Supporting Information for

Chemistry at the Alkyne – Carbene Intersection: A Metallacyclobutene – η^3 -Vinylcarbene Equilibration

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1) Experimental Procedures

Computational Details

The conformational analyses of the molecular systems described in this study, including structural and orbital arrangements as well as property calculations, were carried out using the GAMESS¹ amd GAUSSIAN09² software packages. Structural computations of all compounds were performed using the B97-D dispersion enabled density functional method, using an ultrafine grid, in accord with the ansatz proposed by Grimme.^{3,4} The B97-D exchange-correlation functional is a special re-parameterization of the original B97 hybrid functional of Becke.⁵ which is more neutral to spurious dispersion contamination in the exchange part than the original The Def2-TZVPP basis set⁶ was used for all calculations. Full geometry functional. optimizations were performed and uniquely characterized via second derivatives (Hessian) analysis to determine the number of imaginary frequencies (0=minima; 1=transition state), and effects of zero point energy. From the fully optimized structures, single point NMR computations were performed with the class II NMR methodology, CSGT,⁶ and calibrated against TMS. Effects of solvation were taken into account using the COSMO method,^{7,8} with the dielectric for benzene and solvent radii from Klamt.⁹ Visualization and analysis of structural and property results were obtained using QMView¹⁰ and WEBMO.¹¹ From the fully optimized structures, single point NMR computations were performed with the class II NMR methodology, CSGT,^X and calibrated against TMS.¹²

General Experimental Data. All manipulations were performed under an atmosphere of nitrogen gas or in Vacuum Atmospheres nitrogen box equipped with a Dri-Train MO 40-1

purifier. NMR spectra were recorded on a Varian Mercury 300 (¹H, 300 MHz; ³¹P, 122 MHz; ¹³C 75.5 MHz), a Varian Mercury 400 (¹H, 400 MHz; ³¹P, 163 MHz; ¹³C 100.7 MHz), or a JEOL 500 (¹H, 500MHz; ¹³C, 125.7 MHz; ³¹P, 203.8 MHz) spectrometer. Chemical shifts were referenced to residual protio-solvent signal, and ³¹P NMR chemical shifts were referenced to external 85% H₃PO₄. IR Spectra were recorded on a Nicolet Avatar 320 FT-IR. Benzene and hexanes were distilled over sodium/benzophenone ketyl under an atmosphere of nitrogen. All other reagents were obtained from commercial suppliers and used as received.

Preparation of (*η*⁵-**C**₅**H**₅**)Co**[*η*²-(**TIPS**)**C**≡**C**(**SO**₂**C**₆**H**₄**CH**₃**)**] (**1**-*TIPS*): In a sealed NMR tube under a nitrogen atmosphere, (*η*⁵-**C**₅**H**₅)Co(PPh₃)₂ (25 mg, 0.039 mmol, 0.057 *M*) and protio-toluene (internal standard) were dissolved in dry benzene-*d*₆ (0.69 mL). Triisopropyl-(toluene-4-sulfonylethynyl)-silane (13.0 mg, 0.039 mmol, 0.056 M) was added, and after 24 h at rt a ¹H NMR spectrum of the sample indicated 98% yield of sample **3**-*TIPS*. In a preparative scale experiment, (*η*⁵-C₅H₅)Co(PPh₃)₂ (3.78 g, 5.84 x 10⁻³ mol, 0.29M) was dissolved in dry toluene (20 mL) and triisopropyl-(toluene-4-sulfonylethynyl)-silane (1.87 g, 5.84 x 10⁻³ mol) was added. The reaction was allowed to stir for 20 h at rt. Removal of volatiles and recrystallization from toluene/hexanes (1:10) gave **1**-*TIPS* (3.14 g, 74% yield), as a slightly air-sensitive dark brown crystals. IR (NaCl, neat): 1737 (C≡C) cm⁻¹. ¹H NMR (C₆D₆): δ 0.95 (sept, 3H, TIPS), 1.12 (m, 18H, TIPS), 1.91 (s, 3H, CH₃), 4.62 (s, 5H, C₅H₅), 6.78 (d, 2H, *J* = 8.4 Hz), 7.04 (m, 9H, PPh₃), 7.68 (t, 6H, PPh₃), 7.88 (d, 2H, *J* = 8.0 Hz). ¹³C{¹H} NMR (C₆D₆): δ 12.3 (TIPS), 19.4 (d, *J*_{PC} = 22.8 Hz, TIPS), 21.1 (CH₃), 83.7 (d, *J*_{PC} = 2.3

