Activation reactions of 2-pyridyl and 2-pyrimidinyl alkynes with $Ru_3(CO)_{12}$

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Table S1. Crystal data and structure refinement for **1a, 1b** and **2a**.

Compounds	**1a**	**1b**	**2a**
Formula	$C_{22}H_{10}N_2O_8Ru_3$	$C_{24}H_{10}N_2O_{10}Ru_3$	$C_{22}H_{11}NO_8Ru_3$
Fw (g mol^{-1})	733.53	789.55	720.53
Wavelength(Å)	0.71073	0.71073	0.71073
T (K)	153(2)	153(2)	153(2)
crystal system	triclinic	triclinic	triclinic
space group	P-1	P-1	P-1
a (Å)	8.1837(15)	9.4360(5)	8.1534(15)
b (Å)	9.6603(17)	10.9568(5)	9.9791(19)
c (Å)	15.130(3)	12.7636(6)	14.213(3)
α (°)	97.804(6)	77.1120(10)	91.735(5)
β (°)	94.587(6)	71.3300(10)	94.157(5)
γ (°)	106.052(5)	81.1030(10)	102.600(5)
V (Å3)	1130.1(4)	1213.71(10)	1124.4(4)
Z	2	2	2
Dc (Mg m^{-3}*)*	2.156	2.160	2.128
Absorption coefficient (mm^{-1})	2.031	1.906	2.038
F(0 0 0)	704.0	760.0	692.0
Crystal sizes (mm)	0.140×0.130×0.100	0.140×0.120×0.100	0.150×0.130× 0.100
collected/unique	85076/4427	13622/4645	40777/4338
R_{int}	0.0263	0.0265	0.0283
Data/restraints/parameters	4427/7/316	4645/0/353	4338/0/308
GOF on *F*2	1.153	1.107	1.136
R1, w*R2 [I ≥2σ(I)]*	0.0156, 0.0393	0.0210, 0.0521	0.0163, 0.0411
R1, w*R2 (all data)*	0.0165, 0.0400	0.0216, 0.0525	0.0166, 0.0413
largestdiff. Peak/hole (e. $Å^{-3}$*)*	0.33/-0.53	0.40/-0.73	0.38/-0.57

Table S1. Crystal data and structure refinement for **3a**, **5a**, **6a**.

Compounds	**3a**	**5a**	**6a**
Formula	$C_{22}H_{11}NO_9Ru_3$	$C_{22}H_{15}NO_9Ru_3$	$C_{22}H_{17}NO_9Ru_3$
Fw (g mol^{-1})	736.53	740.56	742.57
Wavelength(Å)	0.71073	0.71073	0.71073
T (K)	296(2)	153(2)	153(2)
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/c$	C2/c	$P2_1/c$
a (Å)	17.721(5)	18.146(3)	13.0521(17)
b (Å)	8.302(2)	10.6229(15)	11.6759(16)
c (Å)	16.368(4)	25.999(5)	16.604(3)
α (°)	90	90	90
β (°)	104.130(9)	105.869(5)	92.248(5)
γ (°)	90	90	90
V (Å3)	2335.2(10)	4820.6(14)	2528.4(6)
Z	4	8	4
Dc (Mg m^{-3}*)*	2.095	2.041	1.951
Absorption coefficient (mm^{-1})	1.968	1.908	1.819
F(0 0 0)	1416.0	2864.0	1440.0
Crystal sizes (mm)	0.150 ×0.120 ×0.110	0.140×0.120×0.100	0.130×0.120×0.100
collected/unique	25457/4582	25735/4421	27996/5171
R_{int}	0.0712	0.0461	0.0445
Data/restraints/parameters	4582/222/371	4421/1/366	5171/1/348
GOF on *F*2	1.401	1.108	1.074
R1, w*R2 [I ≥2σ(I)]*	0.0950, 0.2417	0.0276, 0.0641	0.0207, 0.0442
R1, w*R2 (all data)*	0.0959, 0.2421	0.0342, 0.0693	0.0255, 0.0464
largestdiff. Peak/hole (e. $Å^{-3}$*)*	1.75/-2.83	0.88/-1.79	0.50/-0.65

Table S1. Crystal data and structure refinement for **8a** and **9a**.

Compounds	**8a**	**9a**
Formula	$C_{22}H_{11}BrCl_2N_2O_9Ru_3$	$C_{21}H_9BrN_2O_8Ru_3$
Fw (g mol^{-1})	901.35	800.42
Wavelength(Å)	0.71073	0.71073
T (K)	296(2)	153(2)
crystal system	triclinic	monoclinic
space group	P-1	C2/c
a (Å)	8.0005(16)	35.283(12)
b (Å)	11.922(2)	8.632(3)
c (Å)	14.299(3)	16.713(5)
α (°)	91.869(7)	90
β (°)	94.132(7)	114.304(10)
γ (°)	106.036(7)	90
V (Å3)	1305.4(4)	4639(3)
Z	2	8
Dc (Mg m^{-3})	2.293	2.292
Absorption coefficient (mm^{-1})	3.504	3.702
F(0 0 0)	860.0	3040.0
Crystal sizes (mm)	0.150×0.130×0.100	0.150×0.130×0.110
collected/unique	15372/5137	26215/4561
R_{int}	0.0430	0.0493
Data/restraints/parameters	5137/0/353	4561/0/317
GOF on *F*2	1.025	1.075
R1, w*R2 [I ≥2σ(I)]*	0.0300, 0.0660	0.0205, 0.0484
R1, w*R2 (all data)*	0.0415, 0.0702	0.0259, 0.0510
largestdiff. Peak/hole (e. $Å^{-3}$)	0.82/-0.77	0.44/-0.88

Table S1. Crystal data and structure refinement for **9c** and **10b**.

Compounds	**9c**	**10b**
Formula	$C_{24.5}H_{17}BrCl_2N_2O_8Ru_3$	$C_{38}H_{22}Br_2Fe_2N_4O_6Ru_2$
Fw (g mol^{-1})	921.42	1104.25
Wavelength(Å)	0.71073	0.71073
T (K)	153(2)	296(2)
crystal system	triclinic	triclinic
space group	P-1	P-1
a (Å)	7.6301(14)	10.3905(15)
b (Å)	10.238(2)	13.625(2)
c (Å)	19.359(4)	14.473(2)
α (°)	79.718(6)	114.580(5)
β (°)	86.238(6)	95.293(5)
γ (°)	86.842(6)	99.218(5)
V (Å3)	1483.4(5)	1810.2(5)
Z	2	2
Dc (Mg m^{-3})	2.063	2.026
Absorption coefficient (mm^{-1})	3.083	3.865
F(0 0 0)	886.0	1072.0
Crystal sizes (mm)	0.150×0.130×0.100	0.140×0.110×0.100
collected/unique	17384/5810	20585/7083
R_{int}	0.0241	0.0265
Data/restraints/parameters	5810/30/393	7083/0/487
GOF on *F*2	1.051	1.042
R1, w*R2 [I ≥2σ(I)]*	0.0234, 0.0584	0.0215, 0.0505
R1, w*R2 (all data)*	0.0260, 0.0601	0.0259, 0.0526
largestdiff. Peak/hole (e. $Å^{-3}$)	0.58/-1.05	0.70/-0.85

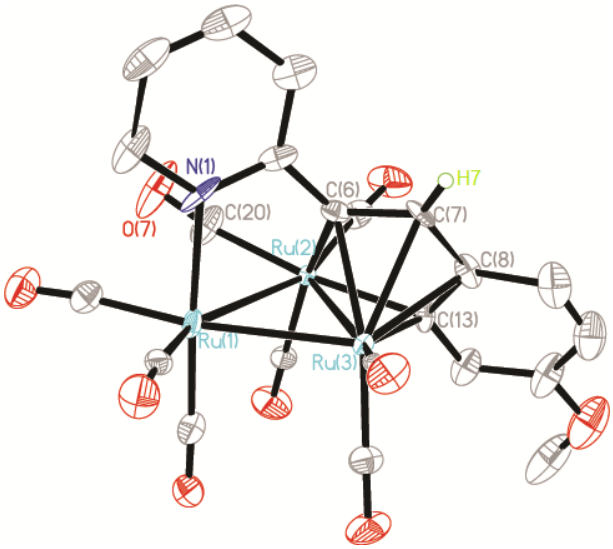

Fig. S1. ORTEP view of cluster **3a** showing 50% ellipsoids. Selected bond lengths (Å) and bond angles (°): C6-C7 = 1.42(2), C7-C8 = 1.46(2),C8-C13 = 1.41(2), Ru2-C6 = 2.119(16), Ru2-C13 = 2.170(15), Ru3-C6 = 2.256(15), Ru3-C7 = 2.286(15), Ru3-C8 = 2.326(16), Ru3-C13 = 2.296(16), N1-Ru1 = 2.179(16), Ru1-Ru2 = 2.8488(18), Ru1-Ru3 = 2.7984(18), Ru2-Ru3 = 2.7657(17), Ru2-Ru1-N1 = 85.0(4), Ru3-Ru1-N1 = 89.4(4).

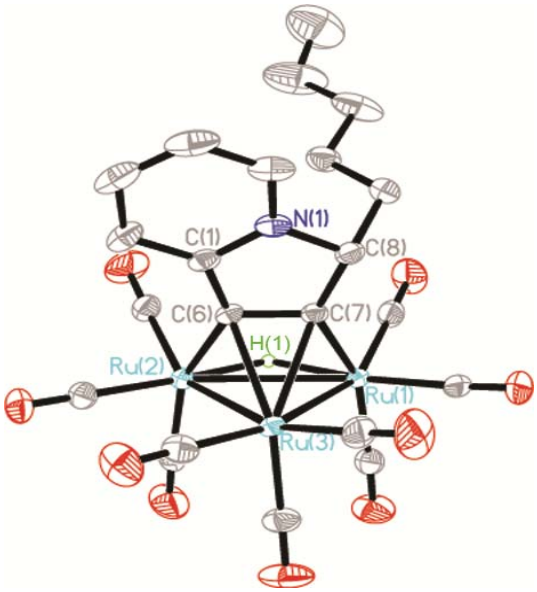

Fig. S2. ORTEP view of cluster **6a** showing 50% ellipsoids. Selected bond lengths (Å) and bond angles (°): C1-C6 = 1.462(3), C6-C7 = 1.410(3), C7-C8 = 1.511(3), C1-N1 = 1.364(3), C8-N1 = 1.501(3), Ru1-C7 = 2.054(2), Ru2-C6 = 2.084(2), Ru3-C6 = 2.227(2), Ru3-C7 = 2.260(2), Ru1-Ru2 = 3.0193(4), Ru1-Ru3 = 2.7497(4), Ru2-Ru3 = 2.7332(4), C1-N1-C8 = 111.26(17).

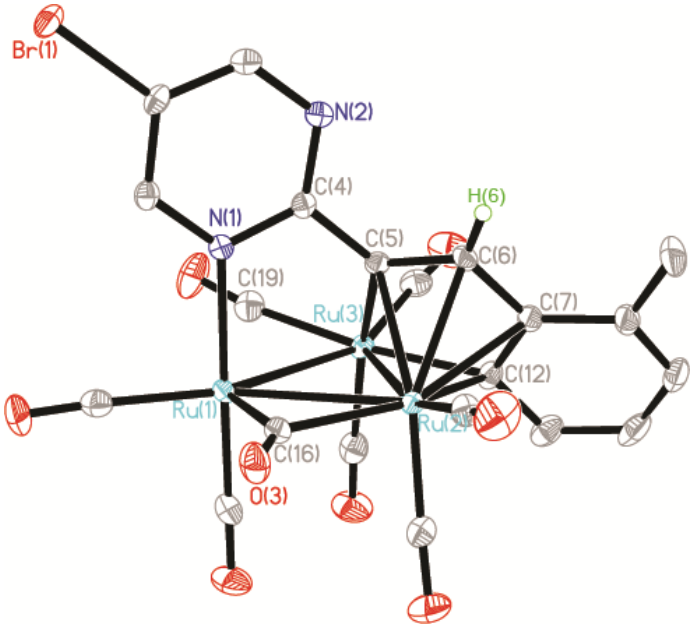

Fig. S3 ORTEP view of cluster **9a** showing 50% ellipsoids. Selected bond lengths (Å) and bond angles (°): Ru1-N1 = 2.165(2), Ru1-C16 = 1.984(3), Ru1-C19 = 2.6996(27), Ru2-C5 = 2.276(3), Ru2-C6 = 2.248(3), Ru2-C7 = 2.329(3), Ru2-C12 = 2.330(3), Ru3-C5 = 2.101(3), Ru3-C12 = 2.099(3), Ru3-C19 = 1.963(3), Ru1-Ru2 = 2.8467(9), Ru2-Ru3 = 2.7862(7), Ru3-Ru1 = 2.8232(7), Ru1-C16-Ru2 = 86.37(10), Ru1-C19-Ru3 = 75.589(84).

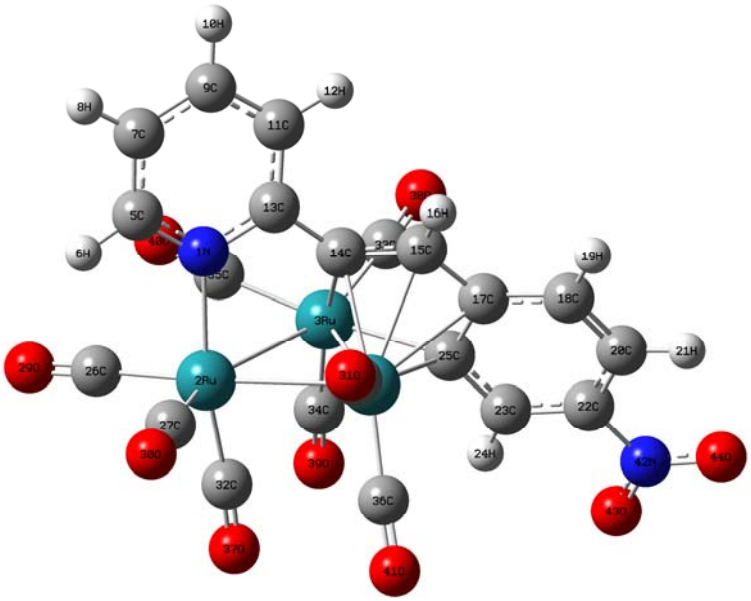

Fig. S4. DFT-optimized structure of **4a** at the level of B3LYP/LanL2DZ/6-31G. Selected bond lengths (Å) and bond angles (°): C14-C15 = 1.40339, Ru3-C14 = 2.12683, Ru3-C25 = 2.20993, Ru4-C14 = 2.31924, Ru4-C15 = 2.37228, Ru4-C17 =2.46869, Ru4-C25 = 2.29002, Ru2-Ru3 = 2.91724, Ru3-Ru4 = 2.82217, Ru2-Ru4 = 2.73458.

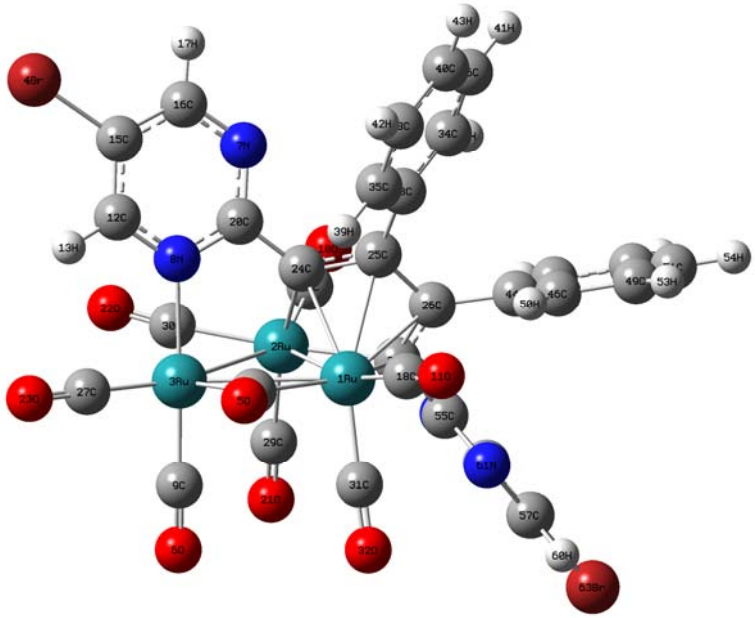

Fig. S5. DFT-optimized structure of **7a** at the level of B3LYP/LanL2DZ/6-31G. Selected bond lengths (Å) and bond angles (°): Ru3-N8 = 2.19081, C24-C25 = 1.40243, C27-C29 = 1.44724, Ru1-C24= 2.33921, Ru1-C25 = 2.34971, Ru1-C27 = 2.47277, Ru1-C29 = 2.45520, Ru1-Ru2 = 2.86914, Ru2-Ru3 = 2.97842, Ru1-Ru3 = 2.99954.

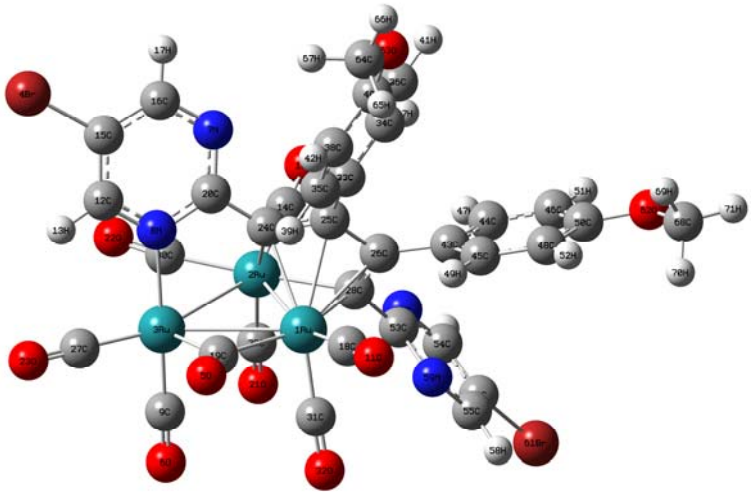

Fig. S6. DFT-optimized structure of **8b** at the level of B3LYP/LanL2DZ/6-31G. Selected bond lengths (Å) and bond angles (°): Ru1-C19 = 2.12095, Ru1-C24 = 2.34383, Ru1-C25 = 2.36048, Ru1-C26 = 2.39225, Ru1-C28 = 2.33763, Ru2-C24 = 2.11286, Ru2-C28 = 2.11007, Ru3-C19 = 2.01905, Ru1-Ru2 = 2.86397, Ru1-Ru3 = 2.98114, Ru2-Ru3 = 2.99449, Ru3-N8 = 2.19013, Ru1-C19-Ru3 = 92.08926.

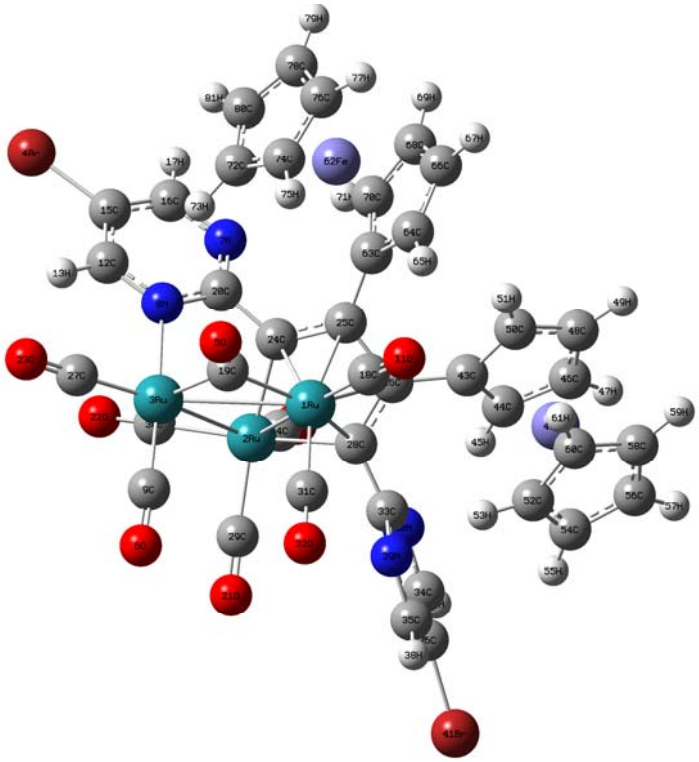

Fig. S7. DFT-optimized structure of **10a** at the level of B3LYP/LanL2DZ/6-31G. Selected bond lengths (Å) and bond angles (°): C24-C25 = 1.41821, C26-C28 = 1.42264, Ru1-C19 = 2.11234, Ru1-C24 = 2.36389, Ru1-C25 = 2.36296, Ru1-C26 = 2.43129, Ru1-C28 = 2.29737, Ru2-C24 = 2.10840, Ru2-C28 = 2.12083, Ru3-C19= 2.03077, Ru3-N8 = 2.18235, Ru1-Ru2 = 2.84947, Ru1-Ru3 = 2.99263, Ru2-Ru3 = 3.02979.

Table S2.DFT optimized structure bond parameters of **1a**

C6-C7 = 1.40888	C7-C8 = 1.45585	C8-C9 = 1.41698	Ru1-N1 = 2.19412
Ru1-C18 = 2.02095	Ru1-C19 = 2.69118	Ru2-C6 = 2.11487	Ru2-C9 = 2.09024
Ru2-C19 = 1.98198	Ru3-C6 = 2.36501	Ru3-C7 = 2.32345	Ru3-C8 = 2.34782
Ru3-C9 = 2.32233	Ru3-C18 = 2.12215	Ru1-Ru2 = 2.97878	Ru1-Ru3 = 2.99446
Ru2-Ru3 =2.88959	Ru1-C18-Ru3 = 92.53253	Ru1-C19-Ru2 = 77.56248	

Table S2.DFT optimized structure bond parameters of **1b**

C6-C7 = 1.45416	C7-C8 = 1.42790	C8-C9 = 1.45547	C6-C10 = 1.44795
C9-C10 = 1.43730	Ru1-Ru3 = 3.02112	Ru1-N1 = 2.21550	Ru1-C7 = 2.06402
Ru2-C6 = 2.29210	Ru2-C7 = 2.41233	Ru2-C8 = 2.45411	Ru2-C9 = 2.39556
Ru2-C10 = 2.29012	Ru2-Ru3 = 2.88077	N1-Ru1-C7 = 77.94061	Ru1-Ru3-Ru2 = 82.74935

Table S2.DFT optimized structure bond parameters of **2a**

C6-C7 = 1.40517	C7-C8 = 1.46018	C8-C9 = 1.44683	Ru1-C16 = 2.02545
Ru1-C18 = 2.68140	Ru1-N1 = 2.19099	Ru2-C6 = 2.10940	Ru2-C9 = 2.13721
Ru2-C18 = 1.97090	Ru3-C6 = 2.36412	Ru3-C7 = 2.33089	Ru3-C8 = 2.45755
Ru3-C9 = 2.46043	Ru3-C16 = 2.08117	Ru1-Ru2 = 3.00097	Ru2-Ru3 = 2.87296
Ru1-Ru3 = 2.99933	Ru1-C16-Ru3 = 93.82401	N1-Ru1-Ru2 = 84.14434	
Ru3-C16-O2 = 135.04245	Ru1-C18-Ru2 = 78.71408		

Table S2.DFT optimized structure bond parameters of **3a**

C6-C7 = 1.40489	C7-C8 = 1.45689	C8-C13 = 1.44765	Ru2-C6 = 2.11637
Ru2-C13 = 2.13619	Ru3-C6 = 2.35510	Ru3-C7 = 2.32811	Ru3-C8 = 2.46680
Ru3-C13 = 2.51426	N1-Ru1 = 2.19263	Ru1-Ru2 = 3.00159	Ru1-Ru3 = 2.99152
Ru2-Ru3 = 2.87883	Ru2-Ru1-N1 = 84.31271	Ru3-Ru1-N1 = 88.41779	

Table S2.DFT optimized structure bond parameters of **5a**

C5-C12 = 1.45376	C6-C13 = 1.54957	C12-C13 = 1.42201	C5-N1 = 1.37627
C6-N1 = 1.55055	Ru1-C12 = 2.27987	Ru1-C13= 2.36373	Ru2-C13 = 2.11467
Ru3-C12 = 2.09530	Ru1-Ru2 = 2.80319	Ru1-Ru3 = 2.78864	Ru2-Ru3 = 3.06394
C5-N1-C6 = 111.12447	Ru2-H12-Ru3 = 116.90216		

Table S2.DFT optimized structure bond parameters of **6a**

C1-C6 = 1.45696	C6-C7 = 1.41993	C7-C8 = 1.52537	C1-N1 = 1.38427
C8-N1 = 1.51957	Ru1-C7 = 2.07089	Ru2-C6 = 2.09811	Ru3-C6 = 2.28849
Ru3-C7 = 2.34115	Ru1-Ru2 = 3.10822	Ru1-Ru3 = 2.81722	Ru2-Ru3 = 2.78354
C1-N1-C8 = 110.53231			

Table S2.DFT optimized structure bond parameters of **8a**

C5-C6 = 1.40330	C6-C7 = 1.45341	C7-C12 = 1.44938	Ru1-C5 = 2.12270
Ru1-C12 = 2.13606	Ru1-C17 = 1.97035	Ru2-C5 = 2.32783	Ru2-C6 = 2.34269
Ru2-C7 = 2.47561	Ru2-C12 = 2.50731	Ru3-N1 = 2.19268	Ru2-C16 = 2.07668
Ru3-C16 = 2.02901	Ru3-C17 = 2.66088	Ru1-Ru2 = 2.87400	Ru1-Ru3 = 2.98116
Ru2-Ru3 = 2.99397	Ru3-C16-Ru2 = 93.63519	Ru1-C17-Ru3 = 78.58520	

Table S2.DFT optimized structure bond parameters of **9a**

Ru1-N1 = 2.19112	Ru1-C16 = 2.02958	Ru1-C19 = 2.68131	Ru2-C5 = 2.33788
Ru2-C6 = 2.34371	Ru2-C7 = 2.46569	Ru2-C12 = 2.45542	Ru3-C5 = 2.11613
Ru3-C12 = 2.13680	Ru3-C19 = 1.97066	Ru1-Ru2 = 2.99873	Ru2-Ru3 = 2.87185
Ru3-Ru1 = 2.98163	Ru1-C16-Ru2 = 93.67261	Ru1-C19-Ru3 = 78.07962	

Table S2.DFT optimized structure bond parameters of **9c**

C5-C6 = 1.44246	C6-C7 = 1.47083	Ru1-C5 = 2.11573	Ru1-C12 = 2.15137
Ru2-C5 = 2.27020	Ru2-C6 = 2.23385	Ru2-C7 = 2.58073	Ru2-C12 = 2.48335
Ru3-C6 = 2.08890	Ru3-N1 = 2.17309	Ru1-Ru2 = 2.81806	Ru2-Ru3 = 2.89560
Ru3-C6-Ru2 = 84.03960	Ru1-Ru2-Ru3 = 114.44136		

Table S2.DFT optimized structure bond parameters of **10b**

C11-C12 = 1.42219	C11-C27 = 1.48028	C27-C28 = 1.42750	Ru1-C11 = 2.42456
Ru1-C12 = 2.29223	Ru1-C27 = 2.48827	Ru1-C28 = 2.27376	Ru1-C35 = 1.94727
Ru2-C12 = 2.13154	Ru2-C28 = 2.14151	Ru2-C35 = 2.49360	Ru1-Ru2 = 2.76409
Ru1-C35-Ru2 = 75.87650			

Table S3. The geometries parameters of **1a**, **1b**, **2a**, **3a**, **4a**, **5a**, **6a**, **7a**, **7b**, **8a**, **8b**, **9a**, **9c** and **10a**.

