Mechanistic studies on the interaction of [(κ^3-*P,P,P*-NP_3)IrH_3] [NP_3 = $N(CH_2CH_2PPh_2)_3$] with HBF_4 and fluorinated alcohols by combined NMR, IR and DFT techniques.

Supporting Information

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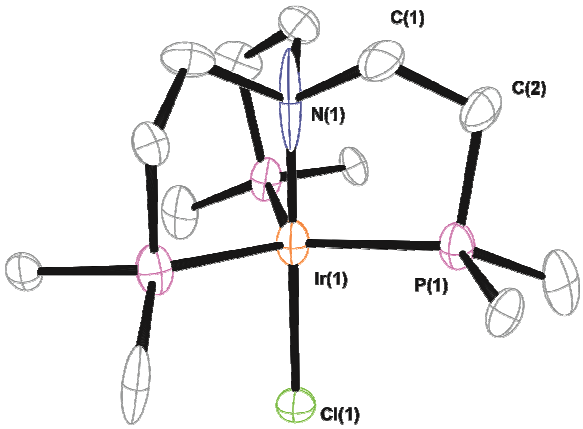


Figure S1. Molecular structure of [(κ^4-NP_3)IrCl] (**1**) (50% probability level). All the hydrogen atoms and the carbon atoms of the phenyl rings on NP_3 (apart from C_{ipso}) are omitted for clarity. Selected bond lengths and angles are given in Table S2.

Table S1. Crystal data and structure refinement for **1**.

CCDC	769848	
Empirical formula	C_{42} H_{42} Cl Ir N P_3	
Formula weight	881.33	
Temperature	150(2) K	
Wavelength	0.71069 Å	
Crystal system	Hexagonal	
Space group	*P* 6_3	
Unit cell dimensions	a = 13.431(9) Å	α= 90°.
	b = 13.431(9) Å	β= 90°.
	c = 11.524(13) Å	γ = 120°.
Volume	1800.3(4) $Å^3$	
Z	2	
Density (calculated)	1.626 Mg/m^3	
Absorption coefficient	3.948 mm^{-1}	
F(000)	880	
Crystal size	0.01 x 0.01 x 0.02 mm^3	
Theta range for data collection	3.92 to 26.46°.	
Index ranges	-9<=h<=16, -14<=k<=15, -6<=l<=14	
Reflections collected	2644	
Independent reflections	1458 [R(int) = 0.0698]	
Completeness to theta = 26.46°	81.7 %	
Refinement method	Full-matrix least-squares on F^2	
Absorption correction	Semi-empirical from equivalents	
Data / restraints / parameters	1458 / 1 / 139	
Goodness-of-fit on F^2	0.852	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.0645	
R indices (all data)	R1 = 0.0785, wR2 = 0.0695	
Absolute structure parameter	0.031(16)	
Largest diff. peak and hole	1.103 and -0.847 e.$Å^{-3}$	

Table S2. Selected bond lengths [Å] and angles [°] for **1**.

C(1)-C(2)	1.506(14)
C(1)-N(1)	1.57(2)
C(2)-P(1)	1.793(13)
C(3)-P(1)	1.828(9)
N(1)-Ir(1)	1.96(4)
P(1)-Ir(1)	2.266(3)
Cl(1)-Ir(1)	2.391(8)
C(2)-C(1)-N(1)	107.7(12)
C(1)-C(2)-P(1)	107.6(9)
C(1)-C(2)-H(2A)	110.2
C(1)-N(1)-Ir(1)	117.0(14)
C(2)-P(1)-Ir(1)	101.3(4)
N(1)-Ir(1)-P(1)	85.04(14)
N(1)-Ir(1)-P(1)#1	85.04(14)
P(1)-Ir(1)-P(1)#1	119.26(4)
N(1)-Ir(1)-P(1)#2	85.04(14)
P(1)-Ir(1)-P(1)#2	119.26(4)
P(1)#1-Ir(1)-P(1)#2	119.26(4)
N(1)-Ir(1)-Cl(1)	180.000(9)
P(1)-Ir(1)-Cl(1)	94.96(14)
P(1)#1-Ir(1)-Cl(1)	94.96(14)
P(1)#2-Ir(1)-Cl(1)	94.96(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x+y,-x+1,z #2 -y+1,x-y+1,z

