

**Electronic Supplementary Information for**  
**An Imine Gallium Lewis Pair Stabilized**  
**Oxophosphinidene via an Unexpected Phosphirene**  
**Rearrangement**

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**Contents:**

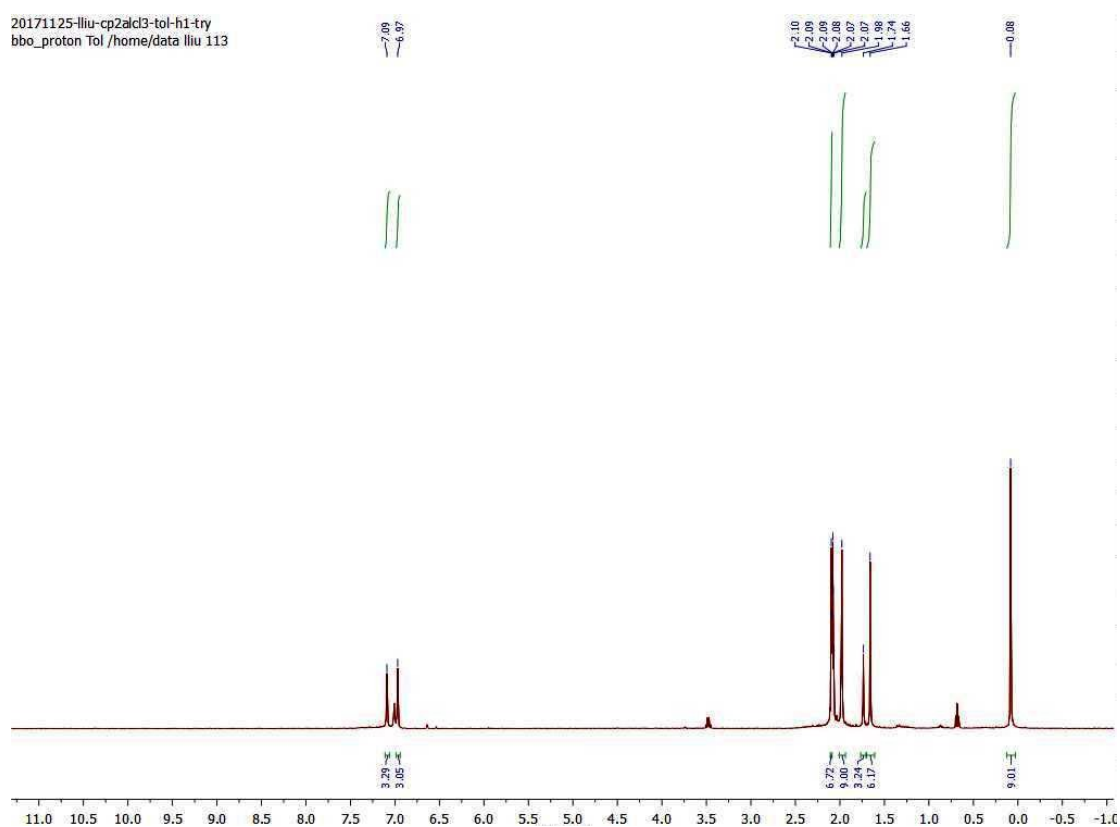
General-----	S2
Experimental Section-----	S3-S6
Details of Single Crystal X-ray Diffraction Study-----	S7-S8
Computational Details-----	S9-S24
References-----	S25

## General:

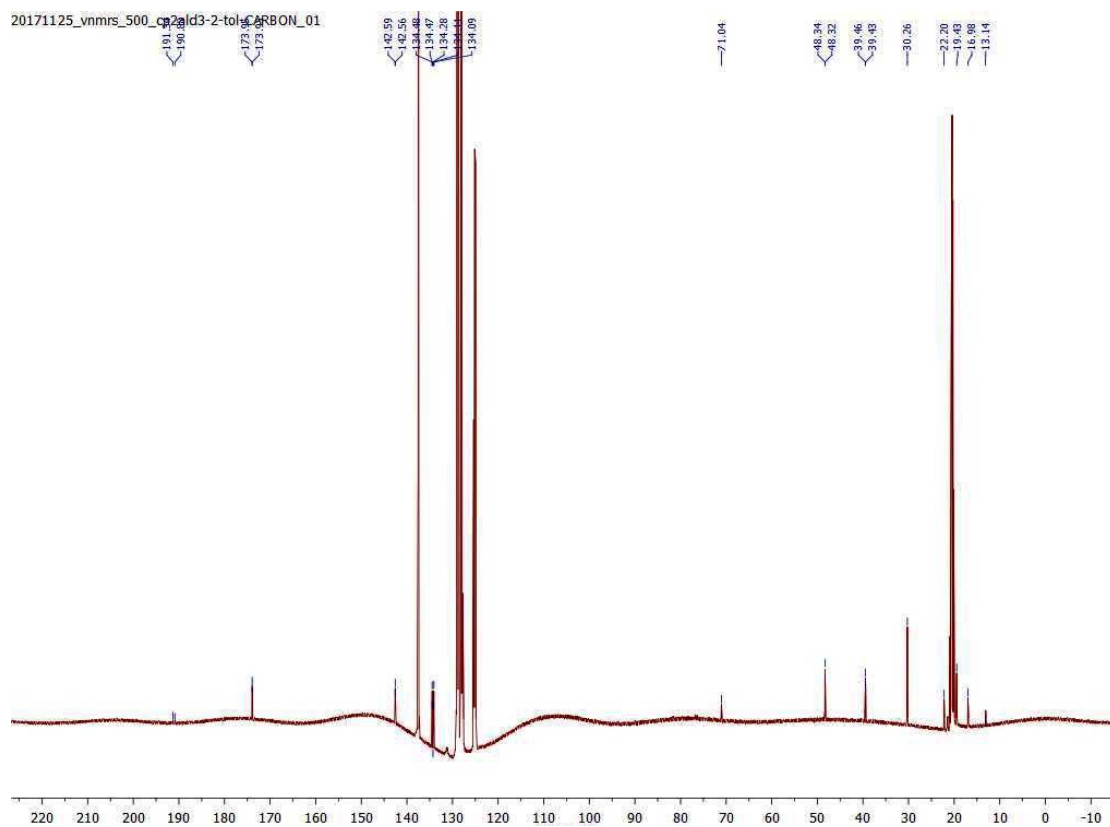
All manipulations were performed under an atmosphere of dry, oxygen-free N<sub>2</sub> by means of standard Schlenk or glovebox techniques (MBraun LABmaster SP drybox and Innovation Technology glovebox both equipped with a -35 °C freezer). Toluene, pentane, and dichloromethane (DCM) were collected from a Grubbs-type column system manufactured by Innovative Technology. These solvents, along with FC<sub>6</sub>H<sub>5</sub>, were dried over 4 Å molecular sieves. Molecular sieves, type 4 Å (pellets, 3.2 mm diameter) purchased from Sigma-Aldrich were activated prior to usage by iteratively heating with 1050 W Haier microwave for 5 min and cooling under vacuo. The process was repeated until no further moisture was released upon heating. Toluene-d<sub>8</sub> (CD<sub>3</sub>C<sub>6</sub>D<sub>5</sub>) and chloroform-d (CDCl<sub>3</sub>), purchased from Cambridge Isotope Laboratories, were degassed and stored over 4 Å molecular sieves in the glovebox for at least 8 h prior to use. AlCl<sub>3</sub> and GaCl<sub>3</sub> were purchased and used directly. Spectra were recorded on a Bruker Avance III 400 MHz and an Agilent DD2 600 MHz spectrometer and spectra were referenced to residual solvents of CDCl<sub>3</sub> (<sup>1</sup>H = 7.26 ppm; <sup>13</sup>C = 77.0 ppm) and CD<sub>3</sub>C<sub>6</sub>D<sub>5</sub> (<sup>1</sup>H (CH<sub>3</sub>) = 2.08 ppm; <sup>13</sup>C (CH<sub>3</sub>C) = 137.5 ppm). Chemical shifts (δ) are reported in ppm and the absolute values of the coupling constants (*J*) are in Hz.