Hz, Cp), 100.5 (Co-C \equiv C), 120.0 (d, $J_{PC} = 13.7$ Hz, Co-C \equiv C), 127.9 (C_m, PPh₃), 128.8 (C_m), 129.1 (C₀), 129.3 (C_P, PPh₃), 143.5 (d, $J_{PC} = 10.7$ Hz, C₀, PPh₃), 135.4 (d, $J_{PC} = 36.5$ Hz), 141.4 (C_P), 142.7 (C_i). ³¹P NMR (C₆D₆): δ 54.91. HRMS (FAB) for C₄₁H₄₈CoPO₂SSi, [MH⁺] Calculated: 722.2208; Found: 722.2221.

Preparation of $(\eta^5-C_5H_5)(PPh_3)Co[\kappa^2-(C,C)-CH(CO_2Et)(Pr_3Si)C=CSO_2Tol]$ (2-*TIPS*): In the glove box, a benzene- d_6 solution (0.75 mL) of **1**-*TIPS* (18 mg, 0.028 mmol, 0.037 M) and 1,3-bis-(trimethylsilyl)-benzene (internal standard) was prepared in an NMR tube. Ethyl diazoacetate (8.2 μ L, 0.069 M) was added by syringe to the NMR tube, and the course of reaction was monitored by ¹H NMR spectroscopy, indicating a 26% yield of **2**-*TIPS*. In a preparative scale reaction, a toluene solution (5 mL) of $(\eta^{5}-C_{5}H_{5})Co[\eta^{2} (TIPS)C \equiv C(SO_2C_6H_4CH_3)$ (1-*TIPS*; 392 mg, 0.542 mmol) and PPh₃ (142.2 mg, 0.542 mmol) was prepared in the glovebox, and ethyl diazoacetate (102.8 µL, 111.6 mg, 0.977 mmol) was added by syringe. After stirring at rt overnight, the volatiles were removed under high vacuum and the residue was subjected to chromatography (alumina, 5% ethyl acetate/hexanes) in the glovebox to give 2-TIPS (51 mg, 12 %) as a orange solid. Recrystallization under a nitrogen atmosphere in hexanes/chloroform (5:1) diffusion gave **2**-*TIPS* as dark orange crystals. IR (NaCl): 1684 cm⁻¹ (C=O). ¹H NMR (C₆D₆): δ 1.18 (t, 3H, J = 6.87 Hz, CH₂CH₃), 1.34 (dd, 18H, I = 7.5, 9.16 Hz, CH₃-TIPS), 1.85 (sept, 3H, I = 8.0 Hz, CH-TIPS), 1.94 (s, 3H, CH₃-Tol), 2.04 (d, 1H, J = 6.87 Hz, [=CH(CO₂Et)]), 4.18 (m, 2H, OCH₂), 4.32 (s, 5H, C₅H₅), 6.82 (d, 2H, J = 8.0 Hz, Tol), 7.07 (m, 9H, PPh₃), 7.71 (m, 6H, PPh₃), 8.00 (d, 2H,