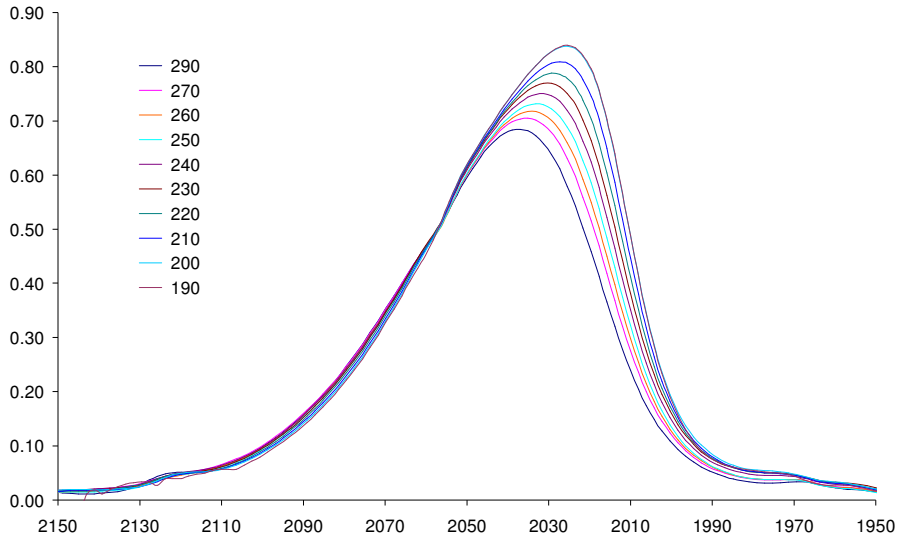


Figure S2. Variable temperature IR spectra (ν_{IrH} region) of $NP_3Ir(H)_3$ (0.01 M) in CH_2Cl_2. d=1.2 mm.

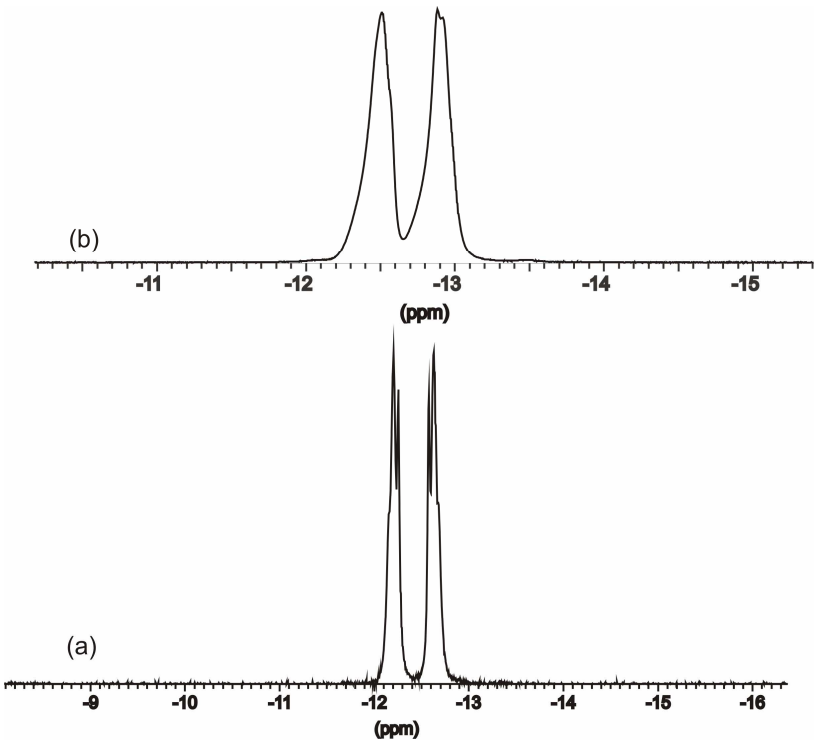


Figure S3. ^1H NMR spectra of (a) (κ^3-NP_3)$Ir(H)_3$ (0.04 M, δ_{MH} region) and (b) the mixture of (κ^3-NP_3)$Ir(H)_3$ and TFE (6 equivalents). CD_2Cl_2, 190 K.

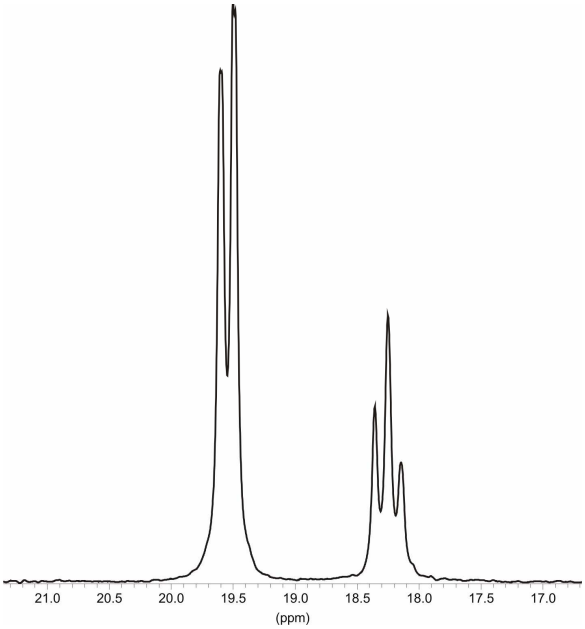


Figure S4. $^{31}P\{^{1}H\}$ spectrum of **5b** (CD_2Cl_2, 298 K).