Cluster **1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.231588	-1.239639	1.263145
2	44	0	-0.765892	0.122635	-1.081844
3	44	0	2.190473	-0.043804	-0.635772
4	8	0	1.246790	1.470102	-3.007450
5	8	0	4.942306	0.790622	-1.689455
6	8	0	-2.293337	2.114515	-2.871265
7	8	0	0.368786	-4.257485	0.466908
8	8	0	2.379717	-2.686936	-2.190359
9	6	0	1.003059	0.818659	-2.025179
10	6	0	3.887285	0.470048	-1.273364
11	6	0	2.302804	-1.672506	-1.606957
12	6	0	-1.712488	1.361205	-2.190619
13	6	0	0.365677	-3.130949	0.781837
14	8	0	3.179216	-1.094645	2.355830
15	8	0	-0.835751	-1.588042	4.131517
16	8	0	-1.081071	-2.163939	-3.105678
17	7	0	2.053348	1.717179	0.665877
18	6	0	-1.494161	1.182697	0.853183
19	1	0	-1.869975	2.199394	0.815051
20	6	0	0.859086	1.877030	1.315242
21	6	0	3.044808	2.623224	0.855668
22	1	0	3.964500	2.454744	0.313571
23	6	0	-2.399366	0.070087	0.603758
24	6	0	-0.923090	-1.277651	-2.355107
25	6	0	-0.408996	-1.481312	3.044722
26	6	0	-3.847359	0.305819	0.380839
27	6	0	2.124472	-1.107089	1.835568
28	6	0	-0.149687	0.833202	1.088103
29	7	0	-4.224112	1.599656	0.204053
30	6	0	0.655462	2.972620	2.171837
31	1	0	-0.294871	3.074304	2.681341
32	6	0	1.679317	3.899440	2.366808
33	1	0	1.532312	4.746352	3.027896
34	6	0	2.896328	3.721379	1.698646

35	1	0	3.716913	4.416732	1.823554
36	6	0	-5.526857	1.878663	0.004019
37	1	0	-5.773135	2.925673	-0.136354
38	6	0	-6.518955	0.893238	-0.029706
39	1	0	-7.555177	1.162806	-0.197995
40	6	0	-4.788972	-0.737447	0.378412
41	1	0	-4.478191	-1.760958	0.549382
42	6	0	-6.136741	-0.438028	0.165383
43	1	0	-6.876162	-1.231675	0.157933
44	6	0	-1.740416	-1.183954	0.572342
45	1	0	-2.322823	-2.073421	0.339870

1	Ru	0.131444
2	Ru	-0.148120
3	Ru	0.185299
4	O	-0.382394
5	O	-0.328787
6	O	-0.295735
7	O	-0.288517
8	O	-0.300697
9	C	0.217560
10	C	0.236552
11	C	0.305395
12	C	0.305549
13	C	0.279176
14	O	-0.304487
15	O	-0.309072
16	O	-0.295440
17	N	-0.589798
18	C	-0.145208
19	H	0.198218
20	C	0.270209
21	C	0.103346
22	H	0.191292
23	C	0.049463
24	C	0.294473
25	C	0.248005
26	C	0.178896
27	C	0.304444
28	C	-0.071470
29	N	-0.422504
30	C	-0.100861
31	H	0.170395
32	C	-0.115313

33	H	0.163158
34	C	-0.123384
35	H	0.164207
36	C	0.024537
37	H	0.154515
38	C	-0.108676
39	H	0.148034
40	C	-0.095306
41	H	0.155157
42	C	-0.123450
43	H	0.151038
44	C	-0.226927
45	H	0.145784

Cluster **1b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.743043	-0.827333	-1.201655
2	44	0	1.233030	0.353347	1.029518
3	44	0	-1.125838	1.780209	0.193685
4	8	0	1.791996	-0.135387	-2.367559
5	1	0	2.795234	-0.040756	-2.445720
6	8	0	-1.719467	-3.402210	-2.914175
7	8	0	-4.829748	-0.248461	-1.228477
8	8	0	-1.207940	0.912546	-3.680669
9	8	0	0.725945	0.647335	4.028009
10	8	0	3.080631	2.787420	0.964533
11	8	0	-2.734480	0.305280	2.412506
12	8	0	-3.607544	3.109606	-1.102970
13	8	0	-0.322911	4.058017	2.138735
14	8	0	0.868781	2.810151	-1.996526
15	7	0	-1.886299	-2.049894	0.640423
16	7	0	4.323071	-0.424605	-1.655214
17	6	0	-3.029102	-2.566679	1.158572
18	1	0	-3.949063	-2.305555	0.654205
19	6	0	-3.034399	-3.385190	2.282003
20	1	0	-3.972077	-3.769827	2.662788
21	6	0	-1.813849	-3.688695	2.902239
22	1	0	-1.786658	-4.321834	3.781955
23	6	0	-0.635716	-3.168395	2.376214
24	1	0	0.321446	-3.388331	2.833502
25	6	0	-0.682094	-2.343816	1.239465

26	6	0	0.460436	-1.756437	0.576069
27	6	0	0.239997	-1.040730	-0.670421
28	6	0	1.539735	-0.710328	-1.160727
29	6	0	2.557115	-1.189883	-0.236956
30	6	0	1.879369	-1.836575	0.853121
31	1	0	2.348442	-2.365165	1.669122
32	6	0	3.991719	-1.054407	-0.488869
33	6	0	4.990607	-1.536719	0.375408
34	1	0	4.718671	-2.036441	1.297438
35	6	0	6.330686	-1.355580	0.035851
36	1	0	7.111990	-1.717556	0.695306
37	6	0	6.659157	-0.701470	-1.159232
38	1	0	7.690788	-0.542781	-1.448714
39	6	0	5.620845	-0.253753	-1.976732
40	1	0	5.817160	0.256132	-2.912891
41	6	0	-1.742921	-2.447122	-2.237649
42	6	0	-3.676141	-0.446973	-1.248733
43	6	0	-1.387252	0.287720	-2.707765
44	6	0	0.912750	0.570785	2.864740
45	6	0	2.327936	1.879500	0.996584
46	6	0	-2.127287	0.826740	1.554472
47	6	0	-2.680628	2.568240	-0.631278
48	6	0	-0.583471	3.189318	1.398273
49	6	0	0.126182	2.381353	-1.204445

1	Ru	0.224073
2	Ru	0.051307
3	Ru	-0.110972
4	O	-0.613119
5	H	0.415354
6	O	-0.300046
7	O	-0.284047
8	O	-0.300179
9	O	-0.334435
10	O	-0.330107
11	O	-0.310789
12	O	-0.302697
13	O	-0.297589
14	O	-0.272982
15	N	-0.615698
16	N	-0.548204
17	C	0.111885
18	H	0.178772
19	C	-0.118639

20	H	0.159299
21	C	-0.123256
22	H	0.158683
23	C	-0.093281
24	H	0.161383
25	C	0.302212
26	C	-0.202607
27	C	0.070325
28	C	0.178852
29	C	-0.024262
30	C	-0.096976
31	H	0.160459
32	C	0.249274
33	C	-0.089428
34	H	0.157523
35	C	-0.119985
36	H	0.154119
37	C	-0.119287
38	H	0.152901
39	C	0.058735
40	H	0.165778
41	C	0.254208
42	C	0.286646
43	C	0.279659
44	C	0.249185
45	C	0.268392
46	C	0.323578
47	C	0.240207
48	C	0.260880
49	C	0.334897

Cluster **2a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.349945	-0.660767	1.483114
2	44	0	1.983383	-0.582191	-0.402420
3	44	0	-0.809422	0.115786	-1.244478
4	7	0	2.225779	1.465373	0.338637
5	8	0	1.552390	0.402715	-3.161174
6	8	0	1.592838	-3.538601	-1.143130
7	8	0	-1.785180	1.727173	-3.681240
8	8	0	-1.501125	-2.591642	-2.518545

9	8	0	4.873793	-0.707212	-1.409969
10	6	0	1.093297	0.103754	-2.087559
11	6	0	-1.418558	1.108458	-2.755087
12	6	0	1.079661	2.080878	0.763991
13	6	0	-0.156915	1.288966	0.701534
14	6	0	2.341956	4.064558	1.353494
15	1	0	2.385290	5.072216	1.751837
16	6	0	1.123697	3.390273	1.274520
17	1	0	0.207057	3.852404	1.619903
18	6	0	-1.191812	-1.563031	-2.051562
19	6	0	1.732560	-2.406503	-0.873344
20	6	0	3.766261	-0.654561	-1.012452
21	8	0	-1.628646	0.028686	4.204741
22	6	0	-2.295944	-0.324170	0.666122
23	6	0	-3.843181	1.487625	-0.150457
24	6	0	-2.538901	1.036639	0.238930
25	6	0	3.407641	2.127827	0.410910
26	1	0	4.280783	1.600386	0.053867
27	6	0	1.472283	-0.802279	2.220603
28	6	0	3.505318	3.422354	0.914164
29	1	0	4.471415	3.909222	0.959456
30	6	0	-3.412153	-1.210599	0.670088
31	1	0	-3.282334	-2.240545	0.983543
32	6	0	-1.130504	-0.250745	3.181394
33	6	0	-4.672050	-0.767504	0.299976
34	1	0	-5.513194	-1.453648	0.320090
35	8	0	2.475699	-0.884736	2.830398
36	8	0	-0.862638	-3.740765	1.504068
37	6	0	-1.337226	1.865360	0.202409
38	1	0	-1.375410	2.886012	-0.168890
39	6	0	-4.074714	2.915889	-0.587388
40	1	0	-5.136586	3.094536	-0.779352
41	1	0	-3.529420	3.152064	-1.511216
42	1	0	-3.749539	3.634568	0.175581
43	6	0	-0.639924	-2.591655	1.516744
44	6	0	-4.885109	0.573671	-0.097226
45	1	0	-5.886369	0.894561	-0.368821

1	Ru	0.136232
2	Ru	0.176384
3	Ru	-0.074827
4	N	-0.590155
5	O	-0.387207
6	O	-0.297277

7	O	-0.307185
8	O	-0.293079
9	O	-0.325230
10	C	0.206843
11	C	0.291594
12	C	0.265502
13	C	-0.069908
14	C	-0.114510
15	H	0.163601
16	C	-0.102445
17	H	0.166390
18	C	0.292293
19	C	0.303874
20	C	0.238968
21	O	-0.308858
22	C	0.016045
23	C	0.169308
24	C	-0.013924
25	C	0.104579
26	H	0.191540
27	C	0.311640
28	C	-0.123093
29	H	0.165223
30	C	-0.198663
31	H	0.151292
32	C	0.245755
33	C	-0.084627
34	H	0.138769
35	O	-0.304526
36	O	-0.296191
37	C	-0.202298
38	H	0.159953
39	C	-0.493382
40	H	0.155971
41	H	0.172653
42	H	0.156205
43	C	0.263856
44	C	-0.192367
45	H	0.135280

Cluster **3a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	44	0	0.286848	1.244544	-0.895981
2	44	0	-2.086154	-0.581326	-0.684764
3	44	0	0.497344	-1.128024	0.720893
4	7	0	-2.655681	0.710166	0.993127
5	8	0	-1.929946	-2.931707	1.111394
6	8	0	-1.206769	-2.144342	-3.180022
7	8	0	1.082939	-2.944752	3.138994
8	8	0	1.628029	-3.143350	-1.304709
9	8	0	-4.942847	-1.634336	-1.025823
10	6	0	-1.392008	-1.979135	0.605021
11	6	0	0.866397	-2.254912	2.216035
12	6	0	-1.621225	1.319490	1.651054
13	6	0	-0.269426	1.059430	1.137570
14	6	0	-3.190628	2.414259	3.139733
15	1	0	-3.396244	3.079051	3.971511
16	6	0	-1.877192	2.179251	2.734148
17	1	0	-1.045521	2.664673	3.229898
18	6	0	1.152823	-2.394361	-0.539811
19	6	0	-1.534193	-1.557292	-2.219796
20	6	0	-3.848823	-1.218042	-0.893799
21	8	0	1.478267	4.090192	-0.827553
22	6	0	2.133069	0.635804	-0.010414
23	6	0	3.292414	0.377710	2.180828
24	6	0	2.103773	0.601820	1.436539
25	6	0	-3.931524	0.938271	1.394317
26	1	0	-4.709876	0.426269	0.846544
27	6	0	-1.463686	1.858694	-1.560197
28	6	0	-4.237318	1.782739	2.458159
29	1	0	-5.271110	1.938606	2.740044
30	6	0	3.385332	0.432910	-0.635985
31	1	0	3.487443	0.450062	-1.714406
32	6	0	1.015552	3.014482	-0.873012
33	6	0	4.541876	0.222164	0.113370
34	8	0	-2.416972	2.397288	-1.992887
35	8	0	1.340793	0.365717	-3.699534
36	6	0	0.782922	0.779208	2.025119
37	1	0	0.650657	0.725894	3.104264
38	6	0	0.915107	0.712539	-2.665917
39	6	0	4.500049	0.201596	1.531409
40	1	0	5.402844	0.047626	2.108849
41	1	0	3.252700	0.362622	3.266413
42	8	0	5.706473	0.048468	-0.615444
43	6	0	6.964471	-0.180626	0.077953

44	1	0	6.927177	-1.098636	0.675374
45	1	0	7.704902	-0.287187	-0.713231
46	1	0	7.226832	0.669925	0.717116

1	Ru	0.134110
2	Ru	0.170503
3	Ru	-0.065588
4	N	-0.589136
5	O	-0.388600
6	O	-0.297476
7	O	-0.306084
8	O	-0.292701
9	O	-0.326180
10	C	0.203184
11	C	0.292603
12	C	0.266912
13	C	-0.077076
14	C	-0.114642
15	H	0.162741
16	C	-0.103427
17	H	0.165978
18	C	0.290981
19	C	0.304410
20	C	0.239074
21	O	-0.309889
22	C	0.036133
23	C	-0.103620
24	C	0.029604
25	C	0.104249
26	H	0.191054
27	C	0.311647
28	C	-0.123331
29	H	0.164366
30	C	-0.219811
31	H	0.166729
32	C	0.246893
33	C	0.323446
34	O	-0.305260
35	O	-0.295853
36	C	-0.206925
37	H	0.160432
38	C	0.262018
39	C	-0.152276
40	H	0.144086

41	H	0.148473
42	O	-0.555861
43	C	-0.175778
44	H	0.156497
45	H	0.180217
46	H	0.153171

Cluster **4a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.695124	-0.528836	0.924531
2	44	0	1.875246	0.722002	-0.706754
3	44	0	-0.242778	-1.282430	-0.787323
4	44	0	-0.397749	1.062803	0.774898
5	6	0	4.012402	-0.618187	1.229385
6	1	0	4.688619	-0.030263	0.622371
7	6	0	4.481022	-1.420829	2.266561
8	1	0	5.542737	-1.468160	2.473164
9	6	0	3.556839	-2.156180	3.018975
10	1	0	3.891570	-2.793599	3.829995
11	6	0	2.199541	-2.061734	2.712037
12	1	0	1.460669	-2.627106	3.267150
13	6	0	1.778531	-1.237554	1.653609
14	6	0	0.383914	-1.071906	1.234152
15	6	0	-0.629309	-0.837184	2.176372
16	1	0	-0.435878	-0.780534	3.246584
17	6	0	-1.970361	-0.616088	1.670806
18	6	0	-3.134456	-0.473791	2.472685
19	1	0	-3.066230	-0.587919	3.549820
20	6	0	-4.353704	-0.217531	1.876096
21	1	0	-5.264218	-0.120815	2.451395
22	6	0	-4.408939	-0.068427	0.472648
23	6	0	-3.293597	-0.172751	-0.344757
24	1	0	-3.415510	-0.041318	-1.412278
25	6	0	-2.023286	-0.454046	0.226276
26	6	0	3.313417	0.209912	-1.889996
27	6	0	2.738690	2.324644	-0.113057
28	6	0	0.403152	2.144831	2.079471
29	8	0	4.180804	-0.070434	-2.623999
30	8	0	3.217848	3.331322	0.241623
31	8	0	0.897437	2.783054	2.939266
32	6	0	0.856573	1.562788	-2.083103

33	6	0	-1.156065	-2.957686	-0.518899
34	6	0	-0.950266	-0.918084	-2.572736
35	6	0	1.392431	-2.099156	-1.431199
36	6	0	-1.064915	2.607405	-0.088331
37	8	0	0.309789	2.103062	-2.966911
38	8	0	-1.668261	-3.992154	-0.330565
39	8	0	-1.423840	-0.674137	-3.613592
40	8	0	2.305428	-2.745305	-1.793441
41	8	0	-1.514740	3.573810	-0.583090
42	7	0	-5.711275	0.215663	-0.144563
43	8	0	-5.760304	0.357740	-1.399386
44	8	0	-6.719913	0.298889	0.614335

1	N	-0.569572
2	Ru	0.069192
3	Ru	0.100532
4	Ru	0.073152
5	C	0.099772
6	H	0.184472
7	C	-0.122691
8	H	0.166843
9	C	-0.117177
10	H	0.166589
11	C	-0.099571
12	H	0.168727
13	C	0.269584
14	C	-0.076123
15	C	-0.184249
16	H	0.164963
17	C	0.102028
18	C	-0.110743
19	H	0.155444
20	C	-0.137886
21	H	0.192343
22	C	0.345347
23	C	-0.193882
24	H	0.208756
25	C	-0.109757
26	C	0.254711
27	C	0.261653
28	C	0.252183
29	O	-0.284803
30	O	-0.285330
31	O	-0.323752

32	C	0.303305
33	C	0.261370
34	C	0.259877
35	C	0.297618
36	C	0.267964
37	O	-0.293319
38	O	-0.295872
39	O	-0.282337
40	O	-0.315928
41	O	-0.305283
42	N	0.052911
43	O	-0.282807
44	O	-0.288253

Cluster **5a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.848612	2.387758	-0.391107
2	44	0	0.448553	0.001299	1.530566
3	44	0	-0.008098	-1.759773	-0.602033
4	44	0	1.879232	0.647729	-0.774169
5	8	0	0.871264	2.501584	3.306992
6	8	0	-1.448198	-1.348886	3.561203
7	8	0	2.977867	-1.554630	2.354101
8	8	0	-1.828019	-3.687120	0.961779
9	8	0	-1.050089	-2.486402	-3.427239
10	8	0	2.360819	-3.794314	-0.411835
11	8	0	1.890759	1.820986	-3.633589
12	8	0	3.106526	3.100980	0.638239
13	8	0	4.591557	-0.922850	-0.858797
14	6	0	-0.413983	3.722948	-0.457273
15	1	0	0.647260	3.929086	-0.464818
16	6	0	-1.349520	4.748671	-0.503535
17	1	0	-1.020337	5.780565	-0.548275
18	6	0	-2.728426	4.451342	-0.494255
19	1	0	-3.471500	5.236692	-0.538351
20	6	0	-3.130362	3.129107	-0.434904
21	1	0	-4.170582	2.835418	-0.433172
22	7	0	-2.202356	2.139807	-0.388060
23	6	0	-2.491665	0.618623	-0.307316
24	6	0	-4.858978	-1.262042	-0.267835
25	1	0	-5.693850	-0.551212	-0.369816

26	1	0	-5.302422	-2.263104	-0.211999
27	6	0	-3.269522	0.223799	-1.600157
28	1	0	-4.055478	0.973331	-1.771651
29	1	0	-2.588645	0.266729	-2.456769
30	6	0	-3.942158	-1.159764	-1.499970
31	1	0	-3.179184	-1.943049	-1.449123
32	1	0	-4.511525	-1.336668	-2.420487
33	6	0	-4.076458	-0.959180	1.022580
34	1	0	-4.750789	-0.958382	1.887757
35	1	0	-3.346285	-1.749293	1.208740
36	6	0	-3.383114	0.412909	0.951811
37	1	0	-2.782266	0.598732	1.846106
38	1	0	-4.173956	1.176261	0.931055
39	6	0	-0.118516	1.130856	-0.366888
40	6	0	-1.047652	0.056548	-0.298519
41	6	0	0.716609	1.556179	2.624909
42	6	0	-0.748551	-0.823521	2.773755
43	6	0	2.026453	-0.962004	1.996598
44	6	0	-1.156854	-2.912487	0.388242
45	6	0	-0.643072	-2.221949	-2.359121
46	6	0	1.456318	-3.055928	-0.466792
47	6	0	1.913559	1.348539	-2.559592
48	6	0	2.636804	2.159480	0.115243
49	6	0	3.593712	-0.316854	-0.805022
50	1	0	1.153907	-0.773935	-1.576714

1	C	0.315939
2	Ru	-0.098405
3	Ru	0.039484
4	Ru	0.072082
5	O	-0.320852
6	O	-0.327091
7	O	-0.319158
8	O	-0.321905
9	O	-0.315777
10	O	-0.286958
11	O	-0.317612
12	O	-0.322392
13	O	-0.281877
14	C	-0.109162
15	H	0.195678
16	C	-0.100940
17	H	0.176829
18	C	-0.155914

19	H	0.172631
20	C	0.161369
21	H	0.198832
22	N	-0.651067
23	C	0.065386
24	C	-0.251422
25	H	0.116332
26	H	0.147344
27	C	-0.232742
28	H	0.123776
29	H	0.171007
30	C	-0.256088
31	H	0.165334
32	H	0.144880
33	C	-0.262629
34	H	0.145194
35	H	0.169676
36	C	-0.241259
37	H	0.180565
38	H	0.120473
39	C	-0.123933
40	C	-0.016807
41	C	0.238011
42	C	0.234355
43	C	0.273190
44	C	0.234326
45	C	0.251842
46	C	0.298469
47	C	0.256679
48	C	0.230992
49	C	0.297765
50	H	0.115551

Cluster **6a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.102468	-1.839549	-0.409257
2	44	0	1.061480	0.219387	1.712561
3	44	0	1.622970	0.456479	-1.003426
4	6	0	3.175009	-0.629636	-0.768270
5	8	0	3.338633	-1.516580	2.980105
6	8	0	-2.421038	-3.320666	0.593532

7	8	0	4.161115	-1.260919	-0.658142
8	8	0	2.424980	2.897534	2.388320
9	6	0	1.445015	-3.237506	-0.047889
10	8	0	-0.245673	-2.607589	-3.374214
11	6	0	-0.094803	-2.316416	-2.247733
12	6	0	-1.445759	-2.778470	0.228637
13	6	0	1.918862	1.873518	2.112080
14	6	0	-0.179437	0.227037	3.182878
15	8	0	2.246314	-4.050327	0.201965
16	6	0	1.481147	0.414440	-2.915270
17	6	0	2.498811	-0.848816	2.515563
18	8	0	1.389955	0.393944	-4.088460
19	8	0	2.987908	3.233743	-0.963405
20	6	0	2.471341	2.177514	-0.969280
21	8	0	-0.967812	0.270900	4.049942
22	6	0	-0.664415	0.062384	-0.697586
23	6	0	-0.209012	1.019635	0.247122
24	6	0	-0.873650	2.283324	-0.042850
25	6	0	-1.717423	0.688357	-1.606484
26	1	0	-1.404823	0.705098	-2.656156
27	7	0	-1.727989	2.128221	-1.120926
28	6	0	-0.797210	3.553188	0.557185
29	1	0	-0.144838	3.693261	1.408296
30	6	0	-1.541220	4.604453	0.036033
31	1	0	-1.477734	5.587061	0.489632
32	6	0	-2.451463	3.145826	-1.650691
33	1	0	-3.073294	2.914140	-2.505347
34	6	0	-2.374890	4.406157	-1.086875
35	1	0	-2.953050	5.219012	-1.505570
36	6	0	-3.128134	0.060806	-1.507987
37	1	0	-3.787259	0.552208	-2.238853
38	1	0	-3.023772	-0.978821	-1.842179
39	6	0	-3.782293	0.097132	-0.116594
40	1	0	-3.114007	-0.365914	0.619677
41	1	0	-3.926055	1.140109	0.202779
42	6	0	-5.142165	-0.626523	-0.097818
43	1	0	-4.997387	-1.675108	-0.397113
44	1	0	-5.807888	-0.176475	-0.851187
45	6	0	-5.832176	-0.586249	1.277888
46	1	0	-5.171902	-1.049418	2.024636
47	1	0	-5.963538	0.461301	1.587713
48	6	0	-7.194318	-1.297904	1.283324
49	1	0	-7.887595	-0.831341	0.571512
50	1	0	-7.659184	-1.261761	2.275016

51	1	0	-7.088446	-2.353237	1.002116
52	1	0	0.266399	-1.349409	1.317444

1	Ru	0.046574
2	Ru	0.081566
3	Ru	-0.089707
4	C	0.269819
5	O	-0.285252
6	O	-0.319605
7	O	-0.316525
8	O	-0.324555
9	C	0.296828
10	O	-0.314705
11	C	0.244696
12	C	0.249796
13	C	0.230876
14	C	0.254859
15	O	-0.283005
16	C	0.232415
17	C	0.298719
18	O	-0.323671
19	O	-0.320171
20	C	0.241057
21	O	-0.315559
22	C	-0.067530
23	C	-0.102003
24	C	0.315239
25	C	-0.044330
26	H	0.204183
27	N	-0.642982
28	C	-0.112576
29	H	0.197388
30	C	-0.101347
31	H	0.176658
32	C	0.160827
33	H	0.198892
34	C	-0.153126
35	H	0.173366
36	C	-0.246978
37	H	0.131052
38	H	0.182636
39	C	-0.263087
40	H	0.174999
41	H	0.123758

42	C	-0.238406
43	H	0.143553
44	H	0.117020
45	C	-0.241644
46	H	0.142246
47	H	0.120767
48	C	-0.407007
49	H	0.129045
50	H	0.135884
51	H	0.139069
52	H	0.099984

Cluster **7a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.378608	-0.050354	-1.325588
2	44	0	1.155064	-0.170698	1.532297
3	44	0	-0.682400	1.642590	0.046794
4	35	0	-6.041602	-1.171136	-0.108813
5	8	0	-0.598020	1.653412	-2.914728
6	8	0	1.269559	3.997441	0.323176
7	7	0	-2.077665	-2.482493	-0.077530
8	7	0	-2.018120	-0.093850	0.030271
9	6	0	0.532470	3.094267	0.206001
10	8	0	1.633175	-2.360817	3.655751
11	8	0	1.524659	-0.978548	-4.259258
12	6	0	-3.370118	-0.054021	-0.009383
13	1	0	-3.844216	0.917105	-0.001759
14	6	0	1.451894	-1.516178	2.866148
15	6	0	-4.112203	-1.230089	-0.069686
16	6	0	-3.423305	-2.443493	-0.117217
17	1	0	-3.943890	-3.390733	-0.191288
18	6	0	1.475090	-0.625882	-3.143314
19	6	0	-0.147239	1.254541	-1.870971
20	6	0	-1.396477	-1.317147	0.015868
21	8	0	3.182822	1.944644	2.600618
22	8	0	-1.263448	0.929391	3.200290
23	8	0	-2.990627	3.593388	-0.471148
24	6	0	0.060147	-1.323374	0.128023
25	6	0	0.813279	-2.224928	-0.638014
26	1	0	0.353473	-2.937623	-1.317647
27	6	0	2.255662	-2.188395	-0.445744

28	6	0	-2.108904	2.839759	-0.268793
29	6	0	2.714062	-1.130369	0.428870
30	6	0	2.396375	1.163781	2.224174
31	6	0	-0.390797	0.587782	2.488267
32	6	0	4.125775	-1.009262	0.598754
33	1	0	4.523146	-0.233641	1.244618
34	6	0	2.658430	1.334174	-1.590155
35	8	0	3.498065	2.137172	-1.733801
36	6	0	3.171763	-3.069785	-1.084553
37	6	0	4.527813	-2.922428	-0.862437
38	1	0	5.233318	-3.601734	-1.329152
39	6	0	5.004739	-1.881123	-0.027371
40	1	0	6.073358	-1.771543	0.128760
41	1	0	2.795197	-3.860963	-1.726412

1	Ru	-0.076221
2	Ru	0.139565
3	Ru	0.171639
4	Br	0.235696
5	O	-0.382446
6	O	-0.294036
7	N	-0.344237
8	N	-0.541434
9	C	0.307488
10	O	-0.300090
11	O	-0.299189
12	C	0.157528
13	H	0.217335
14	C	0.249318
15	C	-0.324905
16	C	0.072894
17	H	0.194387
18	C	0.293165
19	C	0.203467
20	C	0.339601
21	O	-0.294609
22	O	-0.302692
23	O	-0.319672
24	C	-0.041908
25	C	-0.172488
26	H	0.180248
27	C	0.038550
28	C	0.234524
29	C	0.007822