J = 8.0 Hz, Tol). ¹³C{¹H} NMR (C₆D₆): δ -2.11 (d, *J* = 13.07 Hz), 14.3 (*C*H₃-TIPS), 20.6, (*C*H-TIPS) 15.2 (*C*H₃-Tol), 21.2 (OCH₂*C*H₃), 59.2 (O*C*H₂CH₃), 89.3 (C₅H₅), 134.4 (d, *J*_{PC} = 10.0 Hz), 127.2 - 142.7 (PPh₃ and Tol resonances), 174.3 (br, C=O), 181.4 (*C*O₂Et). ¹³C{¹H} NMR (C₇D₈): δ -1.79 (d, J = 10.84 Hz), 14.5 (*C*H₃-TIPS), 21.6, (*C*H-TIPS) 12.8 (*C*H₃-Tol), 15.5 (OCH₂*C*H₃), 59.5 (O*C*H₂CH₃), 89.7 (C₅H₅), 141.5 (d, *J*_{PC} = 27.0 Hz), 128.2 - 135.5 (PPh₃ and Tol resonances), 167.0 (C=O), 181.3 (*C*O₂Et). HRMS (FAB) Calculated for C₄₅H₅₅CoO₄PSSi: 809.2654; Found: 809.2655.

Observation of (η⁵-C₅H₅)Co[η³-CH(CO₂Et)C(Si²Pr₃)C(SO₂Tol)] (3-*E***): In a NMR tube under nitrogen atmosphere, (η⁵-C₅H₅)(PPh₃)Co{κ²-(***C***,***C***)-CH(CO₂Et)(⁷Pr₃Si)C=CSO₂Tol} (2-***TIPS***; 15 mg, 0.019 mmol, 0.023** *M***) and 1,3-bis(trimethylsilyl)benzene (internal standard) were dissolved in dry benzene-***d***₆ (0.85 mL). Ir(N₂)(Cl)(PPh₃)₂ (4**, 5.3 mg, 0.020 mmol, 0.024 M) was added, and after 24 h at rt, a ¹H NMR spectrum of the sample indicated a 99% yield of **3**. IR (NaCl, neat): 1698 cm⁻¹ (C=0). ¹H NMR (C₆D₆): δ 0.96 (t, 3H, *J* = 7.5 Hz, CH₂CH₃), 1.17 (dd, 18H, *J* = 7.5 Hz, CH₃-TIPS), 1.55 (sept, 3H, *J* = 7.5 Hz, CH-TIPS), 1.82 (s, 3H, CH₃-Tol), 3.86 (m, 1H, OCH₂), 3.93 (m, 1H, OCH₂), 4.51 (s, 5H, C₅H₅), 6.02 (s, 1H, [=CH(CO₂Et)]), 6.74 (d, 2H, Tol), 8.15 (d, 2H, Tol). ¹³C{¹H} NMR (C₆D₆): δ 12.4 (CH₃-TIPS), 19.3, (d, *J* = 30.8 Hz, CH-TIPS) 14.6 (CH₃-Tol), 21.8 (OCH₂CH₃), 42.1 (d, *J* = 157.6 Hz, [=*C*(3)H(CO₂Et)]), 60.1 (OCH₂CH₃), 81.4 (C₅H₅), 91.7 (*C*(2)-TIPS), 173.9 (C=0), 251.5 (Co=*C*SO₂Tol), 126.6 - 154.0 (Tol, resonances obscured by resonances of Ir(PPh₃)₃Cl and Ir(H)(Cl)(C₆H₄PPh₂)(PPh₃)₂). 2D-HSQC-NMR (C₆D₆) provided the following ¹H-¹³C correlations (¹H, δ :¹³C, δ): (6.02 : 42.1), (4.51 : 81.4), (3.86 : 60.1), (3.93 : 60.1), (0.96 : 19.3). 2D-HMBC-NMR (C₆D₆) provided the following ¹H-¹³C correlations (¹H, δ :¹³C, δ): (6.02 : 91.7), (6.02 : 251.5). 2D-NOESY-NMR (C₆D₆) provided the following ¹H-¹³C correlations (¹H, δ :¹³C, δ): (6.02 : 1.17, 1.55), (6.74, 8.15 : 1.82, 1.17, 1.55), (4.51 : 1.17, 1.55), (1.55 : 1.17, 1.55), (0.96 : 3.86, 3.93). HRMS (FAB) Calculated for ¹³C¹²C₂₆H₃₉CoO₄SSi: 547.1698; Found: 547.1691.

