Electron-poor Hemilabile Dicationic Palladium NHC Complexes – Synthesis, Structure and Catalytic Activity

Supporting Information

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Supplemental Figures and Tables

a) b)

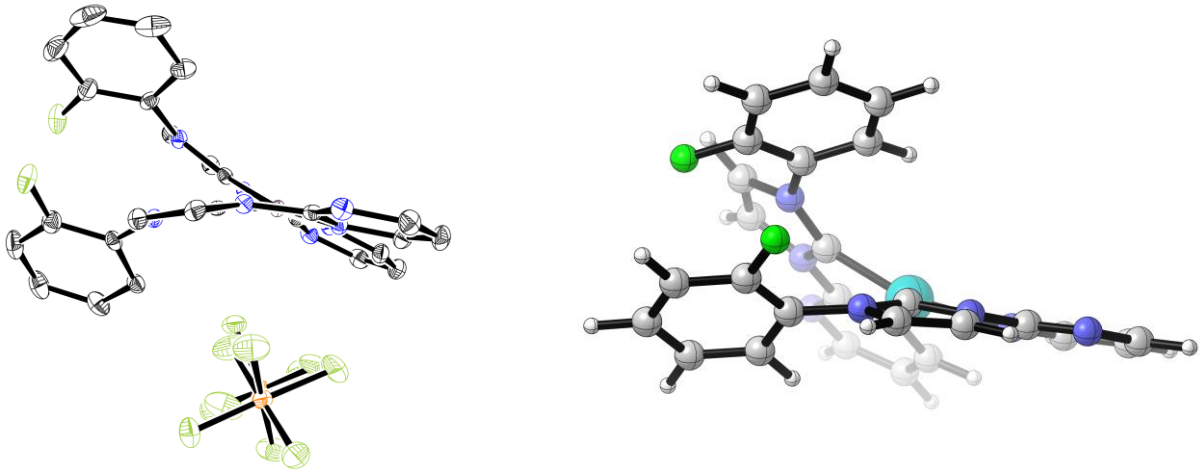


Figure S1. Comparison of solid-state structure and solution structure of (*CN*,*CN*)-**4d**. a) ORTEP representation of (*CN*,*CN*)-**4d**, side-view. Hydrogen atoms and counter ions are omitted for clarity. Ellipsoids are drawn at the 50 % probability level. b) DFT-optimized structure of (*CN*,*CN*)-**4d**, calculated with B3LYP-D3/6-31+G*.

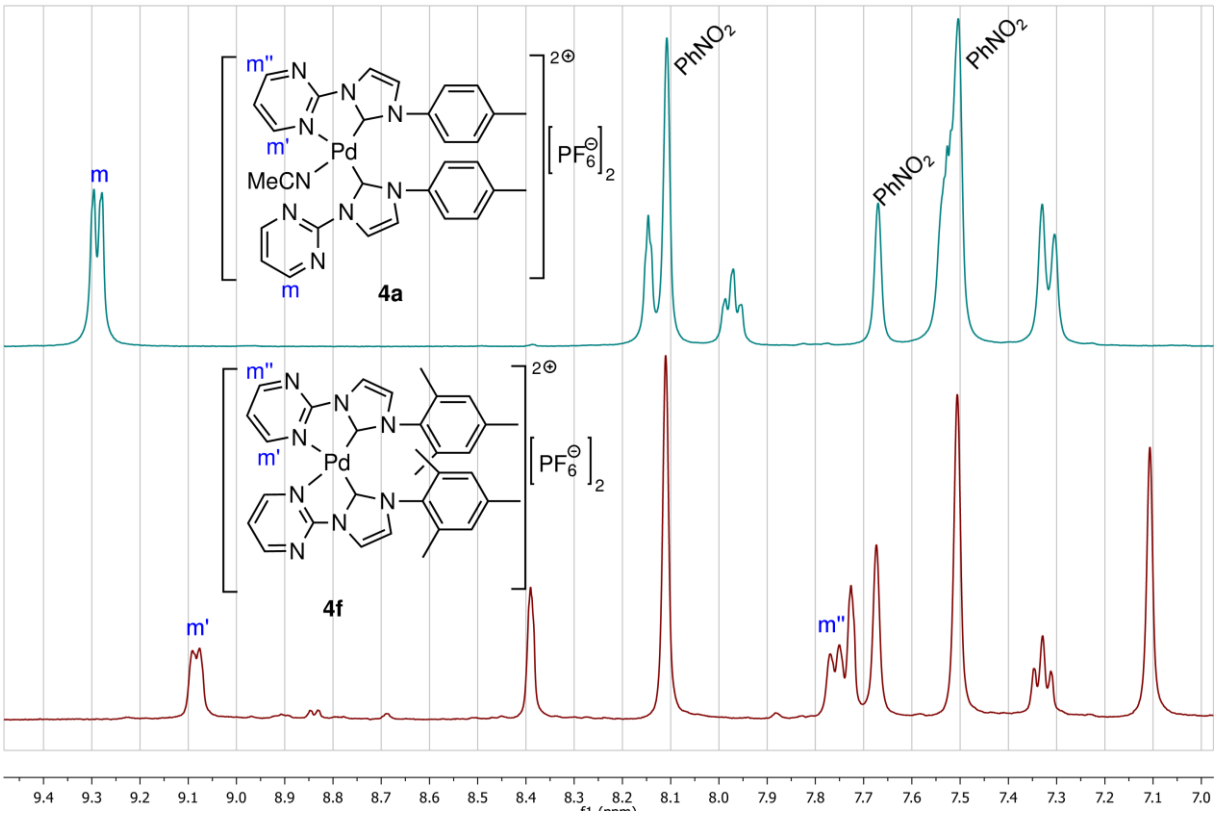


Figure S2. Comparison of the NMR spectra of **4a** (top) and **4f** (bottom) in the aromatic region (solvent: nitrobenzene-*d5*).

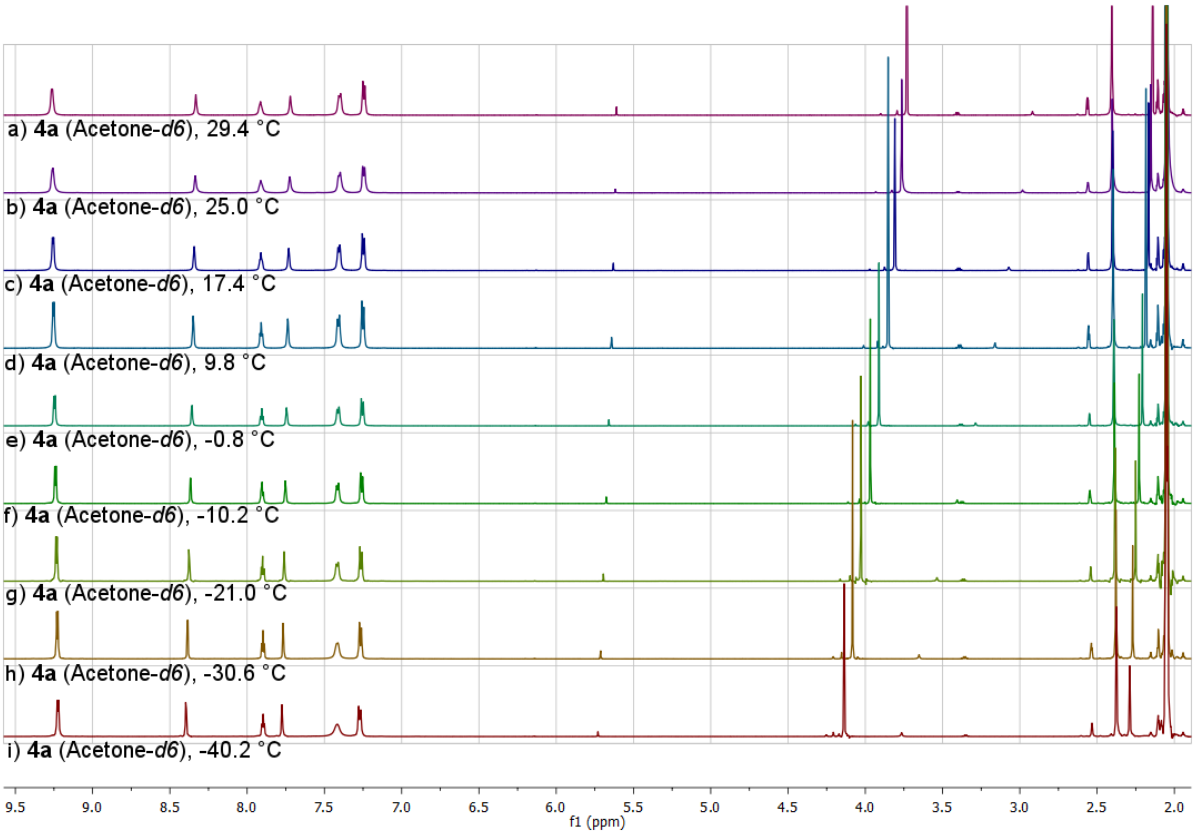


Figure S3. NMR spectrum of **4a** in acetone-*d6* in the temperature range of -40 – 30 °C.

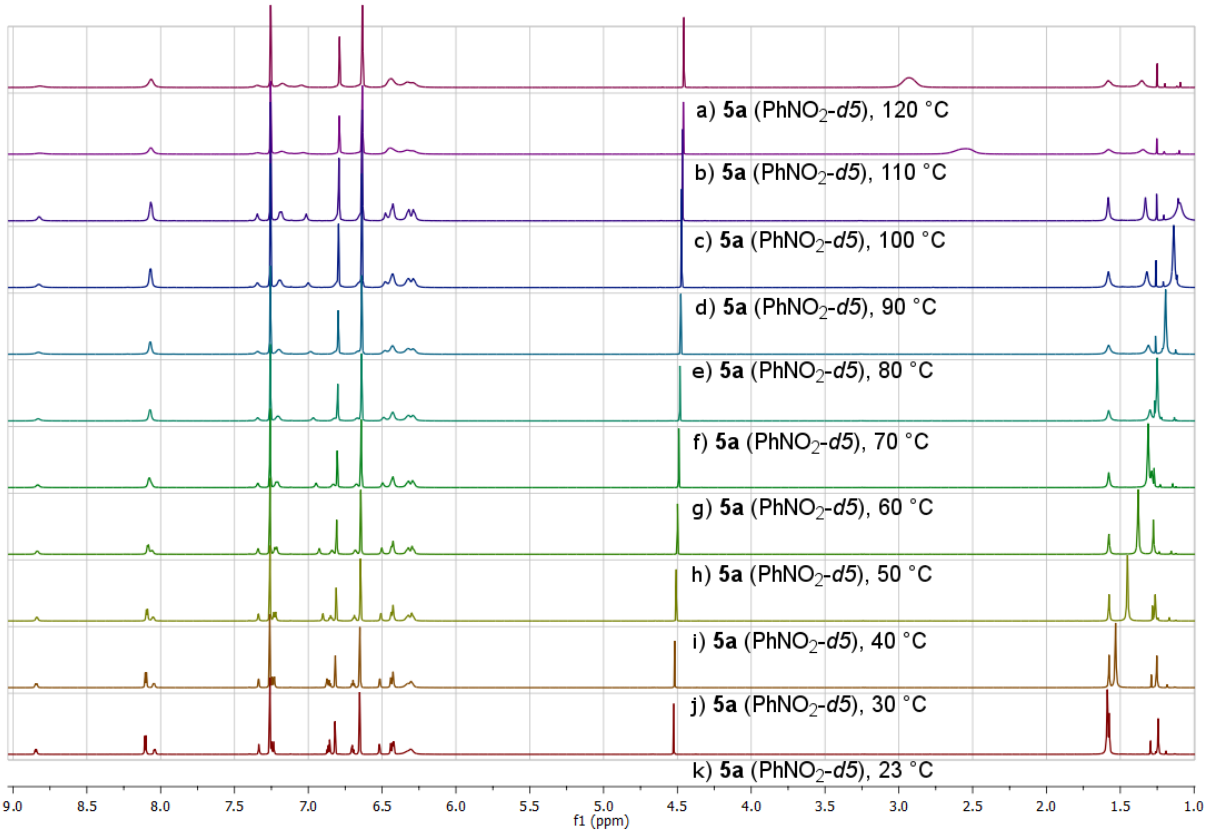


Figure S4. NMR spectrum of **5a** in nitrobenzene-*d5* in the temperature range of 23 – 120 °C.

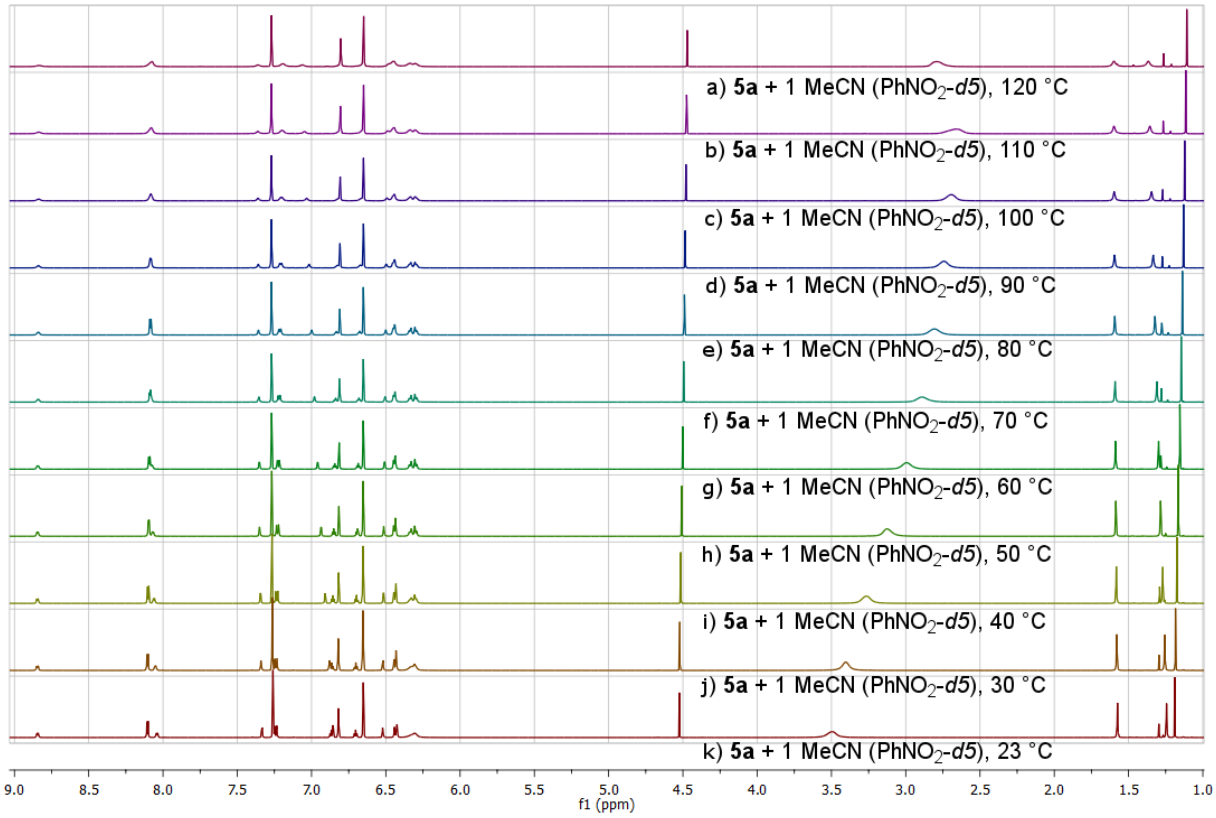


Figure S5. NMR spectrum of **5a** and one equivalent of acetonitrile in nitrobenzene-*d5* in the temperature range of 23 – 120 °C.

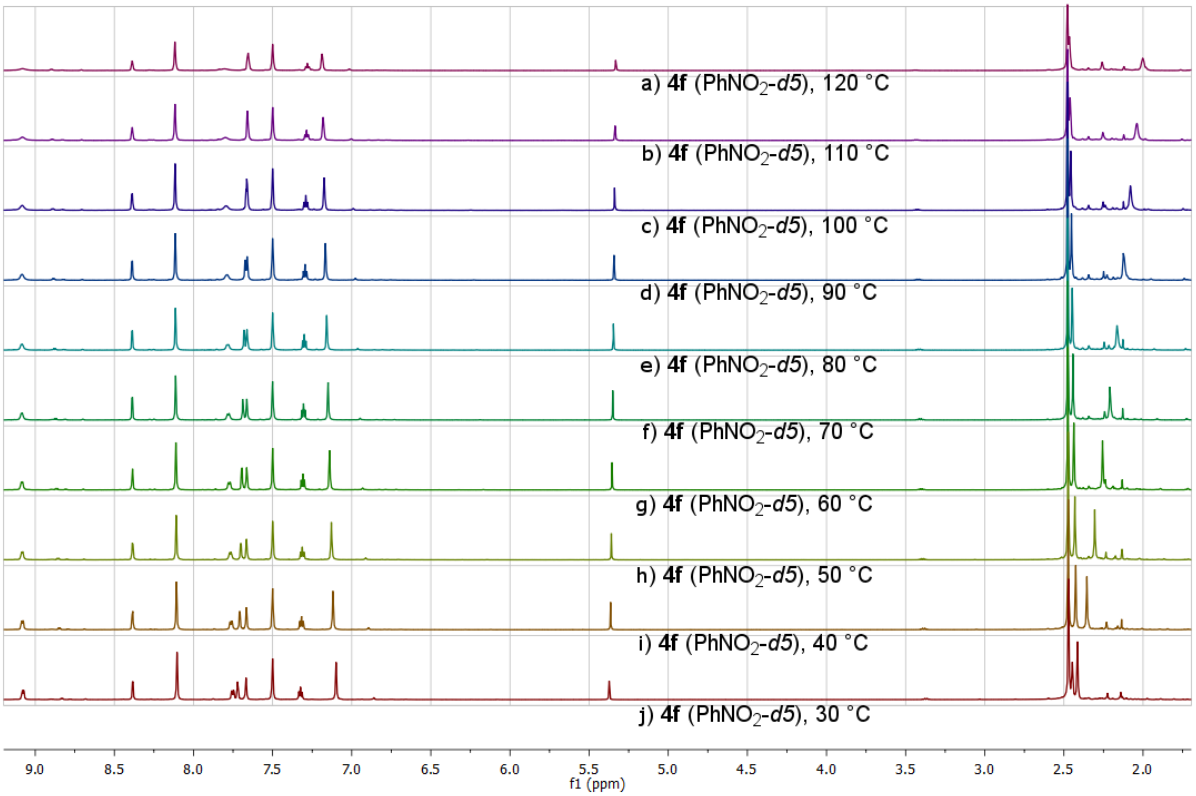


Figure S6. NMR spectrum of **4f** in nitrobenzene-*d5* in the temperature range of 30 – 120 °C.

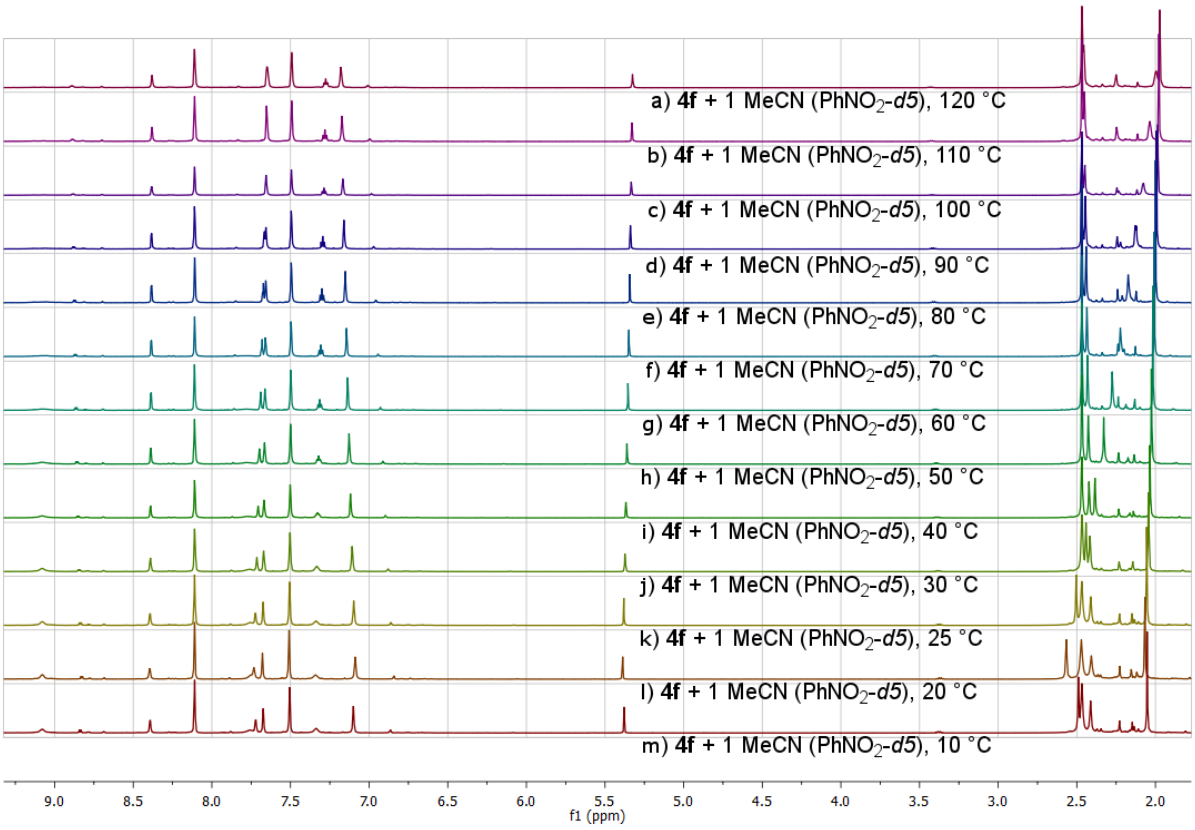


Figure S7. NMR spectrum of **4f** with added acetonitrile (1 equiv) in nitrobenzene-*d5* in the temperature range of 10 – 120 °C.

