000000
H	-2.441235000000	-4.841209000000	2.758646000000
C	-3.545657000000	-2.483411000000	3.560300000000
H	-2.690206000000	-2.259605000000	4.217618000000
H	-4.206378000000	-1.601413000000	3.572891000000
H	-4.103444000000	-3.331238000000	3.996106000000
C	-4.578479000000	-4.407120000000	0.864453000000
H	-4.064479000000	-5.256943000000	1.320899000000
C	-5.583957000000	-4.635722000000	-0.070077000000
C	-6.231331000000	-3.572510000000	-0.686323000000
H	-7.005115000000	-3.769238000000	-1.435411000000
H	-5.857996000000	-5.662558000000	-0.329594000000
C	-5.901729000000	-2.252031000000	-0.368166000000
C	-6.589766000000	-1.098976000000	-1.071713000000
H	-6.304004000000	-0.161995000000	-0.560897000000
C	-6.117661000000	-0.968221000000	-2.517400000000
H	-6.385955000000	-1.862506000000	-3.106721000000
H	-5.024687000000	-0.842049000000	-2.583396000000
H	-6.593098000000	-0.094921000000	-2.997452000000
H	-8.450534000000	-1.303363000000	0.058004000000
C	-8.107635000000	-1.201579000000	-0.985357000000
H	-8.581223000000	-0.302414000000	-1.412938000000
H	-8.492525000000	-2.067952000000	-1.549519000000
H	-1.720173000000	-4.274427000000	1.215530000000
H	-6.185614000000	-0.623985000000	2.399717000000
H	-2.460774000000	1.604913000000	2.785757000000
C	-2.305924000000	2.695242000000	2.877208000000
H	-0.568851000000	2.331070000000	4.111368000000
C	-0.837987000000	2.921474000000	3.221106000000
H	-0.156568000000	2.624182000000	2.410290000000
C	-3.176477000000	3.202296000000	4.028009000000
H	-3.043164000000	4.289687000000	4.163910000000
H	-4.251761000000	3.024560000000	3.864907000000
H	-2.894976000000	2.708900000000	4.972640000000
C	-3.569961000000	2.719525000000	0.640616000000

C	-2.731762000000	3.348446000000	1.577342000000
C	-2.347265000000	4.664128000000	1.306577000000
H	-1.678902000000	5.177116000000	2.003892000000
C	-2.783452000000	5.317413000000	0.164701000000
H	-2.456617000000	6.341806000000	-0.035694000000
C	-3.650774000000	4.684324000000	-0.719532000000
H	-4.011545000000	5.226585000000	-1.597574000000
C	-4.087917000000	3.378773000000	-0.492602000000
C	-5.170511000000	2.772118000000	-1.365358000000
H	-5.035282000000	1.675084000000	-1.370187000000
C	-5.119970000000	3.237450000000	-2.813836000000
H	-5.446578000000	4.286952000000	-2.917412000000
H	-4.109633000000	3.145727000000	-3.239597000000
H	-5.802477000000	2.628354000000	-3.428959000000
C	-6.549320000000	3.081321000000	-0.779236000000
H	-6.721714000000	4.171460000000	-0.751035000000
H	-7.343421000000	2.632275000000	-1.400537000000
H	-6.673974000000	2.700169000000	0.247154000000
H	-0.633601000000	3.979152000000	3.459301000000

4-W (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -5258.902975918

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -5262.759847854

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -5262.785490082

N	5.373737	12.433822	6.091932
C	5.483855	11.393720	5.208607
C	5.430010	13.656358	5.432571
H	5.356454	14.598542	5.980526
C	5.153428	12.402942	7.521092
C	6.254558	12.177626	8.380969
C	7.637788	11.830595	7.836655
H	7.482672	11.019244	7.089743
C	8.319894	13.009165	7.110963
H	9.305690	12.682180	6.727023
H	8.480024	13.857621	7.808341
H	7.741304	13.383587	6.246164
C	8.587155	11.271919	8.903679
H	8.136727	10.428400	9.457994
H	8.888131	12.056060	9.629925
H	9.507742	10.897526	8.416390
C	5.991250	12.241256	9.761667
H	6.807607	12.062602	10.473221
C	4.703316	12.512174	10.246421
H	4.528282	12.551899	11.332217
N	5.636193	11.994631	3.982048
C	5.592859	13.378405	4.105232
H	5.689894	14.027214	3.232718
C	5.792319	11.390353	2.671762
C	4.626259	11.198110	1.889894
C	3.235293	11.575089	2.392402
H	3.255312	11.515938	3.499913
C	2.882336	13.021694	1.986318
H	1.877845	13.298010	2.367416
H	2.869776	13.126183	0.881690
H	3.605064	13.759742	2.383751
C	2.139844	10.612034	1.908219
H	2.408121	9.560479	2.120766
H	1.953234	10.715393	0.819225
H	1.184775	10.834438	2.424886

C	4.807013	10.707543	0.584029
H	3.926731	10.528333	-0.049063
C	6.088316	10.452989	0.079850
H	6.206522	10.065906	-0.943530
C	7.103702	11.163062	2.187558
C	8.342320	11.450330	3.031328
H	8.082642	11.192468	4.079158
C	8.724937	12.945290	2.986789
H	9.621428	13.123508	3.613819
H	8.964382	13.255741	1.948532
H	7.922917	13.607235	3.363130
C	9.565753	10.609673	2.637540
H	9.358807	9.525080	2.638613
H	9.946266	10.892103	1.634068
H	10.383584	10.786420	3.360720
C	7.219557	10.684696	0.868922
H	8.216918	10.469069	0.464720
C	3.840139	12.660322	7.970196
C	2.666287	12.823449	7.010023
H	3.044084	12.677640	5.977751
C	2.073568	14.242349	7.087363
H	1.249516	14.363783	6.354920
H	1.660018	14.451127	8.095649
H	2.837849	15.017464	6.875118
C	1.595806	11.741239	7.242731
H	2.038390	10.731062	7.150232
H	1.140752	11.829275	8.250764
H	0.780935	11.840175	6.496713
C	3.638103	12.713919	9.361883
H	2.627271	12.899776	9.754740
Si	5.516102	9.449153	5.592680
Cl	3.919205	8.912972	4.254241
Cl	4.423050	9.426290	7.439717
W	7.551633	8.032113	5.542516
C	6.293476	6.451828	5.834955
O	5.610907	5.541284	6.119598
C	9.001877	9.467230	5.646274
O	9.872862	10.231921	5.825295
C	7.380720	8.067119	3.508959
O	7.269722	8.103622	2.345901
C	7.632225	8.103357	7.585474
O	7.655086	8.173842	8.750893
Si	9.546352	6.594883	5.263016
Cl	10.889701	7.187179	3.693138
Cl	10.928303	6.542212	6.897613
C	9.357516	4.661480	4.861304
N	8.783092	4.111722	3.739699
C	8.553230	2.753326	3.920524
H	8.112075	2.142768	3.130444
C	8.987536	2.438831	5.177004
N	9.478643	3.612789	5.736420
C	10.215224	3.560622	6.981255
C	9.544030	3.843987	8.191440
C	8.091651	4.304134	8.195338
H	7.979377	5.004327	7.339234
C	7.710768	5.082435	9.459765
H	6.704013	5.525566	9.336269
H	7.675592	4.422059	10.351571
C	7.108502	3.135956	7.979203
H	6.069960	3.519354	7.949589

H	7.285352	2.602385	7.026230
H	7.189801	2.399497	8.805570
C	10.299272	3.727685	9.371856
H	9.827471	3.952250	10.337641
C	11.651262	3.356939	9.332958
C	12.283146	3.093200	8.112035
H	13.348749	2.821108	8.095706
H	12.222869	3.284169	10.270635
C	11.573810	3.184315	6.899483
C	12.274821	2.957182	5.564210
H	11.497520	2.864992	4.778700
C	13.149104	4.170181	5.190575
H	13.956213	4.320685	5.936797
H	12.557567	5.104334	5.150711
H	13.623333	4.013523	4.200164
H	12.449796	0.776207	5.811677
C	13.080851	1.647718	5.544092
H	13.502401	1.470853	4.533699
H	13.933013	1.677642	6.253677
H	8.416368	5.910267	9.658248
H	9.025499	1.492739	5.721990
H	6.372181	4.488671	3.951797
C	6.020930	4.629966	2.910759
H	4.111186	5.380842	3.634267
C	4.913528	5.693406	2.938297
H	5.276387	6.675601	3.283876
C	5.434484	3.288973	2.416634
H	5.037383	3.394747	1.385819
H	6.184427	2.473777	2.393994
H	4.600906	2.966393	3.072914
C	8.554649	4.741126	2.454528
C	7.224418	5.012705	2.058275
C	7.039837	5.578336	0.782073
H	6.022555	5.829789	0.451787
C	8.128045	5.845555	-0.052588
H	7.962075	6.309215	-1.036672
C	9.429163	5.512438	0.348946
H	10.270976	5.698276	-0.331697
C	9.675792	4.929309	1.603885
C	11.066387	4.419599	1.975845
H	11.198325	4.574968	3.064703
C	12.205762	5.174470	1.279252
H	12.236934	4.963156	0.190188
H	12.113472	6.266940	1.426030
H	13.179922	4.855800	1.700854
C	11.182130	2.907056	1.689643
H	11.056992	2.700731	0.606589
H	12.180425	2.532556	1.996433
H	10.422965	2.315303	2.235954
H	4.451809	5.833021	1.939437

4-W (M06/def2-SVP)

E (M06/def2-SVP) = -5255.8440104

E (M06/def2-TZVPP//M06/def2-SVP) = -5259.7060743

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -5259.7266488

N	4.234186000000	1.372830000000	0.952756000000
C	3.921444000000	0.186447000000	0.359443000000
C	5.245543000000	1.199012000000	1.877710000000
H	5.637625000000	2.038966000000	2.446038000000

C	3.736055000000	2.704500000000	0.683792000000
C	2.867029000000	3.298398000000	1.616633000000
C	2.432686000000	2.613565000000	2.898364000000
H	2.589107000000	1.525225000000	2.781477000000
C	3.298693000000	3.095731000000	4.063900000000
H	3.019852000000	2.575184000000	4.994595000000
H	3.156291000000	4.178045000000	4.227741000000
H	4.375456000000	2.931524000000	3.898067000000
C	0.964738000000	2.833746000000	3.247827000000
H	0.279152000000	2.521259000000	2.445917000000
H	0.755001000000	3.892083000000	3.477075000000
H	0.706544000000	2.251915000000	4.146917000000
C	2.474296000000	4.616955000000	1.370875000000
H	1.784620000000	5.105645000000	2.064742000000
C	2.928915000000	5.304807000000	0.256914000000
H	2.593828000000	6.330040000000	0.075780000000
N	4.754815000000	-0.719885000000	0.933915000000
C	5.570515000000	-0.112604000000	1.869436000000
H	6.320376000000	-0.681103000000	2.415688000000
C	5.036321000000	-2.084529000000	0.556132000000
C	6.060361000000	-2.288564000000	-0.378312000000
C	6.762951000000	-1.148955000000	-1.088188000000
H	6.400550000000	-0.194819000000	-0.663802000000
C	8.269893000000	-1.190436000000	-0.862662000000
H	8.757730000000	-0.318151000000	-1.328688000000
H	8.722371000000	-2.094266000000	-1.305549000000
H	8.520613000000	-1.186402000000	0.211527000000
C	6.412916000000	-1.128598000000	-2.573149000000
H	5.323641000000	-1.062779000000	-2.728719000000
H	6.769571000000	-2.041475000000	-3.081012000000
H	6.888536000000	-0.266260000000	-3.070649000000
C	6.391190000000	-3.612952000000	-0.677566000000
H	7.178134000000	-3.819043000000	-1.410541000000
C	5.730343000000	-4.668609000000	-0.062324000000
H	6.004490000000	-5.698742000000	-0.308213000000
C	4.333103000000	-3.124084000000	1.180914000000
C	3.194940000000	-2.838480000000	2.135723000000
H	2.722086000000	-1.895821000000	1.802117000000
C	3.686146000000	-2.623538000000	3.564751000000
H	2.839424000000	-2.356338000000	4.217739000000
H	4.150179000000	-3.545704000000	3.957633000000
H	4.430913000000	-1.815056000000	3.642317000000
C	2.115174000000	-3.908376000000	2.105054000000
H	1.788751000000	-4.128087000000	1.076479000000
H	2.455491000000	-4.847953000000	2.574725000000
H	1.230730000000	-3.570094000000	2.668939000000
C	4.711423000000	-4.427122000000	0.853965000000
H	4.186785000000	-5.270102000000	1.311600000000
C	4.271218000000	3.399336000000	-0.420426000000
C	5.371752000000	2.821148000000	-1.290692000000
H	5.227017000000	1.727219000000	-1.343097000000
C	6.741283000000	3.092133000000	-0.666365000000
H	7.541309000000	2.652151000000	-1.286501000000
H	6.927527000000	4.178253000000	-0.598053000000
H	6.841858000000	2.674606000000	0.348321000000
C	5.356727000000	3.342832000000	-2.720503000000
H	4.357177000000	3.270809000000	-3.173493000000
H	5.688109000000	4.394388000000	-2.775954000000
H	6.052322000000	2.756959000000	-3.342779000000
C	3.824227000000	4.705709000000	-0.622857000000

