Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information for :

Double-Resonance ^{17}O NMR Experiments Reveal Unique Configurational Information for Surface Organometallic Complexes

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1. Experimental

1.1. Synthesis.

Air- and moisture-sensitive synthetic procedures were conducted using standard Schlenk line techniques or in a glovebox under nitrogen atmosphere. Solvents for air- and moisture-sensitive procedures were dried over activated alumina.. All reagents were used without further purification. Ir-POCOP was synthesized according to previous reported procedure.[1,2] All gases, including ultra-high purity ethylene, were purchased from Airgas.

1.1.1. ^{17}O-Enriched Silica.

Davisil silica gel, grade 646, 35-50 mesh, pore size 150 Å, was purchased from Aldrich. Approximately 300 mg of the silica gel was dried at 700 °C overnight under dynamic vacuum in a tube furnace. Following this, the tube was inserted into a wet box and 100 μL of 90% ^{17}O-enriched water (Cortecnet) was added to the tube. The mixture was left to react at room temperature for 6 hours. This procedure was repeated for a total of 5 times. Prior to grafting the sample was dried once more at 700 °C under dynamic vacuum.

1.1.2. Sc{κ^2-(NiPr)$_2$CH}$_2$/Si^{17}O$_2$.

The title compound was prepared in accordance with our earlier studies.[3,4] Briefly, in a glovebox, Sc{κ^2-(N*i*Pr)$_2$CH}$_3$ (50 mg) was dissolved into anhydrous pentane (3 mL) and added to a suspension of the Si^{17}O$_2$ support (100 mg). The mixture was stirred at room temperature for 4 h after which the supernatant was removed by decanting and the solid was washed with pentane (3 x 5 mL). The resulting solid was then dried overnight at room temperature under dynamic vacuum.

1.1.3. Ir(C$_2$H$_4$)(^{tBu4}POCOP)/Si^{17}O$_2$

To an oven-dried 20 mL glass scintillation vial in a glovebox under nitrogen atmosphere was added Ir(C$_2$H$_4$)(^{tBu4}POCOP) (10.0 mg, 0.013 mmol). In another oven-dried 20 mL glass scintillation vial was added 300 mg of Si^{17}O$_2$. To this was added 1 mL of toluene. 3 mL of toluene were used to rinse Ir(C$_2$H$_4$)(^{tBu4}POCOP) into the vial Si^{17}O$_2$. The reaction mixture was sealed with a Teflon cap and shaken on a shaker table (440 rpm) at room temperature for 1 h. It was then filtered on a disposable frit and washed with copious amounts of benzene then pentane, until the filtrate ran clear. The material was dried under reduced pressure to obtain a orange powder. Ir wt % = 2.08 ± 0.16 (by ICP-MS).

1.2. Solid State NMR Spectroscopy.

All solid-state NMR experiments were performed using a Bruker AVANCE III 400 MAS-DNP spectrometer equipped with a triple-resonance 3.2 mm low-temperature MAS probe and a 264 GHz gyrotron. Samples were impregnated with 16 mM solutions of TEKPol,[5] dissolved in dry 1,1,2,2-tetrachloroethane, in a glovebox and packed into 3.2 mm sapphire rotors. Rotors were inserted into a pre-cooled (100 K) NMR probe and spun to a frequency of 10 kHz.

Both the ^{13}C and ^{31}P-based experiments were performed using a ramped cross-polarization pulse sequence employing a 2 ms contact time. Dipolar recoupling was achieved using the REDOR pulse sequence[6] with the ^{13}C and ^{31}P inversion pulses lasting 8 and 10 μs respectively. For recoupling to

^{17}O a phase-modulated ^{17}O saturation pulse lasting 10 rotor periods (1 ms) was applied (i.e. PM-RESPDOR).[7,8] ^{13}C{^{17}O} PM-RESPDOR recoupling was incremented in 400 μs increments from 0 to 2 ms and then 1.2 ms increments from 2.6 to 10 ms. ^{31}P{^{17}O} PM-RESPDOR recoupling was incremented uniformly in 800 μs increments. Each subspectrum was acquired in 512 scans with a 4 s recycle delay for the Sc complex and 1024 scans and a 1.8 s recycle delay for the Ir complex.

^{17}O DNP-enhanced NMR spectra were acquired using the RINEPT-SR412(tt)-QCPMG pulse sequence.[9] The MAS frequency was increased to 12.5 kHz, the effective ^{17}O radiofrequency power was set to 25 kHz, and the QCPMG frequency (spikelet separation) was set to 625 Hz. The ^{1}H radiofrequency powers were set to 80 kHz for the CW decoupling pulses, 100 kHz for the hard pulses, and 132 kHz for the tanh/tan adiabatic $SR4_1^2$ pulses. The total dipolar recoupling time lasted 2.56 ms. For the 1D spectal acquisitions the recycle delays were set to 4 s while this was reduced to 1 s for the HETCOR spectrum acquisition. 1D spectra were acquired in 64 and 128 scans for the Sc and Ir complexes, respectively. The HETCOR spectrum was acquired in 24 scans for each of the 96 t_1 increments of 32.67 μs. 100 kHz of frequency-switched Lee-Goldburg homonuclear decoupling[10] was applied during t_1 for resolution enhancement.

1.3. Density Functional Theory.

We carried out first-principles density functional theory (DFT) calculations on the Ir(POCOP) complex grafted to amorphous silica using the Quantum Espresso (QE) package (http://www.quantum-espresso.org), version 7.1.[11,12,13] Geometry optimizations were carried out with projector augmented wave (PAW) pseudopotentials available from the QE pseudopotential library, implemented with the Perdew, Burke, and Ernzerhof (PBE) functional.[14] The initial structural coordinates were obtained by grafting the Ir complex in both orientations (see main text) onto a periodic amorphous silica model.[15] For all calculations, the plane-wave cutoff energy was converged to 44 Rydberg with a 1x1x1 *k*-point grid, owing to the large unit cell.

The gauge-including projector augmented wave (GIPAW) method[16,17], implemented in QE-GIPAW, version 7.1[18], was used to calculate the NMR magnetic shieldings and electric field gradients. GIPAW pseudopotentials files for each atom were obtained from the distribution of QE-GIPAW except for iridium, which was obtained from ref 19. The computed NMR parameters were extracted using MagresView, version 1.6.2.[20] To convert the calculated magnetic shielding constants to chemical shifts, we used the following equation, $\delta_{iso} \approx \sigma_{ref} - \sigma_{iso}$ where σ_{ref} is the absolute magnetic shielding reference (^{13}C: 186.40 ppm[21]; ^{17}O: 287.50 ppm[22]; ^{31}P: 328.35 ppm[23]) .