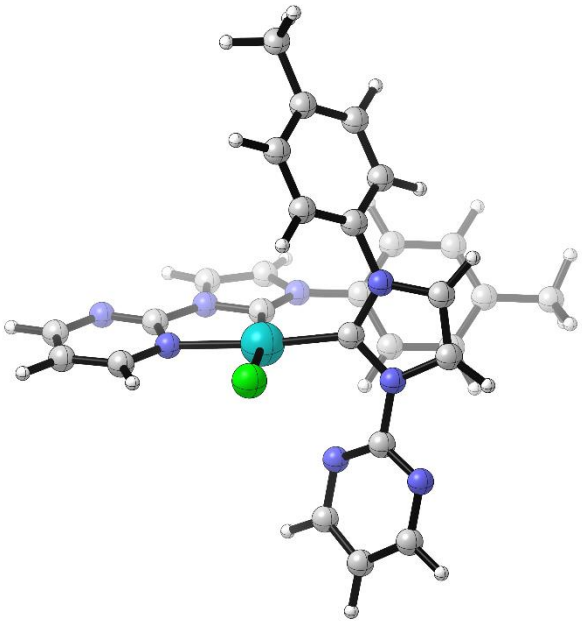
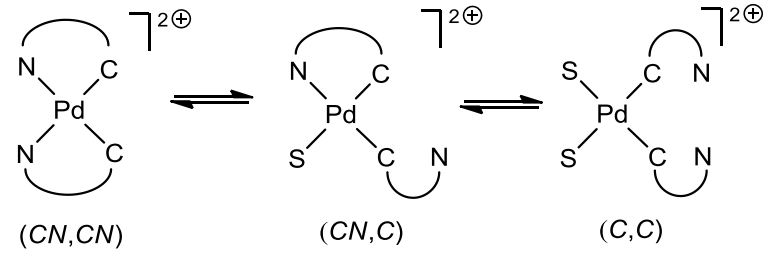


Figure S8: Optimized structure of (*CN*,*C*)-**5a**. Calculated with B3LYP-D3/6-31+G*.

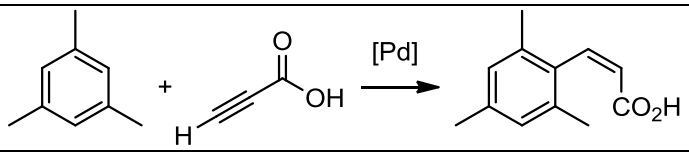
Table 1. Computed energies of the different architectures of the synthesized complexes. Electronic energies (*free energies*) relative to the (*CN*,*CN*)-complex. Calculated with B3LYP-D3(SMD(MeCN))/6-31+G*// B3LYP-D3/6-31+G*.



(*CN*,*CN*) (*CN*,*C*) (*C*,*C*)

		(*CN*,*CN*)		(*CN*,*C*)		(*C*,*C*)	
Complex	Ar =	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
4a	4-Me-Ph	0.0	*0.0*	-8.3	*+0.5*	-8.9	*+9.4*
4b	4-MeO-Ph	0.0	*0.0*	-8.2	*+0.9*	-9.7	*+10.0*
4c	4-F-Ph	0.0	*0.0*	-8.4	*+0.6*	-8.7	*+9.1*
4d	2-F-Ph	0.0	*0.0*	-9.8	*+0.1*	-11.3	*+7.4*
4e	4-NO_2-Ph	0.0	*0.0*	-8.5	*+0.3*	-9.2	*+11.1*
4f	Mes	0.0	*0.0*	-7.3	*+1.5*	-17.8	*+2.4*
4g	4-MeO-2,4-Me_2-Ph	0.0	*0.0*	-6.9	*+3.3*	-18.3	*+2.2*
4h	3,5-$(CF_3)_2$-Ph	0.0	*0.0*	-9.4	*+1.0*	-10.9	*+5.9*
5a	4-Me-Ph	0.0	*0.0*	-14.8	*-8.4*	-11.5	*+4.0*

Table S2. Optimization of the alkyne hydroarylation of mesitylene and propiolic acid.

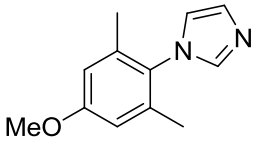


Entry	Catalyst load [mol-%]	Solvent	Temperature [°C]	Reaction time [h]	Yield [%]
	0.1	TFA/DCE (0.5/1.5)	60	24	33
	0.5	TFA/DCE (0.5/1.5)	60	24	30
	0.1	TFA/DCE (1.0/1.0)	60	24	33
	0.1	TFA/hfip (1.5/0.5)	60	24	40
	0.1	TFA/F_3CCH_2OH (1.5/0.5)	60	24	11
	0.1	TFA (1)	60	24	62
	1	TFA (1)	60	1	**69**
	1[b]	TFA (1)	60	1	57
	1[c]	TFA (1)	60	1	31
	0	TFA (1)	60	24	0

b) 2 equivalents of mesitylene, c) 3 equivalents of mesitylene.

Characterization Data and Synthetic Procedures

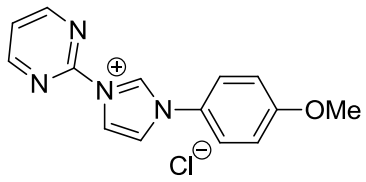
Synthesis of 1-(4-methoxy-2,6-dimethylphenyl)imidazole (**1g**).



The compound was synthesized following a modified literature procedure.[1] In methanol (18 mL), 4-methoxy-2,6-dimethylaniline (3.0 g, 19.8 mmol) is dissolved and glyoxal (2.4 mL, 21 mmol, 1.06 equiv., 40 % aqueous solution) is added. After stirring at room temperature overnight, methanol (70 mL), ammonium chloride (2.12 g, 39.7 mmol, 2 equiv.) and formaldehyde (3.12 mL, 41.7 mmol, 2.1 equiv., 37 % aqueous solution) are added and the mixture is refluxed for 1 h. After addition of phosphoric acid (2.8 mL, 85 % aqueous solution), the mixture is refluxed for another 4 h. After cooling down, the mixture is concentrated under reduced pressure, ice (60 g) is added and the pH value is adjusted to approx. 9 with KOH (40 % aqueous solution). The aqueous phase is extracted with diethyl ether (3 x 40 mL), the combined organic phases are washed with water (15 mL) and brine (15 mL), and dried over magnesium sulfate. The solvent is evaporated under reduced pressure and the raw product purified by colunm chromatography (ethyl acetate) to yield **1g** (2.65 g, 13.1 mmol, 66 %) as a light brown solid. 27 % of the aniline were reisolated. ^{1}H-NMR: (300 MHz, $CDCl_3$) δ ppm 2.00 (s, 6 H, C*H*$_3$), 3.82 (s, 3 H, OC*H*$_3$), 6.68 (s, 2 H, H$_{ar}$), 6.89 (s, 1 H, NC*H*), 7.23 (s, 1 H, NC*H*), 7.44 (s, 1 H, NC*H*N). ^{13}C-NMR: (75.5 MHz, $CDCl_3$) δ ppm 17.6 (s, *C*H$_3$), 55.3 (s, O*C*H$_3$), 113.3 (s, *C*H$_{ar}$), 120.3 (s, N*C*H), 128.8 (s, *i-C*), 129.3 (s, N*C*H), 137.0 (s, *o-C*), 137.7 (s, N*C*HN), 159.3 (s, *p-C*). Elemental analysis calcd. for $C_{12}H_{14}N_2O$ (202.25): C – 71.26 %, H – 6.98 %, N – 13.85 %, found: C – 71.39 %, H – 7.10 %, N – 13.82 %. Mp. 77 °C.

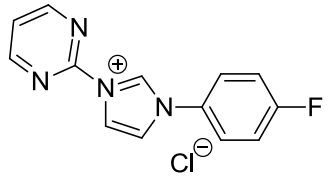
Characterization of the chloride salts

1-(4-Methoxyphenyl)-3-(pyrimidine-2-yl)imidazolium chloride (**2b**)



1b (2.28 g, 13.1 mmol) and 2-chloropyrimidine (1.50 g 13.1 mmol) yield **2b** (2.74 g, 9.51 mmol, 73 %) as a light brown solid. ^{1}H-NMR: (300 MHz, $CDCl_3$) δ ppm 3.87 (s, 3 H, OC*H*$_3$), 7.10 (d, ^{3}J = 9.0 Hz, 2 H, H$_{ar}$), 7.55 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H$_{pym}$), 8.10 (d, ^{3}J = 9.0 Hz, 2 H, H$_{ar}$), 8.25 (t, ^{3}J = 1.8 Hz, 1 H, NC*H*), 8.39 (t, ^{3}J = 1.8 Hz, 1 H, NC*H*), 8.92 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H$_{pym}$), 10.92 (br. s, 1 H, NC*H*N). ^{13}C-NMR: (75.5 MHZ, $CDCl_3$) δ ppm 55.8 (s, O*C*H$_3$), 115.6 (s, *C*H$_{ar}$), 119.5 (s, *p*-C$_{pym}$), 122.2 (s, N*C*H), 123.1 (s, N*C*H), 124.3 (s, *C*H), 127.2 (s, C$_{ar}$), 134.5 (s, NC*H*N), 159.7 (s, *m*-C$_{pym}$), 161.3 (s, *C*H). *One signal was not visible in the spectrum.* Elemental analysis calcd. for $C_{14}H_{13}ClN_4O \cdot 0.25\ H_2O$ (288.73): C – 57.34 %, H – 4.64 %, N – 19.11 %, found: C – 57.43 %, H – 4.67 %, N – 19.07 %. Mp. 255 °C.

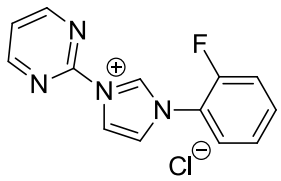
1-(4-Fluorophenyl)-3-(pyrimidine-2-yl)imidazolium chloride (**2c**)



1c (2.0 g, 12.3 mmol) and 2-chloropyrimidine (1.41 g 12.3 mmol) yield **2c** (2.83 g, 10.2 mmol, 83 %) as a brown solid. ^{1}H-NMR: (300 MHz, DMSO-*d*$_6$) δ ppm 7.49 - 7.66 (m, 2 H, H*$_{ar}$*), 7.84 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H$_{pym}$), 7.98 - 8.13 (m, 2 H, H*$_{ar}$*), 8.53 - 8.61 (m,

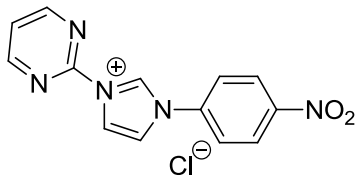
1 H, NC*H*), 8.71 - 8.77 (m, 1 H, NC*H*), 9.12 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H_{pym}), 10.70 (t, ^{3}J = 1.6 Hz, 1 H, NC*H*N). ^{13}C-NMR: (75 MHz, DMSO-d_6) δ ppm 116.9 (d, $^{2}J_{C\text{-}F}$ = 24.0 Hz, *C*H, C_{ar}), 119.8 (s, *C*H, *p*-C_{pym}), 122.8 (s, *C*H, N*C*H), 123.2 (s, *C*H, N*C*H), 125.4 (d, $^{3}J_{C\text{-}F}$ = 9.4 Hz, *C*H, C_{ar}), 131.0 (d, $^{4}J_{C\text{-}F}$ = 3.0 Hz, *C*, C_{ar}), 135.3 (s, *C*H, N*C*HN), 152.1 (s, *C*, *i*-C_{pym}), 160.2 (s, *C*H, *m*-C_{pym}), 162.6 (d, $^{1}J_{C\text{-}F}$ = 245.0 Hz, *C*, C_{ar}). ^{19}F-NMR: (282 MHz, DMSO-*d6*) δ ppm -111.4 (s). Elemental analysis calcd. for $C_{13}H_{10}ClFN_4$ (276.7): C – 56.43 %, H – 3.64 %, N – 20.25 %, found: C – 56.08 %, H – 3.53 %, N – 20.17 %. Mp. 289 °C.

1-(2-Fluorophenyl)-3-(pyrimidine-2-yl)imidazolium chloride (**2d**)



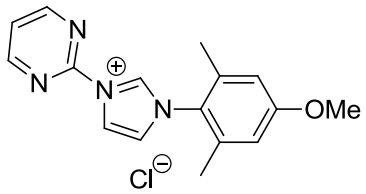
1d (2.0 g, 12.3 mmol) and 2-chloropyrimidine (1.41 g 12.3 mmol) yield **2d** (2.83 g, 10.2 mmol, 81 %) as a brown solid. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 7.49 - 7.57 (m, 1 H, H_{ar}), 7.61 - 7.80 (m, 2 H, H_{ar}), 7.84 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H_{pym}), 7.95 (td, J = 7.8 Hz, J = 1.5 Hz, 1 H, H_{ar}), 8.43 - 8.48 (m, 1 H, NC*H*), 8.74 - 8.78 (m, 1 H, NC*H*), 9.12 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H_{pym}), 10.64 (s, 1 H, NC*H*N). ^{13}C-NMR: (75 MHz, DMSO-d_6) δ ppm 117.2 (d, $^{2}J_{C\text{-}F}$ =19.3 Hz, *C*H, C_{ar}), 119.6 (s, *C*H, *p*-C_{pym}), 122.6 (d, $^{3}J_{C\text{-}F}$ = 12.0 Hz, *C*, C_{ar}), 122.8 (s, *C*H, N*C*H), 125.1 (d, $^{4}J_{C\text{-}F}$ = 2.2 Hz, *C*H, C_{ar}), 125.6 (d, $^{4}J_{C\text{-}F}$ = 3.9 Hz, *C*H, C_{ar}), 127.4 (s, *C*H, N*C*H), 132.9 (d, $^{3}J_{C\text{-}F}$ = 7.7 Hz, *C*H, C_{ar}), 137.2 (s, *C*H, N*C*HN), 152.0 (s, *i*-C_{pym}), 154.9 (d, $^{1}J_{C\text{-}F}$ = 252.0 Hz, *C*, C_{ar}), 160.2 (s, *m*-C_{pym}). ^{19}F-NMR: (282 MHz, DMSO-d_6) δ ppm -124.3 (s). Elemental analysis calcd. for $C_{13}H_{10}ClFN_4$ (276.7): C – 56.43 %, H – 3.64 %, N – 20.25 %, found: C – 56.41 %, H – 3.44 %, N – 20.62 %. Mp. 261 °C.

1-(4-Nitrophenyl)-3-(pyrimidine-2-yl)imidazolium chloride (**2e**)



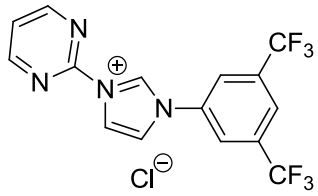
1e (2.0 g, 10.6 mmol) and 2-chloropyrimidine (1.21 g, 10.6 mmol) yield **2e**. The purification of this compound could not be achieved, therefore the crude product was used for further reactions.

1-(4-Methoxy-2,6-dimethylphenyl)-3-(pyrimidine-2-yl)imidazolium chloride (**2g**)



1g (1.25 g, 6.19 mmol) and 2-chloropyrimidine (0.71 g, 6.19 mmol) yield **2g** (0.94 g, 2.96 mmol, 48 %) as a beige solid. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 2.12 (s, 6 H, CH_3), 3.83 (s, 3 H, OCH_3), 6.94 (s, 2 H, H_{ar}), 7.82 (t, ^{3}J = 4.8 Hz, 1 H, *p*-H_{pym}), 8.18 (s, 1 H, NC*H*), 8.77 (s, 1 H, NC*H*), 9.10 (d, ^{3}J = 4.8 Hz, 2 H, *m*-H_{pym}), 10.47 (s, 1 H, NC*H*N). ^{13}C-NMR: (151 MHz, DMSO-d_6) δ ppm 17.4 (s, *C*H_3), 55.6 (s, O*C*H_3), 113.8 (s, *C*H_{ar}), 120.0 (s, *p*-C_{pym}), 122.7 (s, N*C*H), 125.7 (s, N*C*H), 126.6 (s, C_{ar}), 136.2 (s, C_{ar}), 137.4 (s, N*C*HN), 152.4 (s, *i*-C_{pym}), 160.1 (s, *m*-C_{pym}), 160.3 (s, C_{ar}). Elemental analysis calcd. for $C_{16}H_{17}ClN_4O$ (316.79): C – 60.66 %, H – 5.41 %, N – 17.68 %, found: C – 60.28 %, H – 5.31 %, N – 17.61 %. Mp. 275 °C.

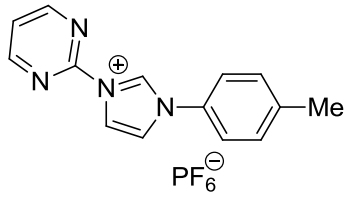
1-(3,5-Bis(trifluoromethyl)phenyl)-3-(pyrimidine-2-yl)imidazolium chloride (**2h**)



1h (3.42 g, 12.2 mmol) and 2-chloropyrimidine (1.40 g, 12.2 mmol) yield **2h** (2.93 g, 7.43 mmol, 61 %) as a beige solid. Deviation from general procedure: After washing with THF, the raw product is dissolved in acetone (10 mL) and precipitated by addition of diethyl ether (40 mL). ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 7.87 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H$_{pym}$), 8.46 (s, 1 H, NC*H*), 8.77 - 8.81 (m, 2 H, H$_{ar}$), 8.82 (s, 2 H, H$_{ar}$), 9.15 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H$_{pym}$), 11.02 (t, ^{3}J = 1.6 Hz, 1 H, NC*H*N). ^{13}C NMR (126 MHz, DMSO-d_6) δ ppm 122.7 (q, ^{1}J = 275.0 Hz, *C*F$_3$), 119.8 (s, *p*-C$_{pym}$), 123.0 (s, N*C*H), 123.2 (s, N*C*H), 123.9 - 124.2 (m, *C*H$_{ar}$), 124.4 - 124.7 (m, *C*H$_{ar}$), 131.6 (q, ^{2}J = 34.0 Hz, C$_{ar}$), 136.0 (s, C$_{ar}$), 136.6 (s, N*C*HN), 152.0 (s, *i*-C$_{pym}$), 160.3 (s, *m*-C$_{pym}$). ^{19}F-NMR: (282 MHz, DMSO-*d6*) δ ppm -61.8 (s). Elemental analysis calcd. for $C_{15}H_9ClF_6N_4$ (394.71): C – 45.65 %, H – 2.30 %, N – 14.19 %, found: C – 45.28 %, H – 2.14 %, N – 14.11 %. Mp. 284 °C (decomp.).

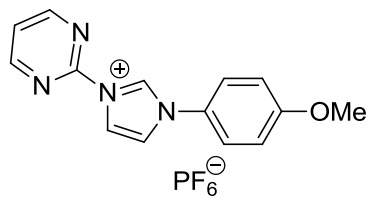
Characterization of the Hexafluorophosphate Salts

1-(4-Methylphenyl)-3-(pyrimidine-2-yl)imidazolium hexafluorophosphate (**3a**)



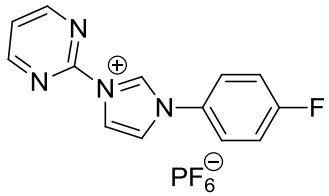
2a (2.0 g, 7.33 mmol) and potassium hexafluorophosphate (2.7 g, 14.7 mmol) yield **3a** (2.03 g, 5.3 mmol, 72 %) as a brown solid. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 2.43 (s, 3 H, C*H*$_3$), 7.49 (d, ^{3}J = 8.3 Hz, 2 H, H$_{ar}$), 7.86 (d, ^{3}J = 8.3 Hz, 2 H, H$_{ar}$), 7.82 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H$_{pym}$), 8.53 (s, 1 H, NC*H*), 8.73 (s, 1 H, NC*H*), 9.11 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H$_{pym}$), 10.66 (s, 1 H, NC*H*N). ^{13}C-NMR: (75.5 MHz, DMSO-d_6) δ ppm 20.6 (s, *C*H$_3$), 119.9 (s, *p*-C$_{pym}$), 122.3 (s, *C*H$_{ar}$), 122.7 (s, N*C*H), 122.8 (s, N*C*H), 130.4 (s, *C*H$_{ar}$), 132.1 (s, C$_{ar}$), 134.7 (s, N*C*HN), 140.3 (s, C$_{ar}$), 152.1 (s, *i*-C$_{pym}$), 160.1 (s, *m*-C$_{pym}$). Elemental analysis calcd. for $C_{14}H_{13}F_6N_4P$ (382.24): C – 43.99 %, H – 3.43 %, N – 14.66 %, found: C – 43.95 %, H – 3.41 %, N – 14.55 %. Mp. 174 °C.

1-(4-Methoxyphenyl)-3-(pyrimidine-2-yl)imidazolium hexafluorophosphate (**3b**)



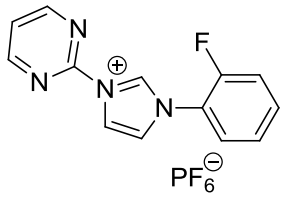
2b (1.44 g, 5 mmol) and potassium hexafluorophosphate (1.84 g, 10 mmol) yield **3b** (1.82 g, 4.57 mmol, 91 %) as a brown solid. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 3.87 (s, 3 H, O*C*H$_3$), 7.22 (d, ^{3}J = 9.1 Hz, 2 H, H$_{ar}$), 7.82 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H$_{pym}$), 7.89 (d, ^{3}J = 9.1 Hz, 2 H, H$_{ar}$), 8.48 (s, 1 H, NC*H*), 8.72 (s, 1 H, NC*H*), 9.11 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H$_{pym}$), 10.61 (s, 1 H, NC*H*N). ^{13}C-NMR: (75.5 MHz, DMSO-d_6) δ ppm 55.8 (s, O*C*H$_3$), 115.0 (s, *C*H$_{ar}$), 119.7 (s, *p*-C$_{pym}$), 122.6 (s, N*C*H), 123.0 (s, N*C*H), 124.1 (s, *C*H$_{ar}$), 127.5 (s, C$_{ar}$), 134.6 (s, N*C*HN), 152.1 (s, i-C$_{pym}$), 160.1 (s, *m*-C$_{pym}$), 160.4 (s, C$_{ar}$). Elemental analysis calcd. for $C_{14}H_{13}F_6N_4OP$ (398.24): C – 42.22 %, H – 3.29 %, N – 14.07 %, found: C – 42.37 %, H – 3.35 %, N – 14.15 %. Mp. 197 °C.

1-(4-Fluorophenyl)-3-(pyrimidine-2-yl)imidazolium hexafluorophosphate (**3c**)



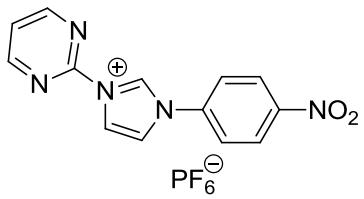
2c (1.0 g, 3.61 mmol) and potassium hexafluorophosphate (1.33 g, 7.23 mmol) yield **3c** (1.21 g, 3.13 mmol, 87 %) as a light brown solid. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 7.58 (t, ^{3}J = 8.8 Hz, 2H, H$_{ar}$), 7.83 (t, ^{3}J = 4.9 Hz, *p*-H$_{pym}$), 7.94 - 8.11 (m, 2H, H$_{ar}$), 8.52 (t, ^{3}J = 2.0 Hz, 1 H, NC*H*), 8.74 (t, ^{3}J = 2.0 Hz, 1 H, NC*H*), 9.12 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H$_{pym}$), 10.69 (t, ^{3}J = 1.7 Hz, 1 H, NC*H*N). ^{13}C-NMR: (75 MHz, DMSO-d_6) δ ppm 116.9 (d, $^{2}J_{C\text{-}F}$ = 24.0 Hz, *C*H$_{ar}$), 119.8 (s, *p*-C$_{pym}$), 122.7 (s, N*C*H), 123.2 (s, N*C*H), 125.4 (d, $^{3}J_{C\text{-}F}$ = 9.4 Hz, *C*H$_{ar}$), 131.0 (d, $^{4}J_{C\text{-}F}$ = 3.0 Hz, C$_{ar}$), 135.3 (s, N*C*HN), 152.1 (s, *i*-C$_{pym}$), 160.2 (s, *m*-C$_{pym}$), 162.6 (d, $^{1}J_{C\text{-}F}$ = 248.0 Hz, C$_{ar}$) ^{19}F-NMR: ^{19}F NMR (282 MHz, DMSO-d_6) δ ppm -106.57 (s, F$_{ar}$), -66.03 (d, ^{1}J = 711.0 Hz, P*F*$_6$). Elemental analysis calcd. for $C_{13}H_{10}F_7N_4P$ (276.7): C – 40.43 %, H – 2.61 %, N – 14.51 %, found: C – 40.12 %, H – 2.26 %, N – 14.46 %. Mp. 166 °C.