Preparation of dicobalt complex [(η⁵-C₅H₅)**Co**]₂[**CH**(**CO**₂**Et**)**C**(**Si**'**P**_{T3})**C**(**SO**₂**Tol**)] (**7**): A benzene-*d*₆ solution (0.65 mL) of (η⁵-C₅H₅)(PPh₃)Co{κ²-(*C*,*C*)-CH(CO₂Et)('Pr₃Si)C=CSO₂Tol} (**2**-*TIPS*; 6 mg, 7.43 x 10⁻³ mmol, 0.011 M), CpCo(PPh₃)₂ (**6**; 5 mg, 8.17 x 10⁻³ mmol), and 1,3-bistrimethylsilyl benzene (as internal standard) were stirred under nitrogen. After 14 h, a ¹H NMR spectrum of the sample indicated formation of the dinuclear complex 7. Chromatographic workup of the reaction mixture under a nitrogen gas atmosphere gave **7** as a green oil in 45% yield. Recrystallization from hexanes/toluene afforded **7** as green crystals. ¹H NMR (C₆D₆): *δ* 0.80 (t, 3H, *J* = 7.45 Hz, CH₂CH₃), 1.17 (d, 9H, *J* = 7.45 Hz, CH₃-TIPS), 1.26 (d, 9H, *J* = 7.45 Hz, CH₃-Tol), 1.89 (sept, 3H, *J* = 7.45 Hz, CH-TIPS), 1.99 (s, 3H, CH₃-Tol), 3.21 (s, 1H, CH), 3.56 (m, 4H, CH₂CH₃), 4.55 (s, 5H, C₅H₅), 5.12 (s, 5H, C₅H₅), 6.97 (d, 2H, *J* = 7.45 Hz, Tol), 21.2 (Tol-CH₃), 36.6 (CHCO₂Et), 62.3 (CO₂CH₂CH₃), 80.6 (C₅H₅), 81.2 (C₅H₅), 97.4 (C1-S), 127.9 – 128.2 (Co, m, p-Tol), 140.8 (C2-Si), 147.5 (C^{ipso-}Tol), 186.6 (C=O). HRMS (FAB) Calculated for C₃₂H₄₄Co₂O₄SSiNa: 693.1286; Found: 693.1285.

(η^{5} -C₅H₅)Co[η^{4} -CH(CO₂Et)=C(SO₂Tol)=C(Si^{*i*}Pr₃)=CH(CO₂Et)] (8): A benzene- d_{6} solution (0.87 mL) of 2-*TIPS* (7 mg, 0.0087 mmol, 9.94 x 10⁻³ M), ethyl diazoacetate (7 µL, 0.035 mmol) and ferrocene (internal standard) was maintained at rt under a nitrogen atmosphere. After 18 h, a ¹H NMR spectrum of the sample indicated the formation of **8** (35%).

In preparative scale reaction cobalt alkyne complex **1**-*TIPS* (242.0 mg, 0.335 mmol, 0.168 M) was dissolved in toluene (3 mL) and ethyl diazoacetate (145.7 µL, 141.9 mg) was added by syringe under a nitrogen atmosphere. The reaction was stirred for 24 h at rt. Evaporation of the volatiles and chromatography on alumina (5% ethyl acetate/hexanes) gave cobalt-diene 8 in 45% yield (95 mg, orange oil). X-ray quality crystals were obtained from 1:10 toluene/hexane at -30 °C under nitrogen. The solid structure of 8 has a large Z and relatively "loose" packing, exhibiting whole molecule disorder. That means the existence of multiple positions for each heavy atom in the molecule (e.g. Co, S, and Si) in all eight molecules of the asymmetric unit. Due to the relative size of these Q peaks (2-3e/A³) and the impossibility to adequately model the disorder for all 8 molecules, the R-1 is high. The light atoms thermals had to be constrained using SIMU (give the name as well as the abbreviations for these terms) because of NPD's, but there are no structural restraints (e.g. DFIX or SAME) used. The reliability of the structural model is without question and the high R-value is simply due to the unresolved problematic disorder. For 8: IR (NaCl, neat): 1708 (C=O), 1730 (C=O) cm⁻¹. ¹H NMR (CDCl₃): δ -0.19 (s, 1H, H_{anti}), 0.83 (d, 9H, CH₃-TIPS), 0.93 (s, 1H, H_{anti}), 0.99 (d, 9H, CH₃-Tol), 1.12 (t, 3H, CH₂CH₃), 1.20 (t, 3H,