30	C	0.263134
31	C	0.310085
32	C	-0.196037
33	H	0.154400
34	C	0.294452
35	O	-0.289741
36	C	-0.086764
37	C	-0.145838
38	H	0.144884
39	C	-0.092234
40	H	0.142977
41	H	0.151383

Cluster **7b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.198276	0.051503	1.394128
2	44	0	0.141010	-1.100929	-1.232926
3	44	0	-1.859928	-2.025912	0.791631
4	35	0	-7.052029	0.300613	-1.260232
5	8	0	-2.009532	-0.688703	3.434703
6	8	0	-0.019072	-4.299135	1.726742
7	7	0	-3.055253	1.491080	-1.469567
8	7	0	-3.115455	-0.495976	-0.142587
9	6	0	-0.718269	-3.422574	1.385777
10	8	0	0.894678	-0.082558	-4.047156
11	8	0	0.269979	1.957994	3.807339
12	6	0	-4.459946	-0.561265	-0.294604
13	1	0	-4.979078	-1.382348	0.178442
14	6	0	0.615812	-0.491854	-2.987814
15	6	0	-5.134651	0.397114	-1.043024
16	6	0	-4.387445	1.414969	-1.640092
17	1	0	-4.851069	2.175463	-2.256603
18	6	0	0.250572	1.248061	2.875390
19	6	0	-1.464797	-0.831294	2.370283
20	6	0	-2.440412	0.549536	-0.718929
21	8	0	2.084597	-3.547744	-1.164791
22	8	0	-2.198242	-2.794835	-2.462613
23	8	0	-4.299296	-3.542258	1.855862
24	6	0	-0.985336	0.558089	-0.568346
25	6	0	-0.273860	1.727542	-0.199534
26	6	0	1.187499	1.541702	-0.185618

27	6	0	-3.363071	-2.961559	1.437708
28	6	0	1.602992	0.211218	-0.467337
29	6	0	1.343506	-2.644599	-1.205742
30	6	0	-1.365851	-2.193126	-1.888184
31	6	0	1.383405	-1.140503	2.290909
32	8	0	2.134239	-1.857519	2.828560
33	6	0	-0.923916	3.050482	0.060052
34	6	0	-0.642554	4.133338	-0.793579
35	6	0	-1.855070	3.232434	1.097871
36	6	0	-1.275506	5.365429	-0.609620
37	1	0	0.067433	4.008272	-1.603589
38	6	0	-2.486757	4.466287	1.281334
39	1	0	-2.080642	2.408594	1.767751
40	6	0	-2.198303	5.537449	0.428657
41	1	0	-1.046965	6.189685	-1.277523
42	1	0	-3.195554	4.590305	2.093779
43	1	0	-2.684304	6.496834	0.573804
44	6	0	2.147425	2.678702	-0.029450
45	6	0	3.039640	2.933633	-1.091439
46	6	0	2.174256	3.529770	1.088893
47	6	0	3.937850	4.003374	-1.029725
48	1	0	3.020204	2.297944	-1.970944
49	6	0	3.077965	4.593899	1.152055
50	1	0	1.497110	3.363012	1.916030
51	6	0	3.962923	4.835029	0.094753
52	1	0	4.613915	4.185053	-1.859076
53	1	0	3.089623	5.233291	2.028726
54	1	0	4.662914	5.662665	0.146828
55	6	0	3.049735	-0.125324	-0.469431
56	6	0	4.905549	-0.829636	-1.670438
57	6	0	5.061442	-0.341481	0.664627
58	6	0	5.683923	-0.744462	-0.516533
59	1	0	5.323316	-1.144696	-2.619006
60	1	0	5.602928	-0.269308	1.600028
61	7	0	3.749862	-0.028862	0.688712
62	7	0	3.591262	-0.528523	-1.647494
63	35	0	7.569863	-1.187702	-0.550885

1	Ru	-0.085800
2	Ru	0.178188
3	Ru	0.196648
4	Br	0.228919
5	O	-0.382324

6	O	-0.295505
7	N	-0.324990
8	N	-0.541722
9	C	0.303469
10	O	-0.302216
11	O	-0.306793
12	C	0.156466
13	H	0.216111
14	C	0.262952
15	C	-0.325031
16	C	0.074594
17	H	0.192700
18	C	0.271815
19	C	0.213319
20	C	0.326032
21	O	-0.291226
22	O	-0.306068
23	O	-0.324556
24	C	-0.028978
25	C	-0.063667
26	C	-0.003040
27	C	0.232274
28	C	-0.050541
29	C	0.279270
30	C	0.303391
31	C	0.299342
32	O	-0.291682
33	C	0.065246
34	C	-0.102987
35	C	-0.148472
36	C	-0.136936
37	H	0.148528
38	C	-0.138328
39	H	0.161276
40	C	-0.114595
41	H	0.133675
42	H	0.137326
43	H	0.132226
44	C	0.053184
45	C	-0.152674
46	C	-0.108340
47	C	-0.134921
48	H	0.165603
49	C	-0.141333

50	H	0.154781
51	C	-0.112560
52	H	0.134662
53	H	0.138659
54	H	0.133743
55	C	0.165734
56	C	0.075956
57	C	0.078652
58	C	-0.298213
59	H	0.185746
60	H	0.187673
61	N	-0.327715
62	N	-0.339763
63	Br	0.192818

Cluster **8a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.069060	0.106860	-1.330887
2	44	0	0.873984	0.053813	1.535993
3	44	0	-1.133515	1.635718	0.001436
4	35	0	-6.190094	-1.700643	-0.075792
5	8	0	-1.057586	1.568052	-2.961189
6	8	0	0.583925	4.174042	0.195472
7	7	0	-2.115224	-2.609514	-0.008276
8	7	0	-2.293926	-0.224413	0.036267
9	6	0	-0.065119	3.202231	0.110832
10	8	0	1.531537	-2.011964	3.734671
11	8	0	1.300042	-0.896788	-4.234558
12	6	0	-3.642829	-0.320331	-0.003955
13	1	0	-4.211431	0.598523	-0.021765
14	6	0	1.276994	-1.214076	2.916800
15	6	0	-4.264096	-1.565666	-0.034007
16	6	0	-3.457848	-2.705127	-0.049970
17	1	0	-3.881429	-3.700988	-0.099909
18	6	0	1.218034	-0.514966	-3.129577
19	6	0	-0.568792	1.245723	-1.907986
20	6	0	-1.552922	-1.379911	0.054465
21	8	0	2.694665	2.381793	2.532372
22	8	0	-1.636879	0.985451	3.169870
23	8	0	-3.626175	3.333338	-0.549198
24	6	0	-0.104120	-1.237449	0.164203

25	6	0	0.738478	-2.084623	-0.571719
26	1	0	0.354305	-2.861548	-1.227572
27	6	0	2.167351	-1.898526	-0.381765
28	6	0	-2.672868	2.675913	-0.334772
29	6	0	2.530342	-0.801355	0.492962
30	6	0	1.985697	1.518986	2.182687
31	6	0	-0.739579	0.702733	2.462057
32	6	0	3.910324	-0.555211	0.681240
33	1	0	4.259756	0.244205	1.323442
34	6	0	2.221399	1.594458	-1.632462
35	8	0	2.988020	2.463748	-1.797572
36	6	0	3.168626	-2.688482	-1.008385
37	6	0	4.506254	-2.426595	-0.782370
38	1	0	5.261303	-3.045662	-1.250007
39	6	0	4.876414	-1.345971	0.060707
40	1	0	2.876761	-3.513612	-1.651626
41	8	0	6.190545	-1.009645	0.331305
42	6	0	7.272709	-1.777333	-0.266801
43	1	0	7.241435	-1.721681	-1.360645
44	1	0	8.184050	-1.307065	0.098930
45	1	0	7.241875	-2.824169	0.055610

1	Ru	-0.069148
2	Ru	0.141061
3	Ru	0.166432
4	Br	0.232778
5	O	-0.383957
6	O	-0.294484
7	N	-0.345676
8	N	-0.540582
9	C	0.307613
10	O	-0.302540
11	O	-0.302345
12	C	0.157003
13	H	0.216860
14	C	0.250693
15	C	-0.324711
16	C	0.072582
17	H	0.193080
18	C	0.290897
19	C	0.200872
20	C	0.340270
21	O	-0.294145
22	O	-0.303647

23	O	-0.321427
24	C	-0.050176
25	C	-0.171444
26	H	0.178643
27	C	0.029285
28	C	0.234111
29	C	0.031467
30	C	0.262915
31	C	0.310782
32	C	-0.219340
33	H	0.167931
34	C	0.291731
35	O	-0.289704
36	C	-0.099487
37	C	-0.152263
38	H	0.146598
39	C	0.325177
40	H	0.153821
41	O	-0.554920
42	C	-0.176973
43	H	0.157519
44	H	0.181710
45	H	0.155141

Cluster **8b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.137893	-0.257662	1.359246
2	44	0	0.042520	-1.600247	-1.168731
3	44	0	-1.995713	-2.291397	0.913315
4	35	0	-7.093615	0.068897	-1.335114
5	8	0	-2.108313	-0.736857	3.437906
6	8	0	-0.262334	-4.560899	2.042107
7	7	0	-3.052373	1.079505	-1.623536
8	7	0	-3.192133	-0.792211	-0.143896
9	6	0	-0.915617	-3.681815	1.624477
10	8	0	0.821148	-0.831105	-4.054209
11	8	0	0.310388	1.828782	3.613004
12	6	0	-4.537693	-0.817572	-0.296530
13	1	0	-5.088829	-1.578746	0.236651
14	6	0	0.532120	-1.145893	-2.965717
15	6	0	-5.173318	0.104613	-1.120473

16	6	0	-4.385921	1.040906	-1.794690
17	1	0	-4.818378	1.765548	-2.473908
18	6	0	0.250608	1.046864	2.741486
19	6	0	-1.562679	-0.989195	2.394297
20	6	0	-2.475804	0.178316	-0.796641
21	8	0	1.905093	-4.097209	-0.914101
22	8	0	-2.353052	-3.303526	-2.268786
23	8	0	-4.498903	-3.628486	2.066291
24	6	0	-1.022523	0.145327	-0.636897
25	6	0	-0.271538	1.313762	-0.353893
26	6	0	1.183713	1.080483	-0.325538
27	6	0	-3.537560	-3.118115	1.613908
28	6	0	1.550403	-0.282768	-0.503202
29	6	0	1.193735	-3.175830	-1.023118
30	6	0	-1.501924	-2.687784	-1.737836
31	6	0	1.276707	-1.428848	2.340757
32	8	0	2.001133	-2.134785	2.927473
33	6	0	-0.875744	2.672337	-0.195302
34	6	0	-0.566586	3.681285	-1.132208
35	6	0	-1.795996	2.971626	0.820036
36	6	0	-1.156348	4.937572	-1.051534
37	1	0	0.135256	3.474002	-1.932065
38	6	0	-2.394771	4.233436	0.913870
39	1	0	-2.049541	2.216388	1.557261
40	6	0	-2.072547	5.219899	-0.026039
41	1	0	-0.925530	5.715596	-1.769409
42	1	0	-3.091882	4.430132	1.718864
43	6	0	2.180995	2.188291	-0.249607
44	6	0	3.118625	2.314247	-1.300289
45	6	0	2.212407	3.144445	0.777244
46	6	0	4.051233	3.345891	-1.314354
47	1	0	3.103691	1.602585	-2.119145
48	6	0	3.151289	4.180105	0.779644
49	1	0	1.507165	3.087358	1.595810
50	6	0	4.075002	4.281714	-0.269273
51	1	0	4.766883	3.449467	-2.121277
52	1	0	3.151304	4.890843	1.596401
53	6	0	2.983358	-0.673625	-0.477715
54	6	0	4.806825	-1.542380	-1.620429
55	6	0	4.985794	-0.890902	0.672472
56	6	0	5.589233	-1.406306	-0.474304
57	1	0	5.209618	-1.943516	-2.542644
58	1	0	5.531224	-0.773155	1.600885
59	7	0	3.688790	-0.521654	0.671347

60	7	0	3.506738	-1.184212	-1.622132
61	35	0	7.454377	-1.931327	-0.471496
62	8	0	5.045693	5.267108	-0.367643
63	8	0	-2.600071	6.504413	-0.028905
64	6	0	-3.548709	6.875042	1.006991
65	1	0	-3.096147	6.805546	2.003065
66	1	0	-3.812799	7.909930	0.793770
67	1	0	-4.446981	6.247837	0.966553
68	6	0	5.136329	6.273310	0.677354
69	1	0	4.211380	6.857320	0.746862
70	1	0	5.358838	5.816834	1.648709
71	1	0	5.959214	6.920488	0.377199

1	Ru	-0.088699
2	Ru	0.179194
3	Ru	0.193747
4	Br	0.225882
5	O	-0.384233
6	O	-0.296387
7	N	-0.324232
8	N	-0.540647
9	C	0.302803
10	O	-0.302137
11	O	-0.311056
12	C	0.155907
13	H	0.215689
14	C	0.262843
15	C	-0.325124
16	C	0.073495
17	H	0.192309
18	C	0.270118
19	C	0.213052
20	C	0.325480
21	O	-0.292359
22	O	-0.307158
23	O	-0.326356
24	C	-0.027538
25	C	-0.064622
26	C	0.002504
27	C	0.231821
28	C	-0.051113
29	C	0.279073
30	C	0.301898
31	C	0.297814

32	O	-0.292765
33	C	0.067223
34	C	-0.107794
35	C	-0.164327
36	C	-0.136011
37	H	0.151016
38	C	-0.148167
39	H	0.162581
40	C	0.290355
41	H	0.147273
42	H	0.139154
43	C	0.059753
44	C	-0.159181
45	C	-0.124131
46	C	-0.132983
47	H	0.166910
48	C	-0.149201
49	H	0.155451
50	C	0.293558
51	H	0.148252
52	H	0.140164
53	C	0.164350
54	C	0.076127
55	C	0.078356
56	C	-0.297441
57	H	0.185603
58	H	0.186403
59	N	-0.327293
60	N	-0.339985
61	Br	0.191888
62	O	-0.558818
63	O	-0.559960
64	C	-0.172706
65	H	0.153268
66	H	0.173443
67	H	0.150113
68	C	-0.173967
69	H	0.153528
70	H	0.153874
71	H	0.174118

Cluster **9a**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	44	0	1.356404	-0.190210	-1.235489
2	44	0	1.056423	0.356911	1.567760
3	44	0	-0.828160	1.659045	-0.340885
4	35	0	-6.028080	-1.410415	0.125906
5	8	0	-0.669746	0.958103	-3.216012
6	8	0	0.985817	4.120900	-0.623603
7	7	0	-2.001741	-2.447299	0.511707
8	7	0	-2.071981	-0.102521	0.047453
9	6	0	0.301192	3.175247	-0.525726
10	8	0	1.584045	-1.245050	4.152605
11	8	0	1.650867	-1.765893	-3.865367
12	6	0	-3.422839	-0.149861	-0.014599
13	1	0	-3.947439	0.766998	-0.242766
14	6	0	1.382720	-0.617921	3.184941
15	6	0	-4.099712	-1.347250	0.198836
16	6	0	-3.346196	-2.495787	0.448689
17	1	0	-3.813961	-3.461786	0.596231
18	6	0	1.544383	-1.164953	-2.864869
19	6	0	-0.223440	0.851568	-2.101986
20	6	0	-1.386008	-1.255718	0.332753
21	8	0	2.939281	2.780088	2.131182
22	8	0	-1.459363	1.686162	2.890896
23	8	0	-3.225391	3.291058	-1.334355
24	6	0	0.065383	-1.149989	0.460916
25	6	0	0.883333	-2.163210	-0.062263
26	1	0	0.468267	-3.034270	-0.558754
27	6	0	2.318752	-2.003538	0.130284
28	6	0	-2.308832	2.661150	-0.947648
29	6	0	2.691784	-0.747587	0.748241
30	6	0	2.207663	1.886513	1.940794
31	6	0	-0.551762	1.235693	2.292330
32	6	0	4.085060	-0.496201	0.914035
33	1	0	4.416144	0.428524	1.373561
34	6	0	2.573435	1.167228	-1.784924
35	8	0	3.378806	1.959438	-2.091505
36	6	0	3.299104	-2.964378	-0.286485
37	6	0	4.634123	-2.658848	-0.069702
38	1	0	5.395949	-3.376823	-0.357812
39	6	0	5.026630	-1.431624	0.516152
40	1	0	6.083298	-1.228175	0.660046
41	6	0	2.885552	-4.270907	-0.923435
42	1	0	3.757787	-4.904162	-1.107860
43	1	0	2.384052	-4.111679	-1.887404

44	1	0	2.192962	-4.834391	-0.285817

1	Ru	-0.078809
2	Ru	0.142951
3	Ru	0.172044
4	Br	0.235103
5	O	-0.382832
6	O	-0.294120
7	N	-0.345098
8	N	-0.541523
9	C	0.307247
10	O	-0.301420
11	O	-0.303160
12	C	0.157657
13	H	0.217400
14	C	0.249089
15	C	-0.325043
16	C	0.072885
17	H	0.193853
18	C	0.290468
19	C	0.204268
20	C	0.339415
21	O	-0.294783
22	O	-0.302856
23	O	-0.320418
24	C	-0.041678
25	C	-0.167992
26	H	0.177427
27	C	-0.013140
28	C	0.234696
29	C	0.011134
30	C	0.264760
31	C	0.310949
32	C	-0.198512
33	H	0.152486
34	C	0.293279
35	O	-0.289922
36	C	0.171303
37	C	-0.192591
38	H	0.137717
39	C	-0.083497
40	H	0.140967
41	C	-0.493753
42	H	0.155956

43	H	0.172788
44	H	0.165303

Cluster **9c**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.728111	2.080942	-0.141377
2	44	0	-0.817558	-1.993109	-0.126732
3	35	0	-5.916747	1.321688	-0.269137
4	44	0	1.120997	-0.312838	1.216090
5	6	0	-0.306470	-0.194616	2.415731
6	8	0	-1.180319	-0.040803	3.190802
7	7	0	-2.043204	-0.207802	-0.307807
8	7	0	-1.831420	2.161943	-0.528878
9	8	0	1.308699	-4.141569	0.477443
10	8	0	-2.768508	-3.223467	2.005255
11	6	0	0.161292	0.722721	-0.561654
12	6	0	-1.275350	0.932412	-0.459902
13	6	0	1.983100	-0.792274	-1.168669
14	6	0	0.543615	-0.621277	-0.919694
15	6	0	2.602968	-1.872100	-1.877261
16	6	0	0.524394	-3.303013	0.246863
17	6	0	-2.025115	-2.803146	1.207826
18	8	0	-0.077360	4.463264	0.809140
19	8	0	2.961748	-1.659934	3.290671
20	6	0	-3.386988	-0.094504	-0.251369
21	1	0	-3.963463	-1.001679	-0.129579
22	8	0	4.307928	3.462971	0.952660
23	6	0	4.183925	0.059180	-0.494166
24	1	0	4.808148	0.790483	0.006933
25	6	0	-3.170212	2.278141	-0.469360
26	1	0	-3.580448	3.279266	-0.522756
27	6	0	2.244019	-1.145799	2.517300
28	6	0	2.774645	0.246278	-0.550229
29	6	0	3.331445	2.970161	0.539560
30	6	0	4.776432	-1.023002	-1.126666
31	1	0	5.855522	-1.140538	-1.107390
32	8	0	1.948031	2.954661	-3.082584
33	6	0	1.824355	-2.848960	-2.733546
34	1	0	2.465039	-3.234116	-3.533489
35	1	0	0.955094	-2.376808	-3.198316
36	1	0	1.467651	-3.716907	-2.168447

37	6	0	0.559911	3.563957	0.428066
38	6	0	3.991989	-1.948170	-1.847720
39	1	0	4.485630	-2.739074	-2.404752
40	6	0	1.870222	2.646600	-1.956454
41	8	0	-1.916847	-3.318107	-2.685824
42	6	0	-3.992240	1.155429	-0.340931
43	6	0	-1.546568	-2.796209	-1.704092
44	1	0	1.643941	1.334493	1.600883

1	Ru	0.063315
2	Ru	0.197689
3	Br	0.222290
4	Ru	-0.108303
5	C	0.277894
6	O	-0.328629
7	N	-0.558148
8	N	-0.354878
9	O	-0.298141
10	O	-0.276846
11	C	-0.004514
12	C	0.355563
13	C	0.001307
14	C	-0.155971
15	C	0.152115
16	C	0.299382
17	C	0.253168
18	O	-0.289832
19	O	-0.306102
20	C	0.151178
21	H	0.207278
22	O	-0.295787
23	C	-0.195318
24	H	0.147462
25	C	0.080287
26	H	0.194873
27	C	0.284772
28	C	-0.009291
29	C	0.287122
30	C	-0.084073
31	H	0.140054
32	O	-0.307345
33	C	-0.492238
34	H	0.153711
35	H	0.173987

36	H	0.168450
37	C	0.315648
38	C	-0.182916
39	H	0.138053
40	C	0.243445
41	O	-0.300150
42	C	-0.329479
43	C	0.243203
44	H	0.125712

Cluster **10a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.101379	-0.686470	1.780554
2	44	0	0.158134	-2.126249	-0.564627
3	35	0	7.319870	-1.915746	0.528903
4	26	0	3.042722	2.868390	-1.232443
5	35	0	-6.871751	-2.254836	-1.813968
6	26	0	-3.375345	2.709809	0.722402
7	6	0	-2.000385	4.238595	0.522484
8	1	0	-2.046341	5.186987	1.034097
9	6	0	-1.499677	2.018343	0.011430
10	6	0	-2.585263	3.936406	-0.753964
11	1	0	-3.150969	4.617781	-1.370240
12	6	0	0.778624	0.816096	0.003089
13	6	0	1.374703	-0.479586	0.063477
14	6	0	-1.345755	3.059530	0.999225
15	1	0	-0.783237	2.969103	1.914817
16	6	0	-2.294948	2.569159	-1.065606
17	1	0	-2.575261	2.030074	-1.955439
18	6	0	-1.224328	-0.542484	-0.212574
19	6	0	-0.699507	0.770786	-0.062573
20	8	0	1.824848	-0.200345	4.146895
21	7	0	-3.107188	-0.436618	-1.724045
22	7	0	-3.346983	-1.622551	0.345134
23	8	0	-2.009394	-4.317462	-1.117549
24	7	0	3.455391	-0.555077	1.361020
25	7	0	3.467981	-1.212365	-0.935040
26	6	0	-2.634589	-0.846686	-0.514508
27	6	0	1.507387	2.102899	-0.005896
28	6	0	2.834396	-0.727324	0.165961
29	6	0	-1.196747	-3.509558	-0.891177

30	6	0	1.119528	-0.386058	3.230690
31	8	0	-2.437487	-0.235148	3.740793
32	8	0	2.434271	-4.281570	-0.493604
33	6	0	-1.558167	-0.403504	2.983145
34	6	0	1.582988	-3.482778	-0.517889
35	6	0	4.756011	-0.898218	1.466723
36	1	0	5.223756	-0.762348	2.434552
37	6	0	-4.578524	-2.023119	-0.031218
38	1	0	-5.131367	-2.639512	0.667329
39	6	0	-4.336712	-0.845354	-2.096034
40	1	0	-4.695096	-0.515631	-3.064167
41	6	0	-5.402913	3.191425	0.756911
42	1	0	-5.901170	3.877078	0.089652
43	6	0	-4.540156	1.247355	1.684366
44	1	0	-4.280270	0.215606	1.844218
45	6	0	-4.792870	3.529114	2.011210
46	1	0	-4.749410	4.513841	2.449443
47	8	0	-0.243358	-3.681206	2.397413
48	8	0	0.628830	-1.291508	-3.486743
49	6	0	2.667800	2.459429	0.785518
50	1	0	3.190780	1.795046	1.451570
51	6	0	2.930761	3.852277	0.600700
52	1	0	3.719018	4.411816	1.079351
53	6	0	1.095933	3.303202	-0.704115
54	1	0	0.262206	3.385333	-1.379678
55	6	0	3.622098	1.497318	-2.709313
56	1	0	3.245546	0.493879	-2.822980
57	6	0	-4.257765	2.327231	2.582912
58	1	0	-3.745847	2.240685	3.527483
59	6	0	5.456607	-1.407664	0.374993
60	6	0	-5.110943	-1.657586	-1.267181
61	6	0	3.079194	2.678943	-3.312512
62	1	0	2.225908	2.717527	-3.971008
63	6	0	1.959057	4.374479	-0.316166
64	1	0	1.892171	5.394447	-0.660419
65	6	0	-0.146482	-2.631674	1.858136
66	6	0	4.770266	-1.544157	-0.832022
67	1	0	5.254377	-1.927300	-1.722454
68	6	0	0.441993	-1.628311	-2.383460
69	6	0	3.878337	3.797189	-2.898090
70	1	0	3.729311	4.825396	-3.188211
71	6	0	-5.244922	1.780293	0.553608
72	1	0	-5.616044	1.219846	-0.288794
73	6	0	4.755480	1.884951	-1.917290

74	1	0	5.393865	1.226132	-1.351846
75	6	0	4.914983	3.306608	-2.035868
76	1	0	5.685836	3.899866	-1.569613

1	Ru	0.075949
2	Ru	0.088330
3	Br	0.197348
4	Fe	0.553191
5	Br	0.193078
6	Fe	0.560936
7	C	-0.195591
8	H	0.152692
9	C	-0.188376
10	C	-0.202894
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12	C	0.159748
13	C	-0.105801
14	C	-0.147985
15	H	0.168996
16	C	-0.152478
17	H	0.181069
18	C	-0.022795
19	C	-0.043597
20	O	-0.311975
21	N	-0.337324
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23	O	-0.291032
24	N	-0.354956
25	N	-0.351738
26	C	0.178125
27	C	-0.183651
28	C	0.204253
29	C	0.288457
30	C	0.289380
31	O	-0.316819
32	O	-0.287993
33	C	0.275915
34	C	0.298641
35	C	0.073259
36	H	0.189495
37	C	0.072326
38	H	0.188691
39	C	0.063064

40	H	0.181084
41	C	-0.197559
42	H	0.152890
43	C	-0.216688
44	H	0.173145
45	C	-0.197133
46	H	0.153290
47	O	-0.336316
48	O	-0.300176
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50	H	0.182995
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57	C	-0.201654
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65	C	0.286521
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67	H	0.188332
68	C	0.264082
69	C	-0.197137
70	H	0.152703
71	C	-0.208453
72	H	0.143764
73	C	-0.217416
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75	C	-0.197172
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Cluster **10b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	44	0	0.158134	-2.126249	-0.564627
3	35	0	7.319870	-1.915746	0.528903
4	26	0	3.042722	2.868390	-1.232443
5	35	0	-6.871751	-2.254836	-1.813968
6	26	0	-3.375345	2.709809	0.722402
7	6	0	-2.000385	4.238595	0.522484
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9	6	0	-1.499677	2.018343	0.011430
10	6	0	-2.585263	3.936406	-0.753964
11	1	0	-3.150969	4.617781	-1.370240
12	6	0	0.778624	0.816096	0.003089
13	6	0	1.374703	-0.479586	0.063477
14	6	0	-1.345755	3.059530	0.999225
15	1	0	-0.783237	2.969103	1.914817
16	6	0	-2.294948	2.569159	-1.065606
17	1	0	-2.575261	2.030074	-1.955439
18	6	0	-1.224328	-0.542484	-0.212574
19	6	0	-0.699507	0.770786	-0.062573
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21	7	0	-3.107188	-0.436618	-1.724045
22	7	0	-3.346983	-1.622551	0.345134
23	8	0	-2.009394	-4.317462	-1.117549
24	7	0	3.455391	-0.555077	1.361020
25	7	0	3.467981	-1.212365	-0.935040
26	6	0	-2.634589	-0.846686	-0.514508
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28	6	0	2.834396	-0.727324	0.165961
29	6	0	-1.196747	-3.509558	-0.891177
30	6	0	1.119528	-0.386058	3.230690
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32	8	0	2.434271	-4.281570	-0.493604
33	6	0	-1.558167	-0.403504	2.983145
34	6	0	1.582988	-3.482778	-0.517889
35	6	0	4.756011	-0.898218	1.466723
36	1	0	5.223756	-0.762348	2.434552
37	6	0	-4.578524	-2.023119	-0.031218
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39	6	0	-4.336712	-0.845354	-2.096034
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41	6	0	-5.402913	3.191425	0.756911
42	1	0	-5.901170	3.877078	0.089652
43	6	0	-4.540156	1.247355	1.684366
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45	6	0	-4.792870	3.529114	2.011210

