A Tridentate and Dianionic N-Heterocyclic Olefin (NHO) with Two Unsymmetrically-Tethered Aryloxide Sidearms on Bismuth: A Fortuitous Followed by Systematic Discovery.

Santu Goswami,[a] Subham Sarkar,[a,b] Anisha Guha Roy,[a] Dibyendu Mallick,[b,*] and Debabrata Mukherjee[a,*]

[a] Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia, 741246, India.

[b] Department of Chemistry, Presidency University, 86/1 College Street, Kolkata, 700073, India.

Table of Contents

1. Characterization Data

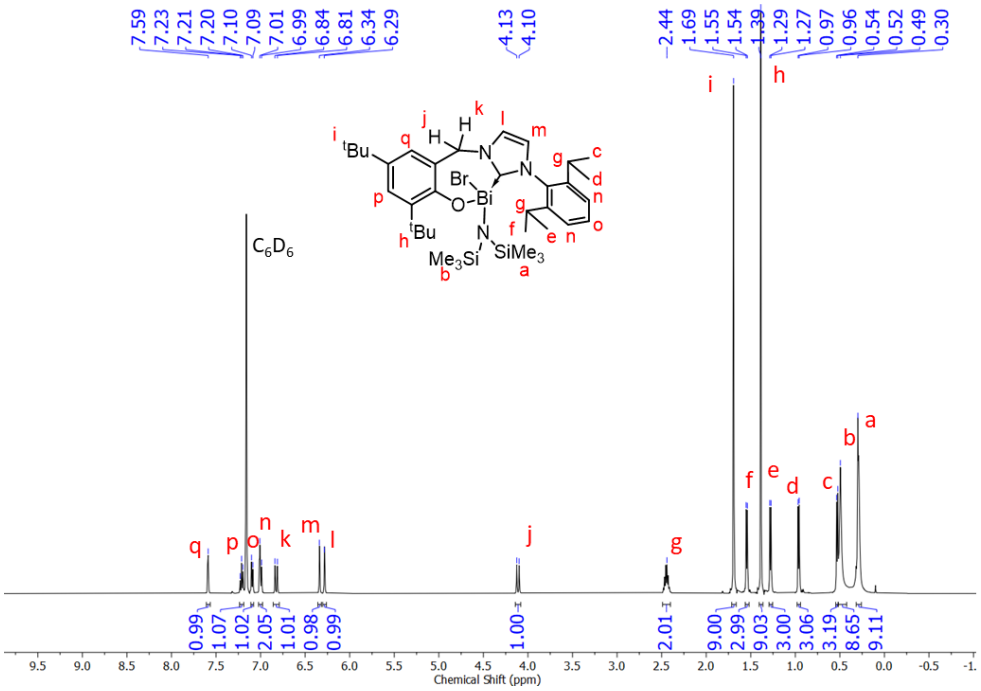


Figure-S1: ^{1}H NMR spectrum of **1** in C_6D_6.

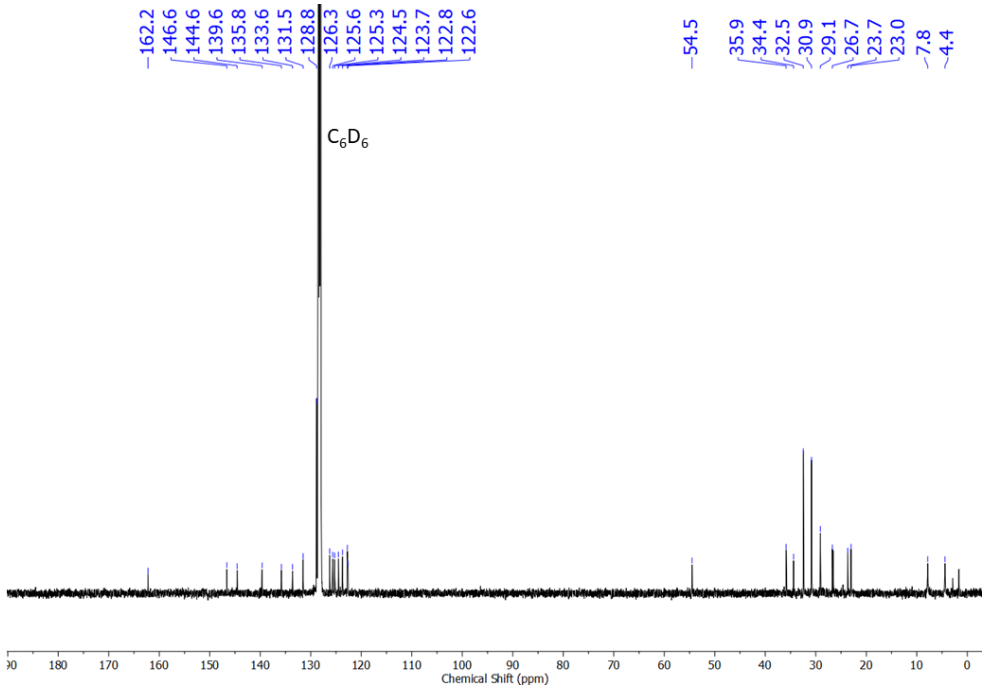


Figure-S2: $^{13}C\{^{1}H\}$ NMR spectrum of **1** in C_6D_6.

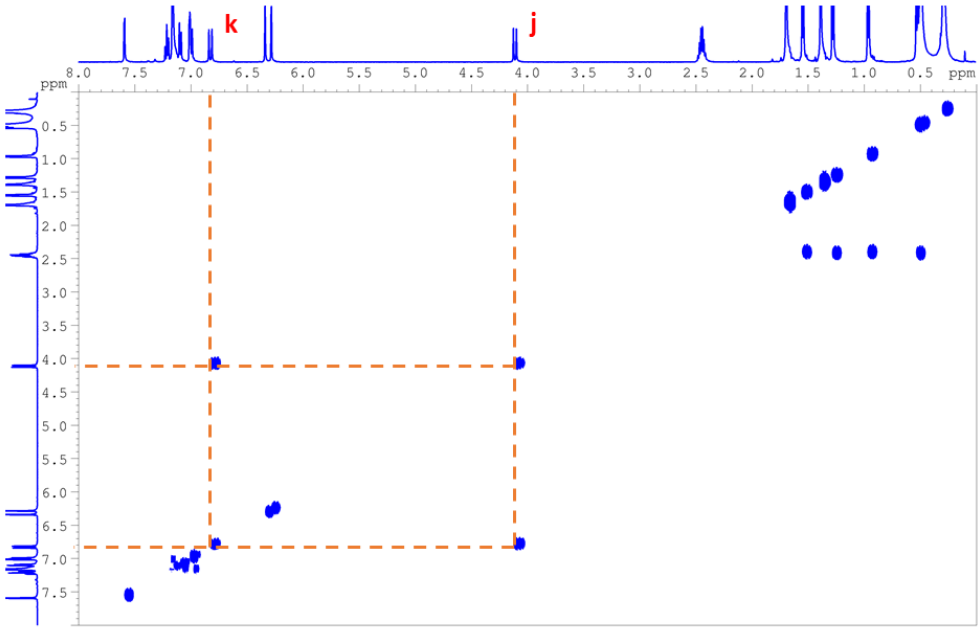


Figure-S3: ^{1}H-^{1}H COSY NMR spectrum of **1** in C_6D_6.

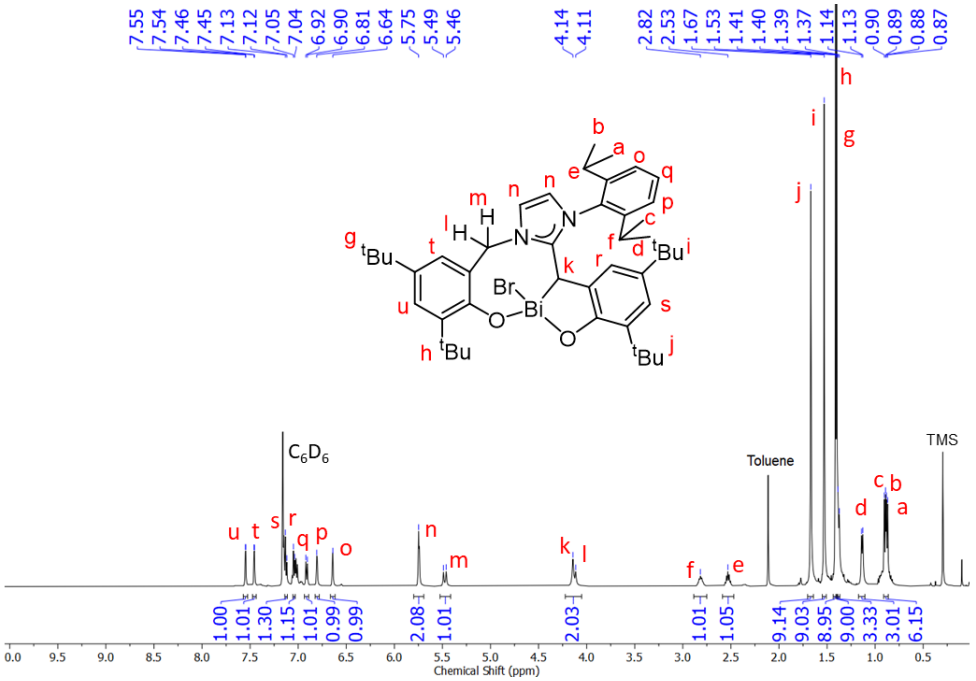


Figure-S4: ^{1}H NMR Spectrum of **2** in C_6D_6.

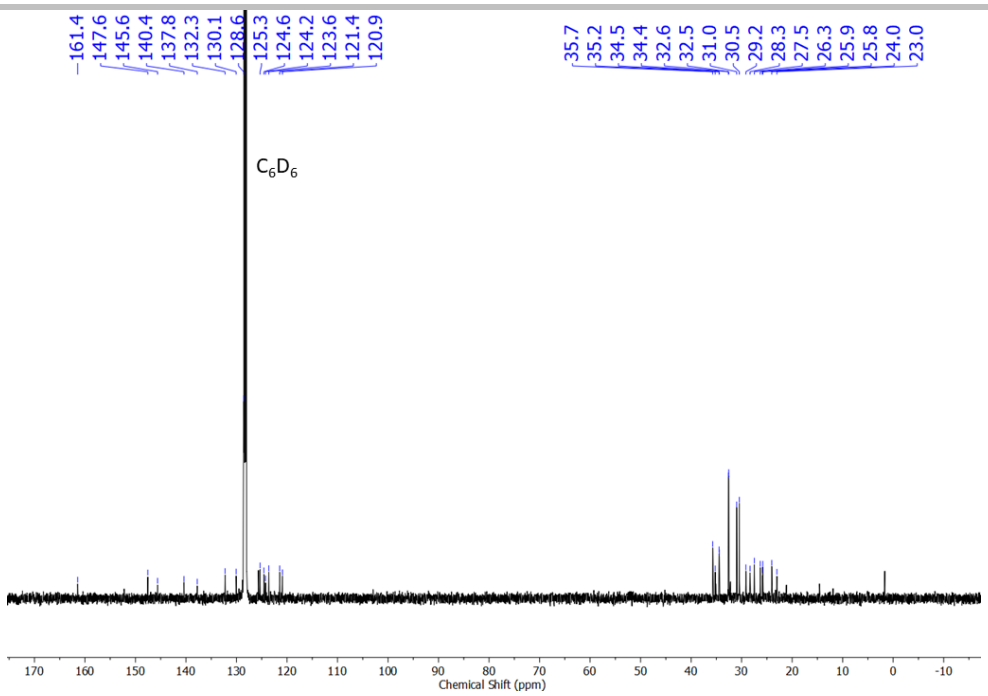


Figure-S5: $^{13}C\{^{1}H\}$ NMR Spectrum of **2** in C_6D_6.

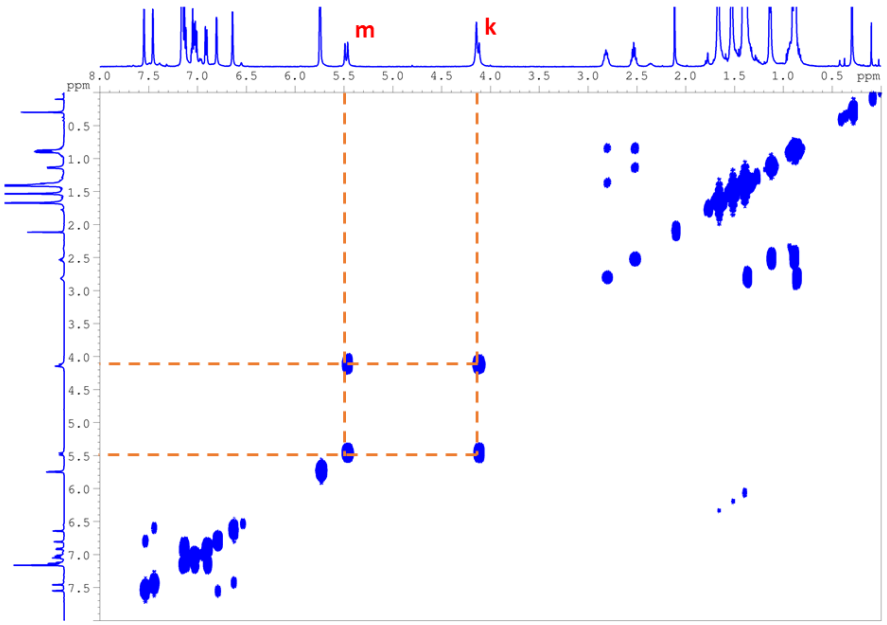


Figure-S6: ^{1}H-^{1}H COSY NMR Spectrum of **2** in C_6D_6.

NMR scale reaction monitoring:

1 h **24 h** **36 h** **48 h**

Figure-S7: NMR scale reaction of LH_2Br, $Bi(HMDS)_3$ and KHMDS in a 2:1:1 ratio leading to **2**. It shows the progress of the reaction along with the consistent partial inhomogeneity.

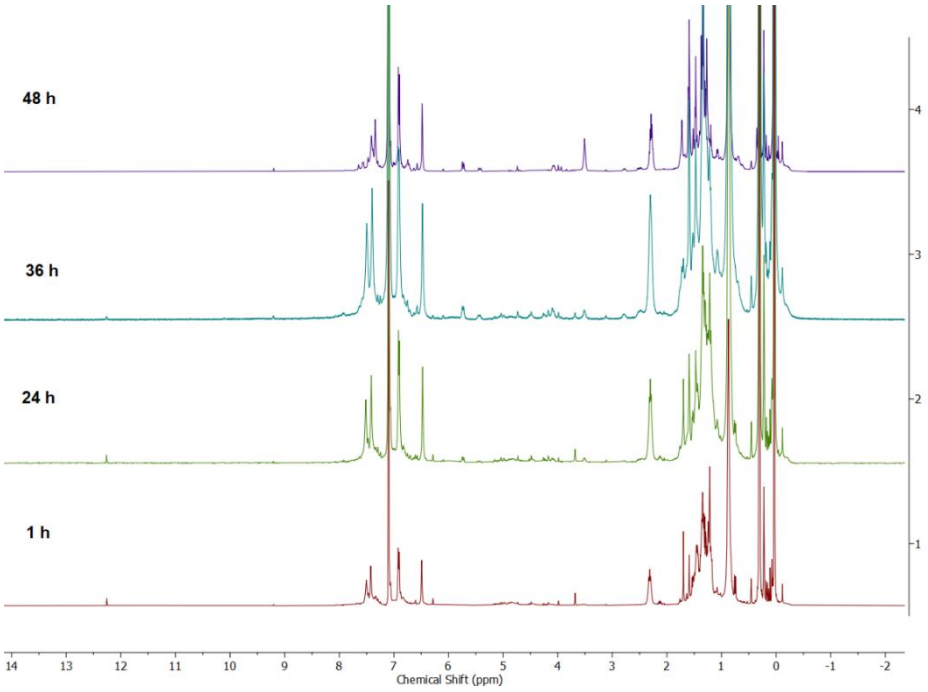


Figure S8: A stacked ^1H NMR plot for the above reaction showing broad and overlapping peaks. A peak at 12.32 ppm, likely of the imidazolium-2-H of LH, is noticed initially that disappears with time.

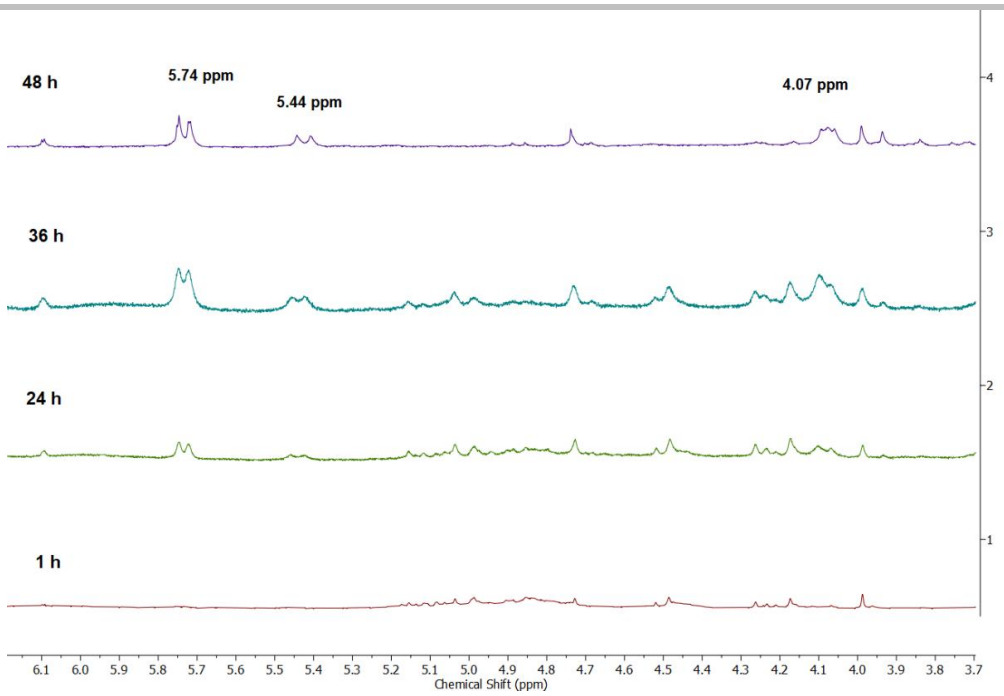


Figure S9: A 'zoomed in' version of the above plot showing 3.6-6.0 ppm region, where the peaks attributed to complex 2 (5.74, 5.44, and 4.07 ppm) are found growing with time.