CH₂CH₃), 1.69 (sept, 3H, CH-TIPS), 2.31 (s, 3H, CH₃), 4.00 (m, 4H, CH₂CH₃), 5.18 (s, 5H, Cp), 7.18 (d, 2H, *J* = 8.02 Hz, Tol), 7.97 (d, 2H, *J* = 8.59 Hz, Tol). HRMS (FAB) Calculated for C₃₁H₄₆O₆SSiCo: 633.2111; Found: 633.2108.

2) FIGURES



Figure S1. Lower Panel: ¹H NMR spectrum of **2**-*TIPS* in benzene-*d*₆ at rt shortly after mixing. Upper Panel: Lower Panel: ¹H NMR spectrum of **2**-*TIPS* in benzene-*d*₆ after 4 days showing equilibrium mixture of **2**-*TIPS* and **3**.



Figure S2. 2D ${}^{13}C{}^{-1}H$ HSQC spectrum of $3{}^{-13}CH$ in C_6D_6 at 298K



Figure S3. 2D ¹H NOESY spectrum of 3^{-13} CH in C₆D₆ at 298K



3-*E*-calc (0 kcal gas phase; 0 kcal in C₆H₆ solution environment)



3-*E*-conf-calc (3.44 kcal gas phase; 1.89 kcal in C_6H_6 solution environment)



3-*Z*-calc (3.77 kcal gas phase; 2.76 kcal C₆H₆ solution environment)



3-*Z*-conf-calc (3.58 kcal gas phase; 3.76 kcal C₆H₆ solution environment)

Figure S4. Computed structures of the η^3 -vinylcarbene complexes with atom numbering and calculated energies. Phenyl ring carbons shown in lighter color for clarity.



3-*C*,*O*-calc (6.37 kcal gas phase; 6.58 kcal C_6H_6 solution environment)

Figure S5. Computed structures of higher energy (6.58 kcal relative to **3**-*E*-*calc* in C₆H₆ solution environment) chelating η^1 -vinylcarbene complex, **3**-*C*,*O*-*calc*, with atom numbering and calculated energies. Phenyl ring carbons shown in lighter color for clarity.



Figure S6. Electrophilic HOMO plots for the η^3 -vinylcarbene complexes.





Figure S7. Nucleophilic LUMO plots for the η^3 -vinylcarbene complexes.



Figure S8. Representaions showing CPK van-der-Waals radii for **3**-*E*-calc (upper panels) and **3**-*E*-conf-calc (lower panels). Left Panels: View for *endo*-approach (*anti* to H3). Right Panels: View for *exo*-approach (*syn* to H3). Green color represents the van-der-Waals radius for C1, yellow for S, tangerine for Si, red for O, magenta for Co, white for H.



Figure S9. Representations showing the CPK van-der-Waals radii for *3-Z-calc* (upper panels) and *3-Z-conf-calc* (lower panels). Right Panel: View for *exo*-approach (*anti* to H3). Left Panel: View for *endo*-approach (*syn* to H3). Green color represents the van-der-Waals radius for C1, yellow for S, tangerine for Si, red for O, magenta for Co, white for H.



Figure S10. Computed structure of **2**-*TIPS*-*calc*, with atom labeling scheme.

3. TABLES

Table S1. Comparison of X-ray Cyrstallographic data for 2-*TIPS* with the computed distances (Å) and angles (deg) for 2-*TIPS-calc.* For labeling see Figure S10 (above).