46	1	0	-4.749410	4.513841	2.449443
47	8	0	-0.243358	-3.681206	2.397413
48	8	0	0.628830	-1.291508	-3.486743
49	6	0	2.667800	2.459429	0.785518
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56	1	0	3.245546	0.493879	-2.822980
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63	6	0	1.959057	4.374479	-0.316166
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66	6	0	4.770266	-1.544157	-0.832022
67	1	0	5.254377	-1.927300	-1.722454
68	6	0	0.441993	-1.628311	-2.383460
69	6	0	3.878337	3.797189	-2.898090
70	1	0	3.729311	4.825396	-3.188211
71	6	0	-5.244922	1.780293	0.553608
72	1	0	-5.616044	1.219846	-0.288794
73	6	0	4.755480	1.884951	-1.917290
74	1	0	5.393865	1.226132	-1.351846
75	6	0	4.914983	3.306608	-2.035868
76	1	0	5.685836	3.899866	-1.569613

1	Ru	0.075949
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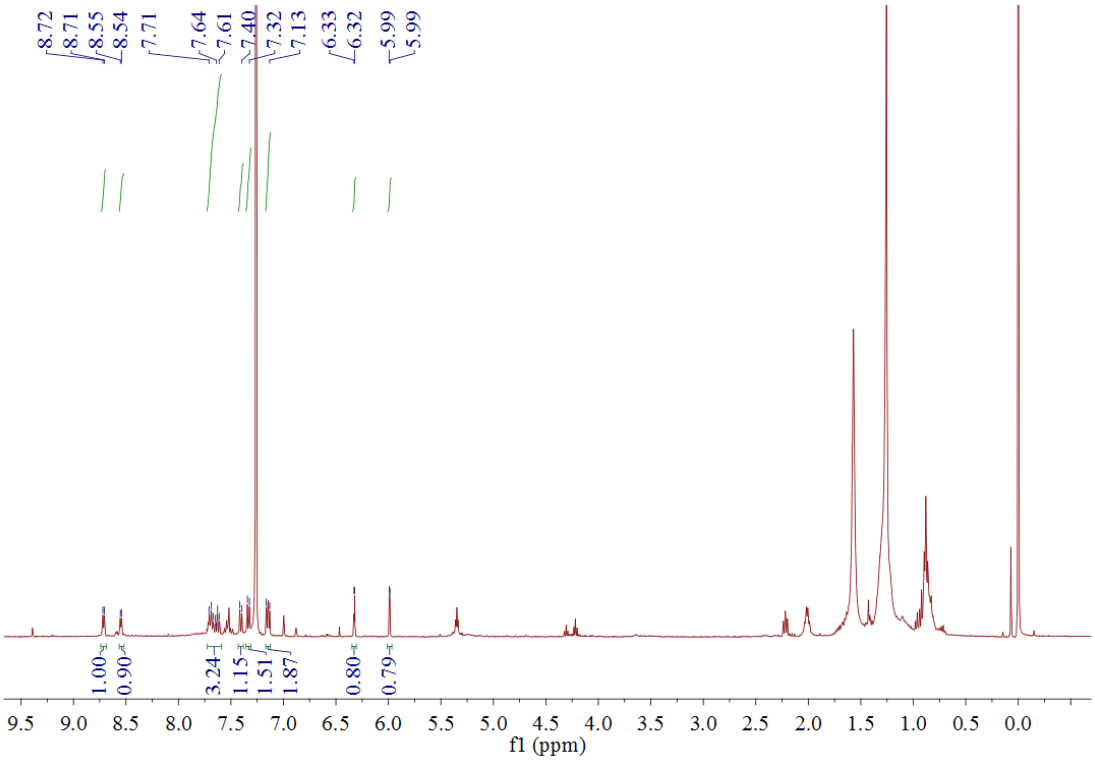
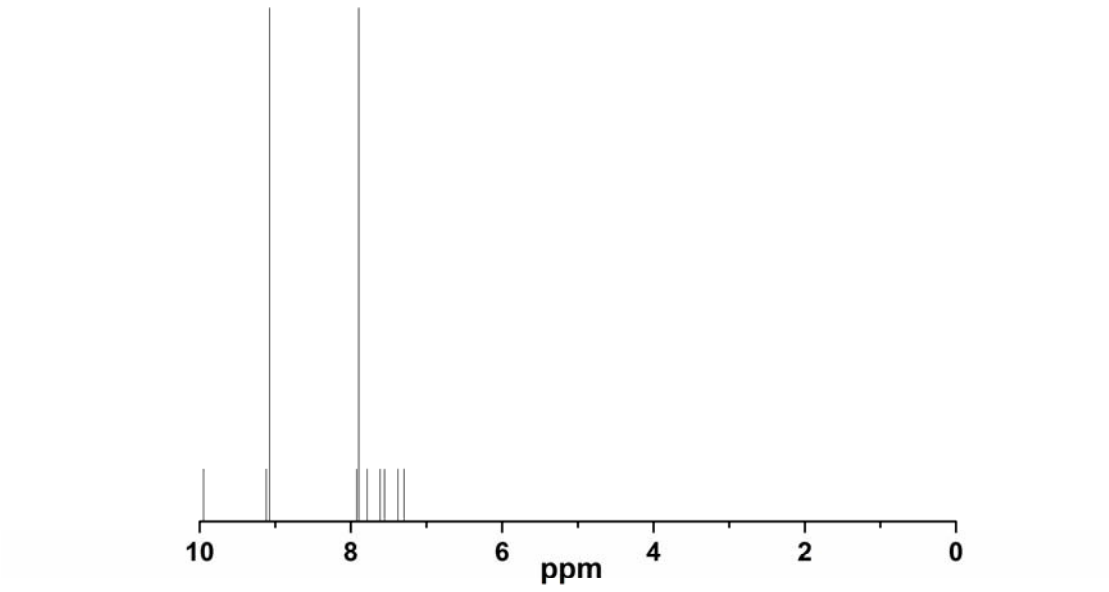
4	Fe	0.553191
5	Br	0.193078
6	Fe	0.560936
7	C	-0.195591
8	H	0.152692
9	C	-0.188376
10	C	-0.202894
11	H	0.151037
12	C	0.159748

13	C	-0.105801
14	C	-0.147985
15	H	0.168996
16	C	-0.152478
17	H	0.181069
18	C	-0.022795
19	C	-0.043597
20	O	-0.311975
21	N	-0.337324
22	N	-0.348974
23	O	-0.291032
24	N	-0.354956
25	N	-0.351738
26	C	0.178125
27	C	-0.183651
28	C	0.204253
29	C	0.288457
30	C	0.289380
31	O	-0.316819
32	O	-0.287993
33	C	0.275915
34	C	0.298641
35	C	0.073259
36	H	0.189495
37	C	0.072326
38	H	0.188691
39	C	0.063064
40	H	0.181084
41	C	-0.197559
42	H	0.152890
43	C	-0.216688
44	H	0.173145
45	C	-0.197133
46	H	0.153290
47	O	-0.336316
48	O	-0.300176
49	C	-0.154685
50	H	0.182995
51	C	-0.205125
52	H	0.150649
53	C	-0.169891
54	H	0.178058
55	C	-0.205617
56	H	0.183274

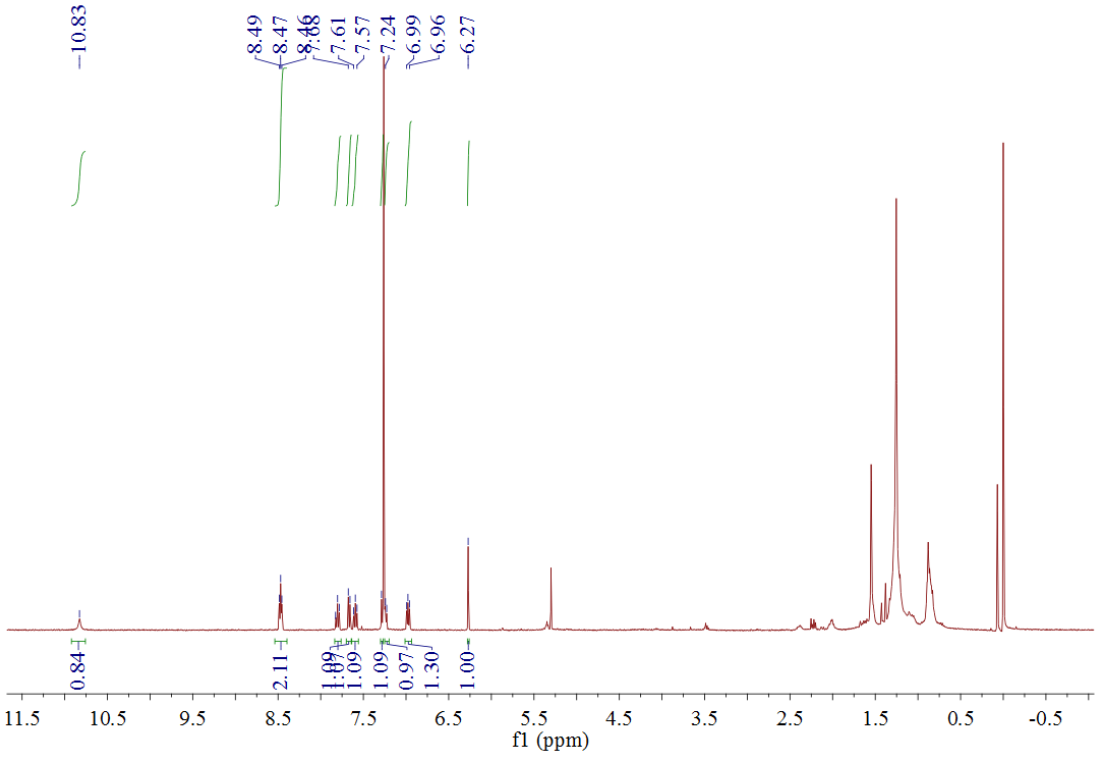
57	C	-0.201654
58	H	0.165540
59	C	-0.298136
60	C	-0.295332
61	C	-0.201632
62	H	0.156182
63	C	-0.190311
64	H	0.151226
65	C	0.286521
66	C	0.072583
67	H	0.188332
68	C	0.264082
69	C	-0.197137
70	H	0.152703
71	C	-0.208453
72	H	0.143764
73	C	-0.217416
74	H	0.141506
75	C	-0.197172
76	H	0.152610



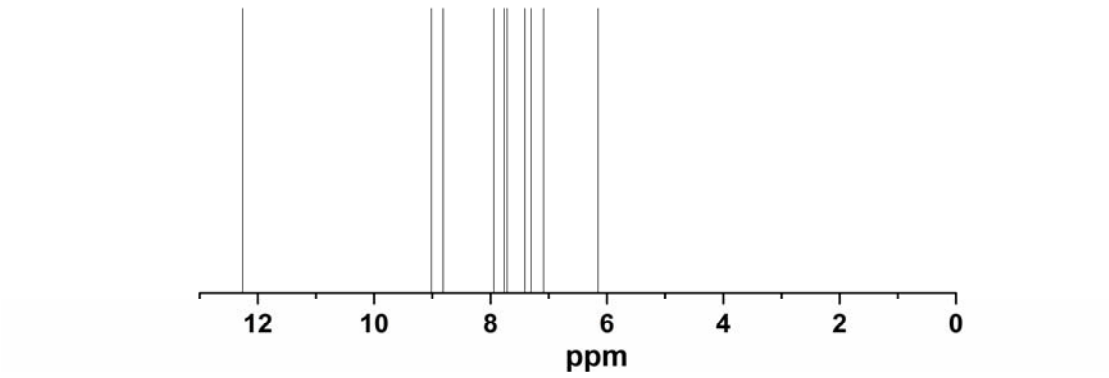
^{1}H NMR spectrum of **1a**.



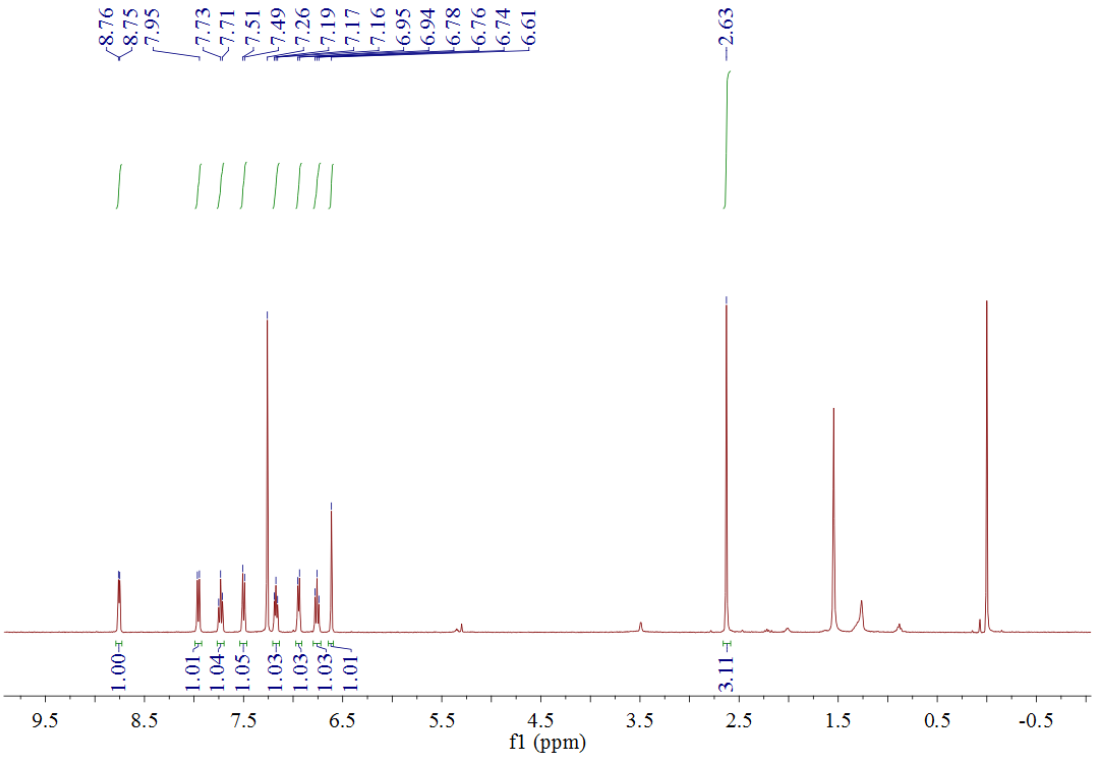
DFT-optimized ^{1}H NMR spectrum of compound **1a** at the level of B3LYP/LanL2DZ/6-311G.



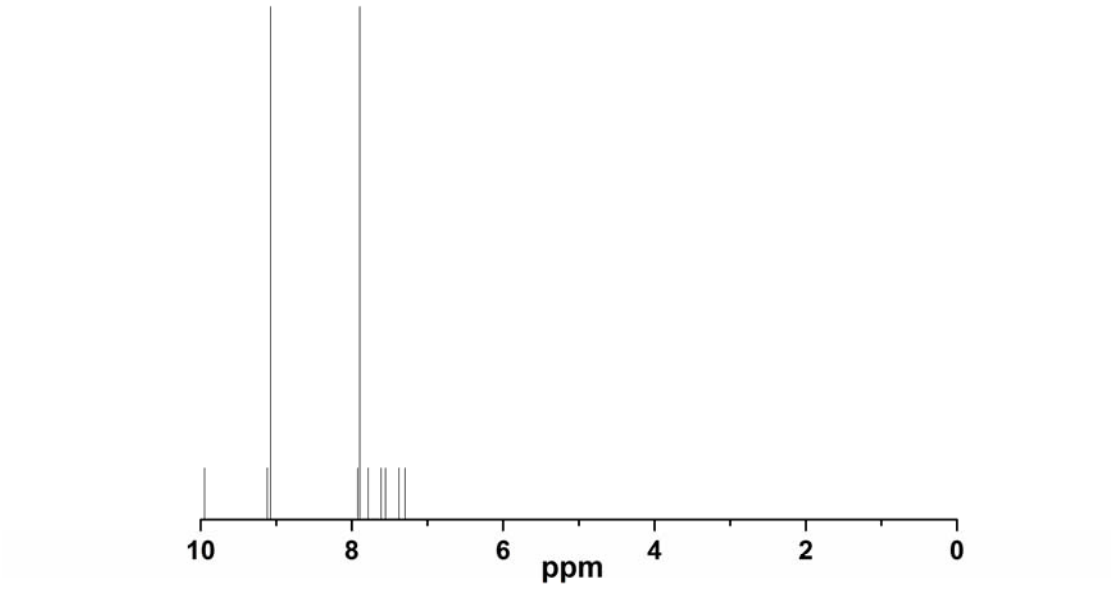
^{1}H NMR spectrum of **1b**.



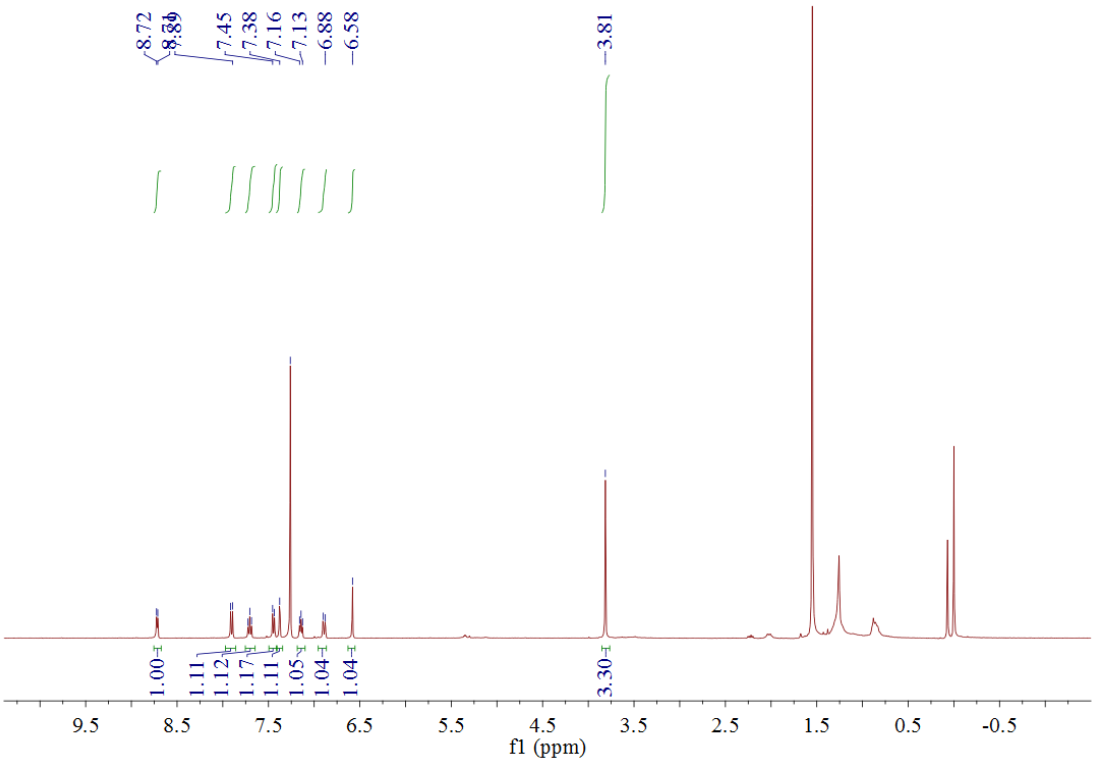
DFT-optimized ^{1}H NMR spectrum of compound **1b** at the level of B3LYP/LanL2DZ/6-311G.



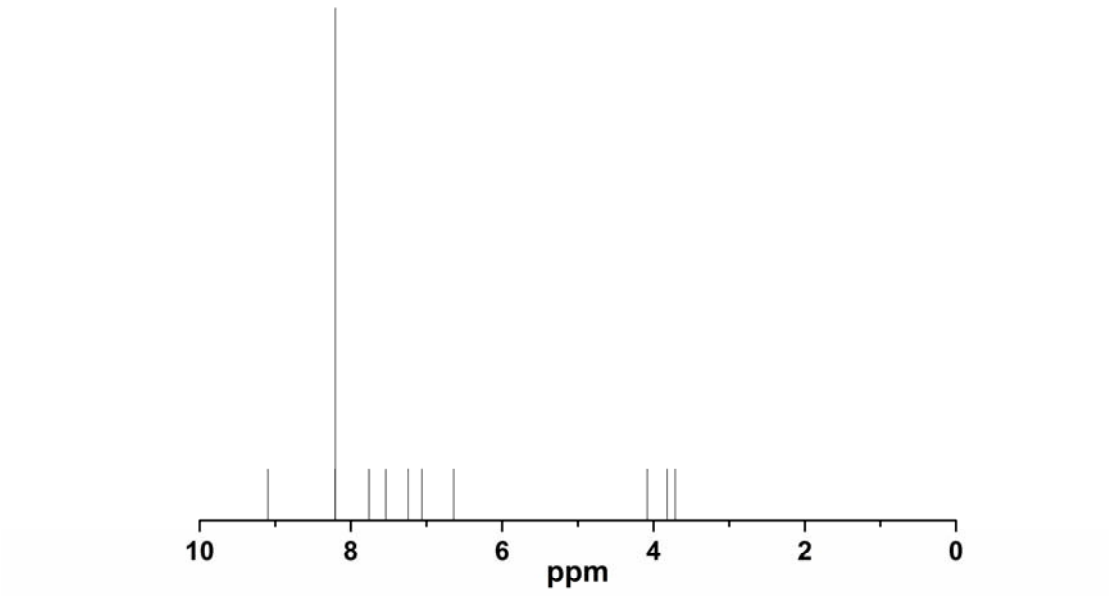
^{1}H NMR spectrum of **2a**.



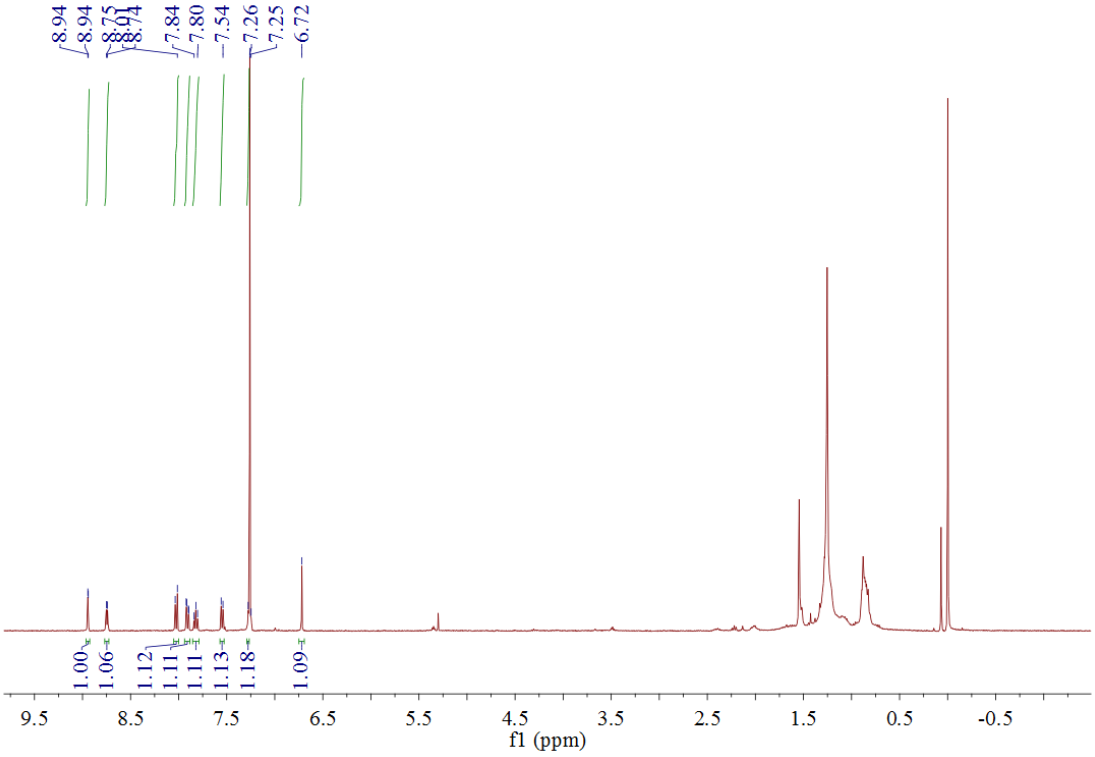
DFT-optimized ^{1}H NMR spectrum of compound **2a** at the level of B3LYP/LanL2DZ/6-311G.



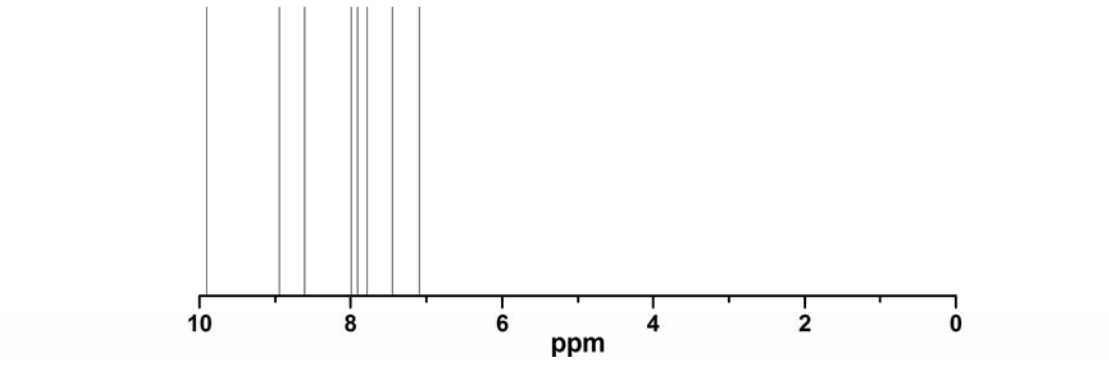
^{1}H NMR spectrum of **3a**.