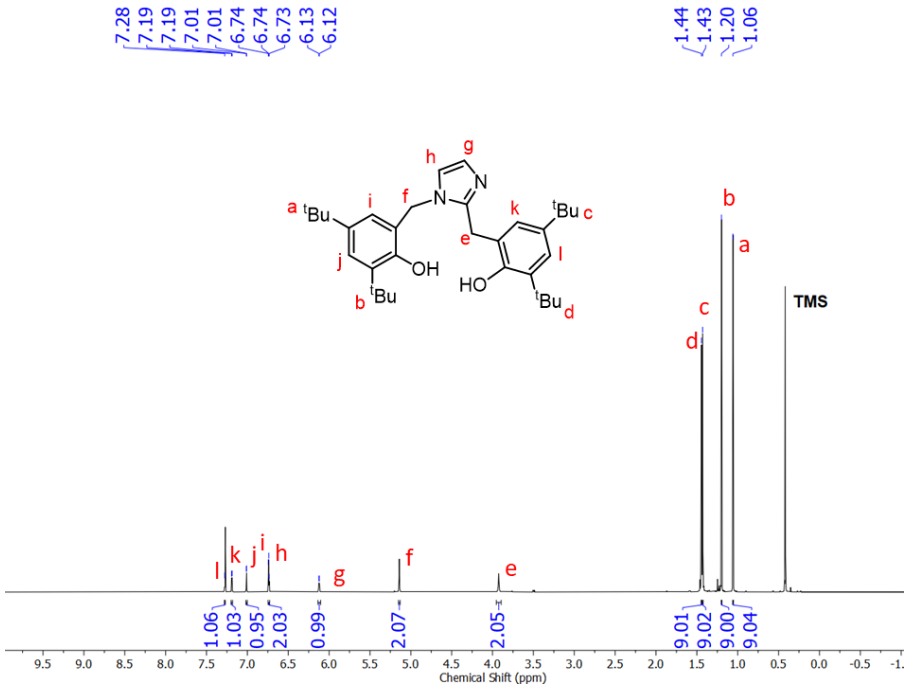


Figure-S10: ^{1}H NMR spectrum of **II** in $CDCl_3$.

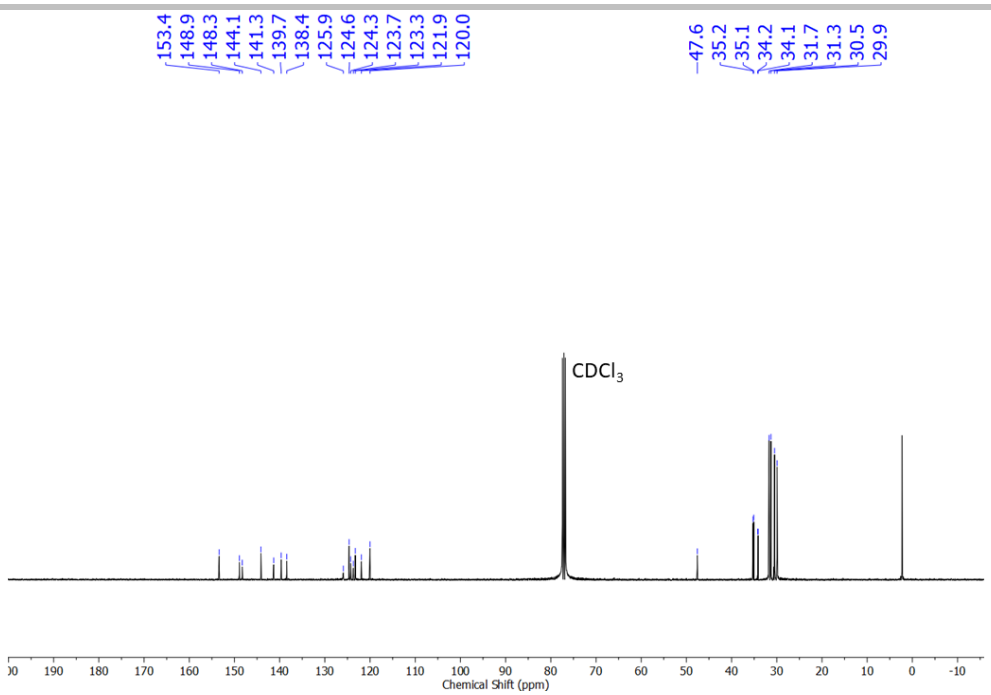


Figure-S11: $^{13}C\{^{1}H\}$ NMR spectrum of **II** in $CDCl_3$.

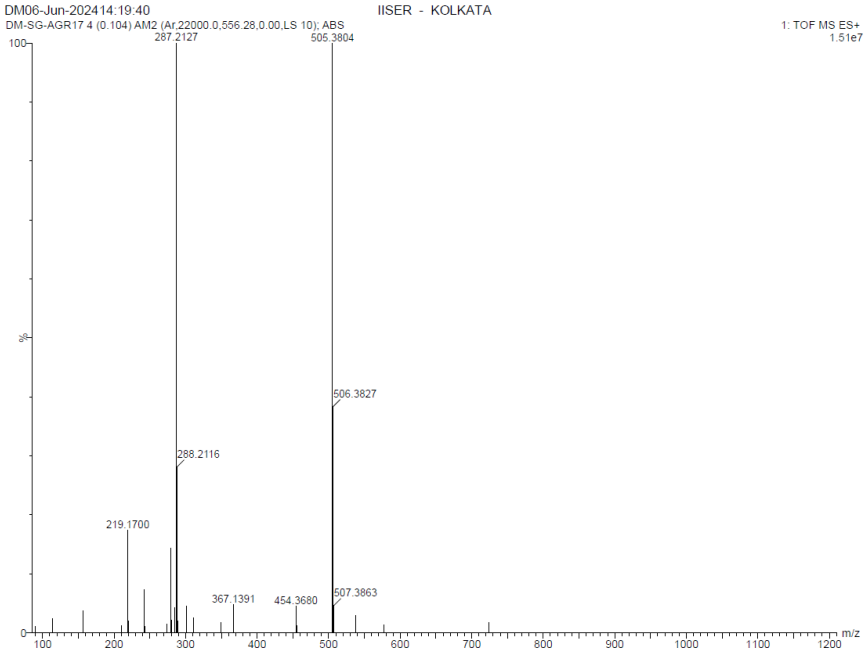


Figure-S12: HRMS spectrum of **II**.

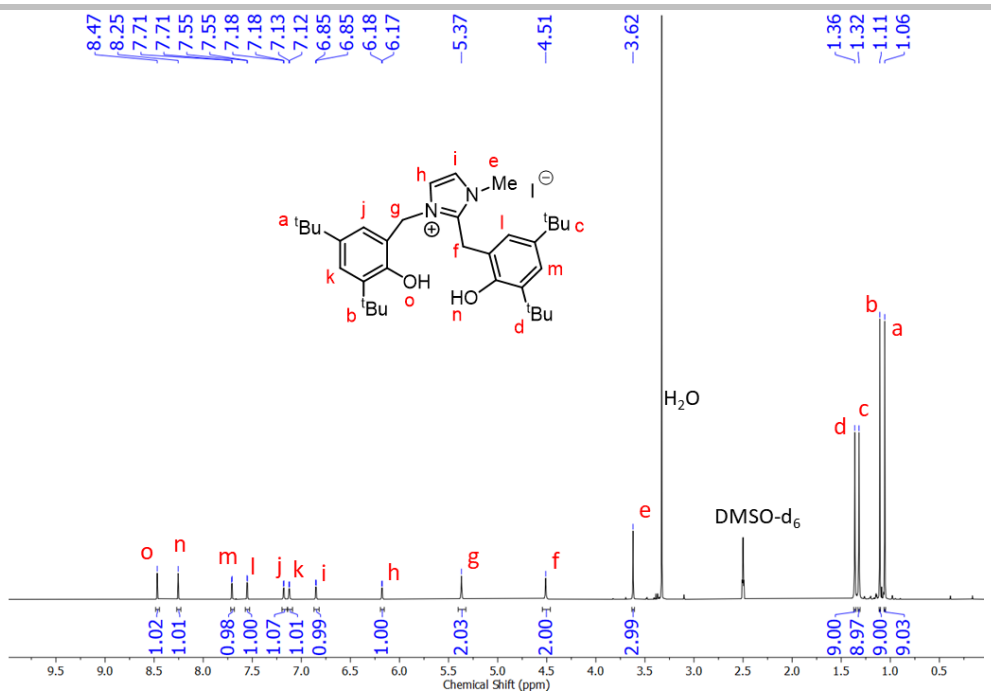


Figure-S13: ^{1}H NMR spectrum of **L'*H*$_3$I** in DMSO-D$_6$.

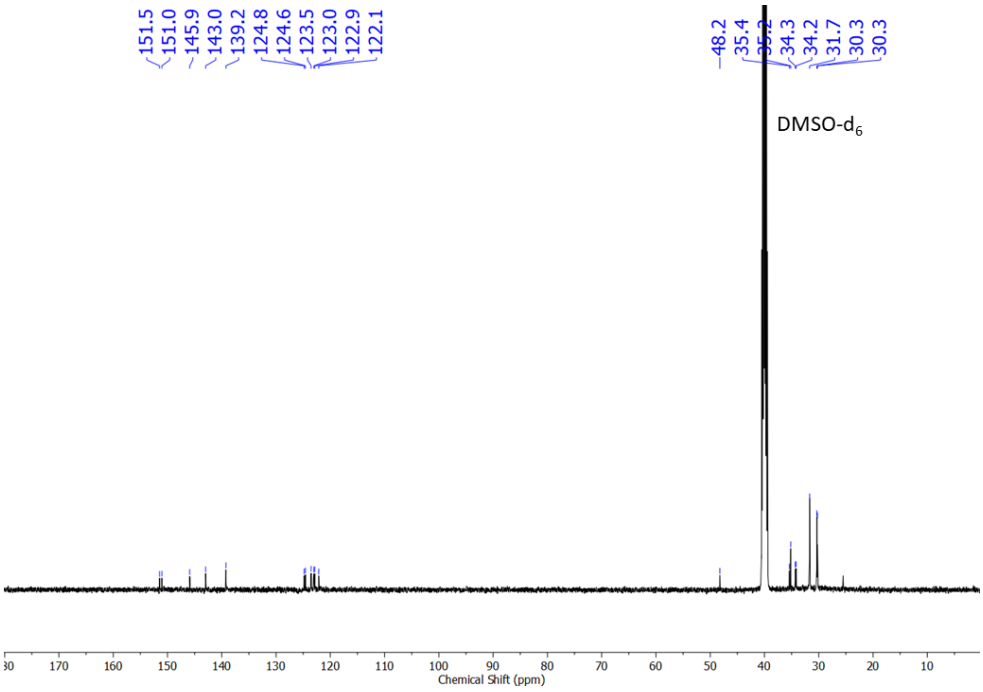


Figure-S14: ^{13}C{^{1}H} NMR spectrum of **L'*H*$_3$I** in DMSO-D$_6$.

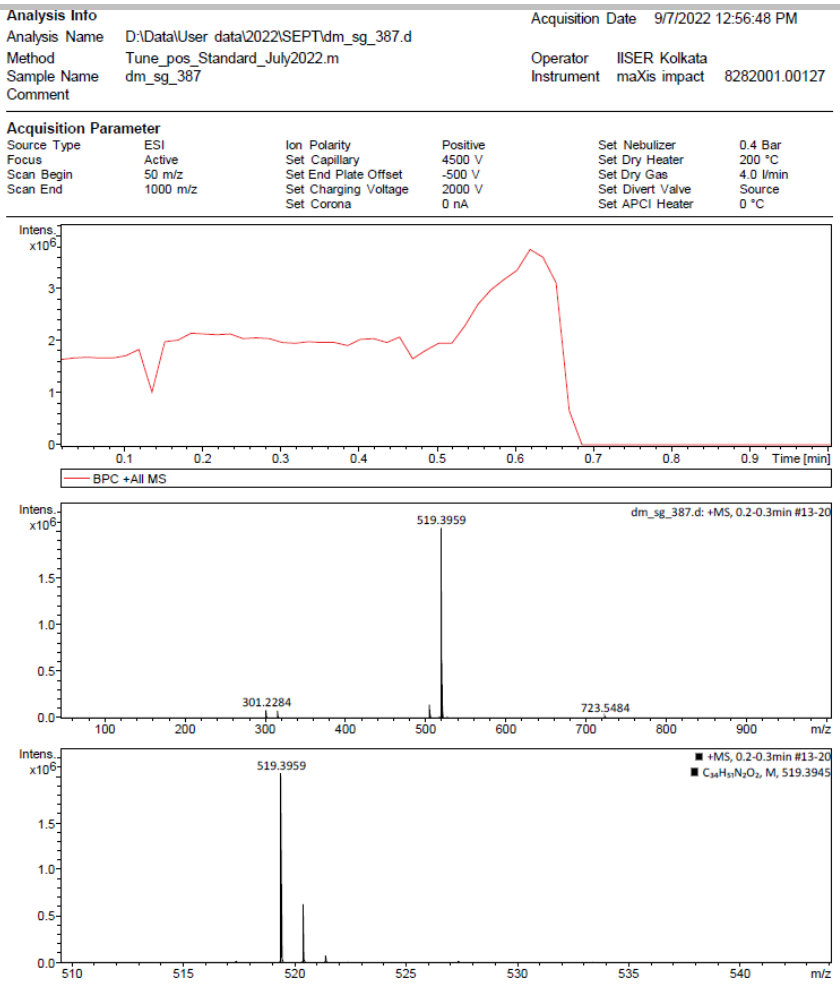


Figure-S15: HRMS spectrum of **L'*H*$_3$I**.

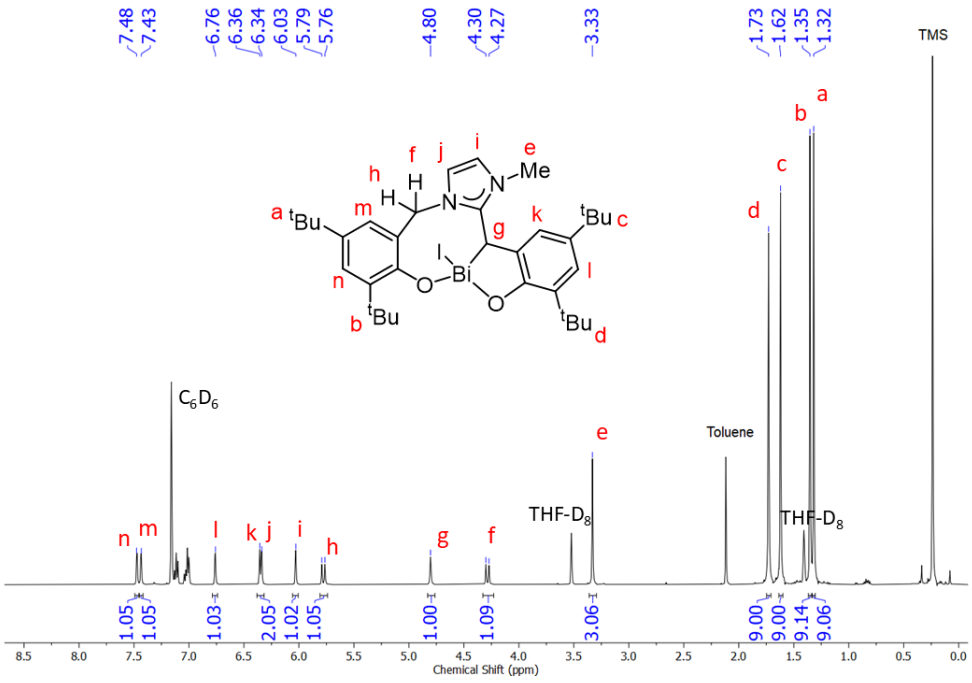


Figure-S16: ^{1}H NMR Spectrum of **3** in THF-D_8 / C_6D_6 (2:5).