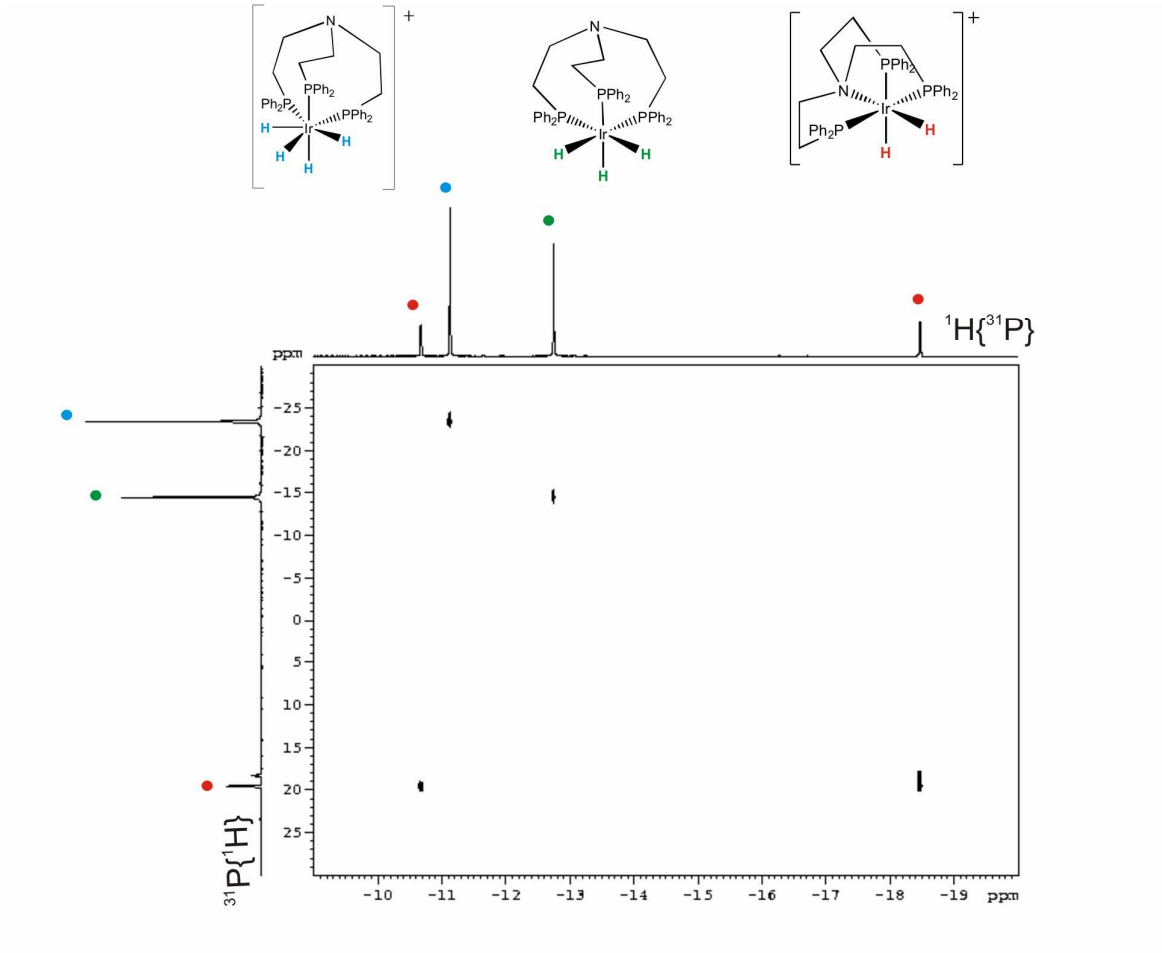


Figure S5. 2D-HETCOR $^{1}H\{^{31}P\}$-$^{31}P\{^{1}H\}$ NMR spectrum of the $NP_3Ir(H)_3$ / $[NP_3Ir(H)_4]^+$ / $[NP_3Ir(H)_2]^+$ mixture (CD_2Cl_2).

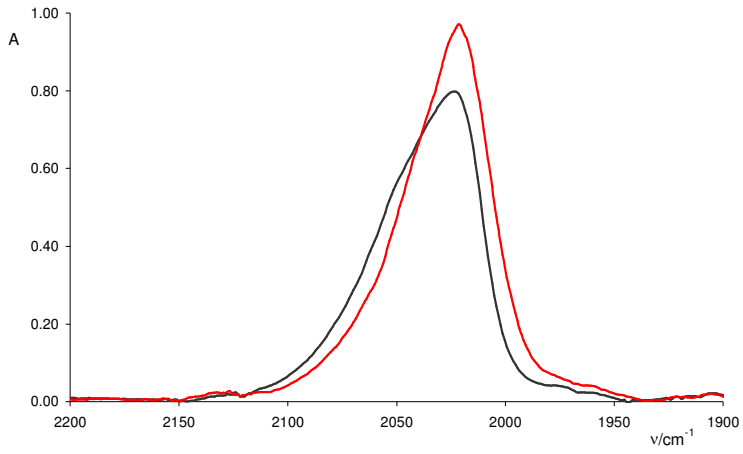
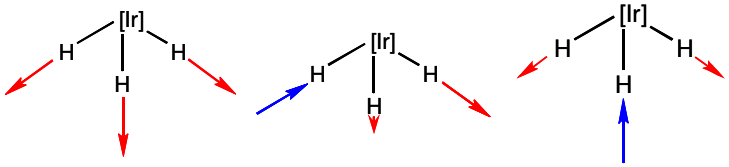