1-(2-Fluorophenyl)-3-(pyrimidine-2-yl)imidazolium hexafluorophosphate (**3d**)



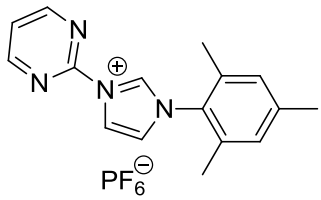
2d (1.0 g, 3.61 mmol) and potassium hexafluorophosphate (1.33 g, 7.23 mmol) yield **3d** (1.20 g, 3.12 mmol, 86 %) as a light brown solid. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 7.44 - 7.58 (m, 1 H, H$_{ar}$), 7.61 - 7.79 (m, 2 H, H$_{ar}$), 7.83 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H$_{pym}$), 7.88 - 8.00 (m, 1 H, H$_{ar}$), 8.39 - 8.48 (m, 1 H, NC*H*), 8.74 - 8.79 (m, 1 H, NC*H*), 9.11 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H$_{pym}$), 10.64 (s, 1 H, NC*H*N). ^{13}C-NMR: (75 MHz, DMSO-d_6) δ ppm 117.2 (d, $^{2}J_{C\text{-}F}$ = 18.0 Hz, *C*H$_{ar}$), 119.6 (s, *p*-C$_{pym}$), 122.6 (d, $^{2}J_{C\text{-}F}$ = 12.0 Hz, C$_{ar}$), 122.8 (s, N*C*H), 125.0 (d, $^{4}J_{C\text{-}F}$ = 2.0 Hz, *C*H$_{ar}$), 125.7 (d, $^{3}J_{C\text{-}F}$ = 4.0 Hz, *C*H$_{ar}$), 127.4 (s, N*C*H), 132.9 (d, $^{3}J_{C\text{-}F}$ = 8.0 Hz, *C*H$_{ar}$), 137.1 (s, 1 C, N*C*HN), 152.1 (s, *i*-C$_{pym}$), 154.9 (d, $^{1}J_{C\text{-}F}$ = 252.0 Hz, 1 C, C$_{ar}$), 160.2 (s, *m*-C$_{pym}$). ^{19}F-NMR: (282 MHz, DMSO-d_6) δ ppm -119.51 (s, F$_{ar}$), -66.03 (d, ^{1}J = 707.0 Hz, P*F*$_6$). Elemental analysis calcd. for $C_{13}H_{10}F_7N_4P$ (276.7): C – 40.43 %, H – 2.61 %, N – 14.51 %, found: C – 40.41 %, H – 2.45 %, N – 14.60 %. Mp. 225 °C.

1-(4-Nitrophenyl)-3-(pyrimidine-2-yl)imidazolium hexafluorophosphate (**3e**)



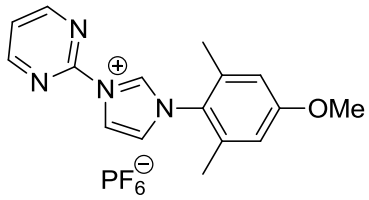
The raw product **2e** and potassium hexafluorophosphate (3.89 g, 21.1 mmol) yield **3e** (0.73 g, 1.77 mmol, 17 % (over two steps)) as a brown solid. Deviation from general procedure: After washing with water, the raw product is dissolved in acetone (20 mL) and precipitated by addition of diethyl ether (60 mL). ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 7.86 (t, ^{3}J = 4.8 Hz, 1 H, *p*-H$_{pym}$), 8.29 (d, ^{3}J = 8.8 Hz, 2 H, H$_{ar}$), 8.55 (d, ^{3}J = 8.8 Hz, 2 H, H$_{ar}$), 8.68 (t, ^{3}J = 2.0 Hz, 1 H, NC*H*), 8.81 (t, ^{3}J = 2.0 Hz, 1 H, H$_{ar}$), 9.14 (d, ^{3}J = 4.8 Hz, 2 H, *m*-H$_{pym}$), 10.87 - 10.95 (m, 1 H, N*C*HN). ^{13}C-NMR: (75 MHz, DMSO-d_6) δ ppm 120.2 (s, *p*-C$_{pym}$), 122.8 (s, N*C*H), 123.0 (s, N*C*H), 124.1 (s, *C*H$_{ar}$), 125.4 (s, *C*H$_{ar}$), 136.1 (s, N*C*HN), 139.1 (s, *C*$_{ar}$), 148.1 (s, *C*$_{ar}$), 152.1 (s, *i*-C$_{pym}$), 160.3 (s, *m*-C$_{pym}$). Elemental analysis calcd. for $C_{13}H_{10}F_6N_5O_2P$ (413.22): C – 37.79 %, H – 2.44 %, N – 16.95 %, found: C – 38.17 %, H – 2.33 %, N – 16.87 %. Mp. 242 °C.

1-(2,4,6-Trimethylphenyl)-3-(pyrimidine-2-yl)imidazolium hexafluorophosphate (**3f**)



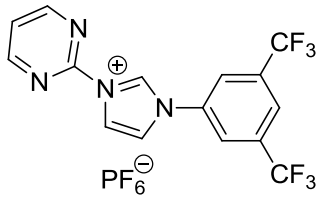
2f (1.68 g, 5.59 mmol) and potassium hexafluorophosphate (2.06 g, 11.2 mmol) yield **3f** (2.06 g, 5.03 mmol, 90 %) as a light brown solid. ^{1}H-NMR (300 MHz, DMSO-d_6) δ ppm 2.11 (s, 6 H, CH_3), 2.36 (s, 3 H, CH_3), 7.18 (s, 2 H, H$_{ar}$), 7.81 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H$_{pym}$), 8.12 - 8.23 (m, 1 H, NC*H*), 8.73 - 8.84 (m, 1 H, NC*H*), 9.09 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H$_{pym}$), 10.44 - 10.53 (m, 1 H, NC*H*). ^{13}C-NMR: (75.5 MHz, DMSO-d_6) δ ppm 17.0 (s, *C*H$_3$), 20.6 (s, *C*H$_3$), 120.1 (s, *p*-C$_{pym}$), 122.6 (s, N*C*H), 125.3 (s, N*C*H),129.2 (s, *C*H$_{ar}$), 131.2 (C$_{ar}$), 134.3 (s, *C*H$_{ar}$), 137.2 (s, N*C*HN), 140.4 (s, C$_{ar}$), 152.3 (s, *i*-C$_{pym}$), 160.0 (s, *m*-C$_{pym}$). Elemental analysis calcd. for $C_{16}H_{17}F_6N_4P \cdot 0.45\ H_2O$ (410.30): C – 45.93 %, H – 4.31 %, N – 13.39 %, found: C – 45.88 %, H – 4.23 %, N – 13.31 %. Mp. 218 °C.

1-(4-Methoxy-2,6-dimethylphenyl)-3-(pyrimidine-2-yl)imidazolium hexafluorophosphate (**3g**)



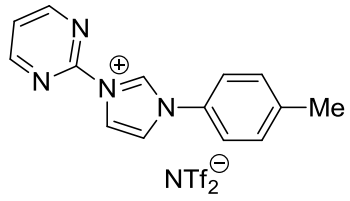
2g (418 mg, 1.32 mmol) and potassium hexafluorophosphate (486 mg, 2.64 mmol) yield **3g** (527 mg, 1.24 mmol, 94 %) as a light grey solid. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 2.12 (s, 6 H, CH_3), 3.83 (s, 3 H, OCH_3), 6.93 (s, 2 H, H$_{ar}$), 7.81 (t, ^{3}J = 5.0 Hz, 1 H, p-H$_{pym}$), 8.16 (s, 1 H, NC*H*), 8.76 (s, 1 H, NC*H*), 9.09 (d, ^{3}J = 5.0 Hz, 2 H, m-H$_{pym}$), 10.45 (s, 1 H, NC*H*N).^{13}C-NMR: (126 MHz, DMSO-d_6) δ ppm 17.4 (s, *C*H$_3$), 55.6 (s, O*C*H$_3$), 113.8 (s, *C*H$_{ar}$), 120.0 (s, *p*-C$_{pym}$), 122.6 (s, N*C*H), 125.6 (s, N*C*H), 126.6 (s, C$_{ar}$), 136.2 (s, C$_{ar}$), 137.4 (s, N*C*HN), 152.3 (s, *i*-C$_{pym}$), 160.0 (s, *m*-C$_{pym}$), 160.2 (s, C$_{ar}$). Elemental analysis calcd. for $C_{16}H_{17}F_6N_4OP$ (426.30): C – 45.08 %, H – 4.02 %, N – 13.14 %, found: C – 45.43 %, H – 3.99 %, N – 13.24 %. Mp. 256 °C.

1-(3,5-Bis(trifluoromethyl)phenyl)-3-(pyrimidine-2-yl)imidazolium hexafluorophosphate (**3h**)



2h (1.0 g, 2.53 mmol) and potassium hexafluorophosphate (0.93 g, 5.07 mmol) yield **3h** (1.20 g, 2.38 mmol, 94 %) as a light brown solid. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 7.86 (t, ^{3}J = 4.7 Hz, 1 H, *p*-H$_{pym}$), 8.47 (s, 1 H, NC*H*), 8.75 (s, 1 H, NC*H*), 8.80 (s, 3 H, H$_{ar}$), 9.14 (d, ^{3}J = 4.7 Hz, 2 H, *m*-H$_{pym}$), 11.01 (s, 1 H, NC*H*N). ^{13}C-NMR: (75 MHz, DMSO-d_6) δ ppm 119.8 (s, *p*-C$_{pym}$), 122.7 (q, ^{1}J = 273.0 Hz, *C*F$_3$), 123.0 (s, N*C*H), 123.2 (s, N*C*H), 123.7 - 124.2 (m, C$_{ar}$), 124.4 - 124.7 (m, C$_{ar}$), 131.7 (q, $^{2}J_{C\text{-}F}$ = 34.0 Hz, *C*$_{ar}$), 136.0 (s, C$_{ar}$), 136.5 (s, N*C*HN), 152.0 (s, C$_{ar}$), 160.3 (s, C$_{ar}$). *One signal was not visible in the spectrum.* ^{19}F-NMR: (282 MHz, DMSO-d_6) δ ppm -66.05 (d, $^{1}J_{F\text{-}P}$ = 707.0 Hz, P*F*$_6$), -57.05 (s, F$_{ar}$). Elemental analysis calcd. for $C_{15}H_9F_{12}N_4P$ (504.22): C – 35.73 %, H – 1.80 %, N – 11.11 %, found: C – 35.83 %, H – 1.67 %, N – 11.51 %. Mp. 267 °C.

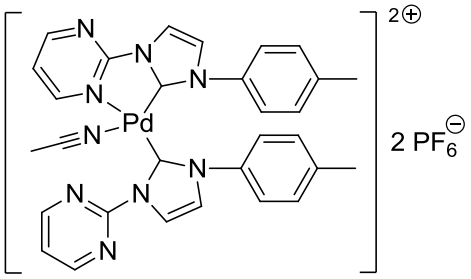
Synthesis of 1-(4-Methylphenyl)-3-(pyrimidine-2-yl)-imidazolium bis(trifluoromethane-sulfonyl)imide (3i)



The imidazolium chloride salt **2a** (0.5 g, 1.83 mmol) is dissolved in water (10 mL) and lithium bis(trifluoromethanesulfonyl)-imide (0.62 mL, 2.02 mmol, 1.1 equiv., 70 % aqueous solution) is added. After addition of DCM (15 mL), the mixture is stirred overnight at room temperature. The phases are separated, the organic phase washed with water (3 x 20 mL) and dried over sodium sulfate. The solvent is evaporated under reduced pressure and the product dried in high vacuum to yield **3i** as a brown solid (860 mg, 1.66 mmol, 91 %). ^{1}H-NMR: (300 MHz, $CDCl_3$) δ ppm 7.42 (d, ^{3}J = 8.3 Hz, 2 H, H_{ar}), 7.56 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H_{pym}), 7.60 (d, ^{3}J = 8.3 Hz, 2 H, H_{ar}), 7.85 (t, ^{3}J = 1.8 Hz, 1 H, NC*H*), 8.44 (t, ^{3}J = 1.8 Hz, 1 H, NC*H*), 8.89 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H_{pym}), 9.78 - 9.88 (m, 1 H, NC*H*N). ^{13}C-NMR: (75 MHz, $CDCl_3$) δ ppm 21.2 (s, *C*H_3), 119.7 (q, $^{1}J_{C\text{-}F}$ = 321.0 Hz, 2 C, *C*F_3), 120.0 (s, *C*H), 122.2 (s, *C*H_{ar}), 122.6 (s, *C*H), 123.1 (s, *C*H), 131.2 (s, *C*H_{ar}), 131.7 (s, *C*), 132.6 (s, N*C*HN), 141.9 (s, *C*), 151.9 (s, *i*-C_{pym}), 159.7 (s, *m*-C_{pym}). ^{19}F-NMR: (282 MHz, DMSO-d_6) δ ppm -79.5 (s). Elemental analysis calcd. for $C_{16}H_{13}F_6N_5O_4S_2$ (517.43): C – 37.14 %, H – 2.53 %, N – 13.54 %, S – 12.39 %, found: C – 37.45 %, H – 2.28 %, N – 13.21 %, S – 12.28 %. Mp. 99 °C.

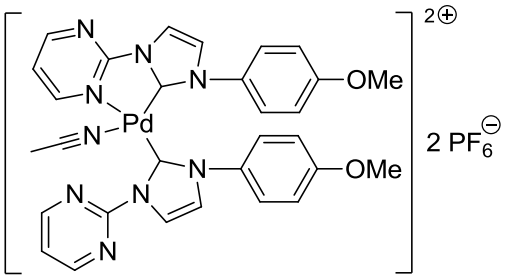
Characterization of the palladium complexes

Acetonitrile bis(1-(pyrimidine-2-yl)-3-(4-methylphenyl)imidazole 2-ylidene)palladium(II) bishexafluorophosphate (**4a**)



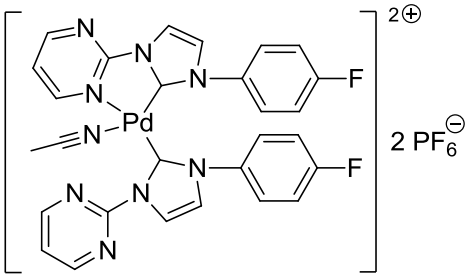
3a (200 mg, 0.52 mmol), Ag_2O (67 mg, 0.29 mmol), and $[Pd(SMe_2)_4][PF_6]_2$ (169 mg, 0.26 mmol) yield **4a** (135 mg, 0.148 mmol, 57 %) as a beige solid. Purification is achieved by slow diffusion of diethyl ether (40 mL) into a DCM solution (10 mL) of the raw product. The resulting solid is filtrated, washed with DCM (3 x 5 mL) and diethyl ether (3 x 15 mL) and dried in high vacuum at 60 °C. ^{1}H-NMR: (500 MHz, DMSO-d_6) δ ppm 2.07 (s, 3 H, C*H*$_3$CN), 2.37 (s, 6 H, C*H*$_3$), 7.25 (br. s, 8 H, H_{ar}), 7.81 (d, ^{3}J = 2.3 Hz, 2 H, NC*H*), 7.85 (t, ^{3}J = 5.0 Hz, 2 H, *p*-H_{pym}), 8.30 (d, ^{3}J = 2.1 Hz, 2 H, NC*H*), 9.11 (d, ^{3}J = 5.0 Hz, 4 H, *m*-H_{pym}). ^{13}C-NMR: (126 MHz, DMSO-d_6) δ ppm 1.2 (s, *C*H_3CN), 20.7 (s, *C*H_3), 120.1 (s, *C*H), 121.5 (s, *C*H), 124.3 (s, 2 *C*H), 125.9 (s, *C*H), 130.1 (s, 2 *C*H), 134.8 (s, *C*), 139.5 (s, *C*), 154.5 (s, C), 154.7 (s, *C*), 159.6 (s, 2 *C*H). *CH$_3$CN was not visible in the spectrum.* Elemental analysis calcd. for $C_{30}H_{27}F_{12}N_9P_2Pd$ (909.95): C – 39.60 %, H – 2.99 %, N – 13.85 %, found: C – 39.77 %, H – 2.96 %, N – 13.71 %. Mp. 230 °C (decomp.).

Acetonitrile bis(1-(pyrimidine-2-yl)-3-(4-methoxyphenyl)imidazol-2-ylidene)palladium(II) bishexafluorophosphate (**4b**)



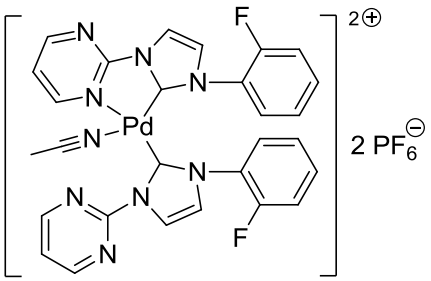
3b (247 mg, 0.62 mmol), Ag_2O (79 mg, 0.34 mmol), and $[Pd(SMe_2)_4][PF_6]_2$ (200 mg, 0.31 mmol) yield 4b (147 mg, 0.163 mmol, 53 %) as a colourless solid. Alternatively, **3b** (266 mg, 0.67 mmol) and palladium acetate (75 mg, 0.33 mmol) yield **4b** (308 mg, 0.33 mmol, 98 %). Purification is achieved by slow diffusion of diethyl ether (40 mL) into an acetone solution (10 mL) of the raw product. The resulting solid is filtrated, washed with diethyl ether (3 x 15 mL) and dried in high vacuum at 60 °C. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 3.83 (s, 3 H, OCH_3), 6.98 (d, ^3J = 8.7 Hz, 2 H, H$_{ar}$), 7.32 (br. s, 2 H, H$_{ar}$), 7.79 (d, ^3J = 2.0 Hz, 1 H, NC*H*), 7.85 (t, ^3J = 5.0 Hz, 1 H, *p*-H$_{pym}$), 8.28 (d, ^3J = 2.0 Hz, 1 H, NC*H*), 9.11 (d, ^3J = 5.0 Hz, 2 H, *p*-H$_{pym}$). ^{13}C-NMR: (126 MHz, DMSO-d_6) δ ppm 55.7 (s, O*C*H$_3$), 114.8 (s, *C*H, C$_{ar}$), 121.4 (s, *C*H), 125.9 (s, *C*H, C$_{ar}$), 126.1 (s, *C*H), 129.7 (s, *C*), 130.1 (s, *C*), 154.7 (s, *C*), 154.8 (br. s, *C*), 159.7 (s, *C*H, *m*-C$_{pym}$). *CH$_3$CN was not visible in the spectrum.* Elemental analysis calcd. for $C_{30}H_{27}F_{12}N_9O_2P_2Pd$ (941.95): C – 38.10 %, H – 2.89 %, N – 13.07 %, found: C – 38.25 %, H – 2.89 %, N – 13.38 %. Mp. 181 °C.

Acetonitrile bis(1-(pyrimidine-2-yl)-3-(4-fluorophenyl)imidazol-2-ylidene)palladium(II) bishexafluorophosphate (**4c**)



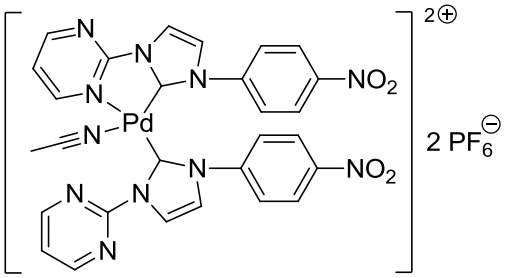
3c (240 mg, 0.62 mmol), Ag_2O (79 mg, 0.34 mmol), and $[Pd(SMe_2)_4][PF_6]_2$ (200 mg, 0.31 mmol) yield **4c** (196 mg, 0.224 mmol, 72 %) as an ivory solid. Alternatively, **3c** (258 mg, 0.67 mmol) and palladium acetate (75 mg, 0.33 mmol) yield **4c** (234 mg, 0.27 mmol, 80 %). Purification is achieved by slow diffusion of diethyl ether (40 mL) into an acetone solution (10 mL) of the raw product. The resulting solid is filtrated, washed with diethyl ether (3 x 15 mL) and dried in high vacuum at 60 °C. ^{1}H-NMR: (500 MHz, DMSO-d_6) δ ppm 7.33 (t, ^3J = 8.7 Hz, 4 H, H$_{ar}$), 7.43 - 7.52 (m, 4 H, H$_{ar}$), 7.86 (t, ^3J = 5.0 Hz, 2 H, *p*-H$_{pym}$), 7.89 (d, ^3J = 2.2 Hz, 2 H, NC*H*), 8.35 (d, ^3J = 2.2 Hz, 2 H, NC*H*), 9.11 (d, ^3J = 5.0 Hz, 4 H, *m*-H$_{pym}$). ^{13}C-NMR: (75 MHz, DMSO-d_6) δ ppm 116.7 (d, $^2J_{C\text{-}F}$ = 23.8 Hz, *C*H, C$_{ar}$), 120.2 (s, *C*H), 121.6 (s, *C*H), 126.1 (s, *C*H), 127.1 (d, $^3J_{C\text{-}F}$ = 9.4 Hz, *C*H, C$_{ar}$), 133.6 (s, *C*, C$_{ar}$), 154.6 (s, *C*), 154.9 (s, *C*), 159.7 (s, *C*H, *m*-C$_{pym}$), 162.0 (d, $^1J_{C\text{-}F}$ = 248.0 Hz, *C*, C$_{ar}$). *CH$_3$CN was not visible in the spectrum.* ^{19}F NMR: (282 MHz, DMSO-d_6) δ ppm -111.49 (s, 2 F, F$_{ar}$), -70.78 (d, $^1J_{F\text{-}P}$ = 710.0 Hz, 12 F, PF_6). Elemental analysis calcd. for $C_{28}H_{21}F_{14}N_9P_2Pd$ (917.87): C – 36.73 %, H – 2.11 %, N – 13.41 %, found: C – 36.64 %, H – 2.31 %, N – 13.73 %. Mp. 212 °C (decomp.).