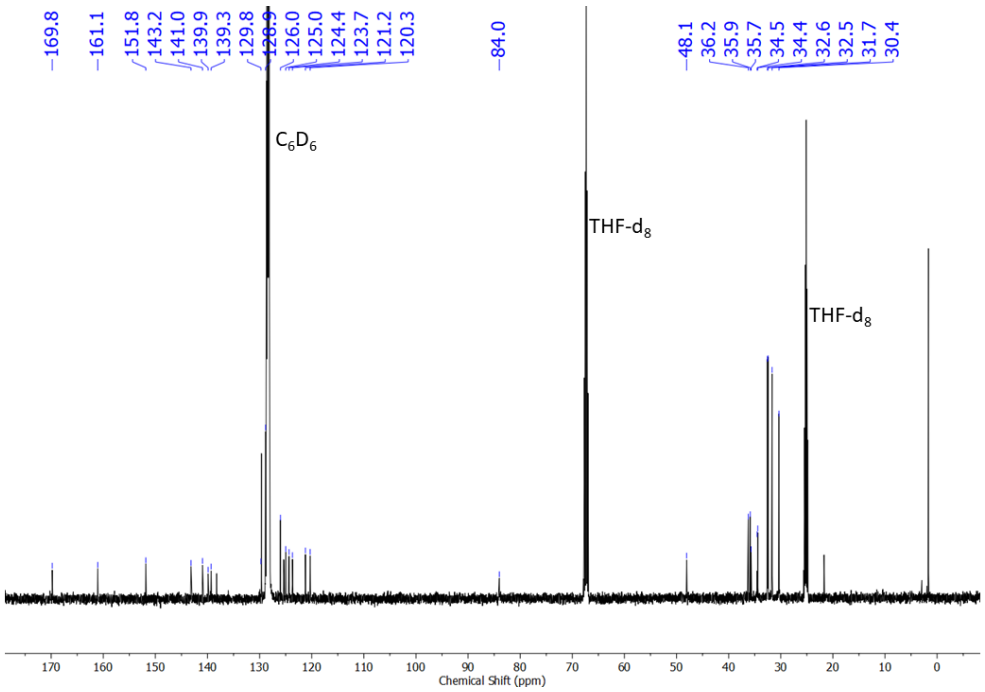


Figure-S17: $^{13}C\{^{1}H\}$ NMR Spectrum of **3** in THF-D_8 / C_6D_6 (2:5).

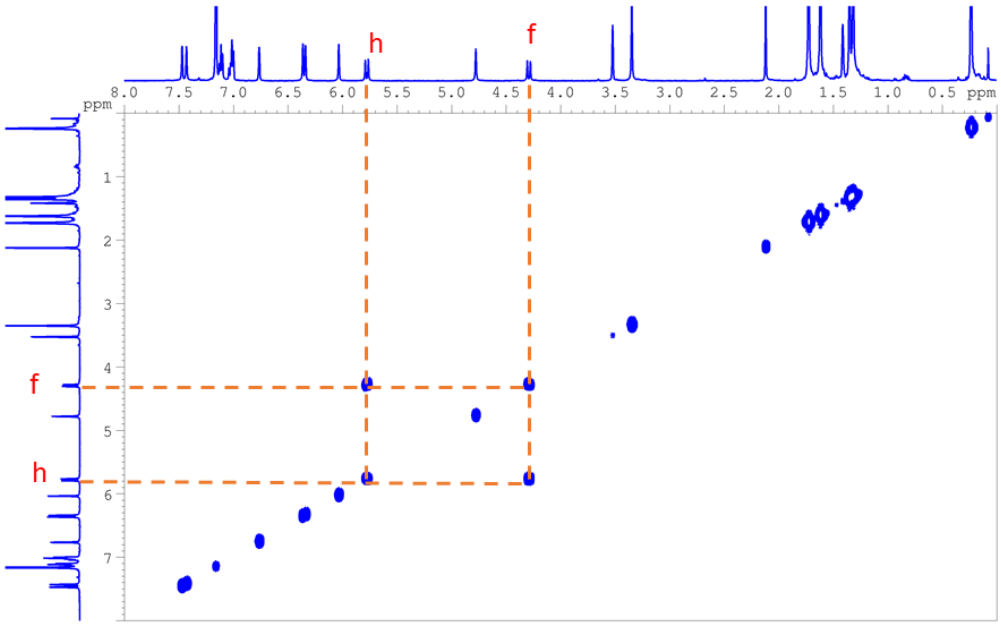


Figure-S18: ^{1}H-^{1}H COSY NMR Spectrum of **3** in THF-D_8 / C_6D_6 (2:5).

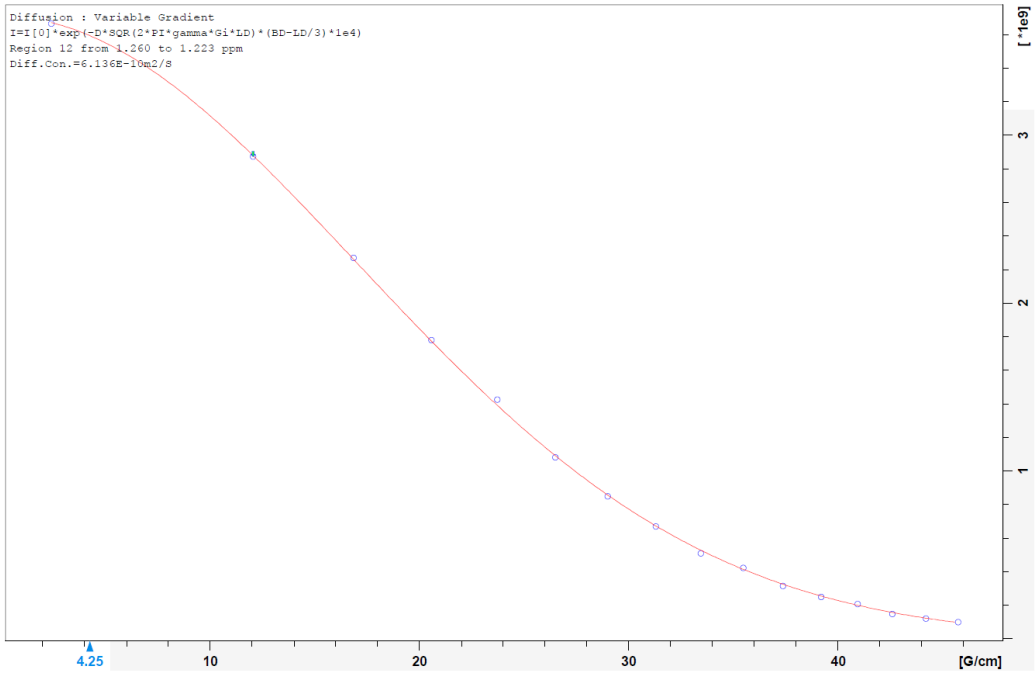


Figure-S19: DOSY analysis of **3** in THF-D_8.

$$r = \frac{kT}{6\pi\eta D}$$

$$= \frac{1.3806488 * 10^{-23} * 300}{6 * \frac{22}{7} * 480.0 * 10^{-6} * 4.993 * 10^{-10}}\ \mathrm{m}$$

$$= 7.45 * 10^{-10}\ \mathrm{m} \quad = 7.45\ \text{Å}$$

From the solid-state structure of the dimeric **3_2**, the crystallographic radius is estimated as (23.2/2) = 11.6 Å. We, therefore, tend to believe that the complex dissociates in its monomeric form in solution.

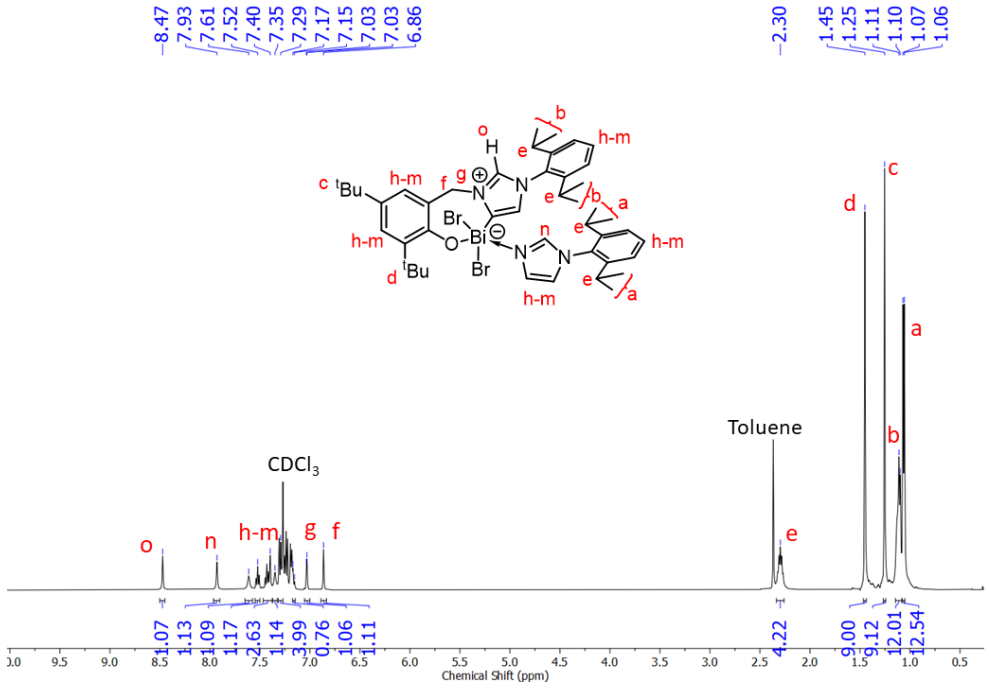


Figure-S20: ^{1}H NMR Spectrum of **4** in $CDCl_3$.

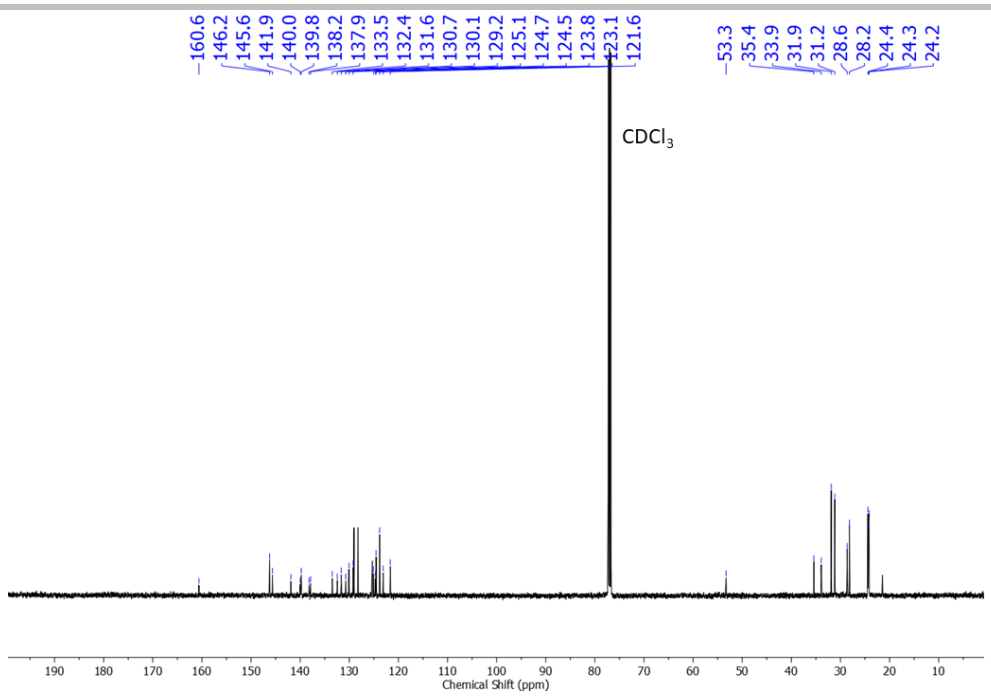


Figure-S21: $^{13}C\{^{1}H\}$ NMR Spectrum of **4** in $CDCl_3$.

3 Crystallographic Data

X-ray diffraction data were collected on a Rigaku XtaLAB Synergy, Dualflex four-circle diffractometer with HyPix3000 detector and Cu-K_α radiation (λ = 1.54184 Å) at 100 K. Data reduction was done with CrysAlis^{PRO}, Agilent Technologies, Version 1.171.37.34. The structures were solved by intrinsic phasing using SHELXT.[1] all refinements were carried out against F^2 with ShelXL[2] as implemented in the program system Olex 2.[3] The non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were included in calculated positions and treated as riding throughout the refinement. Refinement results are given in Table S1. Graphical representations were performed with the program DIAMOND.[4] CCDC-2348036 (**1**), 2348037 (**2**), 2348038 (**3_2**), 2348039 (**4**) contain the supplementary crystallographic data.

Table-S1: Crystallographic data of 1,2,3_2 and 4.

	1•(toluene)$_2$	**2**	**3_2•(thf)$_2$**	**4•(toluene)**
formula	$C_{50}H_{75}BiBrN_3OSi_2$	$C_{45}H_{62}BiBrN_2O_2$	$C_{76}H_{112}Bi_2I_2N_4O_6$	$C_{52}H_{69}BiBr_2N_4O$
Fw /g·mol^{-1}	1079.02	951.85	1849.45	1134.91
crystal. colour, habit	Yellow	Orange	Yellow	Yellow
crystal size / mm^3	0.523 × 0.104 × 0.070	0.41 × 0.02 × 0.05	0.275 × 0.078 × 0.045	0.14 × 0.08 × 0.05
crystal system	monoclinic	Triclinic	triclinic	monoclinic
space group	$P2_1/c$	P-1	P-1	$P2_1/n$
a / Å	20.4928(3)	9.76170(10)	10.8140(2)	14.7082(2)
b / Å	14.7259(2)	14.1831(2)	13.8767(2)	19.7308(2)
c / Å	34.2124(6)	20.8728(2)	15.9783(3)	18.4697(2)
α / °	90	102.6760(10)	98.2010(10)	90
β / °	95.7800	91.5980(10)	106.435(2)	102.8870(10)
γ / °	90	93.5020(10)	99.4120(10)	90
V / Å^3	10272.0(3)	2811.63(6)	2223.14(7)	5224.98(11)
Z	8	2	1	4
d_{calc}/Mg·m^{-3}	1.395	1.124	1.381	1.443
μ (CuKα)/mm^{-1}	8.365	7.194	13.468	8.698
F(000)	4399.0	960.0	916.0	2280.0
2θ range / °	4.334 to 136.836	6.402 to 136.428	5.886 to 136.912	6.646 to 136.606
index ranges	-24 ≤ h ≤ 24, -17 ≤ k ≤ 14, -39 ≤ l ≤ 41	-11 ≤ h ≤ 11, -16 ≤ k ≤ 17, -24 ≤ l ≤ 23	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -18 ≤ l ≤ 19	-17 ≤ h ≤ 17, -23 ≤ k ≤ 23, -22 ≤ l ≤ 22

Reflections collected	71954	63630	58543	66659
independ. reflns (R_{int})	18574 [Rint = 0.0649, Rsigma = 0.0509]	10196 [Rint = 0.0801, Rsigma = 0.0371]	8098 [Rint = 0.0930, Rsigma = 0.0428]	9506 [Rint = 0.0592, Rsigma = 0.0300]
observed reflections	4666	9513	7347	8614
data/ restr./ param.	18574/1604/1082	10196/0/458	8098/0/419	9506/0/508
*R*1, *wR*2 [*I*> 2σ(*I*)]	R1 = 0.0957, wR2 = 0.2617	R1 = 0.0404, wR2 = 0.1127	R1 = 0.0458, wR2 = 0.1230	R1 = 0.0447, wR2 = 0.1181
*R*1, *wR*2 (all data)	R1 = 0.1109, wR2 = 0.2740	R1 = 0.0424, wR2 = 0.1143	R1 = 0.0487, wR2 = 0.1257	R1 = 0.0490, wR2 = 0.1227
GooF-of-fit on F^2	1.050	1.081	1.009	1.035
largest diff. peak, hole/ e·Å^3	10.77/-4.15	2.31/-1.24	4.47/-1.88	4.42/-1.85
CCDC number	2348036	2348037	2348038	2348039

4. DFT Analyses

All the calculations were performed with M06-2X functional[5] as implemented in the Gaussian 16 package.[6] The def2-TZVP[7] basis set was used for optimizing Bi atom while the 6-31G**[8] was used for the rest of the atoms. This combination will be referred to as the M06-2X/B1 level of theory. Optimizations were carried out in gas phase and also in solvent using the SMD solvation model,[9] with toluene as the implicit solvent. The stationary points were characterized by frequency calculations at the same level of theory and the thermal corrections at 298.15 K were obtained as well. Energies were refined by performing single-point energy calculations with def2-TZVPP basis set (B2) on all the atoms,[7] i.e. M06-2X/B2//M06-2X/B1 level of theory. The natural bond orbital (NBO)[10] methods were utilised for calculating the natural charges on gas phase optimized structures at M06-2X/B2//M06-2X/B1 level of theory.

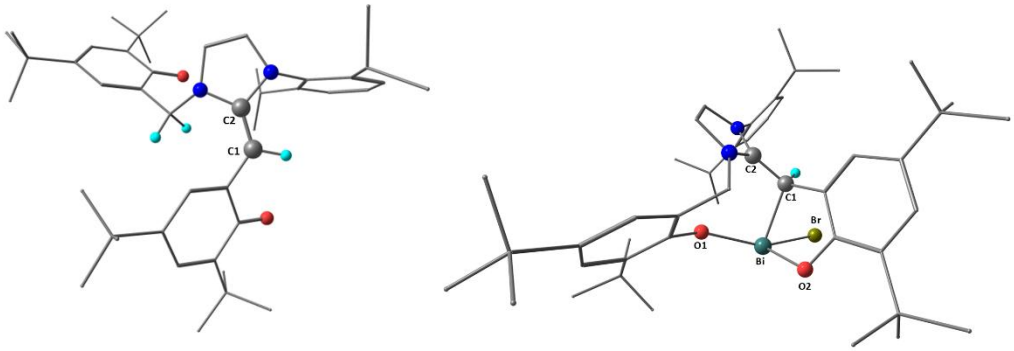


Figure-S22: DFT Optimized gas phase structures of non-metallated [^{Dipp}NHO]$^{2-}$ (*left*) and **2** (*right*).