## Experimental Section:

Synthesis of **2**: A mixture of **1** (30 mg, 0.063 mmol) and AlCl<sub>3</sub> (16.5 mg, 0.126 mmol) was stirring in toluene (2 mL) at room temperature for 12h, giving an orange solution. The solvent was removed under reduced pressure and the residue was washed with pentane (3 mL), yielding **2** as a pale yellow powder (49 mg, 86%). Colorless single crystals were obtained by vapor diffusion of pentane into a saturated FC<sub>6</sub>H<sub>5</sub> solution of **2**. <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>C<sub>6</sub>D<sub>5</sub>): δ (ppm) 7.09 (s, 2H, Ar-H), 6.97 (s, 2H, Ar-H), 2.10 (s, 6H, *p*-Ar-Me), 1.98 (bs, 9H, *o*-Ar-Me and CMe<sub>2</sub>), 1.74 (s, 3H, CMe<sub>2</sub>), 1.66 (s, 6H, *o*-Ar-Me), 0.08 (s, 9H, CMe<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (126 MHz, CD<sub>3</sub>C<sub>6</sub>D<sub>5</sub>): δ (ppm) 191.1 (d, J<sub>C-P</sub> = 57.8 Hz, CP=C*t*Bu), 173.9, 173.9 (C=O), 142.6, 142.5, 134.5, 134.5, 134.1, 134.1 (Ar-C), 71.4 (bs, CP=C*t*Bu), 48.3, 48.3 (CMe<sub>2</sub>), 39.4, 39.4, 30.3 (Ar-Me), 22.2, 19.4, 17.0, 13.1 (CMe<sub>2</sub> and CMe<sub>3</sub>). <sup>31</sup>P{<sup>1</sup>H} NMR (162 MHz, CD<sub>3</sub>C<sub>6</sub>D<sub>5</sub>): δ (ppm) 87.5 (s). Elemental analysis for C<sub>29</sub>H<sub>37</sub>Al<sub>2</sub>Cl<sub>6</sub>N<sub>2</sub>O<sub>2</sub>P: calcd.: C 46.86, H 5.02, N 3.77, found: C 46.98, H 4.88, N 3.64.

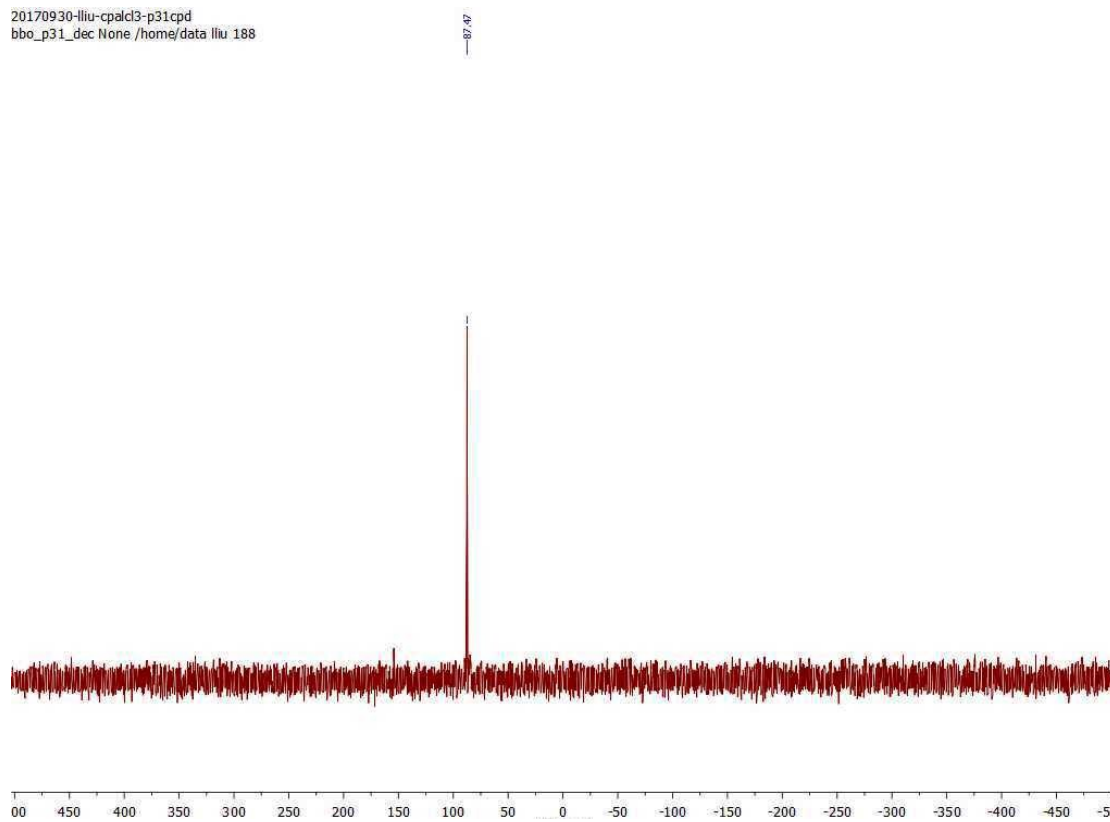


<sup>1</sup>H NMR spectrum of **2** (500 MHz, CD<sub>3</sub>C<sub>6</sub>D<sub>5</sub>).



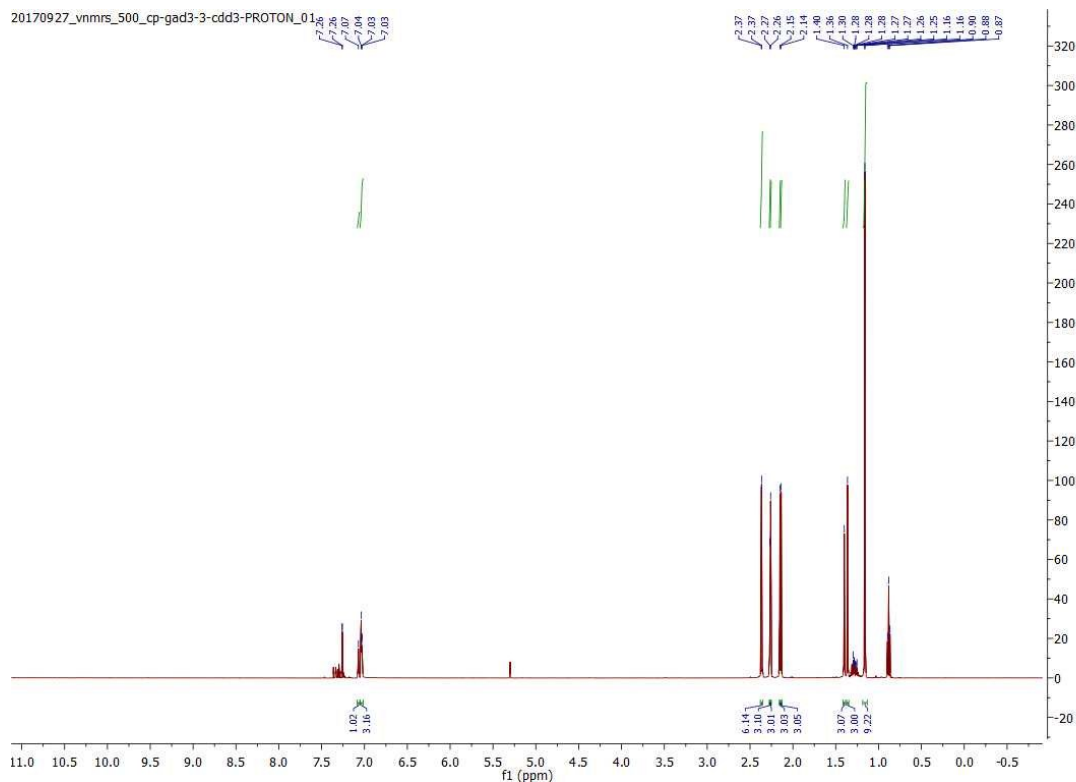
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2** (126 MHz,  $\text{CD}_3\text{C}_6\text{D}_5$ ).