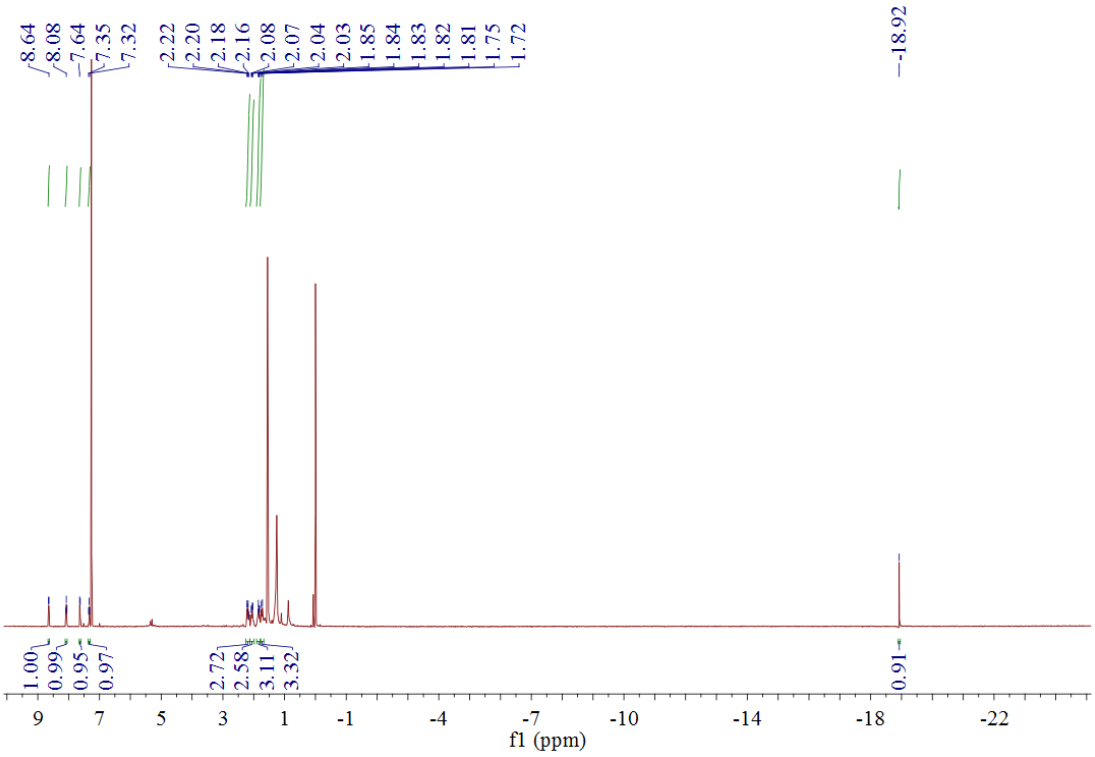
DFT-optimized ^{1}H NMR spectrum of compound **3a** at the level of B3LYP/LanL2DZ/6-311G.



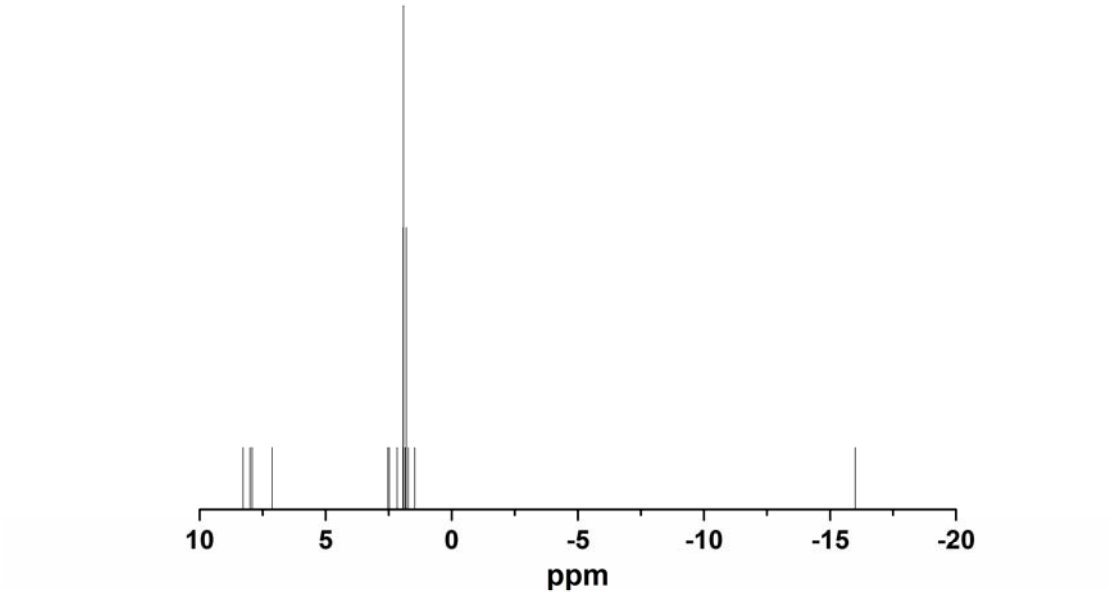
^{1}H NMR spectrum of **4a**.



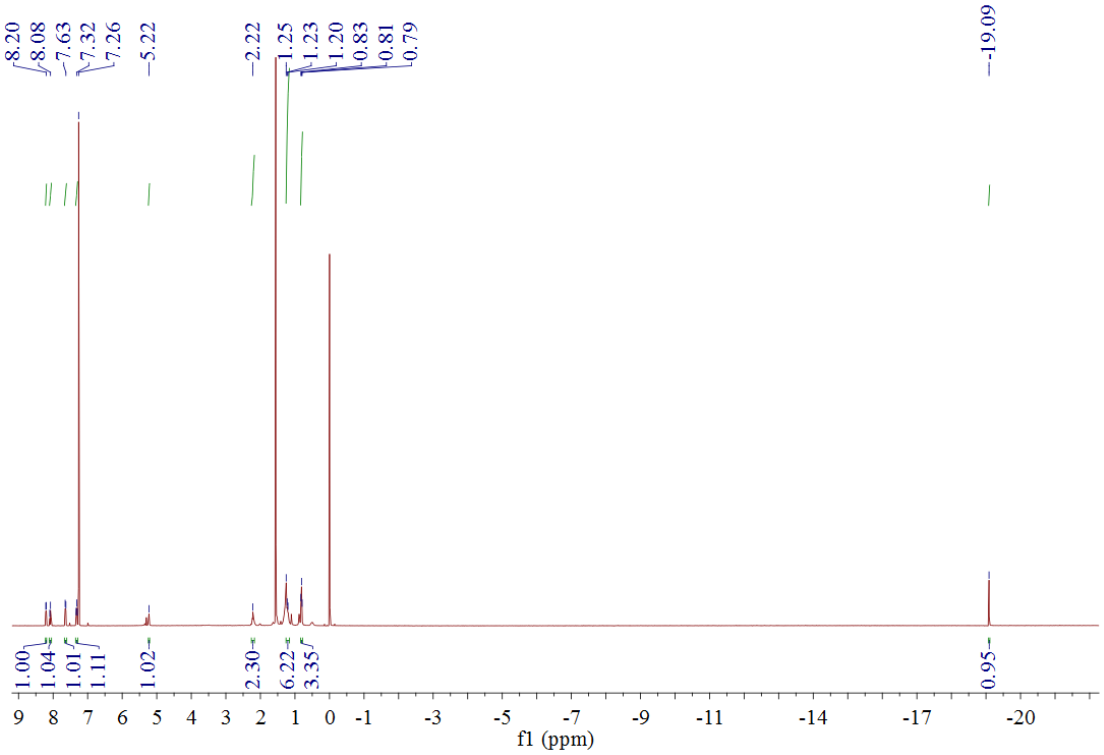
DFT-optimized ^{1}H NMR spectrum of compound **4a** at the level of B3LYP/LanL2DZ/6-311G.



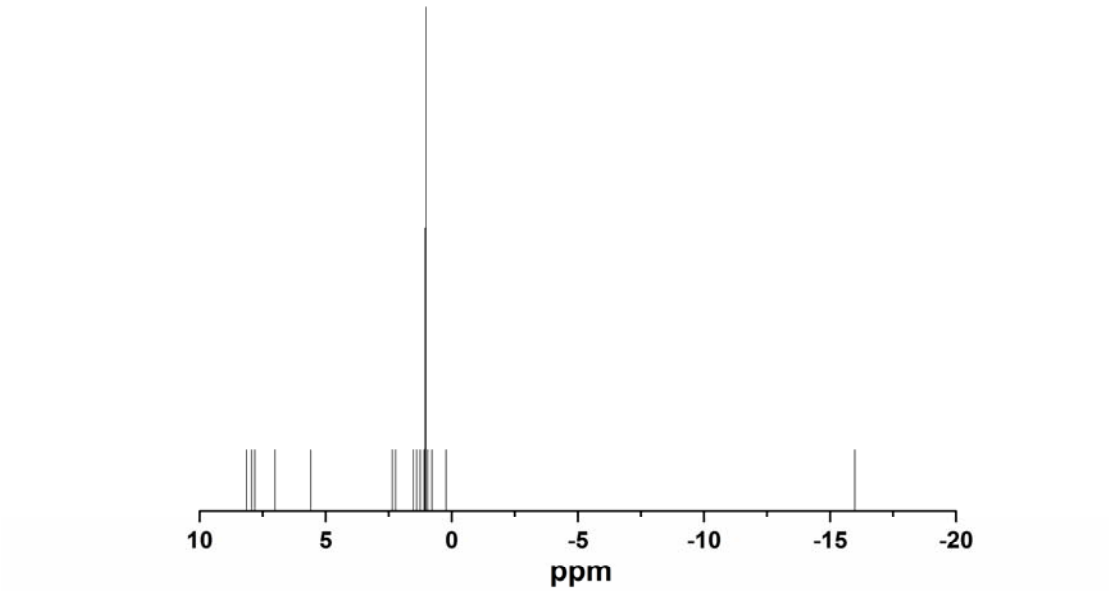
^{1}H NMR spectrum of **5a**.



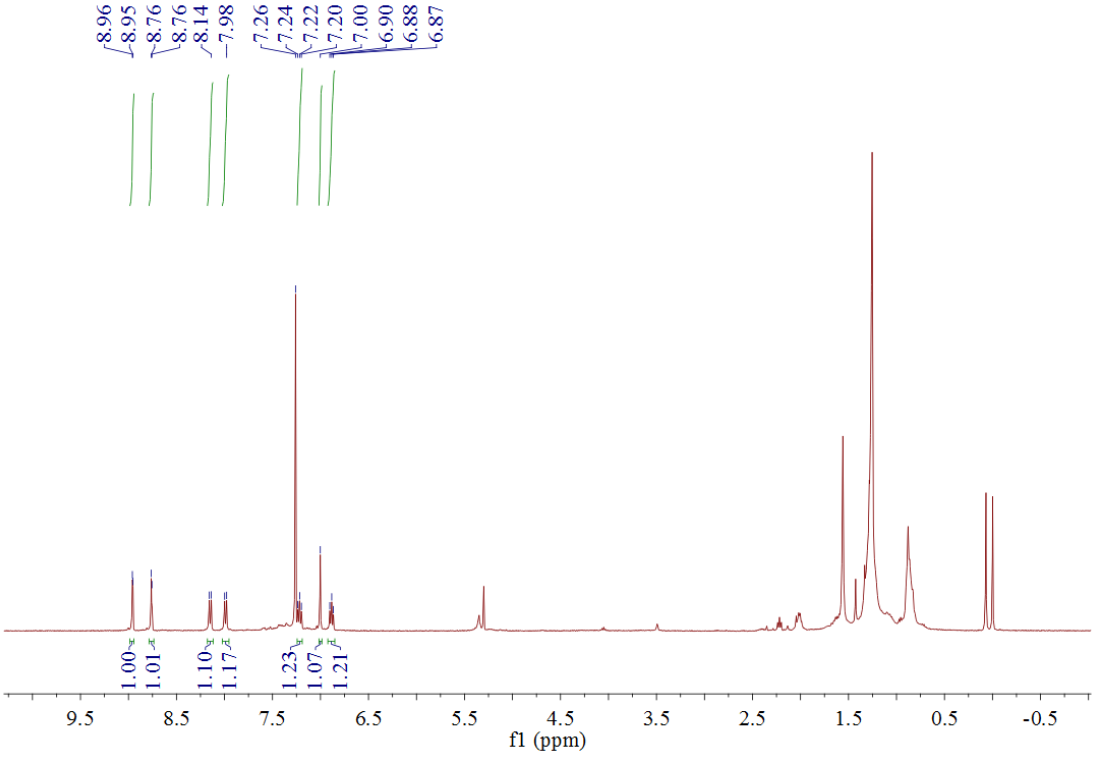
DFT-optimized ^{1}H NMR spectrum of compound **5a** at the level of B3LYP/LanL2DZ/6-311G.



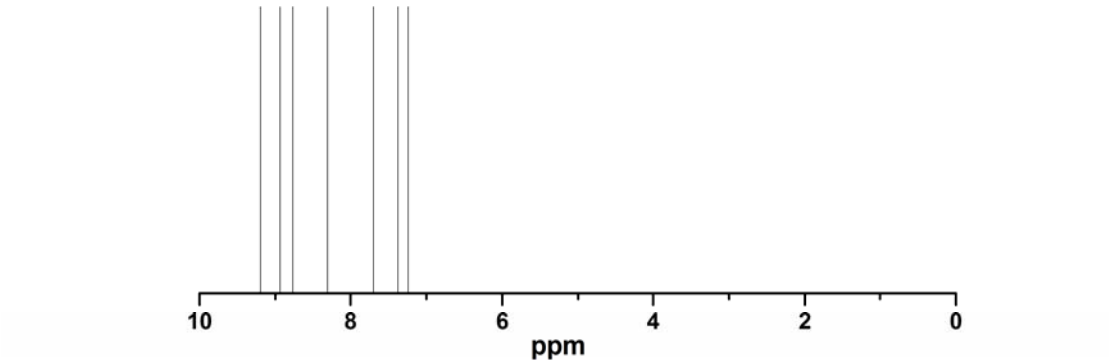
^{1}H NMR spectrum of **6a**.



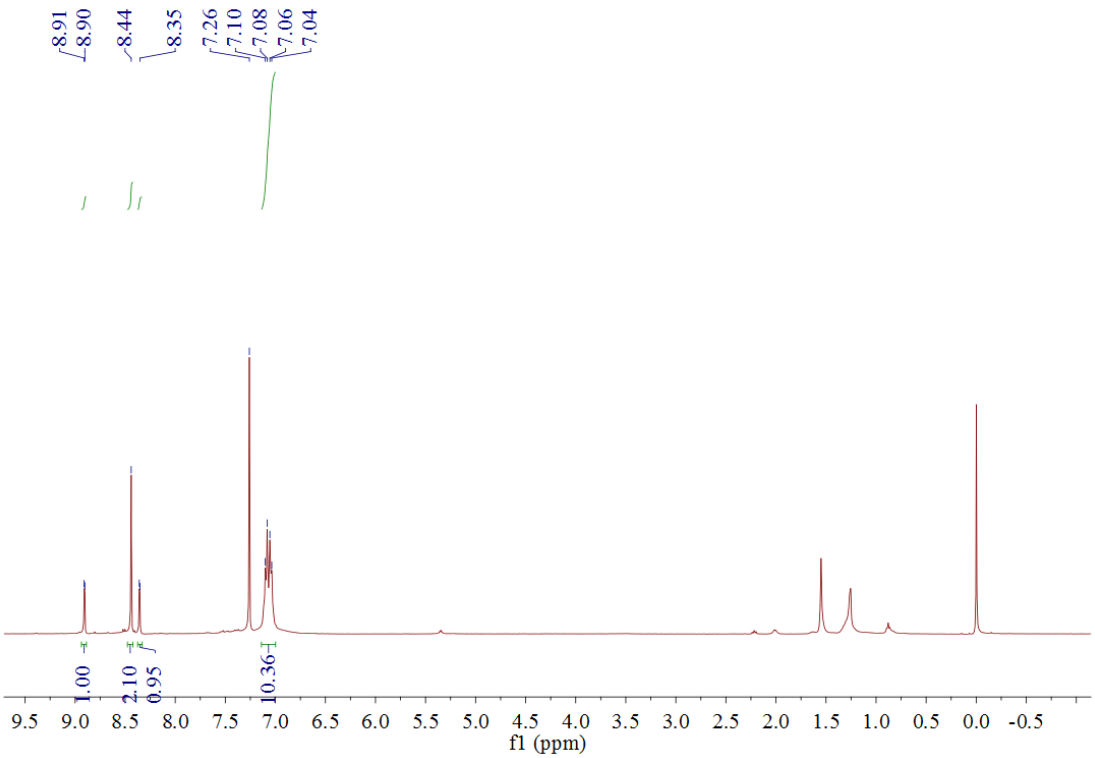
DFT-optimized ^{1}H NMR spectrum of compound **6a** at the level of B3LYP/LanL2DZ/6-311G.



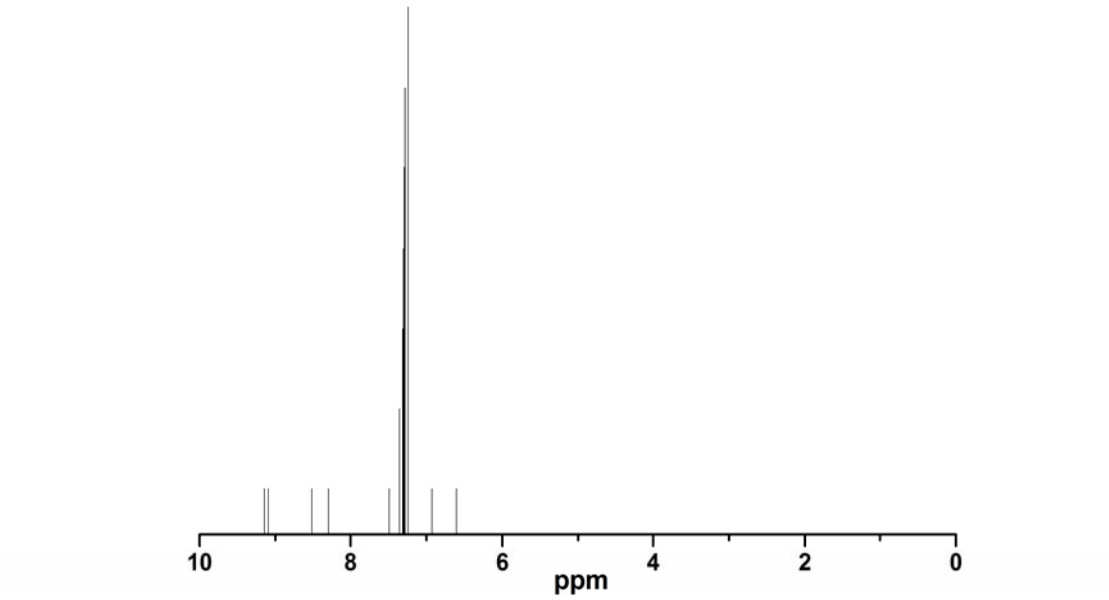
^{1}H NMR spectrum of **7a**.



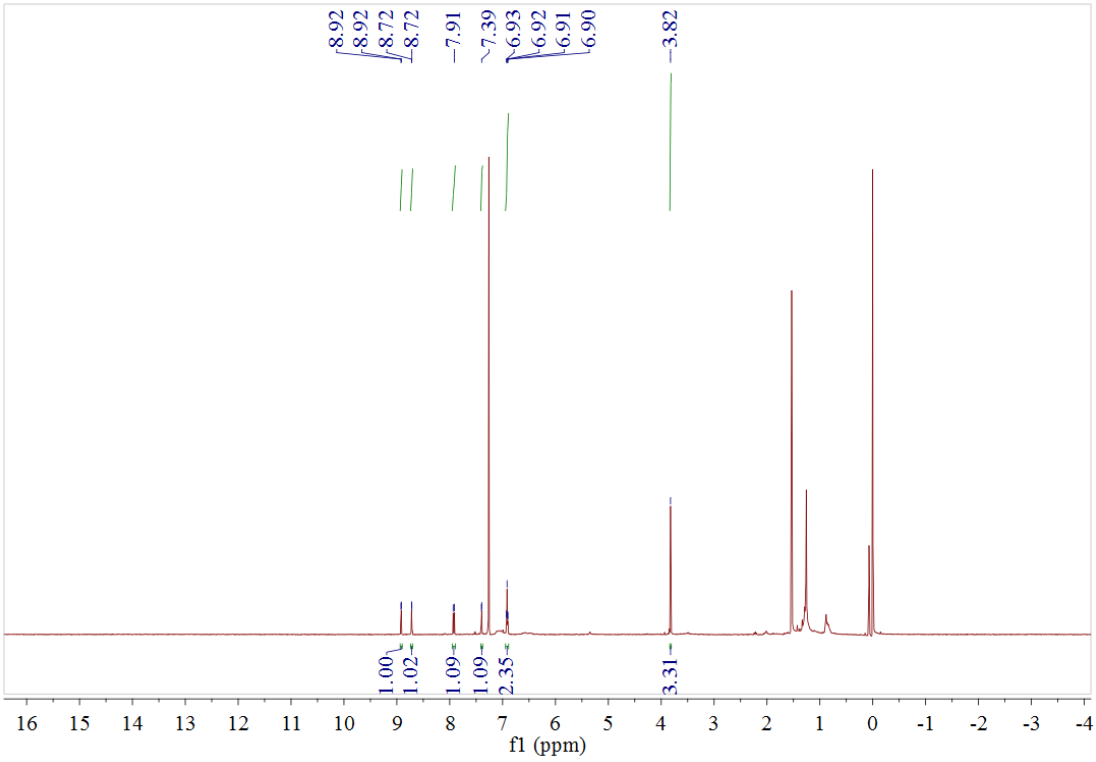
DFT-optimized ^{1}H NMR spectrum of compound **7a** at the level of B3LYP/LanL2DZ/6-311G.



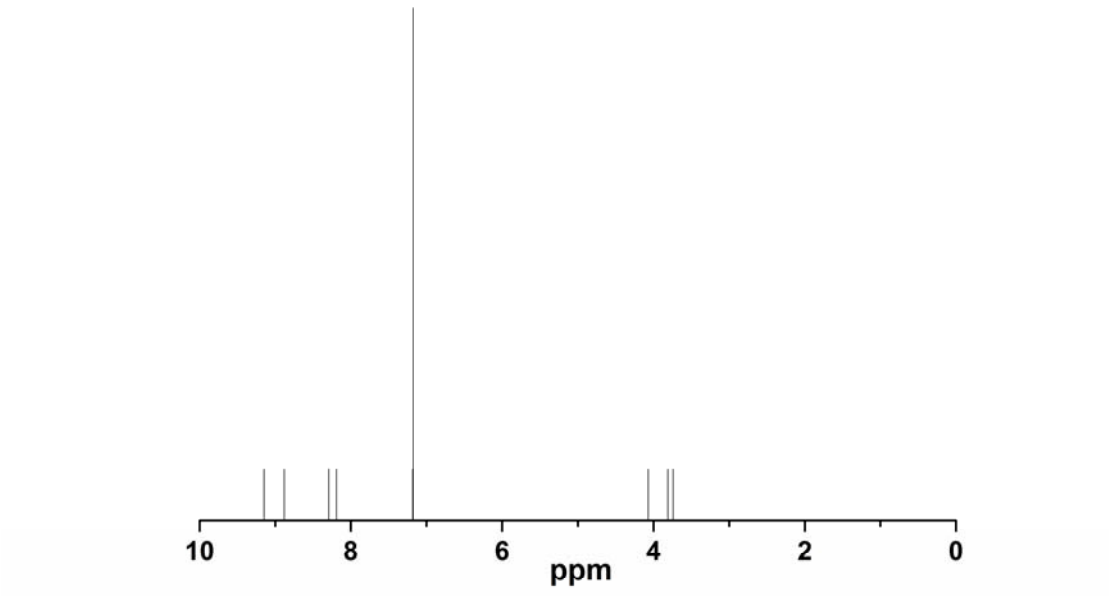
^{1}H NMR spectrum of **7b**.



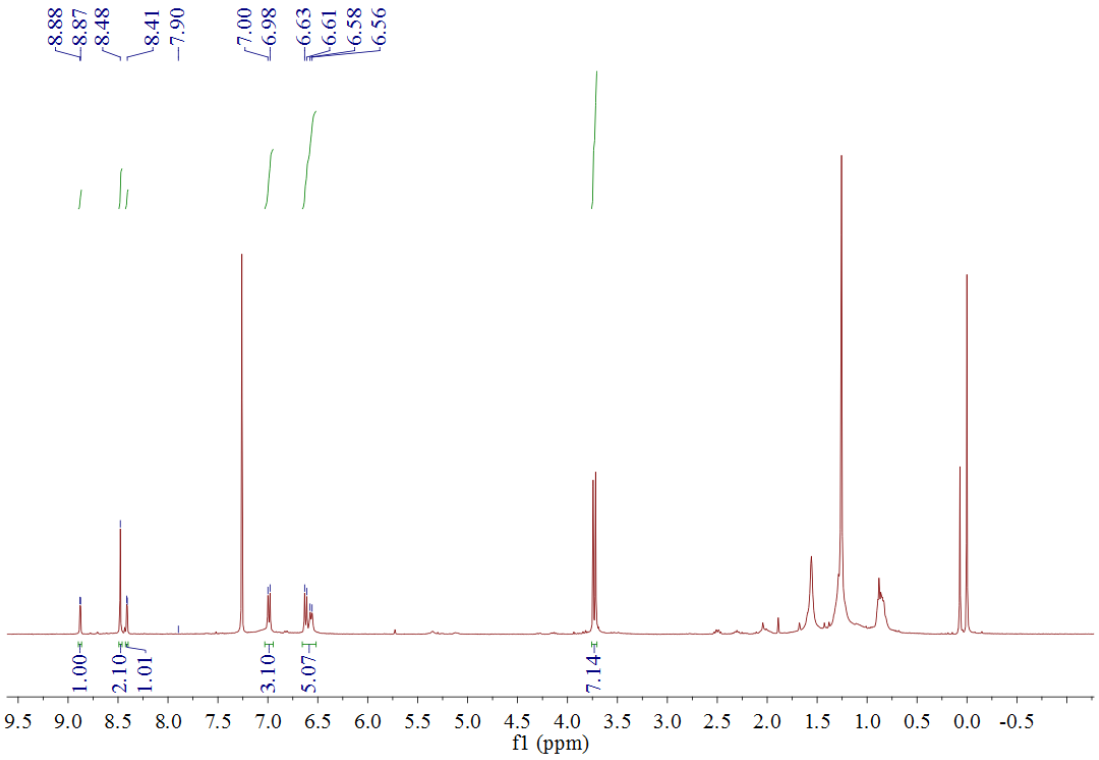
DFT-optimized ^{1}H NMR spectrum of compound **7b** at the level of B3LYP/LanL2DZ/6-311G.



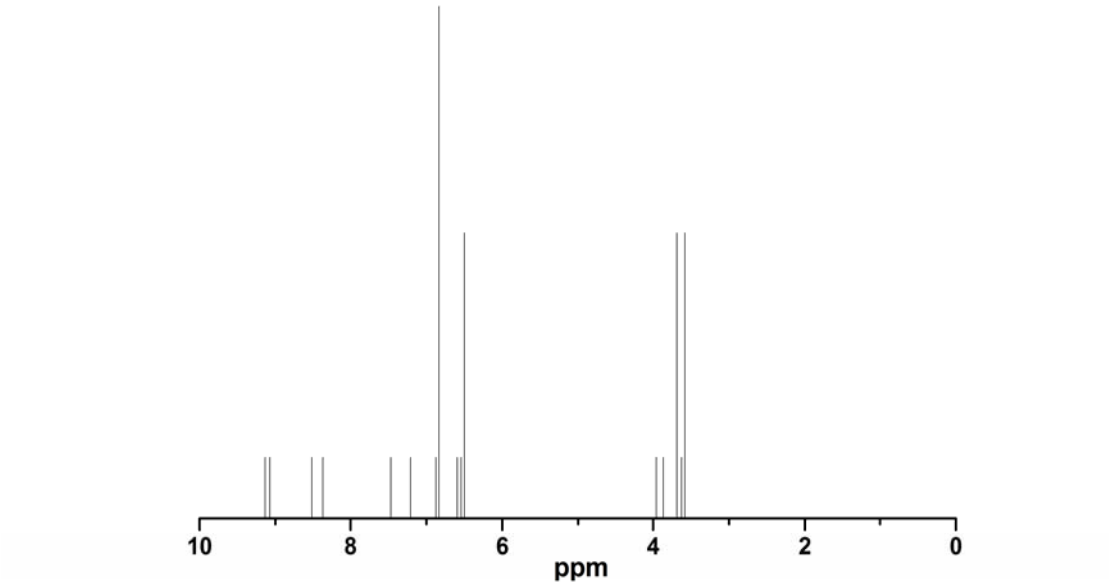
^{1}H NMR spectrum of **8a**.