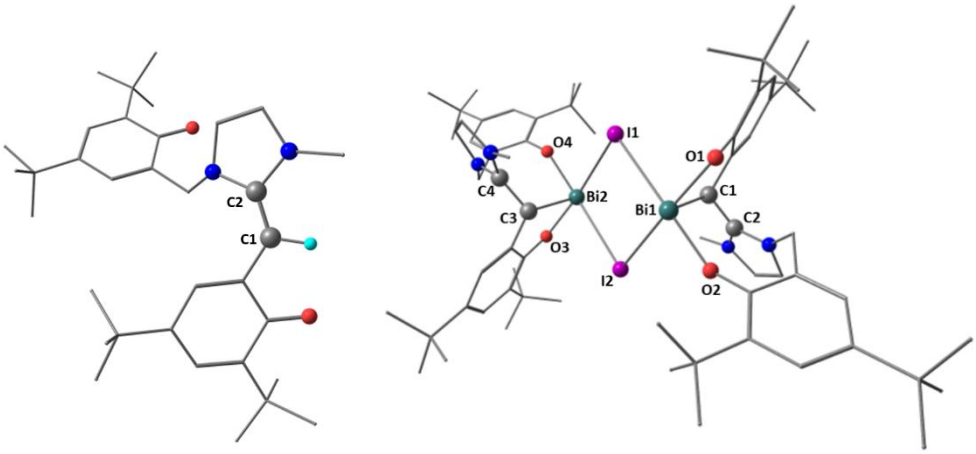


Figure-S23: DFT Optimized gas phase structures of non-metallated [^{Me}NHO]$^{2-}$ (*left*) and **3$_2$** (*right*).

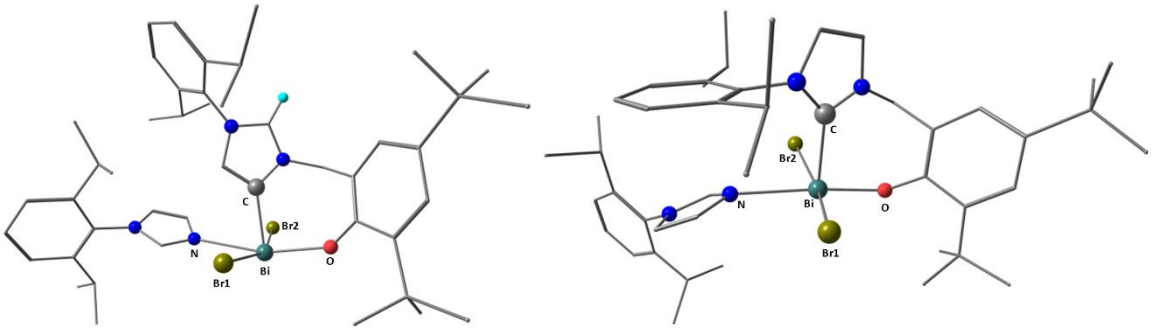
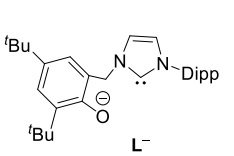


Figure-S24: DFT Optimized gas phase structures of **4** (*left*) and **4'-^{Dipp}Imd** (hypothetical; *right*).

Table-S2: Comparison of the selected observed (from SCXRD data) versus computed (from DFT optimized geometry in gas phase) bond distances (Å).

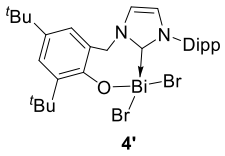
		Obsd.	Calcd.	Δ (Calcd - Obsd)
2	**C1-C2**	1.4673(57)	1.4634	-0.0039
	Bi-C1	2.3099(37)	2.3102	0.0003
	Bi-O1	2.2370(29)	2.3048	0.0678
	Bi-O2	2.1155(32)	2.1084	-0.0071
	Bi-Br	2.8244(7)	2.7710	-0.0534
3_2	**C1-C2 / C3-C4**	1.4738(82)	1.4694	-0.0044
	Bi1-C1 / Bi2-C3	2.2981(46)	2.3092	0.0111
	Bi1-O1 / Bi2-O3	2.1588(32)	2.1579	-0.0009
	Bi2-O2 / Bi2-O4	2.2280(32)	2.1714	-0.0566
	Bi1-I1 / Bi2-I2	3.1972(4)	3.3060	0.1088
	Bi1-I2 / Bi2-I1	3.3270(4)	3.3223	-0.0047
4	**Bi-C**	2.2498(42)	2.2641	0.0143
	Bi-O	2.2001(35)	2.1905	-0.0096
	Bi-N	2.6085(44)	2.6567	0.0482
	Bi-Br1	2.7809(8)	2.8212	0.0403
	Bi-Br2	2.9252(7)	2.8740	-0.0512

The following carbene and 'abnormal' carbene and their corresponding $BiBr_2$ complexes with and without the ^{Dipp}Imd are considered in this calculation. Their corresponding ZPE corrected energies and Gibbs Free energies calculated at M06-2X/B2//M06-2X/B1 level of theory using toluene as solvent (SMD model) are also given below.



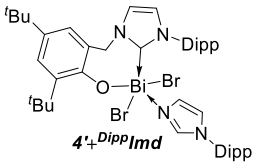
L$^-$

E= -1351.974004 a.u.
G= -1352.036374 a.u.



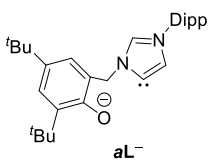
4'

E= -6714.941372 a.u.
G= -6715.014947 a.u.



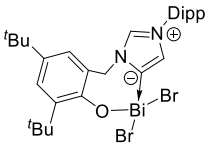
4'*$_+^{Dipp}$*Imd

E= -7407.760182 a.u.
G= -7407.857246 a.u.



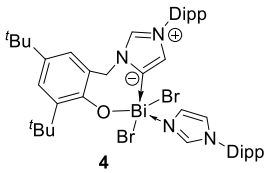
***a*L$^-$**

E= -1351.95473 a.u.
G= -1352.020499 a.u.



4*$_-^{Dipp}$*Imd

E= -6714.936574 a.u.
G= -6715.013769 a.u.



4

E= -7407.765047 a.u.
G= -7407.862547 a.u.

The free energy changes were calculated for the following reactions:

4' + ***a*L$^-$** ⟶ **4–^{Dipp}*imd*** + **L$^-$** ΔG= -9.2 kcal/mol

4+^{Dipp}*imd* + ***a*L$^-$** ⟶ **4** + **L$^-$** ΔG= -13.3 kcal/mol

The bond dissociation energy (BDE) of a metal carbene bond can be estimated as:

$$-BDE = E_{M\text{-}C} - (E_M + E_C) \ldots\ldots\ldots \text{(i)}$$

where $E_{M\text{-}C}$ = electronic energy of the metal carbene complex, E_M = electronic energy of the metal ion and E_C = electronic energy of the free carbene. For normal carbene complex equation **(i)** can be written as: $-BDE^n = E^n_{M\text{-}C} - (E_M + E^n_c) \ldots\ldots\ldots$ **(ii)**

Again, for abnormal carbene complex equation **(i)** can be written as: $-BDE^a = E^a_{M\text{-}C} - (E_M + E^a_c) \ldots\ldots\ldots$ **(iii)**

Where **n** and **a** in the superscript denotes normal and abnormal respectively.
From (ii) and (iii) we can write: $\mathbf{BDE^a - BDE^n = (E^a_c - E^n_c) - (E^a_{M\text{-}C} - E^n_{M\text{-}C})}$ …… **(iv)**
Now, $\mathbf{(E^a_{M\text{-}C} - E^n_{M\text{-}C})}$ can be termed as the rearrangement energy $\mathbf{\Delta E_{rear.}}$ Therefore, equation **(iv)** can be written as:

$$\mathbf{BDE^a - BDE^n = (E^a_c - E^n_c) - \Delta E_{rear}} \text{ …… } \mathbf{(v)}$$

For the free ligands $\mathbf{aL^-}$ and $\mathbf{L^-}$, $\mathbf{(E^a_c - E^n_c)}$ = 0.019274 a.u. = 12.1 kcal/mol
Without ^{Dipp}***Imd***, $\Delta E_{rear.} = (E^a_{M\text{-}C} - E^n_{M\text{-}C})$ = 0.004798 a.u. = 3.0 kcal/mol
Therefore, without ^{Dipp}***Imd***, $\mathbf{(BDE^a - BDE^n)}$= (12.1 – 3.0) kcal/mol = 9.1 kcal/mol
Again, with ^{Dipp}***Imd***, $\Delta E_{rear.} = (E^a_{M\text{-}C} - E^n_{M\text{-}C})$ = -0.004865 a.u. = – 3.0 kcal/mol
Therefore, With ^{Dipp}***Imd***, $\mathbf{(BDE^a - BDE^n)}$= {12.1 – (-3.0)} kcal/mol = 15.1 kcal/mol

NBO analysis:

Table-S3: Selected calculated bond distances (Å) Wiberg bond indices (WBI).

		Calc. bond distance	WBI
$[^{Dipp}NHO]^{2-}$	C1-C2	1.353	1.663
2	C1-C2	1.463	1.093
	Bi-C1	2.310	0.618
$[^{Me}NHO]^{2-}$	C1-C2	1.363	1.590
$\mathbf{3_2}$	C1-C2 / C3-C4	1.469	1.078
	Bi1-C1 / Bi1-C3	2.309	0.588
4	Bi-C1	2.264	0.622
	Bi-N1	2.657	0.152
4'+^{Dipp}Imd	Bi-C1	2.359	0.564
	Bi-N1	2.620	0.160

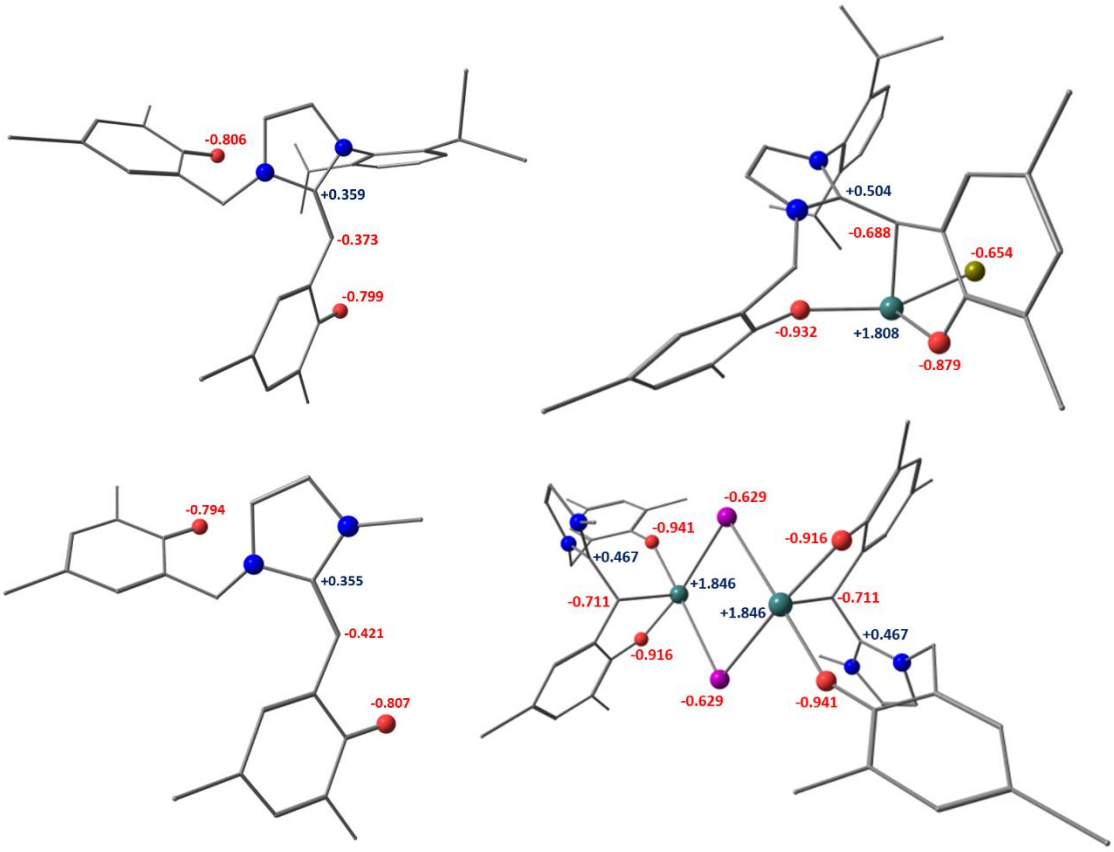


Figure-S25: Natural charges on selected atoms calculated at M062X/B2//M062X/B1 level of theory. The bulky ^{t}Bu groups are not entirely shown for visual clarity.

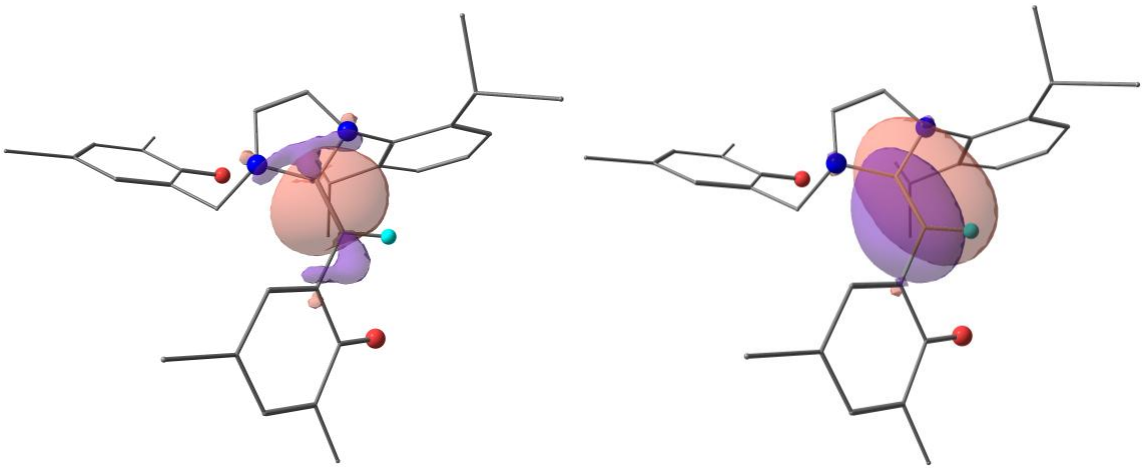


Figure-S26: NBO plots (isovalue=0.030) showing the sigma bond(*left*) and the pi bond (*right*) of the heterocyclic olefin in $[^{Dipp}NHO]^{2-}$. The bulky ^{t}Bu groups are not entirely shown for visual clarity.

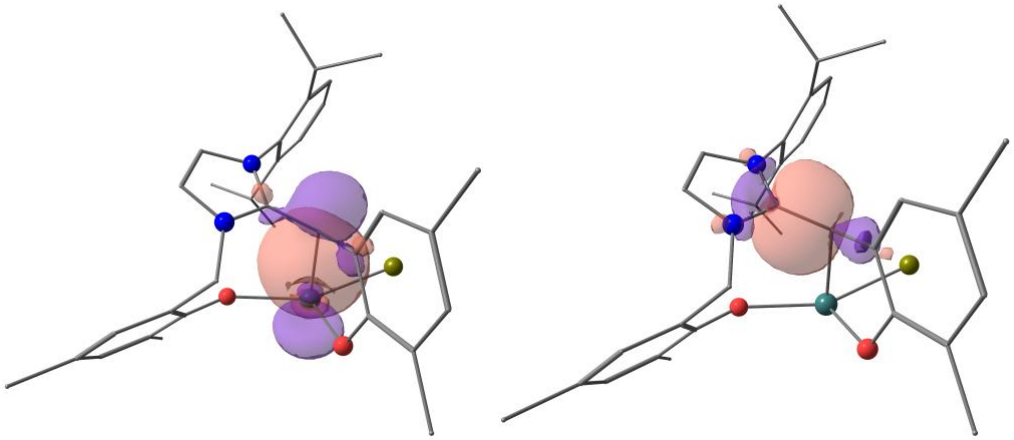


Figure-S27: NBO plots (isovalue=0.030) showing the NHO-Bi bond (*left*) and the sigma bond of the heterocyclic olefin (*right*) in complex **2**. The bulky ^{t}Bu groups are not entirely shown for visual clarity.

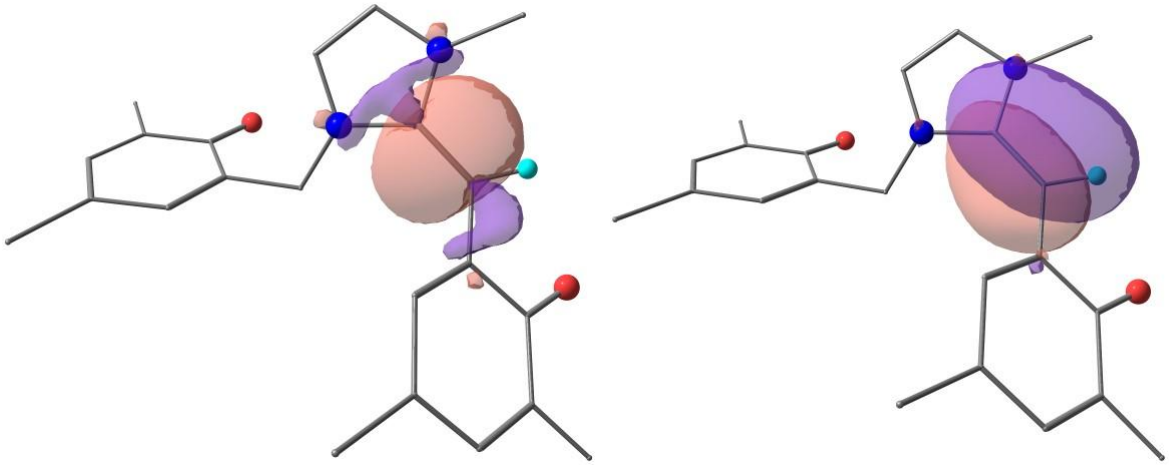


Figure-S28: NBO plots (isovalue=0.030) showing the sigma bond(*left*) and the pi bond (*right*) of the heterocyclic olefin in $[^{Me}NHO]^{2-}$. The bulky ^{t}Bu groups are not entirely shown for visual clarity.