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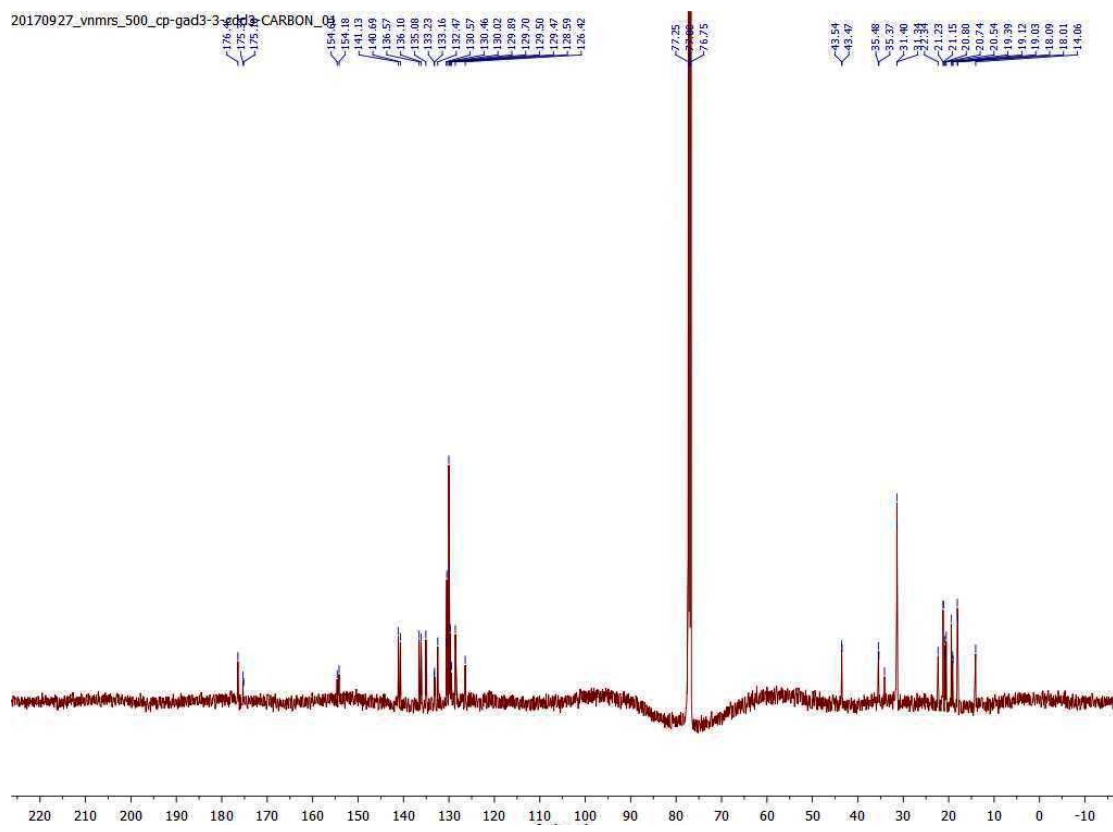


$^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **2** (162 MHz,  $\text{CD}_3\text{C}_6\text{D}_5$ ).

Synthesis of **3**: A mixture of **1** (30 mg, 0.063 mmol) and GaCl<sub>3</sub> (10.9 mg, 0.063 mmol) was stirring in DCM (2 mL) at room temperature for 12h, giving an orange solution. The solvent was removed under reduced pressure and the residue was washed with pentane (3 mL), yielding **3** as a light yellow powder (30.3 mg, 74%). Yellow single crystals were obtained by vapor diffusion of pentane into a saturated FC<sub>6</sub>H<sub>5</sub> solution of **3**. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ (ppm) 7.07 (bs, 1H, Ar-*H*), 7.04 (bs, 2H, Ar-*H*), 7.03 (bs, 1H, Ar-*H*), 2.37 (bs, 6H, Ar-*Me*), 2.27 (s, 3H, Ar-*Me*), 2.26 (s, 3H, Ar-*Me*), 2.15 (s, 3H, Ar-*Me*), 2.14 (s, 3H, Ar-*Me*), 1.40 (s, 3H, CMe<sub>2</sub>), 1.36 (s, 3H, CMe<sub>2</sub>), 1.16 (s, 9H, CMe<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (126 MHz, CDCl<sub>3</sub>): 176.5 (C=O), 175.3 (d, J<sub>C-P</sub> = 20.3 Hz, C=N), 154.4 (d, J<sub>C-P</sub> = 52.2 Hz, CP), 141.1, 140.7, 136.6, 136.1, 135.1, 132.5, 130.6, 130.5, 130.0, 129.9, 129.5, 128.6, 126.4 (C<sub>Ar</sub> and C=CP), 43.5 (d, J<sub>C-P</sub> = 8.4 Hz, CMe<sub>2</sub>), 35.4 (d, J<sub>C-P</sub> = 14.1 Hz, CMe<sub>3</sub>), 31.4 (Me), 31.3 (Me), 21.2 (d, J<sub>C-P</sub> = 10.2 Hz, Ar-*Me*), 20.8 (d, J<sub>C-P</sub> = 9.3 Hz, Ar-*Me*), 20.5 (d, J<sub>C-P</sub> = 4.9 Hz, Ar-*Me*), 19.4 (Ar-*Me*), 19.1 (d, J<sub>C-P</sub> = 9.3 Hz, Ar-*Me*), 18.1 (d, J<sub>C-P</sub> = 9.3 Hz, Ar-*Me*). <sup>31</sup>P{<sup>1</sup>H} NMR (162 MHz, CDCl<sub>3</sub>): δ (ppm) 167.1 (s). Elemental analysis for C<sub>29</sub>H<sub>37</sub>GaCl<sub>3</sub>N<sub>2</sub>O<sub>2</sub>P: calcd.: C 53.37, H 5.71, N 4.29, found: C 53.19, H 5.86, N 4.46.

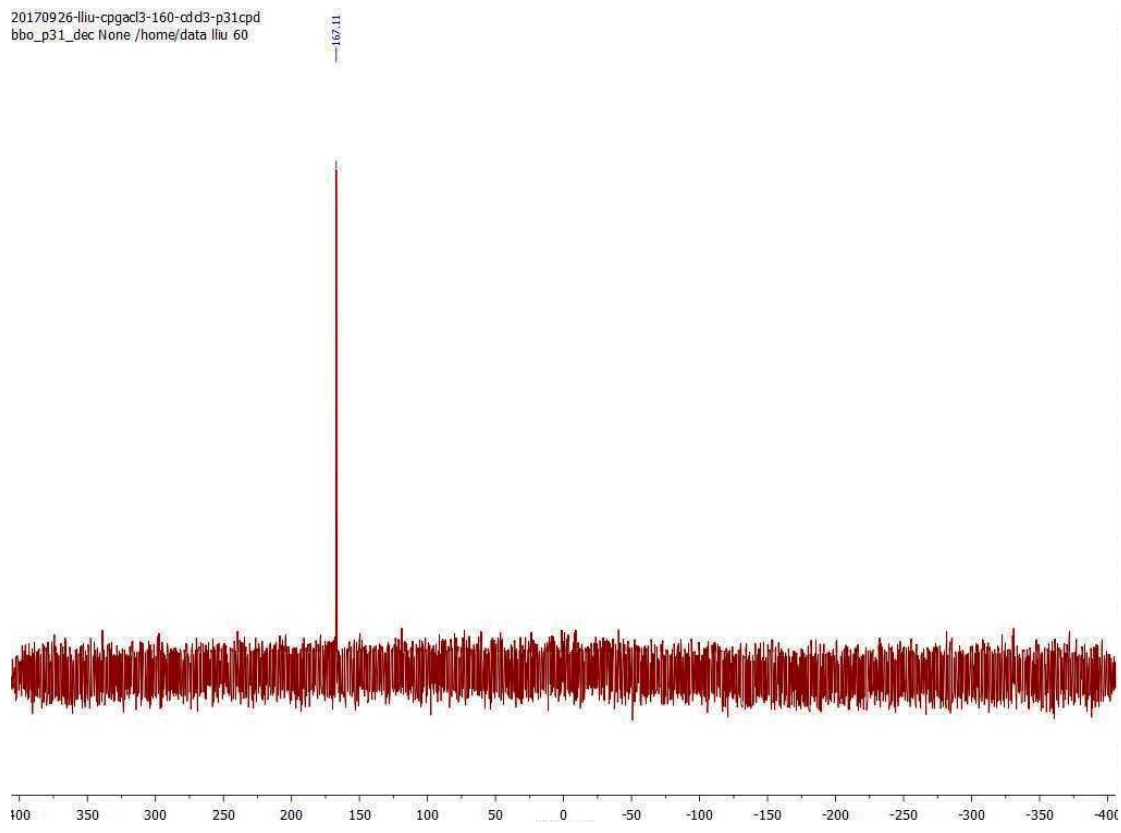


<sup>1</sup>H NMR spectrum of **3** (500 MHz, CDCl<sub>3</sub>).