2. Supplementary Tables and Figures

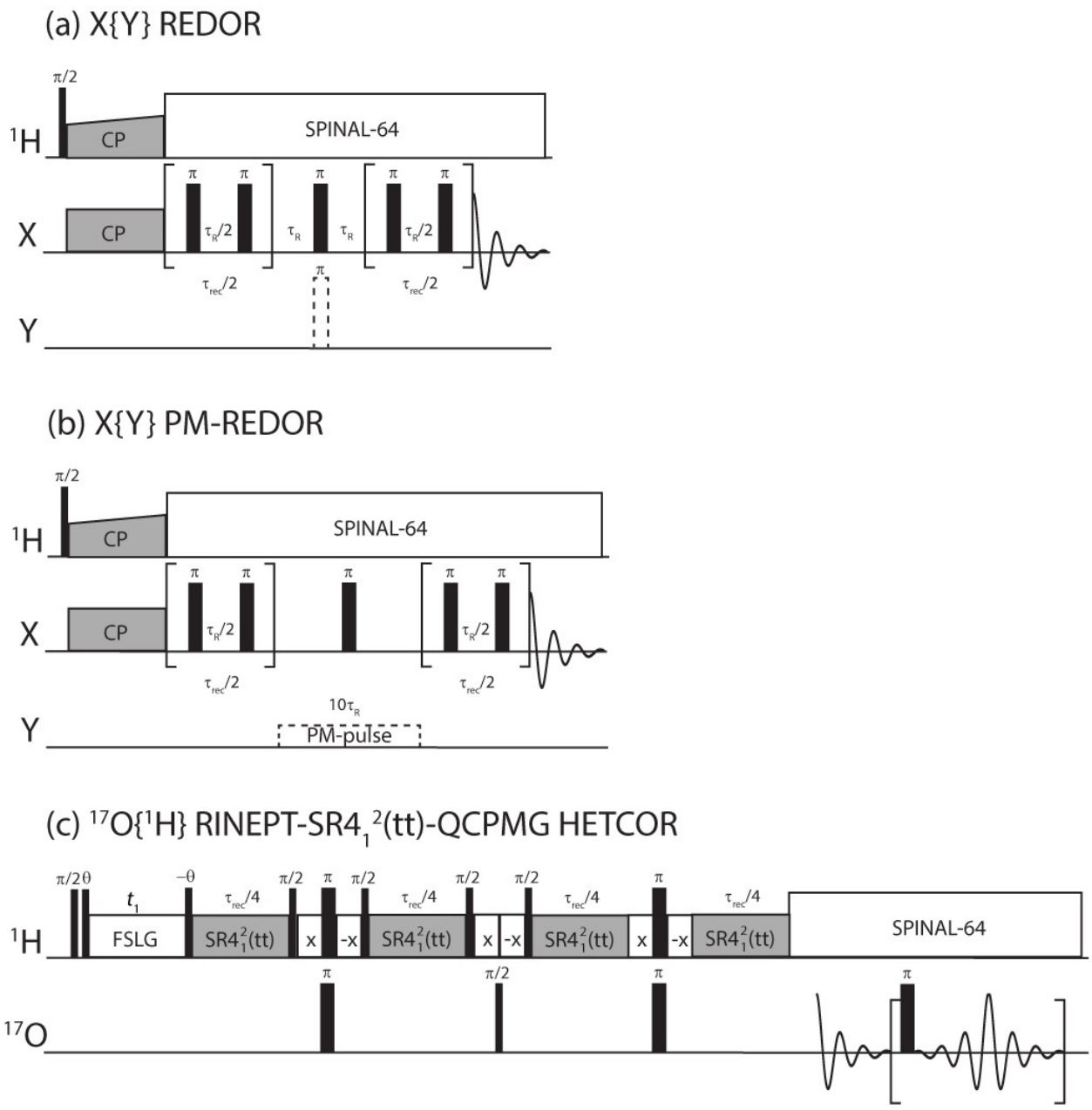

Figure S1. Pulse sequence diagrams for the sequences used in this study. For the phase cycling of the RINEPT-SR4$_1^2$(tt)-QCPMG HETCOR pulse sequence, please refer to the original publication.[9]

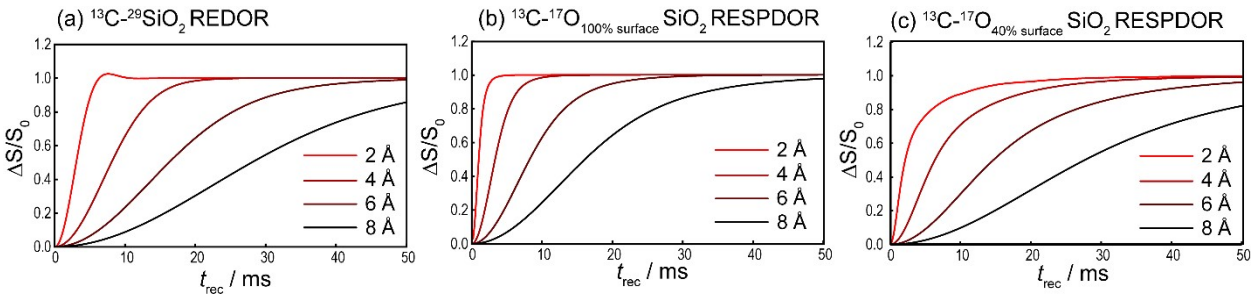

Figure S2. Comparisons of simulated ^{13}C{^{29}Si} REDOR (a) and ^{13}C{^{17}O} RESPDOR (b,c) data from atoms situated at distances of 2, 4, 6, and 8 Å above an amorphous silica surface that is enriched to 100% in ^{29}Si (a), 100 % in ^{17}O (b) and 40% in ^{17}O (c). Comparative dephasing is observed with 40% ^{17}O as is obtained with 100 % ^{29}Si.

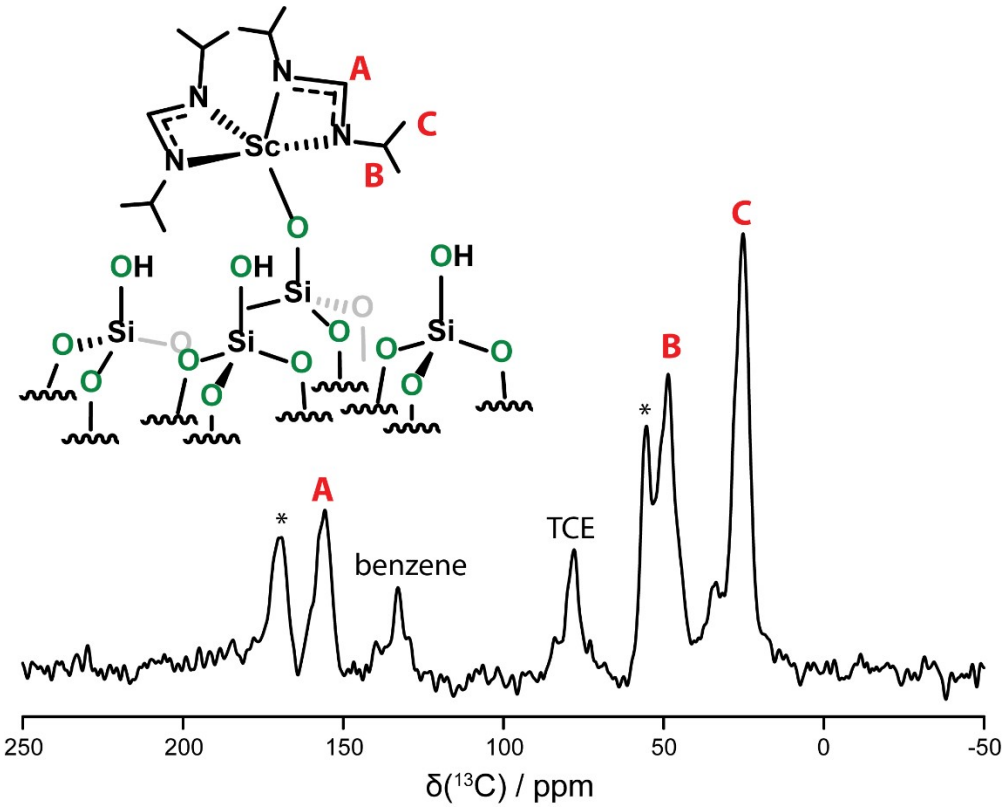

Figure S3. DNP-enhanced ^{13}C CPMAS NMR spectrum acquired on the Sc amidinate complex. The sites are labeled according to the structure on the top. Asterisks denote the positions of resonances from degradation products (free ligand).