Cmpd:	2 -TIPS	2 -TIPS-calc
Co-C1	1.938(3)	1.936
Co-C3	2.055(4)	2.078
C1-C2	1.345(5)	1.349
C2-C3	1.514(3)	1.518
C3-C4	1.465(4)	1.476
C4-O1	1.211(3)	1.220
Co-P	2.201(2)	2.166
Co-Cp ^{cnt}	1.737	1.753
C1-S	1.770(3)	1.780
C2-Si	1.917(4)	1.917
C1-Co-C3	65.8(1)	66.30
Co-C1-C2	102.9(2)	101.97
Co-C1-S1	134.1(2)	133.41
C1-C2-C3	98.6(2)	99.92
C1-S-C12	108.7(1)	107.22
Co-C3-C2	92.0(2)	90.28
Co-C3-C4	112.3(2)	113.41
C1-C2-Si	139.6(2)	138.03
C3-C2-Si	121.8(2)	121.86

Cmpd No:	3 -E- calc	3 -E- conf- calc	3- Z- conf- calc	3 -Z- calc	3 -C,O- calc
Co-C1	1.758	1.759	1.759	1.750	1.863
Co-C2	2.045	2.054	2.059	2.042	-
Co-C3	2.016	2.009	2.024	2.027	-
Co-01	-	-	-	-	1.877
C1-C2	1.405	1.407	1.412	1.412	1.429
C2-C3	1.452	1.449	1.462	1.465	1.402
C3-C4	1.486	1.489	1.481	1.479	1.409
C2-Si	1.914	1.918	1.936	1.928	1.979
S-C1	1.766	1.776	1.756	1.765	1.803
S-C11	1.787	1.800	1.795	1.794	1.811
C4-01	1.216	1.212	1.218	1.217	1.265
C4-02	1.372	1.374	1.368	1.371	1.355
Co1-C1-C2	79.69	80.03	80.13	79.64	126.95
Co1-C1-S	138.44	140.07	141.31	139.13	116.14
Co1-C2-Si	134.05	128.54	137.33	137.91	-
Co1-C2-C1	57.76	57.53	57.34	57.49	-
Co1-C2-C3	67.98	67.44	67.74	68.37	-
Со1-С3-С2	70.12	70.77	70.29	69.42	-

Table S2. Distance (Å) and Angle (deg) Data for Computed Vinylcarbene Structures. See Figure S4 and S5 for computed structures and atom labeling.

S19

Co1-C3-C4	107.75	106.95	113.59	115.58	-
Co1-01-C3	-	-	-	-	128.27
C1-Co1-C2	42.55	42.43	42.53	42.86	-
C1-Co1-C3	74.87	75.01	74.07	73.62	-
C1-Co1-O1	-	-		-	93.86
C2-Co1-C3	41.90	41.78	41.96	42.22	-
C1-C2-C3	107.39	107.44	105.49	104.43	119.90
C1-C2-Si	130.10	131.64	124.56	124.65	128.34
C3-C2-Si	121.96	118.73	129.92	130.91	111.39
C1-S-C11	99.67	103.72	102.43	97.07	103.91
C2-C1-S	136.43	138.35	134.36	139.47	116.91
C2-C3-C4	121.11	121.29	123.69	126.49	124.96
C3-C4-01	127.78	127.75	126.95	128.00	125.39
C3-C4-02	109.30	109.01	110.16	109.48	115.59
Co-C3-C4-O1	-73.84	71.84	46.52	50.07	-
S-C1-C2-Si	-32.89	51.92	-31.47	-36.73	-11.65
C4-C3-C2-Si	131.60	-138.61	-28.13	-28.24	-178.68
H3-C3-C2-Si	-19.89	12.03	126.31	125.98	3.08

4. NBO analysis of 2-*TMS* supporting σ (Co-C)/ π *(CO) hyperconjugation involving the cobalt-(sp³)carbon sigma bond and the π * orbital of the ester carbonyl in 2-*TMS*.

