10.1071/CH19323_AC

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Supplementary Material

Carbon Dioxide Activation by a Palladium Terminal Imido Complex

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Content:

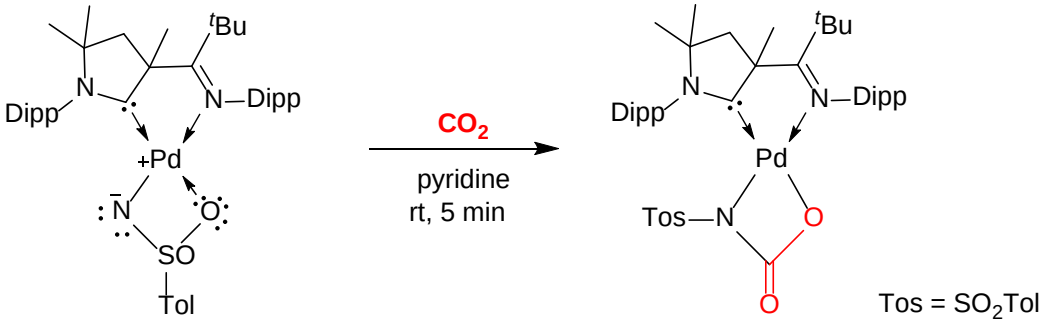
1. General Experimental Details

^{1}H and ^{13}C NMR spectra were recorded on a JEOL ECX 400 or a JEOL ECX 270 instrument operating at 400.18 and 269.71 MHz for ^{1}H and at 100.62 and 67.82 MHz for ^{13}C, respectively at a probe temperature of 23 °C. The chemical shifts δ are calculated in ppm in relation to the applied magnetic field. The solvent residual signals were used as internal reference for the ^{1}H NMR spectra and the solvent signals for ^{13}C NMR spectral data. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, q = quartet, spt = septet, m = multiplet, br = broad signal. All coupling constants *J* are given in Hz.

Infrared (IR) spectra were recorded on a Shimadzu Affinity-1 CE FTIR instrument. Elemental analysis was obtained using Euro EA 3000 (Euro Vector) and EA 1108 (Carlo-Erba) elemental analyzers. Melting points were determined using a Bibby Scientific SMP10 melting point apparatus. Solvents were purified using a two-column solid-state purification system (Glass Contour System, Irvine, CA) and stored over activated molecular sieves. NMR solvents were obtained dry and packaged under argon and stored over activated molecular sieves or a mirror of potassium (C_6D_6). Carbon dioxide used was of 99.8+% grade from Sigma Aldrich, stored in a pressurized gas container. The sulfonimido complex **1** and the bisamido complex **3** were synthesized as reported in the literature.[1] All other reagents were obtained from commercial sources and used as is without further purification.

2. Synthesis and Characterization

Palladium(II) Carbamate Complex **2**



1 **2**

30 mg (0.036 mmol) of **1** were dissolved in pyridine (0.5 mL). CO_2 was introduced by the vessel being frozen, evacuated, filled with CO_2, thawed, and repeated 3 times (3 freeze-pump-thaw cycles). ^{1}H NMR spectroscopic analysis indicated quantitative conversion to **2** within less than 2 minutes. The product was isolated by condensing Et_2O into a solution of **2** in pyridine at –40 °C. The pale yellow solid was dried and gave a yield of 62% (22 mg, 0.026 mmol).

^{1}H NMR (pyridine-D_5, 270 MHz) δ = 8.65 (d, J = 6.3 Hz, 2 H), 8.06 - 8.13 (m, 2 H), 7.50 (d, J = 5.5 Hz, 1 H), 7.25 - 7.41 (m, 3 H), 7.16 - 7.24 (m, 3 H), 7.14 (d, J = 5.5 Hz, 2 H), 6.87 - 6.93 (m, 1 H), 3.38 - 3.49 (m, 1 H), 3.16 - 3.27 (m, 1 H), 2.97 - 3.06 (m, 2 H), 2.81 (dd, J = 13.2, 5.2 Hz, 2 H), 2.33 (d, J = 7.1 Hz, 3 H), 1.98 (d, J = 4.4 Hz, 3 H), 1.79 (t, J = 6.6 Hz, 3 H), 1.67 (t, J = 6.6 Hz, 3 H), 1.47 (d, J = 6.0 Hz, 3 H), 1.24 - 1.37 (m, 21 H), 1.17 (dt, J = 19.0, 6.7 Hz, 3 H), 1.05 (d, J = 7.1 Hz, 6 H) ppm.

^{13}C NMR (pyridine-D_5, 68 MHz) δ = 217.5 (**C** carbene), 192.9 (**C** imine), 165.3 (**C** carboxylate) 145.4 (Ar**C**), 144.8 (Ar**C**), 144.3 (Ar**C**), 138.8 (Ar**C**), 130.7 (Ar**C**), 130.2 (Ar**C**), 126.1 (Ar**C**), 127.9 (Ar**C**), 124.8 (Ar**C**), 80.2 (**C**q), 77.9 (**C**q), 45.1 (**C**H_2), 42.5 (**C**H_2), 30.1 (**C**$(CH_3)_3$), 29.8 (**C**$(CH_3)_3$), 29.0 (**C**H_3/**C**H), 23.6 (**C**H_3/**C**H), 23.5 (**C**H_3/**C**H), 23.2 (**C**H_3/**C**H), 22.3 (**C**H_3/**C**H), 20.9 (**C**H_3/**C**H) ppm.

EA $C_{44}H_{61}N_3O_4PdS$: Calc.: C 63.32, H 7.37, N 5.02, S 3.84; Found: C 62.94, H 7.38, N 4.58, S 3.76%.

m.p. decomposition at 189 °C.

IR: 1677 cm^{-1} (CO stretch)

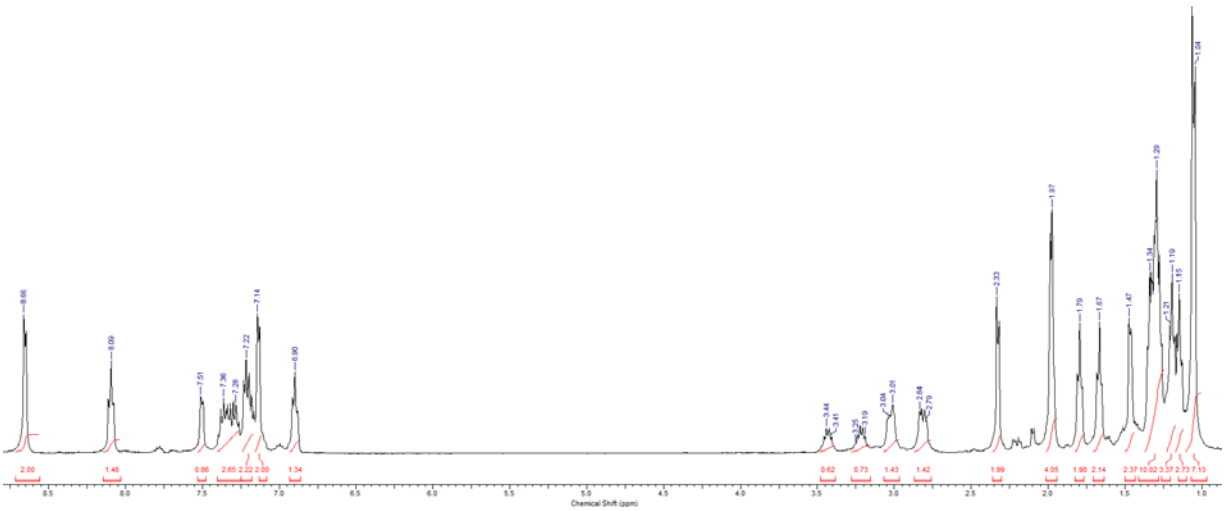


Figure S1. ^{1}H NMR spectrum of **2** (pyridine-D_5, 270 MHz).