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3** (126 MHz,  $\text{CDCl}_3$ ).

20170926-lliu-cpgad3-160-odd3-p31.cpd  
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$^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **3** (162 MHz,  $\text{CDCl}_3$ ).

## Details of Single Crystal X-ray Diffraction Study:

**X-ray Data Collection and Reduction.** Crystals were coated in Paratone-N oil in an N<sub>2</sub> filled glovebox, mounted on a MiTegen Micromount, and placed under a N<sub>2</sub> stream, thus maintaining a dry, O<sub>2</sub>-free environment for each crystal. The data were collected on a Bruker Apex II diffractometer using a graphite monochromator with Mo K $\alpha$  radiation ( $\lambda = 0.71073$  Å). The data were collected at 150(2) K for all crystals. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. Data were corrected for absorption effects using the empirical multiscan method (SADABS).

**Structure Solution and Refinement.** The structures were solved by direct methods using XS and subjected to full-matrix least-squares refinement on F<sup>2</sup> using XL as implemented in the SHELXTL suite of programs. All non-hydrogen atoms were refined with anisotropically thermal parameters. Carbon bound hydrogen atoms were placed in geometrically calculated positions and refined using an appropriate riding model and coupled isotropic thermal parameters.

Table S1. Summary of crystallographic data for compound **2** and **3**.

	<b>2</b>	<b>3</b>
empirical formula	C32 H39.50 Al2 Cl6 F0.50 N2 O2 P	C30 H30 Cl3 Ga N2 O2 P
formula weight	791.28	657.60
crystal system	Monoclinic	Monoclinic
space group	P 21/n	P2 <sub>1</sub>
<i>a</i> (Å)	0.5780(6)	8.6585(4)
<i>b</i> (Å)	17.3535(9)	13.8981(6)
<i>c</i> (Å)	21.099(1)	25.9555(11)
$\alpha$ (deg.)	90	90
$\beta$ (deg.)	96.898(3)	90
$\gamma$ (deg.)	90	90
vol (Å <sup>3</sup> )	3845.0(3)	3123.4(2)
<i>Z</i>	4	4
$\mu$ (mm <sup>-1</sup> )	0.568	1.218
<i>F</i> (000)	1636.0	1348.0
<i>T</i> (K)	150	150
reflections collected	7842	6432

$R_{\text{int}}$	0.0622	0.0690
GOF(F <sup>2</sup> )	1.025	1.057
R1 indices	0.0594	0.0414
[I>2σ(I)]		
wR2 indices (all data)	0.1618	0.0932
CCDC No.	1587367	1587368

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## Computational Details

Calculations were carried out with the Gaussian 09 package.<sup>S1</sup> Geometry optimizations were performed with the M06-2X functional.<sup>S2</sup> The Def2-SVP basis set was used for all the atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide the thermal corrections of Gibbs free energy. Transition states were submitted to intrinsic reaction coordinate (IRC) calculations to determine two corresponding minima.

The single-point energy calculations were performed at the M06-2X/Def2-TZVP level of theory for solution-phase. The gas-phase geometry was used for all the solution phase calculations. The SMD method was used with CH<sub>2</sub>Cl<sub>2</sub>, while Bondi radii<sup>S3</sup> were chosen as the atomic radii to define the molecular cavity. The Gibbs energy corrections from frequency calculations were added to the single-point energies to obtain the Gibbs free energies in solution. All the solution-phase free energies reported in the paper correspond to the reference state of 1 mol/L, 298K. Natural bond orbital (NBO) calculations were carried out using NBO 6.0 program<sup>S4</sup> at the M06-2X/cc-pVTZ level of theory. Optimized structures were visualized by the Chemcraft.<sup>S5</sup>

### Energies of Intermediates and Transition States:

	Solvation Energies (Hartree)	Thermal Corrections of Gibbs Free Energies (Hartree)
<b>1</b>	-1728.626675	0.537346
GaCl <sub>3</sub>	-3305.639854	-0.028083
<b>IN1</b>	-5034.317706	0.531298
<b>TS1</b>	-5034.282545	0.531413
<b>IN2</b>	-5034.320638	0.527951
<b>TS2</b>	-5034.279538	0.535305
<b>IN3</b>	-5034.340451	0.535461

<b>TS3</b>	-5034.29622	0.533856
<b>IN4</b>	-5034.308374	0.533147
<b>TS4</b>	-5034.304333	0.530368
<b>3</b>	-5034.389248	0.532505

**Cartesian**

**Coordinates:**

For mechanistic study:

**1**

7	-1.248542	-0.002521	1.631640	6	-4.053486	1.260958	-1.290626
8	1.815030	0.168039	4.206004	6	-3.212159	2.176232	-0.652568
8	-2.575304	0.726200	3.316023	1	-3.268794	3.234616	-0.920612
7	1.094183	-0.233865	2.096685	6	-2.313793	1.781393	0.339092
6	0.903846	-0.096525	3.454834	6	-1.531782	2.808759	1.108282
6	-0.518581	-0.336373	3.956099	1	-0.581146	2.403156	1.473502
6	-1.548161	0.193466	2.961757	6	-3.184762	-1.943385	0.563842
6	-0.708394	0.348311	5.304132	1	-2.631721	-2.097314	1.499312
1	-0.561001	1.432692	5.214157	6	2.447334	-0.179551	1.607813
1	0.025559	-0.040765	6.019652	6	3.025885	1.075309	1.343686
1	-1.728201	0.169978	5.665075	6	4.307106	1.118154	0.797030
6	-0.724912	-1.859380	4.094855	1	4.755556	2.091779	0.582598
1	-0.606208	-2.385912	3.136557	6	5.041562	-0.046166	0.544783
1	-1.737087	-2.055235	4.476918	6	4.482181	-1.265386	0.918539
1	0.007112	-2.262766	4.809159	1	5.064729	-2.182987	0.798819
6	-2.224331	0.416721	0.662683	6	3.199958	-1.353728	1.473704
6	-3.116800	-0.511388	0.105019	6	2.306492	2.341989	1.714416
6	-4.005856	-0.071111	-0.880151	1	2.113349	2.351573	2.797736
1	-4.692518	-0.794973	-1.328035	6	2.716156	-2.691710	1.967413

