

## **N-heterocyclic imine-based bis-gallium(I) carbene analog featuring a four-membered Ga<sub>2</sub>N<sub>2</sub> ring**

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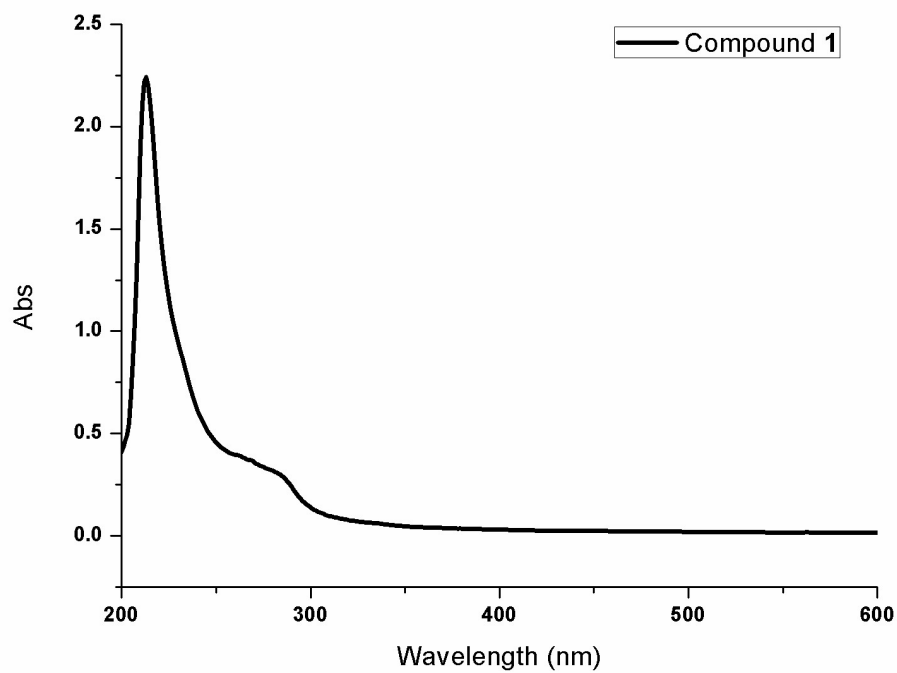
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### **CONTENTS**

1. UV-Vis spectrum of compound **1**
2. Crystal Structure Determination
3. Theoretical calculations
4. References
5. NMR spectra

## 1. UV-Vis spectrum of compound 1



**Figure S1.** UV-Vis absorption spectrum of compound **1** ( $10^{-5}$  M) in hexane (Ultraviolet spectrum was recorded on a Perkin Elmer Lambda 750 UV/Vis spectrophotometer).

## 2. Crystal Structure Determination of Compounds 1, 2, 3, 4, and 5

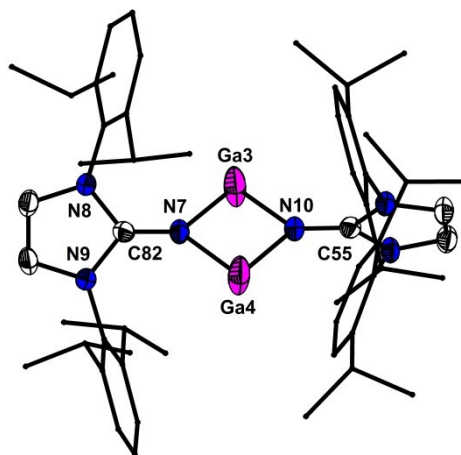
X-ray data collection and structural refinement. Intensity data for compounds **1**, **2**, **3**, **4**, and **5** were collected using a Bruker D8 Venture diffractometer. The crystals of **1**, **2**, **3**, **4**, and **5** were measured at 170 K. The structure was solved by direct phase determination (SHELXS-97)<sup>[S1]</sup> and refined for all data by full-matrix least squares methods on  $F^2$ .<sup>[S2]</sup> All non-hydrogen atoms were subjected to anisotropic refinement. The hydrogen atoms were generated geometrically and allowed to ride in their respective parent atoms; they were assigned appropriate isotropic thermal parameters and included in the structure-factor calculations. CCDC: 2168820-2168824 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallography Data Center via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

**Table S1.** Summary of Data Collection and Structure Refinement of **1**, **2**, **3**, **4**, and **5**.

	<b>1</b>	<b>2·(C<sub>6</sub>H<sub>6</sub>)<sub>2</sub></b>	<b>3·(C<sub>6</sub>H<sub>6</sub>)</b>
Formula	C <sub>54</sub> H <sub>72</sub> Ga <sub>2</sub> N <sub>6</sub>	C <sub>70</sub> H <sub>90</sub> F <sub>6</sub> Ga <sub>2</sub> N <sub>6</sub> O <sub>6</sub> S <sub>2</sub>	C <sub>88</sub> H <sub>94</sub> Ga <sub>2</sub> N <sub>6</sub> O <sub>4</sub>
Fw	944.61	1429.03	1439.13
cryst system	monoclinic	monoclinic	tetragonal
space group	P2 <sub>1</sub> /c	C2/c	P-4
Size (mm <sup>3</sup> )	0.36 × 0.07 × 0.05	0.08 × 0.04 × 0.03	0.48 × 0.32 × 0.29
T, K	170.00	170.00	170.00
<i>a</i> , Å	31.3223(16)	21.4469(7)	19.4930(3)
<i>b</i> , Å	12.3615(6)	17.9353(6)	19.4930(3)
<i>c</i> , Å	30.9147(16)	18.5471(6)	10.5729(3)
α, deg	90	90	90
β, deg	118.4170(10)	105.1940(10)	90
γ, deg	90	90	90
V, Å <sup>3</sup>	10527.6(9)	6884.9(4)	4017.46(17)
Z	8	4	2
ρ <sub>calc</sub> g·cm <sup>-3</sup>	1.192	1.379	1.190
μ, mm <sup>-1</sup>	1.063	0.915	0.723
Refl collected	118009	48398	66333
<i>T</i> <sub>min</sub> / <i>T</i> <sub>max</sub>	0.62/0.746	0.699/0.746	0.636/0.746
Independent refl	23225	7583	8846
[R <sub>int</sub> ]	0.1165	0.0583	0.0410
<i>R</i>	0.0558	0.0307	0.0253
[I>2σ(I)]			
<i>R</i> <sub>w</sub> [I>2σ(I)]	0.1093	0.0755	0.0643

GOF	1.014	1.038	1.040
Largest diff peak/hole[e· Å <sup>-3</sup> ]	0.80/-0.85	0.68/-0.48	0.24/-0.21

	<b>4</b>	<b>5</b>
Formula	C <sub>78</sub> H <sub>92</sub> Ga <sub>2</sub> N <sub>6</sub> S <sub>4</sub>	C <sub>54</sub> H <sub>72</sub> Cl <sub>2</sub> Ge <sub>2</sub> N <sub>6</sub>
Fw	1381.25	1021.25
cryst system	monoclinic	monoclinic
space group	P2 <sub>1</sub> /c	P2 <sub>1</sub> /n
Size (mm <sup>3</sup> )	0.38 × 0.2 × 0.19	0.09 × 0.04 × 0.03
T, K	170.00	170.00
a, Å	12.7756(18)	12.797(2)
b, Å	23.239(3)	13.824(2)
c, Å	12.8137(17)	15.574(2)
α, deg	90	90
β, deg	114.876(5)	103.570(5)
γ, deg	90	90
V, Å <sup>3</sup>	3451.3(8)	2678.2(7)
Z	2	2
ρ <sub>calc</sub> g·cm <sup>-3</sup>	1.329	1.266
μ, mm <sup>-1</sup>	0.950	1.262
Refl collected	46214	23120
T <sub>min</sub> /T <sub>max</sub>	0.525/0.746	0.602/0.746
Independent refl	7593	5886
[R <sub>int</sub> ]	0.092	0.0961
R	0.0596	0.0779
[I>2sigma(I)]		
R <sub>w</sub> [I>2sigma(I)]	0.1618	0.1891
GOF	1.053	1.036
Largest diff peak/hole[e· Å <sup>-3</sup> ]	1.75/-1.31	1.27/-1.04

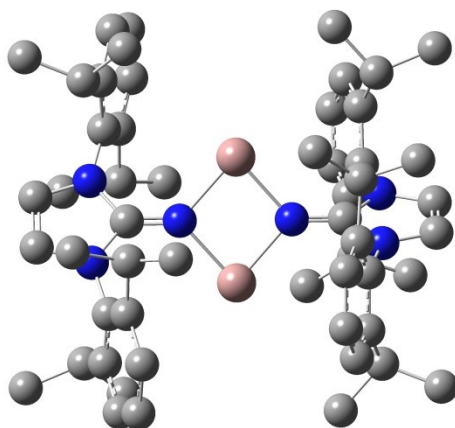


**Figure S2.** Twinned molecular structure of **1** (H atoms are omitted for clarity). Selected bond lengths (Å) and angles (°): Ga3-N7 2.015(3), Ga3-N10 2.014(3), Ga4-N7 2.012(3), Ga4-N10 2.009(3), N7-C82 1.283(4), N10-C55 1.287(4), C82-N8 1.396(4), C82-N9 1.397(4); N7-Ga3-N10 82.20(11), N7-Ga4-N10 82.40(11), Ga3-N7-Ga4 97.64(10), Ga3-N10-Ga4 97.72(11), Ga3-N7-C82 131.6(2), Ga4-N7-C82 130.7(2).

### 3. Theoretical calculations

Gaussian 09E (16 C.01) was used for all density functional theory (DFT) calculations.<sup>[S3]</sup>

Geometry optimization, frequency calculations, and Natural bond order (NBO) analysis on compound **1** was performed at the B3LYP/6-311G(d,p) level of theory.