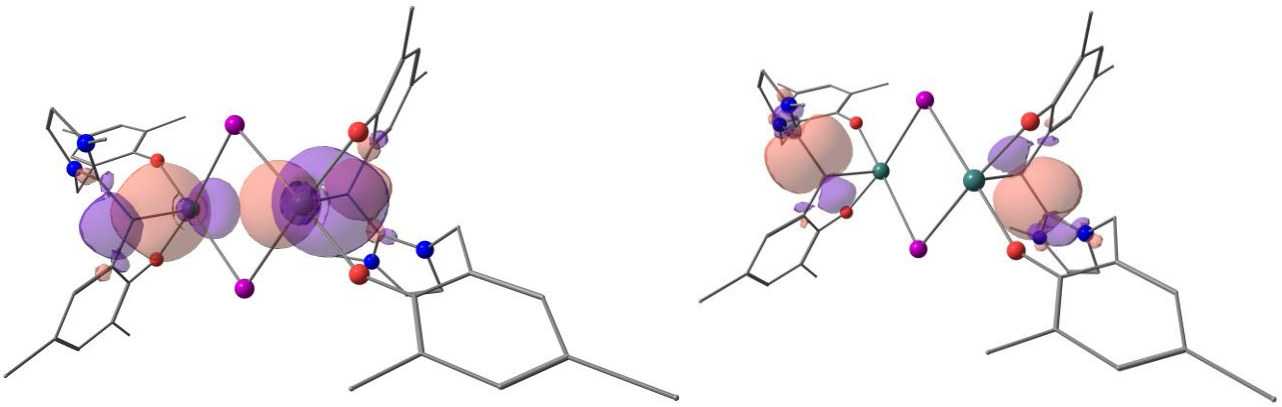


Figure-S29: NBO plots (isovalue=0.030) showing the NHO-Bi bonds (*left*) and the sigma bonds of the heterocyclic olefins (*right*) in complex **3_2.** The bulky ^{t}Bu groups are not entirely shown for visual clarity.

Table-S4: NBO summary:

	NBO (type)	**occupancy**	**Contribution from atomic orbitals**
$[^{Dipp}NHO]^{2-}$	C1-C2 (sigma)	1.979	C1 ($sp^{1.8}$) 48.3% + C2 ($sp^{1.3}$) 51.7%
	C1-C2 (pi)	1.921	C1 (p) 54.9% + C2 (p) 45.1%
2	C1-C2 (sigma)	1.958	C1 ($sp^{2.6}$) 47.4% + C2 ($sp^{1.5}$) 52.6%
	Bi-C1 (sigma)	1.882	Bi (p) 24.7% + C1 (p) 75.3%
$[^{Me}NHO]^{2-}$	C1-C2 (sigma)	1.979	C1 ($sp^{1.8}$) 47.8% + C2 ($sp^{1.3}$) 52.2%
	C1-C2 (pi)	1.903	C1 (p) 57.6% + C2 (p) 42.4%
3_2	C1-C2 / C3-C4 (sigma)	1.974	C1/C3 ($sp^{2.8}$) 47.1% + C2/C4 ($sp^{1.5}$) 52.9%
	Bi1-C1 / Bi2-C3 (sigma)	1.894	Bi1/Bi2 (p) 22.6% + C1/C3 (p) 77.4%

Cartesian coordinates of the optimized structures:

$[^{Dipp}NHO]^{2-}$ (gas phase)
E@B2 = -2011.99780754 a.u.

8	3.744386000	-0.597224000	-1.646450000
8	-2.205272000	1.661376000	-1.423679000
7	1.083070000	2.290172000	1.358057000
7	-0.308908000	0.535546000	0.994706000
6	2.249899000	-1.146528000	0.107439000
6	-0.244322000	2.672310000	1.669739000
1	-0.457595000	3.663409000	2.039695000
6	-3.165281000	-1.256941000	0.495823000
1	-2.657389000	-2.061967000	1.029979000
6	2.114580000	0.279228000	0.405218000
1	3.000647000	0.878338000	0.205490000
6	-4.565059000	-1.226938000	0.445153000
6	-5.137020000	-0.156195000	-0.255211000
1	-6.220162000	-0.094423000	-0.304342000
6	1.633722000	-2.127312000	0.873007000
1	1.012925000	-1.793258000	1.706809000
6	-2.375503000	-0.298935000	-0.115090000
6	1.962809000	3.224133000	0.726038000
6	1.036233000	0.943903000	0.880147000
6	-0.878932000	-0.375327000	-0.030529000
1	-0.562733000	-1.396333000	0.195786000
1	-0.434613000	-0.089705000	-0.992920000
6	-2.949339000	0.794465000	-0.861494000
6	-4.396351000	0.836877000	-0.892494000
6	3.152428000	-1.501055000	-0.973015000
6	-1.051050000	1.625881000	1.466268000
1	-2.116389000	1.534024000	1.607008000
6	1.717663000	3.644620000	-0.592160000
6	2.579940000	4.598907000	-1.141349000
1	2.405522000	4.939380000	-2.159283000
6	3.910813000	4.631026000	0.867820000
1	4.777633000	4.998603000	1.409435000
6	3.076607000	3.677544000	1.452076000
6	3.655777000	5.097788000	-0.418696000

1	4.316093000	5.836272000	-0.866604000
6	3.318046000	-2.917446000	-1.213295000
6	2.631517000	-3.851325000	-0.435309000
1	2.765681000	-4.905159000	-0.660904000
6	3.334906000	3.109665000	2.837673000
1	3.043158000	2.054382000	2.792748000
6	0.590090000	3.060102000	-1.421892000
1	-0.026950000	2.406345000	-0.805177000
6	1.779783000	-3.498888000	0.617295000
6	-5.377740000	-2.325742000	1.131815000
6	-5.019493000	-3.697027000	0.531495000
1	-3.953036000	-3.909893000	0.649552000
1	-5.244956000	-3.711755000	-0.539450000
1	-5.585270000	-4.502156000	1.020215000
6	-5.067183000	2.002626000	-1.624737000
6	-4.630922000	3.328595000	-0.973605000
1	-3.540839000	3.390314000	-0.974618000
1	-4.990301000	3.373731000	0.061345000
1	-5.050234000	4.184966000	-1.520180000
6	1.143211000	2.200912000	-2.565746000
1	1.673612000	2.818983000	-3.303142000
1	0.300574000	1.709911000	-3.063082000
1	1.830418000	1.431118000	-2.196774000
6	-4.640180000	2.000149000	-3.103853000
1	-5.070536000	2.863123000	-3.631215000
1	-4.993309000	1.086404000	-3.595694000
1	-3.551390000	2.037354000	-3.163798000
6	4.248089000	-3.348289000	-2.352180000
6	3.741028000	-2.761654000	-3.682360000
1	2.753716000	-3.172709000	-3.921768000
1	4.427717000	-3.011988000	-4.504419000
1	3.660900000	-1.677756000	-3.582882000
6	-0.362394000	4.138104000	-1.946009000
1	-0.742419000	4.753201000	-1.122774000
1	-1.215735000	3.642939000	-2.416366000
1	0.125719000	4.800733000	-2.673399000
6	5.668340000	-2.818139000	-2.081206000
1	5.619761000	-1.735025000	-1.954585000
1	6.342403000	-3.067865000	-2.913840000
1	6.070402000	-3.270381000	-1.166732000
6	-6.597699000	1.935685000	-1.577069000
1	-6.972007000	1.963873000	-0.547350000
1	-6.977106000	1.023858000	-2.052348000
1	-7.017610000	2.795830000	-2.112917000
6	1.042802000	-4.516328000	1.489853000
6	2.449175000	3.798443000	3.882789000
1	2.664414000	4.873479000	3.913958000
1	2.631572000	3.383925000	4.880955000
1	1.392820000	3.659889000	3.642390000
6	4.804006000	3.184294000	3.254674000
1	5.455505000	2.751108000	2.490770000
1	4.955131000	2.633830000	4.188686000
1	5.121714000	4.219157000	3.430643000
6	-5.062412000	-2.352108000	2.638117000
1	-5.629448000	-3.143910000	3.146640000
1	-5.317587000	-1.391006000	3.095855000
1	-3.997555000	-2.531711000	2.811420000
6	-6.887391000	-2.118568000	0.969676000
1	-7.175830000	-2.119263000	-0.086501000
1	-7.205987000	-1.166458000	1.406719000
1	-7.432740000	-2.925609000	1.473811000
6	4.335471000	-4.870260000	-2.510678000
1	4.717341000	-5.349563000	-1.601748000
1	5.017740000	-5.114132000	-3.335047000
1	3.357629000	-5.308437000	-2.740383000
6	1.227216000	-5.952780000	0.988774000
1	0.867390000	-6.058447000	-0.039725000
1	0.665365000	-6.648122000	1.624606000
1	2.281443000	-6.248031000	1.010261000
6	-0.466626000	-4.209994000	1.502513000
1	-0.661674000	-3.215654000	1.915895000

1	-1.015174000	-4.943046000	2.110451000
1	-0.868659000	-4.227828000	0.484018000
6	1.568074000	-4.446490000	2.935425000
1	2.636569000	-4.684748000	2.959973000
1	1.035765000	-5.152175000	3.589032000
1	1.441951000	-3.439128000	3.342413000

2 (gas phase)
E@B2 = -4800.79476148 a.u.

83	0.021008000	-0.468393000	-1.905505000
35	-2.408186000	-1.190896000	-3.025996000
8	-0.331900000	1.609617000	-1.852915000
8	1.842899000	-0.605658000	-0.500581000
7	-0.659504000	-1.806904000	1.913922000
7	0.464643000	0.038325000	1.868590000
6	-1.755147000	1.135302000	-0.003210000
6	0.226551000	-1.849942000	2.976344000
1	0.262437000	-2.696062000	3.642617000
6	3.601941000	1.594458000	1.802747000
1	3.332678000	2.338101000	2.551837000
6	-1.235579000	-0.289770000	0.024806000
1	-2.046681000	-1.006236000	-0.125053000
6	4.942483000	1.298778000	1.554266000
6	5.203174000	0.327791000	0.582240000
1	6.236109000	0.076542000	0.379747000
6	-2.687534000	1.561817000	0.937764000
1	-3.047878000	0.841950000	1.670849000
6	2.586106000	0.959489000	1.101547000
6	-1.578073000	-2.855730000	1.560278000
6	-0.500047000	-0.647470000	1.238295000
6	1.143178000	1.258186000	1.379669000
1	1.024911000	2.034319000	2.140283000
1	0.618206000	1.577863000	0.480344000
6	2.856972000	-0.015732000	0.112663000
6	4.214422000	-0.342449000	-0.144268000
6	-1.273675000	2.029648000	-0.976984000
6	0.931237000	-0.694490000	2.940283000
1	1.743360000	-0.332544000	3.550059000
6	-1.160873000	-3.809735000	0.621353000
6	-2.057758000	-4.833708000	0.314435000
1	-1.773635000	-5.590169000	-0.409970000
6	-3.697209000	-3.919420000	1.830107000
1	-4.682983000	-3.968944000	2.282101000
6	-2.841404000	-2.869066000	2.165317000
6	-3.308672000	-4.892461000	0.917281000
1	-3.991392000	-5.696778000	0.663848000
6	-1.733445000	3.363615000	-0.998596000
6	-2.666380000	3.738649000	-0.027998000
1	-3.022373000	4.760072000	-0.037346000
6	-3.279980000	-1.799264000	3.149500000
1	-2.555654000	-0.977173000	3.108102000
6	0.217882000	-3.768570000	-0.014272000
1	0.648045000	-2.768622000	0.131044000
6	-3.162872000	2.871726000	0.950017000
6	6.043739000	2.021369000	2.334840000
6	5.946896000	3.534585000	2.077684000
1	4.978275000	3.933257000	2.392947000
1	6.068935000	3.752724000	1.012700000
1	6.726913000	4.067832000	2.632127000
6	4.574837000	-1.408656000	-1.185798000
6	3.923480000	-2.749373000	-0.801865000
1	2.840152000	-2.639532000	-0.731102000
1	4.302495000	-3.094171000	0.166366000
1	4.158184000	-3.513636000	-1.552476000
6	0.168227000	-4.049672000	-1.521751000
1	-0.017558000	-5.109604000	-1.722995000
1	1.133221000	-3.801003000	-1.976717000
1	-0.623864000	-3.480828000	-2.022754000
6	4.084620000	-0.970234000	-2.576368000
1	4.343704000	-1.726997000	-3.325197000

1	4.553506000	-0.025359000	-2.867677000
1	3.002394000	-0.833799000	-2.583713000
6	-1.208493000	4.355610000	-2.042685000
6	0.311946000	4.529516000	-1.873421000
1	0.541948000	4.921161000	-0.876764000
1	0.688395000	5.244462000	-2.613159000
1	0.837142000	3.583180000	-2.006533000
6	1.150605000	-4.763402000	0.690769000
1	1.258217000	-4.522705000	1.752545000
1	2.143564000	-4.744067000	0.233321000
1	0.751931000	-5.780177000	0.611115000
6	-1.528842000	3.842786000	-3.458117000
1	-1.065428000	2.874048000	-3.644577000
1	-1.159631000	4.557195000	-4.202120000
1	-2.610224000	3.739887000	-3.590701000
6	6.087716000	-1.640834000	-1.284823000
1	6.510197000	-1.977979000	-0.332862000
1	6.618757000	-0.736587000	-1.598698000
1	6.283470000	-2.417202000	-2.030806000
6	-4.206828000	3.295176000	1.987334000
6	-3.280384000	-2.348846000	4.581275000
1	-3.982938000	-3.183557000	4.671215000
1	-3.581473000	-1.572308000	5.290085000
1	-2.289447000	-2.711581000	4.868923000
6	-4.652723000	-1.225454000	2.781985000
1	-4.679455000	-0.897735000	1.738455000
1	-4.886111000	-0.368272000	3.421587000
1	-5.446172000	-1.965520000	2.923305000
6	5.869641000	1.752670000	3.839312000
1	6.648628000	2.266698000	4.412859000
1	5.937259000	0.680860000	4.049708000
1	4.899788000	2.108018000	4.200171000
6	7.444628000	1.554925000	1.925986000
1	7.638258000	1.747476000	0.866204000
1	7.583274000	0.485375000	2.112990000
1	8.196223000	2.097219000	2.507768000
6	-1.853379000	5.739065000	-1.892990000
1	-2.939558000	5.697713000	-2.023162000
1	-1.451076000	6.404407000	-2.662585000
1	-1.636102000	6.188683000	-0.918556000
6	-4.493431000	4.799702000	1.939231000
1	-3.585622000	5.386856000	2.110662000
1	-5.216769000	5.060074000	2.717894000
1	-4.920419000	5.098072000	0.977109000
6	-3.709200000	2.949226000	3.400868000
1	-3.538264000	1.874326000	3.518663000
1	-4.450560000	3.251612000	4.148162000
1	-2.769599000	3.466111000	3.618987000
6	-5.519591000	2.542078000	1.714866000
1	-5.898802000	2.777879000	0.716322000
1	-6.282227000	2.820658000	2.450688000
1	-5.372364000	1.459554000	1.769459000

[^{Dipp}NHO]$^{2-}$ (gas phase)
E@B2 = -1584.39662126 a.u.