H	4.196425000000	5.275866000000	-1.478044000000
Si	2.329597000000	-0.183737000000	-0.822506000000
Cl	2.894835000000	-2.071452000000	-1.656326000000
Cl	2.827806000000	1.075713000000	-2.476206000000
W	-0.002443000000	-0.028682000000	0.023092000000
C	-0.420516000000	0.104023000000	-1.984538000000
O	-0.606353000000	0.244142000000	-3.118517000000
C	0.582236000000	-0.198850000000	1.986401000000
O	0.944186000000	-0.371771000000	3.073146000000
C	-0.238323000000	-2.067119000000	0.121882000000
O	-0.381720000000	-3.208438000000	0.230884000000
C	0.142165000000	2.020386000000	-0.026003000000
O	0.203652000000	3.172377000000	-0.081704000000
Si	-2.351240000000	0.173495000000	0.835603000000
Cl	-2.924233000000	-1.036521000000	2.503163000000
Cl	-2.898963000000	2.093001000000	1.612290000000
C	-3.957567000000	-0.190363000000	-0.332075000000
N	-4.349724000000	-1.395476000000	-0.832174000000
C	-5.422311000000	-1.237516000000	-1.688845000000
H	-5.887321000000	-2.093010000000	-2.172898000000
C	-5.696799000000	0.084072000000	-1.742058000000
N	-4.790711000000	0.712183000000	-0.910060000000
C	-4.946658000000	2.125044000000	-0.666594000000
C	-4.132058000000	3.032265000000	-1.362158000000
C	-2.997701000000	2.553840000000	-2.246574000000
H	-2.501665000000	1.724169000000	-1.702845000000
C	-1.932726000000	3.612719000000	-2.482211000000
H	-1.060493000000	3.158921000000	-2.980729000000
H	-2.301942000000	4.420130000000	-3.139169000000
C	-3.485451000000	2.007296000000	-3.587622000000
H	-2.628008000000	1.646044000000	-4.178381000000
H	-4.186690000000	1.163453000000	-3.484413000000
H	-3.993534000000	2.799553000000	-4.165662000000
C	-4.390537000000	4.388120000000	-1.154574000000
H	-3.781489000000	5.138277000000	-1.664279000000
C	-5.400614000000	4.804927000000	-0.291790000000
C	-6.170968000000	3.876751000000	0.395330000000
H	-6.944025000000	4.220693000000	1.090376000000
H	-5.577866000000	5.874325000000	-0.144823000000
C	-5.959844000000	2.506115000000	0.222935000000
C	-6.769823000000	1.504140000000	1.021976000000
H	-6.461347000000	0.484888000000	0.725372000000
C	-6.481493000000	1.626858000000	2.515149000000
H	-6.803299000000	2.607151000000	2.907410000000
H	-5.405423000000	1.516270000000	2.723791000000
H	-7.025910000000	0.849441000000	3.077393000000
H	-8.473460000000	1.516430000000	-0.350443000000
C	-8.260211000000	1.626334000000	0.726188000000
H	-8.830386000000	0.852756000000	1.266633000000
H	-8.655132000000	2.606638000000	1.043740000000
H	-1.577978000000	4.059878000000	-1.540608000000
H	-6.453833000000	0.652653000000	-2.278282000000
H	-2.526798000000	-1.474973000000	-2.525462000000
C	-2.484502000000	-2.558977000000	-2.747011000000
H	-0.724929000000	-2.227533000000	-3.953808000000
C	-1.050848000000	-2.896683000000	-3.142226000000
H	-0.332282000000	-2.785104000000	-2.316252000000
C	-3.398376000000	-2.836713000000	-3.941275000000
H	-3.385599000000	-3.912351000000	-4.190444000000
H	-4.446200000000	-2.552482000000	-3.760883000000

H	-3.050712000000	-2.280745000000	-4.827583000000
C	-3.846679000000	-2.728218000000	-0.577071000000
C	-2.970591000000	-3.301909000000	-1.516741000000
C	-2.600823000000	-4.633042000000	-1.308907000000
H	-1.907377000000	-5.109916000000	-2.006716000000
C	-3.078705000000	-5.348941000000	-0.221294000000
H	-2.762652000000	-6.385243000000	-0.071540000000
C	-3.963848000000	-4.761241000000	0.675262000000
H	-4.345338000000	-5.346808000000	1.516335000000
C	-4.388657000000	-3.441870000000	0.509092000000
C	-5.465927000000	-2.864049000000	1.406525000000
H	-5.330604000000	-1.767775000000	1.433965000000
C	-5.388144000000	-3.362217000000	2.843023000000
H	-5.702503000000	-4.416993000000	2.927917000000
H	-4.371656000000	-3.269153000000	3.254261000000
H	-6.066904000000	-2.774685000000	3.482300000000
C	-6.852773000000	-3.162762000000	0.835899000000
H	-7.019502000000	-4.252386000000	0.773165000000
H	-7.637636000000	-2.739854000000	1.485892000000
H	-6.998668000000	-2.746218000000	-0.173522000000
H	-0.970139000000	-3.928522000000	-3.524411000000

5a-Cr (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -3979.650234218

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3982.115306769

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3982.167014197

N	5.856919	12.589570	5.957724
C	5.785147	11.768148	4.845380
C	5.981344	13.968037	5.678211
C	5.665451	12.153175	7.318468
C	6.787360	12.042480	8.171121
C	8.177071	12.437357	7.694702
H	8.193903	12.318850	6.595097
C	8.404023	13.936714	7.982254
H	9.399633	14.256532	7.607818
H	8.362697	14.136953	9.074489
H	7.620134	14.534333	7.471315
C	9.306180	11.576847	8.278319
H	9.137205	10.497098	8.103908
H	9.422634	11.733433	9.371572
H	10.269469	11.848501	7.802078
C	6.560472	11.653884	9.505252
H	7.417482	11.539318	10.184296
C	5.266609	11.398350	9.970479
H	5.110935	11.073016	11.011086
N	5.875711	12.640644	3.797286
C	5.994099	13.952807	4.291171
H	6.044065	14.772067	3.564518
C	5.610686	12.402391	2.405126
C	4.284832	12.606036	1.957650
C	3.155569	12.923349	2.931246
H	3.615119	13.187370	3.904135
C	2.331521	14.143128	2.487739
H	1.572601	14.394300	3.257031
H	1.790060	13.954749	1.536575
H	2.977458	15.032319	2.341666
C	2.266513	11.687475	3.164909
H	2.858772	10.828707	3.533520
H	1.764780	11.372414	2.225417

H	1.480756	11.913268	3.915247
C	4.029985	12.439702	0.583218
H	3.004870	12.572775	0.204500
C	5.059206	12.094602	-0.301323
H	4.841669	11.964121	-1.373006
C	6.669717	12.045359	1.538022
C	8.061273	11.780694	2.095106
H	7.909927	11.250918	3.057469
C	8.817715	13.086168	2.410758
H	9.797783	12.853634	2.873175
H	8.994517	13.668518	1.481466
H	8.258004	13.723937	3.120622
C	8.909157	10.864640	1.205536
H	8.370825	9.931934	0.952259
H	9.210301	11.370378	0.263179
H	9.837679	10.580867	1.739439
C	6.364758	11.898545	0.173488
H	7.157877	11.604785	-0.528224
C	4.337378	11.968621	7.782989
C	3.144342	12.311441	6.897146
H	3.413216	12.016513	5.863081
C	2.912849	13.837690	6.908856
H	2.111309	14.114294	6.190915
H	2.600351	14.173686	7.920586
H	3.842251	14.379494	6.631715
C	1.859512	11.557852	7.259472
H	2.025769	10.463591	7.283068
H	1.456674	11.876079	8.244564
H	1.073734	11.768764	6.505298
C	4.165511	11.567745	9.119538
H	3.150428	11.393521	9.503774
Si	5.859074	9.832499	4.783216
Cl	5.158706	9.389377	2.801759
Cl	4.106471	9.285289	5.896260
Cr	7.787243	8.570419	5.382351
C	9.225357	7.555793	5.949928
O	10.135338	6.918076	6.317564
C	6.618763	7.104921	5.302279
O	5.912688	6.180829	5.224042
C	8.845643	10.099396	5.226466
O	9.548492	11.018789	5.049460
C	8.155583	8.195443	3.589060
O	8.391755	7.903618	2.483832
C	7.254561	8.809533	7.170669
O	6.923116	8.835981	8.286795

5a-Cr (M06/def2-SVP)

E (M06/def2-SVP) = -3977.7125761

E (M06/def2-TZVPP//M06/def2-SVP) = -3980.1776922

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -3980.2297044

N	-0.048987000000	1.646383000000	1.028849000000
C	0.573907000000	0.618333000000	0.367100000000
C	0.667583000000	2.172812000000	2.119668000000
C	-1.291279000000	2.261640000000	0.653837000000
C	-2.450138000000	1.963896000000	1.390672000000
C	-2.418249000000	1.058739000000	2.603232000000
H	-1.545863000000	0.388505000000	2.508604000000
C	-2.202727000000	1.902557000000	3.859376000000
H	-2.163026000000	1.259861000000	4.756149000000

H	-3.035644000000	2.617850000000	3.989338000000
H	-1.258281000000	2.465657000000	3.784047000000
C	-3.660183000000	0.190962000000	2.756288000000
H	-3.909662000000	-0.357548000000	1.833919000000
H	-4.545160000000	0.789586000000	3.036804000000
H	-3.505376000000	-0.550408000000	3.557406000000
C	-3.634466000000	2.616947000000	1.037586000000
H	-4.554814000000	2.390680000000	1.584819000000
C	-3.662186000000	3.537372000000	0.000784000000
H	-4.603080000000	4.024924000000	-0.273705000000
N	1.732922000000	0.451865000000	1.046447000000
C	1.788280000000	1.379263000000	2.092183000000
H	2.686128000000	1.385703000000	2.715006000000
C	2.915525000000	-0.267188000000	0.679027000000
C	3.889371000000	0.439636000000	-0.043352000000
C	3.661169000000	1.859630000000	-0.522566000000
H	2.731282000000	2.231782000000	-0.057777000000
C	4.776981000000	2.794365000000	-0.072421000000
H	4.552311000000	3.834247000000	-0.363596000000
H	5.747282000000	2.528463000000	-0.528167000000
H	4.899842000000	2.770558000000	1.023133000000
C	3.458232000000	1.911358000000	-2.033258000000
H	2.627833000000	1.259371000000	-2.349647000000
H	4.364756000000	1.587595000000	-2.575869000000
H	3.225914000000	2.942533000000	-2.353207000000
C	5.075852000000	-0.229469000000	-0.355399000000
H	5.849376000000	0.286750000000	-0.934423000000
C	5.282229000000	-1.540849000000	0.052424000000
H	6.216666000000	-2.051406000000	-0.201443000000
C	3.094118000000	-1.594797000000	1.101297000000
C	1.994238000000	-2.322731000000	1.842655000000
H	1.044075000000	-2.027580000000	1.359733000000
C	1.918038000000	-1.896576000000	3.307308000000
H	1.098547000000	-2.427445000000	3.819069000000
H	2.863031000000	-2.141076000000	3.826160000000
H	1.733960000000	-0.816856000000	3.419824000000
C	2.087104000000	-3.836200000000	1.742708000000
H	2.194864000000	-4.176728000000	0.700694000000
H	2.931635000000	-4.233662000000	2.334396000000
H	1.165262000000	-4.289714000000	2.144911000000
C	4.301226000000	-2.214551000000	0.774508000000
H	4.473154000000	-3.252278000000	1.073354000000
C	-1.278712000000	3.247001000000	-0.354384000000
C	0.018573000000	3.728955000000	-0.973507000000
H	0.712158000000	2.869869000000	-1.016600000000
C	0.651661000000	4.788444000000	-0.069981000000
H	1.635562000000	5.098757000000	-0.467186000000
H	0.007127000000	5.685366000000	-0.023676000000
H	0.789388000000	4.411633000000	0.957863000000
C	-0.128783000000	4.264480000000	-2.389967000000
H	-0.652903000000	3.552465000000	-3.046698000000
H	-0.674314000000	5.224964000000	-2.411450000000
H	0.866107000000	4.457459000000	-2.825882000000
C	-2.491872000000	3.856302000000	-0.680090000000
H	-2.521794000000	4.609734000000	-1.472514000000
Si	-0.149506000000	-0.540780000000	-1.036239000000
Cl	1.620499000000	-1.388321000000	-1.888500000000
Cl	-0.618288000000	0.856357000000	-2.582905000000
Cr	-1.871161000000	-2.155380000000	-0.688288000000
C	-3.277281000000	-3.350865000000	-0.498418000000

O	-4.157501000000	-4.090669000000	-0.377689000000
C	-1.901195000000	-2.243027000000	-2.571345000000
O	-1.897992000000	-2.321750000000	-3.719914000000
C	-1.584493000000	-2.064049000000	1.162563000000
O	-1.350331000000	-2.075033000000	2.294927000000
C	-0.598820000000	-3.533449000000	-0.747878000000
O	0.169294000000	-4.391468000000	-0.804654000000
C	-3.063341000000	-0.689018000000	-0.765792000000
O	-3.805055000000	0.184738000000	-0.867603000000