Acetonitrile bis(1-(pyrimidine-2-yl)-3-(2-fluorophenyl)imidazol-2-ylidene)palladium(II) bishexafluorophosphate (**4d**)



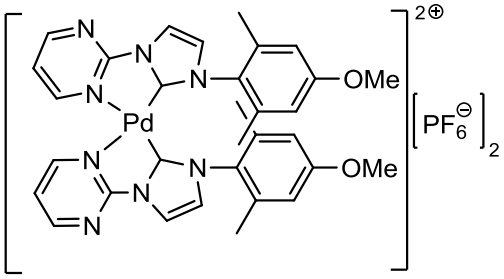
3d (258 mg, 0.67 mmol) and palladium acetate (75 mg, 0.33 mmol) yield **4d** (284 mg, 0.31 mmol, 93 %) as a light brown solid. Purification is achieved by slow diffusion of diethyl ether (40 mL) into an acetone solution (10 mL) of the raw product. The resulting solid is filtrated, washed with diethyl ether (3 x 15 mL) and dried in high vacuum at 60 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 2.07 (s, 3 H, CH_3CN), 7.30 (t, J = 7.3 Hz, 2 H, H$_{ar}$), 7.43 (t, J = 9.2 Hz, 2 H, H$_{ar}$), 7.53 - 7.76 (m, 4 H, H$_{ar}$), 7.85 (t, ^{3}J = 5.1 Hz, 2 H, *p*-H$_{pym}$), 7.94 (t, ^{3}J = 2.1 Hz, 2 H, NC*H*), 8.32 (d, ^{3}J = 2.1 Hz, 2 H, NC*H*), 9.10 (d, ^{3}J = 5.1 Hz, 4 H, *m*-H$_{pym}$). ^{13}C NMR (75 MHz, DMSO-d_6) δ ppm 1.1 (s, *C*H$_3$CN), 117.2 (d, ^{2}J = 19.3 Hz, *C*H$_{ar}$), 120.2 (s, *p*-C$_{pym}$), 121.7 (s, N*C*H), 124.9 (d, ^{2}J = 11.6 Hz, C$_{ar}$), 125.7 (d, ^{3}J = 3.9 Hz, *C*H$_{ar}$), 127.1 (s, N*C*H), 127.6 (s, CH$_{ar}$), 132.4 (d, ^{3}J = 7.7 Hz, *C*H$_{ar}$), 155.4 (d, ^{1}J = 253.0 Hz, *C*F), 154.5 (s, 1 C, *i*-C$_{pym}$), 156.2 (s, C$_{carbene}$), 159.7 (s, *m*-C$_{pym}$). *CH$_3$CN was not visible in the spectrum.* ^{19}F NMR: (282 MHz, DMSO-d_6) δ ppm -123.20 (s, 2 F, F$_{ar}$), -70.78 (d, $^{1}J_{F-P}$ = 710.0 Hz, 12 F, PF_6). Elemental analysis calcd. for $C_{28}H_{21}F_{14}N_9P_2Pd$ (917.87): C – 36.73 %, H – 2.11 %, N – 13.41 %, found: C – 36.70 %, H – 2.19 %, N – 13.39 %. Mp. 268 °C (decomp.).

Acetonitrile Bis(1-(pyrimidine-2-yl)-3-(4-nitrophenyl)imidazol-2-ylidene)palladium(II) bishexafluorophosphate (**4e**)



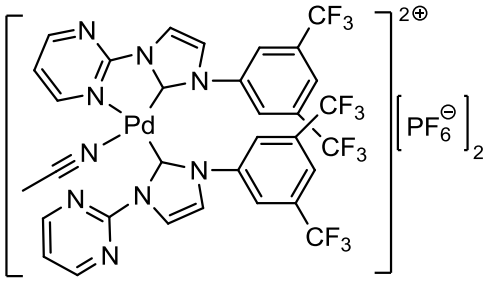
3e (247 mg, 0.62 mmol), Ag_2O (79 mg, 0.34 mmol), and $[Pd(SMe_2)_4][PF_6]_2$ (200 mg, 0.31 mmol) yield **4e** (133 mg, 0.14 mmol, 46 %) as a brown solid. Purification is achieved by slow diffusion of diethyl ether (40 mL) into an acetone solution (10 mL) of the raw product. The resulting solid is filtrated, washed with diethyl ether (3 x 15 mL) and dried in high vacuum at 60 °C. ^{1}H-NMR: (500 MHz, DMSO-d_6) δ ppm 7.74 (d, ^{3}J = 8.7 Hz, 2 H, H$_{ar}$), 7.90 (t, ^{3}J = 5.1 Hz, 1 H, *p*-H$_{pym}$), 7.98 (d, ^{3}J = 2.2 Hz, 1 H, NC*H*), 8.33 (d, ^{3}J = 8.7 Hz, 2 H, H$_{ar}$), 8.40 (d, ^{3}J = 2.2 Hz, 1 H, NC*H*), 9.14 (d, ^{3}J = 5.1 Hz, 2 H, *m*-H$_{pym}$). ^{13}C-NMR: (126 MHz, DMSO-d_6) δ ppm 120.7 (s, *C*H), 121.8 (s, *C*H), 125.0 (s, *C*H), 125.9 (s, *C*H), 126.2 (s, *C*H), 141.7 (s, *C*), 147.6 (s, *C*), 154.5 (s, *C*), 155.3 (s, *C*), 159.9 (s, *m*-C$_{pym}$). *CH$_3$CN was not visible in the spectrum.* Elemental analysis calcd. for $C_{28}H_{21}F_{12}N_{11}O_4P_2Pd \cdot 0.25\ CH_3CN$ (971.89): C – 35.23 %, H – 2.28 %, N – 15.66 %, found: C – 34.85 %, H – 2.23 %, N – 16.04 %. Mp. 236 °C (decomp.).

Bis[1-(pyrimidine-2-yl)-3-((4-methoxy-2,6-trimethylphenyl)-imidazol-2-ylidene)]palladium(II) bishexafluorophosphate (**4g**)



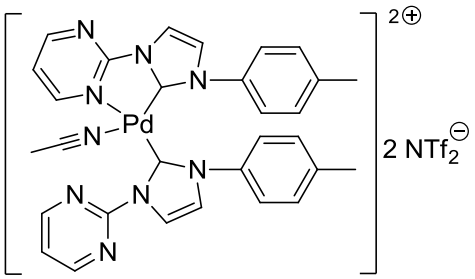
3g (234 mg, 0.62 mmol), Ag_2O (79 mg, 0.34 mmol), and $[Pd(SMe_2)_4][PF_6]_2$ (200 mg, 0.31 mmol) yield **4g** (106 mg, 0.224 mmol, 36 %) as an ivory solid. Alternatively, **3g** (239 mg, 0.56 mmol) and palladium acetate (63 mg, 0.28 mmol) yield **4g** (228 mg, 0.24 mmol, 71 %). Purification is achieved by precipitation from a DCM solution (10 mL) of the raw product by addition of diethyl ether (40 mL). The resulting solid is filtrated, washed with diethyl ether (3 x 15 mL) and dried in high vacuum at 60 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 1.76 (s, 6 H, CH_3), 1.77 (s, 6 H, CH_3'), 3.74 (s, 6 H, OCH_3), 7.73 (t, ^{3}J = 4.9 Hz, 2 H, *p*-H$_{pym}$), 7.78 (d, ^{3}J = 1.7 Hz, 2 H, NC*H*), 8.53 (d, ^{3}J = 1.7 Hz, 2 H, NC*H*), 8.97 (d, ^{3}J = 4.9 Hz, 4 H, *m*-H$_{pym}$). ^{13}C NMR (126 MHz, DMSO-d6) δ ppm 17.8 (s, *C*H$_3$), 18.1 (s, *C*H$_3$'), 55.2 (s, O*C*H$_3$), 113.1 (s, *C*H$_{ar}$), 113.6 (s, *C*H$_{ar}$'), 121.1 (s, *p*-C$_{pym}$), 121.4 (s, N*C*H), 128.0 (s, N*C*H), 128.9 (s, C$_{ar}$), 134.7 (s, C$_{ar}$), 137.5 (s, C$_{ar}$'), 154.0 (s, C$_{carbene}$), 154.8 (s, *i*-C$_{pym}$), 159.0 (s, *m*-C$_{pym}$), 159.2 (s, C$_{ar}$). Elemental analysis calcd. for $C_{32}H_{32}F_{12}N_8O_2P_2Pd$ (957.01): C – 40.16 %, H – 3.37 %, N – 11.71 %, found: C – 40.16 %, H – 3.51 %, N – 11.63 %. Mp. 201 °C .

Acetonitrile-bis[1-(pyrimidine-2-yl)-3-((3,5-(trifluoromethyl)phenyl)-imidazol-2-ylidene)]palladium(II) bishexafluorophosphate (**4h**)



3h (313 mg, 0.62 mmol), Ag_2O (79 mg, 0.34 mmol), and $[Pd(SMe_2)_4][PF_6]_2$ (200 mg, 0.31 mmol) yield **4h** (174 mg, 0.16 mmol, 50 %) as a brown solid. Alternatively, **3h** (337 mg, 0.67 mmol) and palladium acetate (75 mg, 0.33 mmol) yield **4h** (353 mg, 0.31 mmol, 92 %) as a light brown solid. Purification is achieved by precipitation from a DCM solution (10 mL) of the raw product by slow addition of diethyl ether (40 mL). This procedure was repeated twice. The resulting solid is filtrated, washed with diethyl ether (3 x 15 mL) and dried in high vacuum at 60 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 2.08 (s, 3 H, CH_3CN) 7.93 (t, *J*=5.1 Hz, 2 H), 8.11 (d, ^3J = 2.3 Hz, 2 H, *p*-H$_{pym}$), 8.28 (s, 4 H, H$_{ar}$), 8.33 (d, ^3J = 2.3 Hz, 2 H, NC*H*), 8.44 (s, 2 H, NC*H*), 9.16 (d, ^3J = 5.1 Hz, 4 H, *m*-H$_{pym}$). ^{13}C NMR (75 MHz, DMSO-d_6) δ ppm 122.5 (q, ^1J = 273.0 Hz, *C*F$_3$), 120.1 (m, *p*-C$_{pym}$), 121.9 (m, N*C*H), 124.4 - 124.7 (m, *C*H$_{ar}$), 126.0 - 126.3 (m, *C*H$_{ar}$), 126.7 (s, N*C*H), 131.5 (q, ^2J = 34.0 Hz, C$_{ar}$), 138.5 (s, C$_{ar}$), 154.3 (s, C$_{carbene}$), 155.2 (s, *i*-C$_{pym}$), 160.0 (s, *m*-C$_{pym}$). *One signal was not visible in the spectrum.* ^{19}F NMR (282 MHz, DMSO-d_6) δ ppm -70.78 (d, $^1J_{F\text{-}P}$ = 710.0 Hz, 12 F, P*F*$_6$), -61.84 (s, 12 F, C*F*$_3$). Elemental analysis calcd. for $C_{32}H_{19}F_{24}N_9P_2Pd$ (1153.89): C – 33.31 %, H – 1.66 %, N – 10.92 %, found: C – 33.24 %, H – 1.42 %, N – 11.17 %. Mp. 184 °C.

Acetonitrile bis[1-(pyrimidine-2-yl)-3-((4-methylphenyl)-imidazol-2-ylidene)]palladium(II) bis(bis(trifluoromethanesulfonyl)imide) (**4i**)

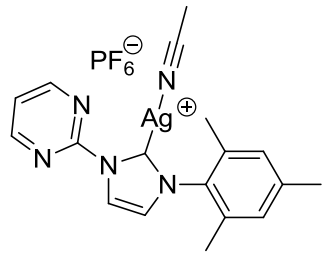


3i (346 mg, 0.67 mmol) and palladium acetate (75 mg, 0.33 mmol) yield **4i** (177 mg, 0.15 mmol, 45 %) as a colourless solid. Purification is achieved by slow diffusion of diethyl ether (40 mL) into a DCM solution (10 mL) of the raw product. The resulting solid is filtrated, washed with diethyl ether (3 x 15 mL) and dried in high vacuum at 60 °C. ^{1}H-NMR: (500 MHz, DMSO-d_6) δ ppm 2.07 (s, 3 H, CH_3CN), 2.37 (s, 6 H, CH_3), 7.26 (br. s, 8 H, H$_{ar}$), 7.81 (d, ^{3}J = 2.3 Hz, 2 H, NC*H*), 7.85 (t, ^{3}J = 5.0 Hz, 2 H, *p*-H$_{pym}$), 8.30 (d, ^{3}J = 2.1 Hz, 2 H, NC*H*), 9.11 (d, ^{3}J = 5.0 Hz, 4 H, *m*-H$_{pym}$). ^{13}C-NMR: (126 MHz, DMSO-d_6) δ ppm 1.1 (s, *C*H$_3$CN), 20.6 (s, *C*H$_3$), 120.0 (s, *C*H), 121.5 (s, *C*H), 124.3 (s, 2 *C*H), 125.9 (s, *C*H), 130.1 (s, 2 *C*H), 134.8 (s, *C*), 139.5 (s, *C*), 154.5 (s, C), 154.7 (s, *C*), 159.6 (s, 2 *C*H). *CH$_3$CN was not visible in the spectrum.* Elemental analysis calcd. for $C_{34}H_{27}F_{12}N_{11}O_8PdS_4$ (1180.32): C – 34.60 %, H – 2.31 %, N – 13.05 %, S – 10.87 %, found: C – 34.53 %, H – 1.93 %, N – 13.03 %, S – 10.93 %. Mp. 250 °C.

Synthesis of Bis[1-(pyrimidine-2-yl)-3-((2,4,6-trimethylphenyl)-imidazol-2-ylidene)]-palladium(II) bishexafluorophosphate (4f) by method C.

The intermediate silver carbene was synthesized by a modified literature procedure.[2] The imidazolium salt **3f** (0.5 g, 1.22 mmol) and silver(I) oxide (155 mg, 0.67 mmol, 0.55 equiv.) are suspended in acetonitrile (20 mL) and stirred at 50 °C for 16 h under the exclusion of light. The suspension is filtered with Celite and the solvent removed under reduced pressure. The residue is dissolved in DCM (5 mL) and the crude product precipitated by addition of diethyl ether (40 mL). The solid is filtrated, washed with diethyl ether (3 x 20 mL) and dried at 50 °C in high vacuum to yield the intermediate silver carbene (483 mg, 0.87 mmol, 71 %).

Acetonitrile [1-(pyrimidine-2-yl)-3-((2,4,6-trimethyl-phenyl)-imidazol-2-ylidene)]silver(I) hexafluorophosphate

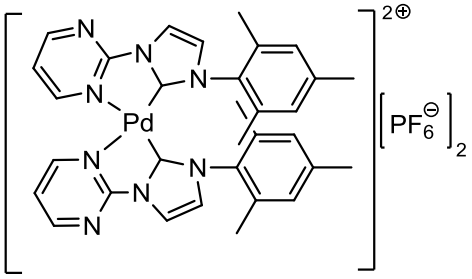


Colourless solid. ^{1}H-NMR: (300 MHz, DMSO-d_6) δ ppm 1.83 (s, 6 H, CH_3), 2.07 (s, 3 H, CH_3CN), 2.34 (s, 3 H, CH_3), 7.04 (s, 2 H, H$_{ar}$), 7.60 (t, ^{3}J = 4.9 Hz, 1 H, *p*-H$_{pym}$), 7.75 (d, ^{3}J = 2.0 Hz, 1 H, NC*H*), 8.44 (d, ^{3}J = 2.0 Hz, 1 H, NC*H*), 8.79 (d, ^{3}J = 4.9 Hz, 2 H, *m*-H$_{pym}$). ^{13}C-NMR: (75.5 MHz, DMSO-d_6) δ ppm 1.1 (s, CH_3CN), 17.1 (s, CH$_3$), 20.6 (s, *C*H$_3$), 119.4 (s, *p*-C$_{pym}$), 121.3 (s, N*C*H), 124.8 (s, N*C*H), 128.9 (s, *C*H$_{ar}$), 134.1 (s, C$_{ar}$), 136.0 (s, C$_{ar}$), 138.6 (s, C$_{ar}$), 154.9 (s, *i*-C$_{pym}$), 159.4 (s, *m*-C$_{pym}$). *CH$_3$CN and* C$_{carbene}$ *were not visible in the spectrum.* Elemental analysis calcd. for $C_{18}H_{19}AgF_6N_5P$ (558.21): C – 38.73 %, H – 3.43 %, N – 12.55 %, found: C – 38.54 %, H – 3.53 %, N – 12.35 %. Mp. 176 °C.

The silver carbene (187 mg, 0.34 mmol) and dichlorocyclooctadiene palladium(II) (48 mg, 0.17 mmol) are then dissolved in acetonitrile (15 mL) and stirred for 16 h at 50 °C under the

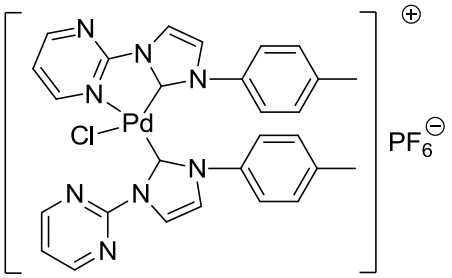
exclusion of light. The mixture is filtered with Celite and the solvent removed under reduced pressure. The residue is dissolved in DCM (5 mL) and the crude product precipitated by addition of diethyl ether (3 mL). The solid is washed with diethyl ether (3 x 5 mL) and dried in high vacuum at 50 °C to yield **4f** (116 mg, 0.13 mmol, 75 %).

Bis[1-(pyrimidin-2-yl)-3-((2,4,6-trimethylphenyl)-imidazol-2-yliden)]palladium(II)-dihexafluorophosphate.



Colourless solid. ^{1}H-NMR (500 MHz, DMSO-d_6) δ ppm 1.74 (s, 6 H, CH_3), 1.78 (s, 6 H, CH_3), 2.19 (s, 6 H, CH_3), 6.73 (s, 2 H, H_{ar}), 6.76 (s, 2 H, H$_{ar}$), 7.77 (t, ^{3}J = 5.0 Hz, 2 H, *p*-H$_{pym}$), 7.80 (d, ^{3}J = 2.1 Hz, 2 H, NCH), 8.52 (d, ^{3}J = 2.1 Hz, 2 H, NCH), 8.99 (d, ^{3}J = 5.0 Hz, 4 H, *m*-H$_{pym}$). ^{13}C-NMR: (75.5 MHz, DMSO-d_6) δ ppm 17.5 (s, CH$_3$), 17.9 (s, CH$_3$), 20.5 (s, CH$_3$), 121.1 (s, *p*-C$_{pym}$), 121.5 (s, NCH), 127.7 (s, NCH), 128.8 (s, CH$_{ar}$), 129.1 (s, CH$_{ar}$'), 132.9 (s, C$_{ar}$), 133.5 (s, C$_{ar}$'), 135.7 (s, C$_{ar}$), 139.5 (s, C$_{ar}$), 154.0 (s, C$_{carbene}$), 154.5 (s, *i*-C$_{pym}$), 158.96 (s, *m*-C$_{pym}$). Elemental analysis calcd. for $C_{32}H_{32}F_{12}N_8P_2Pd$ (925.01): C – 41.55 %, H – 3.49 %, N – 12.11 %, found: C – 41.22 %, H – 3.56 %, N – 12.25 %. Mp. 183 °C.

Synthesis of Chloridobis(1-(pyrimidine-2-yl)-3-(4-methylphenyl)imidazole 2-ylidene)palladium(II)hexafluorophosphate (**5a**)



In a 10 mL crimp vial, the imidazolium salt **2a** (182 mg, 0.67 mmol), the imidazolium salt **3a** (255 mg, 0.67 mmol) and palladium(II) acetate (150 mg, 0.67 mmol) are suspended in acetonitrile (5 mL). Argon is bubbled through the mixture for 30 min. Then, the vial is placed into an aluminium block and heated to 50 °C for 7 days. After cooling to room temperature, silica (20 mg) and Celite (50 mg) are added and the mixture is filtered over Celite. The solvent is removed under reduced pressure and the residue dissolved in DCM (10 mL). The crude product is precipitated by addition of diethyl ether (40 mL). It is washed with diethyl ether (3 x 5 mL) and DCM (3 x 2 mL). The remaining solid is extracted with acetone (3 x 5 mL). The product is precipitated from the combined organic phases by addition of diethyl ether (40 mL), filtered off and dried in high vacuum. The product **5a** (259 mg, 0.34 mmol, 51 %) is obtained as a pale yellow solid. ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 2.33 (s, 6 H, CH_3), 6.85 (d, ^{3}J = 7.7 Hz, 2 H, H$_{ar}$), 7.05 (d, ^{3}J = 7.7 Hz, 2 H, H$_{ar}$), 7.32 (d, ^{3}J = 8.3 Hz, 1 H, H$_{ar}$), 7.64 - 7.74 (m, 2 H, NCH, *p*-H$_{pym}$), 7.74 - 7.83 (m, 3 H, H$_{ar}$, NCH), 7.87 (t, ^{3}J = 5.1 Hz, 1 H, *p*-H$_{pym}$), 8.19 (d, ^{3}J = 2.2 Hz, 1 H, NCH), 8.35 (d, ^{3}J = 2.2 Hz, 1 H, NCH), 9.00 (d, ^{3}J = 5.1 Hz, 2 H, *m*-H$_{pym}$), 9.21 (dd, ^{3}J = 5.4 Hz, ^{4}J = 2.0 Hz, 1 H, *m*-H$_{pym}$), 9.26 (dd, ^{3}J = 5.4 Hz, ^{4}J = 2.0 Hz, 1 H, *m*-H$_{pym}$). ^{13}C NMR (75 MHz, DMSO-d_6) δ ppm 20.6 (s, CH$_3$), 20.6 (s, CH$_3$), 117.7 (s, *p*-C$_{pym}$), 121.0 (s, NCH), 121.3 (s, NCH), 121.4 (s, *p*-C$_{pym}$), 124.3 (s, CH$_{ar}$), 124.5 (s, CH$_{ar}$), 124.6 (s, NCH), 125.6 (s, NCH), 129.4 (s, CH$_{ar}$), 129.6 (s, CH$_{ar}$), 134.0 (s, C$_{ar}$), 136.0 (s, C$_{ar}$), 138.5 (s, C$_{ar}$), 139.5 (s, C$_{ar}$), 154.3 (s, *i*-C$_{pym}$), 156.2 (s, *i*-C$_{pym}$), 157.8 (s, *m*-C$_{pym}$),

158.1 (s, $C_{carbene}$), 159.3 (s, *m*-C_{pym}), 159.6 (s, $C_{carbene}$), 162.0 (s, *m*-C_{pym}). Elem. anal. calcd. for $C_{28}H_{24}ClF_6N_8PPd$ (759.39): C – 44.29 %, H – 3.19 %, N – 14.76 %, found: C – 43.96 %, H – 3.04 %, N – 14.56 %. Mp. 171 °C.