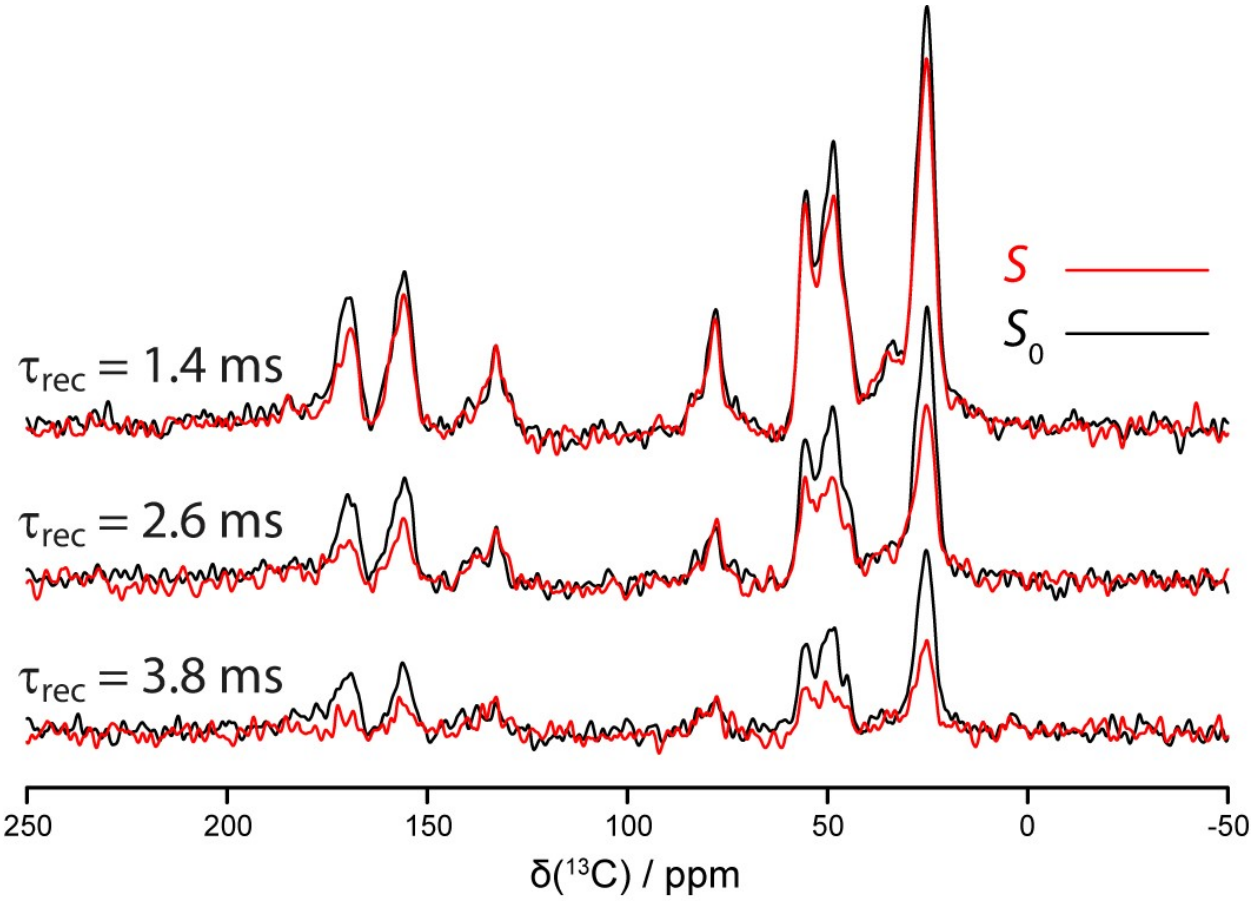

Figure S4. DNP-enhanced $^{13}C\{^{17}O\}$ PM-RESPDOR NMR subspectra acquired on the Sc amidinate complex. The reference signal intensity (S_0) is shown in black while the dephased signal (S) is shown in red.

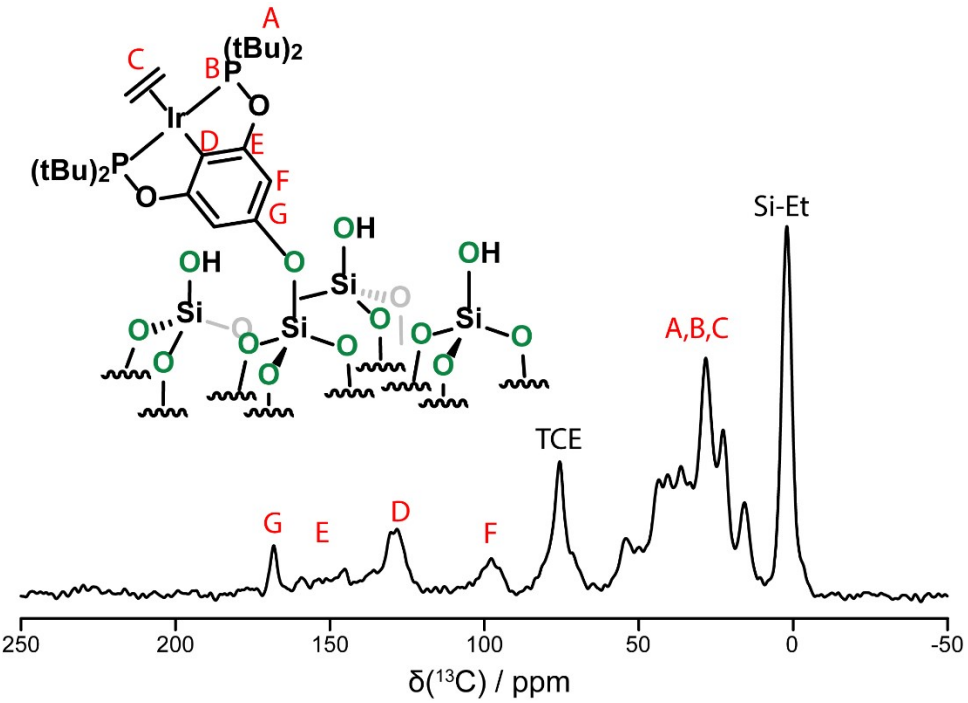

Figure S5. DNP-enhanced ^{13}C CPMAS NMR spectrum acquired on the Ir(POCOP) complex. The sites are labeled according to the structure on the top. An impurity from Si-bound carbon is observed near 0 ppm, presumably due to the insertion of some ethylene into the support.

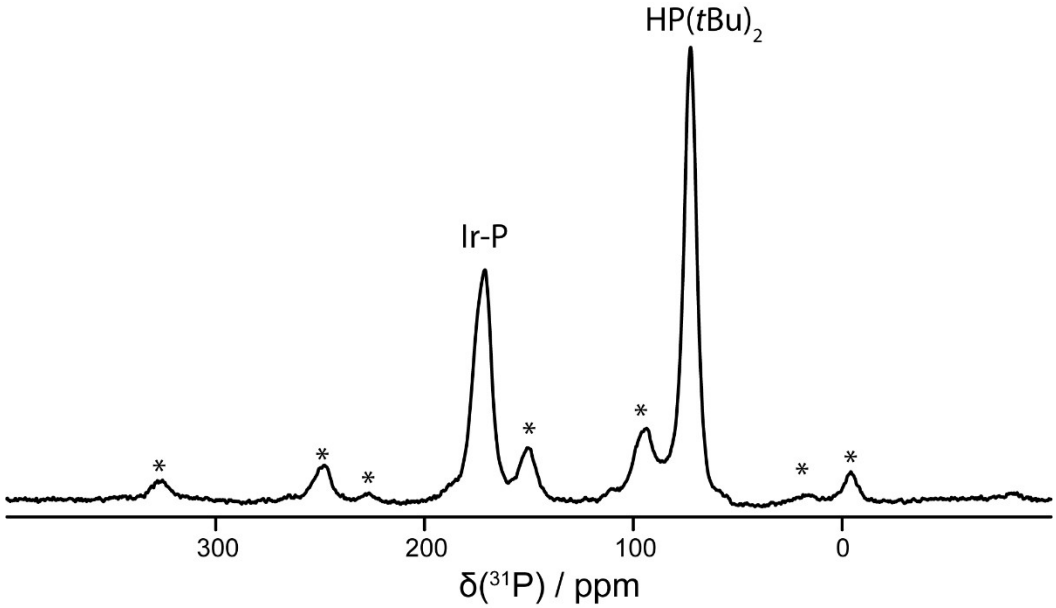

Figure S6. DNP-enhanced ^{31}P CPMAS NMR spectrum acquired on the Ir(POCOP) complex. A resonance is observed at a lower chemical shift corresponding to free phosphine.

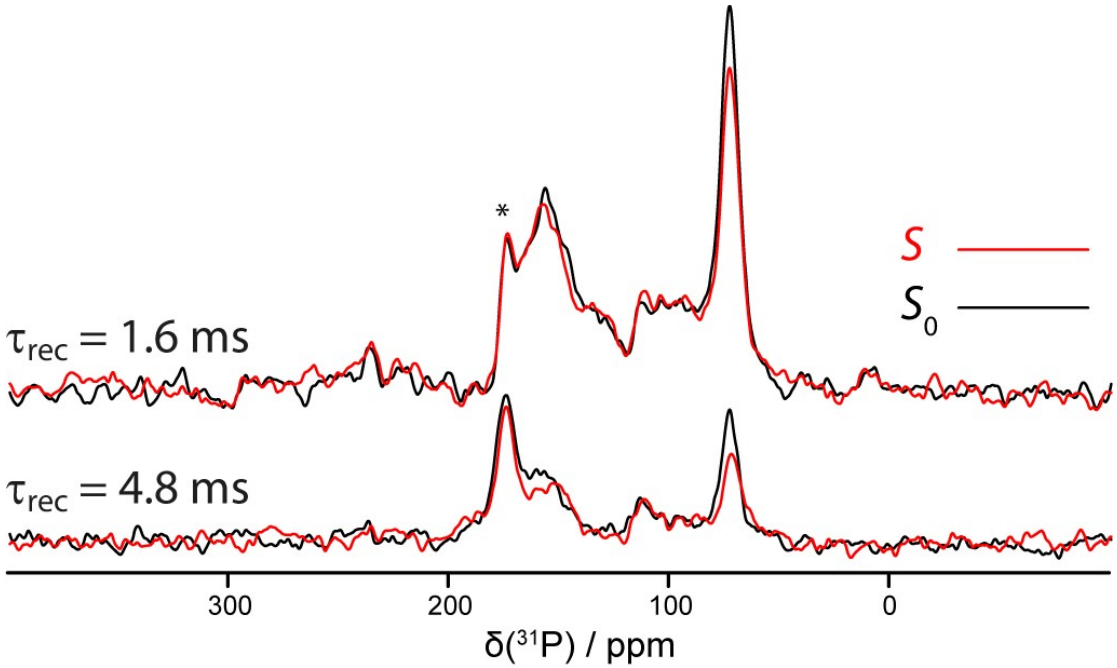

Figure S7. DNP-enhanced $^{13}C\{^{17}O\}$ PM-RESPDOR NMR subspectra acquired on the Ir(POCOP) complex. The reference signal intensity (S_0) is shown in black while the dephased signal (S) is shown in red.