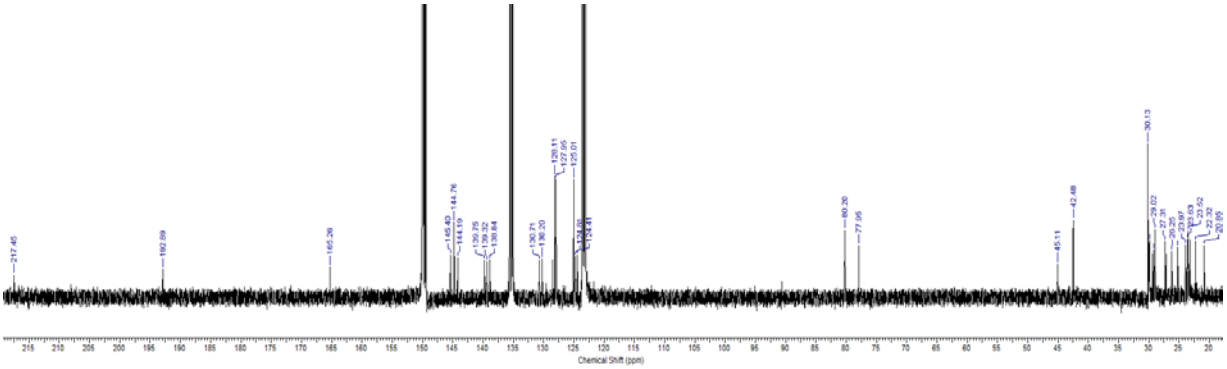
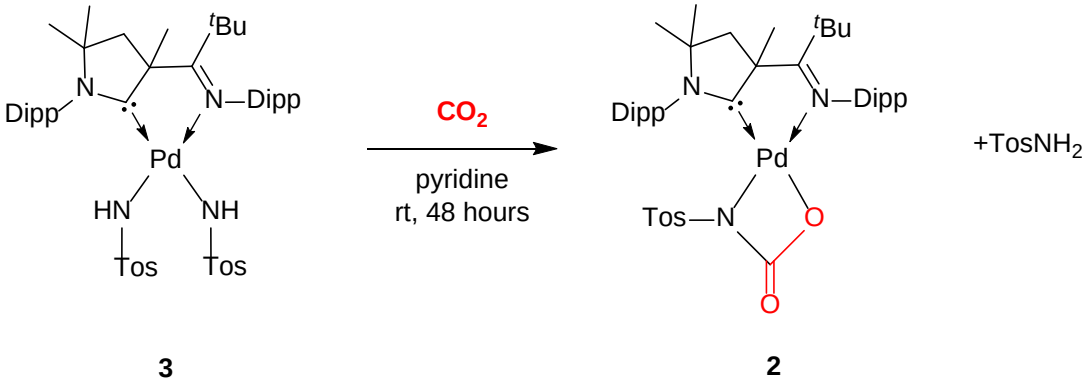


Figure S2. ^{13}C NMR spectrum of **2** (pyridine-D_5, 68 MHz).

<u>Palladium(II) Bisamido Complex **3** + CO_2</u>



3 **2**

30 mg (0.032 mmol) of **3** were suspended in pyridine (0.5 mL). CO_2 was introduced by the vessel being frozen, evacuated, filled with CO_2, thawed, and repeated 3 times (3 freeze-pump-thaw cycles). ^{1}H and ^{13}C NMR spectroscopic analysis indicated a quantitative conversion to a stoichiometric mixture of **2** and tosyl amine after 48 hours.

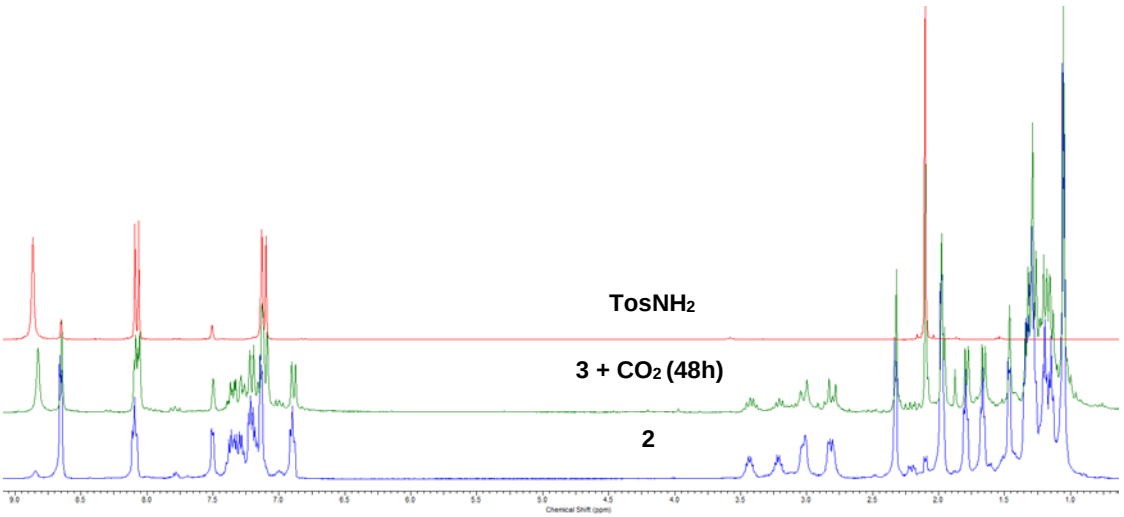


Figure S3. Comparison of the ^{1}H NMR spectra of **2**, the reaction of **3** + CO_2, and $TosNH_2$ (pyridine-D_5, 270 MHz).

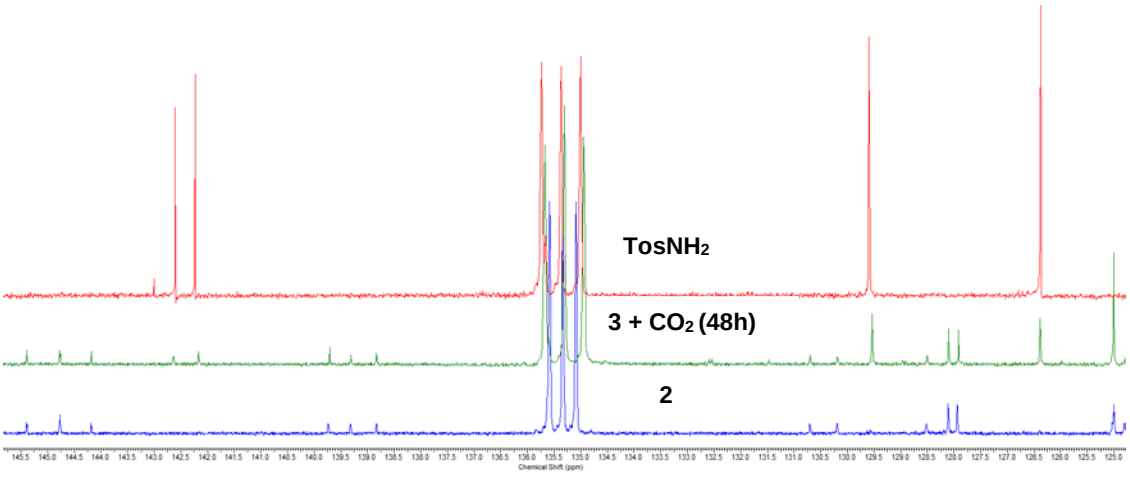


Figure S4. Comparison of the ^{13}C NMR spectra of **2**, the reaction of **3** + CO_2, and $TosNH_2$ (pyridine-D_5, 68 MHz).

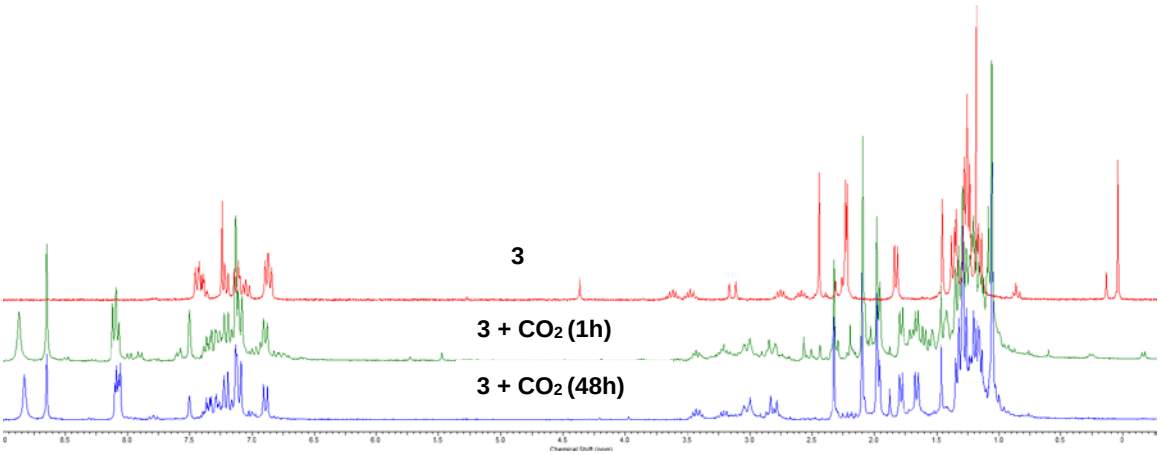


Figure S5. Comparison of the ^{1}H NMR spectra of **3**, the mixture obtained after 1 hour, and the final spectrum of the reaction of **3** + CO_2 after 48 hours (pyridine-D_5, 270 MHz).