Details for the Solid State Structure Determination

Preliminary examination and data collection for single crystals of **4a** were carried out on a NONIUS κ-CCD diffraction system (FR590) equipped with an Oxford Cryosystem cooling system at the window of a fine-focus sealed tube using graphite monochromated Mo K_α radiation (λ = 0.71073 Å). The reflections were merged and corrected from Lorentz, polarization and decay effects. Absorption correction was applied using SADABS.[3] The structures were solved by a combination of direct methods with the aid of difference Fourier synthesis and were refined against all data using SHELXL-97.[4] Hydrogen atoms were assigned to ideal positions using the SHELXL-97 riding model. All non-hydrogen atoms were refined with anisotropic displacement parameters. Full-matrix least-squares refinements were carried out by minimizing $\Sigma w(F_o^2 - F_c^2)^2$ with the SHELXL-97 weighting scheme. Details of the structure determinations are given in the Supporting Information. Neutral-atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from the International Tables for Crystallography. All calculations were performed with the programs COLLECT,[5] DIRAX,[6] EVALCCD,[7] SIR92,[8] SADABS,[3] the SHELXL-97 package,[4] and PLATON. Images of the solid state structures were generated with ORTEP-3[9-10].

Preliminary examination and data collection for single crystals of **4c** and (*CN*,*CN*)-**4d** were carried out on a Bruker Apex II CCD diffractometer. All measurements were performed at 150 K (Cryostream cooler, Oxford Cryosystems) using Mo-K_α radiation (λ = 0.71073 Å). The data were corrected for absorption by the methods included in the diffractometer software. The structures were solved by direct methods (SHELXS97[11]) and refined by full-matrix least squares based on F^2 (SHELXL-2017).[12] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms bonded to carbons (CH_n) were included in their calculated positions and refined as riding atoms with U_{iso} assigned to 1.2 times the U_{eq} value of their bonding atom.

Preliminary examination and data collection for single crystals of compound **5a** was carried out on a Bruker D8 VENTURE (KAPPA goniometer, PHOTON detector) single crystal-diffractometer equipped with an Oxford Cryosystem (Cryostream 800) cooling system at the window of a sealed x-ray tube using monochromated Mo-K_α radiation (λ = 0.71073 Å) (Incoatec IμS3.0 microfocus source equipped with multilayer optics). Intensity data were extracted using the APEX3 suite[13] including the SAINT software package.[14] The reflections were merged and corrected from Lorentz, polarization and decay effects and absorption correction was applied based on multiple scans.[15] The structure was solved by a combination of dual space, [16] direct methods with the aid of difference Fourier synthesis and were refined

against all data using SHELXTL-XTMP.[17] Non-refinable solvent molecules were treated with the SQUEEZE procedure.[18] Hydrogen atoms were assigned to ideal positions using the SHELXTL-XTMP riding model. All non-hydrogen atoms were refined with anisotropic displacement parameters. Full-matrix least-squares refinements were carried out by minimizing $\Sigma w(F_o^2-F_c^2)^2$ with the SHELXTL-XTMP weighting scheme. Neutral-atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from the International Tables for Crystallography. [19] All calculations were performed with the APEX3 suite[13] including SAINT software package,[14] the SHELX program package[20] and PLATON. [21] For the visualization ORTEP3[22-23] was used.

Table S3. Crystal data and structure refinement for **4a**.

Identification code	**4a**	
Empirical formula	C30 H27 F12 N9 P2 Pd	
Formula weight	909.95	
Temperature	123(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.4162(5) Å	α= 90°.
	b = 20.4515(10) Å	β= 98.235(2)°.
	c = 18.6792(9) Å	γ = 90°.
Volume	3560.1(3) $Å^3$	
Z	4	
Density (calculated)	1.698 Mg/m^3	
Absorption coefficient	0.712 mm^{-1}	
F(000)	1816	
Crystal size	0.24 x 0.22 x 0.12 mm^3	
Theta range for data collection	1.48 to 25.36°.	
Index ranges	-11<=h<=11, -24<=k<=24, -22<=l<=22	
Reflections collected	76239	
Independent reflections	6514 [R(int) = 0.0335]	
Completeness to theta = 25.36°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7452 and 0.6124	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6514 / 0 / 490	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0308, wR2 = 0.0772	
R indices (all data)	R1 = 0.0317, wR2 = 0.0782	
Largest diff. peak and hole	1.175 and -0.748 $e.Å^{-3}$	

Table S4. Crystal data and structure refinement for **4c**.

Identification code	**4c**	
Empirical formula	C28 H21 F14 N9 P2 Pd	
Formula weight	917.88	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 16.0292(9) Å	α= 90°.
	b = 11.2624(8) Å	β= 98.024(2)°.
	c = 18.3984(12) Å	γ = 90°.
Volume	3288.9(4) $Å^3$	
Z	4	
Density (calculated)	1.854 Mg/m^3	
Absorption coefficient	0.780 mm^{-1}	
F(000)	1816	
Crystal size	0.395 x 0.088 x 0.034 mm^3	
Theta range for data collection	2.217 to 27.554°.	
Index ranges	-19<=h<=20, -14<=k<=14, -23<=l<=23	
Reflections collected	54110	
Independent reflections	7553 [R(int) = 0.0567]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7553 / 0 / 488	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0349, wR2 = 0.0756	
R indices (all data)	R1 = 0.0536, wR2 = 0.0819	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.748 and -0.597 $e.Å^{-3}$	

Table S5. Crystal data and structure refinement for (*CN*,*CN*)-**4d**.

Identification code	(*CN*,*CN*)-**4d**	
Empirical formula	C26 H18 F14 N8 P2 Pd	
Formula weight	876.82	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.8636(4) Å	α= 75.862(2)°.
	b = 12.5184(7) Å	β= 77.486(2)°.
	c = 16.0803(9) Å	γ = 76.016(2)°.
Volume	1468.45(14) $Å^3$	
Z	2	
Density (calculated)	1.983 Mg/m^3	
Absorption coefficient	0.867 mm^{-1}	
F(000)	864	
Crystal size	0.403 x 0.096 x 0.058 mm^3	
Theta range for data collection	2.368 to 28.552°.	
Index ranges	-10<=h<=10, -16<=k<=16, 0<=l<=21	
Reflections collected	7447	
Independent reflections	7447 [R(int) = ?]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7447 / 0 / 461	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0284, wR2 = 0.0572	
R indices (all data)	R1 = 0.0350, wR2 = 0.0595	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.421 and -0.564 $e.Å^{-3}$	

Table S6. Crystal data and structure refinement for **5a**.

Identification code	**5a**	
Empirical formula	C28 H24 Cl F6 N8 P Pd	
Formula weight	759.37	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.4023(5) Å	α= 90°.
	b = 20.9123(8) Å	β= 111.0550(10)°.
	c = 12.4921(4) Å	γ = 90°.
Volume	3267.4(2) $Å^3$	
Z	4	
Density (calculated)	1.544 Mg/m^3	
Absorption coefficient	0.765 mm^{-1}	
F(000)	1520	
Crystal size	0.407 x 0.207 x 0.104 mm^3	
Theta range for data collection	2.539 to 28.297°.	
Index ranges	-17<=h<=17, -27<=k<=27, -16<=l<=16	
Reflections collected	143203	
Independent reflections	8113 [R(int) = 0.0511]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8113 / 113 / 445	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R_1 = 0.0258, wR_2 = 0.0599	
R indices (all data)	R_1 = 0.0295, wR_2 = 0.0621	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.765 and -0.683 $e.Å^{-3}$	

Cartesian Coordinates for Calculated Structures

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 H     3.901218    -3.355170     0.003790
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 C     3.743330    -2.335993     0.722421
 C     2.363446    -2.326646     0.922459
 C     0.472540    -0.380322    -1.321539
 C     1.615274    -1.767267    -2.713866
 C     0.316959    -2.144854    -2.738701
 C     2.950175    -0.018871    -1.571787
 C     4.110066     1.629092    -0.559647
 C     5.293105     1.147420    -1.116532
 C     5.185209     0.015631    -1.929392
 C    -1.794707    -1.313048    -1.697154
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 C    -3.743070    -2.335803    -0.723257
 C    -2.363208    -2.326300    -0.923438
 C     0.471578     3.369155    -2.275281
 C     0.682552     4.402788    -3.281715
 H     0.192824    -2.920682     3.290341
 H    -2.485753    -2.146116     3.223633
 H    -4.102073     2.500370    -0.089361
 H    -6.250713     1.615255     0.919401
 H    -6.053025    -0.441462     2.396938
 H     2.485821    -2.144429    -3.224903
 H    -0.192703    -2.919161    -3.291809
 H     4.102132     2.500065     0.090917
 H     6.250789     1.615516    -0.918306
 H     6.053091    -0.440213    -2.397214
 H     1.557946     5.005777    -3.017977
 H    -0.195527     5.054674    -3.339057
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 N    -0.311005     2.548688     1.477988
 C    -0.471702     3.367971     2.276820
 C    -0.683861     4.401254     3.283366
 H     0.193808     5.053636     3.341344
 H    -1.559459     5.003795     3.019284
 H    -0.850814     3.939885     4.262484
 H     1.735179    -3.083019     0.462008
 H    -2.102849     0.425214    -2.930036
 H    -4.594814     0.395229    -2.593120
 H     4.220047    -3.085305     0.101535
 H     4.594718     0.394399     2.593382
 H    -4.219678    -3.085376    -0.102602
 H    -1.734846    -3.082803    -0.463330
 H     2.102722     0.424065     2.930109
 N    -5.958583    -1.270447    -1.016039
 O    -6.401316    -2.085288    -0.209591
 O    -6.607357    -0.373648    -1.549598
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 N     2.838691     0.878914     0.853283
 N     3.730331     2.524013    -0.628107
 N     0.297561     1.469942     2.551615
 C    -0.290236    -1.372821    -0.382326
 C     0.069999    -2.925251    -1.984840
 C    -1.248624    -2.966024    -1.689965
 C    -2.755480    -1.777573    -0.119099
 C    -4.060417    -0.704133     1.375763
 C    -5.167653    -1.430860     0.939882
 C    -4.944029    -2.347535    -0.087728
 C     2.074036    -1.703263    -1.156798
 C     2.846377    -2.360631    -0.187425
 C     4.233660    -2.177868    -0.229851
 C     4.846909    -1.373189    -1.196139
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 C     2.646207    -0.909923    -2.166080
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 C     2.755404     1.777717    -0.119092
 C     4.060604     0.703964     1.375321
 C     5.167722     1.430943     0.939553
 C     4.943897     2.347914    -0.087747
 C    -2.074207     1.703298    -1.156481
 C    -2.846626     2.360354    -0.186956
 C    -4.233891     2.177477    -0.229456
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 C    -4.034546     0.745573    -2.150301
 C    -2.646289     0.910165    -2.165977
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 C     0.494835     2.264041     3.367179
 C     0.740409     3.275025     4.388151
 H     0.665070    -3.499973    -2.677766
 H    -2.057033    -3.567908    -2.070226
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 H     6.810605    -1.447429    -0.279727
 H     2.056703     3.568368    -2.069804
 H    -0.665435     3.500403    -2.677171
 H     4.142181    -0.040296     2.163077
 H     6.151913     1.287192     1.371395
 H     5.745055     2.958904    -0.495712
 H    -4.851185     2.688941     0.505975
 H    -4.496255     0.128746    -2.917835
 H    -6.635128     0.199903    -1.532633
 H    -6.781671     1.897839    -1.987032
 H    -6.810765     1.446768    -0.279565
 H     1.783814     3.604575     4.343781
 H     0.538601     2.861367     5.381675
 H     0.086359     4.137665     4.221625
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 C    -1.813691     0.274203    -3.252345
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 H    -1.285167     1.027300    -3.848723
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 H    -1.348262     3.768784     0.524324
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 H     1.347855    -3.769078     0.523499
 H     2.953261    -3.968927     1.240914
 C     1.813692    -0.273620    -3.252311
 H     1.285085    -1.026521    -3.848863
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 H     2.442645     0.304251    -3.934311
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N	-3.716999	-2.540103	-0.549066
N	-0.290298	-1.469538	2.642280
C	0.281275	1.376520	-0.292324
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C	1.224020	2.987776	-1.588686
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C	4.935296	2.357520	-0.020216
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C	-4.030043	0.681476	-2.074067
C	-2.645065	0.886898	-2.081156
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C	-1.224107	-2.987395	-1.589184
C	0.093864	-2.934618	-1.885544
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C	-5.166768	-1.438479	1.002710
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C	2.083102	-1.677031	-1.067933
C	2.871516	-2.314468	-0.090482
C	4.246617	-2.101198	-0.118109
C	4.832430	-1.277581	-1.091748
C	4.030095	-0.681286	-2.074103
C	2.645103	-0.886612	-2.081245
C	-0.485764	-2.260509	3.461297
C	-0.729059	-3.267234	4.486996
H	-0.694622	3.508507	-2.574119
H	2.026398	3.600871	-1.963770
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H	-4.896383	2.580560	0.608353
H	-4.468575	0.064960	-2.849753
H	-2.026511	-3.600398	-1.964361
H	0.694500	-3.508011	-2.574742
H	-4.144168	0.016755	2.246920
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H	4.468678	-0.064671	-2.849680
H	-1.771313	-3.600456	4.443005
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C	0.485806	2.259858	3.461801
C	0.729177	3.266748	4.487319
H	0.530302	2.847479	5.479077
H	1.771358	3.600156	4.443030
H	0.071716	4.127788	4.326071
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H	2.426560	0.277815	-3.883324
H	1.253919	-1.034751	-3.737968
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H	3.013974	-3.899986	1.360291
C	-2.269066	3.198379	0.974833