**Figure S3.** Calculated optimized structures for **1** at B3LYP/6-311G(d,p) level of theory.

**Table S2.** Optimized structures of **1** (atom, x-, y-, z- positions in Å)

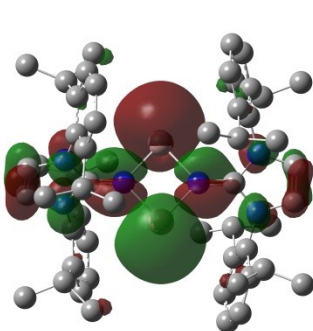
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Ga	0.00567019	1.02452939	1.17763679
N	-1.36718296	0.00062991	-0.00026587
N	-3.52759927	1.08697549	0.20090186
N	-3.52885384	-1.08286177	-0.20282873
N	1.35621550	-0.00036234	-0.00006055
N	3.51722569	-1.03761333	0.37990793
N	3.51888003	1.03367863	-0.37889929
C	-2.65195045	0.00149014	-0.00066468
C	-4.85697572	-0.65800107	-0.12453281
H	-5.67535583	-1.34411807	-0.25226150
C	-4.85621374	0.66375946	0.12192727
H	-5.67379825	1.35094088	0.24903646
C	-3.14883337	-2.44474637	-0.45910978
C	-3.23979693	-2.94339166	-1.77299897
C	-2.91421440	-4.28633874	-1.98638836
H	-2.97450335	-4.69609012	-2.98780819
C	-2.50018378	-5.09802016	-0.94025350
H	-2.24112414	-6.13434639	-1.12818616
C	-2.41798683	-4.58633241	0.34994440
H	-2.09668531	-5.23289537	1.15678673

C	-2.74710653	-3.25695661	0.62161662
C	-3.69779994	-2.08237137	-2.94583145
H	-3.73286658	-1.04660542	-2.60282201
C	-5.12002587	-2.47110271	-3.39580878
H	-5.14742737	-3.50161653	-3.76255999
H	-5.45689818	-1.81753014	-4.20598532
H	-5.83938791	-2.39110729	-2.57697857
C	-2.71969224	-2.13529846	-4.13306241
H	-1.70781459	-1.87171773	-3.81872013
H	-3.03602353	-1.43142560	-4.90878703
H	-2.68678467	-3.12953382	-4.58786441
C	-2.72644680	-2.72588130	2.05130402
H	-2.54479746	-1.65114302	1.99835594
C	-4.09547057	-2.94314318	2.72844581
H	-4.90191053	-2.45981968	2.17269062
H	-4.09055151	-2.52989557	3.74169182
H	-4.32676670	-4.01047406	2.79997811
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H	-1.77117326	-4.38491505	3.12635812
H	-1.56059504	-2.80605500	3.87337889
H	-0.62924932	-3.22555957	2.42992271
C	-3.14604965	2.44826392	0.45807537
C	-2.74225129	3.26037902	-0.62197676
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H	-2.23400379	6.13638394	1.12942603
C	-2.91040247	4.28895621	1.98626814
H	-2.97111797	4.69840396	2.98778471
C	-3.23751832	2.94650352	1.77206878
C	-2.72103444	2.72973165	-2.05182111
H	-2.53973355	1.65491022	-1.99908923
C	-4.08967190	2.94764427	-2.72955610
H	-4.89653695	2.46435311	-2.17440588
H	-4.08437003	2.53478757	-3.74295927
H	-4.32058503	4.01507862	-2.80078520
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H	-1.76495548	4.38879338	-3.12608092
H	-1.55439242	2.81005914	-3.87335099
H	-0.62353298	3.22905097	-2.42944603
C	-3.69751715	2.08561641	2.94423391
H	-3.73371787	1.05003497	2.60077934
C	-5.11952887	2.47601953	3.39340350

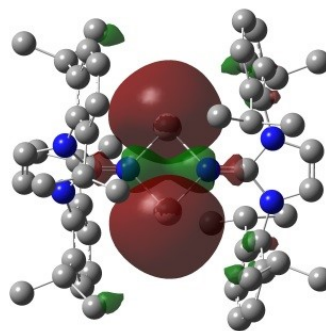
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H	-5.45777354	1.82260975	4.20313938
H	-5.83845439	2.39720897	2.57407606
C	-2.72012634	2.13676005	4.13214684
H	-1.70832947	1.87223630	3.81833817
H	-3.03775874	1.43280261	4.90726215
H	-2.68640197	3.13069626	4.58754270
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C	4.84618387	0.62818380	-0.23228528
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C	4.84516754	-0.63402006	0.23388625
H	5.66303785	-1.28696697	0.48190338
C	3.13674262	2.31055421	-0.91551655
C	2.85361084	2.41277657	-2.29308664
C	2.53857523	3.67500830	-2.80256684
H	2.31672367	3.78561398	-3.85706795
C	2.51153551	4.79517658	-1.98037635
H	2.26587742	5.76613777	-2.39680903
C	2.80190392	4.67393652	-0.62862038
H	2.78111026	5.55554597	0.00085224
C	3.12021440	3.43388043	-0.06561366
C	2.95225335	1.21085488	-3.22690510
H	2.86594657	0.30929794	-2.61809198
C	4.33077243	1.17812516	-3.91814164
H	4.47509553	2.06568883	-4.54179218
H	4.41622425	0.29619703	-4.56006184
H	5.14390065	1.14379538	-3.18931272
C	1.82409417	1.15310484	-4.26898693
H	0.84211346	1.19078034	-3.79369002
H	1.88665586	0.21675776	-4.82987766
H	1.88867378	1.97141575	-4.99218647
C	3.48237691	3.34438864	1.41338726
H	3.46984121	2.28912091	1.69299275
C	4.90976492	3.87379418	1.65962477
H	5.65009232	3.33291914	1.06514056
H	5.18052034	3.76553397	2.71410916
H	4.98482012	4.93425238	1.40038575
C	2.47222624	4.06584086	2.32130836
H	2.47179737	5.14678731	2.15412747
H	2.73173732	3.89872482	3.37089390
H	1.46033296	3.68838313	2.16118185
C	3.13295693	-2.31391973	0.91636948
C	3.11521912	-3.43725779	0.06650236



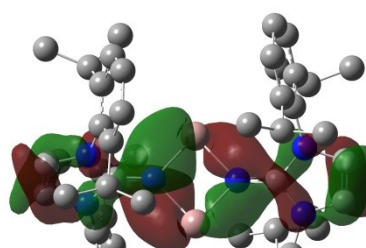
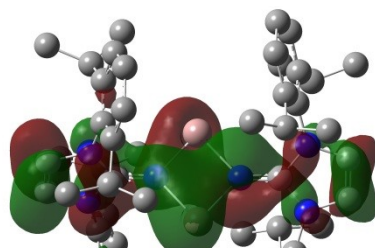
C	2.79459434	-4.67679080	0.62935802
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H	2.25564632	-5.76806403	2.39722246
C	2.53146768	-3.67736724	2.80310001
H	2.30876913	-3.78759420	3.85746055
C	2.84887271	-2.41566433	2.29379042
C	3.47848888	-3.34843048	-1.41227172
H	3.46792379	-2.29315815	-1.69194011
C	4.90515490	-3.88024088	-1.65752397
H	5.64597008	-3.34068289	-1.06245266
H	5.17685349	-3.77233927	-2.71180257
H	4.97822912	-4.94085097	-1.39833931
C	2.46775000	-4.06824757	-2.32083405
H	2.46525347	-5.14916048	-2.15345008
H	2.72838238	-3.90180282	-3.37024817
H	1.45640840	-3.68894304	-2.16155982
C	2.94908636	-1.21391335	3.22765743
H	2.86423934	-0.31220663	2.61886106
C	4.32754065	-1.18329595	3.91913795
H	4.47039620	-2.07115134	4.54271010
H	4.41419777	-0.30156321	4.56116583
H	5.14084938	-1.15010013	3.19046478
C	1.82088695	-1.15451659	4.26959302
H	0.83889821	-1.19082449	3.79420235
H	1.88471514	-0.21821730	4.83041754
H	1.88425646	-1.97286012	4.99286146

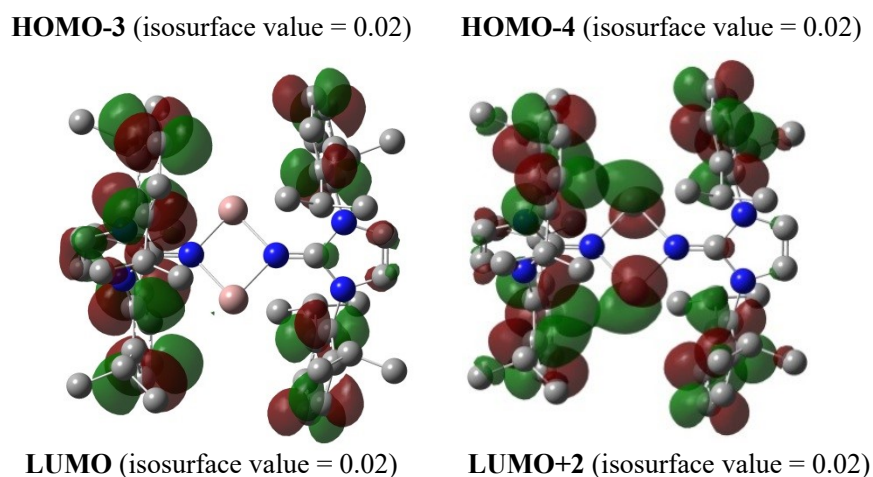


**HOMO** (isosurface value = 0.02)



**HOMO-2** (isosurface value = 0.02)





**Figure S4.** Plots of the frontier orbitals of compounds **1**.

**Table S3.** The NPA charges of **1** calculated at B3LYP/6-311G(d,p) level of theory.

Atom	No	Charge	Core	Valence	Rydberg	Total
Ga	1	0.83813	27.99286	2.10792	0.06109	30.16187
Ga	2	0.83810	27.99286	2.10795	0.06109	30.16190
N	3	-1.43588	1.99943	6.39516	0.04129	8.43588
N	4	-0.45995	1.99916	5.44762	0.01317	7.45995
N	5	-0.45995	1.99916	5.44762	0.01317	7.45995
N	6	-1.45424	1.99943	6.41774	0.03707	8.45424
N	7	-0.45709	1.99917	5.44468	0.01324	7.45709
N	8	-0.45708	1.99917	5.44467	0.01324	7.45708
C	9	0.65902	1.99881	3.30386	0.03831	5.34098
C	10	-0.05652	1.99906	4.03816	0.01930	6.05652
H	11	0.21779	0.00000	0.77910	0.00312	0.78221