Table S1. GIPAW DFT calculated NMR parameters for the Ir and *para*-substituent grafted Ir(POCOP) complex.[a]

Atom	*Para*-grafted	Ir-grafted	*Para*-grafted			Ir-grafted		
	δ_{iso} / ppm		$\lvert C_Q\rvert$ / MHz	η_Q	δ_{obs} / ppm[b]	$\lvert C_Q\rvert$ / MHz	η_Q	δ_{obs} / ppm[b]
C(A)	43.0	42.2						
C(B)	65.5	62.1						
C(C)	57.3							
C(D)	167.8	171.1						
C(E)	186.8	185.2						
C(F)	113.9	116.3						
C(G)	173.5	180.9						
P(B)	239.1	229.1						
P(G)		246.4						
O(linker)[c]	98.4	96.6	10.2	0.2	-116.1	5.2	0.5	37.0

[a]The average of the NMR parameters calculated for structurally equivalent nuclei is presented.
[b]Expected resonance frequency at 54.3 MHz (9.4 T) when accounting for the quadrupole-induced shift.
[c]A lower ^{17}O C_Q value is predicted for a Si-O-Ir oxygen than a Si-O-C oxygen due to the decreased covalency leading to an electronic configuration that more closely resembles the spherically-symmetric $[He]2s^22p^6$ configuration. Covalent, organic, ^{17}O sites generally have C_Q values around 9 MHz[24] while inorganic oxides have far lower C_Q values, with them being largely correlated to covalency.

3. Structure Determination

$^{13}C\{^{17}O\}$ PM-RESPDOR data acquired for the Sc complex was analyzed using the INTERFACES program.[25] Standard RESPDOR dephasing curves were calculated using an amorphous silica model of Comas-Vives[26] that has been surface-^{17}O-enriched to a level of 80%. The potential ^{17}O positions are listed below in XYZ format and were used with the "library_maker.c" program available at https://github.com/fperras/INTERFACES/.

```
O     9.05432     12.41696     -0.05485
O     12.17241     13.01559      0.05005
O     13.03848     10.5663     -0.51512
O     5.79973     15.11999     -0.6108
O     8.26442     15.9683     0.2455
O     4.7548     12.35363     0.25336
O     6.54277     10.37054      0.80931
O     10.84037     8.46746     -0.03708
O     9.41483     6.74966     1.56002
O     2.29011     5.99506     1.09463
O     11.95868     15.47044     -1.10763
O     12.64203     5.42318     0.8076
O     8.08599     2.86349     -0.51615
O     15.48584     2.57038     1.77324
O     18.90838     2.65725     0.56294
O     18.73102     15.77938      0.51374
O     16.2475     16.25349     1.47323
O     19.11442     12.1784     0.53048
O     16.84249     8.38594     0.35963
O     19.21048     8.94457     1.62016
O     0.36671     11.32646     1.01296
O     0.48117     8.72184     0.39414
O     21.87607     8.72184     0.39414
O     21.52584     16.4362     -1.2385
O     2.19918     16.25328     0.51305
O     3.81578     18.74279     0.69381
O     21.87521     2.55969     0.2168
O     0.74326     21.23508     0.67775
O     12.28067     19.29157      0.03501
O     10.36134     17.78729      1.17219
O     6.96297     19.01771     -0.32035
O     16.07335     0.47133     0.20655
O     16.07335     21.86623      0.20655
O     10.85684     0.83098     -0.13891
O     -0.9709     5.15125     0.54244
O     20.424     5.15125     0.54244
```

The initial guess structure given to INTERFACES is described by this MOL2 file:

```
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*****
 21 22 0 0 0
SMALL
GASTEIGER
```

```
@<TRIPOS>ATOM
      1 Sc          0.1998    0.2622    3.0205 Sc      1  UNL11       0.0000
      2 N           1.4236   -1.6838    2.8319 N.3     1  UNL11       0.0000
      3 N          -0.8232   -1.6093    2.6519 N.3     1  UNL11       0.0000
      4 C           0.2806   -2.3523    2.7318 C.3     1  UNL11       0.0000
      5 C           2.7064   -2.3824    2.8979 C.3     1  UNL11       0.0000
      6 C          -2.1889   -2.1331    2.6525 C.3     1  UNL11       0.0000
      7 C           2.5491   -3.8350    3.3673 C.3     1  UNL11       0.0000
      8 C           3.6237   -1.6079    3.8421 C.3     1  UNL11       0.0000
      9 C          -2.2169   -3.5684    3.1899 C.3     1  UNL11       0.0000
     10 C          -3.2175   -1.2454    3.3614 C.3     1  UNL11       0.0000
     11 N          -0.9111    1.1829    4.6146 N.3     1  UNL11       0.0000
     12 N           1.3332    1.3033    4.5053 N.3     1  UNL11       0.0000
     13 C           0.2160    1.6128    5.1632 C.3     1  UNL11       0.0000
     14 C          -2.2756    1.4819    5.0257 C.3     1  UNL11       0.0000
     15 C           2.6803    1.5358    5.0090 C.3     1  UNL11       0.0000
     16 C          -2.6486    2.9611    4.9385 C.3     1  UNL11       0.0000
     17 C          -2.4499    0.9351    6.4472 C.3     1  UNL11       0.0000
     18 C           2.8870    0.9271    6.3966 C.3     1  UNL11       0.0000
     19 C           2.9048    3.0481    5.0186 C.3     1  UNL11       0.0000
     20 Si          0.0000    0.0000    0.0000 Si      1  UNL11       0.0000
     21 O           0.3867    0.9535    1.2185 O.3     1  UNL1        0.0000
@<TRIPOS>BOND
     1     9     6    1
     2     6    10    1
     3     6     3    1
     4    16    14    1
     5    19    15    1
     6     1    12    1
     7     1    11    1
     8     3     4    1
     9    12    15    1
    10    12    13    1
    11    11    14    1
    12    11    13    1
    13    15    18    1
    14    14    17    1
    15     4     2    1
    16     2     5    1
    17     5     7    1
    18     5     8    1
    19     3     1    1
    20     2     1    1
    21     1    21    1
    22    21    20    1
```

And the INTERFACES input file is given below, together with the three experimental PM-RESPDOR datasets. All four N-*i*Pr dihedral angles were sampled in addition to the Sc-amidine dihedrals. The complex's orientation relative to the support was also sampled using a ghost atom.

```
//information on the structure
structure Sc_amidine_SiO.mol2
```

```
support SiO2_80p_17OH
confidence_level 90
cutoff_rmsd 1.5
max_structures 10000

//Structural variables
bend 20 21 1 -40 40 9
revolve 21 1 9
revolve  1 4  4
revolve  1 13 4
revolve  2  5 4
revolve  3  6 4
revolve 11 14 4
revolve 12 15 4

//Constraints
surface_collision_distance 1.2

//REDOR data
surface-REDOR SiO2-methyls.txt 1.0
detected_spins 7 8 9 10 16 17 18 19

surface-REDOR SiO2-iPr.txt 1.0
detected_spins 5 6 14 15

surface-REDOR SiO2-CH.txt 1.0
detected_spins 4 13
```

SiO2-CH.txt

```
0.0008    0.047865738
0.0012    0.126796001
0.0014    0.128778195
0.0016    0.214027892
0.002    0.294988722
0.0026    0.430198384
0.0038    0.49691358
0.005    0.632037262
0.0062    0.656279509
```

SiO2-iPr.txt

```
0.0008    0.031154661
0.0012    0.08350182
0.0014    0.111144264
0.0016    0.145746165
0.002    0.269090488
0.0026    0.332789949
0.0038    0.508944894
0.005    0.569281945
0.0062    0.575598488
0.0074    0.562953995
```