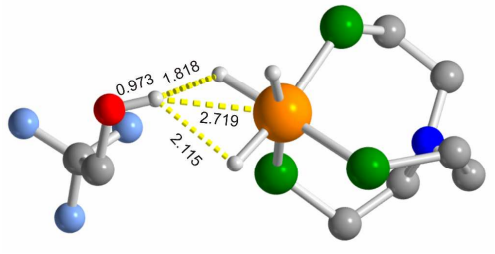
Figure S6. IR spectra (ν_{IrH} region) of NP_3IrH_3 (**3**, 0.005 M, black line) and **3** in the presence of 10 equiv. HFIP. 190 K, CH_2Cl_2. d = 2.2 mm.

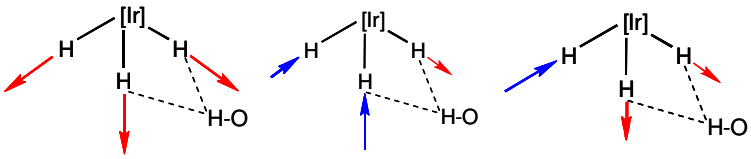
(κ^3-NP_3)IrH_3

3^t



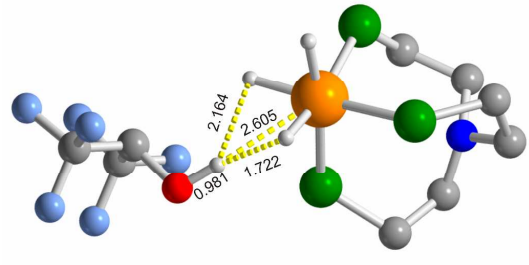
ν, cm^{-1}	2228	2197	2151
A, 10^4 L $mol^{-1}cm^{-2}$	2.63	2.51	2.44

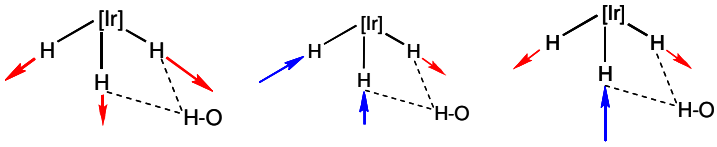




3a^t

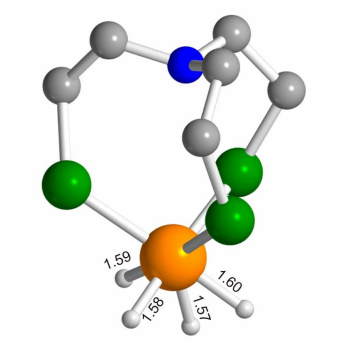
ν, cm^{-1}	2224	2185	2169
A, 10^4 L $mol^{-1}cm^{-2}$	2.85	2.39	2.43

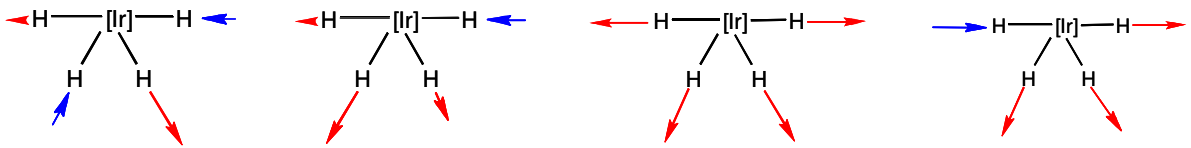




3b^t

ν, cm^{-1}	2218	2144	2113
A, 10^4 L $mol^{-1}cm^{-2}$	3.57	2.22	2.98





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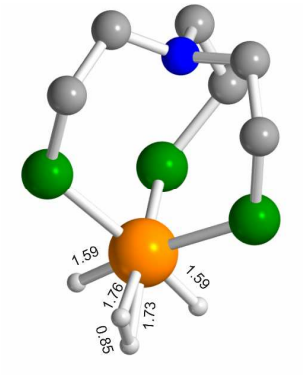
ν, cm^{-1}	2363	2252	2247	2219
A, 10^4 L $mol^{-1}cm^{-2}$	0.61	0.40	0.48	1.52



DIH

ν, cm^{-1}	2968	2254	2225	1844
A, 10^4 L $mol^{-1}cm^{-2}$	0.15	1.36	1.75	0.47

Figure S7. The Ir–H normal modes of the DFT optimized complexes with their frequency and intensity (*A*).

Optimised geometries (*.xyz files plus related absolute internal energy, in the gas-phase and in dichloromethane).

3^t

E(gas) = -419.891364 ha.

E(CH_2Cl_2) = -419.903525 ha.