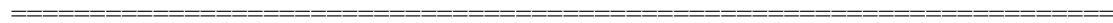
C	12	-0.05654	1.99906	4.03818	0.01930	6.05654
H	13	0.21779	0.00000	0.77909	0.00312	0.78221
C	14	0.14470	1.99862	3.83501	0.02167	5.85530
C	15	0.00444	1.99882	3.97686	0.01988	5.99556
C	16	-0.20652	1.99899	4.19195	0.01559	6.20652
H	17	0.20077	0.00000	0.79562	0.00361	0.79923
C	18	-0.17150	1.99908	4.15684	0.01558	6.17150
H	19	0.19947	0.00000	0.79790	0.00263	0.80053
C	20	-0.20908	1.99899	4.19460	0.01550	6.20908
H	21	0.20251	0.00000	0.79404	0.00345	0.79749
C	22	0.00645	1.99884	3.97558	0.01913	5.99355
C	23	-0.21287	1.99911	4.19797	0.01579	6.21287
H	24	0.20585	0.00000	0.79007	0.00408	0.79415
C	25	-0.55473	1.99926	4.54556	0.00991	6.55473
H	26	0.18963	0.00000	0.80794	0.00243	0.81037
H	27	0.19446	0.00000	0.80331	0.00223	0.80554
H	28	0.19115	0.00000	0.80680	0.00205	0.80885
C	29	-0.56222	1.99929	4.55249	0.01044	6.56222
H	30	0.21735	0.00000	0.78046	0.00219	0.78265
H	31	0.19215	0.00000	0.80573	0.00212	0.80785
H	32	0.18462	0.00000	0.81322	0.00216	0.81538
C	33	-0.20897	1.99913	4.19457	0.01528	6.20897
H	34	0.21207	0.00000	0.78312	0.00481	0.78793
C	35	-0.55631	1.99926	4.54721	0.00984	6.55631
H	36	0.19620	0.00000	0.80170	0.00209	0.80380
H	37	0.19316	0.00000	0.80455	0.00229	0.80684
H	38	0.18911	0.00000	0.80825	0.00264	0.81089
C	39	-0.56822	1.99928	4.55851	0.01042	6.56822
H	40	0.18377	0.00000	0.81379	0.00244	0.81623
H	41	0.19727	0.00000	0.80039	0.00234	0.80273

H	42	0.21308	0.00000	0.78460	0.00232	0.78692
C	43	0.14469	1.99862	3.83502	0.02168	5.85531
C	44	0.00645	1.99884	3.97558	0.01913	5.99355
C	45	-0.20909	1.99899	4.19460	0.01550	6.20909
H	46	0.20252	0.00000	0.79402	0.00345	0.79748
C	47	-0.17150	1.99908	4.15683	0.01558	6.17150
H	48	0.19947	0.00000	0.79790	0.00263	0.80053
C	49	-0.20652	1.99899	4.19194	0.01559	6.20652
H	50	0.20076	0.00000	0.79563	0.00361	0.79924
C	51	0.00443	1.99882	3.97687	0.01988	5.99557
C	52	-0.20898	1.99913	4.19458	0.01527	6.20898
H	53	0.21210	0.00000	0.78308	0.00481	0.78790
C	54	-0.55631	1.99926	4.54721	0.00984	6.55631
H	55	0.19621	0.00000	0.80170	0.00209	0.80379
H	56	0.19316	0.00000	0.80455	0.00229	0.80684
H	57	0.18911	0.00000	0.80825	0.00264	0.81089
C	58	-0.56825	1.99928	4.55855	0.01042	6.56825
H	59	0.18378	0.00000	0.81378	0.00244	0.81622
H	60	0.19728	0.00000	0.80037	0.00234	0.80272
H	61	0.21308	0.00000	0.78460	0.00232	0.78692
C	62	-0.21287	1.99911	4.19797	0.01579	6.21287
H	63	0.20585	0.00000	0.79007	0.00408	0.79415
C	64	-0.55474	1.99926	4.54556	0.00991	6.55474
H	65	0.18963	0.00000	0.80794	0.00243	0.81037
H	66	0.19446	0.00000	0.80331	0.00223	0.80554
H	67	0.19116	0.00000	0.80679	0.00205	0.80884
C	68	-0.56221	1.99929	4.55248	0.01044	6.56221
H	69	0.21735	0.00000	0.78047	0.00219	0.78265
H	70	0.19215	0.00000	0.80572	0.00212	0.80785
H	71	0.18462	0.00000	0.81321	0.00216	0.81538

C	72	0.66455	1.99880	3.29861	0.03804	5.33545
C	73	-0.05496	1.99907	4.03660	0.01930	6.05496
H	74	0.21710	0.00000	0.77981	0.00309	0.78290
C	75	-0.05496	1.99907	4.03659	0.01930	6.05496
H	76	0.21710	0.00000	0.77981	0.00309	0.78290
C	77	0.15113	1.99865	3.82957	0.02065	5.84887
C	78	0.00644	1.99886	3.97527	0.01942	5.99356
C	79	-0.21381	1.99899	4.19929	0.01552	6.21381
H	80	0.20210	0.00000	0.79436	0.00355	0.79790
C	81	-0.17524	1.99908	4.16049	0.01567	6.17524
H	82	0.19947	0.00000	0.79786	0.00267	0.80053
C	83	-0.20855	1.99900	4.19401	0.01555	6.20855
H	84	0.20125	0.00000	0.79511	0.00364	0.79875
C	85	0.00515	1.99885	3.97653	0.01947	5.99485
C	86	-0.20924	1.99912	4.19456	0.01555	6.20924
H	87	0.20952	0.00000	0.78601	0.00447	0.79048
C	88	-0.55557	1.99926	4.54642	0.00990	6.55557
H	89	0.18911	0.00000	0.80835	0.00254	0.81089
H	90	0.19409	0.00000	0.80368	0.00223	0.80591
H	91	0.19487	0.00000	0.80303	0.00210	0.80513
C	92	-0.55984	1.99929	4.55029	0.01026	6.55984
H	93	0.20908	0.00000	0.78900	0.00192	0.79092
H	94	0.19972	0.00000	0.79823	0.00205	0.80028
H	95	0.18308	0.00000	0.81468	0.00224	0.81692
C	96	-0.21137	1.99912	4.19641	0.01585	6.21137
H	97	0.20673	0.00000	0.78918	0.00408	0.79327
C	98	-0.55448	1.99926	4.54532	0.00990	6.55448
H	99	0.19123	0.00000	0.80673	0.00204	0.80877
H	100	0.19449	0.00000	0.80328	0.00223	0.80551
H	101	0.18926	0.00000	0.80826	0.00248	0.81074

C	102	-0.56344	1.99929	4.55358	0.01058	6.56344
H	103	0.18226	0.00000	0.81557	0.00217	0.81774
H	104	0.19427	0.00000	0.80363	0.00210	0.80573
H	105	0.21931	0.00000	0.77824	0.00245	0.78069
C	106	0.15112	1.99865	3.82958	0.02065	5.84888
C	107	0.00516	1.99885	3.97652	0.01948	5.99484
C	108	-0.20855	1.99900	4.19401	0.01555	6.20855
H	109	0.20125	0.00000	0.79511	0.00364	0.79875
C	110	-0.17523	1.99908	4.16048	0.01567	6.17523
H	111	0.19947	0.00000	0.79786	0.00268	0.80053
C	112	-0.21382	1.99899	4.19930	0.01553	6.21382
H	113	0.20210	0.00000	0.79435	0.00354	0.79790
C	114	0.00644	1.99886	3.97528	0.01942	5.99356
C	115	-0.21138	1.99912	4.19641	0.01585	6.21138
H	116	0.20673	0.00000	0.78918	0.00408	0.79327
C	117	-0.55448	1.99926	4.54532	0.00990	6.55448
H	118	0.19122	0.00000	0.80674	0.00204	0.80878
H	119	0.19449	0.00000	0.80328	0.00223	0.80551
H	120	0.18926	0.00000	0.80826	0.00248	0.81074
C	121	-0.56346	1.99929	4.55359	0.01058	6.56346
H	122	0.18226	0.00000	0.81557	0.00217	0.81774
H	123	0.19426	0.00000	0.80364	0.00210	0.80574
H	124	0.21932	0.00000	0.77823	0.00245	0.78068
C	125	-0.20924	1.99912	4.19456	0.01555	6.20924
H	126	0.20952	0.00000	0.78601	0.00447	0.79048
C	127	-0.55557	1.99926	4.54641	0.00990	6.55557
H	128	0.18911	0.00000	0.80835	0.00254	0.81089
H	129	0.19409	0.00000	0.80368	0.00223	0.80591
H	130	0.19487	0.00000	0.80303	0.00210	0.80513
C	131	-0.55986	1.99929	4.55030	0.01026	6.55986

H 132	0.20908	0.00000	0.78899	0.00192	0.79092
H 133	0.19972	0.00000	0.79823	0.00205	0.80028
H 134	0.18308	0.00000	0.81468	0.00224	0.81692



* Total *	0.00000	175.92995	322.75428	1.31578	500.00000
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#### 4. References

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- [S2] Bruker AXS SHELXTL, Madison, WI; SHELX-97G. M. Sheldrick, *Acta Crystallogr. A*, **2008**, *64*, 112–122, *SHELX-2013*, <http://shelx.uni-ac.gwdg.de/SHELX/index.php>.
- [S3] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.