As seen in **Fig. S5**, the reaction shows essentially quantitative conversion of 3 after 1 hour. Additionally observable are the peaks for tosyl amine (**Fig. S3**), indicating abstraction of tosyl amine and complexation of CO_2, leading to the formation of the palladacarbamate product **2**. Full conversion of the product can be observed in the ^{1}H NMR spectrum labelled "48h" (**Fig. S5**) which shows the quantitative conversion of the starting material to a mixture of product and tosyl amine after the course of 48 hours.

4. Solid State Structure

CCDC-1939836 (for **2**) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK (fax: ++44-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

Single crystals of **2** were obtained by vapor diffusion of diethyl ether into a saturated solution of pyridine. The crystals were obtained as colorless blocks. The crystal was measured at 100 K on a Bruker Kappa Photon2 *IμS* Duo diffractometer equipped with QUAZAR focusing Montel optics using Mo*K*α radiation (λ = 0.71073 Å). The structure was solved by direct methods (SHELX XT 2014/5)[2] and refined by full-matrix least-squares procedures on F^2 using SHELXL 2018/3.[3] OLEX2 was used to prepare material for publication.[4] The compound crystallized with a total of three molecules of pyridine per formula unit, all of which were disordered. Two alternative orientations were refined for two of these solvent molecules and resulted in site occupancies of 91.4(8) and 8.6(8) % for the atoms N100 – C105 and N110 – C115 and of 46.7(8) and 53.3(8) % for the atoms N200 – C205 and N210 – C215, respectively. For the third pyridine three orientations were refined and resulted in site occupancies of 42(2), 12.6(3), and 44.9(2) % for the atoms N300 – C305, N310 – C315, and N320 – C325, respectively. Similarity and pseudo-isotropic restraints were applied to the anisotropic displacement parameters of the disordered atoms.

Treatment of hydrogen atoms: All hydrogen atoms were placed in positions of optimized geometry. The isotropic displacement parameters of all hydrogen atoms were tied to those of their corresponding carrier atoms by a factor of 1.2 or 1.5.

Identification code	**2**
Empirical formula	$C_{59}H_{76}N_6O_4PdS$
Formula weight	1071.71
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.1677(7)
b/Å	20.2170(10)
c/Å	21.9331(10)
α/°	90
β/°	105.324(2)
γ/°	90
Volume/Å^3	5631.3(5)

Z	4
ρ_{calc}g/cm^3	1.264
μ/mm^{-1}	0.417
F(000)	2264.0
Crystal size/mm^3	0.18 × 0.15 × 0.13
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.788 to 59.178
Index ranges	-18 ≤ h ≤ 18, -28 ≤ k ≤ 28, -22 ≤ l ≤ 30
Reflections collected	89428
Independent reflections	15781 [R_{int} = 0.0450, R_{sigma} = 0.0337]
Data/restraints/parameters	15781/1021/876
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0372, wR_2 = 0.0828
Final R indexes [all data]	R_1 = 0.0548, wR_2 = 0.0933
Largest diff. peak/hole / e Å^{-3}	0.77/-0.80

Table S1. Details of solid state structure determination.

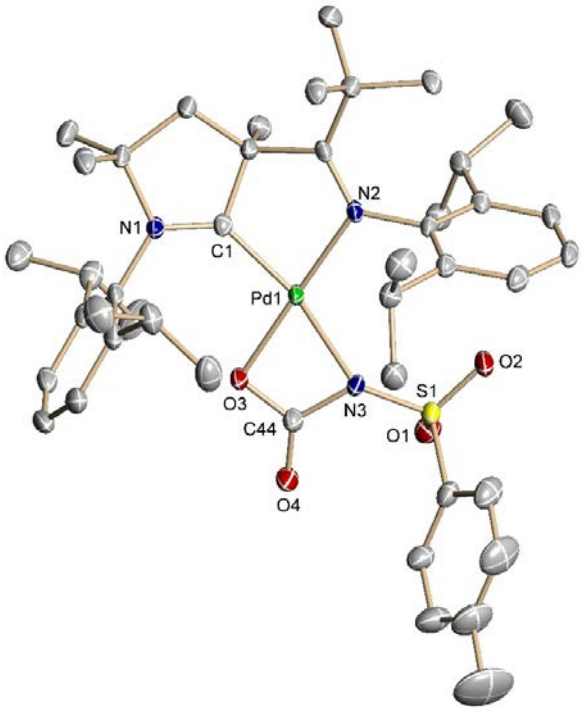


Figure S6. Thermal ellipsoid representation of **2** (50% probability level, hydrogen atoms and solvent molecules omitted for clarity)

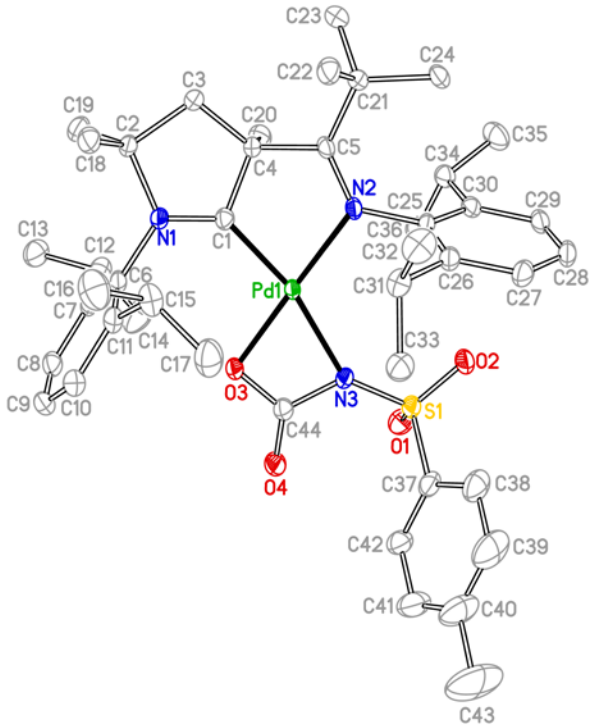


Figure S7. Thermal ellipsoid representation of **2** with the applied numbering scheme (50% probability level, hydrogen atoms and solvent molecules omitted for clarity).

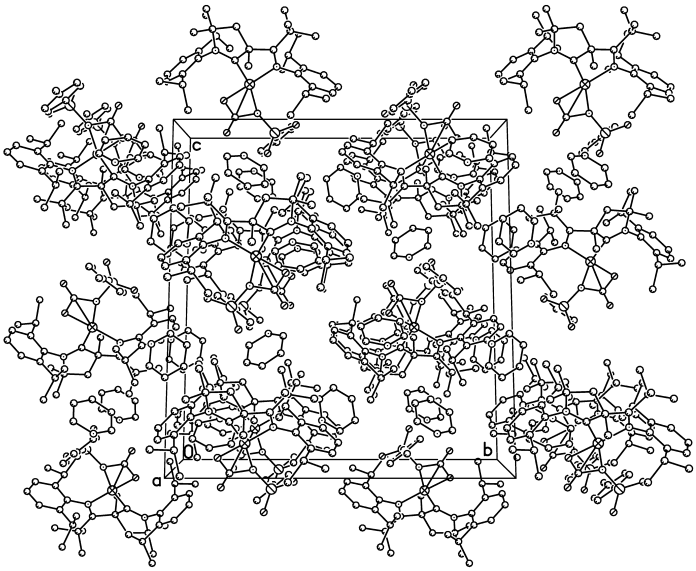


Figure S8. Packing diagram of **2** viewed along the crystallographic *a* axis.