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1	2.910054	3.221803	1.457607	1	-1.483483	0.217223	-2.137467
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1	1.342842	2.426421	1.197477				
1	3.474621	-3.132235	2.630555	<b>IN1</b>			
1	2.557523	-3.396453	1.136650	31	3.871109	-0.705433	-0.220873
1	-1.332998	3.703556	0.503143	15	-1.868660	1.069084	2.383730
1	-2.777356	-2.629420	-0.195277	17	4.391447	1.399190	-0.415864
1	-4.232303	-2.228497	0.735458	17	3.246964	-1.686943	-2.080908
6	6.403104	0.024986	-0.094056	17	5.135709	-1.918826	1.063266
1	6.950163	0.919738	0.232942	8	-1.520216	-3.379932	0.372433
1	7.005929	-0.859189	0.152017	7	-1.789233	-1.131466	0.439587
1	6.315003	0.074476	-1.190500	8	2.204150	-0.684129	0.769126
6	-5.034218	1.711342	-2.341384	7	0.172005	0.237743	0.540460
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1	-6.019276	1.910416	-1.891586	6	-3.450958	-1.354707	-1.357506
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6	0.272449	-0.770213	-0.237541	6	1.239538	-3.267296	0.717115
15	0.001765	-2.299225	0.335459	6	-5.835459	-1.350811	-0.820776
6	0.599101	-0.055648	-1.527999	6	-4.792421	-1.378198	-1.747932
6	0.825828	1.445820	-1.348823	6	0.873646	1.807109	-1.190487
1	1.749370	1.638291	-0.788999	6	1.281169	2.344451	1.166961
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6	1.878322	-0.692671	-2.095200	6	-2.381246	-1.521062	-2.405865
1	2.719615	-0.550790	-1.398276	6	-1.065252	-2.291041	0.622679
1	1.737632	-1.771966	-2.257098	6	0.770970	1.500517	0.174437
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6	1.820871	3.567961	0.763673	1	-4.505071	2.375142	1.237157
6	-2.791259	2.366251	-0.124430	1	-4.838374	3.039734	-0.386412
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6	-2.283821	3.765847	0.261656	1	-2.794110	4.528440	-0.345721
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6	1.333332	1.963260	2.622191	1	-7.649711	-0.300415	-1.318951
6	2.560059	5.220831	-0.989219	1	-7.914109	-1.884565	-0.566387
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1	2.222100	-3.204072	1.203500	1	2.378747	1.982447	2.963761
1	0.756625	-4.218942	0.966164	1	0.943407	0.955532	2.814831
1	1.390214	-3.222984	-0.370621	1	2.453772	5.992189	-0.215109
1	-5.025287	-1.448997	-2.813902	1	3.636266	5.048535	-1.146930
1	-1.388615	-1.667808	-1.966652	1	2.142884	5.606433	-1.928954
1	-2.608443	-2.405877	-3.016205	1	1.517350	3.288762	-2.601818
1	-2.335849	-0.656800	-3.085713				
1	1.248410	-2.019035	3.169157	<b>TS1</b>			
1	-0.397554	-1.321191	3.119660	31	3.737108	-1.058823	-0.447634
1	-0.178473	-3.092681	3.055069	15	-0.968243	1.538256	2.114645
1	-2.788759	1.099605	-1.899404	17	4.602747	0.947072	-0.573511
1	-3.210001	2.800031	-2.193684	17	2.505502	-1.619722	-2.199477
1	-1.516757	2.363039	-1.895591	17	5.133159	-2.618370	0.167063
1	-4.174431	-0.512261	2.981709	8	-1.665036	-3.223952	0.873866
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6	1.012826	-3.399132	0.997777	1	-0.882510	-1.398151	-1.438794
6	-5.491652	-1.452526	-1.453298	1	-1.552433	-2.989709	-1.837923
6	-4.238641	-1.667883	-2.028056	1	-1.725143	-1.641986	-2.986710
6	0.785779	1.927651	-1.278545	1	1.492116	-1.846223	3.228447
6	1.795634	2.056164	0.951623	1	-0.086933	-1.012972	3.301164
6	-2.224250	1.536816	0.957680	1	-0.014929	-2.790919	3.425759
6	0.354561	-2.071003	1.404281	1	-4.051774	1.005038	-1.134760
6	-1.729334	-1.905941	-1.921105	1	-4.164259	2.704761	-1.653854
6	-1.127990	-2.164103	1.028533	1	-2.615361	1.843372	-1.791860
6	1.112885	1.311015	-0.043758	1	-4.050788	0.082949	2.517600
6	0.434359	-1.913163	2.940269	1	-3.953726	-1.677644	2.712624
6	-1.707432	0.268915	1.148555	1	-5.537132	-0.885093	2.523877
6	-3.512926	1.961623	-1.170307	1	-0.194727	1.745219	-3.191043
6	1.161814	-0.924415	0.775443	1	0.653475	0.267265	-2.631082
6	-4.491570	-0.871535	2.191339	1	-0.879827	0.719536	-1.891203
6	0.049320	1.130984	-2.314179	1	2.667401	3.958135	1.437969
6	1.840145	4.001582	-0.540390	1	-4.998278	1.653552	1.089478
6	2.130434	3.391945	0.672364	1	-4.213837	2.904918	2.105287
6	-3.154284	2.466461	0.231574	1	-5.079535	3.367826	0.617323
6	-4.438187	2.599103	1.072532	1	-2.228246	4.223433	1.146488
6	-2.446963	3.826723	0.143068	1	-3.093275	4.548487	-0.376475
6	-6.753476	-1.545569	-2.269851	1	-1.498158	3.739888	-0.409415
6	2.287166	1.473563	2.250855	1	-7.311214	-0.598187	-2.240500
6	2.266924	5.414218	-0.835228	1	-7.417130	-2.328562	-1.874969
6	1.165466	3.242250	-1.509013	1	-6.534506	-1.780731	-3.318880

1	2.396891	2.265214	3.004542	6	-1.133114	-2.090581	0.625599
1	3.268836	1.005133	2.081705	6	1.346232	1.963777	0.577455
1	1.638180	0.688445	2.662334	6	0.034079	-1.608351	2.810091
1	2.524483	5.955249	0.084587	6	-2.029180	0.141445	0.822793
1	3.154843	5.418988	-1.486012	6	-3.429233	1.805927	-1.665633
1	1.474990	5.971123	-1.356103	6	0.962347	-0.391960	0.771347
1	0.928062	3.697188	-2.474897	6	-4.423379	-1.255588	2.288660
				6	0.365637	1.919795	-1.771890
<b>IN2</b>				6	2.919402	4.172351	-0.068897
31	2.898835	-1.038362	-1.408792	6	3.018371	3.569412	1.189866
15	-1.049069	1.244539	1.819564	6	-3.186402	2.342160	-0.248366
17	3.811730	0.776488	-2.183544	6	-4.528921	2.431254	0.497784
17	1.022374	-1.589565	-2.429668	6	-2.515471	3.717844	-0.291092
17	4.240898	-2.679620	-0.955576	6	-7.315239	-2.543487	-1.652962
8	-1.308619	-3.223590	0.270552	6	2.394221	1.781945	2.867545
7	-2.195052	-1.178485	0.538040	6	3.801171	5.336622	-0.434347
8	2.117211	-0.528620	0.291587	6	2.022741	3.637904	-0.992235
7	0.508386	0.848735	0.951338	1	-6.698304	-1.894662	0.928445
6	-4.573452	-1.582582	0.826570	1	2.162959	-2.674762	1.452462
6	-3.462028	-1.576741	-0.025823	1	0.745361	-3.769716	1.446382
6	-3.566649	-1.863088	-1.394072	1	1.298260	-3.046539	-0.065955
6	-5.821081	-1.886658	0.276754	1	-4.935720	-2.387889	-2.960104
6	1.179081	-2.865337	1.008858	1	-1.737448	-0.938646	-2.079176
6	-5.969709	-2.185526	-1.079376	1	-1.725893	-2.700276	-2.130056
6	-4.833701	-2.168017	-1.894312	1	-2.660423	-1.787656	-3.346433
6	1.228761	2.524838	-0.698601	1	0.979944	-1.321765	3.292301
6	2.245495	2.462801	1.533006	1	-0.749561	-0.916821	3.137616
6	-2.318571	1.390616	0.521275	1	-0.235188	-2.612738	3.163906
6	0.234744	-1.681142	1.274031	1	-3.913723	0.818284	-1.629963
6	-2.363858	-1.818538	-2.290561	1	-4.089352	2.493747	-2.215614