## 5. NMR spectrum

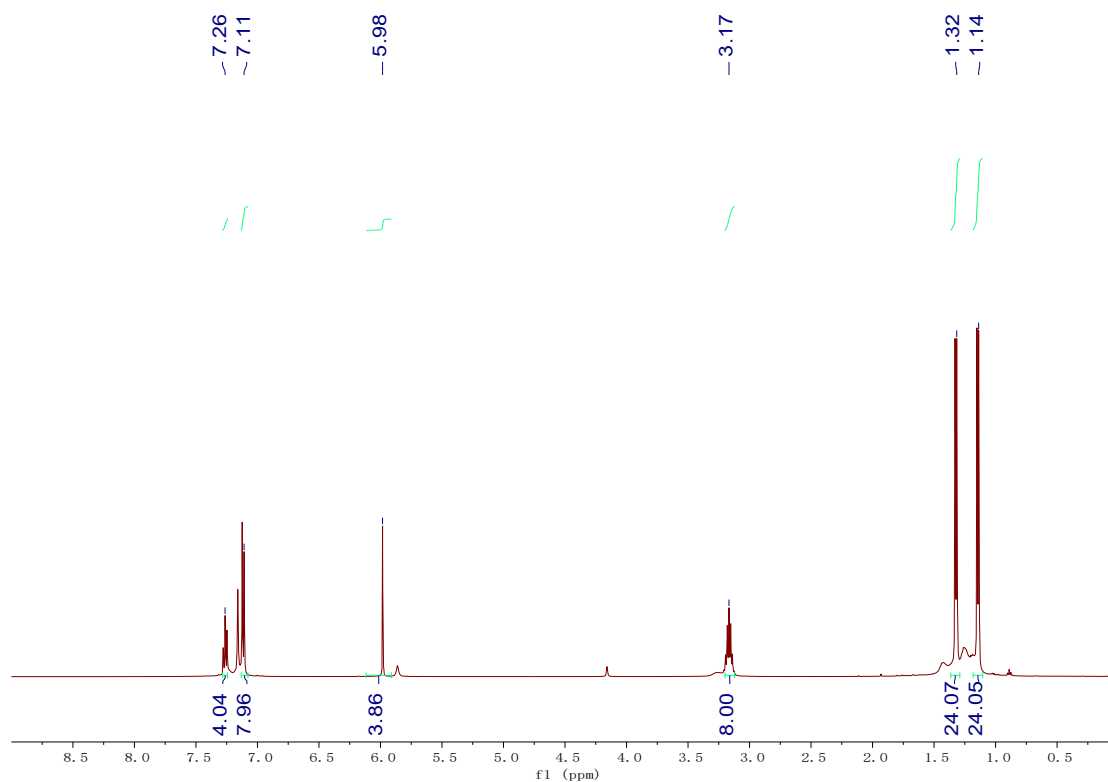


Figure S5. <sup>1</sup>H NMR (500 MHz) spectrum of **1** in C<sub>6</sub>D<sub>6</sub>.

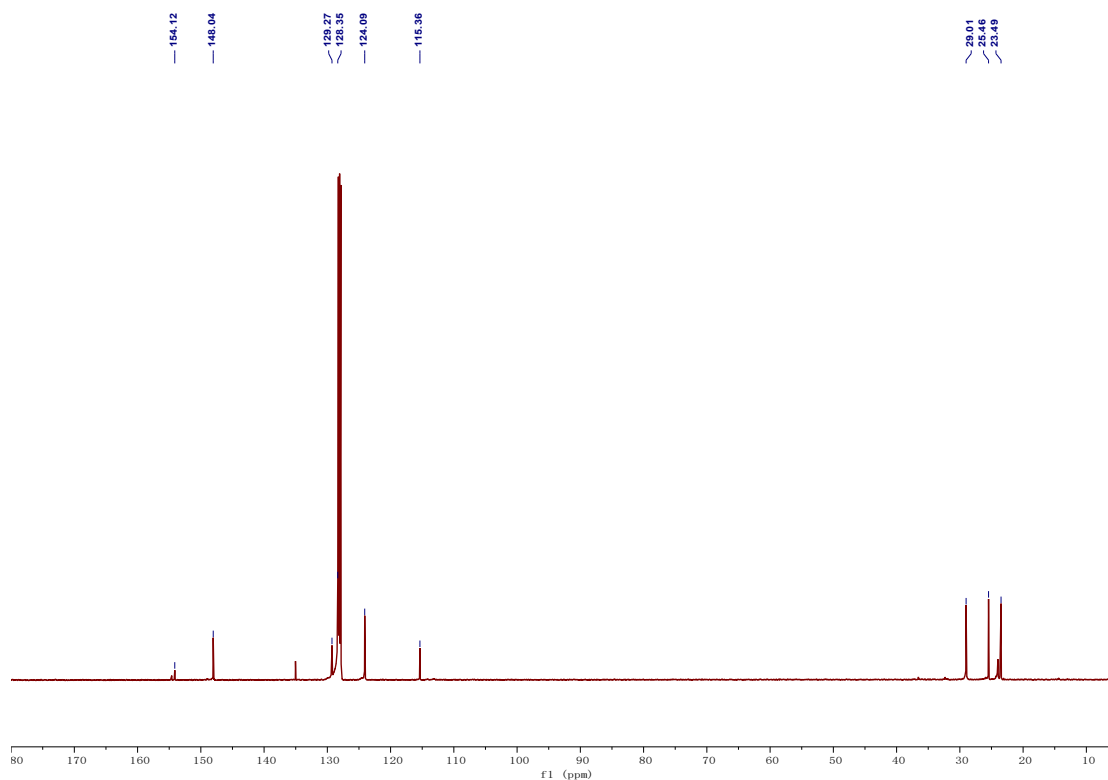


Figure S6. <sup>13</sup>C NMR (126 MHz) spectrum of **1** in C<sub>6</sub>D<sub>6</sub>.

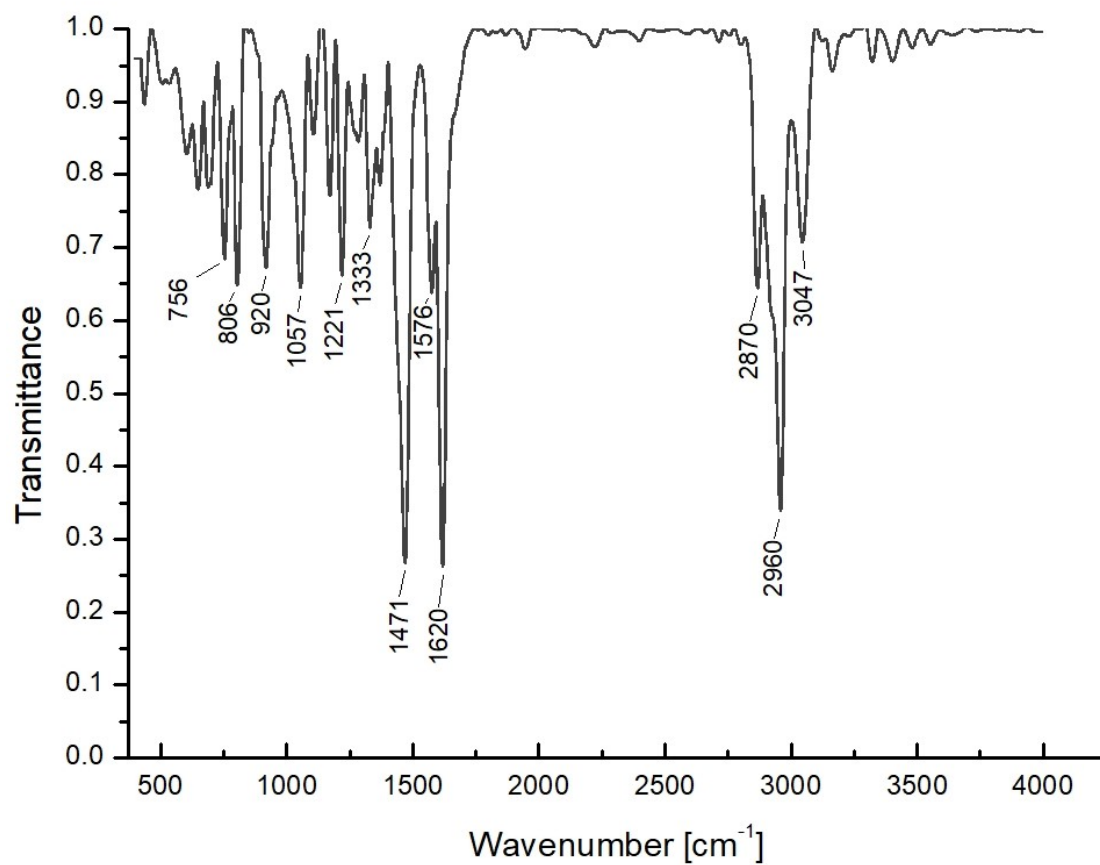


Figure S7. FT-IR spectrum of 1.

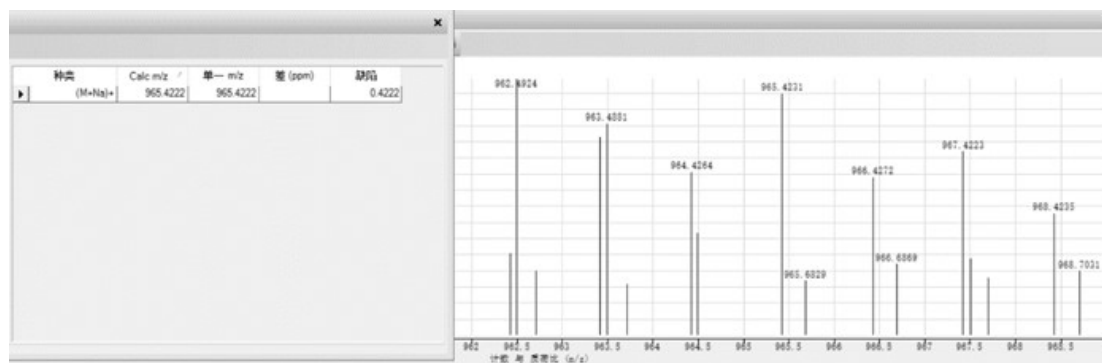


Figure S8. HRMS spectrum of 1.