5a-W (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -3002.363545595

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3004.701954000

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3004.752881966

N	5.770959	12.642455	5.965360
C	5.714407	11.829563	4.847485
C	5.859062	14.025850	5.696292
C	5.615603	12.179463	7.321174
C	6.764767	12.008892	8.127546
C	8.147364	12.362659	7.597180
H	8.136908	12.151511	6.509133
C	8.392300	13.877306	7.768325
H	9.372636	14.161698	7.330812
H	8.401768	14.146194	8.846439
H	7.589123	14.452886	7.260041
C	9.289492	11.552346	8.224113
H	9.129791	10.461511	8.130755
H	9.419796	11.791759	9.300472
H	10.242926	11.796613	7.715325
C	6.570988	11.595656	9.459433
H	7.445145	11.435316	10.105813
C	5.285309	11.369740	9.963456
H	5.156294	11.026001	11.001739
N	5.783971	12.709878	3.807235
C	5.870606	14.021859	4.309309
H	5.909337	14.846429	3.587940
C	5.586632	12.457398	2.408417
C	4.286002	12.662389	1.892317
C	3.115279	13.004694	2.808215
H	3.537078	13.372961	3.764950
C	2.239858	14.135627	2.244725
H	1.461379	14.420898	2.981712
H	1.715604	13.832060	1.313891
H	2.842654	15.037939	2.016422
C	2.280986	11.749717	3.129544
H	2.900384	10.955239	3.586262
H	1.825713	11.328036	2.208466
H	1.462846	12.000431	3.836296
C	4.099037	12.467615	0.510810
H	3.096245	12.600270	0.077141
C	5.168777	12.094409	-0.312381
H	5.003886	11.941619	-1.390494
C	6.686652	12.074622	1.604784
C	8.049162	11.814962	2.235350
H	7.854762	11.254342	3.175058
C	8.770825	13.121544	2.622220
H	9.728256	12.887676	3.128677
H	8.989087	13.726906	1.716812
H	8.167992	13.737760	3.315412

C	8.961347	10.934079	1.374533
H	8.453778	10.003734	1.057940
H	9.313576	11.471433	0.468126
H	9.858650	10.646404	1.957392
C	6.447798	11.899738	0.230298
H	7.271563	11.586236	-0.425738
C	4.300033	12.008384	7.820909
C	3.088829	12.370954	6.968412
H	3.342434	12.112734	5.920144
C	2.846143	13.893959	7.033629
H	2.024929	14.186547	6.344876
H	2.557393	14.195987	8.063065
H	3.765980	14.448090	6.748584
C	1.817988	11.592233	7.328444
H	1.996399	10.499721	7.311934
H	1.430105	11.872524	8.330940
H	1.016220	11.820017	6.596185
C	4.161139	11.584133	9.154176
H	3.155168	11.421799	9.566922
Si	5.816046	9.898603	4.783506
Cl	5.091522	9.433684	2.813463
Cl	4.101813	9.322287	5.944858
W	7.908404	8.498199	5.369651
C	9.447480	7.298473	5.906345
O	10.331345	6.601605	6.231377
C	6.582059	6.920983	5.303942
O	5.838661	6.028613	5.223017
C	9.180742	10.099153	5.208211
O	9.934279	10.976137	5.029936
C	8.225972	8.101212	3.381091
O	8.371753	7.808398	2.261290
C	7.371221	8.716231	7.350595
O	7.033398	8.717612	8.464552

5a-W (M06/def2-SVP)

E (M06/def2-SVP) = -3000.5335286

E (M06/def2-TZVPP//M06/def2-SVP) = -3002.8718326

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -3002.9232215

N	1.255457000000	1.597920000000	1.024358000000
C	1.266582000000	0.387119000000	0.378623000000
C	2.190037000000	1.723630000000	2.068923000000
C	0.454802000000	2.734721000000	0.667819000000
C	-0.653557000000	3.068358000000	1.465923000000
C	-1.005495000000	2.296088000000	2.719845000000
H	-0.577882000000	1.282158000000	2.626278000000
C	-0.340067000000	2.958921000000	3.925574000000
H	-0.565211000000	2.399290000000	4.850121000000
H	-0.716842000000	3.990634000000	4.051462000000
H	0.753108000000	2.991575000000	3.788420000000
C	-2.503483000000	2.151665000000	2.952466000000
H	-3.028222000000	1.727507000000	2.080100000000
H	-2.976201000000	3.120363000000	3.191492000000
H	-2.688334000000	1.484043000000	3.810066000000
C	-1.382039000000	4.211974000000	1.126448000000
H	-2.258290000000	4.485444000000	1.722976000000
C	-1.020650000000	4.996967000000	0.041558000000
H	-1.617214000000	5.876460000000	-0.220813000000
N	2.231396000000	-0.311448000000	1.019987000000
C	2.780941000000	0.483764000000	2.030252000000

H	3.599421000000	0.060463000000	2.617382000000
C	2.870965000000	-1.532825000000	0.638774000000
C	3.997058000000	-1.436698000000	-0.193669000000
C	4.466771000000	-0.112161000000	-0.760941000000
H	3.909902000000	0.694278000000	-0.253274000000
C	5.943762000000	0.131920000000	-0.476442000000
H	6.241352000000	1.139190000000	-0.813249000000
H	6.590748000000	-0.592985000000	-1.001606000000
H	6.160801000000	0.059091000000	0.602333000000
C	4.156667000000	-0.000988000000	-2.250234000000
H	3.079826000000	-0.121555000000	-2.451693000000
H	4.694706000000	-0.770664000000	-2.832469000000
H	4.465583000000	0.987849000000	-2.633114000000
C	4.655589000000	-2.623040000000	-0.527997000000
H	5.524308000000	-2.588368000000	-1.194395000000
C	4.214550000000	-3.846190000000	-0.037813000000
H	4.741077000000	-4.765768000000	-0.312378000000
C	2.400585000000	-2.754000000000	1.145601000000
C	1.159169000000	-2.807260000000	2.008807000000
H	0.501655000000	-1.981642000000	1.678242000000
C	1.489626000000	-2.559542000000	3.478447000000
H	0.570995000000	-2.575722000000	4.088777000000
H	2.168461000000	-3.345133000000	3.857788000000
H	1.975488000000	-1.583168000000	3.631923000000
C	0.376701000000	-4.101441000000	1.848338000000
H	0.200219000000	-4.345654000000	0.788478000000
H	0.897845000000	-4.955160000000	2.317991000000
H	-0.605012000000	-4.015602000000	2.343555000000
C	3.100845000000	-3.908995000000	0.793961000000
H	2.754794000000	-4.880397000000	1.159499000000
C	0.884907000000	3.558181000000	-0.392713000000
C	2.212626000000	3.324830000000	-1.086673000000
H	2.382035000000	2.233821000000	-1.136152000000
C	3.338512000000	3.935613000000	-0.250519000000
H	4.322016000000	3.715755000000	-0.704705000000
H	3.225993000000	5.034199000000	-0.203398000000
H	3.331797000000	3.546685000000	0.781936000000
C	2.270881000000	3.853357000000	-2.511597000000
H	1.427729000000	3.491417000000	-3.120688000000
H	2.273800000000	4.957574000000	-2.540297000000
H	3.204841000000	3.524058000000	-2.997327000000
C	0.108497000000	4.676552000000	-0.703832000000
H	0.403567000000	5.321989000000	-1.536911000000
Si	-0.016145000000	-0.293765000000	-0.930716000000
Cl	0.979210000000	-2.001800000000	-1.754016000000
Cl	0.233408000000	1.057776000000	-2.570893000000
W	-2.518069000000	-0.816103000000	-0.433340000000
C	-4.499542000000	-1.149118000000	-0.147882000000
O	-5.632060000000	-1.325832000000	0.015212000000
C	-2.679007000000	-0.890552000000	-2.497382000000
O	-2.735417000000	-0.964363000000	-3.643939000000
C	-2.101291000000	-0.898577000000	1.583897000000
O	-1.818707000000	-1.034112000000	2.695847000000
C	-2.155101000000	-2.845562000000	-0.500660000000
O	-1.976390000000	-3.981894000000	-0.572076000000
C	-2.847232000000	1.232851000000	-0.555338000000
O	-3.055404000000	2.354710000000	-0.696988000000

5b-Cr (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -3979.658702868

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3982.124184427
 E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3982.175007027

Cr	0.344263	-0.027962	0.070188
O	-2.625501	-0.384780	0.491641
O	0.416848	-3.001564	-0.541916
O	0.184931	0.395329	-2.936923
O	-0.377233	2.866173	0.703782
O	1.157531	-0.779086	2.901542
N	3.298821	1.250196	-0.139598
N	4.603649	-0.418125	-0.558299
C	4.619075	0.932661	-0.355127
C	2.434131	0.129330	-0.204276
C	3.302760	-0.913299	-0.470865
H	3.108405	-1.981412	-0.595383
C	2.867513	2.592941	0.133974
C	2.529761	3.428739	-0.952789
C	2.185622	4.760579	-0.664076
H	1.926554	5.441376	-1.488163
C	2.171455	5.231275	0.654579
H	1.905878	6.280071	0.859744
C	2.476775	4.369386	1.714080
H	2.443022	4.743090	2.748242
C	2.824595	3.028348	1.476654
C	2.556922	2.916204	-2.385070
H	2.495574	1.810599	-2.336793
C	3.880485	3.276549	-3.085511
H	3.880176	2.895007	-4.128368
H	4.760092	2.852296	-2.566288
H	4.019018	4.377459	-3.120032
C	1.345257	3.406785	-3.194545
H	0.395118	3.213922	-2.659220
H	1.298395	2.882702	-4.170044
H	1.407405	4.495532	-3.404518
C	3.139812	2.091337	2.634665
H	3.106252	1.056426	2.239681
C	2.082176	2.190803	3.747344
H	2.230601	1.385094	4.493787
H	1.058064	2.092103	3.338647
H	2.144588	3.161623	4.282411
C	4.554583	2.328759	3.193240
H	5.338406	2.153036	2.427657
H	4.754191	1.647746	4.046775
H	4.673191	3.374112	3.546599
C	5.767758	-1.254092	-0.640128
C	6.248777	-1.644359	-1.911220
C	7.362772	-2.503893	-1.941755
H	7.770637	-2.824038	-2.911356
C	7.966324	-2.945030	-0.755809
H	8.840712	-3.612944	-0.803283
C	7.469629	-2.536172	0.489224
H	7.954810	-2.884841	1.412915
C	6.356092	-1.679520	0.575614
C	5.561623	-1.169466	-3.185202
H	5.101706	-0.188876	-2.946765
C	4.437402	-2.140877	-3.598420
H	4.847321	-3.150217	-3.814707
H	3.923641	-1.775031	-4.511414
H	3.672274	-2.244682	-2.805831
C	6.543070	-0.938698	-4.342694

H	7.363578	-0.265148	-4.029170
H	6.016263	-0.465935	-5.196399
H	6.980218	-1.889818	-4.714516
C	5.773265	-1.269277	1.923404
H	5.143679	-0.373706	1.753255
C	4.852916	-2.374645	2.476627
H	4.043949	-2.617183	1.760156
H	4.372283	-2.045692	3.420639
H	5.423538	-3.305440	2.680919
C	6.855327	-0.856867	2.931060
H	7.515705	-1.705178	3.209604
H	6.384433	-0.484914	3.863624
H	7.475294	-0.040628	2.508275
C	-1.472712	-0.243469	0.326472
C	0.421153	-1.854598	-0.309483
C	0.231353	0.271388	-1.776972
C	0.008002	1.792918	0.457640
C	0.820099	-0.448100	1.833141
Si	6.376501	1.808903	0.029218
Cl	7.140781	1.671316	-2.052145
Cl	5.777199	3.911714	0.002355

5b-Cr (M06/def2-SVP)

E (M06/def2-SVP) = -3977.720824

E (M06/def2-TZVPP//M06/def2-SVP) = -3980.1863836

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -3980.2371945

Cr	-2.664756000000	-1.796795000000	-0.355542000000
O	-5.291468000000	-3.250248000000	-0.546627000000
O	-1.328417000000	-4.490603000000	-0.733197000000
O	-2.312986000000	-1.352157000000	-3.339415000000
O	-4.455933000000	0.657111000000	-0.098812000000
O	-2.275254000000	-2.200489000000	2.628876000000
N	-0.349327000000	0.478929000000	0.037578000000
N	1.494702000000	-0.610257000000	-0.065171000000
C	1.003224000000	0.635746000000	0.113397000000
C	-0.746676000000	-0.857902000000	-0.191066000000
C	0.453942000000	-1.513066000000	-0.249986000000
H	0.679806000000	-2.569880000000	-0.395774000000
C	-1.258960000000	1.582455000000	0.132998000000
C	-1.593689000000	2.277790000000	-1.039751000000
C	-2.428973000000	3.389212000000	-0.919716000000
H	-2.696212000000	3.957946000000	-1.816364000000
C	-2.914791000000	3.790432000000	0.317984000000
H	-3.562327000000	4.669591000000	0.392285000000
C	-2.589849000000	3.068705000000	1.458523000000
H	-2.987888000000	3.382112000000	2.429355000000
C	-1.764536000000	1.945376000000	1.390965000000
C	-1.063153000000	1.875189000000	-2.399878000000
H	-0.655502000000	0.850672000000	-2.315019000000
C	0.074075000000	2.791678000000	-2.842965000000
H	0.438168000000	2.498110000000	-3.843029000000
H	0.929181000000	2.771113000000	-2.149029000000
H	-0.273516000000	3.838912000000	-2.903652000000
C	-2.166065000000	1.837993000000	-3.452621000000
H	-3.037784000000	1.254707000000	-3.113398000000
H	-1.795073000000	1.371721000000	-4.380264000000
H	-2.516178000000	2.852243000000	-3.713667000000
C	-1.453645000000	1.169054000000	2.653950000000
H	-1.003508000000	0.202698000000	2.358287000000