Threshold for printing: 0.50 kcal/mol (Intermolecular threshold: 0.05 kcal/mol) E(2) E(j)-E(i) F(i,j) Donor NBO (i) Acceptor NBO (j) kcal/mol

Csp-Csp bond, Co-C54 and associated Csp-C54 and Csp-Co bonds:



C52C53 pi bond interacts moderately with C54C56 sigma antibond 59. BD (2) C 52 - C 53 /817. BD*(1) C 54 - C 56 4.81 C53-C54 sigma bond interacts strongly with the C52-S sigma* 62. BD (1) C 53 - C 54 /813. BD*(1) C 52 - S 64 14.82 C52-Co sigma bond interacts moderately with S-O sigma* /808. BD*(1) O 50 - S 64 60. BD (1) C 52 -Co 60 6.14 C52-Co sigma bond interacts strongly with the C53-Si sigma* 60. BD (1) C 52 -Co 60 /815. BD*(1) C 53 -Si 65 16.52 C52-Co bond interacts very strongly with the C54-Co sigma* 60. BD (1) C 52 -Co 60 /818. BD*(1) C 54 -Co 60 56.10 C52-Co bond interacts very strongly with Co-P sigma*

60. BD (1) C 52 -Co 60 /825. BD*(1)Co 60 - P 63 52.07 C54-H sigma bond interacts moderately with C56-O sigma* 64. BD (1) C 54 - H 55 /819. BD*(1) C 56 - O 61 6.05 C54-C56 sigma bond interacts weakly with C57-O sigma* 65. BD (1) C 54 - C 56 /824. BD*(1) C 57 - 0 62 4.71 C54-Co sigma bond interacts moderately with C52-S sigma* 66. BD (1) C 54 -Co 60 /813. BD*(1) C 52 - S 64 12.89 C54-Co sigma bond interacts moderately with the C53-Si sigma* 66. BD (1) C 54 -Co 60 /815. BD*(1) C 53 -Si 65 8.64 C54-Co sigma bond interacts strongly with C56-O pi* 66. BD (1) C 54 -Co 60 /820. BD*(2) C 56 - 0 61 26.46 C54-Co sigma bond interacts very strongly Co-P sigma* 66. BD (1) C 54 -Co 60 /825. BD*(1)Co 60 - P 63 49.56 Co-P sigma bond interacts strongly with C52-Co sigma* 73. BD (1)Co 60 - P 63 /812. BD*(1) C 52 -Co 60 27.13 CO-P sigma bond interacts strongly with C54-Co sigma* 73. BD (1)Co 60 - P 63 /818. BD*(1) C 54 -Co 60 23.11 Co-P sigma bond interacts strongly with Co-P sigma* /825. BD*(1)Co 60 - P 63 73. BD (1)Co 60 - P 63 16.75 sulfur oxygen lone pair interactions 122. LP (2) 0 50 /772. BD*(1) C 15 - S 64 17.42 2) 0 50 122. LP (/813. BD*(1) C 52 - S 64 17.84 3) 0 50 /772. BD*(1) C 15 - S 64 123. LP (9.14 3) 0 50 1) 0 51 - S 64 /809. BD*(123. LP (27.13 2) 0 51 /772. BD*(1) C 15 - S 64 125. LP (12.71 125. LP (2) 0 51 /813. BD*(1) C 52 - S 64 16.77 1) C 15 - S 64 12.99 126. LP (3) 0 51 /772. BD*(1) 0 50 - S 64 126. LP (3) 0 51 /808. BD*(23.95 1) C 54 - C 56 131. LP (2) O 61 /817. BD*(20.31 2) 0 61 131. LP (/821. BD*(1) C 56 - O 62 38.60 /819. BD*(1) C 56 - O 61 132. LP (1) 0 62 10.05 1) C 1 - C 57 133. LP (/756. BD*(2) 0 62 7.07 133. LP (2) 0 62 /820. BD*(2) C 56 - O 61 52.20

References

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