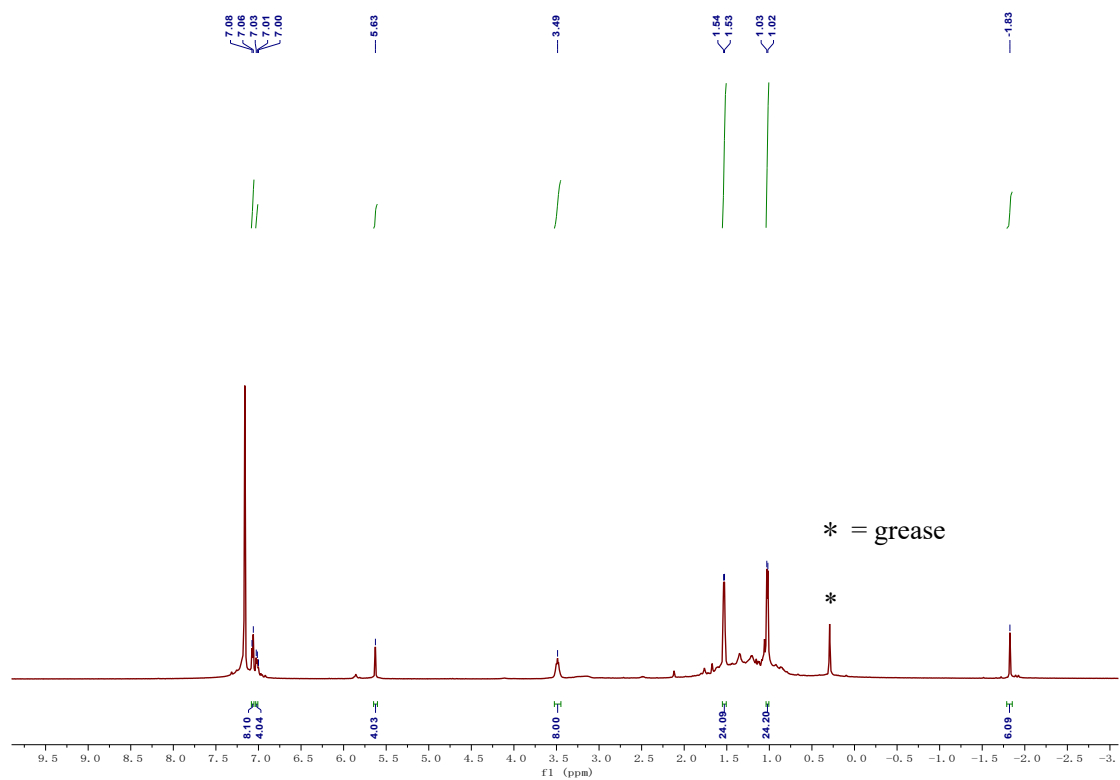


Figure S9.  $^1\text{H}$  NMR (500 MHz) spectrum of **2** in  $\text{C}_6\text{D}_6$ .

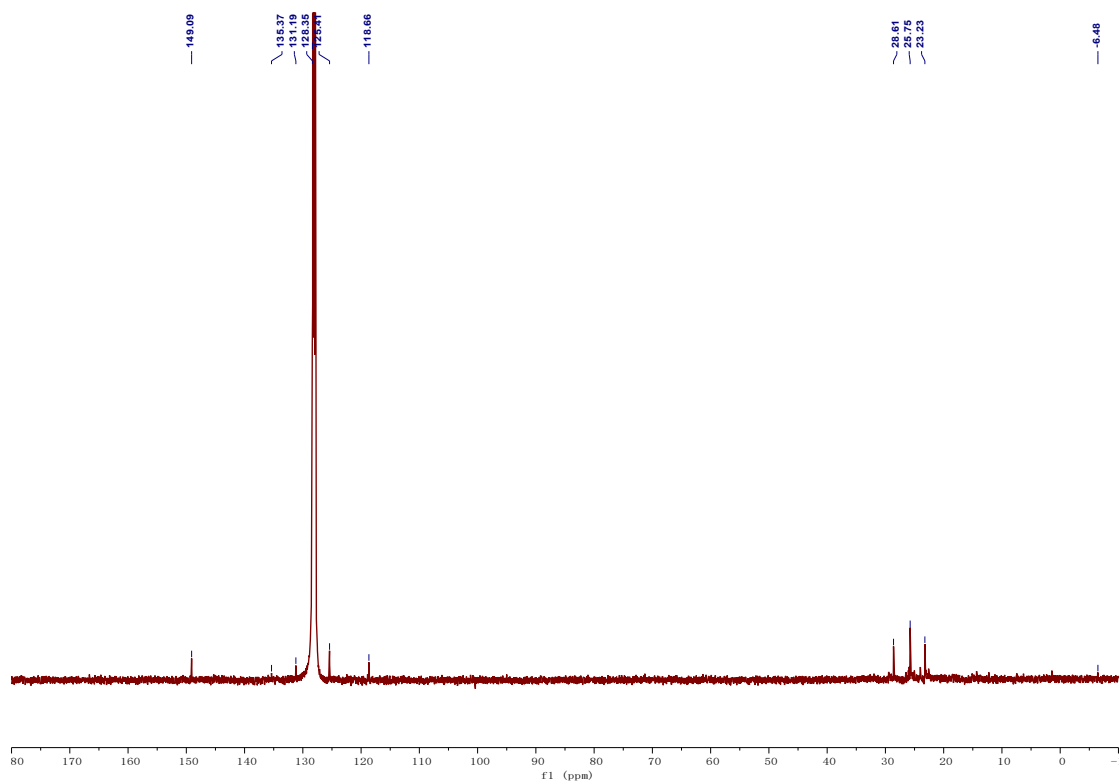


Figure S10.  $^{13}\text{C}$  NMR (126 MHz) spectrum of **2** in  $\text{C}_6\text{D}_6$ .

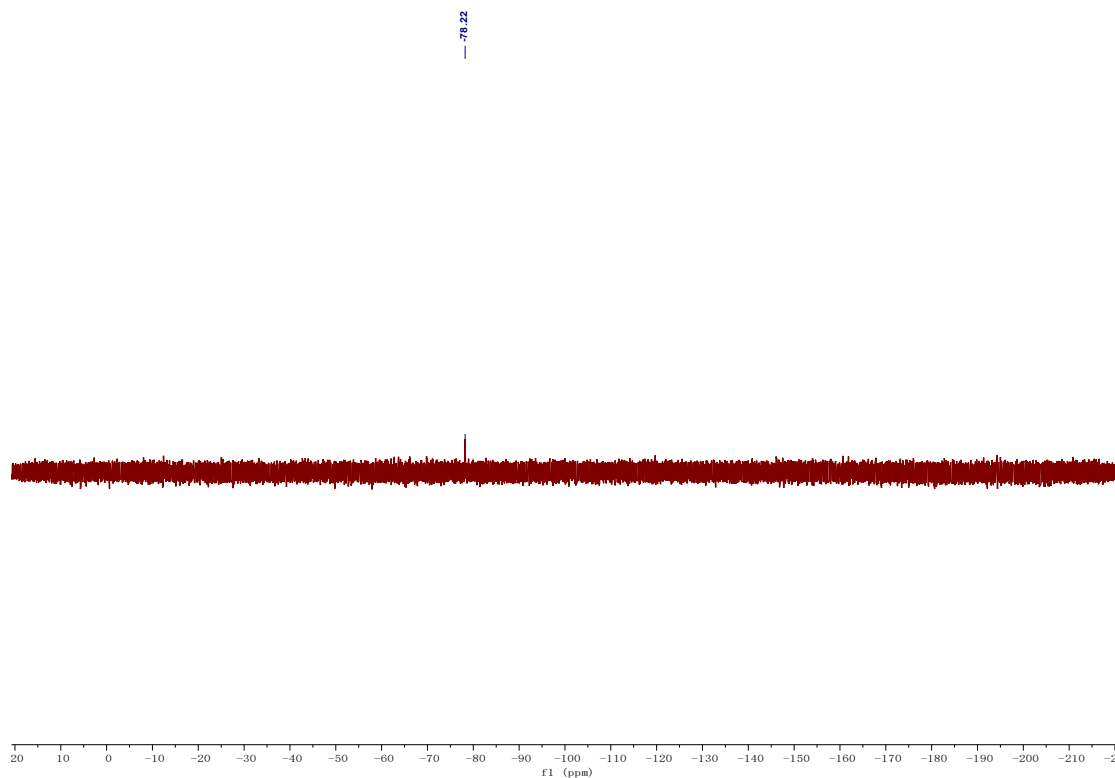


Figure S11.  $^{19}\text{F}$  NMR (470.4 MHz) spectrum of **2** in  $\text{C}_6\text{D}_6$ .