C	-2.721560000000	0.856071000000	3.443402000000
H	-2.503656000000	0.146391000000	4.258413000000
H	-3.500293000000	0.408042000000	2.804148000000
H	-3.147586000000	1.765593000000	3.902596000000
C	-0.447730000000	1.902736000000	3.536137000000
H	0.524567000000	2.045349000000	3.035332000000
H	-0.270275000000	1.342490000000	4.470498000000
H	-0.821335000000	2.906142000000	3.808022000000
C	2.848395000000	-1.036875000000	0.110835000000
C	3.689841000000	-1.150974000000	-1.008854000000
C	4.979094000000	-1.644566000000	-0.794440000000
H	5.663931000000	-1.744265000000	-1.641849000000
C	5.406167000000	-2.008813000000	0.477794000000
H	6.421131000000	-2.392954000000	0.621253000000
C	4.552369000000	-1.885900000000	1.567412000000
H	4.898260000000	-2.176930000000	2.564639000000
C	3.253075000000	-1.397700000000	1.408265000000
C	3.206862000000	-0.806973000000	-2.402211000000
H	2.421657000000	-0.037025000000	-2.291233000000
C	2.595800000000	-2.032403000000	-3.078203000000
H	3.348552000000	-2.835559000000	-3.176087000000
H	2.237083000000	-1.780099000000	-4.090259000000
H	1.740695000000	-2.437121000000	-2.515402000000
C	4.298973000000	-0.212051000000	-3.279853000000
H	4.805767000000	0.624798000000	-2.775191000000
H	3.862965000000	0.169532000000	-4.217864000000
H	5.056640000000	-0.965169000000	-3.561872000000
C	2.308376000000	-1.318938000000	2.590634000000
H	1.471895000000	-0.652221000000	2.313157000000
C	1.712689000000	-2.691850000000	2.891873000000
H	1.187975000000	-3.105775000000	2.015083000000
H	0.982150000000	-2.629055000000	3.715935000000
H	2.501860000000	-3.407209000000	3.185783000000
C	2.966412000000	-0.716618000000	3.823960000000
H	3.771992000000	-1.360035000000	4.219285000000
H	2.225792000000	-0.598432000000	4.632130000000
H	3.388912000000	0.276815000000	3.599432000000
C	-4.280586000000	-2.686905000000	-0.474907000000
C	-1.815653000000	-3.453057000000	-0.587585000000
C	-2.479308000000	-1.506673000000	-2.209211000000
C	-3.705188000000	-0.213475000000	-0.172534000000
C	-2.472416000000	-2.029645000000	1.505070000000
Si	2.246532000000	2.054679000000	0.861375000000
Cl	3.431088000000	2.294946000000	-0.977685000000
Cl	1.000124000000	3.821312000000	0.626985000000

5b-W (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -3002.379861158

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3004.719166538

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3004.769437643

W	0.241850	-0.000277	0.086500
O	-2.902482	-0.377884	0.563772
O	0.351605	-3.144267	-0.596245
O	-0.064765	0.457671	-3.089786
O	-0.416975	3.089688	0.757151
O	1.049768	-0.840584	3.091015
N	3.344163	1.260969	-0.146664
N	4.644940	-0.410400	-0.560887
C	4.663252	0.940950	-0.355513

C	2.474745	0.144146	-0.218455
C	3.341882	-0.901427	-0.481922
H	3.142974	-1.968764	-0.608888
C	2.900317	2.598867	0.129980
C	2.542774	3.428440	-0.955041
C	2.195626	4.759189	-0.665699
H	1.923259	5.437266	-1.487546
C	2.190621	5.231035	0.653060
H	1.923106	6.279091	0.859044
C	2.498014	4.369337	1.712261
H	2.459707	4.741530	2.746753
C	2.847912	3.028906	1.473580
C	2.548505	2.900606	-2.382081
H	2.443750	1.798364	-2.316018
C	3.883197	3.201636	-3.089189
H	3.869695	2.801938	-4.125079
H	4.749162	2.758407	-2.562571
H	4.059978	4.296188	-3.142629
C	1.353059	3.423296	-3.194508
H	0.399032	3.272234	-2.652131
H	1.282689	2.887168	-4.161961
H	1.452622	4.505871	-3.421023
C	3.149087	2.082625	2.627933
H	3.100956	1.050780	2.224487
C	2.086498	2.188018	3.735153
H	2.222161	1.377896	4.479200
H	1.064248	2.100078	3.318655
H	2.153708	3.155884	4.274695
C	4.564223	2.299544	3.192870
H	5.348925	2.123902	2.427943
H	4.754869	1.608770	4.040529
H	4.691889	3.340299	3.556435
C	5.808118	-1.248625	-0.634837
C	6.296069	-1.642060	-1.902184
C	7.408984	-2.503290	-1.924411
H	7.822047	-2.826032	-2.890949
C	8.004879	-2.942808	-0.734044
H	8.878544	-3.612073	-0.774958
C	7.501618	-2.530467	0.507242
H	7.981127	-2.877748	1.434363
C	6.388920	-1.671955	0.585306
C	5.616951	-1.169475	-3.181296
H	5.152819	-0.189879	-2.947042
C	4.498259	-2.144287	-3.601325
H	4.912458	-3.152455	-3.814765
H	3.989171	-1.780516	-4.517789
H	3.728817	-2.250722	-2.813161
C	6.606039	-0.937526	-4.332052
H	7.422819	-0.261952	-4.013264
H	6.084307	-0.466641	-5.189897
H	7.047876	-1.887996	-4.699913
C	5.798553	-1.256944	1.928456
H	5.180236	-0.354555	1.753383
C	4.861077	-2.352520	2.472576
H	4.054467	-2.583859	1.749696
H	4.377404	-2.019944	3.413827
H	5.418862	-3.290456	2.679259
C	6.875419	-0.856483	2.946238
H	7.524399	-1.711590	3.230610
H	6.399852	-0.480220	3.874659

H	7.507871	-0.046509	2.530037
C	-1.751323	-0.232348	0.386447
C	0.339700	-2.000669	-0.349325
C	0.026448	0.333060	-1.932533
C	-0.084565	1.998424	0.514415
C	0.722319	-0.491665	2.025504
Si	6.416033	1.820362	0.034156
Cl	7.187303	1.676393	-2.043665
Cl	5.800529	3.917802	-0.004374

5b-W (M06/def2-SVP)

E (M06/def2-SVP) = -3000.549718

E (M06/def2-TZVPP//M06/def2-SVP) = -3002.8881965

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -3002.9384667

W	-2.678737000000	-1.138555000000	-0.111376000000
O	-5.707416000000	-2.128232000000	-0.083258000000
O	-1.827038000000	-4.220455000000	-0.424550000000
O	-2.510852000000	-0.951597000000	-3.322364000000
O	-3.956069000000	1.821951000000	0.102651000000
O	-2.253035000000	-1.505075000000	3.059610000000
N	0.183447000000	0.715694000000	-0.003967000000
N	1.784309000000	-0.709304000000	-0.019145000000
C	1.541653000000	0.619066000000	0.031555000000
C	-0.466230000000	-0.536587000000	-0.083978000000
C	0.586963000000	-1.411483000000	-0.091551000000
H	0.600485000000	-2.501371000000	-0.125339000000
C	-0.510374000000	1.968238000000	0.056010000000
C	-0.820214000000	2.627819000000	-1.142851000000
C	-1.421974000000	3.883818000000	-1.053837000000
H	-1.664561000000	4.427755000000	-1.972520000000
C	-1.715059000000	4.453115000000	0.178776000000
H	-2.178420000000	5.443429000000	0.227314000000
C	-1.437843000000	3.759675000000	1.349129000000
H	-1.692389000000	4.207350000000	2.315549000000
C	-0.841276000000	2.497995000000	1.313476000000
C	-0.508717000000	2.027725000000	-2.497341000000
H	-0.355200000000	0.941644000000	-2.354009000000
C	0.773330000000	2.611019000000	-3.085087000000
H	0.960646000000	2.192447000000	-4.089314000000
H	1.659622000000	2.412934000000	-2.462143000000
H	0.685582000000	3.707902000000	-3.184595000000
C	-1.668794000000	2.196108000000	-3.473395000000
H	-2.633930000000	1.917516000000	-3.018180000000
H	-1.520195000000	1.558140000000	-4.360099000000
H	-1.753452000000	3.238180000000	-3.829116000000
C	-0.577362000000	1.752082000000	2.606410000000
H	-0.331700000000	0.704662000000	2.348647000000
C	-1.816456000000	1.717651000000	3.495557000000
H	-1.665229000000	1.027965000000	4.342226000000
H	-2.707896000000	1.381315000000	2.939690000000
H	-2.040086000000	2.712445000000	3.919016000000
C	0.610410000000	2.334088000000	3.367108000000
H	1.548175000000	2.281392000000	2.787708000000
H	0.766351000000	1.793219000000	4.317120000000
H	0.440095000000	3.398907000000	3.606535000000
C	3.043638000000	-1.363223000000	0.159682000000
C	3.761100000000	-1.798234000000	-0.967117000000
C	4.941947000000	-2.510338000000	-0.741015000000
H	5.526784000000	-2.861541000000	-1.596868000000

C	5.384215000000	-2.776327000000	0.549771000000
H	6.311779000000	-3.336940000000	0.702841000000
C	4.657642000000	-2.327763000000	1.646835000000
H	5.017305000000	-2.537467000000	2.659109000000
C	3.471893000000	-1.609681000000	1.477314000000
C	3.257531000000	-1.557755000000	-2.374792000000
H	2.601889000000	-0.668949000000	-2.341435000000
C	2.433543000000	-2.748145000000	-2.861047000000
H	3.049419000000	-3.665518000000	-2.874442000000
H	2.063967000000	-2.574307000000	-3.885629000000
H	1.558211000000	-2.939224000000	-2.220895000000
C	4.376528000000	-1.252720000000	-3.361532000000
H	5.029343000000	-0.447951000000	-2.990077000000
H	3.949592000000	-0.926124000000	-4.324233000000
H	4.996270000000	-2.142569000000	-3.572852000000
C	2.666659000000	-1.153317000000	2.677568000000
H	2.016341000000	-0.323066000000	2.349936000000
C	1.759566000000	-2.270548000000	3.186080000000
H	1.057893000000	-2.612354000000	2.407383000000
H	1.156988000000	-1.923226000000	4.042882000000
H	2.354734000000	-3.140812000000	3.517475000000
C	3.542868000000	-0.601835000000	3.793354000000
H	4.167266000000	-1.384825000000	4.259095000000
H	2.914450000000	-0.174776000000	4.592484000000
H	4.203443000000	0.197081000000	3.417357000000
C	-4.605572000000	-1.763209000000	-0.096726000000
C	-2.111758000000	-3.106806000000	-0.308696000000
C	-2.602892000000	-0.995467000000	-2.174131000000
C	-3.434417000000	0.797043000000	0.041006000000
C	-2.453238000000	-1.350576000000	1.934484000000
Si	3.079320000000	1.841751000000	0.535923000000
Cl	4.113338000000	1.654496000000	-1.398801000000
Cl	2.144289000000	3.771341000000	0.186285000000

6-Cr (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -2770.389944738

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2772.436501893

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2772.452517906

Cr	0.330436	0.374430	0.288533
O	0.417679	-2.662052	0.106329
N	0.485885	-0.151578	4.579226
C	-0.850134	-0.160869	4.426172
H	-1.585786	-0.263427	5.227645
O	3.349517	0.336907	0.644997
N	-1.108287	-0.015925	3.104546
C	1.073557	0.001971	3.323756
H	2.161888	0.035740	3.229795
O	0.850887	0.805731	-2.660346
C	0.083169	0.095903	2.347145
O	0.388285	3.336840	0.979828
C	1.177228	-0.251504	5.835933
O	-2.576619	0.477712	-0.619291
C	1.551475	-1.536004	6.293324
C	2.257882	-1.599294	7.509772
H	2.571308	-2.577345	7.903006
C	2.565984	-0.433027	8.224226
H	3.120106	-0.505040	9.172272
C	2.172337	0.824152	7.743790
H	2.419461	1.728295	8.318855