SiO2-methyls.txt

```
0.0012    0.110686831
```

```
0.0014    0.122672406
0.0016    0.1485
0.0020    0.204278151
0.0026    0.334637632
0.0038    0.49707067
0.0050    0.573601629
0.0062    0.73518983
0.0074    0.808431402
0.0086    0.969162996
0.0098    0.775917579
```

The resulting best-fit structure is given by the following MOL2 file.

```
@<TRIPOS>MOLECULE
*****
 26 26 0 0 0
SMALL
GASTEIGER

@<TRIPOS>ATOM
1 Sc 0.2265 1.5089 3.0574 Sc      1  UNL1        0.0000
2 N -0.2913 3.7493 2.8776 N.3      1  UNL1        0.0000
3 N 1.8198 2.9572 2.8371 N.3      1  UNL1        0.0000
4 C 1.0098 4.0149 2.8796 C.3      1  UNL1        0.0000
5 C -1.2836 4.8232 2.8930 C.3      1  UNL1        0.0000
6 C 3.2774 3.0119 2.9472 C.3      1  UNL1        0.0000
7 C -0.7042 6.1368 3.4349 C.3      1  UNL1        0.0000
8 C -2.4681 4.3664 3.7422 C.3      1  UNL1        0.0000
9 C 3.7375 2.4670 4.3041 C.3      1  UNL1        0.0000
10 C 4.0346 2.3534 1.7890 C.3      1  UNL1        0.0000
11 N -1.2876 0.8652 4.4417 N.3      1  UNL1        0.0000
12 N 0.8689 0.2667 4.6752 N.3      1  UNL1        0.0000
13 C -0.3806 0.1905 5.1332 C.3      1  UNL1        0.0000
14 C -2.6887 1.0786 4.7756 C.3      1  UNL1        0.0000
15 C 1.9851 -0.5192 5.1843 C.3      1  UNL1        0.0000
16 C -2.9148 1.8550 6.0721 C.3      1  UNL1        0.0000
17 C -3.3594 -0.2994 4.8145 C.3      1  UNL1        0.0000
18 C 3.1690 0.3605 5.5883 C.3      1  UNL1        0.0000
19 C 2.3716 -1.5163 4.0917 C.3      1  UNL1        0.0000
20 Si -0.4247 0.0000 0.0000 Si      1  UNL1        0.0000
21 O -0.0380 0.9535 1.2185 O.3      1  UNL1        0.0000
22 Si 0.0000 0.0000 0.0000 Si 1 UNL1 0.0000
23 Si 50.0000 50.0000 0.0000 Si 1 UNL1 0.0000
24 Si -50.0000 -50.0000 0.0000 Si 1 UNL1 0.0000
25 Si -50.0000 50.0000 0.0000 Si 1 UNL1 0.0000
26 Si 50.0000 -50.0000 0.0000 Si 1 UNL1 0.0000

@<TRIPOS>BOND
1 9 6 1
2 6 10 1
3 6 3 1
4 16 14 1
5 19 15 1
```

```
6 1 12 1
7 1 11 1
8 3 4 1
9 12 15 1
10 12 13 1
11 11 14 1
12 11 13 1
13 15 18 1
14 14 17 1
15 4 2 1
16 2 5 1
17 5 7 1
18 5 8 1
19 3 1 1
20 2 1 1
21 1 21 1
22 21 20 1
23 22 23 1
24 22 24 1
25 22 25 1
26 22 26 1
```

4. DFT-Optimized Structures

4.1. C-bound Ir(C_2H_4)(^{tBu4}POCOP)/$Si^{17}O_2$

```
data_SiO2-9_IrPOCOP_C-bound
_symmetry_space_group_name_H-M    'P1'
_symmetry_Int_Tables_number       1
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
_cell_length_a                    21.3949
_cell_length_b                    21.3949
_cell_length_c                    34.1700
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
O1     O     0.28735   0.70663   0.08580
O2     O     0.61144   0.61639   0.19966
O3     O     0.15845   0.39231   0.09335
O4     O     0.38526   0.43077   0.15737
O5     O     0.67522   0.84509   0.14258
O6     O     0.05962   0.48344   0.34325
O7     O     0.63825   0.13208   0.19149
Si8    Si    0.35879   0.38763   0.12090
Si9    Si    0.22791   0.65772   0.08674
Si10   Si    0.31000   0.71337   0.31764
```

Si11	Si	0.35839	0.72375	0.09976
Si12	Si	0.26626	0.83559	0.29005
Si13	Si	0.44788	0.57210	0.23455
O14	O	0.19977	0.92020	0.19354
O15	O	0.85351	0.51976	0.09042
O16	O	0.40171	0.76219	0.20949
O17	O	0.52230	0.55540	0.24051
O18	O	0.11019	0.51779	0.20736
O19	O	0.60172	0.62196	0.34939
O20	O	0.43568	0.64711	0.23046
O21	O	0.10917	0.44547	0.27624
Si22	Si	0.61607	0.17786	0.22784
O23	O	0.51745	0.74079	0.23672
O24	O	0.30951	0.97299	0.20178
O25	O	0.31264	0.84921	0.18918
O26	O	0.78707	0.87279	0.23499
O27	O	0.99298	0.26993	0.32631
O28	O	0.97345	0.00346	0.28939
O29	O	-0.00099	0.03270	0.16632
O30	O	0.10409	0.29707	0.12676
Si31	Si	0.90753	0.01977	0.26706
Si32	Si	0.03391	0.76405	0.30769
Si33	Si	0.88341	0.76188	0.31585
O34	O	0.58529	0.71132	0.29975
O35	O	0.79235	0.33029	0.15957
O36	O	0.05429	0.21634	0.26621
O37	O	0.52616	0.68472	0.09212
Si38	Si	0.81714	0.52966	0.13286
Si39	Si	0.41797	0.83751	0.06409
Si40	Si	0.53333	0.38628	0.15975
Si41	Si	0.43352	0.23735	0.34218
Si42	Si	0.65623	0.66717	0.17614
Si43	Si	0.46011	0.71146	0.21001
Si44	Si	0.76228	0.40228	0.15617
O45	O	0.14043	0.60551	0.25535
O46	O	0.54282	0.16457	0.23992
O47	O	0.71931	0.41890	0.19497
O48	O	0.50923	0.94533	0.13254
O49	O	0.25015	0.86064	0.10458
O50	O	0.62941	0.73882	0.17618
O51	O	0.72390	0.88958	0.07435
O52	O	0.70359	0.83313	0.28503
O53	O	0.72729	0.66420	0.19370
Si54	Si	0.85367	0.78307	0.11521
Si55	Si	0.84885	0.91474	0.22570
O56	O	0.21820	0.28551	0.17699
O57	O	0.12077	0.06510	0.10914
O58	O	0.60280	0.15999	0.33178
O59	O	0.84120	0.69655	0.31836
O60	O	0.19352	0.27581	0.25303
O61	O	0.61530	0.52880	0.12696
O62	O	0.33204	0.47172	0.22538
O63	O	0.32262	0.32720	0.13892

O64	O	0.29925	0.96769	0.12334
O65	O	0.49647	0.57895	0.12714
O66	O	0.85067	0.45847	0.30472
O67	O	0.62272	0.04989	0.29846
Si68	Si	0.65234	0.11999	0.30453
Si69	Si	0.76927	1.00102	0.17269
Si70	Si	0.59901	0.56582	0.23570
Si71	Si	0.63370	0.65140	0.31032
Si72	Si	0.95704	0.08443	0.18999
Si73	Si	0.32690	0.14099	0.12525
Si74	Si	0.27103	0.90579	0.20865
O75	O	0.45595	0.13903	0.18413
O76	O	0.46555	0.78421	0.30229
O77	O	0.41461	0.23716	0.38892
O78	O	0.08464	0.82304	0.29672
O79	O	0.31039	0.39726	0.28697
O80	O	0.83661	0.13154	0.35598
O81	O	0.48353	0.69270	0.16558
O82	O	0.98879	0.90384	0.15896
O83	O	0.95519	0.75918	0.29371
O84	O	0.62895	0.59833	0.27514
Si85	Si	0.73583	0.87788	0.12138
Si86	Si	0.78111	0.68288	0.22507
Si87	Si	0.95043	0.84330	0.17523
O88	O	0.79318	0.82699	0.12638
O89	O	0.89135	0.32721	0.29808
O90	O	0.81596	0.45995	0.15445
O91	O	0.62312	0.25485	0.22271
O92	O	0.91329	0.81493	0.13742
O93	O	0.86958	0.07411	0.29141
Si94	Si	0.76682	0.16459	0.35000
Si95	Si	0.13302	0.87396	0.31938
Si96	Si	0.08144	0.02355	0.07691
O97	O	0.43713	0.90010	0.32219
O98	O	0.07897	0.05477	0.30901
O99	O	0.03267	0.42424	0.21132
O100	O	0.57580	0.82901	0.28241
O101	O	-0.00224	0.13759	0.21341
O102	O	0.22336	0.28580	0.10028
Si103	Si	0.46785	0.31892	0.22966
Si104	Si	0.04956	0.27918	0.29427
Si105	Si	0.46946	0.17059	0.22623
Si106	Si	0.20005	0.32464	0.21620
Si107	Si	0.07253	0.64605	0.25764
Si108	Si	0.13599	0.14002	0.11478
O109	O	0.43155	0.86033	0.16568
O110	O	0.40777	0.00065	0.15747
O111	O	0.11958	0.13893	0.22091
O112	O	0.09661	0.95495	0.16753
O113	O	0.25224	0.87935	0.25204
O114	O	0.35341	0.76865	0.13832
O115	O	0.59183	0.02512	0.22266
O116	O	0.31408	0.08168	0.15569