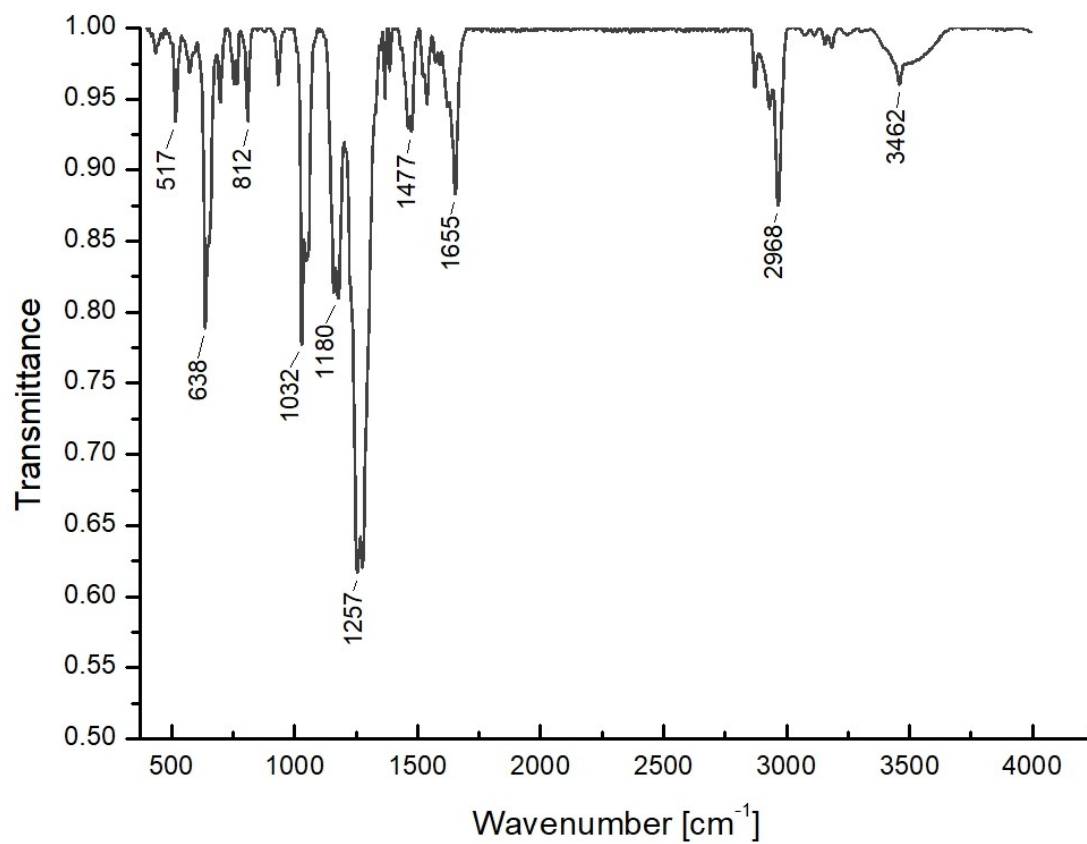


Figure S12. FT-IR spectrum of **2**.

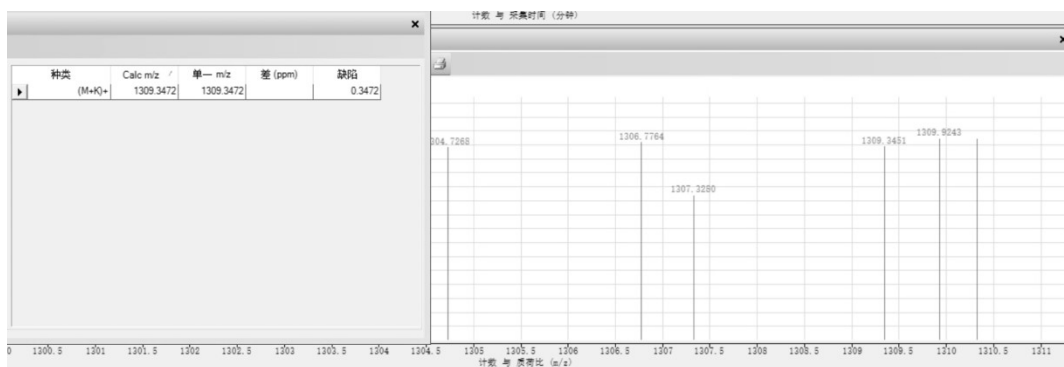


Figure S13. HRMS spectrum of 2.

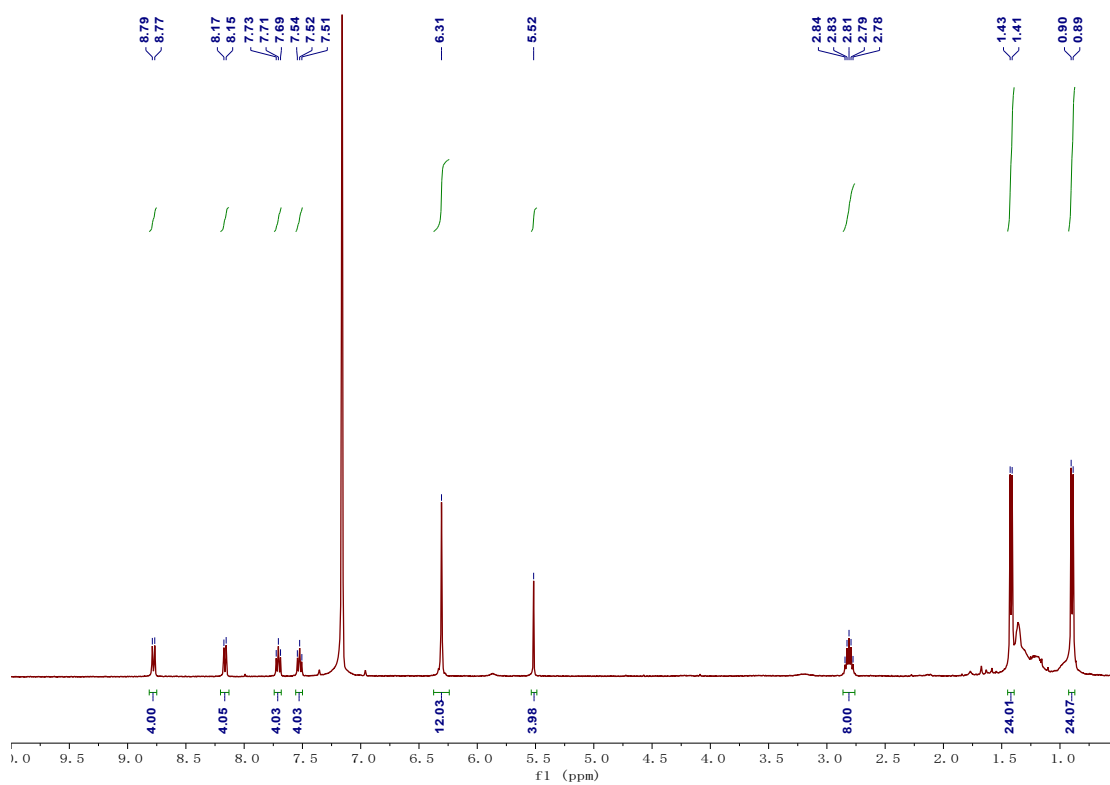


Figure S14. <sup>1</sup>H NMR (500 MHz) spectrum of 3 in C<sub>6</sub>D<sub>6</sub>.

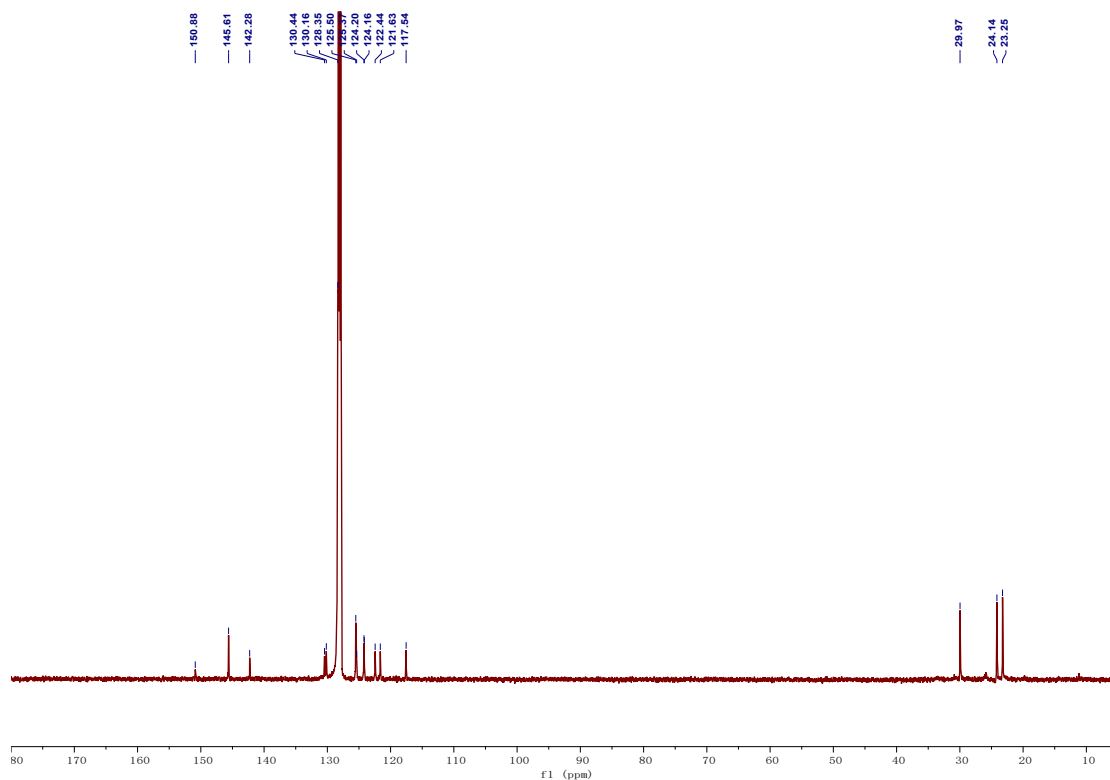


Figure S15.  $^{13}\text{C}$  NMR (126 MHz) spectrum of **3** in  $\text{C}_6\text{D}_6$ .