8	4.395943000	-2.333477000	0.683175000
8	-3.039359000	-2.313237000	1.089148000
7	0.367313000	-3.623911000	-1.802789000
7	-0.439348000	-1.734992000	-0.924855000
6	2.705099000	-0.996843000	-0.322455000
6	-1.000307000	-3.550714000	-2.097822000
1	-1.497475000	-4.332818000	-2.650324000
6	-2.169414000	1.029225000	0.001451000
1	-1.267957000	1.565756000	-0.291195000
6	2.034860000	-2.229368000	-0.721638000
1	2.704301000	-3.084054000	-0.747545000
6	-3.398251000	1.702333000	0.024828000
6	-4.510991000	0.949355000	0.422221000
1	-5.481283000	1.437056000	0.445975000
6	2.288719000	0.271015000	-0.717022000

1	1.383009000	0.332762000	-1.323301000
6	-2.034667000	-0.304100000	0.346335000
6	0.746327000	-2.472217000	-1.094869000
6	-0.683286000	-0.970857000	0.318047000
1	0.114243000	-0.228332000	0.408261000
1	-0.609912000	-1.671253000	1.158775000
6	-3.170390000	-1.089100000	0.775404000
6	-4.442672000	-0.391591000	0.789136000
6	3.966820000	-1.169906000	0.390479000
6	-1.486852000	-2.438640000	-1.531628000
1	-2.498835000	-2.077606000	-1.457873000
6	4.679243000	0.040602000	0.718904000
6	4.185691000	1.285370000	0.319910000
1	4.752692000	2.172492000	0.585109000
6	3.002672000	1.442399000	-0.405843000
6	-3.467110000	3.180618000	-0.361863000
6	-2.596446000	4.015256000	0.594065000
1	-1.554659000	3.683860000	0.560326000
1	-2.950564000	3.903872000	1.623979000
1	-2.624353000	5.080715000	0.326448000
6	-5.688548000	-1.180120000	1.203636000
6	-5.883230000	-2.367948000	0.242698000
1	-4.977212000	-2.976935000	0.244903000
1	-6.069123000	-2.001621000	-0.773978000
1	-6.743719000	-2.979462000	0.550296000
6	-5.506120000	-1.718379000	2.634543000
1	-6.368623000	-2.333146000	2.929925000
1	-5.420546000	-0.885091000	3.341627000
1	-4.593989000	-2.316237000	2.673986000
6	5.991521000	-0.087983000	1.500338000
6	5.728140000	-0.799602000	2.840115000
1	5.062543000	-0.191475000	3.463478000
1	6.668251000	-0.956023000	3.390084000
1	5.250567000	-1.760150000	2.638483000
6	6.996599000	-0.920733000	0.682644000
1	6.538619000	-1.883200000	0.446539000
1	7.928052000	-1.074966000	1.247949000
1	7.243609000	-0.399959000	-0.250265000
6	-6.967250000	-0.335830000	1.175647000
1	-7.173417000	0.052126000	0.171526000
1	-6.903558000	0.515918000	1.862460000
1	-7.820631000	-0.954042000	1.481358000
6	2.540366000	2.797608000	-0.945327000
6	-2.943750000	3.377762000	-1.795681000
1	-2.981894000	4.436566000	-2.086899000
1	-3.545890000	2.798394000	-2.502962000
1	-1.907094000	3.040167000	-1.883008000
6	-4.896572000	3.729964000	-0.301739000
1	-5.310001000	3.650023000	0.709065000
1	-5.559390000	3.185076000	-0.982246000
1	-4.903620000	4.788033000	-0.590678000
6	6.641409000	1.265873000	1.807460000
1	6.894204000	1.810133000	0.890158000
1	7.568562000	1.107949000	2.373637000
1	5.981277000	1.902101000	2.407858000
6	3.273618000	3.970033000	-0.282015000
1	3.150898000	3.941568000	0.805562000
1	2.873138000	4.921690000	-0.652989000
1	4.345635000	3.948055000	-0.502138000
6	1.034225000	2.991261000	-0.708369000
1	0.455448000	2.246049000	-1.260274000
1	0.703288000	3.985015000	-1.041262000
1	0.794105000	2.877540000	0.354223000
6	2.803899000	2.865835000	-2.461368000
1	3.874766000	2.754529000	-2.661263000
1	2.462670000	3.820312000	-2.887878000
1	2.282532000	2.051197000	-2.972760000
6	1.329291000	-4.435344000	-2.483340000
1	0.820100000	-5.043362000	-3.237009000
1	2.085370000	-3.797604000	-2.965333000
1	1.861558000	-5.106993000	-1.797174000

3_2 (gas phase)
E@B2 = -4193.32147599 a.u.

83	-1.188930000	-0.847259000	-1.887492000
53	1.478028000	1.048655000	-1.416089000
8	-1.177485000	-0.132367000	-3.923546000
8	-3.120160000	-1.839468000	-1.916516000
7	-4.189481000	1.487906000	-0.178850000
7	-4.614264000	0.581892000	-2.094625000
6	-1.371086000	1.192398000	-4.069962000
6	-4.488452000	-0.006341000	-3.442738000
1	-3.454527000	0.119665000	-3.757830000
1	-5.121249000	0.580453000	-4.113875000
6	-3.674711000	5.724640000	-4.203481000
1	-3.999715000	5.377604000	-3.218165000
1	-4.271660000	5.203884000	-4.958414000
1	-3.892187000	6.796157000	-4.270410000
6	-2.180261000	3.286346000	-3.137200000
1	-2.604353000	3.821771000	-2.288703000
6	-3.501736000	2.182016000	0.905871000
1	-2.765484000	1.519571000	1.364367000
1	-4.248496000	2.465256000	1.646412000
1	-3.020045000	3.081997000	0.518813000
6	-2.174899000	5.466821000	-4.425474000
6	-4.880292000	-1.453142000	-3.445054000
6	-5.956424000	-1.904678000	-4.197131000
1	-6.516597000	-1.183377000	-4.790301000
6	-1.062564000	1.850678000	-5.280687000
6	-4.458433000	-3.706222000	-2.635794000
6	-3.629893000	1.103283000	-1.344341000
6	-1.924015000	1.925880000	-3.000342000
6	-6.312809000	-3.253253000	-4.205831000
6	-1.366766000	6.216263000	-3.352785000
1	-1.553103000	7.293825000	-3.418173000
1	-0.295277000	6.040319000	-3.484543000
1	-1.637679000	5.888699000	-2.344926000
6	-5.796332000	0.604833000	-1.390466000
1	-6.701305000	0.190906000	-1.805018000
6	-5.546553000	-4.114029000	-3.414944000
1	-5.812699000	-5.162450000	-3.400102000
6	-1.335461000	3.218298000	-5.362401000
1	-1.097096000	3.726722000	-6.287136000
6	-5.533449000	1.174773000	-0.190021000
1	-6.170583000	1.382417000	0.653480000
6	-3.681837000	-4.702126000	-1.765368000
6	-7.497934000	-3.725928000	-5.052264000
6	-3.774615000	-4.285685000	-0.286290000
1	-3.207447000	-4.987190000	0.335622000
1	-4.817626000	-4.304582000	0.046103000
1	-3.377484000	-3.282413000	-0.126785000
6	-2.206300000	1.216349000	-1.690392000
1	-1.673997000	1.696259000	-0.865584000
6	-1.892498000	3.965322000	-4.319606000
6	-4.108941000	-2.334751000	-2.660189000
6	-2.208578000	-4.755148000	-2.205369000
1	-1.721327000	-3.788870000	-2.069243000
1	-2.129154000	-5.039571000	-3.259442000
1	-1.665996000	-5.494888000	-1.606843000
6	-1.790753000	6.032691000	-5.796486000
1	-2.353258000	5.551197000	-6.602581000
1	-0.722577000	5.906424000	-5.997849000
1	-2.012929000	7.103746000	-5.825850000
6	-0.447113000	1.075679000	-6.450559000
6	-4.238963000	-6.127163000	-1.882218000
1	-3.655855000	-6.791555000	-1.237538000
1	-4.172033000	-6.511028000	-2.905541000
1	-5.282890000	-6.182570000	-1.557975000
6	0.895568000	0.462524000	-6.013456000
1	1.593538000	1.250223000	-5.712595000
1	1.340449000	-0.090750000	-6.848339000

1	0.761649000	-0.218024000	-5.172011000
6	-8.775280000	-2.998484000	-4.599680000
1	-8.987607000	-3.210619000	-3.547377000
1	-9.633124000	-3.324866000	-5.197536000
1	-8.681281000	-1.914528000	-4.714301000
6	-7.736364000	-5.233942000	-4.924292000
1	-6.867001000	-5.807856000	-5.259766000
1	-8.589178000	-5.523867000	-5.545581000
1	-7.961032000	-5.519943000	-3.891938000
6	-0.174729000	1.979398000	-7.659094000
1	-1.094200000	2.429283000	-8.047805000
1	0.266511000	1.379783000	-8.460984000
1	0.529440000	2.781699000	-7.416506000
6	-7.230512000	-3.405182000	-6.532455000
1	-7.095615000	-2.331499000	-6.692173000
1	-8.071240000	-3.734783000	-7.152588000
1	-6.325397000	-3.912454000	-6.879119000
6	-1.413049000	-0.033664000	-6.905061000
1	-1.621462000	-0.732926000	-6.094562000
1	-0.975512000	-0.588246000	-7.742642000
1	-2.358730000	0.401709000	-7.245312000
83	1.188930000	0.847259000	1.887492000
53	-1.478028000	-1.048655000	1.416089000
8	1.177485000	0.132367000	3.923546000
8	3.120160000	1.839468000	1.916516000
7	4.189481000	-1.487906000	0.178850000
7	4.614264000	-0.581892000	2.094625000
6	1.371086000	-1.192398000	4.069962000
6	4.488452000	0.006341000	3.442738000
1	3.454527000	-0.119665000	3.757830000
1	5.121249000	-0.580453000	4.113875000
6	3.674711000	-5.724640000	4.203481000
1	3.999715000	-5.377604000	3.218165000
1	4.271660000	-5.203884000	4.958414000
1	3.892187000	-6.796157000	4.270410000
6	2.180261000	-3.286346000	3.137200000
1	2.604353000	-3.821771000	2.288703000
6	3.501736000	-2.182016000	-0.905871000
1	2.765484000	-1.519571000	-1.364367000
1	4.248496000	-2.465256000	-1.646412000
1	3.020045000	-3.081997000	-0.518813000
6	2.174899000	-5.466821000	4.425474000
6	4.880292000	1.453142000	3.445054000
6	5.956424000	1.904678000	4.197131000
1	6.516597000	1.183377000	4.790301000
6	1.062564000	-1.850678000	5.280687000
6	4.458433000	3.706222000	2.635794000
6	3.629893000	-1.103283000	1.344341000
6	1.924015000	-1.925880000	3.000342000
6	6.312809000	3.253253000	4.205831000
6	1.366766000	-6.216263000	3.352785000
1	1.553103000	-7.293825000	3.418173000
1	0.295277000	-6.040319000	3.484543000
1	1.637679000	-5.888699000	2.344926000
6	5.796332000	-0.604833000	1.390466000
1	6.701305000	-0.190906000	1.805018000
6	5.546553000	4.114029000	3.414944000
1	5.812699000	5.162450000	3.400102000
6	1.335461000	-3.218298000	5.362401000
1	1.097096000	-3.726722000	6.287136000
6	5.533449000	-1.174773000	0.190021000
1	6.170583000	-1.382417000	-0.653480000
6	3.681837000	4.702126000	1.765368000
6	7.497934000	3.725928000	5.052264000
6	3.774615000	4.285685000	0.286290000
1	3.207447000	4.987190000	-0.335622000
1	4.817626000	4.304582000	-0.046103000
1	3.377484000	3.282413000	0.126785000
6	2.206300000	-1.216349000	1.690392000
1	1.673997000	-1.696259000	0.865584000
6	1.892498000	-3.965322000	4.319606000

6	4.108941000	2.334751000	2.660189000
6	2.208578000	4.755148000	2.205369000
1	1.721327000	3.788870000	2.069243000
1	2.129154000	5.039571000	3.259442000
1	1.665996000	5.494888000	1.606843000
6	1.790753000	-6.032691000	5.796486000
1	2.353258000	-5.551197000	6.602581000
1	0.722577000	-5.906424000	5.997849000
1	2.012929000	-7.103746000	5.825850000
6	0.447113000	-1.075679000	6.450559000
6	4.238963000	6.127163000	1.882218000
1	3.655855000	6.791555000	1.237538000
1	4.172033000	6.511028000	2.905541000
1	5.282890000	6.182570000	1.557975000
6	-0.895568000	-0.462524000	6.013456000
1	-1.593538000	-1.250223000	5.712595000
1	-1.340449000	0.090750000	6.848339000
1	-0.761649000	0.218024000	5.172011000
6	8.775280000	2.998484000	4.599680000
1	8.987607000	3.210619000	3.547377000
1	9.633124000	3.324866000	5.197536000
1	8.681281000	1.914528000	4.714301000
6	7.736364000	5.233942000	4.924292000
1	6.867001000	5.807856000	5.259766000
1	8.589178000	5.523867000	5.545581000
1	7.961032000	5.519943000	3.891938000
6	0.174729000	-1.979398000	7.659094000
1	1.094200000	-2.429283000	8.047805000
1	-0.266511000	-1.379783000	8.460984000
1	-0.529440000	-2.781699000	7.416506000
6	7.230512000	3.405182000	6.532455000
1	7.095615000	2.331499000	6.692173000
1	8.071240000	3.734783000	7.152588000
1	6.325397000	3.912454000	6.879119000
6	1.413049000	0.033664000	6.905061000
1	1.621462000	0.732926000	6.094562000
1	0.975512000	0.588246000	7.742642000
1	2.358730000	-0.401709000	7.245312000

4 (gas phase)
E@B2 = -7408.69827797 a.u.

83	-0.552203000	-2.185255000	0.469933000
35	-0.260973000	-2.375940000	3.269591000
35	-0.115798000	-1.228974000	-2.204942000
8	-2.740459000	-2.145722000	0.561892000
7	-0.060162000	2.203966000	1.008059000
7	-1.460035000	0.710546000	1.701126000
6	-3.370380000	-3.035366000	-2.264647000
1	-2.585846000	-3.288212000	-1.551344000
1	-3.009154000	-2.205440000	-2.877846000
1	-3.528038000	-3.904866000	-2.912607000
6	-0.554904000	0.037476000	0.900688000
6	-1.277248000	3.940861000	-0.947613000
1	-1.937738000	3.380786000	-0.273750000
6	-4.684756000	-2.680984000	-1.548936000
6	0.322034000	0.991559000	0.471328000
1	1.173628000	0.915485000	-0.189047000
6	1.734999000	3.780030000	1.481826000
6	-5.410971000	0.931848000	-0.370788000
6	0.567325000	3.476039000	0.767369000
6	-3.678325000	-0.016813000	1.035714000
6	-4.538775000	1.025456000	0.709677000
1	-4.521729000	1.926096000	1.324185000
6	-1.153160000	2.001116000	1.752697000
1	-1.700593000	2.769263000	2.277638000
6	-2.728933000	0.132792000	2.190327000
1	-3.119195000	0.821067000	2.943966000
1	-2.485370000	-0.820812000	2.662714000
6	2.311645000	5.030118000	1.249119000
1	3.212774000	5.312658000	1.782751000

6	-0.025534000	4.335490000	-0.172006000
6	-5.045937000	-3.797032000	-0.551559000
1	-5.109242000	-4.757744000	-1.074949000
1	-6.017156000	-3.597046000	-0.087451000
1	-4.292752000	-3.874766000	0.233913000
6	2.304337000	2.817608000	2.512197000
1	2.071928000	1.795397000	2.192206000
6	-5.412166000	-0.277267000	-1.075430000
1	-6.108199000	-0.386261000	-1.896232000
6	0.605394000	5.565069000	-0.376342000
1	0.188370000	6.267929000	-1.088289000
6	-4.569533000	-1.353393000	-0.787330000
6	-6.301124000	2.120123000	-0.742699000
6	-3.627940000	-1.195505000	0.262472000
6	-5.787045000	-2.634251000	-2.615597000
1	-5.572718000	-1.890607000	-3.390341000
1	-6.767448000	-2.413628000	-2.181349000
1	-5.852071000	-3.611835000	-3.102257000
6	-0.934503000	3.012927000	-2.124300000
1	-0.248059000	3.517208000	-2.813182000
1	-1.845742000	2.760987000	-2.674063000
1	-0.480105000	2.070249000	-1.806556000
6	1.752677000	5.910387000	0.329974000
1	2.218064000	6.875680000	0.158137000
6	1.634456000	3.051877000	3.874030000
1	2.012680000	2.341560000	4.614140000
1	0.549436000	2.930103000	3.814442000
1	1.842870000	4.066329000	4.229359000
6	-2.066201000	5.152638000	-1.448788000
1	-2.264426000	5.871339000	-0.648359000
1	-3.024050000	4.820631000	-1.855973000
1	-1.533982000	5.670316000	-2.253151000
6	3.825459000	2.910697000	2.644302000
1	4.137894000	3.857882000	3.094952000
1	4.321855000	2.811670000	1.673674000
1	4.183140000	2.110009000	3.297659000
6	-7.190660000	2.505893000	0.450422000
1	-7.825019000	3.361206000	0.193285000
1	-6.595061000	2.782105000	1.325290000
1	-7.836472000	1.669905000	0.734326000
6	-7.209265000	1.813424000	-1.937804000
1	-7.883491000	0.978354000	-1.724055000
1	-6.628140000	1.566262000	-2.831508000
1	-7.822805000	2.690015000	-2.167601000
6	-5.404510000	3.314248000	-1.115471000
1	-6.010579000	4.181932000	-1.399622000
1	-4.755636000	3.052193000	-1.958133000
1	-4.765840000	3.609399000	-0.275994000
7	2.030419000	-1.577730000	0.607918000
7	3.942471000	-0.713180000	-0.058783000
6	2.798311000	-1.330431000	-0.434275000
1	2.551297000	-1.548852000	-1.464649000
6	2.705378000	-1.108293000	1.709702000
1	2.277297000	-1.201263000	2.698139000
6	3.897185000	-0.564814000	1.312853000
1	4.711955000	-0.108413000	1.853099000
6	6.006712000	-2.655253000	-0.577333000
1	5.316175000	-2.643969000	0.272196000
6	5.012307000	-0.332172000	-0.935976000
6	6.027060000	-1.265122000	-1.189375000
6	7.034261000	0.366798000	-2.668447000
1	7.827597000	0.641747000	-3.356118000
6	7.039193000	-0.888545000	-2.074451000
1	7.836775000	-1.588435000	-2.302821000
6	6.020738000	1.276001000	-2.386047000
1	6.036797000	2.253725000	-2.855082000
6	3.855126000	1.924524000	-1.225579000
1	3.458952000	1.698254000	-0.225002000
6	4.985437000	0.948104000	-1.509466000
6	5.478971000	-3.669917000	-1.600687000
1	6.135884000	-3.705736000	-2.476033000