Ir	-1.313800	-0.001613	0.005066
P	-0.188485	2.015883	0.131466
P	-0.156569	-1.132022	1.664609
P	-0.178618	-0.898772	-1.804140
N	2.297048	0.009188	-0.004745
C	1.525166	-0.597832	2.284233
H	1.434946	0.449323	2.590661
H	1.794840	-1.181997	3.167383
C	2.587387	-0.653542	-1.274361
H	3.573864	-1.146613	-1.252313
H	2.640853	0.113279	-2.052884
C	2.601287	-0.754834	1.203295
H	3.584550	-0.475398	1.617708
H	2.669424	-1.811383	0.926858
C	1.515639	-1.678277	-1.664675
H	1.444930	-2.468171	-0.909877
H	1.779950	-2.148448	-2.615174
C	1.499138	2.290772	-0.626452
H	1.418142	2.036177	-1.688181
H	1.762662	3.349334	-0.558702
C	2.579868	1.441928	0.054050

H	3.562382	1.674334	-0.390688
H	2.640256	1.730308	1.107652
H	-2.353033	0.547678	1.086445
H	-2.350232	0.624614	-1.034029
H	-2.350267	-1.216645	-0.029566
H	0.083018	-0.066806	-2.937483
H	-0.829721	-1.938168	-2.524571
H	0.084350	2.574953	1.419275
H	-0.843275	3.162966	-0.396828
H	-0.804941	-1.299824	2.919736
H	0.144728	-2.515230	1.462116

5^{t}

E(gas) = -419.122015 ha.

E(CH_2Cl_2) = -419.183827 ha.

Ir	0.367987	4.767649	4.357316
H	-0.462693	5.189245	5.606010
H	0.040127	6.255267	3.871390
P	0.859952	2.610531	5.082797
P	-1.446117	4.258003	3.083439
P	2.305017	5.697016	5.113953
C	2.722677	5.182125	2.420087
H	2.276068	6.136333	2.139069
H	3.396252	4.868093	1.614119
N	1.586803	4.195576	2.529671
C	2.312910	2.187230	3.991613

H	3.193555	2.616540	4.473215
H	2.474158	1.110470	3.918043
C	2.091942	2.767950	2.587619
H	3.019611	2.705007	2.008329
H	1.354628	2.147858	2.076559
C	-0.676787	3.702499	1.474674
H	-0.606741	2.612451	1.504506
H	-1.307521	3.959273	0.622216
C	3.508694	5.364539	3.721064
H	4.213565	6.190308	3.612311
H	4.091624	4.476459	3.968727
C	0.699003	4.359250	1.316216
H	1.212176	3.950031	0.437794
H	0.569843	5.431212	1.166232
H	-2.352573	5.281858	2.725398
H	-2.357991	3.213115	3.381905
H	1.337332	2.291127	6.378567
H	-0.026456	1.515206	4.895642
H	3.010270	5.252470	6.263173
H	2.363959	7.093857	5.322064

3a^{t}

E(gas) = -872.653314 ha.

E(CH_2Cl_2) = -872.662511 ha.

Ir	4.533731	4.242172	4.353935
P	5.530975	4.123432	6.452548
P	3.435726	6.259816	4.632488

P	2.727693	2.852455	4.795185
N	2.528207	4.808923	7.304780
C	3.112623	7.015254	6.308748
H	4.071088	7.057170	6.835445
H	2.753630	8.039901	6.187103
C	1.499618	3.780919	7.157132
H	0.565287	4.072561	7.664156
H	1.853958	2.873545	7.655575
C	2.093049	6.190359	7.104116
H	1.885287	6.689015	8.064896
H	1.148072	6.170834	6.552638
C	1.201773	3.454266	5.688075
H	0.847839	4.345396	5.160092
H	0.417326	2.696459	5.624717
C	4.592509	3.581677	7.973991
H	4.146239	2.607775	7.749333
H	5.291402	3.443334	8.802464
C	3.509273	4.593370	8.367136
H	3.022851	4.265877	9.300740
H	3.986333	5.553449	8.586234
H	5.780987	5.108036	3.866675
H	5.341882	2.932497	3.905741
H	4.120631	4.277309	2.809738
H	2.944140	1.662343	5.556927
H	2.109017	2.219316	3.682921
H	6.135138	5.300266	6.985572
H	6.669263	3.282284	6.586216
H	3.996460	7.384384	3.970365
H	2.117004	6.393566	4.098750

H	6.692073	4.039342	2.712458
O	7.579137	3.773834	2.412593
C	8.221484	3.023016	3.434661
C	9.042831	3.904244	4.329350
H	8.899314	2.308799	2.971362
H	7.510225	2.487498	4.066599
F	10.054002	4.555836	3.666182
F	8.287940	4.874488	4.967342
F	9.629764	3.141623	5.330206

3b^{t}

E(gas) = -1209.684181 ha.

E(CH_2Cl_2) = -1209.691087 ha.