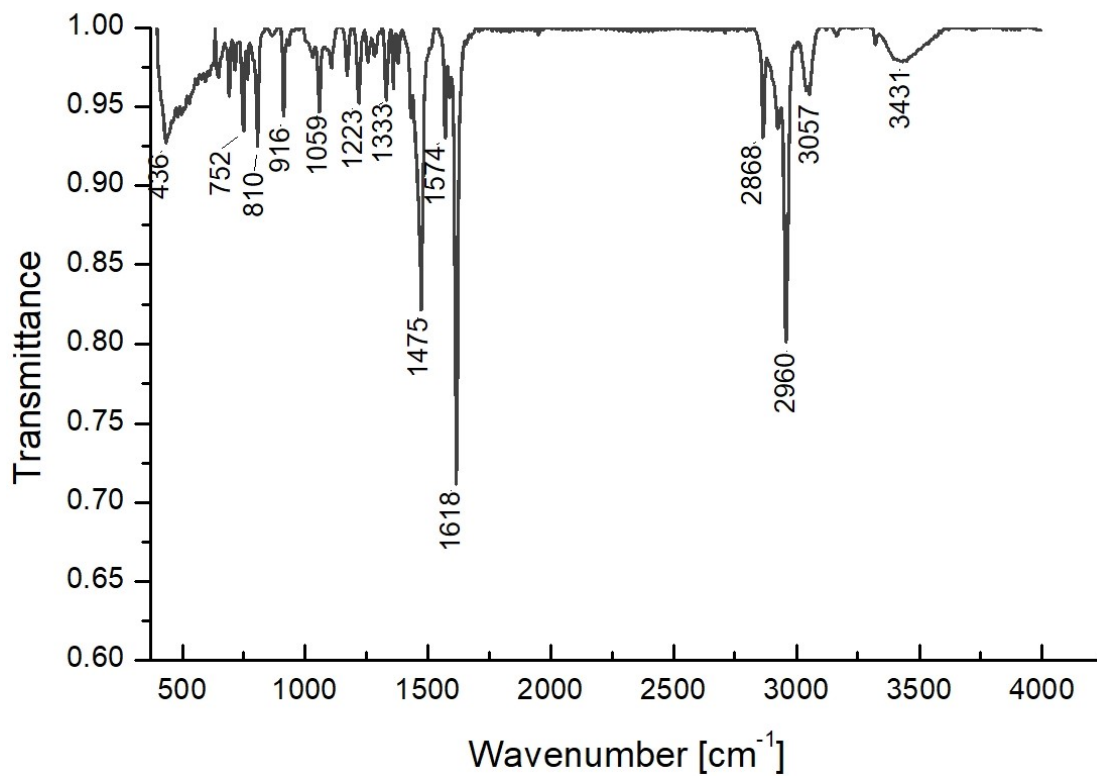


Figure S16. FT-IR spectrum of **3**.

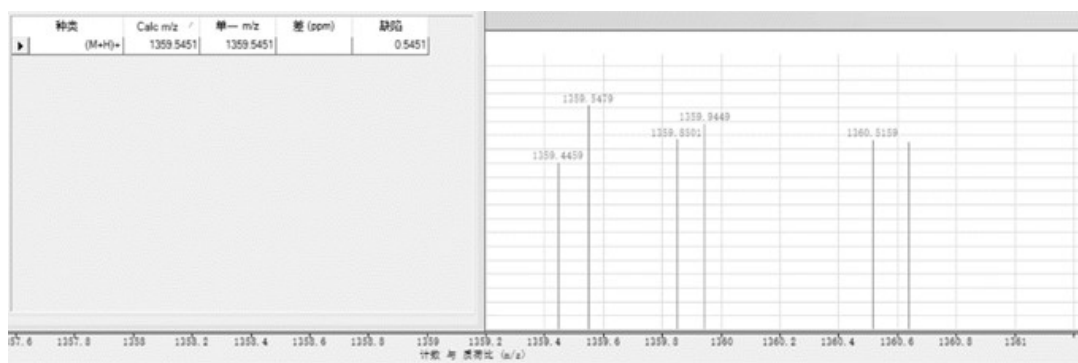


Figure S17. HRMS spectrum of **3**.

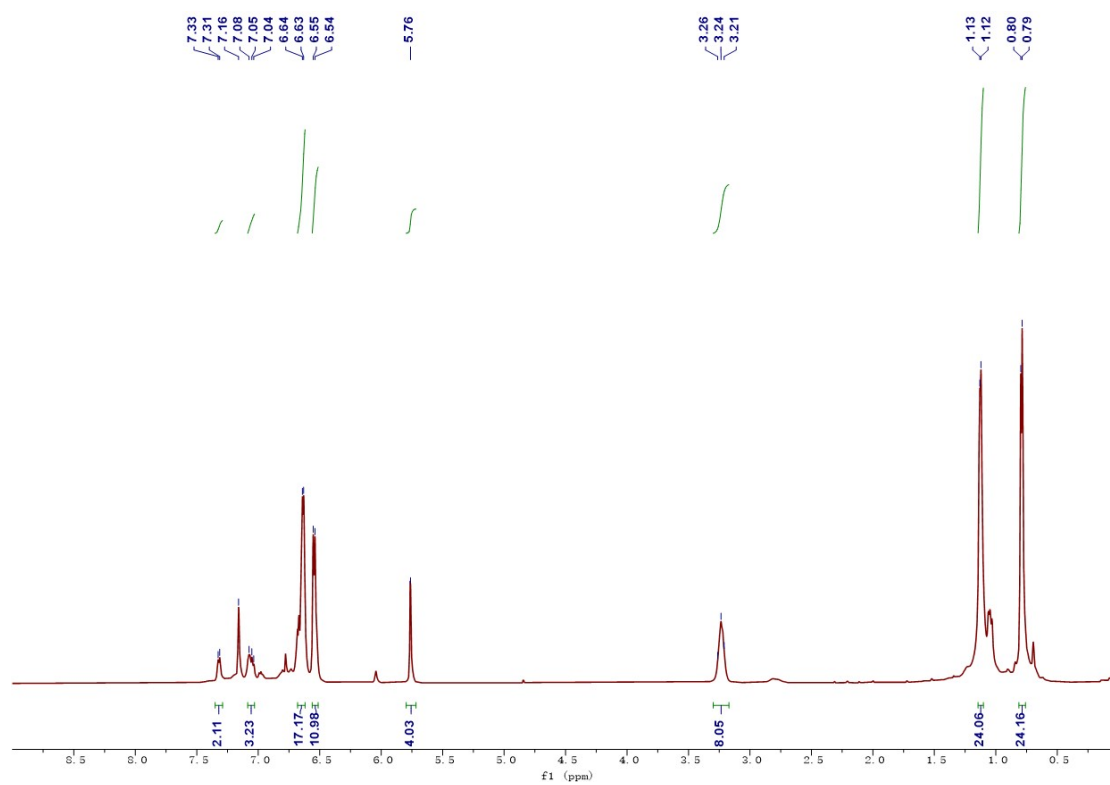


Figure S18. <sup>1</sup>H NMR (500 MHz) spectrum of **4** in C<sub>6</sub>D<sub>6</sub>.

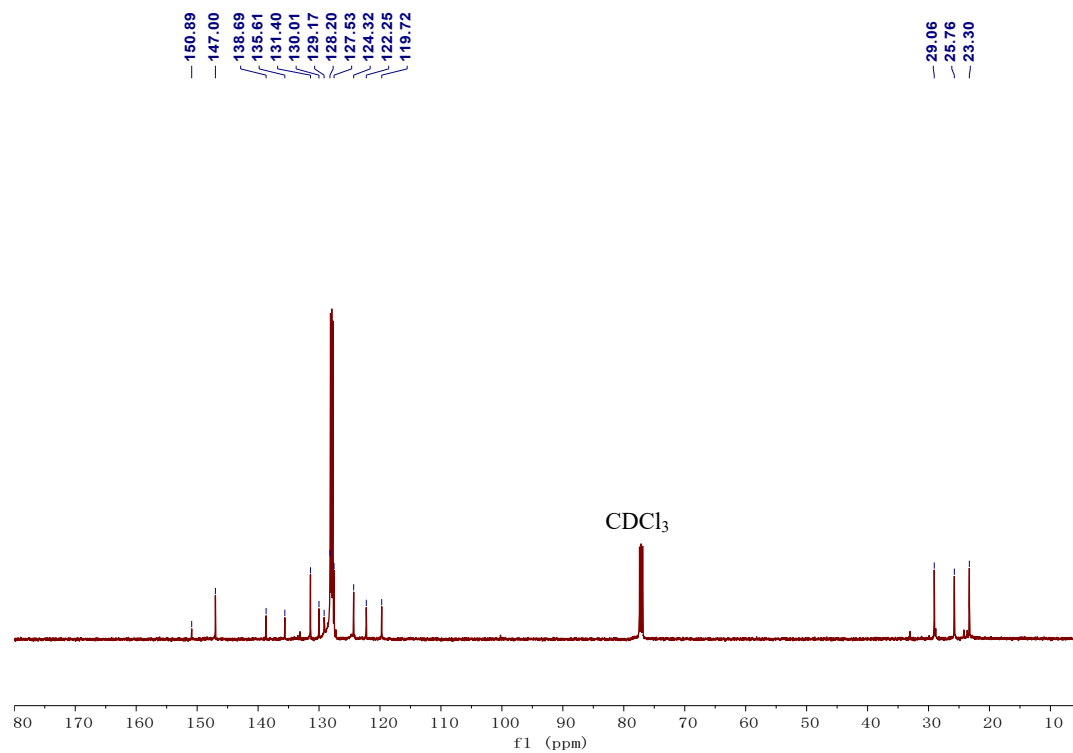


Figure S19. <sup>13</sup>C NMR (126 MHz) spectrum of **4** in C<sub>6</sub>D<sub>6</sub>.