1	-2.486978	1.714467	-2.224354	17	-1.283409	3.184122	0.072881
1	-4.211347	-0.184148	2.438061	8	-1.576091	-1.351625	-3.084101
1	-3.590595	-1.818028	2.736065	7	-1.690234	-0.918651	-0.838698
1	-5.341281	-1.497148	2.838640	8	0.802043	0.959587	-1.016963
1	-0.102585	2.702157	-2.386053	7	1.651197	-0.714960	0.406253
1	0.987236	1.304217	-2.441432	6	-3.682348	-2.096369	-0.096945
1	-0.421696	1.270642	-1.365715	6	-3.122799	-0.996652	-0.761469
1	3.725084	3.968076	1.922062	6	-3.903516	0.019393	-1.322339
1	-5.021164	1.446712	0.528135	6	-5.067467	-2.126525	0.064851
1	-4.384904	2.787419	1.528703	6	1.226790	-0.804836	-3.113986
1	-5.196384	3.135508	-0.021529	6	-5.884380	-1.109493	-0.440193
1	-2.377791	4.117698	0.724419	6	-5.286743	-0.057954	-1.138524
1	-3.138031	4.423423	-0.860408	6	3.992001	-0.301299	-0.330129
1	-1.526874	3.660507	-0.769804	6	3.446872	-2.396930	0.793690
1	-8.131506	-2.203456	-1.002510	6	-0.952317	-0.098316	1.476135
1	-7.408962	-3.634424	-1.766752	6	0.502494	-1.237365	-1.836165
1	-7.454035	-2.096686	-2.647098	6	-3.280625	1.135003	-2.111781
1	3.097992	2.328631	3.506947	6	-1.015939	-1.155264	-2.043990
1	2.782816	0.759944	2.730829	6	3.033043	-1.129277	0.302145
1	1.434296	1.707514	3.401632	6	0.795646	-2.705216	-1.519664
1	4.064106	5.932879	0.449689	6	-0.907744	-0.594214	0.233533
1	4.738737	4.975684	-0.884905	6	-2.152938	-0.844471	3.479148
1	3.313121	5.994126	-1.165824	6	0.855660	-0.262113	-0.699985
1	1.950046	4.081066	-1.988756	6	-2.813633	-3.224977	0.393894
				6	3.718789	1.092763	-0.823946
				6	5.732136	-1.998454	-0.001155
<b>TS2</b>				6	4.780347	-2.786239	0.637929
31	0.839917	2.656870	-0.070354	6	-1.902286	0.364487	2.557411
15	0.426573	-1.267463	1.499149	6	-1.238843	1.481655	3.374562
17	1.959392	3.962782	-1.395533	6	-3.238405	0.853716	1.985998
17	1.700445	2.299583	1.914783				

6	-7.380313	-1.169665	-0.276848	1	-3.824698	0.030284	1.555290
6	2.556693	-3.397531	1.492635	1	-7.663613	-1.771365	0.596769
6	7.162633	-2.445563	-0.136047	1	-7.847547	-1.626810	-1.162810
6	5.303800	-0.765217	-0.477053	1	-7.807667	-0.164798	-0.159874
1	-5.522458	-2.969778	0.590517	1	3.092854	-4.349029	1.594400
1	2.311073	-0.951497	-3.002203	1	1.628462	-3.598660	0.943104
1	0.861163	-1.419239	-3.946553	1	2.270391	-3.070471	2.502083
1	1.024750	0.249683	-3.336580	1	7.229480	-3.534507	-0.264345
1	-5.914707	0.736260	-1.549960	1	7.649882	-1.964570	-0.994445
1	-2.318471	1.446580	-1.684299	1	7.739582	-2.182117	0.763991
1	-3.095443	0.796824	-3.142857	1	6.021630	-0.108244	-0.973588
1	-3.939762	2.011767	-2.141006				
1	1.871315	-2.866712	-1.364947	<b>IN3</b>			
1	0.241817	-3.048540	-0.632334	31	0.688294	2.636518	-0.279859
1	0.467113	-3.316049	-2.371630	15	0.990264	-0.150939	1.958146
1	-1.217710	-1.226306	3.917669	17	1.959953	4.014290	-1.364319
1	-2.808157	-0.534658	4.306424	17	1.591818	2.296168	1.843384
1	-2.652795	-1.661343	2.936558	17	-1.327284	3.369615	0.159485
1	-2.050834	-2.884275	1.110538	8	-1.528076	-1.454858	-3.082021
1	-2.282911	-3.695378	-0.448981	7	-1.612694	-0.786223	-0.876901
1	-3.419034	-3.995980	0.886405	8	0.732959	0.996593	-1.119946
1	4.657010	1.566653	-1.135533	7	1.611325	-0.546744	0.466903
1	3.033603	1.136082	-1.679087	6	-3.481746	-2.155468	-0.140388
1	3.306171	1.701231	-0.010861	6	-3.025718	-0.982753	-0.751265
1	5.077227	-3.763756	1.025710	6	-3.897382	-0.019936	-1.274401
1	-0.261959	1.162996	3.765260	6	-4.859744	-2.305948	0.035493
1	-1.082458	2.378244	2.761434	6	1.367443	-0.895264	-3.022336
1	-1.893551	1.738801	4.220687	6	-5.762985	-1.340418	-0.414469
1	-3.081431	1.620822	1.216289	6	-5.264475	-0.216750	-1.082411
1	-3.827630	1.299677	2.801621	6	3.931767	-0.409590	-0.413055



6	3.211156	-2.339251	0.909805	1	0.229881	-3.005782	-0.493642
6	-0.725958	-0.081353	1.414640	1	0.440727	-3.380771	-2.219428
6	0.549810	-1.268431	-1.795110	1	-1.103918	-1.473894	3.741084
6	-3.360822	1.165547	-2.023468	1	-2.743388	-0.889536	4.122507
6	-0.952132	-1.171609	-2.074683	1	-2.477828	-1.890097	2.676368
6	2.933727	-1.091469	0.308515	1	-1.683517	-2.847658	0.867011
6	0.786292	-2.732697	-1.401540	1	-2.094998	-3.727222	-0.619433
6	-0.723965	-0.402933	0.084784	1	-3.033291	-4.009198	0.864675
6	-2.041422	-1.097159	3.300355	1	4.688028	1.368539	-1.346584
6	0.645685	-0.276198	-0.615865	1	2.985051	1.035715	-1.742011
6	-2.521773	-3.240099	0.272106	1	3.417498	1.658773	-0.145510
6	3.741340	0.982415	-0.949485	1	4.677858	-3.880970	1.181328
6	5.460658	-2.286720	-0.037547	1	-0.336752	1.025154	3.904924
6	4.470012	-2.910853	0.722300	1	-1.150511	2.230286	2.868122
6	-1.803242	0.179642	2.478739	1	-2.026911	1.453962	4.216776
6	-1.290171	1.288279	3.417543	1	-2.981078	1.431851	1.126263
6	-3.139878	0.667591	1.899679	1	-3.725866	1.124172	2.711505
6	-7.246800	-1.511995	-0.222743	1	-3.739529	-0.149691	1.483564
6	2.205742	-3.076644	1.760253	1	-7.472517	-2.382713	0.406032
6	6.793833	-2.949151	-0.261772	1	-7.749723	-1.652330	-1.191224
6	5.170922	-1.037226	-0.582150	1	-7.687561	-0.622409	0.249115
1	-5.236006	-3.206054	0.527764	1	2.429467	-4.151264	1.769203
1	2.436834	-1.067185	-2.831318	1	1.177089	-2.945471	1.398907
1	1.053461	-1.527125	-3.864556	1	2.236068	-2.725581	2.803795
1	1.211980	0.156163	-3.289380	1	6.706227	-3.754988	-1.006534
1	-5.962643	0.532041	-1.465226	1	7.537843	-2.231634	-0.630996
1	-2.580908	1.687355	-1.450770	1	7.175576	-3.397782	0.665765
1	-2.911943	0.831665	-2.971696	1	5.943282	-0.509757	-1.147045
1	-4.160456	1.881677	-2.248951				
1	1.854573	-2.921935	-1.235740	<b>TS3</b>			