Computational Details

All DFT calculations were performed using ORCA 4.0.1.[5] All geometry optimizations were performed at the PBE0-D3(BJ)/def2-SVP level of theory[6] using the def2 quasi relativistic effective core potential (28 core electrons) and the related def2-SVP valence basis set for palladium,[7] and applying the D3 dispersion correction[8] with Becke-Johnson damping.[9] We chose the PBE0 functional, because it shows excellent performance for organometallic chemistry with palladium and ligand substitution reactions.[10] Tighter than default convergence criteria (tightopt) were chosen for both the optimization of the structural parameters as well as the scf (tightscf) and a more accurate than default grid value of 6 (FinalGrid7, Gridx6) were used. The RIJCOSX approximation in conjunction with the related def2/J auxiliary basis[11] set was used to speed up the calculations.[12] All structures were verified to be true minima by the absence of negative eigenvalues in the harmonic vibrational frequency analysis. The energies of all structures were corrected by single-point calculations at the PBE0-D3BJ/def2-TZVPP level of theory.[6b] Implicit correction for solvent effects was conducted by the SMD solvation model within the framework of the CPCM module (solvent: PYRIDINE).[13]

Denominator	**Imag [cm^{-1}]**	***E* in [H]**	***G* in [H]**	***E*(TZVPP) in [H]**
1	-	-2472.92473	-2472.06253	-2475.26364
2	-	-2661.2098	-2660.33384	-2663.77007
3	-	-3308.1117	-3307.12542	-3311.13172
1^{CO2}	-	-2661.17125	-2660.29812	-2663.73557
ts1_1^{CO2}	-141	-2661.17103	-2660.29779	-2663.73393
ts1-2	-191	-2661.13617	-2660.2722	-2663.69435
ts1^{CO2}-2	-46	-2661.16345	-2660.28683	-2663.72777
ts2-2^{CO2}	-127	-3496.35561	-3495.35691	-3499.58317
CO_2	-	-188.24434	-188.254519	-188.468628
TosNH_2	-	-835.117131	-835.022457	-835.82264

Table S2. Energies and imaginary frequencies of calculated structures.

XYZ Coordinates

CO_2

O	3.31236	5.80258	10.78084
C	3.45104	6.53098	11.67201
O	3.58972	7.25938	12.56317

$TosNH_2$

S	2.38624	4.17703	9.61632
O	1.93984	5.13030	8.60961
O	3.38351	3.15101	9.34472
N	2.95083	5.05754	10.91692
C	0.94174	3.36548	10.25598
C	1.08282	2.13156	10.88673
H	2.07043	1.67177	10.95655
C	-0.05163	1.50528	11.39547
H	0.03989	0.53640	11.89106
C	-1.30250	2.10964	11.26483
C	-1.42783	3.33846	10.61707
H	-2.41069	3.80157	10.50462
C	-0.30084	3.97529	10.10322
H	-0.37145	4.92723	9.57381
H	-2.18983	1.61357	11.66479
H	3.89583	4.76594	11.15594
H	2.88291	6.05551	10.73133

1

Pd	6.17702	5.43358	8.29904
S	6.52269	5.30151	10.87842
O	7.33304	4.52548	9.78420
O	6.08780	4.44319	11.98127
N	5.47715	6.10173	10.05453
N	6.87992	4.56589	6.53097
N	3.80108	6.76174	7.08220
C	8.25793	7.45317	10.84772
C	9.22787	8.28434	11.39866
C	9.69481	8.05181	12.69416
C	9.19065	6.98476	13.43587
C	8.22370	6.14311	12.88630
C	7.76639	6.38170	11.59301
C	9.66619	6.28646	7.51940
C	10.93471	5.47354	5.49942
C	9.62641	5.39120	6.27949
C	5.83633	1.64412	8.98294
C	5.68469	0.69317	6.65634
C	6.07888	1.90946	7.49600
C	9.23774	3.97811	6.67094
C	10.21600	3.03643	6.98605
C	9.87731	1.75542	7.41059
C	8.54118	1.41057	7.55076
C	7.51864	2.31774	7.25624

C	7.88474	3.58662	6.77576
C	7.79535	3.40620	3.90479
C	6.56493	5.27935	2.89991
C	5.32268	3.31324	3.85711
C	6.52765	4.25955	4.04672
C	6.42711	7.41001	5.42006
C	3.01038	8.53481	5.50211
C	1.80336	6.38234	5.64180
C	2.88852	3.81454	9.60051
C	0.86416	4.11105	8.13919
C	2.25643	4.64362	8.47888
C	5.40871	9.37001	9.49483
C	3.78863	10.74290	8.13177
C	4.31419	9.33893	8.42429
C	2.25605	6.10597	8.88143
C	1.47347	6.49359	9.97223
C	1.53534	7.78123	10.48561
C	2.42863	8.69585	9.94439
C	3.23498	8.36345	8.85342
C	3.08812	7.07829	8.29595
C	6.35387	4.93707	5.41641
C	5.48163	6.19683	5.58982
C	4.18066	6.36982	4.78944
C	3.17321	7.03781	5.74423
C	5.00152	6.24747	7.03435
H	7.86623	7.63581	9.84557
H	9.61593	9.12504	10.81816
H	9.55118	6.80555	14.45177
H	7.80630	5.30121	13.44145
H	10.44449	5.94531	8.21888
H	9.87990	7.33270	7.24717
H	8.71318	6.25223	8.06685
H	10.94039	4.79486	4.63221
H	11.09291	6.49934	5.13288
H	8.83737	5.78104	5.61661
H	6.11140	2.51361	9.59507
H	4.77781	1.40397	9.16256
H	6.43478	0.78639	9.32822
H	6.24025	-0.20328	6.97367
H	4.61222	0.47302	6.77585
H	5.88842	0.83804	5.58443
H	5.43525	2.75536	7.20195
H	8.27618	0.41551	7.91537
H	7.82895	3.02777	2.87161
H	8.70857	3.98998	4.07629
H	7.81170	2.54326	4.57941
H	6.59104	4.73342	1.94515
H	5.69181	5.94072	2.87069
H	7.47330	5.89866	2.94502
H	5.20826	2.63964	4.71679
H	4.37435	3.84343	3.70546

H	5.49451	2.69381	2.96354
H	7.25528	7.34938	6.13874
H	6.83318	7.45295	4.40111
H	5.88652	8.34667	5.61048
H	2.35150	8.97574	6.26221
H	3.96330	9.07786	5.51501
H	2.54278	8.68952	4.51886
H	1.39139	6.57316	4.63984
H	1.86464	5.29632	5.78567
H	1.10590	6.79643	6.38355
H	2.25676	3.83653	10.50221
H	2.98949	2.76340	9.29050
H	3.87494	4.21128	9.87801
H	0.36318	4.69663	7.35497
H	0.92899	3.06595	7.79792
H	0.21009	4.11972	9.02474
H	2.89832	4.53314	7.59067
H	5.69428	8.34417	9.77567
H	6.29030	9.92281	9.13115
H	5.04854	9.87579	10.40486
H	3.37976	11.21337	9.03923
H	4.60610	11.38914	7.77597
H	2.99408	10.74813	7.37088
H	4.77712	8.94958	7.50709
H	0.82138	5.75688	10.44602
H	0.91350	8.06064	11.33926
H	2.52672	9.68531	10.39572
H	3.77900	5.39585	4.49062
H	4.30822	6.97171	3.88029
H	10.45141	8.71056	13.12773
H	11.80228	5.22223	6.12852
H	11.26864	3.31176	6.90303
H	10.66010	1.03323	7.65233

$\mathbf{1}^{CO2}$

Pd	6.07764	5.37486	8.66232
S	6.96544	5.67105	11.14270
O	7.53203	4.73889	10.04636
O	6.96497	5.11036	12.48043
N	5.60143	6.14368	10.47615
N	6.71545	4.45984	6.92678
N	3.75465	6.85232	7.35108
C	8.00537	8.04139	10.16779
C	8.93972	9.07304	10.15780
C	9.95069	9.11218	11.11978
C	10.02394	8.12275	12.09939
C	9.09478	7.08381	12.11663
C	8.09971	7.04923	11.14299
C	9.78088	5.92340	7.66532
C	10.76097	4.87987	5.58935
C	9.52742	4.98782	6.48144