C	1.464181	0.945693	6.533076
C	1.244743	-2.787451	5.478871
H	0.449198	-2.527018	4.750559
C	0.709770	-3.940684	6.342835
H	0.404194	-4.790260	5.699772
H	-0.170526	-3.627890	6.939386
H	1.478097	-4.323301	7.045612
C	2.482736	-3.214022	4.664554
H	3.325570	-3.480949	5.335182
H	2.825411	-2.400720	3.995488
H	2.251006	-4.096043	4.033935
C	1.066289	2.305360	5.969395
H	0.265452	2.136817	5.219979
C	2.254312	2.947502	5.224778
H	2.623898	2.292129	4.412342
H	3.098550	3.140375	5.918470
H	1.953406	3.911997	4.768300
C	0.493529	3.248278	7.039330
H	-0.349798	2.780380	7.585672
H	0.121985	4.179809	6.567361
H	1.259635	3.544303	7.785046
C	-2.458821	0.021396	2.607438
C	-3.064868	-1.195605	2.222564
C	-4.398290	-1.135876	1.778653
H	-4.904249	-2.058504	1.460676
C	-5.082906	0.085346	1.720831
H	-6.123205	0.111320	1.363112
C	-4.446531	1.276102	2.094550
H	-4.989490	2.229263	2.021408
C	-3.113468	1.271701	2.543943
C	-2.401915	2.557273	2.943759
H	-1.312638	2.362160	2.881819
C	-2.707965	3.718260	1.985096
H	-2.535560	3.422514	0.932483
H	-2.049993	4.581307	2.206413
H	-3.757772	4.065207	2.078830
C	-2.723064	2.935544	4.403504
H	-2.172735	3.851243	4.701933
H	-2.442738	2.127370	5.108880
H	-3.807828	3.129883	4.534198
C	-2.302249	-2.511932	2.293229
H	-1.222369	-2.265883	2.252181
C	-2.603157	-3.432053	1.100735
H	-2.475315	-2.896562	0.140443
H	-3.637184	-3.832889	1.138813
H	-1.910649	-4.296530	1.100123
C	-2.563601	-3.229056	3.633240
H	-3.637510	-3.486486	3.742567
H	-2.282816	-2.597189	4.499865
H	-1.977510	-4.168684	3.695967
C	2.188132	0.348270	0.527946
C	0.363082	-1.498011	0.157131
C	0.647412	0.638243	-1.522853
C	0.344041	2.207537	0.690437
C	-1.497889	0.425931	-0.179362

6-Cr (M06/def2-SVP)

E (M06/def2-SVP) = -2768.6437656

E (M06/def2-TZVPP//M06/def2-SVP) = -2770.7080065

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -2770.7197085

Cr	-2.104822000000	-0.394803000000	-1.793065000000
O	-1.397531000000	-3.243991000000	-1.018475000000
N	1.807039000000	0.091447000000	0.005521000000
C	1.070899000000	0.294069000000	1.092338000000
H	1.456720000000	0.465950000000	2.098122000000
O	-0.348718000000	-0.715986000000	-4.247808000000
N	-0.221421000000	0.232676000000	0.739134000000
C	0.944944000000	-0.091379000000	-1.064548000000
H	1.355642000000	-0.262640000000	-2.060137000000
O	-4.456504000000	-1.081551000000	-3.551353000000
C	-0.367543000000	-0.020520000000	-0.638687000000
O	-2.208426000000	2.595918000000	-2.334458000000
C	3.236048000000	0.031519000000	-0.042794000000
O	-4.223725000000	-0.131655000000	0.381434000000
C	3.850760000000	-1.224047000000	0.109753000000
C	5.243609000000	-1.261695000000	0.021511000000
H	5.762435000000	-2.218793000000	0.131401000000
C	5.979425000000	-0.102462000000	-0.206392000000
H	7.069695000000	-0.157169000000	-0.272701000000
C	5.339611000000	1.122575000000	-0.348668000000
H	5.930427000000	2.027098000000	-0.526769000000
C	3.947225000000	1.218244000000	-0.271884000000
C	3.043264000000	-2.491716000000	0.305202000000
H	2.052527000000	-2.208249000000	0.709031000000
C	3.682792000000	-3.449655000000	1.300986000000
H	3.009848000000	-4.299246000000	1.497459000000
H	3.902758000000	-2.958849000000	2.263046000000
H	4.625286000000	-3.873799000000	0.914813000000
C	2.804940000000	-3.183670000000	-1.035626000000
H	3.764237000000	-3.480923000000	-1.494247000000
H	2.277925000000	-2.529895000000	-1.748570000000
H	2.194066000000	-4.091372000000	-0.903428000000
C	3.263376000000	2.559293000000	-0.430367000000
H	2.171123000000	2.405882000000	-0.349495000000
C	3.531838000000	3.153138000000	-1.808620000000
H	3.210318000000	2.468923000000	-2.610458000000
H	4.605337000000	3.362103000000	-1.955863000000
H	2.988706000000	4.103365000000	-1.936358000000
C	3.675886000000	3.515519000000	0.683440000000
H	3.447086000000	3.099905000000	1.679394000000
H	3.149356000000	4.479095000000	0.588168000000
H	4.758752000000	3.725484000000	0.652414000000
C	-1.263865000000	0.377743000000	1.715146000000
C	-1.641816000000	-0.749280000000	2.461310000000
C	-2.631676000000	-0.570548000000	3.430888000000
H	-2.955388000000	-1.424768000000	4.033616000000
C	-3.215925000000	0.672591000000	3.635641000000
H	-3.992102000000	0.789572000000	4.397303000000
C	-2.828875000000	1.767315000000	2.871171000000
H	-3.308827000000	2.736267000000	3.036145000000
C	-1.844659000000	1.644466000000	1.888955000000
C	-1.416540000000	2.834760000000	1.057864000000
H	-0.993160000000	2.446762000000	0.113325000000
C	-2.584198000000	3.738292000000	0.687238000000
H	-3.422461000000	3.157452000000	0.269465000000
H	-2.273501000000	4.472881000000	-0.072215000000
H	-2.959067000000	4.304561000000	1.557160000000
C	-0.320652000000	3.624032000000	1.769645000000
H	0.004253000000	4.483191000000	1.159017000000

H	0.568055000000	3.003639000000	1.978820000000
H	-0.686247000000	4.014979000000	2.735570000000
C	-1.014711000000	-2.110873000000	2.249203000000
H	-0.474909000000	-2.092729000000	1.283497000000
C	-2.056857000000	-3.219986000000	2.160626000000
H	-2.860216000000	-2.969691000000	1.450010000000
H	-2.523177000000	-3.421473000000	3.140276000000
H	-1.589667000000	-4.156928000000	1.817497000000
C	-0.000292000000	-2.416466000000	3.348683000000
H	-0.492503000000	-2.443599000000	4.336543000000
H	0.799913000000	-1.658833000000	3.405100000000
H	0.473768000000	-3.398832000000	3.184773000000
C	-1.006429000000	-0.589194000000	-3.309901000000
C	-1.725493000000	-2.182625000000	-1.326787000000
C	-3.559879000000	-0.814860000000	-2.875883000000
C	-2.194406000000	1.462062000000	-2.132522000000
C	-3.366029000000	-0.215775000000	-0.382834000000

6-W (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -1793.109764275

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1795.030383446

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1795.046343721

W	0.038908	0.138770	0.106644
O	0.136413	-3.085275	0.085081
N	0.546142	-0.091888	4.551475
C	-0.798791	-0.094320	4.504640
H	-1.468728	-0.137582	5.367015
O	3.256531	0.113262	0.280187
N	-1.158531	-0.032975	3.201324
C	1.034268	-0.027986	3.246586
H	2.112026	-0.015163	3.063991
O	0.329317	0.333892	-3.079820
C	-0.030458	0.012456	2.347129
O	0.166221	3.339342	0.484118
C	1.332910	-0.136951	5.754363
O	-3.129312	0.187225	-0.503002
C	1.723642	-1.402679	6.249271
C	2.520434	-1.415655	7.410183
H	2.849549	-2.377653	7.829452
C	2.898794	-0.219774	8.036523
H	3.522866	-0.252582	8.942316
C	2.487833	1.017680	7.520782
H	2.791897	1.945957	8.025939
C	1.690466	1.089082	6.362608
C	1.339045	-2.689736	5.528721
H	0.503457	-2.451999	4.838661
C	0.837535	-3.779144	6.490258
H	0.476115	-4.657206	5.918318
H	0.002345	-3.412600	7.120077
H	1.640888	-4.137418	7.166109
C	2.512522	-3.190912	4.663123
H	3.391642	-3.440965	5.292446
H	2.828067	-2.424207	3.928795
H	2.222162	-4.100602	4.099627
C	1.271949	2.425229	5.759414
H	0.425380	2.231766	5.068854
C	2.419014	3.015339	4.914474
H	2.730066	2.317352	4.112867
H	3.307261	3.227393	5.544843

H	2.102577	3.962786	4.433329
C	0.775133	3.424251	6.816506
H	-0.038956	2.993411	7.433143
H	0.386062	4.338318	6.324933
H	1.587896	3.742805	7.500992
C	-2.540320	-0.012387	2.797070
C	-3.179614	-1.244930	2.536800
C	-4.545348	-1.200121	2.202706
H	-5.080499	-2.135511	1.986012
C	-5.225195	0.022423	2.119929
H	-6.291834	0.036168	1.850055
C	-4.550186	1.229230	2.345929
H	-5.088820	2.181694	2.240321
C	-3.184187	1.239676	2.682352
C	-2.420596	2.539506	2.899818
H	-1.347390	2.315079	2.732474
C	-2.816826	3.624302	1.886642
H	-2.765679	3.238570	0.850130
H	-2.127560	4.488137	1.960708
H	-3.845272	4.000797	2.064572
C	-2.573739	3.041267	4.349336
H	-1.983602	3.966790	4.508851
H	-2.226384	2.287682	5.084608
H	-3.635214	3.267753	4.580814
C	-2.409969	-2.557502	2.604748
H	-1.340737	-2.311534	2.442391
C	-2.821286	-3.534685	1.493250
H	-2.790556	-3.044687	0.500884
H	-3.844708	-3.933491	1.650428
H	-2.127485	-4.397616	1.465609
C	-2.534637	-3.205993	3.997759
H	-3.591183	-3.458832	4.224213
H	-2.174549	-2.530611	4.799769
H	-1.939706	-4.140668	4.050307
C	2.090395	0.121563	0.231511
C	0.076588	-1.920499	0.070146
C	0.216386	0.262307	-1.919425
C	0.095292	2.186266	0.322751
C	-2.001845	0.165361	-0.205758

6-W (M06/def2-SVP)

E (M06/def2-SVP) = -1791.4710999

E (M06/def2-TZVPP//M06/def2-SVP) = -1793.4083817

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -1793.4204562

W	2.112703000000	-1.194601000000	-0.552322000000
O	1.981549000000	0.197171000000	-3.455539000000
N	-2.194657000000	-0.027421000000	0.005007000000
C	-1.637712000000	1.068723000000	0.510086000000
H	-2.177876000000	1.927232000000	0.911709000000
O	0.592977000000	-3.769522000000	-1.741483000000
N	-0.306027000000	0.933169000000	0.434851000000
C	-1.175235000000	-0.874771000000	-0.400537000000
H	-1.418715000000	-1.836532000000	-0.853437000000
O	4.892724000000	-2.622849000000	-1.194083000000
C	0.054863000000	-0.299433000000	-0.141314000000
O	1.941642000000	-2.501126000000	2.389414000000
C	-3.601132000000	-0.263717000000	-0.124589000000
O	3.881606000000	1.254704000000	0.578907000000
C	-4.237297000000	0.159499000000	-1.303316000000

C	-5.605036000000	-0.103040000000	-1.417704000000
H	-6.141388000000	0.210779000000	-2.318985000000
C	-6.294155000000	-0.760849000000	-0.405141000000
H	-7.363771000000	-0.959793000000	-0.517165000000
C	-5.633905000000	-1.167288000000	0.748953000000
H	-6.189914000000	-1.687133000000	1.535488000000
C	-4.268181000000	-0.926049000000	0.919211000000
C	-3.489479000000	0.849483000000	-2.424522000000
H	-2.454718000000	1.038691000000	-2.084753000000
C	-4.105222000000	2.200639000000	-2.768068000000
H	-3.499768000000	2.718924000000	-3.529453000000
H	-4.166015000000	2.854795000000	-1.882177000000
H	-5.124469000000	2.095735000000	-3.177220000000
C	-3.394155000000	-0.054641000000	-3.649555000000
H	-4.391933000000	-0.277887000000	-4.064989000000
H	-2.909692000000	-1.013492000000	-3.403828000000
H	-2.802791000000	0.427762000000	-4.444550000000
C	-3.550365000000	-1.399173000000	2.166172000000
H	-2.539794000000	-0.949641000000	2.172961000000
C	-3.372904000000	-2.914706000000	2.138483000000
H	-2.825689000000	-3.244881000000	1.240933000000
H	-4.350386000000	-3.427283000000	2.141629000000
H	-2.810001000000	-3.258609000000	3.021291000000
C	-4.255554000000	-0.949080000000	3.439846000000
H	-4.405570000000	0.142677000000	3.459554000000
H	-3.661825000000	-1.226041000000	4.326033000000
H	-5.244734000000	-1.424833000000	3.551425000000
C	0.578614000000	1.957776000000	0.913825000000
C	0.987917000000	2.960679000000	0.020380000000
C	1.803932000000	3.973943000000	0.527428000000
H	2.145551000000	4.773160000000	-0.137063000000
C	2.197250000000	3.975925000000	1.860621000000
H	2.839933000000	4.777171000000	2.236108000000
C	1.794743000000	2.956039000000	2.714404000000
H	2.128343000000	2.959180000000	3.756626000000
C	0.979652000000	1.917819000000	2.258366000000
C	0.542857000000	0.808222000000	3.190834000000
H	0.216625000000	-0.045488000000	2.567035000000
C	1.679310000000	0.313462000000	4.077386000000
H	2.591320000000	0.107617000000	3.494316000000
H	1.391195000000	-0.620981000000	4.584828000000
H	1.936506000000	1.047841000000	4.859814000000
C	-0.647116000000	1.252728000000	4.037510000000
H	-0.975198000000	0.443752000000	4.711313000000
H	-1.510412000000	1.552554000000	3.418803000000
H	-0.376517000000	2.121286000000	4.663384000000
C	0.559597000000	2.959552000000	-1.431879000000
H	0.253738000000	1.928143000000	-1.688942000000
C	1.694465000000	3.340959000000	-2.373550000000
H	2.607220000000	2.760244000000	-2.163589000000
H	1.948610000000	4.412143000000	-2.297616000000
H	1.407367000000	3.148695000000	-3.419511000000
C	-0.648400000000	3.868961000000	-1.642522000000
H	-0.405232000000	4.911086000000	-1.370632000000
H	-1.513213000000	3.560702000000	-1.029832000000
H	-0.966116000000	3.862054000000	-2.698888000000
C	1.136857000000	-2.846710000000	-1.316241000000
C	2.050446000000	-0.308072000000	-2.422750000000
C	3.889742000000	-2.100462000000	-0.958995000000
C	2.026093000000	-2.040159000000	1.337198000000