1	5.438117000	-4.670811000	-1.161883000
1	4.475275000	-3.404742000	-1.943645000
6	7.380301000	-3.081155000	-0.050492000
1	7.791777000	-2.339292000	0.638894000
1	7.295431000	-4.033669000	0.479347000
1	8.097653000	-3.224257000	-0.864303000
6	4.322946000	3.381696000	-1.220362000
1	4.608669000	3.711289000	-2.224052000
1	3.505846000	4.026914000	-0.888482000
1	5.179524000	3.533658000	-0.556250000
6	2.712717000	1.754922000	-2.238156000
1	2.266632000	0.754876000	-2.223469000
1	1.919943000	2.481121000	-2.024986000
1	3.078475000	1.943306000	-3.252910000

4'+^{Dipp}Imd (gas phase)
E@B2 = -7408.69930166

83	0.462159000	-0.911263000	-0.204075000
35	-0.605504000	-0.764608000	-2.852653000
35	1.130541000	-0.227610000	2.401501000
8	2.440078000	-1.640450000	-0.747798000
7	0.597778000	2.514008000	-0.275212000
7	2.133774000	1.603675000	-1.470426000
6	3.281449000	-3.154361000	1.763741000
1	2.326767000	-2.930355000	1.288650000
1	3.468583000	-2.381110000	2.513818000
1	3.190552000	-4.120478000	2.273023000
6	2.347711000	2.961638000	-1.526138000
6	-1.744026000	2.676618000	-1.935677000
1	-0.903477000	2.020470000	-2.179734000
6	4.418073000	-3.220626000	0.731116000
6	1.376020000	3.537743000	-0.781476000
1	1.142426000	4.570662000	-0.584392000
6	-0.662254000	3.125663000	1.747172000
6	6.286532000	-0.042864000	-0.444760000
6	-0.659369000	2.796463000	0.383730000
6	4.028791000	0.010075000	-1.321233000
6	5.300384000	0.560799000	-1.221328000
1	5.519637000	1.473266000	-1.775004000
6	1.073457000	1.313817000	-0.695250000
6	2.983765000	0.635292000	-2.195343000
1	3.443176000	1.202157000	-3.008076000
1	2.317204000	-0.113124000	-2.630723000
6	-1.896026000	3.453839000	2.318258000
1	-1.940363000	3.701148000	3.373710000
6	-1.807715000	2.857254000	-0.426696000
6	4.042031000	-4.211256000	-0.386093000
1	3.827922000	-5.195861000	0.044969000
1	4.869455000	-4.321777000	-1.094341000
1	3.161313000	-3.867764000	-0.930854000
6	0.610853000	3.228618000	2.570200000
1	1.365081000	2.584648000	2.109993000
6	5.946260000	-1.244852000	0.185088000
1	6.708374000	-1.746684000	0.765886000
6	-3.008474000	3.200182000	0.195866000
1	-3.913238000	3.274133000	-0.400285000
6	4.686883000	-1.845888000	0.104344000
6	7.674165000	0.595318000	-0.335255000
6	3.684834000	-1.167775000	-0.631230000
6	5.656112000	-3.775092000	1.448367000
1	5.961033000	-3.137949000	2.285059000
1	6.506336000	-3.887977000	0.768236000
1	5.420289000	-4.764339000	1.851824000
6	-1.520773000	4.040304000	-2.609376000
1	-2.357290000	4.712032000	-2.388709000
1	-1.456927000	3.917935000	-3.694400000
1	-0.601854000	4.523078000	-2.268626000
6	-3.056819000	3.478600000	1.557486000
1	-4.003319000	3.738666000	2.022186000
6	0.423175000	2.763136000	4.017560000

1	1.400575000	2.665448000	4.497379000
1	-0.067465000	1.789600000	4.065850000
1	-0.157466000	3.487567000	4.598727000
6	-2.991918000	2.020378000	-2.528039000
1	-3.242174000	1.094823000	-2.005957000
1	-2.804731000	1.766617000	-3.574485000
1	-3.858128000	2.690683000	-2.493738000
6	1.120341000	4.678540000	2.569206000
1	0.366859000	5.347290000	2.998441000
1	1.352698000	5.037876000	1.563949000
1	2.029468000	4.757647000	3.172244000
6	8.309757000	0.689529000	-1.732552000
1	9.303659000	1.146188000	-1.670470000
1	7.702730000	1.298138000	-2.409203000
1	8.413265000	-0.304911000	-2.176638000
6	8.614348000	-0.212794000	0.564925000
1	8.780038000	-1.220687000	0.171849000
1	8.219496000	-0.300056000	1.581884000
1	9.585884000	0.287532000	0.623027000
6	7.540882000	2.008577000	0.256661000
1	8.524842000	2.483103000	0.339526000
1	7.090654000	1.968299000	1.252927000
1	6.911875000	2.646957000	-0.370897000
7	-1.963522000	-0.222950000	0.507832000
7	-4.116073000	-0.674925000	0.596320000
6	-2.999780000	-0.683018000	-0.168013000
1	-2.976923000	-1.022086000	-1.196172000
6	-2.422377000	0.085882000	1.764543000
1	-1.753496000	0.469019000	2.520803000
6	-3.760551000	-0.183223000	1.835228000
1	-4.482192000	-0.096831000	2.631925000
6	-6.021337000	1.244345000	-0.384641000
1	-4.931217000	1.337510000	-0.393371000
6	-5.413138000	-1.153582000	0.211300000
6	-6.351471000	-0.232928000	-0.276565000
6	-7.905449000	-2.076202000	-0.511485000
1	-8.887007000	-2.440315000	-0.797480000
6	-7.609359000	-0.723144000	-0.629451000
1	-8.363600000	-0.039762000	-1.006304000
6	-6.951667000	-2.965984000	-0.032007000
1	-7.195574000	-4.020317000	0.050365000
6	-4.630848000	-3.498245000	0.846649000
1	-3.864189000	-2.925589000	1.379612000
6	-5.683632000	-2.522678000	0.348406000
6	-6.551492000	1.875365000	-1.673930000
1	-7.645272000	1.909125000	-1.689105000
1	-6.197502000	2.908274000	-1.755012000
1	-6.211456000	1.326749000	-2.556335000
6	-6.539177000	2.004854000	0.842810000
1	-6.096738000	1.618908000	1.765340000
1	-6.292719000	3.069245000	0.764455000
1	-7.627544000	1.913918000	0.922181000
6	-5.203248000	-4.525056000	1.828414000
1	-5.889813000	-5.217890000	1.332439000
1	-4.392404000	-5.121499000	2.254825000
1	-5.740878000	-4.039698000	2.647047000
6	-3.958489000	-4.203395000	-0.339732000
1	-3.489174000	-3.489216000	-1.021973000
1	-3.188342000	-4.895166000	0.013323000
1	-4.697148000	-4.776528000	-0.909737000
1	3.161043000	3.387478000	-2.090913000

L^{-} (in toluene)
E@B2 = -1352.62767266 a.u.

8	-3.377744000	-2.888885000	-0.349541000
7	2.391375000	-0.737208000	0.249695000
7	0.470740000	-1.557453000	-0.093535000
6	-6.153445000	-2.010460000	-1.055021000
1	-5.440409000	-2.811211000	-1.257461000
1	-6.207623000	-1.354564000	-1.931677000

1	-7.150091000	-2.441921000	-0.891259000
6	0.586625000	-1.419312000	1.278200000
6	4.725912000	-2.348696000	-0.273753000
1	3.756838000	-2.601019000	-0.713706000
6	-5.695659000	-1.215159000	0.180550000
6	1.813489000	-0.896774000	1.505118000
1	2.321226000	-0.624349000	2.417976000
6	3.671909000	1.328126000	0.121541000
6	-2.731206000	1.236846000	-0.245008000
6	3.642982000	-0.072130000	0.050922000
6	-1.910174000	-1.043767000	-0.497570000
6	-1.696125000	0.324057000	-0.474222000
1	-0.678104000	0.685402000	-0.636339000
6	1.566299000	-1.131748000	-0.777091000
6	-0.771673000	-2.008891000	-0.722983000
1	-1.064750000	-2.980216000	-0.314681000
1	-0.535561000	-2.147468000	-1.782267000
6	4.905448000	1.967929000	-0.034842000
1	4.952555000	3.052687000	0.013719000
6	4.798717000	-0.832037000	-0.202158000
6	-5.695202000	-2.146954000	1.405400000
1	-6.691909000	-2.580171000	1.563454000
1	-5.421198000	-1.589911000	2.309017000
1	-4.972102000	-2.949487000	1.251598000
6	2.411248000	2.155200000	0.319971000
1	1.570213000	1.468730000	0.456500000
6	-4.006487000	0.690108000	-0.039908000
1	-4.829757000	1.372805000	0.144158000
6	6.006304000	-0.150146000	-0.355264000
1	6.915675000	-0.708288000	-0.553432000
6	-4.279982000	-0.676051000	-0.053930000
6	-2.435323000	2.738824000	-0.229010000
6	-3.214389000	-1.626356000	-0.303412000
6	-6.723694000	-0.107168000	0.434444000
1	-6.807967000	0.575898000	-0.418202000
1	-6.475423000	0.485599000	1.322062000
1	-7.710687000	-0.554999000	0.599516000
6	4.779641000	-2.950464000	1.136704000
1	5.724170000	-2.689002000	1.627440000
1	4.709047000	-4.042054000	1.092018000
1	3.958280000	-2.585141000	1.758845000
6	6.062692000	1.237813000	-0.265449000
1	7.012753000	1.749599000	-0.387095000
6	2.118550000	2.997870000	-0.926343000
1	1.198646000	3.576741000	-0.789256000
1	1.995900000	2.360095000	-1.806491000
1	2.932763000	3.703552000	-1.126779000
6	5.815072000	-2.965346000	-1.152055000
1	5.848084000	-2.498290000	-2.140578000
1	5.617999000	-4.032844000	-1.287490000
1	6.806826000	-2.874942000	-0.695430000
6	2.503702000	3.036548000	1.569132000
1	3.304978000	3.778025000	1.476785000
1	2.699238000	2.438981000	2.464621000
1	1.564625000	3.578484000	1.720314000
6	-1.403101000	3.055573000	0.867902000
1	-1.141951000	4.122444000	0.868708000
1	-0.484256000	2.478531000	0.719233000
1	-1.797707000	2.796876000	1.856228000
6	-3.688638000	3.576963000	0.042422000
1	-4.129895000	3.337329000	1.015565000
1	-4.452438000	3.415656000	-0.725492000
1	-3.433106000	4.642802000	0.043164000
6	-1.858165000	3.168981000	-1.588500000
1	-1.613387000	4.239365000	-1.593873000
1	-2.579197000	2.976663000	-2.389980000
1	-0.946192000	2.611552000	-1.824654000
1	-0.210911000	-1.688495000	1.953704000

***a*L**$^{-}$ (in toluene)
E@B2 = -1352.60768786 a.u.

8	0.788588000	0.911142000	-2.123854000
7	-2.279392000	-0.951670000	-0.032994000
7	-0.589604000	-1.816780000	-1.035665000
6	2.908673000	2.965306000	-2.560011000
1	2.054791000	2.509036000	-3.063244000
1	3.831906000	2.564377000	-2.994191000
1	2.895767000	4.049688000	-2.732065000
6	-1.181857000	-2.938742000	-0.413789000
6	-1.431468000	0.890241000	2.036638000
1	-0.729270000	0.775861000	1.204525000
6	2.848662000	2.655528000	-1.053700000
6	-2.257118000	-2.336539000	0.208339000
1	-3.038038000	-2.752630000	0.831487000
6	-4.534312000	-0.036590000	-0.063357000
6	3.799600000	-0.903803000	0.135257000
6	-3.234312000	-0.007601000	0.460766000
6	1.762326000	-1.035114000	-1.196825000
6	2.757111000	-1.636653000	-0.441127000
1	2.707903000	-2.717222000	-0.300961000
6	-1.235456000	-0.671599000	-0.816787000
1	-0.911744000	0.293384000	-1.195429000
6	0.661822000	-1.856240000	-1.812595000
1	0.445712000	-1.478959000	-2.816658000
1	0.923720000	-2.914211000	-1.861057000
6	-5.471665000	0.858602000	0.461749000
1	-6.485179000	0.857850000	0.069675000
6	-2.845592000	0.898127000	1.468779000
6	1.577324000	3.286115000	-0.458450000
1	1.563404000	4.370090000	-0.632435000
1	1.539281000	3.116303000	0.624116000
1	0.695322000	2.836727000	-0.918193000
6	-4.934396000	-0.964550000	-1.199395000
1	-4.082208000	-1.606678000	-1.435590000
6	3.786863000	0.479521000	-0.093393000
1	4.583110000	1.075434000	0.339523000
6	-3.816678000	1.775358000	1.951881000
1	-3.554788000	2.490845000	2.723694000
6	2.812616000	1.137679000	-0.842637000
6	4.878268000	-1.616050000	0.956548000
6	1.733256000	0.383392000	-1.433710000
6	4.057378000	3.321786000	-0.387373000
1	5.004793000	2.939105000	-0.782881000
1	4.058243000	3.176272000	0.698569000
1	4.029684000	4.401173000	-0.577266000
6	-1.240791000	-0.310349000	2.974909000
1	-1.934970000	-0.244348000	3.820736000
1	-0.219637000	-0.321834000	3.368363000
1	-1.410839000	-1.257975000	2.458009000
6	-5.119304000	1.753583000	1.460335000
1	-5.856903000	2.445621000	1.855432000
6	-5.277169000	-0.155234000	-2.455573000
1	-5.518356000	-0.825666000	-3.286517000
1	-4.435772000	0.474809000	-2.758383000
1	-6.142880000	0.494374000	-2.284721000
6	-1.060306000	2.184196000	2.760999000
1	-1.231678000	3.065597000	2.135597000
1	0.000477000	2.158344000	3.024826000
1	-1.624739000	2.304611000	3.692427000
6	-6.100295000	-1.873744000	-0.798557000
1	-7.004494000	-1.294476000	-0.580588000
1	-5.855059000	-2.464422000	0.089000000
1	-6.336996000	-2.566079000	-1.612435000
6	4.231607000	-2.354487000	2.140511000
1	4.989395000	-2.879756000	2.735540000
1	3.501483000	-3.093965000	1.798546000
1	3.707595000	-1.650310000	2.794868000
6	5.919319000	-0.641980000	1.517890000
1	5.459806000	0.099891000	2.179428000
1	6.443418000	-0.107237000	0.718779000
1	6.667888000	-1.191650000	2.099627000

6	5.613083000	-2.640438000	0.074874000
1	6.384967000	-3.169733000	0.647918000
1	6.094433000	-2.142953000	-0.773464000
1	4.921575000	-3.387579000	-0.326349000

4 (in toluene)
E@B2 = -7408.74914526 a.u.

83	-0.548622000	-2.011447000	0.582678000
35	-0.326118000	-2.061915000	3.419065000
35	-0.145944000	-1.305479000	-2.167846000
8	-2.745175000	-2.028747000	0.645800000
7	-0.136082000	2.404123000	0.810513000
7	-1.568489000	0.957129000	1.527763000
6	-3.399814000	-3.202739000	-2.077759000
1	-2.560792000	-3.294067000	-1.388414000
1	-3.149809000	-2.424052000	-2.804110000
1	-3.503063000	-4.153543000	-2.613750000
6	-0.602680000	0.231371000	0.853313000
6	-0.901181000	3.775298000	-1.607896000
1	-1.601765000	3.176868000	-1.015352000
6	-4.706982000	-2.880172000	-1.336279000
6	0.295605000	1.158143000	0.407839000
1	1.197934000	1.042110000	-0.174728000
6	1.525122000	4.092736000	1.390097000
6	-5.654761000	0.765821000	-0.454892000
6	0.531977000	3.643107000	0.510790000
6	-3.786114000	0.086167000	0.939285000
6	-4.740622000	1.025715000	0.563565000
1	-4.768062000	1.977724000	1.092969000
6	-1.275486000	2.253780000	1.492696000
1	-1.859424000	3.053494000	1.921974000
6	-2.828211000	0.396352000	2.056232000
1	-3.243093000	1.143880000	2.735659000
1	-2.559261000	-0.495568000	2.626529000
6	2.187730000	5.275063000	1.046119000
1	2.957013000	5.664499000	1.706975000
6	0.176748000	4.308287000	-0.674869000
6	-4.942521000	-3.925245000	-0.230989000
1	-4.959681000	-4.932042000	-0.664512000
1	-5.904576000	-3.753383000	0.263575000
1	-4.153093000	-3.882932000	0.521248000
6	1.863376000	3.374496000	2.686623000
1	1.291805000	2.441974000	2.730054000
6	-5.591762000	-0.500025000	-1.048041000
1	-6.313378000	-0.735859000	-1.818835000
6	0.882676000	5.474122000	-0.976314000
1	0.648116000	6.020709000	-1.883482000
6	-4.658178000	-1.481467000	-0.703361000
6	-6.669725000	1.836136000	-0.868574000
6	-3.690234000	-1.161723000	0.285003000
6	-5.850803000	-3.012284000	-2.350440000
1	-5.727675000	-2.329503000	-3.197947000
1	-6.828762000	-2.826423000	-1.894390000
1	-5.859990000	-4.032494000	-2.746758000
6	-0.295783000	2.851253000	-2.673957000
1	0.461738000	3.385353000	-3.258714000
1	-1.077494000	2.507845000	-3.357979000
1	0.163744000	1.960669000	-2.236294000
6	1.877051000	5.951179000	-0.127100000
1	2.409274000	6.862430000	-0.381186000
6	1.462711000	4.235472000	3.890804000
1	1.658518000	3.698787000	4.823527000
1	0.400593000	4.496232000	3.863004000
1	2.036138000	5.168122000	3.910971000
6	-1.705939000	4.895759000	-2.272046000
1	-2.075822000	5.620871000	-1.541200000
1	-2.565994000	4.466869000	-2.793282000
1	-1.112003000	5.433245000	-3.018021000
6	3.346942000	3.000695000	2.758826000
1	3.988040000	3.887592000	2.721232000