C	5.49189	1.83656	9.55133
C	5.18006	0.71988	7.30868
C	5.71558	1.94932	8.04228
C	9.01521	3.64923	6.97790
C	9.91259	2.63517	7.31047
C	9.47476	1.42012	7.82775
C	8.11972	1.21261	8.04054
C	7.17635	2.19776	7.73491
C	7.63842	3.39946	7.17208
C	7.39309	3.11774	4.31349
C	6.44293	5.13994	3.29230
C	4.93916	3.40069	4.36581
C	6.27991	4.16296	4.46390
C	6.69081	7.29604	5.97479
C	3.63918	8.96143	6.01387
C	1.95772	7.21138	5.61149
C	2.45445	3.37658	8.32282
C	0.54407	4.31576	6.99125
C	1.91514	4.60973	7.60208
C	4.60020	9.21972	10.63005
C	3.03992	10.43277	9.09970
C	3.77971	9.11328	9.34358
C	1.89281	5.81478	8.52726
C	0.95790	5.84243	9.56075
C	0.93365	6.87832	10.48395
C	1.85220	7.91109	10.38743
C	2.81159	7.94501	9.37133
C	2.81048	6.88391	8.44649
C	6.23373	4.88718	5.81295
C	5.54370	6.25933	5.99226
C	4.38366	6.70358	5.08915
C	3.40662	7.45163	6.00678
C	4.91126	6.24965	7.38680
H	7.19235	8.00294	9.43961
H	8.87303	9.85854	9.40108
H	10.80660	8.16171	12.86073
H	9.12026	6.30415	12.88038
H	10.59817	5.53623	8.29301
H	10.06048	6.93261	7.32352
H	8.89878	6.00004	8.31569
H	10.60803	4.17513	4.75721
H	11.00671	5.86456	5.16312
H	8.73514	5.44044	5.86578
H	5.83859	2.73492	10.07900
H	4.42287	1.71532	9.77704
H	6.03033	0.96866	9.96355
H	5.66024	-0.20336	7.66907
H	4.09780	0.61458	7.47994
H	5.35226	0.77541	6.22216
H	5.14376	2.82224	7.69140
H	7.77734	0.26853	8.47002

H	7.30917	2.68658	3.30433
H	8.39253	3.56067	4.40587
H	7.31538	2.29819	5.03582
H	6.41942	4.57066	2.35149
H	5.65603	5.89818	3.23174
H	7.41685	5.65057	3.33924
H	4.84588	2.67725	5.18761
H	4.05651	4.05175	4.39343
H	4.91265	2.84468	3.41614
H	7.42766	7.07063	6.75562
H	7.19111	7.29566	4.99606
H	6.30290	8.30570	6.15496
H	2.91414	9.46046	6.66599
H	4.64377	9.24546	6.34810
H	3.49513	9.34630	4.99399
H	1.77029	7.72076	4.65488
H	1.73130	6.14835	5.47775
H	1.26766	7.62580	6.35958
H	1.76689	3.05704	9.12050
H	2.57182	2.54234	7.61233
H	3.40543	3.60240	8.81872
H	0.09698	5.19683	6.50768
H	0.62203	3.51106	6.24302
H	-0.16332	3.97209	7.76082
H	2.61358	4.82174	6.77768
H	5.09850	8.27076	10.86192
H	5.35138	10.02003	10.53088
H	3.95867	9.46777	11.48867
H	2.43825	10.69991	9.98188
H	3.75315	11.25438	8.92837
H	2.34816	10.39210	8.24526
H	4.48668	8.94397	8.51738
H	0.25592	5.01310	9.66521
H	0.21204	6.86502	11.30330
H	1.85300	8.70069	11.14048
H	3.86304	5.84371	4.65412
H	4.70861	7.34873	4.26300
H	10.67925	9.92657	11.11176
H	11.64619	4.54597	6.15162
H	10.98139	2.80219	7.16699
H	10.19670	0.64089	8.08156
C	4.25485	5.66455	11.25590
O	4.03544	6.37332	12.21158
O	3.74332	4.70847	10.69789

2

Pd	4.18424	5.49991	12.77462
S	2.59741	4.05854	10.07575
O	3.21731	4.58531	8.86260
O	3.02867	2.75082	10.57111
O	3.23834	7.10578	12.05754

O	1.82460	7.01556	10.31313
N	5.49889	7.46820	14.56930
N	5.00569	3.80741	13.66044
N	2.74948	5.10740	11.32488
C	5.40939	6.29148	14.01823
C	6.54885	7.58693	15.63931
C	6.98679	6.11529	15.79630
H	6.50772	5.70300	16.69027
H	8.07267	6.05200	15.94205
C	6.51183	5.38936	14.52295
C	5.93557	3.96205	14.54297
C	4.66794	8.58570	14.19596
C	5.09888	9.43311	13.15729
C	4.30853	10.54738	12.86610
H	4.61309	11.22093	12.06248
C	3.12570	10.79104	13.55084
H	2.52074	11.66580	13.30235
C	2.68517	9.89385	14.51459
H	1.72095	10.05698	15.00067
C	3.43504	8.76411	14.84902
C	6.29590	9.12972	12.27457
H	6.84151	8.28904	12.72324
C	7.26565	10.30396	12.15489
H	6.80627	11.14988	11.62103
H	8.15497	10.00532	11.57857
H	7.60162	10.67486	13.13489
C	5.83203	8.66244	10.89194
H	5.13334	7.81998	10.97392
H	6.69728	8.36254	10.28004
H	5.30442	9.46941	10.36015
C	2.83521	7.73708	15.79118
H	3.59613	6.96640	15.98659
C	2.41005	8.33292	17.13239
H	3.23342	8.86255	17.63375
H	2.05125	7.53948	17.80635
H	1.58404	9.04983	17.00780
C	1.66059	7.03167	15.10974
H	0.84216	7.73796	14.90116
H	1.26458	6.23316	15.75660
H	1.96641	6.59488	14.14953
C	7.68004	8.51653	15.21076
H	7.29223	9.52349	15.00508
H	8.21313	8.16256	14.31985
H	8.40709	8.59666	16.03167
C	5.94590	8.13021	16.92801
H	6.73294	8.18482	17.69427
H	5.14306	7.48596	17.30810
H	5.54323	9.14246	16.78048
C	7.61292	5.39363	13.43442
H	7.20816	5.05798	12.47105
H	8.44404	4.73778	13.72517

H	8.01072	6.40768	13.29867
C	6.45058	2.91529	15.54535
C	5.65998	3.16235	16.84898
H	5.86976	4.13330	17.31353
H	5.93059	2.38532	17.57995
H	4.57910	3.09587	16.66874
C	7.95593	3.07364	15.80420
H	8.53990	2.81220	14.90904
H	8.24983	2.37290	16.59908
H	8.24949	4.07607	16.13275
C	6.24406	1.43779	15.17923
H	5.19058	1.15004	15.10040
H	6.69960	0.83928	15.98313
H	6.74268	1.16740	14.24088
C	4.42264	2.56064	13.27744
C	3.15767	2.20773	13.77056
C	2.62923	0.97561	13.37355
H	1.65086	0.66980	13.75166
C	3.31729	0.14459	12.50247
C	4.54396	0.54641	11.98494
C	5.11749	1.76310	12.34385
C	2.34010	3.10747	14.67753
H	2.95032	3.99551	14.91579
C	1.96783	2.42149	15.99263
H	1.26692	1.58960	15.82263
H	1.47125	3.13287	16.67115
H	2.84435	2.00524	16.51205
C	1.08725	3.59431	13.94664
H	1.35334	4.13294	13.02609
H	0.49591	4.26439	14.58877
H	0.44375	2.74492	13.66941
C	6.42508	2.22400	11.72581
H	7.00924	2.72285	12.51884
C	7.29166	1.08184	11.20611
H	7.45874	0.30473	11.96866
H	8.27287	1.46771	10.89074
H	6.83958	0.60121	10.32521
C	6.17983	3.25177	10.61862
H	5.56468	2.82501	9.81502
H	7.13657	3.59480	10.19332
H	5.63053	4.13145	10.98585
C	0.84355	3.92996	9.77732
C	0.16093	2.84430	10.32285
H	0.71649	2.11246	10.91269
C	-1.20560	2.71532	10.08244
H	-1.75411	1.86748	10.50021
C	-1.86878	3.66120	9.30062
C	-1.16761	4.73622	8.75277
H	-1.68899	5.47394	8.13812
C	0.19841	4.87687	8.98419
H	0.76808	5.71667	8.58599