C 3.206199000000 0.407677000000 0.187393000000

8-Cr (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -2770.413972790

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2772.457943691

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2772.471303505

Cr	5.622710	9.803063	4.939723
N	5.625078	12.757975	6.017223
C	5.624585	11.895688	4.939719
C	5.625692	14.095647	5.622293
H	5.626124	14.909252	6.351293
C	5.625358	12.399614	7.410022
C	6.868685	12.258630	8.069408
C	8.185787	12.393373	7.317440
H	7.968794	12.220458	6.244146
C	8.752787	13.820685	7.450360
H	9.698742	13.921047	6.879813
H	8.965350	14.063187	8.512269
H	8.043125	14.579853	7.066398
C	9.218477	11.341835	7.752512
H	8.789348	10.321752	7.729616
H	9.593631	11.534070	8.778863
H	10.092177	11.357585	7.071674
C	6.841349	11.985501	9.449022
H	7.787961	11.858776	9.993542
C	5.626110	11.857639	10.133751
H	5.626407	11.637757	11.211967
O	5.619157	6.781373	4.939756
C	5.620543	7.947969	4.939759
O	2.578615	9.835978	4.939810
C	3.744300	9.847735	4.939767
O	5.622243	9.232737	1.952909
C	5.622526	9.578484	3.065857
N	5.624999	12.758007	3.862242
C	5.625640	14.095668	4.257213
H	5.626020	14.909294	3.528238
C	5.625180	12.399688	2.469436
C	4.382172	12.260867	1.809034
C	3.064674	12.397707	2.559920
H	3.280677	12.225565	3.633534
C	2.499245	13.825472	2.425226
H	1.552960	13.927354	2.994955
H	2.287733	14.067212	1.362932
H	3.209411	14.584271	2.808998
C	2.031262	11.346784	2.125033
H	2.459357	10.326297	2.149268
H	1.657164	11.538383	1.098178
H	1.157019	11.364081	2.805136
C	4.410157	11.987693	0.429436
H	3.463766	11.862625	-0.115856
C	5.625730	11.857645	-0.254271
H	5.625946	11.637733	-1.332481
C	6.868459	12.258698	1.809966
C	8.185607	12.393420	2.561862
H	7.968639	12.220657	3.635185
C	8.752731	13.820665	2.428744
H	9.698719	13.921011	2.999241
H	8.965274	14.063016	1.366796
H	8.043154	14.579944	2.812641

C	9.218186	11.341729	2.126898
H	8.788966	10.321686	2.149963
H	9.593317	11.533780	1.100504
H	10.091915	11.357501	2.807698
C	6.841022	11.985531	0.430362
H	7.787592	11.858791	-0.114226
C	4.382399	12.260830	8.070530
C	3.064833	12.397724	7.319776
H	3.280686	12.225411	6.246159
C	2.499595	13.825577	7.454346
H	1.553255	13.927499	6.884716
H	2.288239	14.067486	8.516633
H	3.209809	14.584236	7.070388
C	2.031345	11.346993	7.754948
H	2.459314	10.326452	7.730834
H	1.657387	11.538805	8.781814
H	1.157027	11.364282	7.074941
C	4.410489	11.987694	9.450134
H	3.464138	11.862667	9.995505
O	8.666886	9.828750	4.939654
C	7.501235	9.843395	4.939666
O	5.622390	9.233110	7.926637
C	5.622625	9.578574	6.813601

8-Cr (M06/def2-SVP)

E (M06/def2-SVP) = -2768.6663734

E (M06/def2-TZVPP//M06/def2-SVP) = -2770.7279707

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -2770.7368905

Cr	-0.000008000000	0.000029000000	1.764509000000
N	-1.069402000000	-0.000046000000	-1.215337000000
C	-0.000006000000	-0.000060000000	-0.361911000000
C	-0.675227000000	-0.000027000000	-2.545203000000
H	-1.402434000000	-0.000192000000	-3.354858000000
C	-2.463894000000	-0.000461000000	-0.885486000000
C	-3.126370000000	1.232281000000	-0.770634000000
C	-2.385837000000	2.547699000000	-0.884074000000
H	-1.317455000000	2.347117000000	-0.679860000000
C	-2.492624000000	3.107848000000	-2.299985000000
H	-1.936882000000	4.055913000000	-2.391416000000
H	-3.547166000000	3.307287000000	-2.559735000000
H	-2.091047000000	2.407024000000	-3.050156000000
C	-2.858969000000	3.569221000000	0.141415000000
H	-2.864971000000	3.148396000000	1.160213000000
H	-3.877474000000	3.930760000000	-0.081369000000
H	-2.196308000000	4.449275000000	0.142465000000
C	-4.505066000000	1.204412000000	-0.551626000000
H	-5.052311000000	2.146784000000	-0.453299000000
C	-5.188438000000	-0.001449000000	-0.449304000000
H	-6.268558000000	-0.001848000000	-0.277586000000
O	-0.000045000000	-0.000500000000	4.776869000000
C	-0.000055000000	-0.000203000000	3.624184000000
O	0.001132000000	-3.041830000000	1.653960000000
C	0.000714000000	-1.891187000000	1.694917000000
O	2.993947000000	0.000963000000	2.290719000000
C	1.887668000000	0.000707000000	1.972732000000
N	1.069358000000	0.000011000000	-1.215384000000
C	0.675126000000	0.000022000000	-2.545228000000
H	1.402283000000	0.000092000000	-3.354925000000
C	2.463888000000	0.000349000000	-0.885578000000

C	3.126384000000	-1.232371000000	-0.770627000000
C	2.385942000000	-2.547803000000	-0.884122000000
H	1.317521000000	-2.347394000000	-0.679926000000
C	2.493072000000	-3.107870000000	-2.300035000000
H	1.937736000000	-4.056161000000	-2.391576000000
H	3.547733000000	-3.306909000000	-2.559618000000
H	2.091384000000	-2.407177000000	-3.050262000000
C	2.859190000000	-3.569316000000	0.141308000000
H	2.865409000000	-3.148361000000	1.160061000000
H	3.877611000000	-3.930994000000	-0.081641000000
H	2.196434000000	-4.449316000000	0.142520000000
C	4.505052000000	-1.204441000000	-0.551520000000
H	5.052329000000	-2.146781000000	-0.453040000000
C	5.188418000000	0.001429000000	-0.449249000000
H	6.268524000000	0.001818000000	-0.277445000000
C	3.125469000000	1.233570000000	-0.770770000000
C	2.383990000000	2.548454000000	-0.884171000000
H	1.315767000000	2.347148000000	-0.679788000000
C	2.490163000000	3.108701000000	-2.300083000000
H	1.933849000000	4.056447000000	-2.391325000000
H	3.544536000000	3.308770000000	-2.560032000000
H	2.088846000000	2.407706000000	-3.050240000000
C	2.856602000000	3.570338000000	0.141205000000
H	2.863065000000	3.149634000000	1.160051000000
H	3.874873000000	3.932474000000	-0.081717000000
H	2.193438000000	4.450008000000	0.142208000000
C	4.504175000000	1.206759000000	-0.551667000000
H	5.050677000000	2.149555000000	-0.453310000000
C	-3.125468000000	-1.233644000000	-0.770633000000
C	-2.384009000000	-2.548517000000	-0.884220000000
H	-1.315711000000	-2.347307000000	-0.680095000000
C	-2.490661000000	-3.108522000000	-2.300198000000
H	-1.934588000000	-4.056369000000	-2.391830000000
H	-3.545147000000	-3.308352000000	-2.559884000000
H	-2.089463000000	-2.407381000000	-3.050283000000
C	-2.856414000000	-3.570420000000	0.141199000000
H	-2.862447000000	-3.149714000000	1.160053000000
H	-3.874806000000	-3.932411000000	-0.081409000000
H	-2.193351000000	-4.450163000000	0.141951000000
C	-4.504171000000	-1.206802000000	-0.551596000000
H	-5.050685000000	-2.149591000000	-0.453236000000
O	-0.001207000000	3.041921000000	1.653871000000
C	-0.000778000000	1.891258000000	1.694798000000
O	-2.994036000000	-0.000312000000	2.290561000000
C	-1.887707000000	-0.000318000000	1.972718000000

8-W (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -1793.137234379

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1795.054556322

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -1795.067853699

W	5.624975	9.729355	4.939917
N	5.625031	12.833866	6.017826
C	5.624975	11.973783	4.939757
C	5.624944	14.170500	5.622984
H	5.624969	14.985216	6.350954
C	5.625189	12.459790	7.406814
C	6.868836	12.304199	8.061497
C	8.181747	12.400547	7.295787
H	7.949174	12.193991	6.230985

C	8.773605	13.821112	7.376775
H	9.715480	13.886781	6.794582
H	9.000704	14.093911	8.428251
H	8.073329	14.579457	6.974524
C	9.199810	11.343900	7.752118
H	8.750033	10.332284	7.765200
H	9.590442	11.559152	8.768002
H	10.065517	11.321281	7.061418
C	6.841311	12.036930	9.442341
H	7.787209	11.902801	9.986144
C	5.625501	11.918170	10.128159
H	5.625626	11.704301	11.207529
O	5.624898	6.528601	4.940158
C	5.624932	7.695612	4.940064
O	2.399643	9.682149	4.940193
C	3.564813	9.721631	4.940070
O	5.624704	9.225598	1.760972
C	5.624798	9.521515	2.888172
N	5.624857	12.833724	3.861572
C	5.624838	14.170411	4.256240
H	5.624757	14.985032	3.528163
C	5.624803	12.459466	2.472631
C	4.381206	12.303777	1.817873
C	3.068233	12.400218	2.583467
H	3.300736	12.193890	3.648329
C	2.476308	13.820737	2.502143
H	1.534382	13.886478	3.084246
H	2.249280	14.093312	1.450593
H	3.176513	14.579199	2.904297
C	2.050260	11.343423	2.127266
H	2.500092	10.331828	2.114431
H	1.659704	11.558445	1.111303
H	1.184495	11.320902	2.817898
C	4.408838	12.036321	0.437065
H	3.462980	11.902118	-0.106793
C	5.624700	11.917476	-0.248644
H	5.624660	11.703466	-1.327986
C	6.868352	12.303800	1.817773
C	8.181387	12.400280	2.583257
H	7.949001	12.193834	3.648120
C	8.773180	13.820858	2.502013
H	9.715150	13.886626	3.084041
H	9.000092	14.093551	1.450469
H	8.072941	14.579218	2.904300
C	9.199409	11.343619	2.126870
H	8.749663	10.331987	2.113979
H	9.589860	11.558771	1.110894
H	10.065234	11.321107	2.817426
C	6.840614	12.036346	0.436968
H	7.786431	11.902158	-0.106965
C	4.381694	12.304197	8.061781
C	3.068601	12.400544	7.296378
H	3.300935	12.194099	6.231503
C	2.476690	13.821071	7.377637
H	1.534680	13.886753	6.795665
H	2.249818	14.093763	8.429191
H	3.176843	14.579486	6.975301
C	2.050706	11.343792	7.752852
H	2.500549	10.332203	7.765731
H	1.660308	11.558924	8.768853

H	1.184832	11.321188	7.062358
C	4.409535	12.036936	9.442623
H	3.463759	11.902813	9.986644
O	8.850296	9.681978	4.939695
C	7.685133	9.721535	4.939744
O	5.625296	9.226021	8.118922
C	5.625177	9.521808	6.991690

8-W (M06/def2-SVP)