31	1.051687	2.873346	-0.226200	6	3.772747	-3.856257	0.278626
15	0.985182	-0.084568	1.900907	6	-1.791734	0.507189	2.538708
17	2.579919	3.586065	-1.607837	6	-1.081137	1.125060	3.752711
17	1.463749	3.301645	1.901554	6	-2.722307	1.563364	1.929491
17	-1.003474	3.373779	-0.818535	6	-7.167634	-2.024952	-0.150607
8	-1.565015	-1.427940	-2.929283	6	1.310422	-3.862213	0.767392
7	-1.661926	-0.581905	-0.786839	6	6.245517	-4.004581	-0.199493
8	1.235723	1.003853	-0.124222	6	4.994137	-1.818704	0.014959
7	1.336934	-1.100717	0.573606	1	-4.955322	-3.443271	0.598828
6	-3.353314	-2.158746	-0.033308	1	1.737045	1.005001	-2.696372
6	-3.048682	-0.924850	-0.620247	1	0.527994	0.340925	-3.843576
6	-4.037040	-0.071378	-1.125628	1	0.016247	1.448100	-2.548148
6	-4.699874	-2.492220	0.125404	1	-6.154339	0.216391	-1.311444
6	0.709351	0.631557	-2.800212	1	-3.044251	1.846547	-1.218271
6	-5.719834	-1.644038	-0.311132	1	-3.081118	0.956914	-2.749775
6	-5.368243	-0.446700	-0.942024	1	-4.560774	1.745908	-2.151126
6	3.838775	-1.045372	0.203228	1	2.394884	-1.521031	-2.383156
6	2.596411	-3.138496	0.470085	1	1.176726	-2.673495	-1.786202
6	-0.743452	0.091208	1.510021	1	1.023012	-2.003405	-3.427757
6	0.489877	-0.596310	-1.901134	1	-1.954537	-1.491415	3.413726
6	-3.664791	1.192082	-1.845722	1	-3.287757	-0.384730	3.829048
6	-0.995051	-0.942769	-2.000706	1	-3.227165	-1.119309	2.213607
6	2.621931	-1.728059	0.395504	1	-1.523708	-2.614529	1.042397
6	1.326051	-1.774376	-2.397189	1	-1.717816	-3.466189	-0.507137
6	-0.783485	-0.208188	0.166482	1	-2.669704	-3.972593	0.906570
6	-2.611170	-0.699952	3.019903	1	5.062475	0.705237	0.301749
6	0.645289	-0.221657	-0.417951	1	3.632877	0.912308	-0.731565
6	-2.257725	-3.101458	0.382086	1	3.456517	0.945250	1.017826
6	3.999507	0.454741	0.197781	1	3.743136	-4.947665	0.329942
6	4.987622	-3.210646	0.030995	1	-0.464215	0.382419	4.284642

1	-0.437914	1.966626	3.453372	6	0.748434	0.718548	-2.744559
1	-1.830389	1.499235	4.464871	6	-5.708386	-1.705757	-0.347972
1	-2.152451	2.441659	1.594181	6	-5.365718	-0.474051	-0.913423
1	-3.459198	1.885985	2.680597	6	3.819605	-1.159720	-0.015670
1	-3.275606	1.156922	1.070684	6	2.572313	-3.162398	0.619035
1	-7.295250	-2.801000	0.615019	6	-0.734856	0.112938	1.484336
1	-7.570752	-2.416528	-1.097178	6	0.505865	-0.534842	-1.894931
1	-7.776328	-1.155073	0.131385	6	-3.668957	1.220880	-1.726412
1	1.464556	-4.948330	0.762936	6	-0.990930	-0.878323	-2.021964
1	0.530702	-3.614287	0.033735	6	2.610068	-1.776735	0.359217
1	0.910744	-3.571449	1.750863	6	1.325078	-1.715338	-2.415935
1	6.201104	-4.531673	-1.164539	6	-0.788435	-0.228509	0.178904
1	7.131397	-3.356975	-0.208258	6	-2.504038	-0.863979	2.993315
1	6.380993	-4.765103	0.582660	6	0.637481	-0.261398	-0.399727
1	5.941166	-1.296517	-0.141084	6	-2.231475	-3.182579	0.230768
				6	3.956151	0.315751	-0.286858
<b>IN4</b>				6	4.939710	-3.338965	0.078656
31	1.022083	2.978348	-0.164463	6	3.732616	-3.919953	0.473511
15	1.110288	0.217726	1.709341	6	-1.757593	0.409115	2.568065
17	2.665948	3.528671	-1.470394	6	-1.039068	0.988172	3.794844
17	1.297215	3.451403	1.957852	6	-2.757374	1.449828	2.042790
17	-0.979938	3.435294	-0.896442	6	-7.153347	-2.100379	-0.192624
8	-1.526493	-1.302656	-3.004555	6	1.285193	-3.819438	1.036586
7	-1.658331	-0.611214	-0.813765	6	6.176529	-4.177668	-0.102916
8	1.187384	1.032473	0.071258	6	4.956941	-1.964639	-0.152778
7	1.356410	-1.097719	0.551792	1	-4.931288	-3.550692	0.454766
6	-3.338568	-2.232223	-0.130890	1	1.784481	1.071460	-2.647785
6	-3.039005	-0.970051	-0.657201	1	0.553976	0.466347	-3.795480
6	-4.036214	-0.088632	-1.091262	1	0.065889	1.534648	-2.466482
6	-4.682201	-2.575382	0.029369	1	-6.157309	0.208888	-1.231554

1	-3.047705	1.828657	-1.053773	1	6.277418	-4.915606	0.704954
1	-3.085449	1.049400	-2.644553	1	5.895022	-1.487477	-0.446962
1	-4.565688	1.794834	-1.990178				
1	2.397435	-1.478674	-2.420848	<b>TS4</b>			
1	1.173803	-2.617434	-1.807258	31	1.037364	3.023983	-0.208552
1	0.994903	-1.929986	-3.441063	15	1.088970	0.367432	1.630866
1	-1.799395	-1.643646	3.321818	17	2.386833	3.484695	-1.855916
1	-3.176667	-0.636004	3.834420	17	1.658429	3.720211	1.775592
1	-3.116065	-1.262809	2.172829	17	-1.092438	3.361478	-0.638210
1	-1.525823	-2.727938	0.943018	8	-1.491009	-1.777529	-2.903756
1	-1.660333	-3.460356	-0.670383	7	-1.660163	-0.835915	-0.809720
1	-2.631496	-4.102037	0.676445	8	1.194204	1.139548	0.094649
1	4.996617	0.556525	-0.536515	7	1.403689	-1.071153	0.574985
1	3.325947	0.648424	-1.123006	6	-3.438438	-2.224248	0.098976
1	3.672338	0.929256	0.581356	6	-3.056705	-1.104637	-0.647608
1	3.692931	-4.993487	0.675205	6	-3.987233	-0.248579	-1.247686
1	-0.336084	0.258801	4.229570	6	-4.803610	-2.439740	0.300604
1	-0.478314	1.899385	3.536425	6	0.628319	0.466355	-2.684904
1	-1.774730	1.244563	4.570578	6	-5.766259	-1.586154	-0.243871
1	-2.234462	2.359998	1.713473	6	-5.339573	-0.505941	-1.023969
1	-3.470912	1.719908	2.836236	6	3.848967	-1.152793	0.006382
1	-3.331320	1.049076	1.194668	6	2.604022	-3.137583	0.723760
1	-7.276474	-2.874403	0.576056	6	-0.761422	0.143182	1.412689
1	-7.547846	-2.502196	-1.138702	6	0.504231	-0.832244	-1.863860
1	-7.772977	-1.236078	0.082155	6	-3.523682	0.898463	-2.100130
1	1.435914	-4.890088	1.222831	6	-0.982330	-1.237620	-1.963858
1	0.516784	-3.703085	0.258553	6	2.650482	-1.766637	0.416275
1	0.875584	-3.355524	1.945807	6	1.405624	-1.933424	-2.411558
1	6.133549	-4.733660	-1.052099	6	-0.796284	-0.345262	0.160047
1	7.081422	-3.556550	-0.119020	6	-1.751945	-0.430955	3.616551