Si117	Si	0.04083	0.49450	0.19353
O118	O	0.40689	0.35098	0.25053
O119	O	0.51359	0.20416	0.12934
O120	O	0.68490	0.32890	0.05586
O121	O	0.84675	0.70839	0.12867
O122	O	0.85027	0.68436	0.20483
O123	O	0.61734	0.24906	0.09969
O124	O	0.38875	0.76642	0.06411
Si125	Si	0.37485	0.81057	0.17577
O126	O	0.41956	0.03676	0.31183
O127	O	0.27089	0.59180	0.27261
O128	O	0.24131	0.12872	0.22725
Si129	Si	0.46653	0.97345	0.31869
Si130	Si	0.63910	0.86000	0.26358
Si131	Si	0.26577	0.27573	0.13967
Si132	Si	0.64592	0.05091	0.09704
Si133	Si	0.59120	0.99772	0.26854
Si134	Si	0.16485	0.46748	0.09054
Si135	Si	0.53999	0.51681	0.11626
Si136	Si	0.46264	0.00637	0.12394
O137	O	0.74313	0.54831	0.12674
O138	O	0.62929	0.03726	0.14367
O139	O	0.82811	0.96625	0.19341
O140	O	0.16536	0.40978	0.33975
O141	O	0.06373	0.72144	0.14321
O142	O	0.66322	0.64427	0.13038
O143	O	0.70971	0.02043	0.20099
O144	O	0.63926	0.84495	0.21647
Si145	Si	0.80340	0.26559	0.13251
Si146	Si	0.68241	0.25916	0.07585
O147	O	0.41671	0.36004	0.09376
O148	O	0.50714	0.27003	0.06208
O149	O	0.90472	0.86843	0.21035
O150	O	0.53934	0.33161	0.12695
O151	O	0.40150	0.14932	0.11512
O152	O	0.76425	0.75136	0.24259
O153	O	0.63298	0.98384	0.07273
O154	O	0.17904	0.53621	0.32412
O155	O	0.05248	0.67698	0.21517
Si156	Si	0.58858	0.23562	0.33724
Si157	Si	0.40320	0.82724	0.31669
Si158	Si	0.05730	0.18391	0.22236
Si159	Si	0.13433	0.01555	0.28480
O160	O	0.86957	0.95357	0.26504
O161	O	0.18499	0.04290	0.18371
O162	O	0.31895	0.09806	0.28838
O163	O	0.01794	0.59868	0.27363
O164	O	0.91030	0.11898	0.15859
Si165	Si	0.83812	0.12769	0.14292
Si166	Si	0.96957	0.54489	0.25791
Si167	Si	0.29429	0.91707	0.08728
Si168	Si	0.89458	0.12518	0.32371
Si169	Si	0.24223	0.58553	0.31912

Si170	Si	0.02806	0.96724	0.14905
O171	O	0.42792	0.12833	0.25599
O172	O	0.18160	0.15132	0.15367
O173	O	0.11759	-0.00121	0.23903
O174	O	0.33900	0.85934	0.29817
Si175	Si	0.15035	0.97846	0.19717
Si176	Si	0.24726	0.11564	0.27522
Si177	Si	0.04744	0.53877	0.10697
Si178	Si	0.78742	0.07723	0.06758
O179	O	0.29059	0.12873	0.08262
O180	O	0.86426	0.27848	0.10484
O181	O	0.86759	0.78365	0.06773
O182	O	0.07227	0.70291	0.29049
O183	O	0.47831	0.83861	0.09495
O184	O	0.43616	0.00544	0.07867
O185	O	0.20634	0.84765	0.32074
O186	O	0.79524	0.06967	0.15911
Si187	Si	0.35690	0.33167	0.28478
Si188	Si	0.08918	0.68010	0.10580
O189	O	0.95388	0.66988	0.16522
O190	O	0.31229	0.27133	0.27311
O191	O	0.91793	0.04610	0.22296
O192	O	0.81213	0.57704	0.32665
O193	O	0.36222	0.66338	0.30024
O194	O	0.51175	0.24405	0.33925
Si195	Si	0.18230	0.11635	0.19681
Si196	Si	0.27657	0.43464	0.24817
Si197	Si	0.15344	0.31611	0.09186
Si198	Si	0.53476	0.76439	0.28173
Si199	Si	0.24102	0.25585	0.28868
O200	O	0.72344	0.11838	0.32300
O201	O	0.89685	0.56280	0.26924
O202	O	0.98009	0.55067	0.08537
O203	O	0.51922	0.98009	0.28252
O204	O	0.40286	0.66192	0.10888
O205	O	0.40907	0.16764	0.32659
O206	O	0.47996	0.35996	0.19012
O207	O	0.03474	0.49731	0.14628
O208	O	0.09618	0.49842	0.07962
O209	O	0.21500	0.57388	0.19428
Si210	Si	0.70889	0.39877	0.06834
Si211	Si	0.87717	0.66132	0.16234
Si212	Si	0.49411	0.87012	0.13825
Si213	Si	0.34383	0.58909	0.29284
O214	O	0.98209	0.26500	0.12920
O215	O	0.19253	0.49470	0.13291
O216	O	0.36679	0.89234	0.07621
O217	O	0.31085	0.52515	0.15447
O218	O	0.71926	0.40563	0.11626
O219	O	0.16336	0.69665	0.09772
Si220	Si	0.64896	0.42314	0.21443
Si221	Si	0.87687	0.39235	0.32413
Si222	Si	0.77284	0.81687	0.26619

Si223	Si	0.62490	0.81580	0.17330
O224	O	0.61833	0.27708	0.30090
O225	O	0.45026	0.24492	0.22294
O226	O	0.23027	0.18156	0.29849
O227	O	0.71142	0.66467	0.31855
O228	O	0.53028	0.32435	0.25705
O229	O	0.39971	0.30050	0.32123
O230	O	0.29822	0.20639	0.14243
Si231	Si	0.60514	0.30748	0.25752
Si232	Si	0.46968	0.14304	0.13734
Si233	Si	0.54311	0.26372	0.10435
O234	O	0.60009	0.39676	0.18178
O235	O	0.53109	0.50085	0.06948
O236	O	0.25545	0.37661	0.22016
O237	O	0.64561	0.37279	0.25155
O238	O	0.03584	0.97451	0.10121
O239	O	0.85541	0.58767	0.15455
Si240	Si	0.47693	0.65346	0.12366
Si241	Si	0.98465	0.47599	0.32981
O242	O	0.67187	0.57400	0.06430
O243	O	0.63160	0.49625	0.22783
O244	O	0.06891	0.17610	0.12165
O245	O	0.88005	0.26847	0.36706
O246	O	0.83378	0.12108	0.09476
O247	O	0.49983	0.07367	0.12690
O248	O	0.63587	0.93537	0.27110
O249	O	0.24180	0.60925	0.12240
O250	O	0.05827	0.23974	0.18930
O251	O	0.74881	0.94875	0.13952
O252	O	0.81482	0.19877	0.15673
Si253	Si	0.91676	0.26474	0.32358
Si254	Si	0.00835	0.03804	0.32619
Si255	Si	0.33145	0.00624	0.15981
Si256	Si	0.36239	0.49052	0.18344
O257	O	0.22980	0.29991	0.32789
O258	O	0.72087	0.06445	0.09017
O259	O	0.31481	0.43414	0.09293
O260	O	0.83395	0.81230	0.29578
O261	O	0.08139	0.60546	0.11678
O262	O	0.90449	0.19515	0.30392
O263	O	0.13417	0.36273	0.21622
O264	O	0.03829	0.34108	0.26690
O265	O	0.66258	0.15642	0.26320
Si266	Si	0.16515	0.33238	0.34505
Si267	Si	0.12939	0.47071	0.32061
Si268	Si	0.67371	0.57353	0.11307
Si269	Si	0.23786	0.55013	0.15128
Si270	Si	0.17250	0.54504	0.22981
Si271	Si	0.01439	0.71321	0.17982
Si272	Si	0.78546	0.64401	0.30749
O273	O	0.21591	0.48577	0.25038
O274	O	0.78382	0.63141	0.26017
O275	O	0.74182	0.25185	0.10562