C	1.781193	1.447005	2.957756
C	3.010113	0.694921	2.496511
H	3.054501	0.775076	1.406604
C	2.972789	-0.781474	2.829569
O	4.122066	1.263389	3.120066
H	4.752764	1.542381	2.422224
F	1.853064	2.748563	2.521229
F	1.655220	1.467353	4.323499
F	0.626163	0.899284	2.439501
F	2.857321	-1.021339	4.175582
F	4.144181	-1.377610	2.403207
F	1.937274	-1.429465	2.194714
H	5.892100	2.439007	1.492243
Ir	6.428104	1.352386	0.435821
P	8.368576	2.620678	0.358558

P	7.125869	-0.127561	2.112630
P	6.905297	-0.035431	-1.350800
H	5.752551	2.368857	-0.589918
H	4.960875	0.715307	0.433432
C	9.886134	2.086913	-0.588484
H	9.011567	2.963270	1.587320
H	8.234888	3.946778	-0.133014
C	8.925739	-0.316956	2.571684
H	6.565129	0.034607	3.406628
H	6.810895	-1.509403	1.959273
C	8.041705	-1.509883	-1.223199
H	7.477214	0.557181	-2.517633
H	5.798269	-0.644523	-2.000023
H	9.568054	1.835348	-1.605130
H	10.586890	2.922362	-0.655983
C	10.562425	0.883449	0.079318
H	9.322968	0.682688	2.772321
H	9.002038	-0.895956	3.495081
C	9.724014	-1.002555	1.456957
C	9.496920	-1.074781	-1.013710
H	7.693908	-2.114433	-0.380317
H	7.956282	-2.115781	-2.128174
N	9.667418	-0.267298	0.193246
H	11.480751	0.625093	-0.472226
H	10.873702	1.170120	1.088370
H	10.765250	-1.149406	1.786320
H	9.307806	-2.000009	1.287380
H	10.147887	-1.963760	-0.997536
H	9.812444	-0.472834	-1.871434

TETRA

E(gas) = -420.278032 ha.

E(CH_2Cl_2) = -420.336394 ha.

Ir	5.720338	3.055980	5.373178
P	6.708605	5.212056	5.709124
P	4.944258	3.405553	3.160708
P	3.614382	3.593138	6.349300
N	3.938005	6.069869	4.433786
C	4.889773	5.078885	2.365225
H	5.867157	5.549229	2.504579
H	4.731296	4.952974	1.292084
C	2.695126	5.978578	5.210544
H	1.870928	6.514329	4.719027
H	2.854824	6.468536	6.174719
C	3.774351	5.931853	2.980207
H	3.744413	6.911389	2.483427
H	2.810342	5.453670	2.785798
C	2.283982	4.520929	5.448307
H	2.088636	4.010506	4.501873
H	1.369732	4.470285	6.043555
C	5.697883	6.728542	6.068499
H	5.060442	6.511623	6.930618
H	6.370193	7.540271	6.353437
C	4.858088	7.136611	4.853079
H	4.316367	8.066019	5.079313
H	5.525754	7.359724	4.016091

H	6.927804	2.269727	5.998792
H	5.938242	2.699685	6.917415
H	5.191472	1.572911	5.184314
H	3.688373	4.352227	7.546288
H	2.914558	2.465388	6.838827
H	7.516540	5.694702	4.643425
H	7.679853	5.270901	6.739905
H	5.626369	2.625493	2.199537
H	3.622394	2.947003	2.920851
H	7.007987	2.661010	4.521613

DIH

E(gas) = -420.278620 ha.

E(CH_2Cl_2) = -420.337211 ha.

Ir	0.104480	4.815609	5.124922
H	-1.305908	4.264069	5.604231
H	-0.485557	6.250252	5.475968
P	0.697624	2.547021	4.702164
P	-0.948834	5.172374	3.142773
P	2.050698	5.972526	4.370408
C	2.942103	4.773687	1.998147
H	2.712897	5.672441	1.420235
H	3.765313	4.263226	1.478595
N	1.740476	3.930012	2.038415
C	2.149627	2.037980	3.667691
H	3.047111	2.449969	4.130171
H	2.234890	0.949526	3.702599
C	2.000644	2.492629	2.208873

H	2.904920	2.201275	1.655618
H	1.170087	1.940347	1.759736
C	-0.716126	4.057390	1.684645
H	-0.880180	3.026796	2.010356
H	-1.488740	4.296416	0.949406
C	3.428868	5.207773	3.390051
H	4.228416	5.944749	3.285826
H	3.829456	4.369562	3.961408
C	0.678118	4.231027	1.067719
H	0.752220	3.600028	0.171482
H	0.793908	5.265464	0.736293
H	-0.658098	6.437564	2.567157
H	-2.354256	5.263696	3.254446
H	0.888065	1.747886	5.858448
H	-0.332940	1.776741	4.099844
H	2.769524	6.682775	5.365263
H	1.726411	7.071653	3.527954
H	0.171280	4.788638	6.857083
H	0.982083	4.664897	6.640580

3^t•••$(HFIP)_2$

E(gas) = -1999.496994 ha.

E(CH_2Cl_2) = -1999.476133 ha.