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 C    -1.435338    -1.270570     2.855853
 C    -2.760088     0.599308     1.903184
 C    -3.960059     2.218816     0.886400
 C    -5.037069     1.954594     1.730514
 C    -4.857351     0.941166     2.674789
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 C     3.502359    -2.338700     0.187676
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 C     0.189554    -1.749776    -2.699126
 C     2.761482     0.607582    -1.896853
 C     3.952199     2.236429    -0.884086
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 C    -2.783195    -0.199152    -1.840952
 C    -4.116126    -0.389333    -1.470972
 C    -4.481949    -1.455714    -0.649036
 C    -3.499357    -2.338631    -0.191010
 C    -2.164675    -2.167853    -0.556540
 C     0.172430     3.796996    -2.330473
 C     0.214969     4.820499    -3.367874
 H     0.327069    -2.584100     3.163773
 H    -2.263288    -1.597146     3.463084
 H    -4.014415     2.982169     0.115581
 H    -5.969929     2.501726     1.651447
 H    -5.640214     0.662958     3.375441
 H     2.272523    -1.590218    -3.457678
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 H     4.000720     3.004755    -0.117850
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 H     0.503251     4.370663    -4.323889
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 C    -0.189500     3.794581     2.334576
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 F     4.086211    -2.948968    -2.014680
 F     5.036180    -4.047137    -0.389176
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 N    -2.895377    -1.029093    -0.772318
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 C    -0.794194     0.422115    -1.445653
 C    -0.516935     1.844988    -3.176610
 C    -1.807473     1.439817    -3.225025
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 C     3.435302     2.705400    -1.434895
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 C     5.752284     1.703805    -1.196741
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 C     2.402516     0.765233     2.137164
 C     2.087471    -2.386640     0.482494
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 C    -1.528987    -2.628380     2.787367
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 H    -2.618107     1.666986    -3.899706
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 H    -6.138922    -0.722190    -2.748815
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 H     4.288111    -0.582115    -1.541800
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 H     2.633323    -5.738559    -1.095310
 H     4.440740    -4.600005     0.278002
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 H    -2.857312     2.866899     2.778114
 H     0.337525     5.347850     1.322261
 H     1.769338     3.345109     1.048368
 H    -2.041090     6.233368     1.475617
 H    -2.015579     5.951255     3.217915
 H    -3.298584     5.237188     2.234341
 H    -1.807031    -4.487232     3.725912
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(CN,C)-4b.xyz
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   69
HF= -1929.055045 Hartree
NImag=0
Pd     1.200694    -0.848309    -0.106517
 N     1.909575     0.512207     2.281272
 N    -0.213081     0.867296     2.143847
 N     3.110117    -0.863747     0.875377
 N     4.191822     0.195898     2.721519
 N    -1.555012    -1.500837    -1.217385
 N    -1.012324     0.559433    -1.595971
 N    -0.540295    -3.215042     0.032096
 N    -2.659406    -3.539701    -1.021898
 N     1.832728    -1.911065    -1.833032
 C     0.801737     0.250499     1.511182
 C     0.258514     1.531027     3.288766
 C     1.591162     1.310771     3.376707
 C     3.146049    -0.064658     1.961898
 C     4.265061    -1.462522     0.531328
 C     5.426042    -1.260705     1.270261
 C     5.339535    -0.405957     2.373538
 C    -1.608792     0.798184     1.809143
 C    -2.226204    -0.452306     1.680809
 C    -3.579132    -0.520818     1.387946
 C    -4.338858     0.658569     1.246539
 C    -3.716592     1.909411     1.408608
 C    -2.349289     1.971912     1.687732
 C    -0.584562    -0.566894    -0.986427
 C    -2.602982    -0.940817    -1.952383
 C    -2.259193     0.345140    -2.191128
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 C    -1.579327    -2.833020    -0.706416
 C    -0.600425    -4.467267     0.513454
 C    -1.679271    -5.311544     0.254880
 C    -2.704555    -4.788628    -0.536629
 C    -0.316921     1.817331    -1.634805
 C     1.013457     1.880839    -2.072113
 C     1.670885     3.101699    -2.102539
 C     1.003553     4.282026    -1.717114
 C    -0.339157     4.214718    -1.304696
 C    -0.991053     2.980104    -1.264200
 C     2.116880    -2.468910    -2.805684
 C     2.471193    -3.174008    -4.031100
 H    -0.416620     2.066334     3.938221
 H     2.334783     1.615889     4.096299
 H     4.232250    -2.102596    -0.343434
 H     6.356533    -1.745625     0.997844
 H     6.202386    -0.192599     2.998575
 H    -1.642778    -1.357166     1.818065
 H    -4.084267    -1.475981     1.285776
 H    -4.281579     2.830035     1.322876
 H    -1.863009     2.936971     1.797690
 H    -3.471241    -1.518575    -2.222744
 H    -2.760957     1.125046    -2.742119
 H     0.241378    -4.788460     1.121822
 H    -1.721827    -6.320748     0.649397
 H    -3.585376    -5.371969    -0.791984
 H     1.518680     0.982590    -2.411733
 H     2.696377     3.178734    -2.449267
 H    -0.880895     5.108409    -1.018469
 H    -2.022833     2.924835    -0.932073
 H     2.702179    -4.220840    -3.806594
 H     3.345686    -2.704208    -4.493885
 H     1.632677    -3.136090    -4.734879
 O    -5.642262     0.477345     0.960219
 C    -6.518014     1.611884     0.893582
 H    -6.225358     2.284994     0.078518
 H    -7.507992     1.202892     0.693290
 H    -6.527446     2.152390     1.847169
 C     1.118199     6.672357    -1.491026
 H     1.895317     7.419491    -1.650466
 H     0.276561     6.865289    -2.166694
 H     0.782793     6.706608    -0.447284
 O     1.733030     5.412027    -1.789667
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(CN,C)-4c.xyz
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HF= -1898.459836 Hartree
NImag=0
Pd    -0.995881    -0.714447     0.146692
 N    -1.951853     0.657422    -2.148521
 N     0.131424     1.204126    -2.107023
 N    -2.950154    -0.859162    -0.728346
 N    -4.217725     0.149521    -2.481890
 N     1.868395    -1.196445     1.043152
 N     1.190911     0.777447     1.609117
 N     0.907710    -2.910368    -0.251119
 N     3.123514    -3.109755     0.618722
 N    -1.437643    -1.896458     1.853421
 C    -0.786690     0.473092    -1.446532
 C    -0.458715     1.858518    -3.201412
 C    -1.768071     1.516565    -3.228876
 C    -3.115287    -0.037573    -1.785144
 C    -4.028307    -1.568617    -0.345508
 C    -5.240332    -1.450364    -1.017620
 C    -5.288886    -0.561290    -2.095926
 C     1.543432     1.261309    -1.842501
 C     2.283124     0.076251    -1.825646
 C     3.656980     0.128785    -1.597749
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 C     4.256061     1.374188    -1.417967
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 C     0.814058    -0.335068     0.940355
 C     2.912571    -0.606522     1.760724
 C     2.485706     0.626453     2.116020
 C     1.965442    -2.486346     0.435150
 C     1.035153    -4.119744    -0.822253
 C     2.198077    -4.879128    -0.701219
 C     3.235823    -4.317503     0.046434
 C     0.405945     1.970825     1.779094
 C    -0.888390     1.893565     2.302746
 C    -1.639969     3.057798     2.458426
 C    -1.066545     4.276483     2.101663
 C     0.232264     4.373784     1.607128
 C     0.973679     3.203781     1.443244
 C    -1.622037    -2.524987     2.807025
 C    -1.851930    -3.318491     4.007686
 H     0.127070     2.478326    -3.862744
 H    -2.574963     1.775439    -3.896833
 H    -3.893029    -2.227710     0.504838
 H    -6.108810    -2.023707    -0.713776
 H    -6.199196    -0.408180    -2.669134
 H     1.784996    -0.872837    -1.994264
 H     4.266576    -0.768395    -1.576688
 H     4.051532     3.512105    -1.337868
 H     1.567556     3.415635    -1.706811
 H     3.837271    -1.129601     1.941184
 H     2.959595     1.403084     2.696188
 H     0.178597    -4.475696    -1.389105
 H     2.293737    -5.854243    -1.165985
 H     4.180517    -4.834024     0.194764
 H    -1.296770     0.936849     2.609688
 H    -2.643465     3.037628     2.870084
 H     0.642746     5.347564     1.361425
 H     1.983762     3.248601     1.050096
 H    -1.998021    -4.370045     3.738082
 H    -2.742246    -2.954900     4.532021
 H    -0.987521    -3.237649     4.675709
 F    -1.789254     5.398282     2.250347
 F     5.578798     1.425303    -1.191637
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(CN,C)-4d.xyz
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HF= -1898.460752 Hartree
NImag=0
Pd    0.909431     0.643453    -0.017801
 N     1.876345    -1.310814    -1.835308
 N    -0.228185    -1.756971    -1.750240
 N     2.886268     0.502993    -0.833376
 N     4.169682    -0.974886    -2.199543
 N    -1.950040     1.388095     0.721691
 N    -1.302549    -0.402457     1.740485
 N    -0.995794     2.694893    -0.986616
 N    -3.130653     3.235048    -0.061015
 N     1.345602     2.233252     1.302497
 C     0.699855    -0.914429    -1.252579
 C     0.368865    -2.689849    -2.616935
 C     1.690402    -2.409214    -2.672486
 C     3.053649    -0.576933    -1.623567
 C     3.977556     1.257647    -0.607378
 C     5.205116     0.929315    -1.173556
 C     5.253962    -0.216270    -1.973646
 C    -1.645128    -1.671369    -1.564729
 C    -2.329968    -0.483835    -1.835545
 C    -3.715950    -0.434636    -1.685220
 C    -4.421419    -1.577478    -1.290634
 C    -3.746594    -2.775549    -1.038826
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 C    -2.365942    -2.804714    -1.181171
 C    -0.910765     0.511548     0.824570
 C    -2.997484     1.007682     1.566759
 C    -2.589409    -0.112190     2.205249
 C    -2.022861     2.509884    -0.162087
 C    -1.095964     3.753488    -1.807455
 C    -2.205188     4.598268    -1.797400
 C    -3.218252     4.287936    -0.887319
 C    -0.531737    -1.524278     2.193908
 C     0.663546    -1.332130     2.890687
 C     1.416291    -2.401735     3.353383
 C     0.949949    -3.700228     3.125803
 C    -0.256505    -3.913017     2.449757
 C    -0.998273    -2.825281     1.987929
 C     1.533161     3.038889     2.109965
 C     1.768067     4.048334     3.133963
 H    -0.216403    -3.450399    -3.109340
 H     2.507690    -2.858640    -3.214764
 H     3.839671     2.122842     0.031435
 H     6.084736     1.538079    -0.997688
 H     6.175478    -0.542188    -2.448232
 H    -1.767118     0.382946    -2.165972
 H    -4.247993     0.487312    -1.898392
 H    -4.269497    -3.680676    -0.746774
 H    -3.910244     1.577673     1.620542
 H    -3.070844    -0.725481     2.951337
 H    -0.263120     3.914272    -2.487331
 H    -2.280052     5.449566    -2.465016
 H    -4.122266     4.886244    -0.809722
 H     2.335364    -2.209173     3.897327
 H    -0.621205    -4.921445     2.283628
 H    -1.938474    -2.973587     1.468512
 H     2.158566     4.964401     2.678265
 H     2.491261     3.672147     3.865556
 H     0.828710     4.277137     3.648768
 F     1.086872    -0.065432     3.130039
 F    -1.691432    -3.952805    -0.941235
 H    -5.502068    -1.544091    -1.191602
 H     1.526423    -4.544880     3.490415
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(CN,C)-4e.xyz
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HF= -2108.978848 Hartree
NImag=0
Pd     0.884703    -1.262516    -0.112110
 N     1.963594    -0.339040     2.350505
 N     0.080826     0.698686     2.250626
 N     2.674403    -1.942747     0.854310
 N     4.015760    -1.402405     2.753453
 N    -1.922327    -0.972235    -1.248098
 N    -0.771036     0.830316    -1.555407
 N    -1.512166    -2.956159    -0.048645
 N    -3.603372    -2.577429    -1.139588
 N     1.173113    -2.378548    -1.890704
 C     0.843525    -0.185792     1.575620
 C     0.729285     1.111160     3.427097
 C     1.912919     0.457611     3.491607
 C     2.954162    -1.266677     1.986950
 C     3.579117    -2.861845     0.466222
 C     4.733602    -3.088928     1.208147
 C     4.914563    -2.319847     2.362046
 C    -1.249480     1.112661     1.905217
 C    -2.222036     0.136396     1.677907
 C    -3.507081     0.528662     1.312782
 C    -3.789606     1.890291     1.217160
 C    -2.842678     2.872160     1.502582
 C    -1.549080     2.475483     1.843880
 C    -0.713765    -0.397590    -0.986487
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 C    -2.741053    -0.092771    -1.962594
 C    -2.019068     1.034329    -2.154721
 C    -2.366657    -2.252687    -0.785704
 C    -1.966291    -4.145445     0.383237
 C    -3.246622    -4.605754     0.078874
 C    -4.044725    -3.766351    -0.702521
 C     0.273700     1.816017    -1.536422
 C     1.570003     1.470068    -1.930461
 C     2.581180     2.427460    -1.876320
 C     2.264355     3.714998    -1.447145
 C     0.967398     4.084107    -1.095414
 C    -0.038635     3.119225    -1.137935
 C     1.286703    -2.958406    -2.885452
 C     1.427238    -3.690580    -4.137559
 H     0.263547     1.804897     4.110377
 H     2.707983     0.462200     4.221341
 H     3.353557    -3.404661    -0.444842
 H     5.461531    -3.830762     0.899578
 H     5.792286    -2.432793     2.992492
 H    -1.968088    -0.913197     1.779023
 H    -3.742423    -0.365702    -2.254237
 H    -2.255073     1.947989    -2.678463
 H    -1.279359    -4.730536     0.989297
 H    -3.606761    -5.565059     0.434002
 H    -5.057445    -4.038261    -0.988075
 H    -1.052653     3.374901    -0.850467
 H     1.320260    -4.765453    -3.955471
 H     2.412105    -3.496478    -4.576128
 H     0.653491    -3.368896    -4.843231
 H     1.782268     0.472088    -2.296865
 H    -0.781052     3.217328     2.039845
 H    -4.284873    -0.198049     1.108783
 H    -3.114749     3.920017     1.440877
 H     3.596826     2.195034    -2.174894
 H     0.760214     5.103344    -0.789468
 N     3.347793     4.728141    -1.364379
 O     3.030745     5.857440    -1.004848
 O     4.482918     4.354971    -1.649187
 N    -5.141869     2.304374     0.766081
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 O    -5.896861     1.412600     0.382863
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(CN,C)-4f.xyz
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   79
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 N    -0.342771     0.591606     2.394390
 N     2.637684    -1.590342     1.010819
 N     3.741378    -1.141058     3.078877
 N    -1.685790    -0.630829    -1.633080
 N    -0.408867     1.095034    -1.926728
 N    -1.426753    -2.718183    -0.569499
 N    -3.517724    -2.060335    -1.515124
 N     1.353383    -2.155490    -1.769356
 C     0.612685    -0.027146     1.678412
 C     0.088997     0.801765     3.712590
 C     1.339399     0.298549     3.826175
 C     2.746630    -1.010546     2.222922
 C     3.659378    -2.377867     0.626521
 C     4.757031    -2.583806     1.455116
 C     4.752421    -1.934327     2.693608
 C    -1.688270     0.902221     1.965478
 C    -2.617664    -0.148857     1.876864
 C    -3.910262     0.176660     1.458694
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 C    -2.035557     2.246829     1.778823
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 C    -1.477693     1.210753    -2.818870
 C    -2.238729    -1.876410    -1.200177
 C    -1.974296    -3.887396    -0.201191
 C    -3.302767    -4.205373    -0.475363
 C    -4.047516    -3.236060    -1.152403
 C     0.603235     2.128109    -1.782253
 C     1.937136     1.873532    -2.139818
 C     2.883358     2.880489    -1.900853
 C     2.531867     4.124737    -1.373735
 C     1.172547     4.372123    -1.131592
 C     0.187378     3.406031    -1.345614
 C     1.496474    -2.862063    -2.672977
 C     1.673371    -3.738268    -3.823837
 H    -0.551924     1.281182     4.436106
 H     2.032738     0.240121     4.650664
 H     3.571126    -2.836528    -0.351767
 H     5.578454    -3.222302     1.150494
 H     5.572043    -2.044538     3.398477
 H    -4.648006    -0.617186     1.366717
 H    -3.647246     3.552509     1.226957
 H    -3.215112    -0.148741    -3.087640
 H    -1.553249     2.043564    -3.499120
 H    -1.320698    -4.578757     0.325246
 H    -3.735705    -5.155327    -0.181571
 H    -5.091188    -3.394269    -1.412023
 H     3.919970     2.691395    -2.171731
 H     0.868497     5.357463    -0.784915
 H     2.182004    -4.659885    -3.521768
 H     2.273138    -3.232218    -4.588156
 H     0.696327    -3.994400    -4.247519
 C    -2.278167    -1.548748     2.332006
 H    -2.188910    -1.579062     3.425810
 H    -3.067907    -2.250518     2.051161
 H    -1.337510    -1.915493     1.914807
 C    -1.041168     3.357543     2.021844
 H    -1.474276     4.328181     1.771762
 H    -0.741536     3.403393     3.075340
 H    -0.128610     3.227365     1.429459
 C    -1.266906     3.789169    -1.199002
 H    -1.883846     2.988436    -0.787640
 H    -1.370415     4.665660    -0.555831
 H    -1.690339     4.064611    -2.173286
 C     2.387615     0.621888    -2.856498
 H     2.974569    -0.035497    -2.205104
 H     1.547161     0.046875    -3.249861
 H     3.030197     0.896874    -3.699929
 C     3.561168     5.200646    -1.128235
 H     3.375374     6.071474    -1.768558
 H     4.575953     4.845858    -1.330865
 C    -5.711529     1.816144     0.781604
 H    -6.078063     1.097911     0.039800
 H    -5.795452     2.821145     0.357347
 H     3.524157     5.551460    -0.089973
 H    -6.387270     1.764254     1.644846
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(CN,C)-4g.xyz
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   81
HF= -2086.332280 Hartree
NImag=0
Pd     0.708715    -1.288387    -0.065176
 N     1.655844    -0.616679     2.531437
 N    -0.168168     0.521433     2.372231
 N     2.289972    -2.242355     1.030836
 N     3.554694    -1.903559     3.027266
 N    -1.749926    -0.441597    -1.664389
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N	-0.114732	0.956568	-1.926571
N	-2.013439	-2.485410	-0.520313
N	-3.847166	-1.445269	-1.640434
N	0.842114	-2.618379	-1.719180
C	0.642937	-0.282499	1.662521
C	0.339755	0.708684	3.666882
C	1.487380	-0.000619	3.770631
C	2.566528	-1.627206	2.199027
C	3.118826	-3.237380	0.664437
C	4.191192	-3.610272	1.467619
C	4.371377	-2.902860	2.660359
C	-1.465698	0.994648	1.953115
C	-2.528215	0.067603	1.918010
C	-3.763489	0.521864	1.472739
C	-3.957255	1.871892	1.124004
C	-2.907226	2.790580	1.275576
C	-1.645008	2.360275	1.706312
C	-0.506154	-0.119997	-1.195582
C	-2.133541	0.435705	-2.682456
C	-1.104565	1.294224	-2.852601
C	-2.582532	-1.522540	-1.236772
C	-2.825862	-3.487969	-0.148892
C	-4.172901	-3.524278	-0.502257
C	-4.643826	-2.455665	-1.270105
C	1.095834	1.736707	-1.750693
C	2.356308	1.184101	-2.061636
C	3.493405	1.939760	-1.787721
C	3.399126	3.238267	-1.266378
C	2.132607	3.810793	-1.075908
C	0.969194	3.076346	-1.332010
C	0.822310	-3.358279	-2.607139
C	0.797186	-4.280216	-3.735502
H	-0.183509	1.319681	4.385675
H	2.187259	-0.145940	4.578730
H	2.897506	-3.724415	-0.278576
H	4.855924	-4.416187	1.178084
H	5.185084	-3.133292	3.342648
H	-4.618043	-0.146067	1.427291
H	-3.059568	3.844883	1.076475
H	-3.092478	0.349940	-3.166034
H	-0.973178	2.113407	-3.540734
H	-2.372721	-4.276462	0.447169
H	-4.821040	-4.340084	-0.201364
H	-5.678568	-2.397954	-1.598055
H	4.480852	1.550436	-2.018592
H	2.035269	4.840136	-0.750630
H	0.834278	-5.314411	-3.377099
H	1.657169	-4.095230	-4.388201
H	-0.124069	-4.135968	-4.310155
O	-5.194789	2.184119	0.687886
C	-5.522661	3.551145	0.409769
H	-4.901387	3.945815	-0.403674
H	-6.568017	3.542702	0.101504
H	-5.408293	4.170500	1.307170
C	4.570206	5.224637	-0.586540
H	5.620245	5.495965	-0.478455
H	4.097289	5.874123	-1.332766
H	4.061901	5.326830	0.380172
O	4.571150	3.860259	-1.023828
C	-2.365520	-1.332573	2.462057
H	-2.146946	-1.297706	3.536975
H	-3.285646	-1.907748	2.332586
H	-1.553710	-1.880748	1.977253
C	-0.529504	3.350127	1.948924
H	-0.819385	4.352378	1.627856
H	-0.286752	3.414515	3.016095
H	0.389554	3.071751	1.421879
C	-0.365950	3.780584	-1.241472
H	-1.156716	3.148732	-0.831248