O276	O	0.98435	0.47837	0.28119
O277	O	0.25043	0.66243	0.33519
O278	O	0.27046	0.75800	0.28613
O279	O	0.11101	0.29348	0.32119
O280	O	0.40366	0.55374	0.27308
O281	O	0.72760	0.17442	0.39142
Si282	Si	0.93756	0.28328	0.09155
Si283	Si	0.64193	0.05392	0.18996
Si284	Si	0.07981	0.39389	0.24404
Si285	Si	0.91510	0.53237	0.06249
Si286	Si	0.05306	0.24509	0.14128
O287	O	0.42124	0.53604	0.19526
O288	O	0.04704	0.69538	0.06643
O289	O	0.98186	0.53627	0.21091
O290	O	0.51548	0.45568	0.14184
O291	O	0.99276	0.78470	0.19306
O292	O	0.14052	0.94453	0.30154
O293	O	0.55431	0.83435	0.15757
O294	O	0.19888	0.05834	0.28814
H295	H	0.70576	0.59740	0.05126
H296	H	0.56628	0.47418	0.05958
H297	H	0.31267	0.47488	0.10727
H298	H	0.44269	0.39374	0.08221
O299	O	0.36001	0.76644	0.33982
O300	O	0.31202	0.55419	0.33258
H301	H	0.41872	0.27823	0.40183
O302	O	0.15880	0.32421	0.39254
H303	H	0.15602	0.28074	0.40195
O304	O	0.77633	0.23770	0.33218
O305	O	0.96373	0.09821	0.34028
O306	O	0.89967	0.78763	0.36134
O307	O	0.93389	0.53302	0.34213
O308	O	0.94696	0.41121	0.34398
O309	O	0.81666	0.36764	0.35103
O310	O	0.02394	0.76481	0.35624
O311	O	0.10000	0.89037	0.36247
O312	O	0.01656	0.98908	0.36402
O313	O	0.49916	0.98031	0.36219
H314	H	0.51380	0.02295	0.36835
O315	O	0.65184	0.44603	0.05417
O316	O	0.77505	0.41170	0.04480
H317	H	0.80231	0.44498	0.05544
H318	H	0.66460	0.49114	0.05211
O319	O	0.68069	0.20286	0.04296
H320	H	0.72057	0.18324	0.03345
H321	H	0.31092	0.09762	0.06539
O322	O	0.13016	0.29359	0.04820
H323	H	0.14074	0.24848	0.04471
O324	O	0.21076	0.49009	0.05393
H325	H	0.25157	0.46742	0.05473
H326	H	0.23980	0.82499	0.08744
H327	H	0.46670	0.29250	0.06522
O328	O	0.44219	0.85635	0.02004

H329	H	0.46694	0.82394	0.00656
O330	O	0.22260	0.62258	0.04439
H331	H	0.21772	0.57588	0.04559
H332	H	0.41313	0.96672	0.07118
H333	H	0.02399	0.73529	0.06751
H334	H	0.86386	0.74253	0.05487
H335	H	0.68910	0.92102	0.07051
H336	H	0.52884	0.73085	0.09331
O337	O	0.26730	0.95125	0.04768
H338	H	0.22276	0.96562	0.04981
O339	O	0.89235	0.59044	0.03380
O340	O	0.92650	0.46665	0.03755
H341	H	0.91986	0.59777	0.01104
H342	H	0.97083	0.45332	0.03679
H343	H	0.58880	0.97017	0.07221
O344	O	0.82143	0.01093	0.05544
H345	H	0.79662	0.97245	0.06039
O346	O	0.77753	0.12037	0.02718
H347	H	0.77541	0.09539	0.00295
O348	O	0.16837	0.16881	0.07498
H349	H	0.21385	0.15684	0.07245
O350	O	0.04040	0.06526	0.04552
O351	O	0.13514	0.98625	0.05014
H352	H	1.00046	0.08260	0.05529
O353	O	0.94688	0.23310	0.05500
O354	O	0.95630	0.35537	0.07894
H355	H	0.97544	0.24826	0.03439
H356	H	0.92368	0.37976	0.06502
H357	H	0.11776	0.96976	0.02542
O358	O	0.60457	0.10832	0.07924
H359	H	0.62931	0.14004	0.06403
Si360	Si	0.87135	0.53324	0.31163
Si361	Si	0.39454	0.10688	0.29688
O362	O	0.63061	0.25823	0.37581
Si363	Si	0.80525	0.29311	0.36246
O364	O	0.75281	0.29446	0.39800
Si365	Si	0.69383	0.24267	0.40234
O366	O	0.66720	0.24219	0.44734
H367	H	0.69682	0.22822	0.46765
Si368	Si	0.02584	0.91299	0.36584
Si369	Si	0.96943	0.81927	0.36552
O370	O	-0.01908	0.87702	0.33234
O371	O	-0.00826	0.86838	0.40133
Ir372	Ir	0.65651	0.55526	0.52322
C373	C	0.63980	0.57775	0.46638
C374	C	0.60411	0.53906	0.44168
C375	C	0.59199	0.55310	0.40263
C376	C	0.65274	0.64927	0.41026
C377	C	0.66363	0.63252	0.44918
C378	C	0.66473	0.55988	0.58732
C379	C	0.68473	0.50049	0.57441
O380	O	0.58072	0.48363	0.45647
H381	H	0.65456	0.45992	0.57966

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H382   H     0.61864   0.56580   0.60102
P383   P     0.59624   0.47390   0.50463
C384   C     0.51649   0.46679   0.52490
C385   C     0.62406   0.39258   0.50371
O386   O     0.69905   0.67277   0.47193
H387   H     0.69986   0.59382   0.59700
H388   H     0.73470   0.48913   0.57270
P389   P     0.71006   0.64620   0.51806
C390   C     0.79627   0.64314   0.52024
C391   C     0.69038   0.71722   0.54616
C392   C     0.61700   0.60837   0.38756
H393   H     0.56378   0.52238   0.38407
H394   H     0.67092   0.69320   0.39837
H395   H     0.61067   0.37026   0.47578
H396   H     0.60367   0.36601   0.52828
H397   H     0.67542   0.39210   0.50625
H398   H     0.50751   0.41896   0.53558
H399   H     0.48225   0.47824   0.50184
H400   H     0.51038   0.50019   0.54915
H401   H     0.81554   0.65872   0.49191
H402   H     0.81084   0.59449   0.52542
H403   H     0.81485   0.67349   0.54364
H404   H     0.66157   0.70445   0.57166
H405   H     0.66309   0.74916   0.52749
H406   H     0.73249   0.74195   0.55644
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4.2. Ir-bound Ir(C_2H_4)(^{tBu4}POCOP)/$Si^{17}O_2$