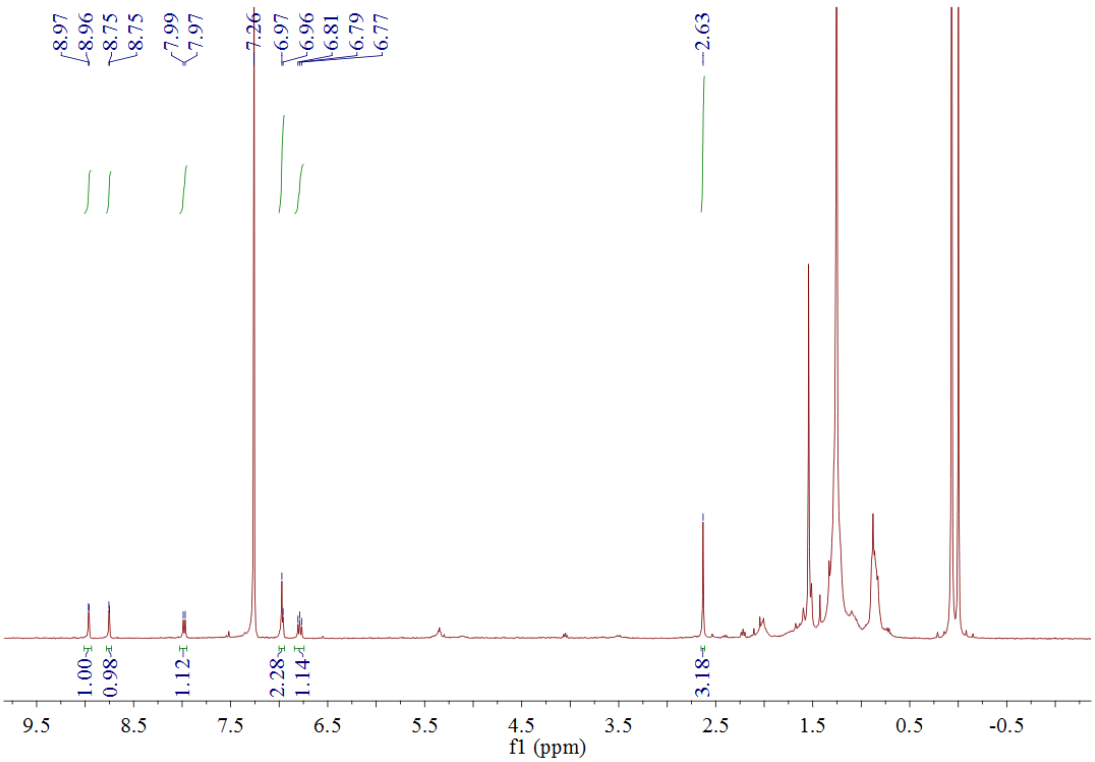
DFT-optimized ^{1}H NMR spectrum of compound **8a** at the level of B3LYP/LanL2DZ/6-311G.



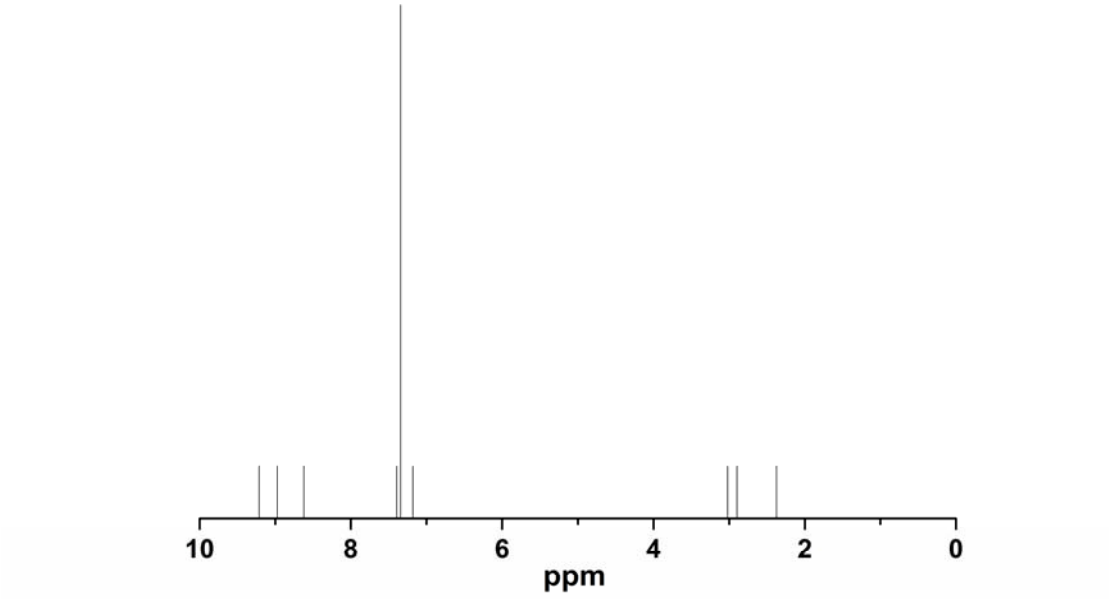
^{1}H NMR spectrum of **8b**.



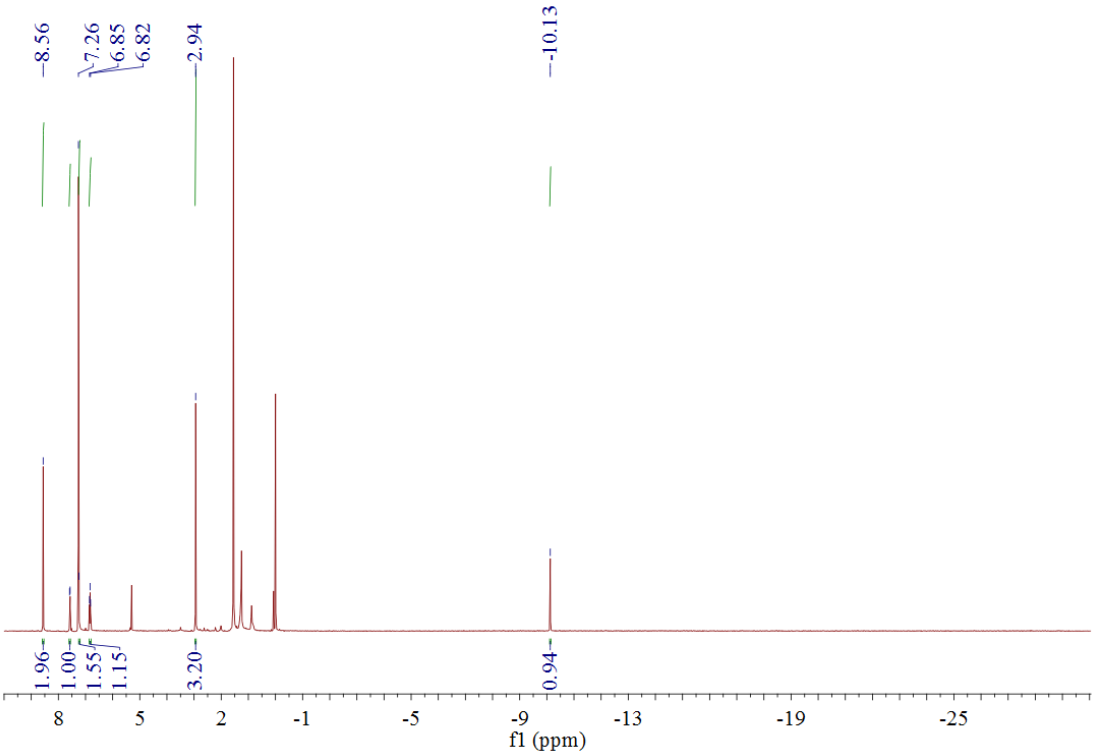
DFT-optimized ^{1}H NMR spectrum of compound **8b** at the level of B3LYP/LanL2DZ/6-311G.



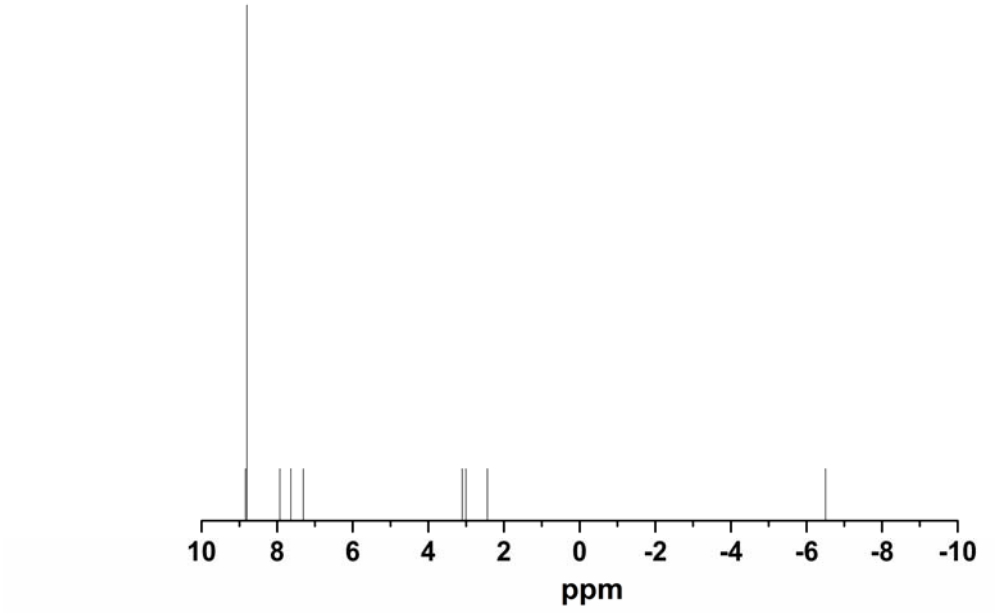
^{1}H NMR spectrum of **9a**.



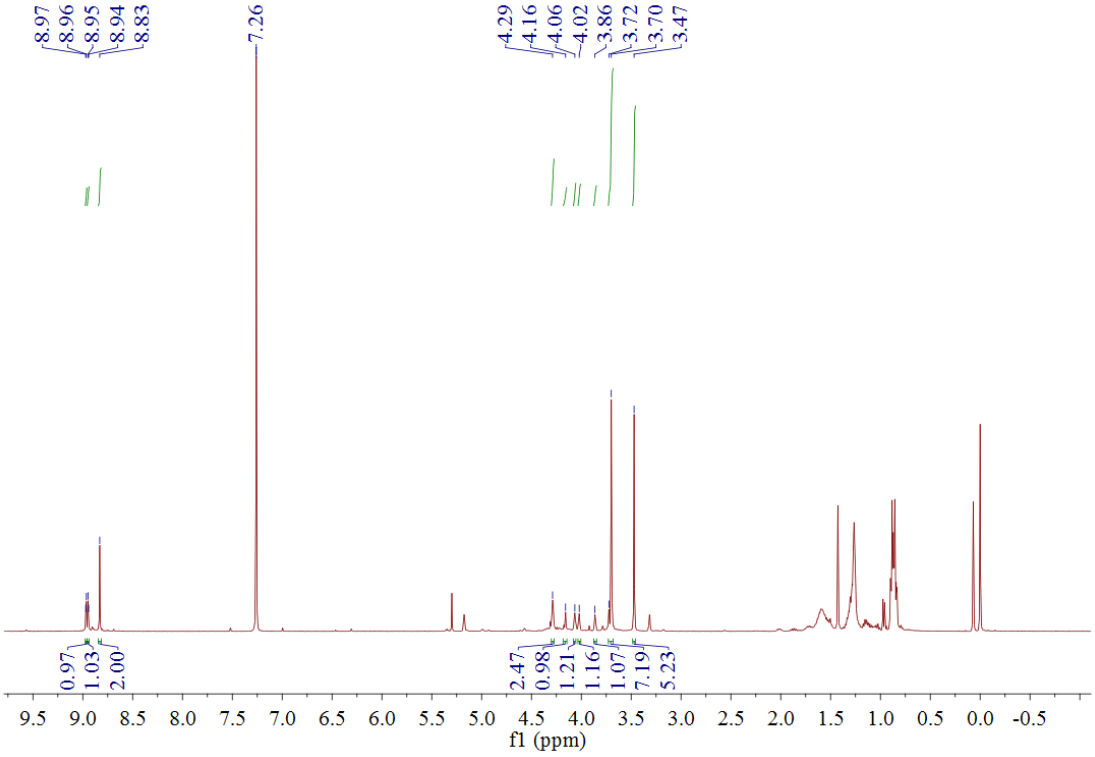
DFT-optimized ^{1}H NMR spectrum of compound **9a** at the level of B3LYP/LanL2DZ/6-311G.



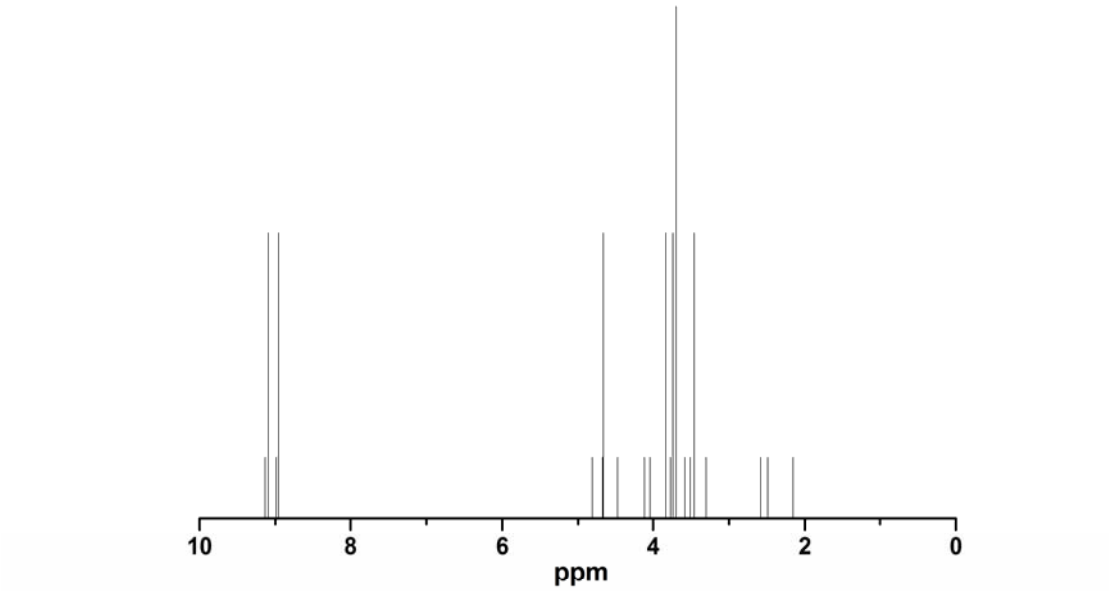
^{1}H NMR spectrum of **9c**.



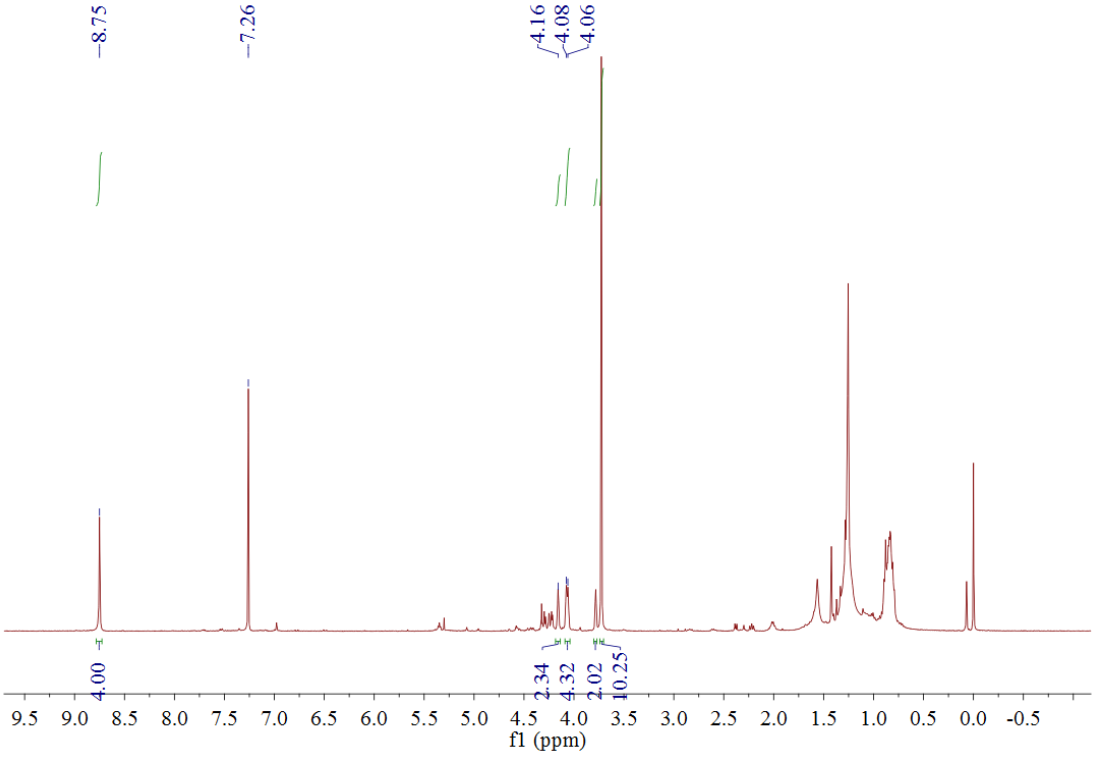
DFT-optimized ^{1}H NMR spectrum of compound **9c** at the level of B3LYP/LanL2DZ/6-311G.



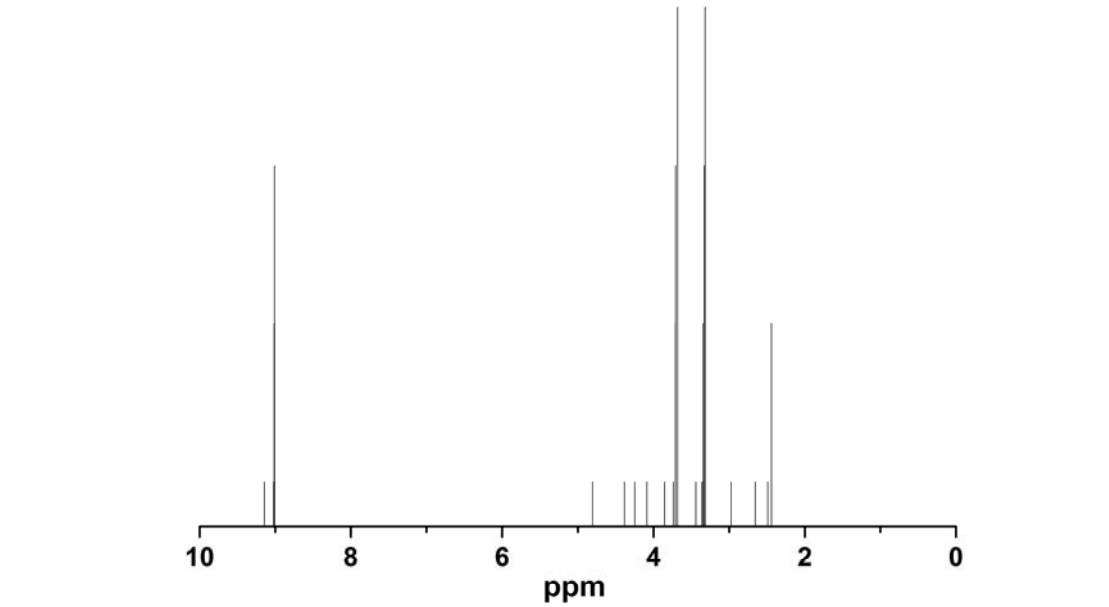
^{1}H NMR spectrum of **10a**.



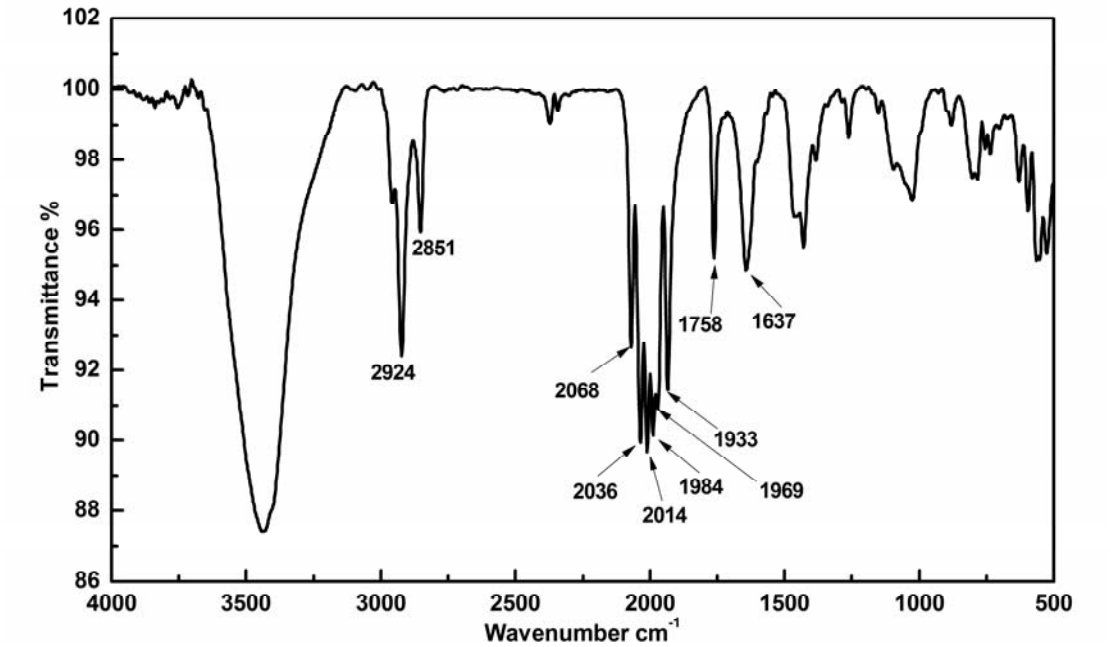
DFT-optimized ^{1}H NMR spectrum of compound **10a** at the level of B3LYP/LanL2DZ/6-311G.



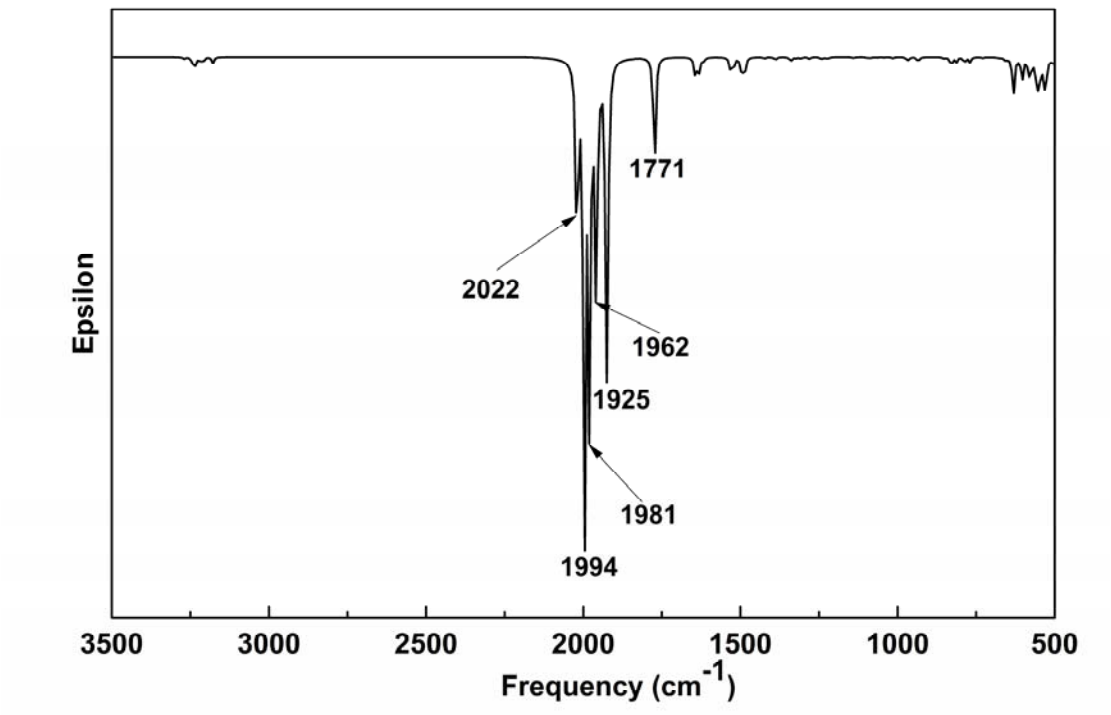
^{1}H NMR spectrum of **10b**.



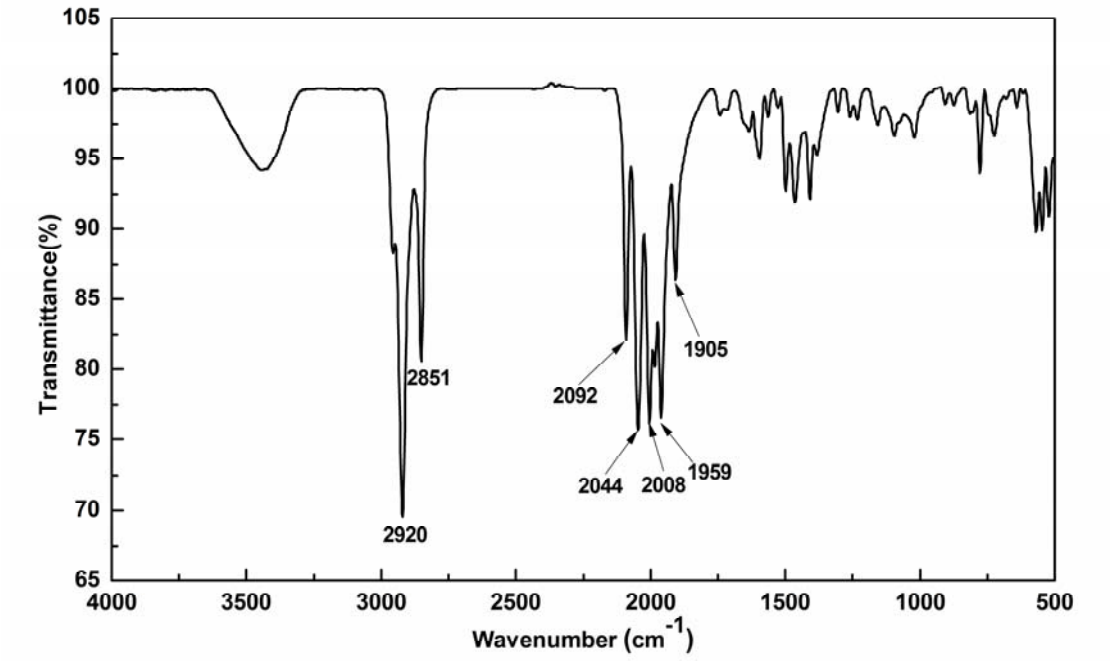
DFT-optimized ^{1}H NMR spectrum of compound **10b** at the level of B3LYP/LanL2DZ/6-311G.