C	2.52671	6.47903	11.13337
H	-2.94045	3.55779	9.11251
H	2.88587	-0.81308	12.20290
H	5.05675	-0.09748	11.27009

3

Pd	5.56047	5.09678	8.61444
S	4.14593	3.80200	11.41434
S	7.58650	6.24073	10.44582
O	8.35397	6.50862	9.21233
O	7.96698	5.03147	11.18453
O	4.30848	5.16450	11.95623
O	4.64295	2.65078	12.16681
N	6.01054	6.37188	10.09725
N	4.67775	3.76028	9.90409
N	5.39648	3.77527	6.97815
N	5.92534	7.47268	6.81071
C	7.12936	8.79291	11.40138
C	7.41502	9.87481	12.23009
C	8.41701	9.77273	13.19559
C	9.12943	8.58199	13.34387
C	8.84738	7.49146	12.52437
C	7.85459	7.61347	11.55435
C	1.50259	4.61533	11.50439
C	0.13132	4.41368	11.34687
C	-0.35662	3.15376	11.00276
C	0.52666	2.08483	10.83283
C	1.89603	2.27772	10.99029
C	2.37495	3.54971	11.30599
C	7.52971	2.09064	9.30227
C	7.75003	0.26623	7.58595
C	7.06663	1.58938	7.93145
C	1.80912	4.29183	7.84234
C	1.54243	3.14805	5.60439
C	2.52172	3.59316	6.68773
C	5.55261	1.49903	7.83135
C	4.88514	0.36158	8.29496
C	3.50054	0.24903	8.21987
C	2.75235	1.28469	7.67416
C	3.36581	2.44970	7.20857
C	4.76598	2.53680	7.28608
C	5.66033	1.83503	4.67185
C	7.30144	3.43948	3.81752
C	4.83519	3.92941	3.66215
C	5.95195	3.33762	4.54728
C	8.17329	5.10143	6.44168
C	6.13819	8.92772	4.71776
C	4.33763	7.24170	4.95901
C	2.77116	7.28426	9.53711
C	2.02495	8.37958	7.41958
C	3.21951	7.76743	8.15788

C	9.10955	9.36481	8.39757
C	8.40745	10.71031	6.42505
C	8.06349	9.48973	7.28800
C	4.36564	8.75680	8.26356
C	4.12899	9.91485	9.01245
C	5.09874	10.89196	9.17555
C	6.34811	10.71076	8.60240
C	6.65092	9.57474	7.84636
C	5.63524	8.60222	7.66654
C	5.96313	4.12265	5.87388
C	6.72561	5.44594	6.00392
C	6.73028	6.46854	4.85320
C	5.78725	7.57759	5.30387
C	6.15008	6.23103	7.18161
H	4.82758	2.77978	9.67158
H	5.48332	6.07930	10.93894
H	6.34284	8.84281	10.64791
H	6.84616	10.80166	12.12103
H	9.90404	8.49802	14.11000
H	9.37167	6.53976	12.63008
H	1.91456	5.58460	11.78959
H	-0.56044	5.24521	11.50269
H	0.14261	1.09199	10.58474
H	2.59958	1.45050	10.87719
H	7.14576	1.44535	10.10811
H	8.62880	2.09025	9.35772
H	7.19529	3.11186	9.52717
H	7.39089	-0.15464	6.63343
H	8.83741	0.41575	7.50748
H	7.40109	2.32568	7.18338
H	2.53533	4.59999	8.60541
H	1.26301	5.17836	7.48398
H	1.08571	3.62135	8.33171
H	0.77283	2.47387	6.01060
H	1.01922	4.01838	5.17841
H	2.04830	2.61590	4.78366
H	3.20602	4.32995	6.23890
H	1.66446	1.20039	7.62845
H	5.77035	1.39404	3.66956
H	6.36883	1.32754	5.33656
H	4.64573	1.61711	5.02170
H	7.20404	2.94788	2.83826
H	7.63774	4.46638	3.63557
H	8.09084	2.91164	4.37210
H	3.86313	3.89481	4.17224
H	5.01885	4.96441	3.35281
H	4.75504	3.32034	2.74906
H	8.17337	4.38909	7.27635
H	8.74936	4.69832	5.59955
H	8.66323	6.00833	6.82036
H	5.56070	9.73468	5.19074

H	7.20480	9.15303	4.80936
H	5.88868	8.91604	3.64680
H	4.20814	7.22336	3.86696
H	4.04131	6.26241	5.36186
H	3.65512	7.99655	5.36624
H	2.46132	8.12702	10.17371
H	1.90625	6.61404	9.44015
H	3.56609	6.74203	10.06121
H	2.30075	8.83160	6.45554
H	1.25552	7.61443	7.23259
H	1.55772	9.17402	8.02195
H	3.56896	6.88510	7.60094
H	8.96751	8.44253	8.97155
H	10.11809	9.34566	7.95435
H	9.06373	10.22634	9.08186
H	8.57782	11.59522	7.05742
H	9.34189	10.53089	5.87070
H	7.62223	10.97385	5.70391
H	8.13252	8.57944	6.67247
H	3.15216	10.04650	9.48142
H	4.88496	11.78797	9.76285
H	7.12465	11.46277	8.75519
H	6.42918	6.07457	3.87923
H	7.74684	6.87336	4.74042
H	8.63813	10.62341	13.84503
H	-1.43150	2.99855	10.88125
H	7.58834	-0.49149	8.36789
H	5.46614	-0.45480	8.72688
H	3.00430	-0.64950	8.59344

ts1^{CO2}-2

Pd	6.21032	5.20352	8.63309
S	6.85520	6.24678	11.02361
O	7.59984	5.09816	10.35857
O	6.73850	6.17014	12.46876
N	5.48885	6.38326	10.16776
N	7.06042	4.00718	7.18893
N	4.20259	6.49024	6.81746
C	7.79549	8.26104	9.35336
C	8.53079	9.41583	9.10999
C	9.23012	10.03483	10.14811
C	9.18923	9.50008	11.43390
C	8.45392	8.34323	11.68870
C	7.76744	7.73177	10.64349
C	10.04292	5.63481	8.13786
C	11.25778	4.25835	6.41559
C	9.92114	4.51139	7.10811
C	5.39756	1.33942	9.83611
C	5.55595	0.42015	7.50186
C	5.89706	1.59910	8.41645
C	9.32017	3.27150	7.74303

C	10.15041	2.35185	8.38223
C	9.63557	1.21844	9.00154
C	8.26623	0.99780	8.99900
C	7.38259	1.89276	8.38845
C	7.92872	3.01670	7.74266
C	8.14085	2.28054	4.97722
C	7.60871	4.20895	3.54549
C	5.78039	2.67824	4.36481
C	7.10511	3.38626	4.73884
C	7.28608	6.67240	5.72361
C	4.33976	8.32109	5.11569
C	2.62899	6.57151	4.85000
C	2.56052	3.10823	8.18623
C	1.00589	4.01696	6.45597
C	2.29610	4.27898	7.23995
C	4.59616	9.45002	9.73334
C	3.27486	10.26693	7.77588
C	3.98318	9.05475	8.38865
C	2.24236	5.60447	7.98326
C	1.22900	5.77090	8.92843
C	1.09978	6.94505	9.65371
C	1.99432	7.98205	9.44547
C	3.03808	7.87548	8.52327
C	3.14635	6.67542	7.79154
C	6.80084	4.27287	5.95491
C	6.12530	5.65332	5.80094
C	5.06537	5.90267	4.71865
C	4.03366	6.84342	5.35972
C	5.34571	5.90886	7.08756
H	7.22449	7.77440	8.56085
H	8.55188	9.84215	8.10412
H	9.72727	9.98879	12.24922
H	8.38825	7.91244	12.68951
H	10.76095	5.35685	8.92465
H	10.39273	6.56808	7.66815
H	9.08586	5.82373	8.64062
H	11.20342	3.42382	5.69938
H	11.57280	5.15951	5.86712
H	9.22661	4.85204	6.32596
H	5.60117	2.19825	10.48751
H	4.30743	1.19269	9.82815
H	5.85319	0.43130	10.26157
H	6.01282	-0.51044	7.87514
H	4.46632	0.26463	7.46662
H	5.91272	0.56665	6.47147
H	5.36893	2.49116	8.04527
H	7.86092	0.11352	9.49477
H	8.26598	1.73533	4.02949
H	9.12071	2.67687	5.26571
H	7.83077	1.55922	5.74099
H	7.72280	3.54083	2.67891