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 H    -0.287311     4.677461    -0.623619
 H    -0.690853     4.112463    -2.235498
 C     2.531814    -0.139348    -2.771742
 H     2.940029    -0.909712    -2.107924
 H     1.593395    -0.512050    -3.186530
 H     3.239823    -0.017671    -3.598414
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(CN,C)-4h.xyz
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HF= -3048.212626 Hartree
NImag=0
Pd     1.451113    -1.382362     0.105733
 N     1.954455     0.290562     2.340597
 N    -0.142932     0.610763     1.974985
 N     3.246161    -1.299824     1.282340
 N     4.196108     0.066260     2.993912
 N    -1.074038    -1.983518    -1.495308
 N    -0.449246     0.068209    -1.750645
 N    -0.633413    -3.614469     0.138799
 N    -1.835540    -4.153717    -1.856325
 N     2.208756    -2.687889    -1.370624
 C     0.920752    -0.086918     1.527960
 C     0.231718     1.440442     3.046325
 C     1.550774     1.238495     3.276588
 C     3.211440    -0.327128     2.215764
 C     4.423785    -1.932320     1.121458
 C     5.529973    -1.594113     1.893881
 C     5.366977    -0.570590     2.832274
 C    -1.500195     0.481572     1.524640
 C    -2.084634    -0.785261     1.470201
 C    -3.416145    -0.889166     1.070496
 C    -4.154587     0.247436     0.724666
 C    -3.547508     1.500176     0.791974
 C    -2.217875     1.630432     1.203023
 C    -0.161279    -1.071987    -1.070083
 C    -1.942486    -1.414792    -2.429844
 C    -1.556271    -0.126562    -2.583624
 C    -1.179551    -3.340515    -1.041132
 C    -0.785364    -4.881691     0.559942
 C    -1.478479    -5.832229    -0.188452
 C    -1.993089    -5.411587    -1.416998
 C     0.259189     1.304892    -1.599001
 C     1.653668     1.299150    -1.589438
 C     2.340057     2.472507    -1.280993
 C     1.651765     3.664245    -1.047137
 C     0.257977     3.664768    -1.135027
 C    -0.449558     2.489548    -1.402634
 C     2.582337    -3.378347    -2.220313
 C     3.049732    -4.248593    -3.291088
 H    -0.489536     2.064429     3.551913
 H     2.233297     1.648527     4.005047
 H     4.453891    -2.710282     0.366866
 H     6.477867    -2.105259     1.769280
 H     6.183186    -0.246636     3.472045
 H    -1.513985    -1.666836     1.738466
 H    -2.736907    -1.988762    -2.878864
 H    -1.940390     0.660425    -3.214698
 H    -0.349819    -5.123154     1.525965
 H    -1.614558    -6.847518     0.167661
 H    -2.540743    -6.085185    -2.070713
 H    -1.533855     2.502276    -1.430153
 H     3.348748    -5.219045    -2.880341
 H     3.908221    -3.791315    -3.795098
 H     2.246616    -4.400374    -4.020552
 H    -5.192167     0.157740     0.420849
 H     2.188807     4.576619    -0.812842
 H     2.202082     0.392936    -1.816357
 H    -1.755029     2.610516     1.256183
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 C    -4.283764     2.744145     0.340583
 C    -4.068749    -2.249733     0.969046
 C     3.838465     2.383030    -1.117377
 C    -0.535611     4.919280    -0.833115
 F    -1.531521     5.097622    -1.719970
 F    -1.113985     4.804677     0.401093
 F     0.231769     6.018740    -0.818946
 F     4.436690     3.578176    -1.082714
 F     4.131470     1.742739     0.064687
 F     4.406830     1.641388    -2.094347
 F    -5.607114     2.550192     0.248739
 F    -4.053980     3.781505     1.166478
 F    -3.832997     3.109075    -0.897517
 F    -5.356355    -2.222349     1.339522
 F    -3.427958    -3.175554     1.719151
 F    -4.027283    -2.698052    -0.321496
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(CN,CN)-4a.xyz
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HF= -1645.836636 Hartree
NImag=0
Pd    -1.409894     0.000000     0.000000
 N    -0.699064    -2.654441     0.778435
 N     1.054907    -1.499913     1.281401
 N    -2.725249    -1.721826     0.180272
 N    -2.529027    -4.084860     0.486530
 N    -0.699064     2.654440    -0.778434
 N     1.054907     1.499913    -1.281401
 N    -2.725249     1.721826    -0.180272
 N    -2.529027     4.084860    -0.486530
 C    -0.146413    -1.401951     0.681979
 C     1.272260    -2.821236     1.708029
 C     0.174894    -3.547679     1.393696
 C    -2.048858    -2.857110     0.464277
 C    -4.019115    -1.877488    -0.165029
 C    -4.623536    -3.128859    -0.173845
 C    -3.826485    -4.223099     0.178002
 C     1.970137    -0.434942     1.592039
 C     1.490395     0.776771     2.096840
 C     2.397241     1.778719     2.440406
 C     3.783699     1.581239     2.324897
 C     4.234845     0.344383     1.835163
 C     3.342450    -0.658992     1.464393
 C     4.759857     2.644614     2.762673
 C    -0.146413     1.401951    -0.681979
 C     0.174895     3.547679    -1.393696
 C     1.272260     2.821236    -1.708028
 C    -2.048858     2.857110    -0.464277
 C    -4.019115     1.877489     0.165029
 C    -4.623535     3.128860     0.173844
 C    -3.826484     4.223099    -0.178002
 C     1.970137     0.434941    -1.592039
 C     1.490395    -0.776771    -2.096841
 C     2.397241    -1.778719    -2.440407
 C     3.783699    -1.581239    -2.324898
 C     4.234845    -0.344384    -1.835162
 C     3.342451     0.658991    -1.464392
 C     4.759857    -2.644614    -2.762674
 H     2.173630    -3.099109     2.231302
 H    -0.087012    -4.580980     1.560558
 H    -4.562830    -0.980435    -0.437927
 H    -5.667436    -3.245828    -0.442086
 H    -4.223845    -5.234065     0.207148
 H     0.426368     0.922735     2.250933
 H     2.022443     2.716936     2.841409
 H     5.301883     0.165859     1.732350
 H     3.711915    -1.590347     1.046311
 H     4.330243     3.647983     2.680558
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 H     5.681939     2.613911     2.173288
 H     5.041057     2.493972     3.813118
 H    -0.087011     4.580980    -1.560558
 H     2.173631     3.099109    -2.231300
 H    -4.562830     0.980436     0.437926
 H    -5.667436     3.245829     0.442085
 H    -4.223845     5.234065    -0.207149
 H     0.426369    -0.922734    -2.250934
 H     2.022443    -2.716935    -2.841411
 H     5.301883    -0.165860    -1.732349
 H     3.711915     1.590346    -1.046309
 H     5.681940    -2.613910    -2.173290
 H     5.041056    -2.493973    -3.813119
 H     4.330244    -3.647984    -2.680558
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(CN,CN)-4b.xyz
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   63
HF= -1796.258712 Hartree
NImag=0
Pd    -1.716706     0.000000    -0.000000
 N    -1.005718     2.567798    -1.028741
 N     0.750544     1.370082    -1.415256
 N    -3.032322     1.695690    -0.347840
 N    -2.837187     4.018065    -0.882860
 N    -1.005719    -2.567798     1.028742
 N     0.750543    -1.370082     1.415256
 N    -3.032322    -1.695690     0.347839
 N    -2.837187    -4.018065     0.882860
 C    -0.452244     1.329980    -0.811412
 C     0.967891     2.645602    -1.964795
 C    -0.129764     3.398611    -1.722870
 C    -2.355701     2.798519    -0.739854
 C    -4.326978     1.883327    -0.022155
 C    -4.932310     3.128920    -0.136456
 C    -4.135107     4.184296    -0.591868
 C     1.663718     0.280747    -1.616108
 C     1.182309    -0.983498    -1.987551
 C     2.074731    -2.016909    -2.224806
 C     3.464792    -1.795220    -2.133729
 C     3.940028    -0.515925    -1.793828
 C     3.036365     0.512434    -1.530152
 C    -0.452245    -1.329980     0.811413
 C    -0.129765    -3.398611     1.722871
 C     0.967890    -2.645602     1.964795
 C    -2.355702    -2.798519     0.739854
 C    -4.326978    -1.883327     0.022154
 C    -4.932310    -3.128920     0.136456
 C    -4.135108    -4.184295     0.591867
 C     1.663717    -0.280747     1.616108
 C     1.182309     0.983498     1.987550
 C     2.074730     2.016909     2.224805
 C     3.464791     1.795220     2.133728
 C     3.940028     0.515925     1.793828
 C     3.036365    -0.512434     1.530153
 H     1.869535     2.873603    -2.510892
 H    -0.390463     4.411735    -1.986862
 H    -4.870602     1.016684     0.335876
 H    -5.976771     3.270628     0.117175
 H    -4.533230     5.187202    -0.720280
 H     0.118123    -1.144369    -2.122616
 H     1.727199    -2.998707    -2.529943
 H     5.002201    -0.315628    -1.720913
 H     3.410603     1.484411    -1.223542
 H    -0.390464    -4.411734     1.986863
 H     1.869535    -2.873603     2.510893
 H    -4.870602    -1.016683    -0.335877
 H    -5.976771    -3.270627    -0.117176
 H    -4.533231    -5.187202     0.720280
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 H     0.118123     1.144369     2.122615
 H     1.727199     2.998707     2.529942
 H     5.002201     0.315627     1.720914
 H     3.410603    -1.484411     1.223543
 C     5.668061     2.708876     2.441079
 H     6.061143     2.421307     1.458355
 H     6.055936     3.688732     2.718029
 H     5.956157     1.969213     3.196863
 C     5.668061    -2.708876    -2.441079
 H     6.061143    -2.421308    -1.458355
 H     6.055936    -3.688732    -2.718029
 H     5.956157    -1.969213    -3.196863
 O     4.241561    -2.861655    -2.397025
 O     4.241560     2.861655     2.397024
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(CN,CN)-4c.xyz
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HF= -1765.661666 Hartree
NImag=0
Pd     1.395008     0.000000     0.000000
 N     0.712192     2.690318     0.679869
 N    -1.060147     1.585172     1.220683
 N     2.721495     1.715028     0.094211
 N     2.554899     4.088629     0.319642
 N     0.712194    -2.690318    -0.679870
 N    -1.060146    -1.585172    -1.220684
 N     2.721496    -1.715028    -0.094210
 N     2.554901    -4.088629    -0.319642
 C     0.140451     1.444441     0.624423
 C    -1.253614     2.923115     1.606017
 C    -0.144036     3.618582     1.266325
 C     2.061991     2.866834     0.345845
 C     4.011594     1.843912    -0.277472
 C     4.628592     3.087634    -0.338666
 C     3.849461     4.202407    -0.011272
 C    -1.997415     0.549436     1.558635
 C    -1.539316    -0.654765     2.104489
 C    -2.457290    -1.636739     2.472421
 C    -3.817184    -1.372871     2.315797
 C    -4.289087    -0.164087     1.809357
 C    -3.365453     0.802966     1.419286
 C     0.140452    -1.444441    -0.624423
 C    -0.144034    -3.618582    -1.266326
 C    -1.253612    -2.923115    -1.606019
 C     2.061992    -2.866834    -0.345845
 C     4.011595    -1.843911     0.277474
 C     4.628593    -3.087633     0.338667
 C     3.849463    -4.202406     0.011272
 C    -1.997414    -0.549437    -1.558635
 C    -1.539315     0.654765    -2.104488
 C    -2.457290     1.636739    -2.472419
 C    -3.817183     1.372870    -2.315796
 C    -4.289086     0.164085    -1.809358
 C    -3.365452    -0.802967    -1.419287
 H    -2.147939     3.235467     2.122191
 H     0.135814     4.652461     1.397812
 H     4.541036     0.932383    -0.529487
 H     5.669084     3.183699    -0.627883
 H     4.258102     5.209239    -0.021315
 H    -0.479510    -0.811595     2.271899
 H    -2.139935    -2.576998     2.910938
 H    -5.357108     0.001046     1.714914
 H    -3.713492     1.734579     0.984443
 H     0.135817    -4.652461    -1.397814
 H    -2.147936    -3.235468    -2.122194
 H     4.541036    -0.932382     0.529489
 H     5.669085    -3.183698     0.627885
 H     4.258105    -5.209238     0.021315
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 H    -0.479509     0.811596    -2.271896
 H    -2.139935     2.576998    -2.910935
 H    -5.357108    -0.001048    -1.714916
 H    -3.713491    -1.734582    -0.984445
 F    -4.702504     2.315720    -2.673628
 F    -4.702504    -2.315721     2.673629
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(CN,CN)-4d.xyz
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   55
HF= -1765.661146 Hartree
NImag=0
Pd    -1.335259     0.000003    -0.000027
 N    -0.603165     2.729433    -0.410324
 N     1.134482     1.637553    -1.077556
 N    -2.640866     1.739681     0.046937
 N    -2.423645     4.120435     0.071716
 N    -0.603214    -2.729428     0.410324
 N     1.134450    -1.637575     1.077554
 N    -2.640888    -1.739641    -0.046973
 N    -2.423724    -4.120401    -0.071683
 C    -0.066396     1.472838    -0.487271
 C     1.367234     3.004204    -1.322853
 C     0.278674     3.689444    -0.906027
 C    -1.953966     2.897976    -0.073338
 C    -3.937016     1.857486     0.399060
 C    -4.531569     3.101210     0.576588
 C    -3.722853     4.226573     0.387459
 C     1.992031     0.600552    -1.569963
 C     3.378287     0.714203    -1.425975
 C     4.245804    -0.232314    -1.949810
 C     3.714135    -1.327730    -2.634304
 C     2.330248    -1.456373    -2.797812
 C     1.470627    -0.487712    -2.280310
 C    -0.066421    -1.472842     0.487262
 C     0.278607    -3.689452     0.906037
 C     1.367188    -3.004232     1.322838
 C    -1.954016    -2.897949     0.073336
 C    -3.937041    -1.857425    -0.399097
 C    -4.531622    -3.101140    -0.576591
 C    -3.722933    -4.226517    -0.387428
 C     1.991997    -0.600586     1.569985
 C     3.378251    -0.714211     1.425961
 C     4.245768     0.232293     1.949820
 C     3.714099     1.327664     2.634386
 C     2.330213     1.456279     2.797933
 C     1.470594     0.487636     2.280398
 H     2.281167     3.344003    -1.782882
 H     0.030258     4.739350    -0.922646
 H    -4.490738     0.936147     0.538568
 H    -5.577278     3.189188     0.849009
 H    -4.111517     5.235418     0.496801
 H     5.314240    -0.103556    -1.811700
 H     1.922720    -2.292565    -3.357110
 H     0.401055    -0.548036    -2.451380
 H     0.030169    -4.739353     0.922670
 H     2.281119    -3.344043     1.782862
 H    -4.490737    -0.936076    -0.538636
 H    -5.577332    -3.189102    -0.849013
 H    -4.111622    -5.235356    -0.496741
 H     5.314202     0.103557     1.811674
 H     1.922686     2.292437     3.357283
 H     0.401024     0.547938     2.451494
 F     3.877749    -1.776692     0.753680
 F     3.877787     1.776730    -0.753768
 H     4.384590    -2.072620    -3.051344
 H     4.384553     2.072544     3.051445
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   59
HF= -1976.178843 Hartree
NImag=0
Pd    -1.875887     0.000000     0.000001
 N    -1.238137    -2.558873     1.108246
 N     0.564975    -1.434341     1.461280
 N    -3.219610    -1.662903     0.334285
 N    -3.099453    -3.969473     0.944397
 N    -1.238134     2.558873    -1.108244
 N     0.564979     1.434340    -1.461275
 N    -3.219609     1.662904    -0.334287
 N    -3.099451     3.969473    -0.944401
 C    -0.636910    -1.354413     0.850186
 C     0.723228    -2.695889     2.061350
 C    -0.407605    -3.403488     1.839456
 C    -2.586889    -2.767334     0.783216
 C    -4.501942    -1.833607    -0.049768
 C    -5.137981    -3.062924     0.074855
 C    -4.387943    -4.119261     0.603123
 C     1.545597    -0.395191     1.601421
 C     1.138123     0.909502     1.898791
 C     2.098475     1.907393     2.045829
 C     3.444985     1.566627     1.924938
 C     3.863519     0.259792     1.685610
 C     2.899514    -0.731009     1.511640
 C    -0.636907     1.354413    -0.850182
 C    -0.407600     3.403488    -1.839453
 C     0.723233     2.695889    -2.061344
 C    -2.586887     2.767335    -0.783217
 C    -4.501941     1.833608     0.049763
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 C    -4.387941     4.119261    -0.603130
 C     1.545600     0.395190    -1.601416
 C     1.138126    -0.909501    -1.898791
 C     2.098478    -1.907392    -2.045831
 C     3.444987    -1.566628    -1.924935
 C     3.863522    -0.259794    -1.685601
 C     2.899517     0.731007    -1.511630
 H     1.609705    -2.947436     2.622507
 H    -0.716303    -4.394107     2.136486
 H    -5.008148    -0.969553    -0.464180
 H    -6.171693    -3.191786    -0.225961
 H    -4.813917    -5.108386     0.747949
 H     3.206592    -1.745036     1.277295
 H    -0.716298     4.394107    -2.136483
 H     1.609711     2.947436    -2.622499
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 H     3.206595     1.745033    -1.277281
 H     0.087975     1.137335     2.040255
 H     0.087979    -1.137333    -2.040260
 H     1.820684    -2.929737    -2.275365
 H     4.921361    -0.033290    -1.614094
 H     4.921358     0.033287     1.614107
 H     1.820681     2.929738     2.275360
 N     4.466438     2.639587     2.040032
 O     5.641901     2.304238     1.940611
 O     4.053655     3.785639     2.200077
 N     4.466441    -2.639588    -2.040029
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 O     4.053658    -3.785638    -2.200090
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N	-2.920795	-1.673792	0.023915
N	-2.838310	-4.046612	0.277797
N	-0.982850	2.693039	-0.741309
N	0.788554	1.633978	-1.370007
N	-2.920811	1.673755	-0.023899
N	-2.838343	4.046586	-0.277695
C	-0.345644	-1.473191	0.662532
C	0.866565	-2.944607	1.870759
C	-0.236478	-3.614758	1.472396
C	-2.310066	-2.838494	0.325599
C	-4.182223	-1.766153	-0.444135
C	-4.828271	-2.992342	-0.541197
C	-4.108572	-4.124592	-0.142959
C	1.780974	-0.648606	1.749157
C	1.409919	0.408746	2.600800
C	2.430127	1.253429	3.055982
C	3.774865	1.045850	2.727680
C	4.095460	-0.043756	1.907990
C	3.121229	-0.907142	1.401855
C	-0.345675	1.473185	-0.662526
C	-0.236497	3.614782	-1.472308
C	0.866539	2.944639	-1.870702
C	-2.310089	2.838473	-0.325537
C	-4.182243	1.766092	0.444145
C	-4.828303	2.992272	0.541244
C	-4.108608	4.124542	0.143053
C	1.780915	0.648612	-1.749189
C	1.409871	-0.408648	-2.600949
C	2.430073	-1.253327	-3.056147
C	3.774801	-1.045811	-2.727760
C	4.095387	0.043706	-1.907946
C	3.121155	0.907070	-1.401779
H	1.697786	-3.255358	2.482680
H	-0.579986	-4.623758	1.639705
H	-4.661763	-0.840172	-0.741533
H	-5.846147	-3.063015	-0.907717
H	-4.547090	-5.118510	-0.169902
H	2.168548	2.072463	3.722015
H	5.136864	-0.229772	1.655357
H	-0.579995	4.623794	-1.639571
H	1.697768	3.255407	-2.482604
H	-4.661779	0.840097	0.741508
H	-5.846182	3.062924	0.907757
H	-4.547133	5.118456	0.170029
H	2.168507	-2.072288	-3.722275
H	5.136784	0.229666	-1.655242
C	-0.003083	-0.625867	-3.094427
H	-0.580262	-1.257301	-2.407554
H	-0.550949	0.314836	-3.214891
H	0.008740	-1.127487	-4.066266
C	3.527437	2.086318	-0.547804
H	4.503191	1.905350	-0.092651
H	3.619716	3.004192	-1.141440
H	2.814809	2.277180	0.260047
C	-0.003059	0.626091	3.094151
H	-0.580143	1.257506	2.407180
H	-0.550993	-0.314566	3.214662
H	0.008724	1.127799	4.065945
C	3.527549	-2.086487	0.548028
H	4.503371	-1.905609	0.092989
H	3.619706	-3.004318	1.141744
H	2.815015	-2.277374	-0.259901
C	4.850035	1.979090	3.225401
H	4.556334	2.475947	4.155081
H	5.051260	2.764110	2.483521
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 N    3.238784     1.656227     0.131711
 N    3.175640     4.005494     0.551371
 N    1.310991    -2.638559    -0.917676
 N   -0.488102    -1.573189    -1.447162
 N    3.238787    -1.656225    -0.131708
 N    3.175646    -4.005492    -0.551365
 C    0.655999     1.436982     0.749766
 C   -0.551129     2.850565     2.029262
 C    0.567846     3.525224     1.691450
 C    2.638725     2.801143     0.515425
 C    4.498197     1.771195    -0.335412
 C    5.152444     2.995923    -0.350195
 C    4.443830     4.101789     0.131179
 C   -1.511342     0.593087     1.733990
 C   -1.188376    -0.544281     2.507365
 C   -2.228391    -1.388828     2.879118
 C   -3.561132    -1.103386     2.539879
 C   -3.855967     0.053849     1.807461
 C   -2.837372     0.915684     1.394536
 C    0.656003    -1.436984    -0.749768
 C    0.567854    -3.525225    -1.691451
 C   -0.551122    -2.850569    -2.029264
 C    2.638729    -2.801141    -0.515422
 C    4.498199    -1.771190     0.335416
 C    5.152448    -2.995918     0.350202
 C    4.443835    -4.101785    -0.131171
 C   -1.511338    -0.593091    -1.733995
 C   -1.188372     0.544278    -2.507368
 C   -2.228387     1.388826    -2.879120
 C   -3.561128     1.103386    -2.539879
 C   -3.855963    -0.053850    -1.807463
 C   -2.837369    -0.915687    -1.394541
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 H    6.168191     3.084858    -0.717003
 H    4.891807     5.090889     0.172380
 H   -2.035103    -2.271801     3.479704
 H   -4.878450     0.296207     1.544285
 H    0.926747    -4.514631    -1.926105
 H   -1.385737    -3.135486    -2.648018
 H    4.967789    -0.864613     0.699538
 H    6.168195    -3.084850     0.717010
 H    4.891814    -5.090884    -0.172370
 H   -2.035098     2.271800    -3.479704
 H   -4.878446    -0.296208    -1.544287
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 H   -6.092506     1.711534    -1.663975
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 H   -6.388865    -2.586766     3.191468
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 C     0.210830     0.848746    -2.992631
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 H     0.172620     1.437757    -3.912697
 C    -3.195743    -2.163943    -0.620249
 H    -4.161012    -2.041781    -0.125636
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 H    -2.458090    -2.395505     0.152970
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 N     3.457624    -1.483449    -1.019381
 N     3.131882    -3.454388    -2.334969
 N     1.379572     1.953926     1.921796
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 N     3.131882     3.454387     2.334966
 C     0.921654    -0.857747    -1.258735
 C    -0.592346    -1.539566    -2.785079
 C     0.447375    -2.406658    -2.853863
 C     2.720668    -2.347596    -1.756473
 C     4.748646    -1.824218    -0.832378
 C     5.284138    -2.976502    -1.397554
 C     4.424585    -3.772050    -2.161549
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 C    -0.993476     3.027279    -1.281949
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 C    -3.077469     1.824845    -1.272734
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 C     2.720668     2.347595     1.756470
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 C     5.284140     2.976497     1.397556
 C     4.424586     3.772047     2.161548
 C    -1.013419    -0.639877     1.597844
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 C    -0.993482    -3.027279     1.281955
 C    -2.381177    -3.031205     1.150351
 C    -3.077473    -1.824842     1.272731
 C    -2.404178    -0.618657     1.481159
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 H     0.630045    -3.274108    -3.469557
 H     5.346209    -1.154501    -0.223588
 H     6.325662    -3.240231    -1.251650
 H     4.765742    -4.683823    -2.644146
 H    -2.959343    -0.312294    -1.534053
 H     0.630043     3.274111     3.469550
 H    -1.507709     1.487548     3.355077
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 H     0.763393    -1.859567     1.703814
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 C    -0.173745     4.286237    -1.114079
 C    -4.581256    -1.807248     1.078923
 C    -0.173752    -4.286239     1.114090
 F    -5.167242     0.869612    -1.844838
 F    -4.866780     1.514564     0.221003
 F    -5.135834     2.997196    -1.357575
 F    -0.922998     5.389549    -1.024006
 F     0.569991     4.195062     0.037331
 F     0.710412     4.441068    -2.122567
 F    -5.167245    -0.869603     1.844828
 F    -4.866782    -1.514565    -0.221010
 F    -5.135840    -2.997189     1.357576
 F    -0.923006    -5.389550     1.024026
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 H    -3.983442     3.502467     0.213624
 H    -3.983442     2.179940    -0.977185
 N    -0.980880     2.497446     0.000000

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 N    -2.863058     0.626556     0.794011
 N    -3.770810    -1.206091     2.022269
 N     2.050899    -0.523843    -1.748957
 N     0.089369    -1.425458    -1.847322
 N     2.933971     1.316675    -0.585014
 N     4.333329    -0.086066    -1.914293
 C    -0.263661    -0.585423     1.285144
 C     0.039667    -2.394548     2.604692
 C    -1.289037    -2.150765     2.567095
 C    -2.777986    -0.496699     1.493015
 C    -4.106154     1.104314     0.621446
 C    -5.231482     0.459055     1.128382
 C    -5.004598    -0.723320     1.835113
 C     2.082934    -1.354284     1.640609
 C     2.807889    -0.353470     2.283967
 C     4.197890    -0.335712     2.156059
 C     4.871532    -1.303174     1.394824
 C     4.110669    -2.297930     0.755769
 C     2.723101    -2.334441     0.879769
 C     6.376122    -1.302898     1.284341
 C     0.771484    -0.415969    -1.266234
 C     2.150346    -1.604671    -2.628117
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 C     3.171036     0.284324    -1.388181
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 C    -2.994201    -3.208461    -0.779534
 C    -1.647732    -2.895838    -0.954496
 C    -5.458367    -2.754043    -1.131860
 H     0.616449    -3.140514     3.129487
 H    -2.125891    -2.641215     3.035042
 H    -4.183947     2.040029     0.075548
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 H     6.811793    -2.045548     1.964715
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 H     0.543511    -3.000039    -3.260770
 H     3.821360     2.896502     0.411071
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 H     6.341498     0.380092    -2.030009
 H    -1.999796     0.004940    -2.714927
 H    -4.392322    -0.572416    -2.405977
 H    -3.265404    -4.108245    -0.233722
 H    -0.871781    -3.539792    -0.549675
 H    -5.652270    -3.175635    -0.139508
 H    -5.745073    -3.516446    -1.867231
 H    -6.118179    -1.893185    -1.277802
 N    -0.485122     2.416320     1.430318
 C    -0.921026     3.314426     2.011405
 C    -1.498912     4.452162     2.710506
 H    -0.711584     5.147383     3.019773
 H    -2.189110     4.965746     2.031945
 H    -2.045017     4.112841     3.596858
 C    -0.633308     2.735831    -1.630933
 C     0.574027     2.789573    -1.772488
 H     1.624524     2.876190    -1.947392
 C    -2.071060     2.996213    -1.562420
 O    -2.590157     3.636825    -0.675592
 O    -2.706929     2.462311    -2.615847
 H    -3.640037     2.756219    -2.605969

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 N     2.685611     0.897218    -0.645565
 N     3.265930     0.552449    -2.934865
 N    -1.581034    -1.708696     1.351262
 N     0.464443    -2.201672     0.845311
 N    -2.817971     0.293146     1.510940
 N    -3.820685    -1.821886     1.972863
 C    -0.038806     0.343628    -1.437254
 C    -0.688994    -0.043439    -3.560767
 C     0.648836     0.147611    -3.588502
 C     2.416921     0.628260    -1.917110
 C     3.981973     1.088274    -0.357561
 C     4.973648     1.044119    -1.337499
 C     4.555105     0.772270    -2.639080
 C    -2.496328     0.028698    -1.854183
 C    -3.203066     1.236200    -1.748418
 C    -4.572841     1.161500    -1.470739
 C    -5.230615    -0.062378    -1.304419
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C	-4.482910	-1.241576	-1.428357
C	-3.116255	-1.225669	-1.722834
C	-6.715578	-0.119602	-1.043015
C	-0.399711	-1.163042	0.911469
C	-1.434554	-3.083617	1.559017
C	-0.154974	-3.384899	1.244556
C	-2.814337	-1.031442	1.616181
C	-3.988665	0.893398	1.781138
C	-5.115997	0.177966	2.178231
C	-4.975127	-1.207949	2.263816
C	1.883999	-2.138117	0.555946
C	2.756038	-1.863493	1.621341
C	4.126780	-1.846067	1.341766
C	4.626247	-2.127863	0.064273
C	3.715953	-2.434805	-0.956049
C	2.335418	-2.460885	-0.733507
C	6.112730	-2.150584	-0.196502
H	-1.399281	-0.243116	-4.348317
H	1.364810	0.138866	-4.393371
H	4.215683	1.270733	0.686616
H	6.018570	1.204816	-1.096589
H	5.254544	0.720493	-3.469454
H	-5.142451	2.085381	-1.396855
H	-4.981461	-2.201196	-1.313878
H	-6.974691	-0.949791	-0.376912
H	-7.264884	-0.275663	-1.980197
H	-7.086271	0.809740	-0.598973
H	-2.255133	-3.686545	1.910542
H	0.386686	-4.317823	1.274968
H	-4.005610	1.975524	1.682035
H	-6.053642	0.671663	2.407617
H	-5.797606	-1.849846	2.568643
H	4.820059	-1.624382	2.149496
H	4.089657	-2.676136	-1.948501
H	6.344530	-1.891987	-1.235046
H	6.519107	-3.153524	-0.013598
H	6.649496	-1.459560	0.461930
N	0.306243	2.829613	0.082390
C	0.511779	3.958390	-0.053064
C	0.767331	5.382915	-0.210888
H	1.026557	5.815637	0.761309
H	1.596013	5.540746	-0.909202
H	-0.126353	5.883217	-0.598905
C	1.391570	-2.885487	-1.832419
H	1.898534	-2.890579	-2.800992
H	1.014557	-3.900989	-1.655746
H	0.520039	-2.233304	-1.909554
C	2.256784	-1.687257	3.034369
H	1.372304	-1.048445	3.088633
H	1.984499	-2.659130	3.466705
H	3.027675	-1.242764	3.666544
C	-2.536087	2.580624	-1.909810
H	-2.107091	2.912540	-0.957457
H	-1.724795	2.558654	-2.644592
H	-3.260814	3.333953	-2.231823
C	-2.358548	-2.517415	-1.913512
H	-1.932065	-2.591593	-2.920762
H	-1.528522	-2.613365	-1.208701
H	-3.017510	-3.377558	-1.770750
C	0.822411	1.625207	2.783202
C	-0.312507	1.267527	3.037809
H	-1.301902	0.982957	3.327403
C	2.212381	2.077708	2.712362
O	3.161777	1.330309	2.747541
O	2.280340	3.418115	2.623578
H	3.221668	3.679407	2.686460

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HF=-1911.7638918 Hartree
NImag=0
 N                -1.39251000   -0.96806300   -2.54475800
 N                 0.67075700   -0.34868300   -2.52307000
 N                -2.75117300   -1.14716300   -0.68481700
 N                -3.56962500   -1.79209500   -2.83175400
 N                 1.84344800   -0.13829900    1.26758400
 N                 0.99414200    1.83648800    1.04260100
 N                 0.87043600   -2.26227400    1.12262100
 N                 3.20070300   -2.01040300    1.57947200
 C                -0.39875700   -0.50485300   -1.72347600
 C                 0.35071200   -0.70533400   -3.84096100
 C                -0.94745700   -1.09620700   -3.85779500
 C                -2.64844200   -1.32214500   -2.01770200
 C                -3.91699200   -1.51218800   -0.11908600
 C                -4.95593400   -2.02517100   -0.88999400
 C                -4.73611800   -2.14293200   -2.26426700
 C                 2.00510900    0.03730100   -2.12143000
 C                 2.92443900   -0.96242200   -1.80117200
 C                 4.22712800   -0.60080900   -1.45899900
 C                 4.62899700    0.74507800   -1.44361700
 C                 3.68074300    1.72581000   -1.77718100
 C                 2.37241300    1.38249000   -2.12197800
 C                 6.05176100    1.12135000   -1.11162800
 C                 0.73431300    0.52820500    0.84034400
 C                 2.80735700    0.76252600    1.72425600
 C                 2.27150500    1.99762800    1.58801600
 C                 1.98164300   -1.55666100    1.31857700
 C                 1.00682700   -3.59703600    1.17593300
 C                 2.23679300   -4.20000400    1.43605000
 C                 3.32265700   -3.34460800    1.64379700
 C                 0.06622000    2.91727200    0.83284700
 C                -0.20160800    3.78682700    1.89444300
 C                -1.11853200    4.82339800    1.71404300
 C                -1.78192900    5.00830000    0.48823500
 C                -1.49612100    4.11457600   -0.55739600
 C                -0.57437200    3.07836900   -0.39720700
 C                -2.74136300    6.15599100    0.29457100
 H                 1.08692600   -0.64463400   -4.62810000
 H                -1.59289700   -1.44956400   -4.64708600
 H                -3.99227300   -1.39606000    0.95503900
 H                -5.89437600   -2.32168700   -0.43543500
 H                -5.49926700   -2.52834400   -2.93477100
 H                 2.62261900   -2.00615500   -1.82176000
 H                 4.94348600   -1.37642200   -1.20302600
 H                 3.97070700    2.77326400   -1.77953500
 H                 1.65536700    2.14901000   -2.39944600
 H                 6.12043000    2.14058400   -0.71860900
 H                 6.67889700    1.07563800   -2.01133300
 H                 6.48856500    0.43658900   -0.37725100
 H                 3.76318900    0.42447800    2.08953100
 H                 2.67155400    2.97551800    1.80629400
 H                 0.09975200   -4.17673200    1.02290400
 H                 2.34411000   -5.27802600    1.48634500
 H                 4.31564600   -3.72643400    1.86651600
 H                 0.28836200    3.64663800    2.85423100
 H                -1.32359800    5.49766700    2.54136400
 H                -1.98916500    4.24072900   -1.51780000
 H                -0.35444300    2.40624300   -1.21844300
 H                -3.45411900    5.95716200   -0.51161700
 H                -2.19319400    7.07007100    0.03179300
 H                -3.30481400    6.36782800    1.20905000
 C                -2.05351600    0.67811500    2.06123300
 C                -1.78653300   -0.47075000    2.39199700
 H                -2.29958400    1.71513900    1.92706500
 Pd               -0.97900100   -0.30103600    0.20033100
 C                -1.70125300   -1.84523300    2.90437300
 O                -2.22352500   -2.77742000    2.33357100
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 O                -1.00403400   -1.89314900    4.03970800
 H                -1.01878200   -2.80813400    4.38854600