E (M06/def2-SVP) = -1791.4958274

E (M06/def2-TZVPP//M06/def2-SVP) = -1793.4299816

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -1793.4392068

W	-0.000872000000	-0.027332000000	1.600843000000
N	-1.070185000000	0.042579000000	-1.544661000000
C	0.000246000000	0.014743000000	-0.692810000000
C	-0.675610000000	0.088302000000	-2.872483000000
H	-1.401562000000	0.119668000000	-3.682743000000
C	-2.462853000000	0.019611000000	-1.203775000000
C	-3.140118000000	1.241927000000	-1.063181000000
C	-2.429330000000	2.573428000000	-1.179786000000
H	-1.346130000000	2.391783000000	-1.048939000000
C	-2.632229000000	3.173499000000	-2.568939000000
H	-2.117287000000	4.144450000000	-2.657313000000
H	-3.705263000000	3.342851000000	-2.766183000000
H	-2.247820000000	2.514097000000	-3.364600000000
C	-2.861901000000	3.556113000000	-0.098400000000
H	-2.840459000000	3.097122000000	0.903306000000
H	-3.885215000000	3.930609000000	-0.272914000000
H	-2.192360000000	4.430891000000	-0.081421000000
C	-4.515670000000	1.191987000000	-0.826419000000
H	-5.073829000000	2.125722000000	-0.707735000000
C	-5.182610000000	-0.023494000000	-0.734493000000
H	-6.260088000000	-0.040551000000	-0.548059000000
O	-0.002181000000	-0.048392000000	4.785622000000
C	-0.001845000000	-0.042683000000	3.631583000000
O	0.001606000000	-3.250007000000	1.498567000000
C	0.001625000000	-2.099378000000	1.541552000000
O	3.182391000000	-0.035773000000	2.074257000000
C	2.062839000000	-0.030168000000	1.806229000000
N	1.070738000000	0.041432000000	-1.544723000000
C	0.675857000000	0.087862000000	-2.872556000000
H	1.401210000000	0.120514000000	-3.683191000000
C	2.463536000000	0.024793000000	-1.203648000000
C	3.116523000000	-1.215343000000	-1.101519000000
C	2.378295000000	-2.528138000000	-1.254727000000
H	1.302890000000	-2.329141000000	-1.090620000000
C	2.535800000000	-3.078536000000	-2.670010000000
H	1.985133000000	-4.027002000000	-2.785350000000
H	3.598948000000	-3.276008000000	-2.893480000000
H	2.160935000000	-2.376633000000	-3.432715000000
C	2.816255000000	-3.561744000000	-0.224325000000
H	2.820600000000	-3.145925000000	0.796258000000
H	3.830324000000	-3.942825000000	-0.434813000000
H	2.135129000000	-4.427622000000	-0.232391000000
C	4.492304000000	-1.200182000000	-0.863824000000
H	5.031052000000	-2.148378000000	-0.774343000000
C	5.183423000000	-0.001734000000	-0.732413000000
H	6.260827000000	-0.012372000000	-0.545078000000
C	3.134001000000	1.251262000000	-1.064590000000

C	2.415755000000	2.578663000000	-1.183622000000
H	1.333712000000	2.391280000000	-1.050606000000
C	2.613442000000	3.175723000000	-2.574893000000
H	2.093056000000	4.143559000000	-2.665546000000
H	3.685288000000	3.350341000000	-2.773993000000
H	2.231504000000	2.511583000000	-3.367724000000
C	2.844744000000	3.566685000000	-0.105809000000
H	2.825432000000	3.110886000000	0.897387000000
H	3.866344000000	3.944904000000	-0.282194000000
H	2.171508000000	4.438707000000	-0.091593000000
C	4.509487000000	1.209719000000	-0.826607000000
H	5.061867000000	2.146961000000	-0.708585000000
C	-3.108648000000	-1.224384000000	-1.104117000000
C	-2.361272000000	-2.531403000000	-1.261685000000
H	-1.288388000000	-2.326682000000	-1.087985000000
C	-2.503571000000	-3.069325000000	-2.683310000000
H	-1.947249000000	-4.013962000000	-2.802931000000
H	-3.563754000000	-3.269247000000	-2.918394000000
H	-2.124585000000	-2.357681000000	-3.435026000000
C	-2.800321000000	-3.576227000000	-0.243343000000
H	-2.814081000000	-3.168330000000	0.780397000000
H	-3.810550000000	-3.961592000000	-0.464277000000
H	-2.113754000000	-4.437745000000	-0.253518000000
C	-4.484528000000	-1.217852000000	-0.867214000000
H	-5.017587000000	-2.169397000000	-0.779598000000
O	-0.005972000000	3.196551000000	1.544566000000
C	-0.004629000000	2.045477000000	1.574372000000
O	-3.184608000000	-0.054385000000	2.071074000000
C	-2.064843000000	-0.041590000000	1.804289000000

10-Cr (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -3242.021130303

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3244.584857365

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -3244.584857365

Cr	0.231927	0.066587	-0.124120
O	-2.770281	-0.104581	-0.432145
O	0.221656	-2.970932	-0.266511
O	0.884000	0.099996	-3.091906
O	-0.385078	3.044364	0.013706
O	0.259878	-0.174850	2.908191
O	7.848171	1.614993	-1.071553
O	6.556986	3.700618	0.681321
N	3.253365	1.154094	0.079189
N	4.513007	-0.554568	-0.154195
C	4.583293	0.803824	-0.020421
C	2.341229	0.069925	-0.006767
C	3.188738	-1.014919	-0.146968
H	2.964293	-2.079721	-0.254745
C	2.871137	2.527815	0.225232
C	2.722753	3.322727	-0.935443
C	2.354725	4.671945	-0.767257
H	2.218269	5.309932	-1.652340
C	2.135521	5.203154	0.510116
H	1.831864	6.255005	0.622244
C	2.278403	4.392476	1.645426
H	2.079344	4.814001	2.640968
C	2.646053	3.039545	1.526533
C	2.950224	2.738230	-2.322196
H	2.850714	1.639174	-2.231220

C	4.382477	3.027857	-2.810339
H	4.544271	2.622922	-3.829912
H	5.125183	2.544667	-2.143498
H	4.589003	4.118329	-2.834763
C	1.903231	3.211753	-3.341433
H	0.877424	3.064540	-2.952571
H	1.995084	2.633051	-4.281575
H	2.024750	4.285541	-3.595172
C	2.804326	2.139426	2.744233
H	2.555079	1.112691	2.411246
C	1.851111	2.498696	3.891017
H	1.893086	1.721221	4.678871
H	0.803781	2.561539	3.538057
H	2.117714	3.466818	4.365382
C	4.270058	2.115474	3.219403
H	4.943590	1.814297	2.392987
H	4.401713	1.395333	4.052897
H	4.585180	3.116402	3.583172
C	5.628695	-1.381193	-0.493522
C	5.904736	-1.590222	-1.867864
C	6.976831	-2.443196	-2.196038
H	7.211534	-2.635281	-3.253894
C	7.742457	-3.056751	-1.193420
H	8.572518	-3.724758	-1.469521
C	7.457033	-2.821225	0.159937
H	8.070234	-3.301566	0.936449
C	6.391546	-1.979662	0.537063
C	5.051028	-0.934766	-2.946522
H	4.441561	-0.153124	-2.451750
C	4.071567	-1.947744	-3.568618
H	4.612537	-2.755012	-4.105594
H	3.393961	-1.442232	-4.285403
H	3.439115	-2.415964	-2.790051
C	5.904567	-0.233501	-4.014580
H	6.570102	0.523211	-3.553607
H	5.254857	0.284012	-4.748675
H	6.537136	-0.947105	-4.582698
C	6.103938	-1.652287	1.996234
H	5.053981	-1.297864	2.046724
C	6.239080	-2.864444	2.929282
H	5.614294	-3.711470	2.582831
H	5.914622	-2.597788	3.955208
H	7.287780	-3.220809	3.001120
C	7.002019	-0.485421	2.454103
H	8.075786	-0.760741	2.393563
H	6.776075	-0.194790	3.500027
H	6.837725	0.404400	1.813841
C	-1.608863	-0.036517	-0.309435
C	0.252866	-1.804955	-0.208376
C	0.593473	0.114610	-1.959406
C	-0.050269	1.926246	-0.034229
C	0.233929	-0.062374	1.746197
C	8.720310	0.469863	-0.905949
H	8.089838	-0.408457	-0.683988
H	9.403100	0.651584	-0.044202
C	9.485729	0.376333	-2.220472
H	8.863109	-0.139315	-2.979588
H	10.438242	-0.178897	-2.122196
C	9.676064	1.860804	-2.577673
H	10.528355	2.287594	-2.009401

H	9.867663	2.034458	-3.654118
C	8.353178	2.486194	-2.115216
H	8.464180	3.510038	-1.701851
H	7.599932	2.519007	-2.932297
C	5.721582	4.878593	0.525883
H	4.718477	4.549506	0.200797
H	6.162816	5.528510	-0.263650
C	5.739497	5.554989	1.891825
H	4.983020	5.083197	2.550567
H	5.514566	6.637030	1.833746
H	7.279223	5.317070	3.479323
C	7.165525	5.249226	2.380112
H	7.892115	5.950636	1.919674
C	7.390140	3.824203	1.860940
H	8.442074	3.614883	1.576015
H	7.065953	3.060368	2.600793
Li	6.228584	2.011383	-0.140259

10-Cr (M06/def2-SVP)

E (M06/def2-SVP) = -3239.8989132

E (M06/def2-TZVPP//M06/def2-SVP) = -3242.4826153

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -3242.5030692

Cr	-3.787046000000	-0.989117000000	-0.019913000000
O	-6.763178000000	-1.338084000000	-0.322927000000
O	-3.650861000000	-3.966312000000	0.560066000000
O	-3.041538000000	-1.578502000000	-2.902055000000
O	-4.426776000000	1.923450000000	-0.622573000000
O	-3.787120000000	-0.469616000000	2.973305000000
O	4.014425000000	0.485783000000	-0.652779000000
O	2.463571000000	2.924034000000	0.071807000000
N	-0.754903000000	0.182528000000	0.000269000000
N	0.501883000000	-1.474958000000	0.420773000000
C	0.563356000000	-0.156880000000	0.134028000000
C	-1.662424000000	-0.887859000000	0.180653000000
C	-0.816572000000	-1.931572000000	0.455569000000
H	-1.028658000000	-2.981392000000	0.664553000000
C	-1.127349000000	1.534702000000	-0.270621000000
C	-1.201145000000	1.976604000000	-1.602738000000
C	-1.553205000000	3.309627000000	-1.836544000000
H	-1.631152000000	3.671259000000	-2.866793000000
C	-1.821180000000	4.175300000000	-0.782573000000
H	-2.107151000000	5.211952000000	-0.985030000000
C	-1.743101000000	3.718029000000	0.528374000000
H	-1.974958000000	4.399294000000	1.353556000000
C	-1.404959000000	2.391702000000	0.809450000000
C	-0.899863000000	1.051964000000	-2.761772000000
H	-1.018425000000	0.015976000000	-2.398874000000
C	0.547979000000	1.218723000000	-3.216847000000
H	0.768731000000	0.581693000000	-4.090165000000
H	1.251818000000	0.929547000000	-2.413990000000
H	0.755609000000	2.266719000000	-3.501121000000
C	-1.863442000000	1.241178000000	-3.925563000000
H	-2.910359000000	1.225406000000	-3.580897000000
H	-1.743113000000	0.429012000000	-4.660179000000
H	-1.691576000000	2.194363000000	-4.455599000000
C	-1.344506000000	1.902185000000	2.239886000000
H	-1.460196000000	0.803658000000	2.218777000000
C	-2.468305000000	2.464227000000	3.100750000000
H	-2.527311000000	1.918146000000	4.055716000000