H	6.92430	5.01278	3.24972
H	8.59665	4.64656	3.75365
H	5.29088	2.24491	5.24844
H	5.06415	3.33695	3.85987
H	6.00748	1.85604	3.66975
H	7.94544	6.56364	6.59319
H	7.87028	6.53020	4.80548
H	6.90062	7.69857	5.72060
H	3.54553	8.95264	5.52818
H	5.28820	8.64799	5.55699
H	4.38299	8.50274	4.03191
H	2.56256	6.90914	3.80531
H	2.37862	5.50645	4.87834
H	1.88075	7.12422	5.43592
H	1.68892	2.93199	8.83606
H	2.73134	2.18558	7.60804
H	3.41500	3.31119	8.84620
H	0.70411	4.86086	5.82042
H	1.11886	3.12494	5.81945
H	0.17189	3.81784	7.14596
H	3.13595	4.31892	6.52810
H	5.01709	8.56804	10.23108
H	5.38779	10.20132	9.58711
H	3.83806	9.89258	10.39756
H	2.54239	10.67934	8.48693
H	3.99702	11.06621	7.54549
H	2.72059	10.02685	6.85698
H	4.80832	8.74943	7.72774
H	0.53794	4.94623	9.11255
H	0.31329	7.04216	10.40470
H	1.90650	8.89297	10.03975
H	4.55213	4.97035	4.46150
H	5.47214	6.33221	3.79397
H	9.80340	10.94428	9.95348
H	12.05699	4.02887	7.13650
H	11.22721	2.52885	8.39724
H	10.30567	0.51119	9.49516
C	4.43071	5.38132	10.65894
O	3.57796	5.79594	11.40257
O	4.65027	4.26663	10.12003

ts1_2

Pd	3.21707	6.67774	12.45283
S	2.70049	5.67727	9.91947
O	2.88127	7.18005	10.11281
O	3.57931	5.06773	8.91394
O	0.79461	6.68911	12.41220
O	-0.05595	4.56108	12.06439
N	3.06335	8.96512	14.41677
N	5.06727	5.96761	13.19706
N	2.71728	5.04863	11.35700

C	3.72231	8.10747	13.68218
C	3.90212	9.80937	15.33431
C	5.23437	9.03594	15.29249
H	5.28464	8.40033	16.18151
H	6.08680	9.72679	15.32987
C	5.19944	8.18766	14.00462
C	5.74473	6.74045	13.97481
C	1.63024	9.08372	14.33687
C	1.05319	9.92096	13.36415
C	-0.34221	10.00267	13.32446
H	-0.81465	10.64189	12.57547
C	-1.13470	9.26960	14.19638
H	-2.22327	9.34549	14.14332
C	-0.54210	8.41302	15.11540
H	-1.17259	7.80600	15.76874
C	0.84622	8.29092	15.20002
C	1.85517	10.66658	12.31510
H	2.92068	10.52515	12.53830
C	1.56450	12.16692	12.32745
H	0.52842	12.37589	12.01898
H	2.22614	12.69099	11.62084
H	1.70505	12.61262	13.32376
C	1.61642	10.07119	10.92708
H	1.90624	9.01205	10.87888
H	2.21197	10.61102	10.17473
H	0.55674	10.15748	10.63804
C	1.42975	7.25405	16.14311
H	2.52103	7.38223	16.15877
C	0.91591	7.40970	17.57347
H	1.06404	8.42986	17.95669
H	1.43561	6.71029	18.24651
H	-0.15947	7.18493	17.64098
C	1.17290	5.84200	15.61868
H	0.09628	5.63902	15.50922
H	1.59162	5.09288	16.30846
H	1.64402	5.70094	14.63747
C	4.01328	11.23637	14.80167
H	3.02563	11.71611	14.77209
H	4.44857	11.28444	13.79639
H	4.65228	11.82333	15.47702
C	3.32529	9.87855	16.74180
H	3.95889	10.53685	17.35351
H	3.29426	8.89635	17.22793
H	2.30929	10.29938	16.73417
C	5.86209	8.92456	12.81556
H	5.66066	8.39674	11.87492
H	6.94681	9.00818	12.96013
H	5.45316	9.93893	12.72255
C	6.97042	6.34394	14.82190
C	6.44598	6.08552	16.25486
H	6.18073	6.99929	16.79857

H	7.23805	5.58734	16.83388
H	5.57148	5.42021	16.24443
C	8.02903	7.45488	14.84281
H	8.48376	7.58594	13.84937
H	8.83350	7.16317	15.53411
H	7.64482	8.42396	15.18099
C	7.70013	5.06063	14.40009
H	7.06815	4.16777	14.45393
H	8.54295	4.92172	15.09461
H	8.11013	5.12207	13.38632
C	5.44805	4.69754	12.67806
C	4.80982	3.53819	13.14683
C	5.13414	2.32042	12.54648
H	4.65517	1.40675	12.90562
C	6.02992	2.25767	11.48909
C	6.62839	3.42287	11.02289
C	6.36393	4.66283	11.60288
C	3.80770	3.57139	14.28029
H	3.61995	4.63202	14.51443
C	4.35746	2.89935	15.54029
H	4.52001	1.82332	15.37013
H	3.64565	2.99784	16.37591
H	5.32012	3.32710	15.85880
C	2.47774	2.94584	13.86391
H	2.13459	3.38579	12.91767
H	1.71321	3.10094	14.64127
H	2.58030	1.85827	13.72146
C	7.05344	5.90915	11.07533
H	7.13272	6.62089	11.91303
C	8.48284	5.64726	10.60395
H	9.08091	5.11422	11.35988
H	8.98535	6.60089	10.37983
H	8.50390	5.05161	9.67876
C	6.24235	6.58807	9.97310
H	6.08083	5.90656	9.12596
H	6.76726	7.48731	9.61111
H	5.23875	6.88520	10.30607
C	1.05940	5.51742	9.21883
C	0.66356	4.27655	8.71837
H	1.38650	3.45905	8.68286
C	-0.64397	4.10569	8.27363
H	-0.96300	3.13456	7.88716
C	-1.54673	5.16974	8.31829
C	-1.13560	6.41224	8.79929
H	-1.83629	7.25091	8.82158
C	0.17101	6.59150	9.25060
H	0.51649	7.55332	9.63185
C	0.50197	5.57233	12.16057
H	-2.57299	5.03045	7.96997
H	6.25788	1.29974	11.01654
H	7.32414	3.36635	10.18460

ts1_1^{CO2}

Pd	6.20243	5.42881	8.53705
S	7.05119	5.65737	11.02835
O	7.61956	4.73581	9.91509
O	6.99197	5.04737	12.34682
N	5.73346	6.19866	10.35139
N	6.86101	4.51730	6.80011
N	3.86766	6.86981	7.20939
C	8.25768	7.99916	10.19116
C	9.24211	8.98135	10.25491
C	10.21849	8.93020	11.25126
C	10.20648	7.89994	12.19097
C	9.22624	6.91069	12.13348
C	8.26556	6.96557	11.12645
C	9.88403	6.01269	7.60884
C	10.93011	5.01742	5.54347
C	9.67338	5.09116	6.40623
C	5.66464	1.84563	9.38393
C	5.35901	0.75314	7.12875
C	5.88286	1.97971	7.87547
C	9.17146	3.73653	6.86957
C	10.07654	2.72428	7.18634
C	9.64731	1.49181	7.66840
C	8.29294	1.26536	7.86481
C	7.34201	2.24824	7.57525
C	7.79557	3.46673	7.04269
C	7.63114	3.22691	4.17423
C	6.62661	5.22520	3.16427
C	5.17040	3.42220	4.19461
C	6.48018	4.23107	4.32411
C	6.77243	7.36770	5.83679
C	3.61976	8.92839	5.80970
C	2.04283	7.06896	5.47715
C	2.65285	3.45817	8.42158
C	0.68594	4.25660	7.07863
C	2.06261	4.62427	7.63315
C	4.83531	9.30120	10.33949
C	3.23742	10.54745	8.87192
C	3.95105	9.21105	9.09507
C	2.03401	5.88725	8.47658
C	1.10352	5.97999	9.51081
C	1.08393	7.07253	10.36662
C	2.00828	8.09297	10.20630
C	2.96252	8.06258	9.18500
C	2.94836	6.95026	8.32174
C	6.38931	4.94126	5.68056
C	5.66101	6.29252	5.85440
C	4.48894	6.69176	4.94528
C	3.47844	7.40870	5.85152
C	5.03438	6.28667	7.25101