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(CN,C)-I1f.xyz
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HF=-2069.048655 Hartree
NImag=0
 N                 0.35153300    2.70381700   -1.20007300
 N                -1.40727600    1.53428200   -1.64757000
 N                 1.55929900    2.51361100    0.76174600
 N                 2.00625500    4.30470300   -0.75121500
 N                -1.49396200   -1.71453400    0.53527900
 N                 0.35481400   -2.07582300   -0.53530400
 N                -2.12321800   -0.11915200    2.14958400
 N                -3.57534100   -1.91877200    1.55231500
 C                -0.35068100    1.59026300   -0.81736600
 C                -1.35192000    2.59209800   -2.56853000
 C                -0.24893700    3.32863400   -2.29217400
 C                 1.37426800    3.21133000   -0.37798400
 C                 2.47608600    2.99885800    1.61837600
 C                 3.18630500    4.15990400    1.33049700
 C                 2.92144200    4.78251000    0.10803800
 C                -2.62036000    0.76037300   -1.44574500
 C                -3.52704700    1.26521600   -0.49313100
 C                -4.73721500    0.58634200   -0.33315700
 C                -5.05041900   -0.55658900   -1.08156400
 C                -4.12890900   -0.99744500   -2.03835400
 C                -2.90858800   -0.34554800   -2.25747300
 C                -6.34051000   -1.30376000   -0.85560400
 C                -0.27827300   -1.16956100    0.24655100
 C                -1.63296200   -2.95293400   -0.09989400
 C                -0.47434900   -3.17663400   -0.76128000
 C                -2.46000300   -1.20529000    1.45907100
 C                -3.04672600    0.31867500    3.02184300
 C                -4.26408200   -0.33351600    3.20565100
 C                -4.47924200   -1.47949400    2.43706200
 C                 1.78167100   -2.10500200   -0.82430100
 C                 2.57523800   -2.90665500    0.02278600
 C                 3.94155000   -2.99583000   -0.26017800
 C                 4.52208600   -2.32096200   -1.34275900
 C                 3.69436100   -1.52943700   -2.14891200
 C                 2.31678600   -1.41436500   -1.92203900
 C                 5.99304800   -2.47619700   -1.64697000
 H                -2.12429500    2.71943400   -3.31194200
 H                 0.16086900    4.22413900   -2.73319700
 H                 2.62317400    2.44220700    2.53745000
 H                 3.91613000    4.55730600    2.02679300
 H                 3.44380500    5.68439700   -0.19924300
 H                -5.45960800    0.96694700    0.38449500
 H                -4.37457700   -1.86071300   -2.65275900
 H                -6.76756900   -1.66339700   -1.79738600
 H                -7.08967100   -0.67995600   -0.35848600
 H                -6.16251900   -2.18445800   -0.22383100
 H                -2.53237900   -3.53631200    0.00540100
 H                -0.14307200   -4.01499100   -1.35476800
 H                -2.78985800    1.21161100    3.58642900
 H                -4.99893900    0.02113600    3.92001200
 H                -5.39177000   -2.06339200    2.52430800
 H                 4.56952500   -3.60068700    0.38897000
 H                 4.12645600   -1.00192800   -2.99658200
 H                 6.37910800   -1.63723500   -2.23493100
 H                 6.16587100   -3.38934900   -2.23089000
 H                 6.58815000   -2.56455000   -0.73161300
 C                 1.08596800   -0.25196100    2.81347800
 C                 2.14110900   -0.27901000    2.18962200
 H                 0.22976900   -0.30951400    3.45728600
 Pd                0.52115200    0.61461800    0.72471400
 C                 3.54132300   -0.46087800    1.77975800
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 O                  4.28832400   -1.17741700    2.39585300
 O                  3.84060100    0.26818800    0.69330200
 H                  4.74857800    0.03975200    0.40975800
 C                  1.99516400   -3.66603500    1.19426900
 H                  1.23309700   -3.08833200    1.72795300
 H                  1.52374700   -4.60138300    0.86824900
 H                  2.77968000   -3.92564600    1.90955700
 C                  1.47203200   -0.61420800   -2.88069500
 H                  0.60762800   -0.16612100   -2.39374600
 H                  2.06024800    0.18447500   -3.34311300
 H                  1.09660400   -1.25071600   -3.69156200
 C                 -1.97443400   -0.84312600   -3.33367000
 H                 -1.37029000   -0.04305900   -3.77014500
 H                 -1.28581600   -1.59677200   -2.93614100
 H                 -2.54061500   -1.31401000   -4.14235700
 C                 -3.22500100    2.51133200    0.30574700
 H                 -3.02082000    3.36958300   -0.34592600
 H                 -4.07265400    2.77840400    0.94206700
 H                 -2.34978500    2.37101800    0.95063400

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TS1a.xyz
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HF=-2340.663539 Hartree
NImag=1
 Pd                -0.62184600    0.98874700   -0.04288700
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 N                 -3.40264400    0.92463000   -1.67375500
 N                 -0.36767300    3.10093300   -0.35705300
 N                 -1.41112800    4.93604400   -1.47594200
 N                 -1.71963700   -1.64528000    1.01148600
 N                 -0.24115300   -1.96967800   -0.52919700
 N                 -2.62744800    0.28594800    2.00656200
 N                 -3.27279700   -1.89726100    2.72335700
 C                 -2.26356300    1.45386600   -1.19439500
 C                 -4.17830000    1.90105700   -2.31908500
 C                 -3.50257100    3.07284400   -2.24113600
 C                 -1.32699700    3.66710300   -1.12103000
 C                  0.59988000    3.91775300    0.09575900
 C                  0.60344600    5.27282800   -0.22154100
 C                 -0.43856900    5.74269300   -1.02433300
 C                 -3.81643500   -0.44263800   -1.48459800
 C                 -4.81938000   -0.72344100   -0.55579500
 C                 -5.20829700   -2.04768300   -0.35497100
 C                 -4.61116500   -3.09815700   -1.07073400
 C                 -3.61050500   -2.78208900   -2.00287600
 C                 -3.21234100   -1.46195500   -2.21879200
 C                 -5.05746900   -4.52415300   -0.85944900
 C                 -0.90224000   -0.98996200    0.13533000
 C                 -1.56686000   -3.02907000    0.89014700
 C                 -0.64181100   -3.23063700   -0.07270000
 C                 -2.59030600   -1.04164300    1.96891600
 C                 -3.45403600    0.81758600    2.91826100
 C                 -4.22351400    0.03109000    3.77404100
 C                 -4.09067600   -1.35192800    3.63274400
 C                  0.78658100   -1.77502700   -1.51096700
 C                  1.96090700   -2.52642300   -1.42084400
 C                  2.97494000   -2.33518600   -2.35954200
 C                  2.85080700   -1.39130800   -3.38998200
 C                  1.66097300   -0.64860900   -3.45805500
 C                  0.62922700   -0.84240200   -2.53954600
 C                  3.94053900   -1.21102400   -4.41868800
 H                 -5.12529100    1.65466200   -2.77468600
 H                 -3.72379800    4.06565700   -2.60013500
 H                  1.35483500    3.45787300    0.72258000
 H                  1.38047600    5.93357800    0.14557400
 H                 -0.50782400    6.78706500   -1.31663100
 H                 -5.27601400    0.08286200    0.01115100
 H                 -5.98424300   -2.26913100    0.37307900
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 H                -3.14071900   -3.57764100   -2.57527300
 H                -2.44668400   -1.22673700   -2.95144200
 H                -5.29101400   -4.71893400    0.19290100
 H                -4.29372100   -5.23919800   -1.18139600
 H                -5.96673700   -4.73332200   -1.43745500
 H                -2.14375100   -3.71140500    1.49114300
 H                -0.25718300   -4.14003500   -0.50658600
 H                -3.49189700    1.90392000    2.95553800
 H                -4.88712800    0.46833800    4.51191100
 H                -4.64772900   -2.04623100    4.25670900
 H                 2.09215800   -3.23719800   -0.61044900
 H                 3.88228400   -2.92881300   -2.28965500
 H                 1.52996800    0.08018400   -4.25405300
 H                -0.28793200   -0.27114100   -2.61881800
 H                 4.01006200   -0.17115600   -4.75498200
 H                 3.73982700   -1.82634900   -5.30517000
 H                 4.91823500   -1.51302000   -4.02870300
 C                 1.03663500    0.70084500    1.19905800
 C                 2.20311500    0.30235100    0.75632300
 H                 2.55557500    0.03831600   -0.23134200
 C                 3.61504300    0.02778400    1.95025900
 C                 4.57955000    0.93245800    1.35659000
 C                 3.76013500   -1.40961900    1.81355000
 C                 5.49898600    0.42494500    0.44678200
 C                 4.71345100   -1.90411300    0.93122500
 C                 5.52535700   -0.98227600    0.20509900
 H                 3.16972600    0.35968300    2.88685600
 C                 0.67233400    0.92448200    2.61137900
 O                 0.35128300    0.05336400    3.39554500
 O                 0.69184800    2.24394600    2.93813000
 H                 0.40337500    2.32812000    3.86887100
 C                 2.82495200   -2.28611400    2.59972900
 H                 3.37892200   -2.84684300    3.36469700
 H                 2.04995100   -1.70031500    3.09844500
 H                 2.32986300   -3.02406600    1.95828900
 C                 4.91830000   -3.39396200    0.75968300
 H                 5.98032900   -3.65578600    0.80389200
 H                 4.41543000   -3.96545100    1.54079500
 H                 4.53811700   -3.75275600   -0.20493700
 C                 6.48664700   -1.50803100   -0.82673600
 H                 7.49208900   -1.60606000   -0.39045100
 H                 6.20294200   -2.49065800   -1.20436100
 H                 6.57844700   -0.82750700   -1.67713300
 C                 6.48192300    1.32776200   -0.26666200
 H                 6.52443800    2.32141200    0.18131800
 H                 7.49667800    0.91817800   -0.23781700
 H                 6.21464700    1.45547000   -1.32413000
 C                 4.47597400    2.39197400    1.70497700
 H                 5.36305400    2.71829400    2.26373600
 H                 4.41400300    3.01982200    0.80871800
 H                 3.59746500    2.58839700    2.32581200

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HF=-2497.943271 Hartree
NImag=1
 Pd               -0.45526900    0.63397800    0.63817600
 N                -2.69323400    0.85172100    2.44314300
 N                -3.22595200   -0.90706600    1.32607900
 N                -0.59978400    1.84429300    2.42910700
 N                -2.29189600    2.61247100    3.93276300
 N                -0.55256500   -1.52963700   -1.57793400
 N                -1.26900300    0.41701700   -2.19336800
 N                 0.67163600   -2.29682100    0.28510500
 N                 0.20809400   -3.72522900   -1.57036700
 C                -2.25425700    0.01978500    1.44423200
 C                -4.27115900   -0.64829800    2.22826300
 C                -3.94108900    0.46090100    2.93111800
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C	-1.83739000	1.83453000	2.96868900
C	0.26582000	2.73420200	2.94460100
C	-0.10658600	3.59175400	3.97568200
C	-1.42017600	3.50040300	4.43672000
C	-3.09751100	-2.16637600	0.62205500
C	-2.34499400	-3.16995600	1.26343800
C	-2.24006100	-4.40861700	0.62755700
C	-2.85261900	-4.66074800	-0.60792500
C	-3.61863700	-3.64465500	-1.18761200
C	-3.77361600	-2.38809200	-0.58539700
C	-2.67788900	-5.98811100	-1.30313700
C	-0.70766600	-0.23788300	-1.14751200
C	-1.06396900	-1.67975600	-2.87554200
C	-1.50632000	-0.46146400	-3.25444800
C	0.13798600	-2.57473400	-0.90193900
C	1.31968700	-3.30673000	0.88188900
C	1.44427300	-4.56532000	0.29710500
C	0.86399700	-4.72003500	-0.96404000
C	-1.32089100	1.86206600	-2.33925300
C	-0.30150400	2.44736600	-3.11620100
C	-0.32005100	3.83507300	-3.27830300
C	-1.30310200	4.63912100	-2.68636200
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O	2.30321600	3.13280800	-1.38241100
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C	0.25487200	5.65532200	0.69793300
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C	-2.50094000	-0.15042300	-0.46557800
H	-2.29074100	-0.47210400	-1.48558500
C	-3.92302100	-0.27389800	-0.01161000
C	-4.30652600	-1.30749300	0.86943000
C	-4.86917200	0.66143100	-0.48122100
C	-5.65068400	-1.39064100	1.28883200
C	-6.20648100	0.57679500	-0.05250300
C	-6.60237600	-0.47223600	0.80298100
C	-1.75797800	0.89698200	1.62356300
O	-2.06923300	2.05455600	1.86132800
O	-1.52322400	0.00582400	2.62516100
H	-1.72358700	0.45811500	3.46773300
C	-3.30788400	-2.34810300	1.33985500
H	-2.34765200	-2.24529100	0.83671900
H	-3.11216700	-2.26618800	2.41571800
H	-3.67485300	-3.36373900	1.14837700
C	-6.08512800	-2.46989400	2.26330100
H	-6.59438600	-3.29936800	1.75137000
H	-5.24365000	-2.89813500	2.81085200
H	-6.78476700	-2.07713800	3.00851600
C	-8.05899900	-0.61245900	1.20321300
H	-8.33699800	-1.65737800	1.36441400
H	-8.27829500	-0.07195400	2.13579200
H	-8.73240500	-0.22021700	0.43703700
C	-7.22479000	1.61230000	-0.49271700
H	-7.86189200	1.23899000	-1.30750700
H	-7.88948400	1.89318100	0.33065200
H	-6.75468900	2.53215600	-0.84650600
C	-4.44573100	1.76212000	-1.43650600
H	-3.44142100	1.59123100	-1.83165500
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HF=-2497.6528012 Hartree

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N	0.09095200	-2.38767500	0.08808500
N	1.40307400	-1.53541200	1.57889300
N	-0.57256900	-1.70969200	-2.06527800
N	-1.38923800	-3.73270200	-1.09890600
C	1.75679700	1.61556200	-1.06328000
C	3.32797900	2.57669200	-2.40647800
C	2.36623800	3.50934300	-2.23715600
C	0.23149400	3.50691100	-0.96026600
C	-1.68998900	3.24593200	0.25968100
C	-1.97268800	4.59586600	0.06331900
C	-1.07884700	5.33158600	-0.71158800
C	3.81144400	0.28333000	-1.65128400
C	3.56606100	-0.77224000	-2.54114600
C	4.51455100	-1.80025300	-2.59766400
C	5.68583500	-1.76832200	-1.83027500
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C	4.96658400	0.35766300	-0.85736000
C	6.68214300	-2.90098800	-1.89426800
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C	0.35801000	-3.40520000	1.00889400
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C	-1.31811800	-1.94242900	-3.15256100
C	-2.14143700	-3.06124600	-3.26847700
C	-2.12530100	-3.95205000	-2.19423900
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C	2.23954200	0.31908700	3.02465300
C	3.34589400	0.95380600	3.60600500
C	4.65512500	0.50655300	3.40672400
C	4.85077200	-0.61558600	2.59466100
C	3.78787900	-1.27194600	1.96825700
C	5.82828900	1.22799800	4.02537000
H	4.25138000	2.59758200	-2.96418800
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H	-2.32372200	2.59561200	0.85159900
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H	-1.24246000	6.38352700	-0.93069100
H	4.34639400	-2.63130700	-3.27923200
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H	6.43958400	-3.67123900	-1.14893500
H	7.70010400	-2.55450800	-1.68684400
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H	1.63699000	-3.29855600	2.81105500
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H	-2.74766200	-3.23824200	-4.14996900
H	-2.71421800	-4.86597400	-2.20135700
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H	5.86020500	-0.98746000	2.43329500
H	6.22651800	1.98355300	3.33399100
H	6.64578300	0.53827100	4.26140400
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C	-1.77952600	0.07771400	0.52672800
C	-2.75536700	-0.08027500	-0.38109000
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C	-4.22236100	-0.22423800	-0.11453200
C	-4.76036000	-1.36334800	0.52410800
C	-5.07369200	0.81907700	-0.54769300
C	-6.15137600	-1.43782200	0.74994000
C	-6.45863800	0.73889000	-0.31398100
C	-7.00005400	-0.40578500	0.30649300
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 H                  5.35562200    2.46019700   -0.49029700
 H                  4.35268300    1.67960500    0.73864600
 C                  2.35164300   -0.76637600   -3.43537900
 H                  1.42728500   -0.74592500   -2.85084900
 H                  2.34998000    0.11579400   -4.08909400
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 C                  0.85041800    0.80343000    3.34436500
 H                  0.41986500    1.37518800    2.51451400
 H                  0.17911700   -0.03592000    3.53384700
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 C                  4.05779200   -2.47615600    1.09648200
 H                  5.12705900   -2.56868200    0.89905600
 H                  3.73067100   -3.40846400    1.56945600
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 H                 -8.83144600   -1.57156000    0.41181200
 C                 -6.75022500   -2.63763900    1.46049400
 H                 -6.00956000   -3.19283400    2.03844600
 H                 -7.53864800   -2.33589100    2.15761200
 H                 -7.20346700   -3.34526600    0.75094000
 C                 -3.88954800   -2.54169100    0.91104800
 H                 -4.26146500   -3.46795700    0.45509900
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 N                 -0.37991900   -1.71638600    2.45830000
 N                 -1.68568200   -2.76274400    4.16573100
 N                 -0.63861500    0.15905100   -2.29891500
 N                 -1.73898400    1.61524800   -1.14306000
 N                 -0.33480600   -2.16467000   -2.14876000
 N                  1.02907200   -0.83070800   -3.59121500
 C                 -2.57050500   -1.30251300    0.99924500
 C                 -4.72150900   -1.85281800    1.45674600
 C                 -3.99458400   -2.23931100    2.53091900
 C                 -1.53436800   -2.14105500    3.01091700
 C                  0.74575000   -1.98956900    3.14296300
 C                  0.69776900   -2.65767200    4.36472700
 C                 -0.55774500   -3.01585200    4.84989200
 C                 -4.24999300   -0.82289200   -0.76609900
 C                 -3.55279500   -1.23673500   -1.90247900
 C                 -3.96772500   -0.78269300   -3.15289700
 C                 -5.08793600    0.05326900   -3.29534300
 C                 -5.77788900    0.43578100   -2.13601200
 C                 -5.36246700    0.01097800   -0.87241100
 C                 -5.54793000    0.49692300   -4.66341900
 C                 -1.10123500    0.42154300   -1.04173900
 C                 -0.95211600    1.19970000   -3.17205900
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C	-3.98743800	3.59904800	1.87388000
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C	-3.71641700	2.84735000	-0.42952500
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H	-5.77400900	-1.94936300	1.24147500
H	-4.26281500	-2.72528400	3.45515200
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H	1.61004100	-2.88548400	4.90382300
H	-0.68048400	-3.52480900	5.80217600
H	-2.69140600	-1.88906000	-1.80402200
H	-3.41978300	-1.09903000	-4.03743700
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H	-0.63851900	1.18424800	-4.20310100
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H	-4.45570600	5.38467800	2.99071900
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C	1.95633500	0.87589400	-0.45759800
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C	2.98233900	1.94032000	-0.38659500
C	2.63644100	3.25147800	0.00427200
C	4.31416800	1.59122300	-0.69680700
C	3.65142600	4.22121400	0.10841000
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C	4.98253700	3.88649900	-0.21616000
C	1.59083800	0.83745500	1.95809600
O	0.78053100	1.37551700	2.69756900
O	2.86402900	0.60031700	2.34227300
H	2.99211000	0.99907500	3.22463600
C	2.95366700	-2.79684600	0.41715700
O	3.30156500	-2.59899800	1.56939300
O	2.06781800	-2.16416700	-0.28730100
H	1.66548800	-1.08384200	0.24861300
C	3.58904700	-3.95575100	-0.40914400
F	4.51688100	-4.62248000	0.28196100
F	2.62982600	-4.84417200	-0.78960800
F	4.16424200	-3.47823900	-1.54043500
C	1.18722800	3.63877900	0.23083800
H	0.50619400	2.87431500	-0.14433400
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C	3.31609900	5.62827000	0.56633000
H	2.37961700	5.66629900	1.12692400
H	4.09462800	6.03001300	1.22226400
H	3.21839000	6.32223900	-0.28102100
C	6.05834100	4.95463300	-0.18020700
H	5.65675500	5.94374000	-0.41446300
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 C                 -2.21077100   -1.62605200    1.03056400
 C                 -4.14332700   -2.76788500    1.39033800
 C                 -3.26117600   -3.23877000    2.29676100
 C                 -0.86574900   -2.73997800    2.72278700
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 C                  1.50375200   -3.17498400    3.84703200
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 C                 -4.16088800   -1.68338100   -1.72317800
 C                 -5.02904300   -1.16305200   -2.68913600
 C                 -5.97263800   -0.17489100   -2.37903000
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C	5.69725600	2.42226600	-0.74990600
C	5.54897800	3.71745900	-0.21118200
C	1.98531000	0.68655200	2.10631000
O	1.22224600	0.79152800	3.05408400
O	3.32618800	0.74435600	2.27397500
H	3.49915200	0.93527800	3.21551400
C	3.33584500	-2.59908600	0.13271500
O	3.90498500	-2.34614200	1.18023400
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F	4.87206500	-4.41185100	-0.23770100
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H	-3.54430300	1.51415300	-2.42894600
C	-3.24873200	-2.84506000	-2.02666800
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H	-2.21670600	-2.62218600	-1.74597800
H	-3.56429300	-3.73992200	-1.47336100
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H	-5.99052200	1.15861600	1.42324200
H	-5.52283100	-0.42995500	2.04702500
H	-4.28552400	0.77450200	1.67476400
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C	6.72173900	4.67879700	-0.22765900
H	6.39296900	5.71914000	-0.29049400
H	7.33774500	4.58585200	0.67868100
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C	7.05876200	1.95673800	-1.23168900
H	7.86245100	2.35880400	-0.60808900
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C	3.35889700	-1.59321200	-0.86838300
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