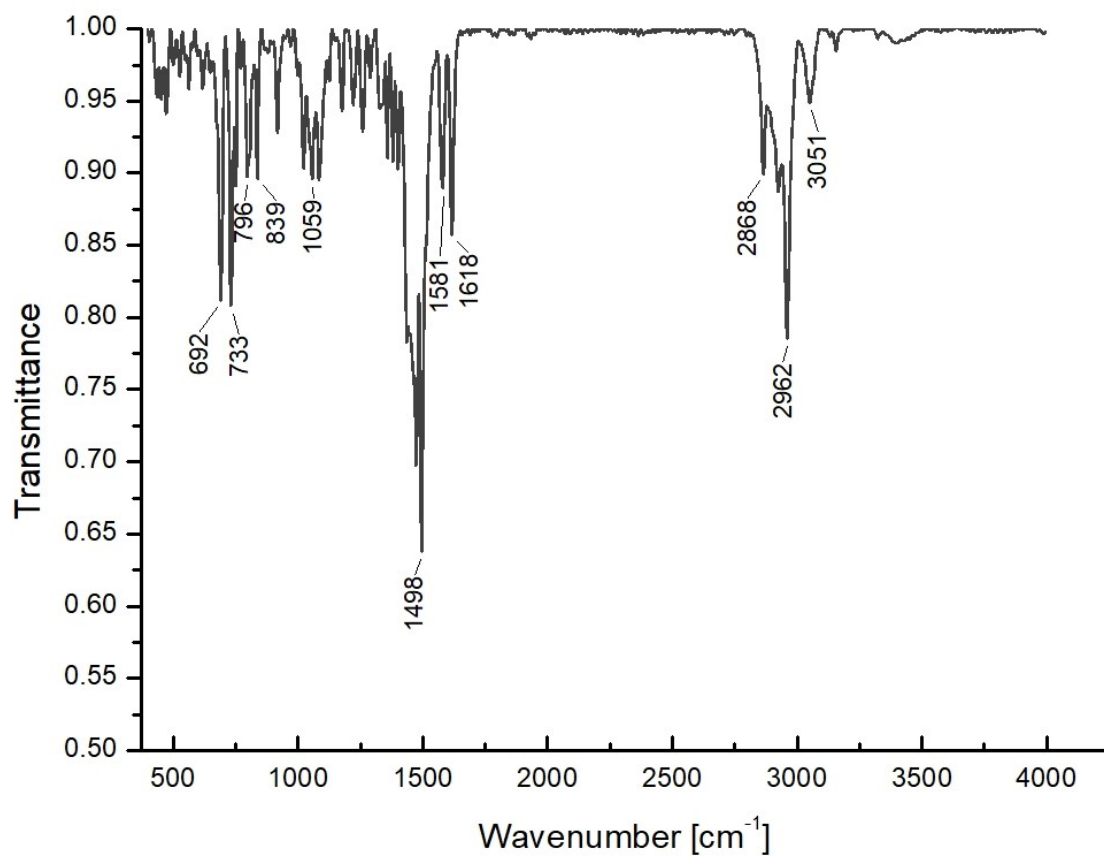


Figure S20. FT-IR spectrum of **4**.



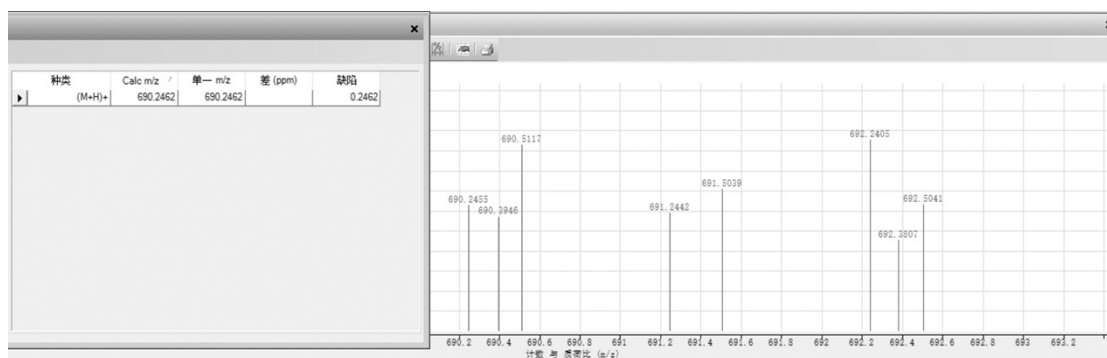


Figure S21. HRMS spectrum of **4**.

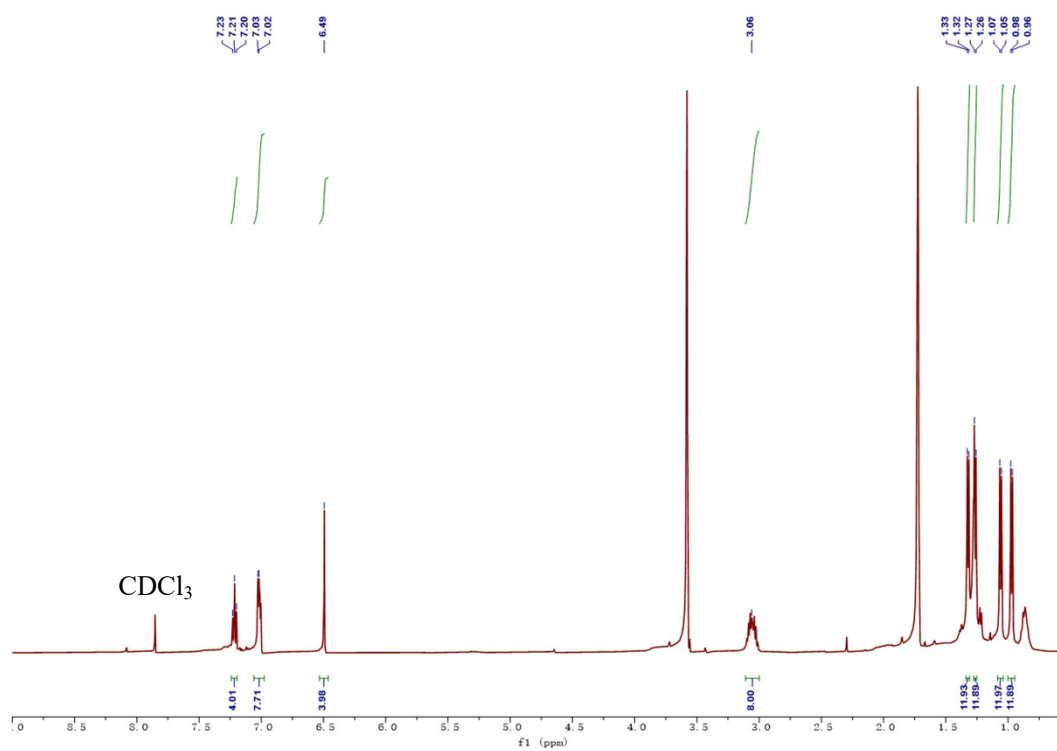


Figure S22. <sup>1</sup>H NMR (500 MHz) spectrum of **5** in THF-*d*<sub>8</sub>.

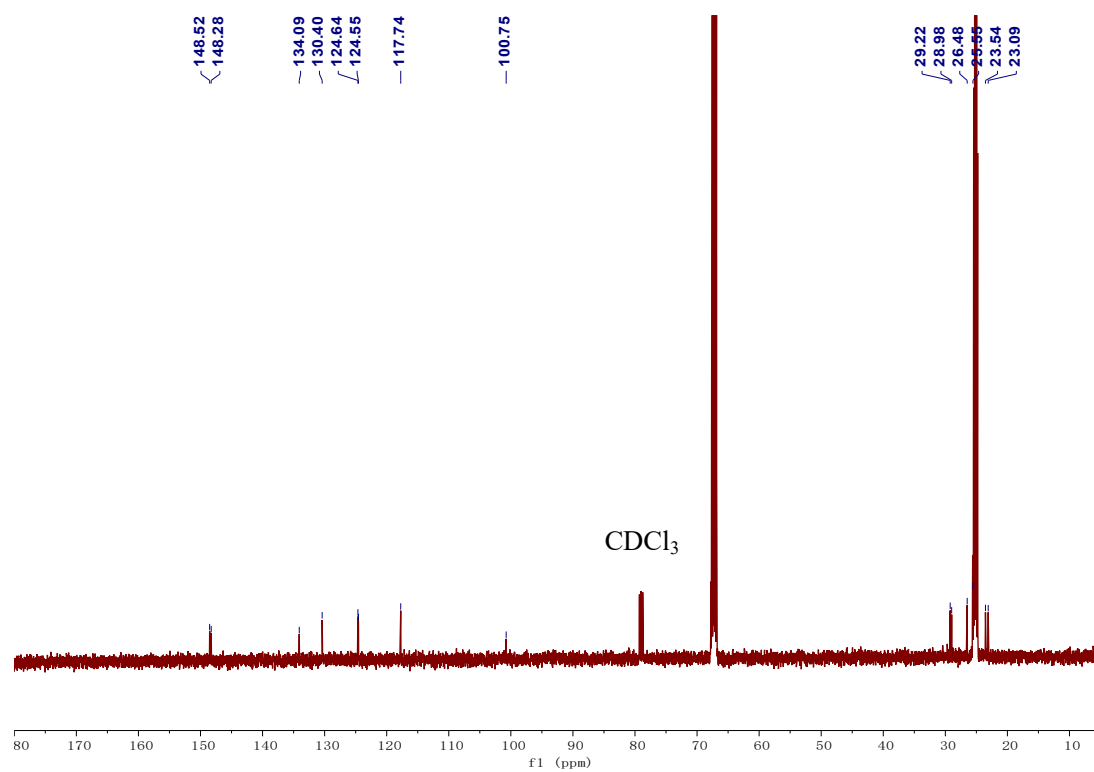


Figure S23. <sup>13</sup>C NMR (126 MHz) spectrum of **5** in THF-*d*<sub>8</sub>.

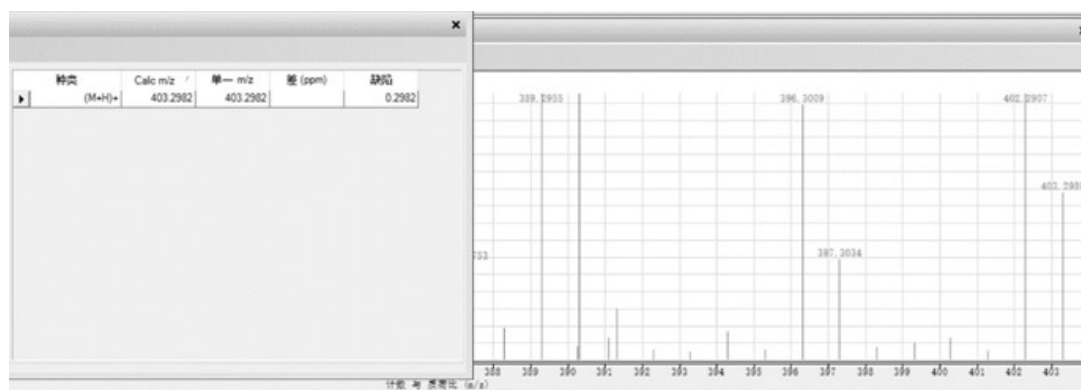


Figure S24. HRMS spectrum of **5**.