H	-3.445428000000	2.366048000000	2.600573000000
H	-2.312752000000	3.531322000000	3.338594000000
C	0.017205000000	2.209079000000	2.855957000000
H	0.831688000000	1.735462000000	2.279745000000
H	0.073199000000	1.841459000000	3.894900000000
H	0.198100000000	3.300318000000	2.877873000000
C	1.629643000000	-2.322164000000	0.591161000000
C	2.095788000000	-3.049168000000	-0.518776000000
C	3.183625000000	-3.906832000000	-0.328973000000
H	3.562769000000	-4.492024000000	-1.174001000000
C	3.784076000000	-4.035379000000	0.919530000000
H	4.628048000000	-4.718961000000	1.051881000000
C	3.308184000000	-3.302044000000	2.001966000000
H	3.789923000000	-3.410040000000	2.979766000000
C	2.219315000000	-2.435468000000	1.862423000000
C	1.467596000000	-2.896235000000	-1.887927000000
H	0.595985000000	-2.226396000000	-1.786680000000
C	0.956158000000	-4.223879000000	-2.432002000000
H	1.775662000000	-4.946335000000	-2.591429000000
H	0.450413000000	-4.077605000000	-3.400242000000
H	0.230776000000	-4.684434000000	-1.742115000000
C	2.442764000000	-2.229786000000	-2.852656000000
H	2.801671000000	-1.266837000000	-2.444983000000
H	1.962623000000	-2.035555000000	-3.826069000000
H	3.323613000000	-2.868970000000	-3.045079000000
C	1.731393000000	-1.616538000000	3.038890000000
H	0.774743000000	-1.146367000000	2.747176000000
C	1.469489000000	-2.469094000000	4.273967000000
H	0.776143000000	-3.295839000000	4.052792000000
H	1.020558000000	-1.859345000000	5.074794000000
H	2.397507000000	-2.906739000000	4.680932000000
C	2.719271000000	-0.493534000000	3.342465000000
H	3.715315000000	-0.894385000000	3.603371000000
H	2.376278000000	0.123969000000	4.189561000000
H	2.845418000000	0.172527000000	2.469710000000
C	-5.621106000000	-1.201082000000	-0.205197000000
C	-3.684893000000	-2.834459000000	0.342589000000
C	-3.373688000000	-1.344528000000	-1.821594000000
C	-4.100577000000	0.840780000000	-0.392363000000
C	-3.822612000000	-0.655533000000	1.835753000000
C	4.867527000000	-0.480520000000	-0.027429000000
H	4.240793000000	-1.286548000000	0.383971000000
H	5.409911000000	0.001718000000	0.810917000000
C	5.817405000000	-0.909574000000	-1.121143000000
H	5.323795000000	-1.648810000000	-1.776304000000
H	6.742905000000	-1.361334000000	-0.735046000000
C	6.033049000000	0.404961000000	-1.858502000000
H	6.748468000000	1.037662000000	-1.304829000000
H	6.417376000000	0.286637000000	-2.882190000000
C	4.642837000000	1.017498000000	-1.824994000000
H	4.643482000000	2.120137000000	-1.767009000000
H	4.046769000000	0.722525000000	-2.710350000000
C	1.815828000000	4.018023000000	-0.587467000000
H	0.805490000000	3.701568000000	-0.890924000000
H	2.389496000000	4.282435000000	-1.498955000000
C	1.843412000000	5.141192000000	0.423586000000
H	1.018976000000	5.012048000000	1.147786000000
H	1.736808000000	6.135242000000	-0.035204000000
H	3.295985000000	5.390000000000	2.073994000000
C	3.194267000000	4.911486000000	1.088781000000

H	4.005077000000	5.295995000000	0.445455000000
C	3.250308000000	3.395653000000	1.168779000000
H	4.269661000000	2.977221000000	1.083201000000
H	2.804485000000	3.022549000000	2.111123000000
Li	2.229271000000	1.033049000000	-0.189346000000

10-W (BP86+D3(BJ)/def2-SVP)

E (BP86+D3(BJ)/def2-SVP) = -2264.741385948

E (BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2267.178939733

E (PCM(THF)-BP86+D3(BJ)/def2-TZVPP//BP86+D3(BJ)/def2-SVP) = -2267.178939733

W	0.139391	0.095621	-0.122121
O	-3.030872	-0.081366	-0.549920
O	0.164681	-3.127758	-0.174433
O	0.855016	0.036647	-3.262475
O	-0.414372	3.270642	-0.051582
O	-0.031116	-0.071788	3.093985
O	7.856809	1.637085	-1.156995
O	6.597955	3.692082	0.720304
N	3.304787	1.167810	0.100342
N	4.563939	-0.539509	-0.136942
C	4.632848	0.821228	-0.017624
C	2.392859	0.081930	0.040247
C	3.240934	-1.002862	-0.102938
H	3.015863	-2.069217	-0.196451
C	2.910052	2.539606	0.230495
C	2.772810	3.322952	-0.938927
C	2.414945	4.676987	-0.785880
H	2.291979	5.308734	-1.677443
C	2.180897	5.218523	0.484396
H	1.885301	6.273790	0.584774
C	2.286690	4.411356	1.626733
H	2.061788	4.838611	2.614118
C	2.647668	3.055506	1.523402
C	2.982188	2.715780	-2.319112
H	2.880109	1.618315	-2.205489
C	4.404944	2.994802	-2.838440
H	4.546145	2.576194	-3.855497
H	5.159587	2.518448	-2.180265
H	4.613251	4.084356	-2.881744
C	1.915167	3.172929	-3.325566
H	0.897596	3.030593	-2.913519
H	1.988934	2.579865	-4.258309
H	2.029656	4.242905	-3.597374
C	2.747237	2.147745	2.742178
H	2.438121	1.139349	2.399528
C	1.806160	2.557933	3.881270
H	1.797612	1.778287	4.667982
H	0.766620	2.679820	3.520062
H	2.121894	3.509162	4.359767
C	4.204216	2.033998	3.231458
H	4.871899	1.709970	2.408808
H	4.285420	1.294931	4.054701
H	4.569317	3.009828	3.616322
C	5.677460	-1.364683	-0.487888
C	5.936628	-1.576582	-1.865257
C	7.007645	-2.426661	-2.204086
H	7.229677	-2.621743	-3.264031
C	7.788799	-3.033382	-1.209258
H	8.618086	-3.698748	-1.493904

C	7.519941	-2.794760	0.146907
H	8.145012	-3.270216	0.916839
C	6.455627	-1.956643	0.534863
C	5.064067	-0.928315	-2.933200
H	4.487922	-0.122311	-2.437382
C	4.043989	-1.934184	-3.500151
H	4.551644	-2.764248	-4.034778
H	3.353782	-1.430726	-4.206228
H	3.427095	-2.371080	-2.691726
C	5.894740	-0.270777	-4.045665
H	6.593504	0.480100	-3.626334
H	5.230575	0.245276	-4.767696
H	6.489530	-1.010868	-4.620492
C	6.183628	-1.625449	1.996296
H	5.127366	-1.292333	2.060616
C	6.358372	-2.827212	2.935969
H	5.748542	-3.690888	2.604219
H	6.041627	-2.560123	3.964169
H	7.415747	-3.159134	2.996596
C	7.063261	-0.436370	2.432440
H	8.141615	-0.689149	2.357164
H	6.847017	-0.143275	3.479789
H	6.869312	0.444649	1.788358
C	-1.874267	-0.009513	-0.386132
C	0.179048	-1.960548	-0.153196
C	0.543015	0.086103	-2.137068
C	-0.131068	2.137673	-0.075191
C	0.009738	0.008214	1.929854
C	8.745201	0.509000	-0.963608
H	8.127747	-0.370235	-0.709933
H	9.432945	0.725492	-0.113767
C	9.500834	0.385327	-2.281213
H	8.877975	-0.159975	-3.019095
H	10.460565	-0.155779	-2.174710
C	9.670990	1.860602	-2.683696
H	10.524259	2.312954	-2.137213
H	9.849866	2.004284	-3.766728
C	8.345983	2.485881	-2.226232
H	8.453315	3.520851	-1.840170
H	7.585534	2.491672	-3.037013
C	5.764493	4.875113	0.589537
H	4.773913	4.560523	0.214348
H	6.232368	5.560964	-0.152678
C	5.729845	5.488365	1.984937
H	4.947240	4.989609	2.590910
H	5.508620	6.572579	1.967414
H	7.203866	5.174376	3.620176
C	7.134410	5.155890	2.515334
H	7.880983	5.873309	2.115597
C	7.374619	3.754510	1.943125
H	8.437432	3.549453	1.698675
H	7.010354	2.961240	2.631464
Li	6.270020	2.037983	-0.170384

10-W (M06/def2-SVP)

E (M06/def2-SVP) = -2262.7263926

E (M06/def2-TZVPP//M06/def2-SVP) = -2265.183035

E (PCM(THF)-M06/def2-TZVPP//M06/def2-SVP) = -2265.202605

W	-3.485208000000	-0.618481000000	0.005171000000
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O	-6.611641000000	-0.862775000000	-0.580703000000
O	-3.595404000000	-3.674990000000	1.009988000000
O	-2.451998000000	-1.652934000000	-2.857906000000
O	-3.832066000000	2.417646000000	-1.016768000000
O	-3.809187000000	0.328021000000	3.067190000000
O	4.442295000000	0.125977000000	-0.866750000000
O	3.205226000000	2.800048000000	0.036198000000
N	-0.233977000000	0.357744000000	0.075907000000
N	0.896369000000	-1.357291000000	0.610091000000
C	1.054874000000	-0.072584000000	0.221851000000
C	-1.219663000000	-0.622790000000	0.342598000000
C	-0.453435000000	-1.705167000000	0.690343000000
H	-0.744596000000	-2.715946000000	0.980470000000
C	-0.515517000000	1.700098000000	-0.322741000000
C	-0.494335000000	2.031024000000	-1.688837000000
C	-0.748911000000	3.359083000000	-2.047910000000
H	-0.747678000000	3.640404000000	-3.105864000000
C	-1.024180000000	4.321082000000	-1.084206000000
H	-1.235961000000	5.351676000000	-1.384479000000
C	-1.053900000000	3.969889000000	0.261848000000
H	-1.291382000000	4.731844000000	1.010814000000
C	-0.806281000000	2.656755000000	0.669215000000
C	-0.192022000000	1.000153000000	-2.756288000000
H	-0.353649000000	0.002093000000	-2.310898000000
C	1.269967000000	1.084549000000	-3.188617000000
H	1.491854000000	0.359359000000	-3.990181000000
H	1.951944000000	0.859412000000	-2.348608000000
H	1.513571000000	2.093456000000	-3.569167000000
C	-1.113353000000	1.114897000000	-3.964363000000
H	-2.172462000000	1.154915000000	-3.663180000000
H	-0.988937000000	0.241871000000	-4.624924000000
H	-0.897031000000	2.014395000000	-4.566623000000
C	-0.819744000000	2.277758000000	2.135272000000
H	-1.083407000000	1.205741000000	2.191985000000
C	-1.849241000000	3.049863000000	2.946600000000
H	-1.937606000000	2.623066000000	3.958517000000
H	-2.847551000000	3.012096000000	2.480897000000
H	-1.570400000000	4.111824000000	3.065685000000
C	0.574103000000	2.435050000000	2.738236000000
H	1.317791000000	1.837533000000	2.181783000000
H	0.588396000000	2.108623000000	3.792393000000
H	0.892322000000	3.495213000000	2.713765000000
C	1.955448000000	-2.291864000000	0.772244000000
C	2.299391000000	-3.107102000000	-0.321172000000
C	3.313219000000	-4.052893000000	-0.135317000000
H	3.599410000000	-4.707000000000	-0.966240000000
C	3.956816000000	-4.180952000000	1.091000000000
H	4.739290000000	-4.934742000000	1.220775000000
C	3.606694000000	-3.355079000000	2.155181000000
H	4.125191000000	-3.461970000000	3.113503000000
C	2.598522000000	-2.395710000000	2.018410000000
C	1.612479000000	-2.975348000000	-1.664939000000
H	0.895723000000	-2.137979000000	-1.600654000000
C	0.811777000000	-4.225911000000	-2.009651000000
H	1.463474000000	-5.110969000000	-2.114532000000
H	0.272860000000	-4.091308000000	-2.961518000000
H	0.063071000000	-4.448193000000	-1.232381000000
C	2.612246000000	-2.629725000000	-2.762879000000
H	3.169410000000	-1.707201000000	-2.518075000000
H	2.096164000000	-2.471620000000	-3.724439000000

H	3.349225000000	-3.438472000000	-2.916733000000
C	2.269465000000	-1.447732000000	3.152334000000
H	1.268012000000	-1.021817000000	2.956204000000
C	2.228059000000	-2.129773000000	4.512645000000
H	1.557369000000	-3.003377000000	4.508928000000
H	1.865792000000	-1.428846000000	5.281841000000
H	3.226698000000	-2.471943000000	4.835408000000
C	3.266858000000	-0.291421000000	3.156433000000
H	4.296520000000	-0.661224000000	3.312482000000
H	3.041709000000	0.432023000000	3.958453000000
H	3.242342000000	0.253748000000	2.194818000000
C	-5.479096000000	-0.766413000000	-0.363055000000
C	-3.536638000000	-2.579889000000	0.654232000000
C	-2.898015000000	-1.277436000000	-1.861520000000
C	-3.646318000000	1.340438000000	-0.648280000000
C	-3.729295000000	-0.002026000000	1.965545000000
C	5.263211000000	-0.830749000000	-0.188936000000
H	4.605876000000	-1.557343000000	0.312523000000
H	5.868985000000	-0.313929000000	0.582557000000
C	6.143171000000	-1.409777000000	-1.272600000000
H	5.588864000000	-2.177016000000	-1.841602000000
H	7.057909000000	-1.876374000000	-0.878403000000
C	6.404310000000	-0.178668000000	-2.131039000000
H	7.186727000000	0.446736000000	-1.667397000000
H	6.728915000000	-0.409704000000	-3.156187000000
C	5.060986000000	0.532928000000	-2.092392000000
H	5.140201000000	1.634115000000	-2.106501000000
H	4.408282000000	0.228075000000	-2.932469000000
C	2.615514000000	3.920289000000	-0.634892000000
H	1.612505000000	3.633664000000	-0.987547000000
H	3.235131000000	4.182923000000	-1.516015000000
C	2.620805000000	5.027501000000	0.393807000000
H	1.757533000000	4.909177000000	1.072550000000
H	2.563167000000	6.030429000000	-0.054077000000
H	3.984711000000	5.211568000000	2.124657000000
C	3.927355000000	4.753047000000	1.126403000000
H	4.781652000000	5.128796000000	0.536619000000
C	3.944875000000	3.235139000000	1.181238000000
H	4.959446000000	2.800051000000	1.140725000000
H	3.444359000000	2.853125000000	2.092231000000
Li	2.809124000000	0.930767000000	-0.223766000000

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