1	3.629716000	2.338972000	1.935407000
1	3.553777000	2.477614000	3.697332000
6	-7.534711000	2.229652000	0.339922000
1	-8.265104000	2.994988000	0.054232000
1	-6.929846000	2.635678000	1.156436000
1	-8.080057000	1.362730000	0.725843000
6	-7.600518000	1.351808000	-1.984626000
1	-8.187179000	0.481817000	-1.672427000
1	-7.043542000	1.084371000	-2.888293000
1	-8.302327000	2.149215000	-2.249231000
6	-5.917895000	3.078027000	-1.376666000
1	-6.624493000	3.861275000	-1.673720000
1	-5.298730000	2.826969000	-2.244010000
1	-5.262178000	3.493478000	-0.604645000
7	2.018749000	-1.438630000	0.682847000
7	4.061586000	-0.946037000	0.031884000
6	2.814587000	-1.292360000	-0.359799000
1	2.521178000	-1.400877000	-1.395216000
6	2.782583000	-1.179085000	1.796413000
1	2.356865000	-1.240668000	2.787552000
6	4.056825000	-0.868432000	1.408266000
1	4.945801000	-0.604252000	1.960261000
6	5.963202000	-3.046945000	-0.647041000
1	5.111487000	-3.091858000	0.037969000
6	5.150678000	-0.626927000	-0.847321000
6	6.062490000	-1.632984000	-1.192929000
6	7.188344000	-0.007827000	-2.596986000
1	7.986670000	0.233842000	-3.291599000
6	7.086582000	-1.293454000	-2.080725000
1	7.808146000	-2.050695000	-2.373902000
6	6.274819000	0.973067000	-2.225233000
1	6.367603000	1.975037000	-2.632755000
6	4.240830000	1.759749000	-0.932527000
1	3.703417000	1.402069000	-0.046342000
6	5.239254000	0.686789000	-1.334746000
6	5.712180000	-4.052238000	-1.775964000
1	6.547809000	-4.066559000	-2.483468000
1	5.600453000	-5.061200000	-1.368092000
1	4.803219000	-3.805778000	-2.332129000
6	7.219203000	-3.418068000	0.148753000
1	7.394653000	-2.712072000	0.965830000
1	7.112596000	-4.418425000	0.578613000
1	8.108087000	-3.422277000	-0.490598000
6	4.929991000	3.073678000	-0.554751000
1	5.415378000	3.535751000	-1.420244000
1	4.188985000	3.785440000	-0.177204000
1	5.688214000	2.921664000	0.219417000
6	3.203498000	1.994877000	-2.036652000
1	2.639748000	1.084102000	-2.267921000
1	2.494798000	2.771191000	-1.724995000
1	3.688001000	2.332062000	-2.959669000

4'+^{Dipp}Imd (in toluene)
E@B2 = -7408.74438859 a.u.

83	0.456887000	-0.873502000	-0.227809000
35	-0.553480000	-0.771598000	-2.908976000
35	1.130792000	-0.256366000	2.406223000
8	2.440069000	-1.629437000	-0.763081000
7	0.609170000	2.546760000	-0.289198000
7	2.163595000	1.634959000	-1.459749000
6	3.250400000	-3.217349000	1.713581000
1	2.303519000	-2.954356000	1.242366000
1	3.447503000	-2.479863000	2.496817000
1	3.136225000	-4.200628000	2.185024000
6	2.371871000	2.993342000	-1.523070000
6	-1.744028000	2.697579000	-1.940683000
1	-0.903960000	2.039675000	-2.182364000
6	4.393569000	-3.264590000	0.687993000
6	1.389534000	3.570351000	-0.792634000
1	1.151560000	4.604575000	-0.604869000

6	-0.644594000	3.157385000	1.737112000
6	6.298365000	-0.073752000	-0.392063000
6	-0.646763000	2.828868000	0.372868000
6	4.047742000	0.020116000	-1.289425000
6	5.324117000	0.555998000	-1.164703000
1	5.556998000	1.477623000	-1.696442000
6	1.093208000	1.346750000	-0.697448000
6	3.022215000	0.667620000	-2.173161000
1	3.501796000	1.236822000	-2.971457000
1	2.361024000	-0.073628000	-2.628085000
6	-1.874714000	3.493871000	2.311704000
1	-1.915860000	3.742620000	3.367131000
6	-1.798904000	2.890041000	-0.432480000
6	4.015636000	-4.222706000	-0.455942000
1	3.792729000	-5.218058000	-0.054042000
1	4.843743000	-4.321946000	-1.165793000
1	3.138649000	-3.860901000	-0.995600000
6	0.630031000	3.240344000	2.560776000
1	1.374648000	2.587776000	2.097099000
6	5.942586000	-1.287668000	0.206187000
1	6.695660000	-1.810143000	0.781055000
6	-2.996865000	3.237764000	0.194002000
1	-3.905334000	3.305999000	-0.397153000
6	4.678022000	-1.875053000	0.099337000
6	7.691317000	0.549672000	-0.255328000
6	3.686404000	-1.170604000	-0.627947000
6	5.620979000	-3.850211000	1.398001000
1	5.927850000	-3.240599000	2.254566000
1	6.476245000	-3.954471000	0.722421000
1	5.373844000	-4.848140000	1.773683000
6	-1.523951000	4.053598000	-2.628732000
1	-2.362571000	4.726428000	-2.417932000
1	-1.458371000	3.920486000	-3.712906000
1	-0.607162000	4.544765000	-2.293230000
6	-3.038130000	3.523761000	1.554484000
1	-3.981226000	3.789847000	2.022779000
6	0.433906000	2.770628000	4.005140000
1	1.409423000	2.648148000	4.484425000
1	-0.080302000	1.808708000	4.051503000
1	-0.129054000	3.504064000	4.592465000
6	-2.997069000	2.037643000	-2.516736000
1	-3.241638000	1.112799000	-1.989813000
1	-2.824971000	1.784918000	-3.566544000
1	-3.863350000	2.706938000	-2.473684000
6	1.163872000	4.680508000	2.568445000
1	0.422359000	5.361226000	3.000591000
1	1.405996000	5.041866000	1.566087000
1	2.073201000	4.740777000	3.174340000
6	8.342077000	0.667590000	-1.643349000
1	9.340053000	1.112928000	-1.561870000
1	7.749554000	1.297286000	-2.314133000
1	8.443295000	-0.317295000	-2.110079000
6	8.615069000	-0.284777000	0.637206000
1	8.780025000	-1.285952000	0.226038000
1	8.211299000	-0.390743000	1.649236000
1	9.590205000	0.206361000	0.716538000
6	7.565476000	1.951924000	0.362640000
1	8.553053000	2.415625000	0.465480000
1	7.105600000	1.899634000	1.354485000
1	6.950091000	2.610495000	-0.258086000
7	-1.978370000	-0.227337000	0.476708000
7	-4.124625000	-0.702233000	0.596892000
6	-3.017071000	-0.712475000	-0.179482000
1	-3.006794000	-1.066014000	-1.202264000
6	-2.428594000	0.097248000	1.733280000
1	-1.758872000	0.503584000	2.476563000
6	-3.762750000	-0.185042000	1.822821000
1	-4.477315000	-0.088656000	2.625193000
6	-6.027275000	1.236495000	-0.362609000
1	-4.936486000	1.328133000	-0.364719000
6	-5.431076000	-1.170758000	0.227173000

6	-6.365675000	-0.239441000	-0.250652000
6	-7.943352000	-2.066175000	-0.466834000
1	-8.932183000	-2.419451000	-0.742048000
6	-7.633154000	-0.716339000	-0.589005000
1	-8.384515000	-0.024745000	-0.956986000
6	-6.994735000	-2.965803000	0.004322000
1	-7.249743000	-4.017466000	0.090803000
6	-4.678487000	-3.527939000	0.867389000
1	-3.873326000	-2.963718000	1.348936000
6	-5.717301000	-2.536303000	0.371225000
6	-6.548559000	1.864034000	-1.657121000
1	-7.642431000	1.899094000	-1.679356000
1	-6.193868000	2.896796000	-1.739563000
1	-6.205571000	1.313573000	-2.537907000
6	-6.553492000	2.003478000	0.856655000
1	-6.123810000	1.620861000	1.787000000
1	-6.304902000	3.067327000	0.776483000
1	-7.643398000	1.917609000	0.926217000
6	-5.248085000	-4.494920000	1.909208000
1	-5.983263000	-5.176588000	1.470331000
1	-4.443274000	-5.108207000	2.324592000
1	-5.728899000	-3.959560000	2.732701000
6	-4.077541000	-4.301101000	-0.313349000
1	-3.621460000	-3.629007000	-1.046181000
1	-3.308977000	-4.997291000	0.035824000
1	-4.852571000	-4.879918000	-0.827269000
1	3.187442000	3.420191000	-2.084584000

4–^{Dipp}Imd (in toluene)
E@B2 = -6715.59516387 a.u.

83	0.830072000	-2.256354000	0.340997000
35	-0.170528000	-3.522966000	-1.979609000
35	0.541629000	-1.169678000	2.931112000
8	2.325427000	-1.129193000	-0.664174000
7	-2.568384000	0.544702000	-0.250763000
7	-0.768873000	0.031086000	-1.327691000
6	4.117522000	-0.635412000	1.706281000
1	3.574943000	-1.523199000	1.377659000
1	3.452190000	-0.047840000	2.344987000
1	4.962199000	-0.978107000	2.314230000
6	-0.732955000	-0.703790000	-0.155082000
6	-2.412460000	3.045259000	1.180372000
1	-1.641222000	2.694796000	0.485056000
6	4.639128000	0.187081000	0.515031000
6	-1.874067000	-0.369228000	0.516698000
1	-2.247218000	-0.691834000	1.476653000
6	-5.008188000	0.539251000	-0.213490000
6	2.551480000	3.027962000	-1.079328000
6	-3.808792000	1.184506000	0.110315000
6	1.489548000	0.904297000	-1.585456000
6	1.552295000	2.288130000	-1.707820000
1	0.797114000	2.790550000	-2.310563000
6	-1.869162000	0.774682000	-1.365878000
1	-2.144086000	1.470966000	-2.143616000
6	0.371885000	0.149251000	-2.255850000
1	0.012047000	0.678017000	-3.140236000
1	0.661799000	-0.864316000	-2.540685000
6	-6.192775000	1.176932000	0.165139000
1	-7.145198000	0.710910000	-0.069932000
6	-3.739674000	2.411164000	0.791041000
6	5.349209000	-0.746615000	-0.481504000
1	6.151701000	-1.293952000	0.026060000
1	5.795759000	-0.171657000	-1.299497000
1	4.651835000	-1.470826000	-0.906880000
6	-5.057550000	-0.794453000	-0.940160000
1	-4.033498000	-1.122276000	-1.144166000
6	3.514517000	2.310750000	-0.362651000
1	4.316854000	2.864212000	0.106001000
6	-4.953039000	3.001060000	1.146953000
1	-4.951646000	3.948355000	1.675528000

6	3.501391000	0.920047000	-0.212781000
6	2.551706000	4.556027000	-1.183728000
6	2.428055000	0.209563000	-0.798385000
6	5.686202000	1.165741000	1.063813000
1	5.262233000	1.838693000	1.816748000
1	6.139295000	1.770538000	0.271929000
1	6.488637000	0.596548000	1.542566000
6	-2.002730000	2.591141000	2.588412000
1	-2.756780000	2.896218000	3.321713000
1	-1.047332000	3.044455000	2.868469000
1	-1.883779000	1.505835000	2.649928000
6	-6.165219000	2.391751000	0.836802000
1	-7.095967000	2.870506000	1.124134000
6	-5.782180000	-0.660100000	-2.283774000
1	-5.768591000	-1.614845000	-2.817115000
1	-5.308040000	0.093367000	-2.919746000
1	-6.828127000	-0.370204000	-2.140846000
6	-2.442145000	4.573480000	1.099913000
1	-2.801415000	4.922659000	0.127350000
1	-1.434994000	4.969797000	1.255120000
1	-3.081374000	5.006262000	1.875569000
6	-5.717321000	-1.867797000	-0.067559000
1	-6.761702000	-1.617961000	0.145357000
1	-5.195813000	-1.980603000	0.887197000
1	-5.700914000	-2.833020000	-0.581620000
6	2.610325000	4.979826000	-2.659958000
1	2.604739000	6.072203000	-2.742341000
1	1.754612000	4.599530000	-3.225907000
1	3.521701000	4.605326000	-3.136349000
6	3.742230000	5.186719000	-0.455327000
1	4.696285000	4.850406000	-0.873886000
1	3.733316000	4.952626000	0.613972000
1	3.699168000	6.275531000	-0.557764000
6	1.257768000	5.097223000	-0.550559000
1	1.233824000	6.191557000	-0.599602000
1	1.190480000	4.798114000	0.500735000
1	0.369816000	4.718889000	-1.067847000

4' (in toluene)
E@B2 = -6715.60041439 a.u.

83	0.657656000	-1.270246000	-0.629633000
35	1.548315000	-3.049602000	1.373646000
35	-0.366334000	0.879161000	-2.063271000
8	-1.259151000	-1.794272000	0.048397000
7	1.912302000	1.283311000	1.072459000
7	0.206604000	0.474965000	2.103214000
6	-2.670193000	-1.853398000	-2.668450000
1	-1.691488000	-2.185774000	-2.316499000
1	-2.558486000	-0.850491000	-3.086689000
1	-2.980541000	-2.534721000	-3.468885000
6	0.684722000	1.505411000	2.881164000
6	4.231756000	-0.445793000	1.227971000
1	3.245965000	-0.734304000	1.603259000
6	-3.717087000	-1.881609000	-1.543723000
6	1.767886000	2.011129000	2.237791000
1	2.450955000	2.801260000	2.502647000
6	2.852038000	2.533499000	-0.818828000
6	-4.223126000	0.992699000	0.997277000
6	2.964009000	1.474798000	0.099299000
6	-2.130285000	-0.126462000	1.495038000
6	-3.099810000	0.819983000	1.804878000
1	-2.969908000	1.422955000	2.702019000
6	0.953281000	0.336954000	1.000983000
6	-0.968082000	-0.359371000	2.423632000
1	-1.241536000	-0.110234000	3.449913000
1	-0.637659000	-1.401036000	2.387823000
6	3.884542000	2.676841000	-1.748012000
1	3.831187000	3.475772000	-2.479954000
6	4.063362000	0.598978000	0.136359000
6	-3.743447000	-3.284347000	-0.908733000

1	-3.953840000	-4.038038000	-1.676126000
1	-4.526999000	-3.348885000	-0.146535000
1	-2.786029000	-3.524283000	-0.441792000
6	1.705924000	3.531149000	-0.787754000
1	0.840039000	3.036235000	-0.336739000
6	-4.364950000	0.124684000	-0.089825000
1	-5.255966000	0.210485000	-0.696728000
6	5.060408000	0.785374000	-0.824652000
1	5.921492000	0.125528000	-0.832212000
6	-3.426927000	-0.854135000	-0.437098000
6	-5.253279000	2.073542000	1.340780000
6	-2.251796000	-0.920701000	0.340370000
6	-5.084898000	-1.640839000	-2.196604000
1	-5.131148000	-0.671100000	-2.703235000
1	-5.901613000	-1.693117000	-1.469673000
1	-5.262537000	-2.416203000	-2.948060000
6	5.020535000	0.161662000	2.396528000
1	6.020986000	0.464299000	2.068944000
1	5.130249000	-0.571157000	3.201492000
1	4.518456000	1.043928000	2.805566000
6	4.969911000	1.809181000	-1.758828000
1	5.754906000	1.936809000	-2.497619000
6	1.294551000	4.003157000	-2.185535000
1	0.346031000	4.544205000	-2.122811000
1	1.159313000	3.163305000	-2.868647000
1	2.034243000	4.691164000	-2.608489000
6	4.905426000	-1.727446000	0.735804000
1	4.416208000	-2.124063000	-0.158662000
1	4.838417000	-2.494363000	1.511436000
1	5.965352000	-1.569451000	0.510913000
6	2.088539000	4.752127000	0.062416000
1	2.958713000	5.256742000	-0.371108000
1	2.338309000	4.487730000	1.092760000
1	1.260836000	5.467429000	0.088806000
6	-5.835968000	1.806843000	2.738228000
1	-6.574109000	2.574519000	2.995570000
1	-5.059881000	1.819589000	3.509507000
1	-6.330193000	0.830893000	2.774365000
6	-6.410244000	2.111782000	0.337806000
1	-6.969295000	1.170521000	0.327162000
1	-6.057392000	2.314989000	-0.678326000
1	-7.107868000	2.908497000	0.614475000
6	-4.565177000	3.448562000	1.333614000
1	-5.286805000	4.237237000	1.573818000
1	-4.135708000	3.662957000	0.350038000
1	-3.757726000	3.498459000	2.070523000
1	0.221406000	1.778245000	3.815915000

5. References

1. G. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv.*, 2015, **71**, 3-8.
2. G. Sheldrick, *Acta Crystallogr., Sect. C: Struct. Chem.*, 2015, **71**, 3-8.
3. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.
4. K. Brandenburg, Diamond Version 4.6.0, Crystal Impact GbR, Bonn, 2019.
5. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
6. https://gaussian.com/dl/g16_c01.enw.
7. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.
8. V. A. Rassolov, M. A. Ratner, J. A. Pople, P. C. Redfern and L. A. Curtiss, *J. Comput. Chem.*, 2001, **22**, 976-984.
9. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.
10. E. D. Glendening, C. R. Landis and F. Weinhold, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2011, **2**, 1-42.