C	-3.755058	-2.279447	-0.808376
C	-2.417696	-2.190948	-0.106078
H	-1.712633	-2.831030	-0.643808
C	-2.452651	-2.649233	1.337265
O	-2.018262	-0.851083	-0.108326

H	-1.106270	-0.776463	-0.496008
F	-3.632929	-1.798650	-2.087499
F	-4.720243	-1.546846	-0.163011
F	-4.192469	-3.582041	-0.891504
F	-3.162547	-1.776248	2.128168
F	-1.161788	-2.687492	1.827368
F	-2.990523	-3.901509	1.488794
H	-0.033223	0.403756	-1.180830
Ir	1.270426	-0.498218	-0.925198
P	2.437662	1.476362	-1.271190
P	1.141139	-0.336156	1.417767
P	3.093084	-1.926883	-0.976482
H	1.168013	-0.677883	-2.505810
H	0.354373	-1.822846	-0.919309
C	4.285596	1.595950	-1.054614
H	2.059659	2.622782	-0.514743
H	2.302012	2.057705	-2.559326
C	2.241204	0.810080	2.392663
H	-0.114506	-0.039948	2.005043
H	1.396394	-1.534529	2.147941
C	4.235989	-2.195573	0.473221
H	4.083492	-1.678096	-1.973487
H	2.829908	-3.276646	-1.331696
H	4.741575	0.790966	-1.638986
H	4.636414	2.545310	-1.466050
C	4.679355	1.485408	0.423736
H	2.154114	1.802438	1.944762
H	1.869619	0.876106	3.417609
C	3.694421	0.326376	2.383844

C	5.072091	-0.941744	0.756126
H	3.615857	-2.448756	1.338119
H	4.888443	-3.047391	0.267818
N	4.236430	0.227771	1.026960
H	5.768529	1.616678	0.524837
H	4.212887	2.307365	0.974623
H	4.309264	0.990754	3.011531
H	3.742376	-0.666888	2.840107
H	5.766520	-1.141656	1.587662
H	5.689387	-0.722477	-0.120495
F	-1.582607	4.111735	1.436133
C	-1.127457	3.120850	0.606955
C	-2.195282	2.121381	0.222073
F	-0.094202	2.477397	1.264794
F	-0.571266	3.720312	-0.503901
H	-1.753815	1.466987	-0.532778
C	-3.416317	2.760538	-0.405580
O	-2.587020	1.432654	1.375265
F	-4.094261	3.577540	0.461488
F	-4.276841	1.767887	-0.812475
F	-3.080098	3.507972	-1.514331
H	-2.609451	0.487340	1.154233

DIH•[AHA]

E(gas) = -1999.469519 ha.

E(CH_2Cl_2) = -1999.450595 ha.

C	1.749250	3.272801	1.183613
C	2.566486	2.149414	0.572175

H	3.547828	2.183267	1.072816
C	2.849754	2.372053	-0.902295
O	1.893151	0.968627	0.738100
H	0.389256	0.396426	-0.662876
F	1.613756	3.058685	2.539873
F	0.464873	3.337990	0.668308
F	2.313398	4.519488	1.023088
F	1.695718	2.432645	-1.658281
F	3.589544	1.310761	-1.387171
F	3.569156	3.518513	-1.158571
H	0.278684	-0.085740	-1.346557
Ir	-1.371728	0.319134	-0.974528
P	-1.814478	-2.032540	-0.785576
P	-1.264096	0.736866	1.368423
P	-3.521490	0.914106	-1.298852
H	-1.360961	0.205145	-2.567405
H	-1.065132	1.844016	-1.244430
C	-3.546704	-2.660800	-0.505352
H	-1.166824	-2.779405	0.230721
H	-1.426179	-2.829119	-1.892833
C	-1.980486	-0.465088	2.589961
H	0.050600	0.930642	1.846268
H	-1.892448	1.935845	1.804812
C	-4.727335	1.180442	0.085127
H	-4.289741	0.040369	-2.118474
H	-3.680388	2.103761	-2.048973
H	-4.214189	-2.202224	-1.239822
H	-3.559139	-3.739377	-0.676515
C	-4.007108	-2.346989	0.923390

H	-1.539495	-1.442861	2.376395
H	-1.656130	-0.172807	3.591425
C	-3.508812	-0.513617	2.523304
C	-5.151958	-0.156792	0.703189
H	-4.244896	1.819861	0.829318
H	-5.595054	1.716281	-0.307999
N	-3.999550	-0.909142	1.198577
H	-5.001846	-2.785614	1.095942
H	-3.323950	-2.828854	1.628785
H	-3.893312	-1.187147	3.304048
H	-3.905112	0.481695	2.746787
H	-5.890555	0.023988	1.498607
H	-5.654682	-0.759182	-0.059413
F	2.026320	-3.647324	1.025396
C	1.839749	-2.447701	0.386649
C	3.093520	-1.596097	0.240298
F	0.869112	-1.761723	1.101674
F	1.264716	-2.730665	-0.848955
H	2.918097	-0.941694	-0.622334
C	4.297026	-2.445100	-0.095968
O	3.337469	-0.881752	1.395379
F	4.729340	-3.212495	0.954610
F	5.343650	-1.650545	-0.491634
F	4.006226	-3.302761	-1.145461
H	2.738908	-0.016342	1.252119