6	0.603109	-0.545518	-0.392578	1	3.268045	0.620764	-1.113914
6	-2.402847	-3.170195	0.643551	1	3.730594	0.949097	0.549870
6	3.960857	0.313421	-0.318505	1	3.725024	-4.968658	0.816412
6	4.966435	-3.329358	0.170471	1	-0.262390	1.920524	3.427432
6	3.763991	-3.900572	0.589199	1	-1.291045	2.714998	2.207963
6	-1.747701	0.593573	2.471402	1	-1.956804	2.292962	3.808412
6	-1.280008	1.959167	3.007770	1	-3.150989	1.408296	1.018892
6	-3.165462	0.773076	1.917754	1	-3.785657	1.271624	2.677736
6	-7.236175	-1.833926	-0.029521	1	-3.643141	-0.183091	1.669836
6	1.311407	-3.770889	1.162695	1	-7.712049	-2.174032	-0.961745
6	6.222149	-4.151088	0.050922	1	-7.749529	-0.914093	0.284022
6	4.982926	-1.961810	-0.111476	1	-7.405098	-2.601996	0.736090
1	-5.120980	-3.300575	0.894193	1	1.450289	-4.838381	1.373222
1	1.643600	0.878134	-2.617090	1	0.537287	-3.667509	0.386648
1	0.397987	0.230770	-3.732463	1	0.914614	-3.281486	2.064680
1	-0.082854	1.229137	-2.332561	1	5.996953	-5.225077	0.028783
1	-6.082912	0.160465	-1.468976	1	6.778618	-3.894098	-0.860948
1	-2.801531	1.532629	-1.564417	1	6.889515	-3.964632	0.906176
1	-3.024493	0.517702	-3.005346	1	5.917099	-1.498106	-0.438566
1	-4.369844	1.522952	-2.411989				
1	2.451934	-1.602014	-2.446484	<b>3</b>			
1	1.351758	-2.850495	-1.809359	31	1.245728	2.956806	0.817559
1	1.065194	-2.168584	-3.428848	15	1.062761	-0.061978	1.993311
1	-0.743368	-0.558363	4.041731	17	3.166840	3.889547	0.369784
1	-2.417448	-0.091637	4.424881	17	-0.093596	4.232895	1.990743
1	-2.107852	-1.411349	3.266210	17	0.187141	2.232199	-1.015003
1	-1.635968	-2.642848	1.231139	8	-1.831423	-2.238920	-2.696846
1	-1.888589	-3.686143	-0.183735	7	-1.784780	-1.138418	-0.675894
1	-2.865692	-3.933278	1.281793	8	1.594303	1.411748	1.837080
1	4.981575	0.547837	-0.643618	7	1.527244	-0.826348	0.376328

6	-3.853720	-2.212006	0.011294	1	2.054004	-1.203903	-2.758895
6	-3.212648	-1.110103	-0.566630	1	0.571148	-1.500231	-3.721056
6	-3.923310	-0.052077	-1.146002	1	0.721353	-0.005021	-2.746612
6	-5.246717	-2.191466	0.094428	1	-5.887406	0.749660	-1.476889
6	0.963228	-1.076672	-2.786008	1	-2.455062	1.540235	-1.213914
6	-5.991733	-1.123497	-0.413151	1	-2.645689	0.637588	-2.726225
6	-5.315107	-0.073812	-1.042529	1	-3.895370	1.806703	-2.233132
6	3.776082	-0.677031	-0.633373	1	1.825747	-3.401740	-1.519119
6	3.141069	-2.607457	0.750788	1	0.259578	-3.855623	-0.773140
6	-0.718175	-0.085911	1.446976	1	0.398584	-3.760914	-2.544498
6	0.309149	-1.833782	-1.619442	1	-2.034756	-1.495658	3.382632
6	-3.194135	1.048325	-1.863891	1	-3.339785	-0.322580	3.689603
6	-1.217561	-1.776494	-1.775984	1	-3.249729	-1.140108	2.116130
6	2.842917	-1.371920	0.144473	1	-2.246349	-3.072934	1.182111
6	0.734293	-3.309201	-1.601003	1	-2.576873	-3.898121	-0.360824
6	-0.809686	-0.705410	0.239774	1	-3.683225	-4.112708	1.016973
6	-2.648432	-0.705121	2.923425	1	3.998616	0.812084	-2.169458
6	0.478188	-1.113601	-0.320773	1	2.437564	0.898403	-1.318228
6	-3.047388	-3.387100	0.494739	1	3.910169	1.461672	-0.522837
6	3.506523	0.688904	-1.195099	1	4.637468	-4.128024	0.964666
6	5.349044	-2.520034	-0.285613	1	-0.494280	0.367587	4.202668
6	4.396603	-3.162602	0.512713	1	-0.460167	1.948614	3.355004
6	-1.769694	0.448988	2.414804	1	-1.872048	1.476711	4.314253
6	-1.094576	1.097612	3.636162	1	-2.024873	2.322723	1.311726
6	-2.639792	1.509920	1.723621	1	-3.327869	1.946585	2.463418
6	-7.491459	-1.096262	-0.281135	1	-3.245230	1.067252	0.924094
6	2.161899	-3.314654	1.652520	1	-7.959740	-0.644646	-1.166026
6	6.706230	-3.134043	-0.503108	1	-7.790998	-0.497348	0.592853
6	5.019703	-1.286248	-0.842622	1	-7.900094	-2.106627	-0.149230
1	-5.762644	-3.036077	0.557719	1	2.419635	-4.377661	1.739812

1	1.125204	-3.244007	1.293472	6	1.436730	-2.206909	-1.316573
1	2.181321	-2.875009	2.661442	6	-4.138989	-3.240930	1.230943
1	6.641020	-4.227863	-0.578101	1	-4.334325	-4.037227	1.953507
1	7.175844	-2.749022	-1.417363	6	1.710613	1.266554	1.951154
1	7.373542	-2.898906	0.340180	6	-2.693566	-1.536315	0.357875
1	5.753754	-0.763005	-1.460203	6	-0.340898	-1.254276	-0.148838

For NBO analysis:

**3**

31	-1.469390	2.919595	-0.301796	1	-3.943868	0.880762	-1.143773
17	-3.448435	3.511171	-1.004349	1	-3.906910	-0.236352	-2.518471
15	-1.063249	0.413342	1.722042	1	-2.397541	0.233616	-1.699252
17	-0.301977	1.780801	-1.830366	6	0.896610	-0.585914	0.251448
17	-0.274027	4.596556	0.445074	6	-6.387127	-3.722541	0.190703
8	-1.718377	1.713525	1.123414	1	-6.232342	-4.667484	-0.352409
8	2.108813	-2.892170	-2.036010	1	-7.169111	-3.159228	-0.334403
7	1.924418	-1.204336	-0.482027	1	-6.755112	-3.975039	1.194301
6	5.458334	-1.637266	0.520804	6	0.727653	0.371876	1.202394
1	6.047200	-2.240235	1.217077	6	3.375952	-2.843291	1.317074
6	4.076791	-1.812363	0.473958	1	4.065645	-3.295892	2.040374
7	-1.426146	-0.850449	0.424335	1	2.978148	-3.645813	0.675081
6	3.341317	-1.010498	-0.409726	1	2.531262	-2.405228	1.871397
6	-3.646189	-1.173078	-0.600683	6	3.136486	0.625014	-2.312895
6	5.343670	0.016732	-1.221107	1	2.628064	-0.080518	-2.988948
1	5.839658	0.718530	-1.895636	1	3.770917	1.283369	-2.918856
6	-5.104706	-2.937536	0.264649	1	2.355210	1.234573	-1.834870
6	-2.930683	-2.551449	1.305203	6	2.489499	2.146071	0.960569
6	3.955333	-0.126223	-1.301602	1	3.142684	1.539803	0.321554
6	6.107269	-0.717793	-0.311983	1	3.124669	2.844959	1.525457
6	-0.086988	-2.322675	-1.162477	1	1.810137	2.738895	0.332096

6	2.688366	0.410344	2.772813	1	-0.312772	-2.654092	-3.270259
1	2.147023	-0.271129	3.447301	6	7.602888	-0.557058	-0.240735
1	3.314174	1.072931	3.389497	1	7.926259	-0.342563	0.787957
1	3.355157	-0.174798	2.128100	1	7.949011	0.258928	-0.887499
6	-1.939077	-2.874001	2.393326	1	8.108642	-1.481452	-0.557579
1	-2.023567	-2.149046	3.217316				
1	-0.897611	-2.837362	2.042782				
1	-2.126619	-3.875542	2.800308				
6	-0.425318	-3.749593	-0.711729				
1	-0.019327	-4.438685	-1.464888				
1	-1.512145	-3.889225	-0.637396				
1	0.038802	-3.989509	0.255858				
6	0.958237	2.184339	2.931147				
1	0.241430	2.840124	2.419011				
1	1.683726	2.830580	3.445050				
1	0.430408	1.602992	3.704263				
6	-0.747035	-1.988844	-2.511216				
1	-0.558654	-0.943847	-2.797138				
1	-1.830866	-2.158564	-2.455905				



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