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_cell_angle_gamma    88.6455
loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  H1       1.0000 0.14255  0.08986  0.33920
  H2       1.0000 0.12544  0.84326  0.27981
  H3       1.0000 0.24322  0.63036  0.31227
  H4       1.0000 0.12474  0.53184  0.27938
  H5       1.0000 0.48233  0.66402  0.31943
  H6       1.0000 0.30970  0.93434  0.31477
  H7       1.0000 0.45777  0.00093  0.43244
  H8       1.0000 0.52949  0.15025  0.31871
  H9       1.0000 0.61823  0.29883  0.30380
  H10      1.0000 0.67603  0.61777  0.53055
```

H11	1.0000	0.88051	0.36150	0.33286
H12	1.0000	0.75989	0.85615	0.29752
H13	1.0000	0.55360	0.94476	0.32603
H14	1.0000	0.74594	0.68924	0.30270
H15	1.0000	0.97013	0.74867	0.28907
H16	1.0000	0.53342	0.50124	0.31094
O1	1.0000	0.48536	0.47859	0.47146
O2	1.0000	0.38017	0.04918	0.36436
O3	1.0000	0.37822	0.02393	0.43224
O4	1.0000	0.00350	0.00274	0.37524
O5	1.0000	0.26047	0.32164	0.37622
O6	1.0000	0.18274	0.44450	0.33079
O7	1.0000	0.20882	0.49901	0.39489
O8	1.0000	0.44431	0.39330	0.41157
O9	1.0000	0.19767	0.10260	0.40098
O10	1.0000	0.47764	0.30446	0.35353
O11	1.0000	0.40074	0.20183	0.40589
O12	1.0000	0.03329	0.38525	0.37826
O13	1.0000	0.39306	0.55262	0.35853
O14	1.0000	0.42501	0.85568	0.36442
O15	1.0000	0.21054	0.93153	0.37087
O16	1.0000	0.39484	0.58357	0.42168
O17	1.0000	0.22557	0.68143	0.38232
O18	1.0000	0.06122	0.60398	0.34168
O19	1.0000	0.99823	0.71753	0.39501
O20	1.0000	0.09807	0.79098	0.33973
O21	1.0000	0.78309	0.06875	0.39855
O22	1.0000	0.67654	0.20276	0.35835
O23	1.0000	0.87620	0.11781	0.33854
O24	1.0000	0.86566	0.25901	0.38615
O25	1.0000	0.80934	0.45788	0.38438
O26	1.0000	0.63375	0.57230	0.35776
O27	1.0000	0.80090	0.94520	0.35043
O28	1.0000	0.63217	0.78589	0.34558
O29	1.0000	0.62062	0.51768	0.41960
O30	1.0000	0.61798	0.93554	0.38902
O31	1.0000	0.81820	0.85066	0.40673
O32	1.0000	0.85471	0.75541	0.34847
O33	1.0000	0.78211	0.64965	0.40092
O34	1.0000	0.97794	0.94106	0.31084
Si1	1.0000	0.48764	0.49171	0.43250
Si2	1.0000	0.13697	0.03619	0.37176
Si3	1.0000	0.16742	0.41131	0.37008
Si4	1.0000	0.39641	0.30884	0.38703
Si5	1.0000	0.34062	0.09615	0.40137
Si6	1.0000	0.51111	0.57319	0.33704
Si7	1.0000	0.30740	0.58231	0.38988
Si8	1.0000	0.15402	0.55347	0.31457
Si9	1.0000	0.33263	0.94080	0.35146
Si10	1.0000	0.09639	0.69823	0.36568
Si11	1.0000	0.03834	0.82908	0.30497
Si12	1.0000	0.57453	0.24030	0.33259
Si13	1.0000	0.91981	0.00212	0.34174
Si14	1.0000	0.89599	0.36881	0.36986
Si15	1.0000	0.80067	0.16261	0.37102
Si16	1.0000	0.75753	0.95097	0.38941
Si17	1.0000	0.55778	0.88324	0.35611

Si18	1.0000	0.74845	0.77636	0.32225
Si19	1.0000	0.71223	0.54820	0.39075
Si20	1.0000	0.86029	0.74282	0.38909
C1	1.0000	0.47443	0.47856	0.59602
C2	1.0000	0.49812	0.48002	0.63014
C3	1.0000	0.60655	0.44722	0.64093
C4	1.0000	0.69012	0.41521	0.61790
C5	1.0000	0.66259	0.41772	0.58393
C6	1.0000	0.55518	0.44996	0.57173
O35	1.0000	0.74433	0.38606	0.56077
Ir1	1.0000	0.51709	0.44904	0.52236
O36	1.0000	0.63303	0.44103	0.67466
H17	1.0000	0.77396	0.38839	0.62642
O37	1.0000	0.36458	0.50534	0.58568
H18	1.0000	0.43257	0.50482	0.64777
P1	1.0000	0.34312	0.50185	0.54439
C7	1.0000	0.29992	0.63512	0.53709
P2	1.0000	0.70710	0.40358	0.52070
C8	1.0000	0.75640	0.28060	0.50358
H19	1.0000	0.76893	0.66775	0.50010
C9	1.0000	0.88376	0.25708	0.51030
C10	1.0000	0.72897	0.27612	0.46606
C11	1.0000	0.68350	0.20407	0.52181
C12	1.0000	0.19655	0.67102	0.55787
C13	1.0000	0.27901	0.65387	0.49969
C14	1.0000	0.40644	0.69257	0.54792
C15	1.0000	0.22130	0.41380	0.54242
C16	1.0000	0.27386	0.30888	0.54479
C17	1.0000	0.16456	0.42574	0.50798
C18	1.0000	0.13740	0.42715	0.57179
C19	1.0000	0.79955	0.51199	0.50830
C20	1.0000	0.85689	0.49763	0.47411
C21	1.0000	0.88984	0.53023	0.53518
H20	1.0000	0.79366	0.48169	0.45471
H21	1.0000	0.92318	0.43903	0.47413
H22	1.0000	0.89886	0.56634	0.46704
H23	1.0000	0.85103	0.54762	0.55954
H24	1.0000	0.94061	0.59369	0.52739
H25	1.0000	0.94828	0.46696	0.53848
H26	1.0000	0.94029	0.30683	0.49685
H27	1.0000	0.90436	0.18195	0.50150
H28	1.0000	0.90376	0.26038	0.53711
H29	1.0000	0.69678	0.20533	0.54897
H30	1.0000	0.70924	0.13052	0.51258
H31	1.0000	0.59143	0.21508	0.51664
H32	1.0000	0.78612	0.32110	0.45100
H33	1.0000	0.63965	0.29951	0.46093
H34	1.0000	0.74029	0.19959	0.45745
H35	1.0000	0.42681	0.68220	0.57450
H36	1.0000	0.38855	0.77143	0.54364
H37	1.0000	0.48281	0.67175	0.53315
H38	1.0000	0.19686	0.62519	0.49109
H39	1.0000	0.34743	0.62155	0.48401
H40	1.0000	0.27645	0.73385	0.49530
H41	1.0000	0.11603	0.63843	0.54957
H42	1.0000	0.18640	0.75126	0.55476
H43	1.0000	0.20826	0.65592	0.58463

H44	1.0000	0.22920	0.42368	0.48790
H45	1.0000	0.11415	0.49448	0.50576
H46	1.0000	0.10659	0.36427	0.50373
H47	1.0000	0.18185	0.41364	0.59560
H48	1.0000	0.06887	0.37304	0.56956
H49	1.0000	0.09673	0.50045	0.57293
H50	1.0000	0.32627	0.29033	0.52277
H51	1.0000	0.20318	0.25655	0.54608
H52	1.0000	0.32677	0.29860	0.56734
C22	1.0000	0.71822	0.60290	0.50642
H53	1.0000	0.65224	0.59516	0.48705
H54	1.0000	0.49092	0.34376	0.53389
C23	1.0000	0.50930	0.48294	0.73206
H55	1.0000	0.92926	0.56919	0.69691
C24	1.0000	0.51126	0.54473	0.76420
C25	1.0000	0.52916	0.37339	0.73989
C26	1.0000	0.76285	0.54204	0.71894
C27	1.0000	0.80436	0.45122	0.73860
C28	1.0000	0.77135	0.63549	0.74049
H56	1.0000	0.79334	0.38321	0.72425
H57	1.0000	0.75931	0.44407	0.76258
H58	1.0000	0.89670	0.45722	0.74427
H59	1.0000	0.74046	0.70120	0.72682
H60	1.0000	0.86215	0.64671	0.74700
H61	1.0000	0.72316	0.63117	0.76400
H62	1.0000	0.58969	0.53107	0.77887
H63	1.0000	0.43757	0.52589	0.78007
H64	1.0000	0.50391	0.62411	0.75895
H65	1.0000	0.60800	0.35877	0.75423
H66	1.0000	0.45662	0.34676	0.75487
H67	1.0000	0.81296	0.61835	0.67282
P3	1.0000	0.61205	0.53877	0.70047
C29	1.0000	0.38936	0.49641	0.71607
H68	1.0000	0.32315	0.47590	0.73430
H69	1.0000	0.37955	0.44878	0.69413
H70	1.0000	0.53365	0.32938	0.71689
C30	1.0000	0.84123	0.55536	0.68828
H71	1.0000	0.84407	0.48971	0.67236
H72	1.0000	0.37184	0.57304	0.70843

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