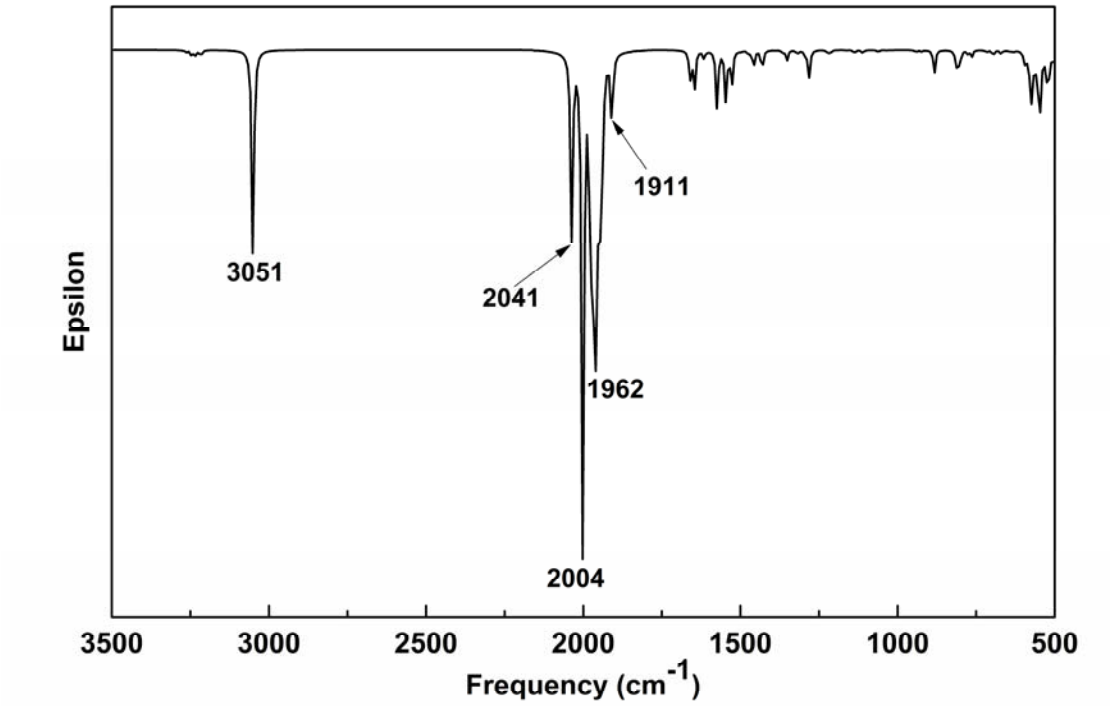
FT-IR spectrum of compound **1a**.



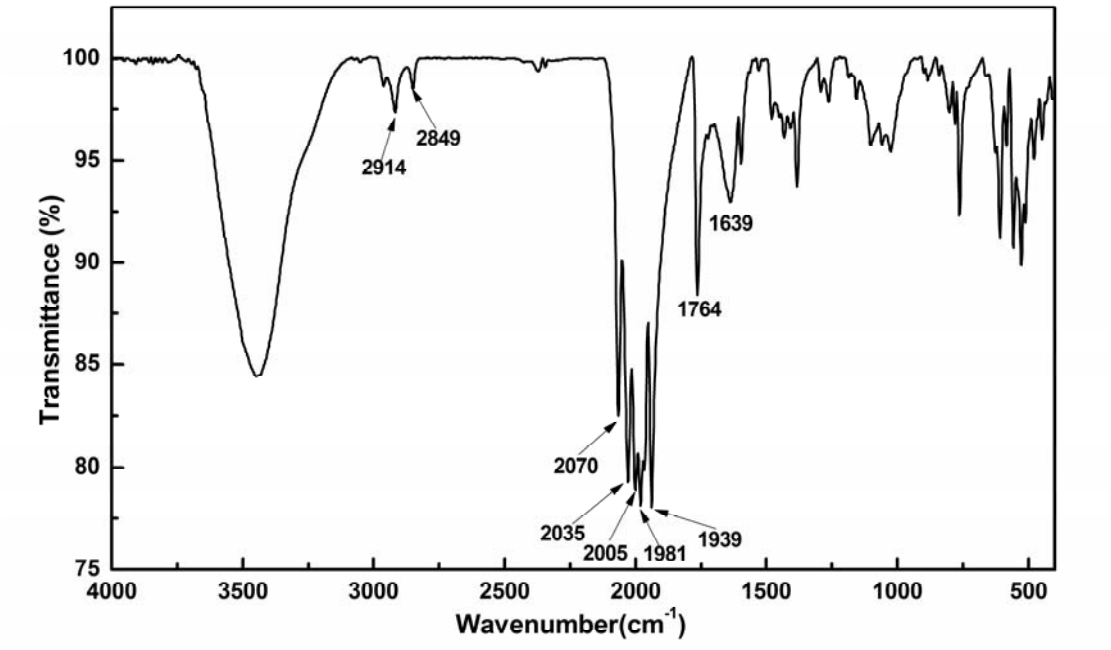
DFT-optimized IR spectrum of compound **1a** at the level of B3LYP/LanL2DZ/6-31G.



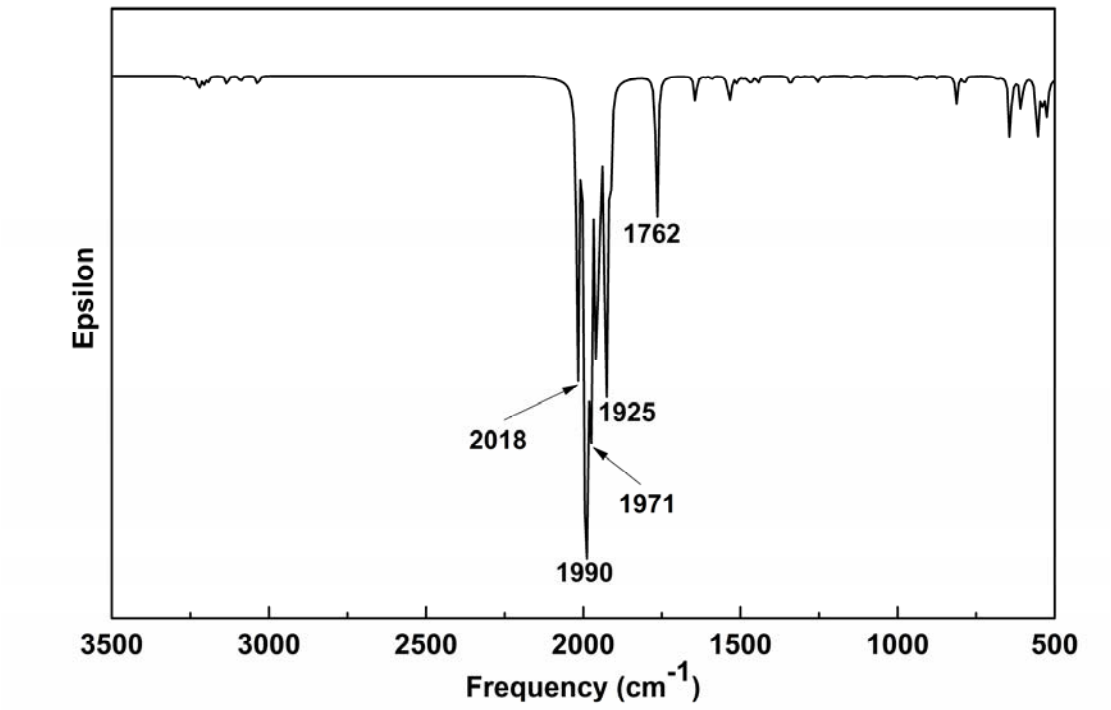
FT-IR spectrum of compound **1b**.



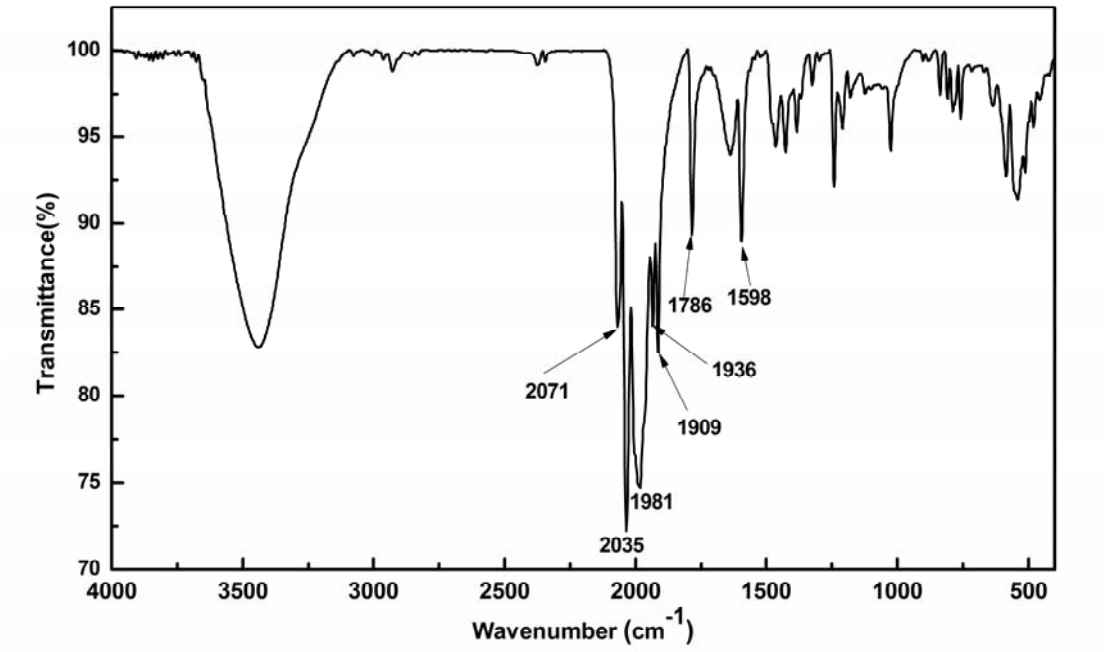
DFT-optimized IR spectrum of compound **1b** at the level of B3LYP/LanL2DZ/6-31G.



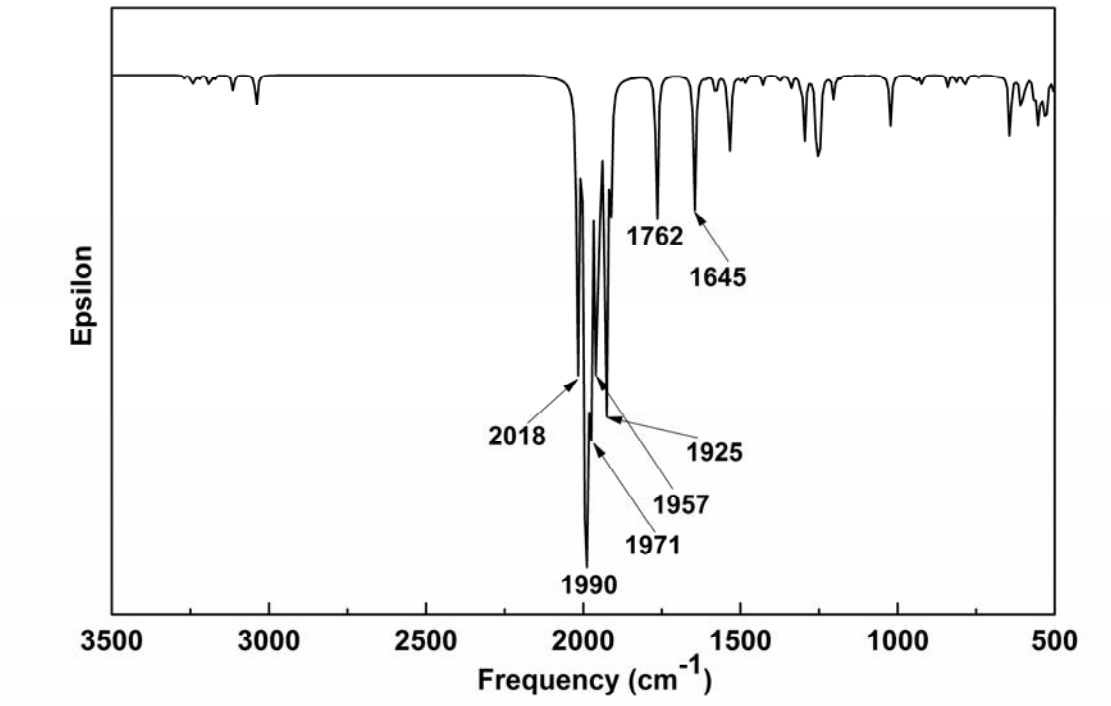
FT-IR spectrum of compound **2a**.



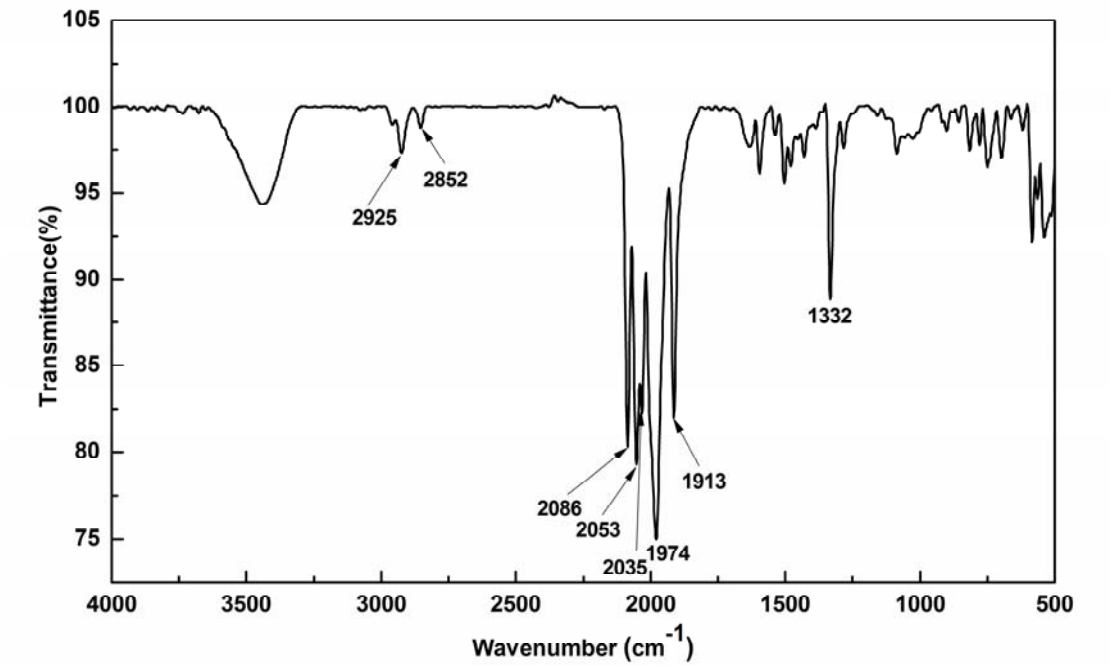
DFT-optimized IR spectrum of compound **2a** at the level of B3LYP/LanL2DZ/6-31G.



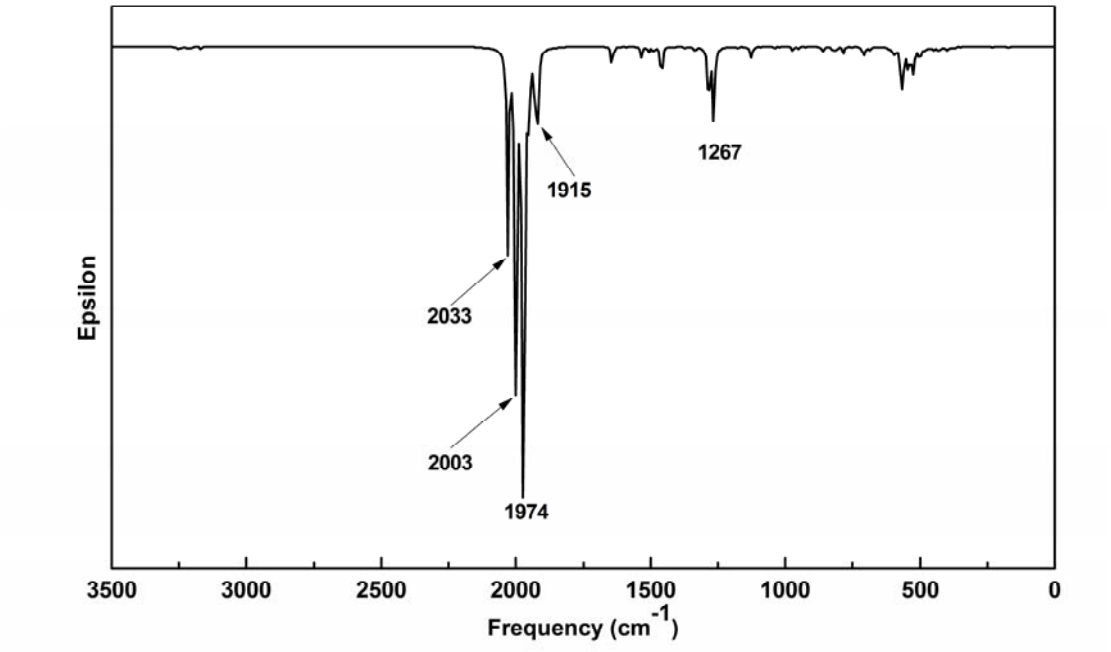
FT-IR spectrum of compound **3a**.



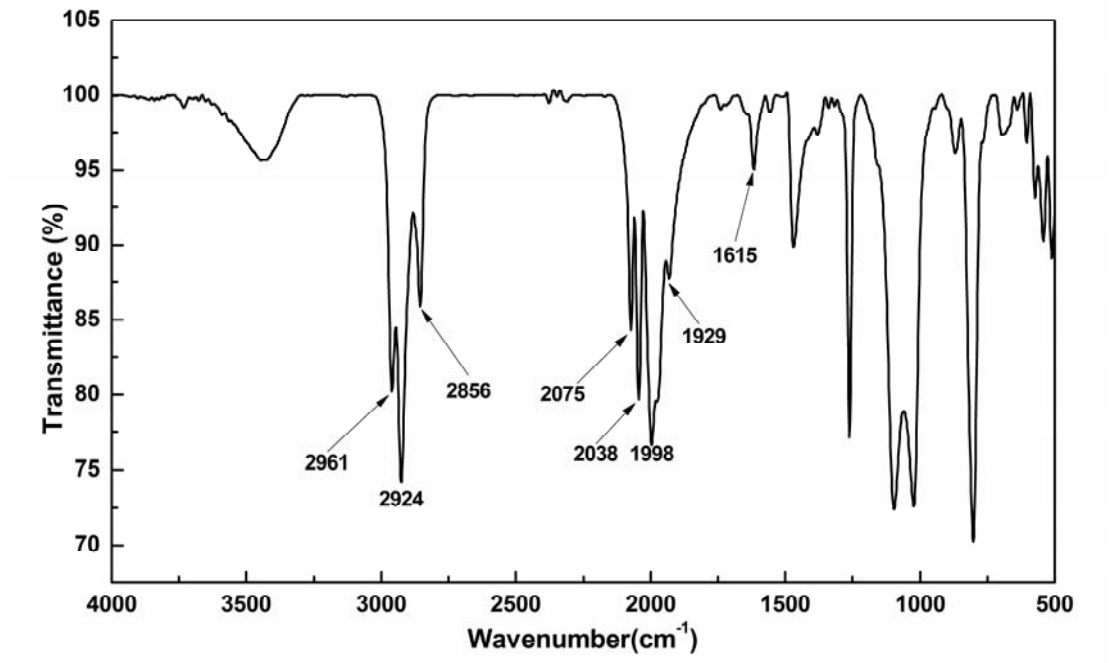
DFT-optimized IR spectrum of compound **3a** at the level of B3LYP/LanL2DZ/6-31G.



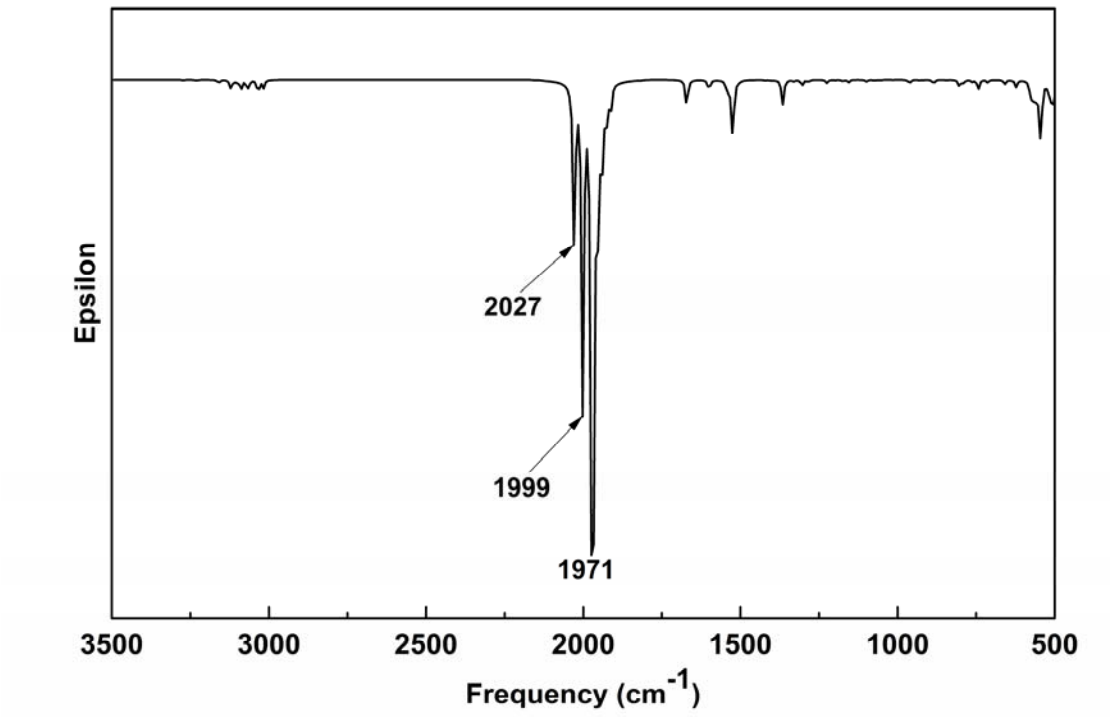
FT-IR spectrum of compound **4a**.



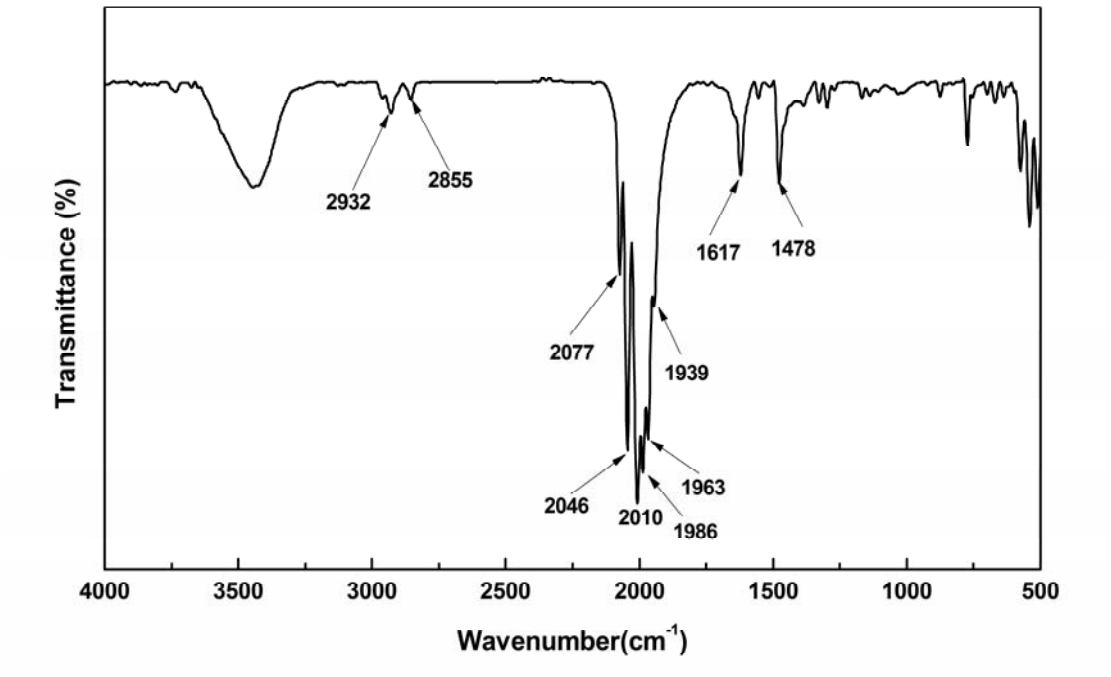
DFT-optimized IR spectrum of compound **4a** at the level of B3LYP/LanL2DZ/6-31G.



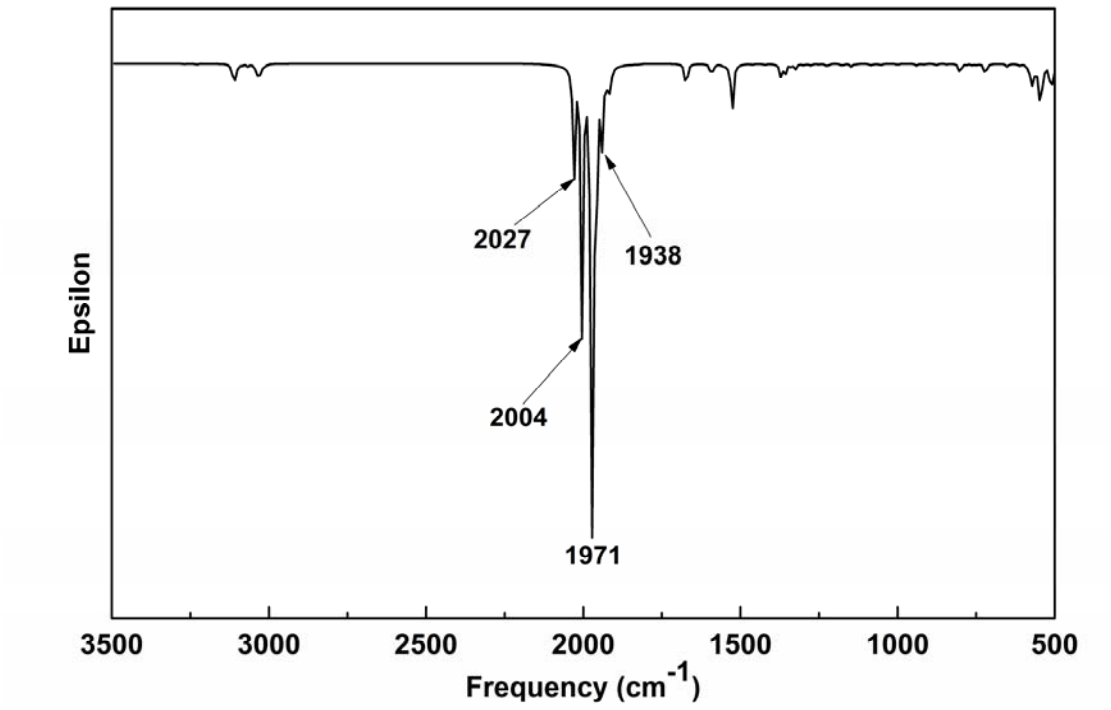
FT-IR spectrum of compound **5a**.



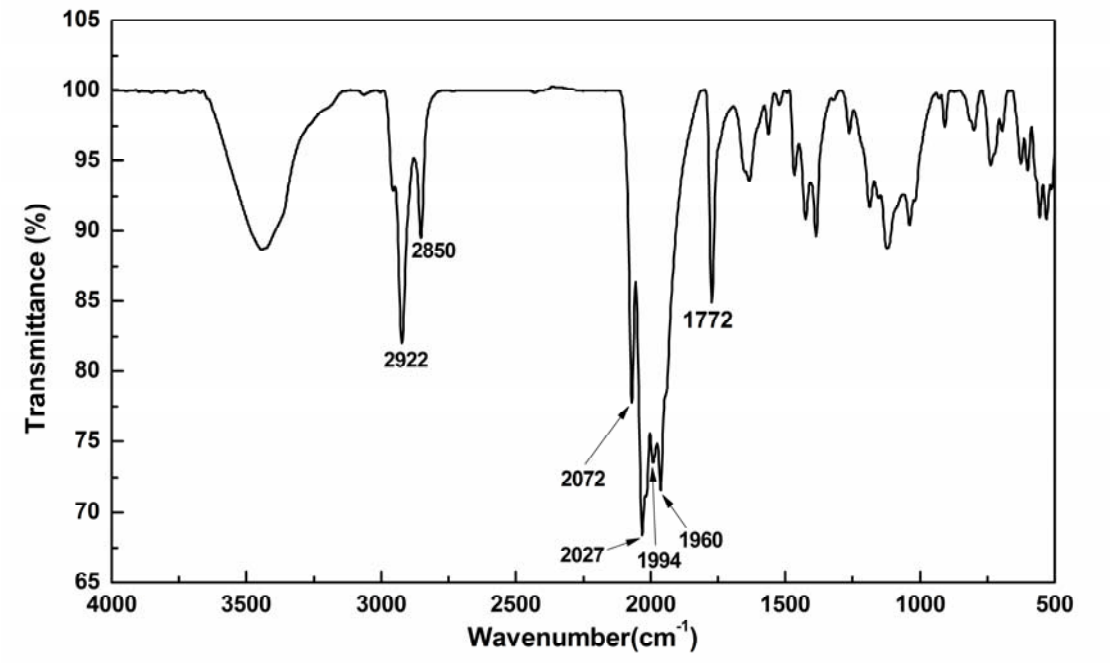
DFT-optimized IR spectrum of compound **5a** at the level of B3LYP/LanL2DZ/6-31G.