H	7.46964	8.03248	9.43567
H	9.24107	9.79910	9.53002
H	10.96242	7.86803	12.97930
H	9.18378	6.10073	12.86410
H	10.68902	5.62752	8.25333
H	10.15952	7.02997	7.28835
H	8.98464	6.06891	8.23669
H	10.81210	4.32101	4.69868
H	11.16813	6.01210	5.13651
H	8.88802	5.54077	5.77906
H	6.00998	2.73977	9.92075
H	4.59856	1.70343	9.61187
H	6.21587	0.97972	9.78297
H	5.84311	-0.17021	7.48340
H	4.27640	0.63881	7.29320
H	5.53634	0.81855	6.04378
H	5.30225	2.85163	7.53580
H	7.95734	0.30765	8.26881
H	7.57368	2.80817	3.15793
H	8.61342	3.70293	4.28362
H	7.57407	2.39424	4.88325
H	6.63333	4.66509	2.21773
H	5.81706	5.95873	3.10038
H	7.58328	5.76555	3.22821
H	5.09489	2.68129	5.00230
H	4.26360	4.03918	4.22172
H	5.17641	2.88232	3.23526
H	7.51717	7.16586	6.61708
H	7.27126	7.38842	4.85770
H	6.34848	8.36229	6.02275
H	2.89389	9.40165	6.48071
H	4.62015	9.27903	6.08927
H	3.40890	9.27494	4.78767
H	1.82076	7.52802	4.50266
H	1.87877	5.98976	5.38583
H	1.33286	7.47110	6.21321
H	2.01871	3.20335	9.28372
H	2.73869	2.56949	7.77553
H	3.63200	3.72202	8.83726
H	0.20483	5.09472	6.55286
H	0.76909	3.41033	6.37859
H	0.00608	3.94134	7.88442
H	2.73510	4.79634	6.77880
H	5.34080	8.34656	10.53346
H	5.58296	10.10086	10.21175
H	4.23854	9.53613	11.23330
H	2.66739	10.83310	9.76906
H	3.96862	11.34876	8.68235
H	2.52532	10.52629	8.03344
H	4.61356	9.01760	8.23861
H	0.40206	5.15920	9.67055

H	0.36277	7.11371	11.18554
H	2.01655	8.92578	10.91134
H	4.00412	5.81205	4.50911
H	4.79470	7.34549	4.11861
H	10.98649	9.70595	11.30229
H	11.80672	4.69290	6.12451
H	11.14471	2.90548	7.05667
H	10.37524	0.71378	7.90836
C	4.26612	5.84812	11.30601
O	4.18302	6.68433	12.15788
O	3.73325	4.87616	10.84275

ts3_3^{CO2}

Pd	5.82612	4.79958	8.76103
S	3.88359	4.13450	11.48612
S	7.82421	6.00550	10.59651
O	8.68247	6.57413	9.55819
O	7.97523	4.58045	10.91066
O	4.60289	5.26061	12.12318
O	3.74216	2.88463	12.23722
N	6.21231	6.27966	10.16672
N	4.53630	3.84747	10.05216
N	5.97359	3.06963	7.56927
N	6.80175	6.49831	6.45657
C	8.99549	7.92749	12.13952
C	9.22850	8.58158	13.34583
C	8.52403	8.20806	14.48991
C	7.58505	7.17738	14.43618
C	7.34923	6.50301	13.24138
C	8.06030	6.89820	12.10802
C	2.00946	6.07567	10.92804
C	0.71904	6.49574	10.61078
C	-0.33011	5.57818	10.55470
C	-0.09671	4.22914	10.82587
C	1.18675	3.79499	11.14860
C	2.22652	4.72356	11.18712
C	6.87015	1.44614	11.34533
C	8.32836	0.97271	9.35456
C	7.03589	1.62871	9.83790
C	2.04566	3.10361	7.27079
C	2.81236	1.84623	5.23064
C	3.25197	2.52639	6.52696
C	5.80990	1.16503	9.07208
C	5.15002	-0.00585	9.45179
C	3.96351	-0.39969	8.84355
C	3.37925	0.41856	7.88547
C	3.99674	1.60083	7.46570
C	5.25660	1.91173	8.00644
C	6.76687	0.50490	6.07361
C	8.73119	1.79930	5.40019
C	6.48591	2.25296	4.35804

C	7.22143	1.91936	5.67453
C	8.91334	4.14945	7.59102
C	7.97546	7.29230	4.33358
C	6.03321	5.77179	4.23649
C	2.92760	6.47500	7.71474
C	2.89982	6.88582	5.25156
C	3.79622	6.68932	6.47703
C	8.96631	9.39715	8.43838
C	9.09860	9.85874	6.00880
C	8.47945	8.93228	7.06454
C	4.74725	7.85583	6.68156
C	4.16376	9.11158	6.86892
C	4.92786	10.24098	7.10731
C	6.30798	10.13064	7.16555
C	6.95971	8.91027	6.97528
C	6.15674	7.76839	6.72684
C	6.89330	3.06471	6.65945
C	7.71063	4.36315	6.63646
C	8.18436	4.98264	5.31154
C	7.26232	6.16601	5.04849
C	6.85844	5.46577	7.25943
H	4.34382	2.87312	9.82530
H	5.64082	5.92668	10.97143
H	9.51833	8.20523	11.22389
H	9.95850	9.39294	13.39021
H	7.02964	6.89210	15.33216
H	6.60645	5.70324	13.18515
H	2.84233	6.78292	10.94983
H	0.53651	7.55303	10.40449
H	-0.92088	3.51225	10.79464
H	1.39687	2.74958	11.38351
H	6.93074	0.38691	11.64390
H	7.67421	1.98944	11.86209
H	5.91186	1.85385	11.69690
H	8.55208	1.20950	8.30469
H	9.17603	1.32887	9.95941
H	7.12763	2.71334	9.68080
H	2.35638	3.61419	8.19289
H	1.50012	3.82133	6.63933
H	1.34343	2.30295	7.55019
H	2.04678	1.07873	5.42196
H	2.36963	2.58319	4.54269
H	3.64647	1.35165	4.71159
H	3.92304	3.36303	6.27123
H	2.41044	0.14569	7.46125
H	7.15333	-0.18437	5.30755
H	7.16908	0.18572	7.04067
H	5.67913	0.38887	6.10487
H	8.87455	1.06372	4.59529
H	9.21258	2.72901	5.07963
H	9.26689	1.42319	6.28325

H	5.41005	2.38741	4.52890
H	6.86282	3.14974	3.85534
H	6.61262	1.40793	3.66458
H	8.59646	3.74183	8.55845
H	9.65720	3.48663	7.13346
H	9.37599	5.12214	7.80516
H	7.34089	8.18587	4.26048
H	8.91712	7.55922	4.82365
H	8.20852	6.95854	3.31185
H	6.34447	5.46599	3.22708
H	5.47942	4.94217	4.69652
H	5.35253	6.62523	4.13316
H	2.41471	7.40234	8.00531
H	2.16259	5.71394	7.52185
H	3.52573	6.16613	8.57915
H	3.46030	7.14606	4.34202
H	2.32700	5.96688	5.04975
H	2.16959	7.69115	5.42413
H	4.38751	5.77414	6.32944
H	8.50716	8.81387	9.23871
H	10.06209	9.30030	8.49308
H	8.71568	10.45697	8.60139
H	8.88292	10.91005	6.25312
H	10.19462	9.75000	6.00550
H	8.73289	9.68376	4.98935
H	8.84766	7.90482	6.91987
H	3.07549	9.19295	6.85361
H	4.44617	11.20773	7.26874
H	6.90705	11.01594	7.38473
H	8.20077	4.30506	4.45499
H	9.21153	5.34902	5.45232
H	8.70501	8.72904	15.43325
H	-1.33866	5.91720	10.30504
H	8.28083	-0.12452	9.44933
H	5.56618	-0.60601	10.26252
H	3.46806	-1.32270	9.15248
C	5.65867	7.94641	10.07842
O	4.46879	7.89928	9.92054
O	6.57500	8.70295	10.23648

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