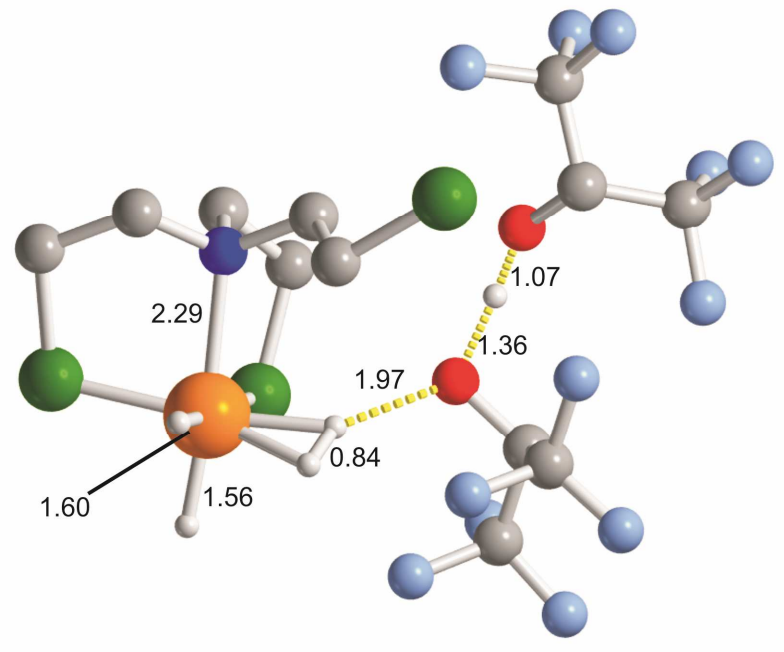


Figure S8. Optimized geometry of **(κ^3-*P,P,N*-NP_3)-DIH•[AHA].** Selected bond lengths reported (Å). Atom color code: see Figure 8 in the main text. Hydrogen atoms on the $N(CH_2CH_2PH_2)_3$ ligand and on HFIP omitted for clarity.

(κ^3-*P,P,N*-NP_3)-DIH•[AHA]

E(gas) = -1998.910550 ha.

E(CH_2Cl_2) = -1999.453231 ha.

C	-0.556698	3.394582	-0.616700
C	-1.353449	2.237224	-0.046744
H	-2.359339	2.321985	-0.480162
C	-1.534057	2.336988	1.457144
O	-0.720379	1.049665	-0.341779
H	1.087621	0.992283	0.450392
F	-0.518136	3.293566	-1.994390
F	0.756296	3.399246	-0.183644

F	-1.092029	4.625797	-0.317052
F	-0.326707	2.276861	2.135584
F	-2.284990	1.264435	1.899717
F	-2.175971	3.480467	1.866740
H	1.609841	1.295096	1.040585
Ir	2.698402	0.288445	0.169068
P	-1.359179	-1.845627	2.802684
P	1.903110	0.555619	-2.031066
P	4.571735	-0.860068	-0.224270
H	3.128467	0.043197	1.689879
H	3.465785	1.640537	0.254252
C	0.339670	-1.414150	2.097438
H	-1.055109	-3.197958	3.162943
H	-1.108839	-1.344910	4.116936
C	0.891805	-0.979112	-2.293870
H	1.079740	1.620025	-2.451581
H	2.832365	0.509427	-3.109513
C	4.127760	-2.662514	-0.000370
H	5.687735	-0.649236	0.617426
H	5.229840	-0.844679	-1.484478
H	0.411350	-0.327549	2.121300
H	1.125168	-1.823052	2.732491
C	0.403311	-1.919587	0.660389
H	-0.127402	-0.773080	-1.967198
H	0.847356	-1.255491	-3.348565
C	1.530942	-2.111040	-1.489080

C	2.700675	-2.771488	0.560299
H	4.230526	-3.172186	-0.958932
H	4.827328	-3.134129	0.691172
N	1.737175	-1.780619	-0.029848
H	0.127096	-2.982454	0.614692
H	-0.321754	-1.367604	0.065046
H	0.912432	-3.014552	-1.553424
H	2.509835	-2.343351	-1.915366
H	2.313765	-3.784505	0.388489
H	2.717944	-2.588050	1.631807
F	-3.839025	-2.832137	-1.759608
C	-3.444139	-2.443516	-0.503140
C	-3.265358	-0.946358	-0.375627
F	-2.242847	-3.081412	-0.242004
F	-4.360867	-2.942373	0.394951
H	-2.993085	-0.751090	0.668673
C	-4.549428	-0.183305	-0.636874
O	-2.299777	-0.543530	-1.286778
F	-5.007430	-0.318017	-1.922218
F	-4.317357	1.164530	-0.421387
F	-5.569199	-0.555062	0.210805
H	-1.631471	0.177983	-0.852528