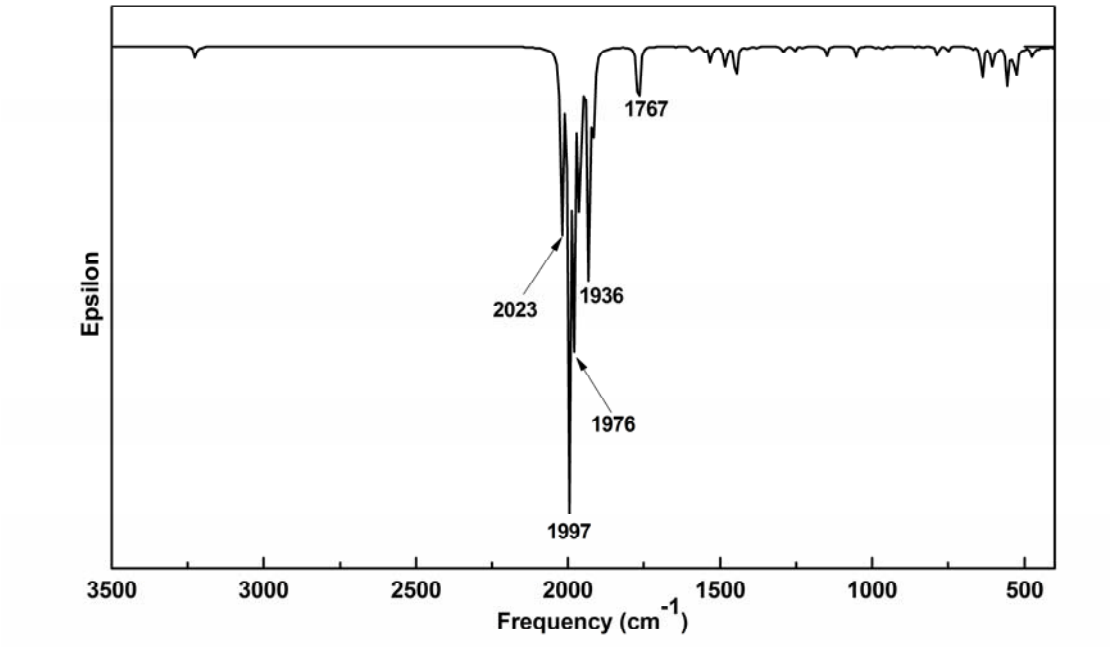
FT-IR spectrum of compound **6a**.



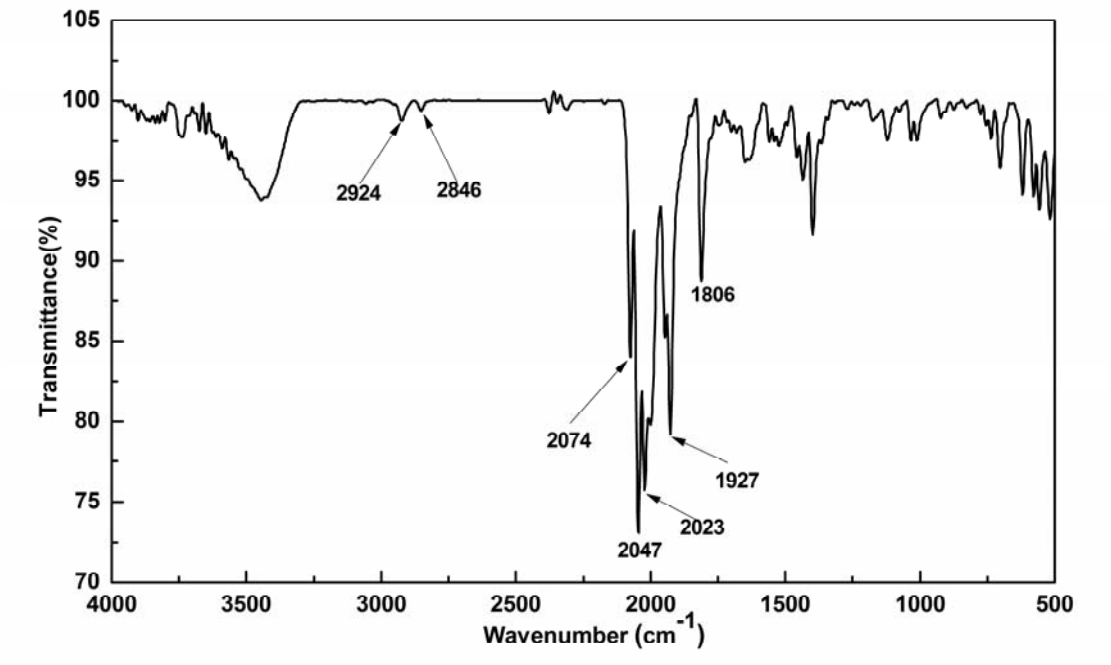
DFT-optimized IR spectrum of compound **6a** at the level of B3LYP/LanL2DZ/6-31G.



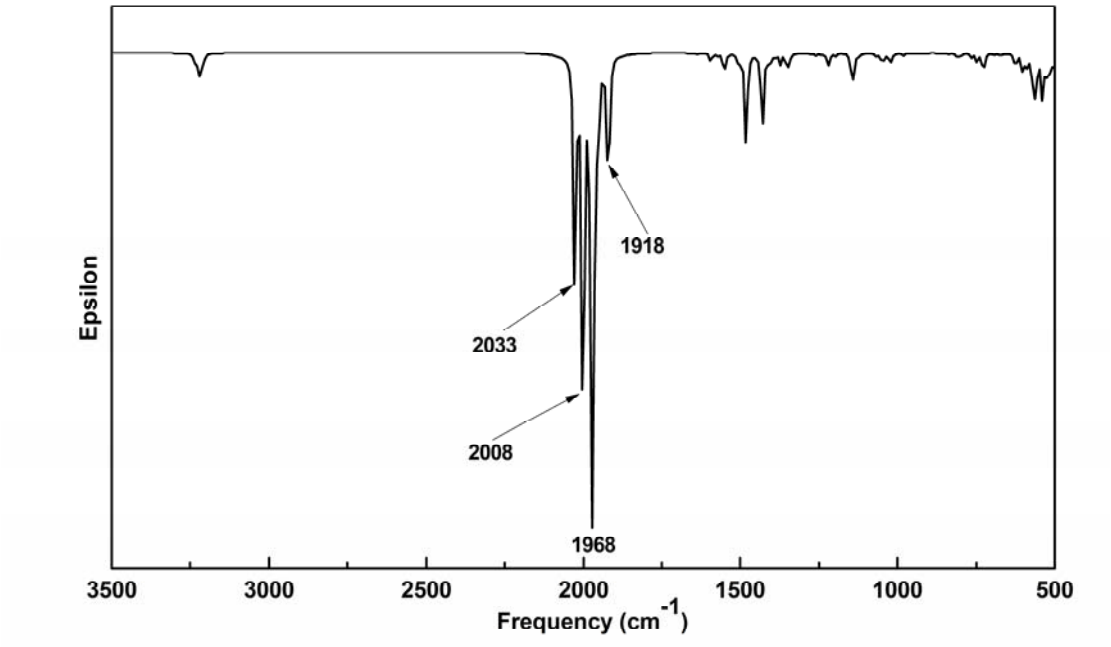
FT-IR spectrum of compound **7a**.



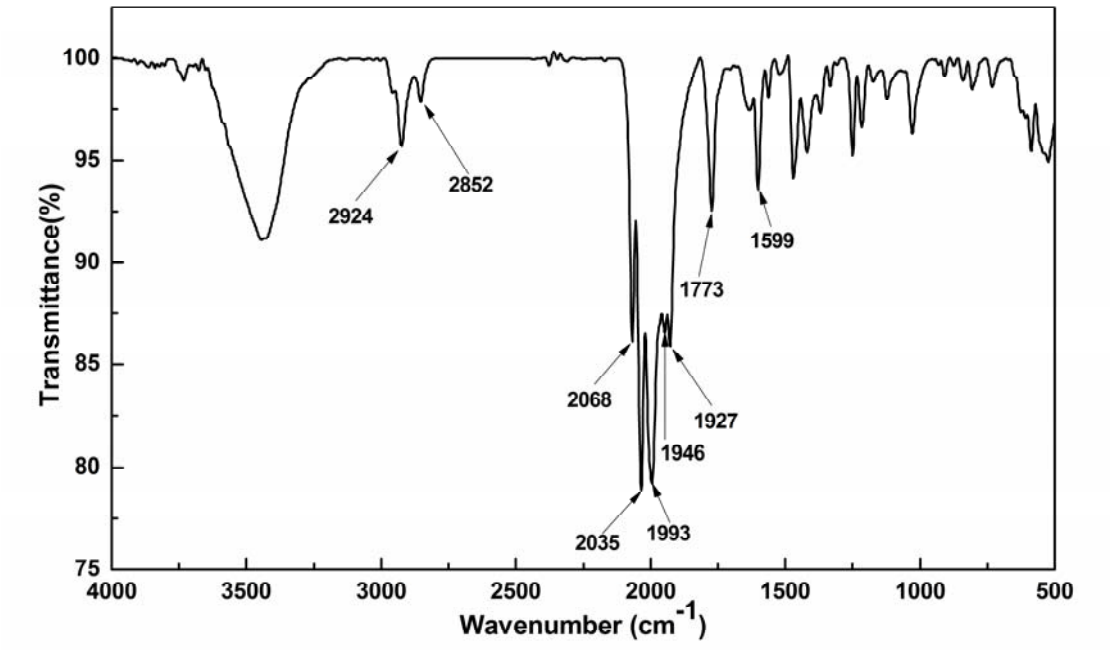
DFT-optimized IR spectrum of compound **7a** at the level of B3LYP/LanL2DZ/6-31G.



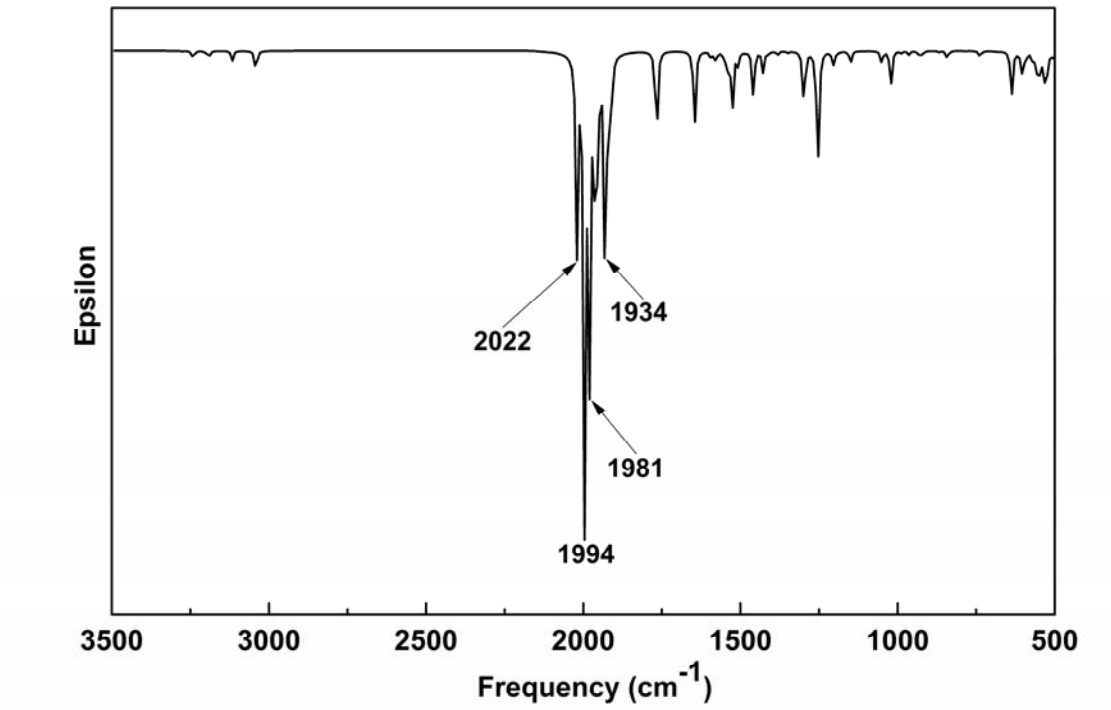
FT-IR spectrum of compound **7b**.



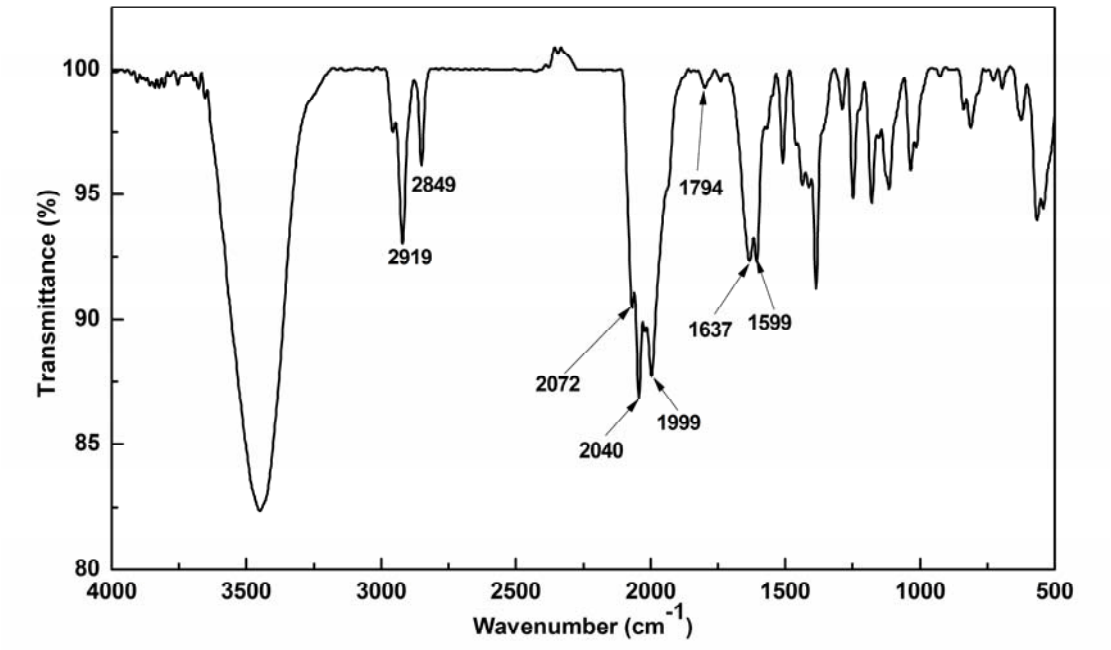
DFT-optimized IR spectrum of compound **7b** at the level of B3LYP/LanL2DZ/6-31G.



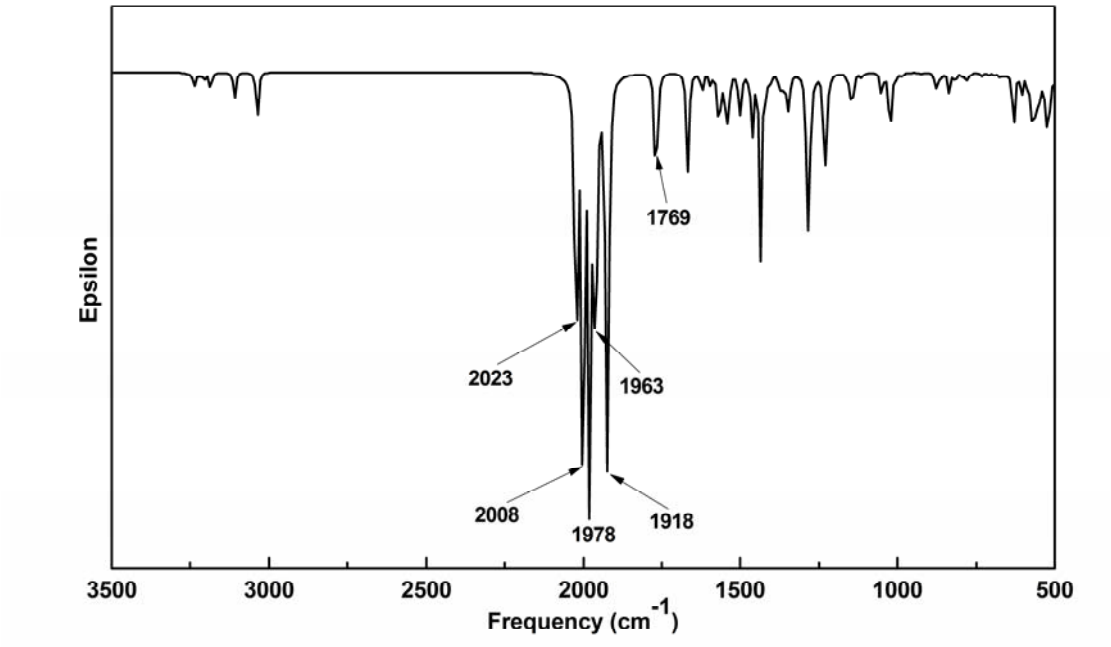
FT-IR spectrum of compound **8a**.



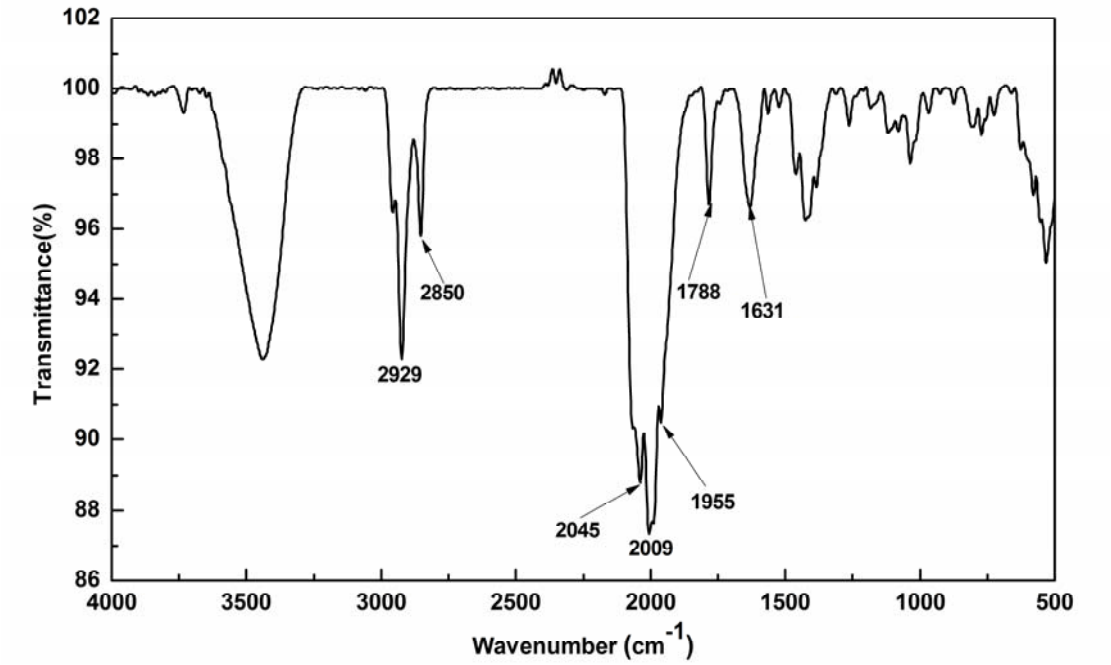
DFT-optimized IR spectrum of compound **8a** at the level of B3LYP/LanL2DZ/6-31G.



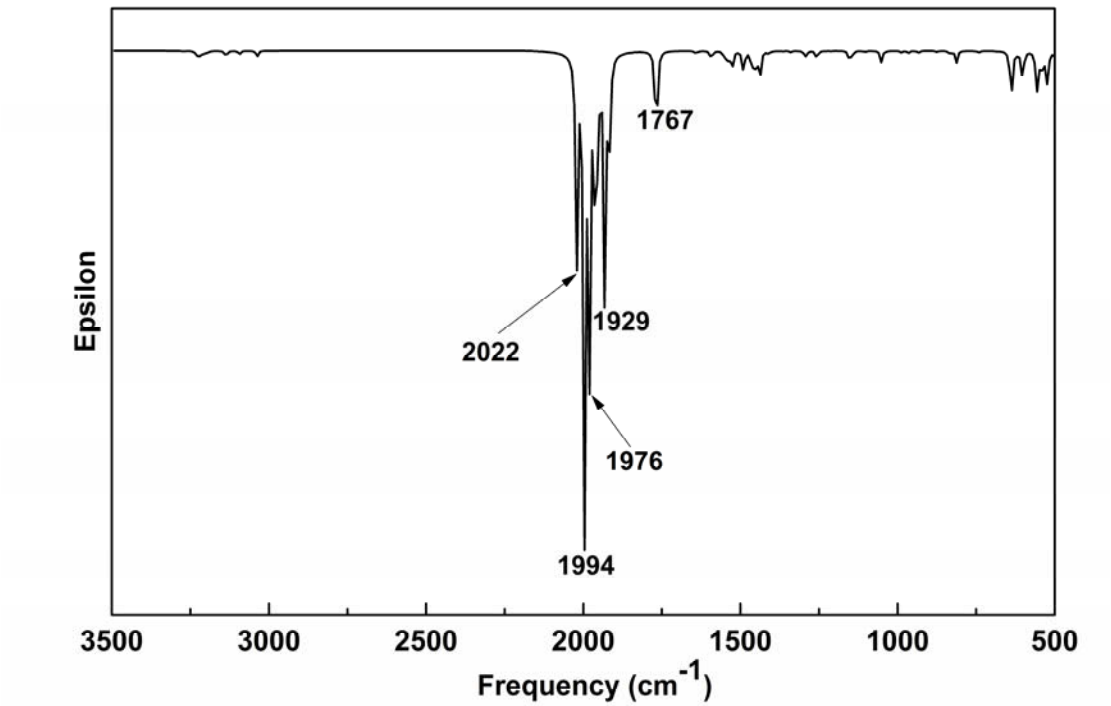
FT-IR spectrum of compound **8b**.



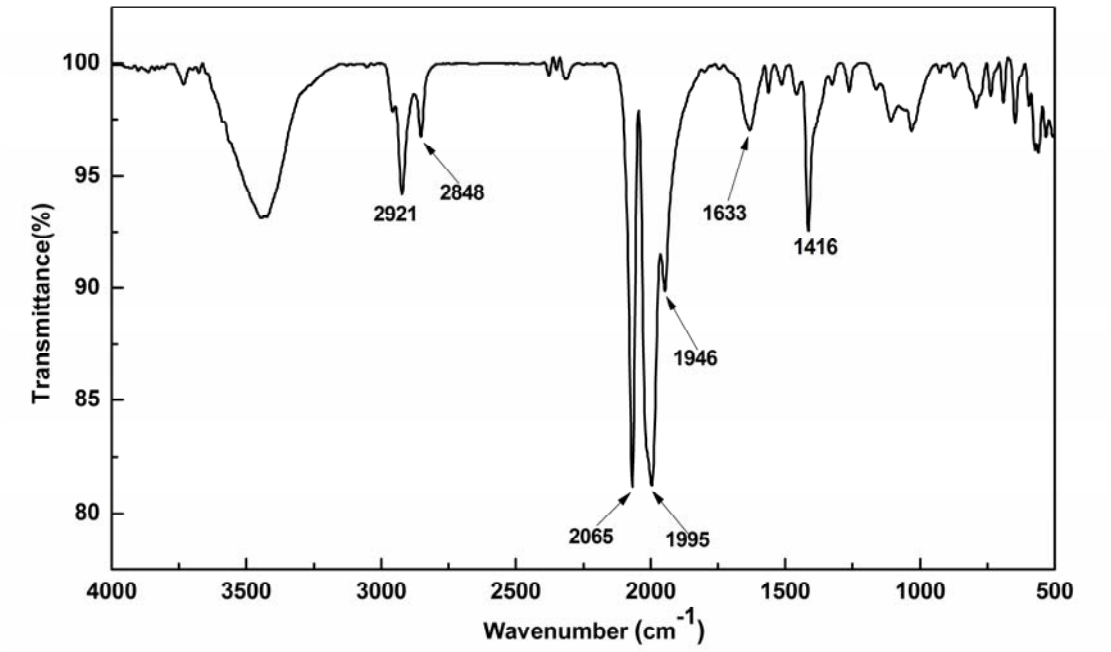
DFT-optimized IR spectrum of compound **8b** at the level of B3LYP/LanL2DZ/6-31G.



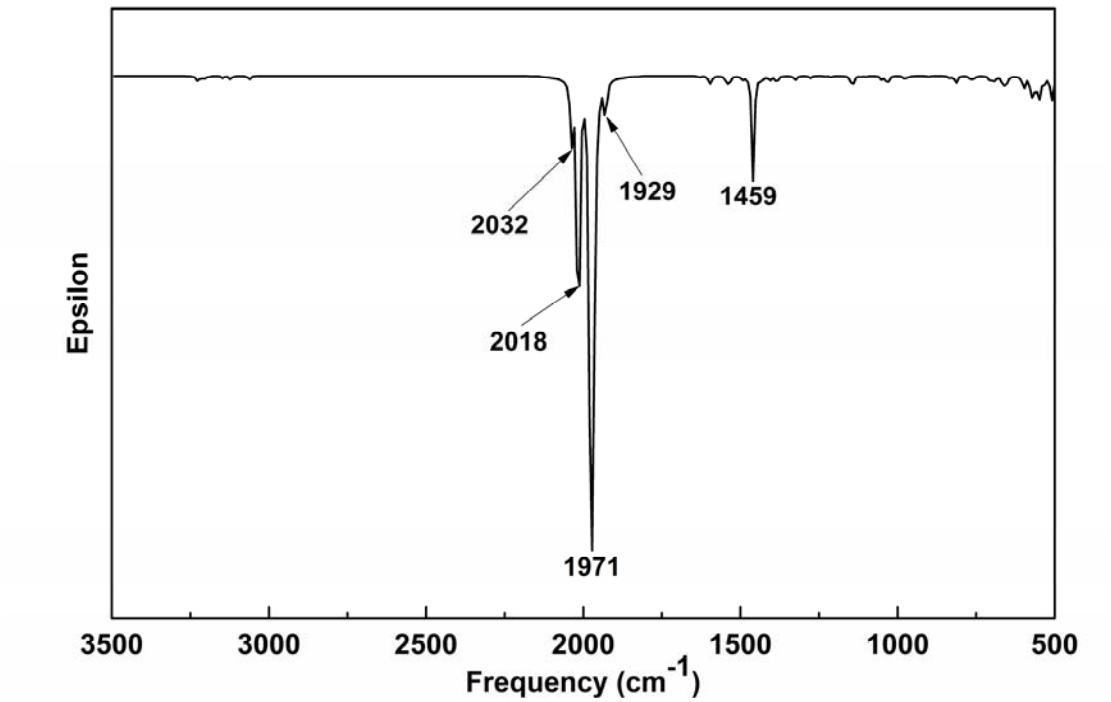
FT-IR spectrum of compound **9a**.



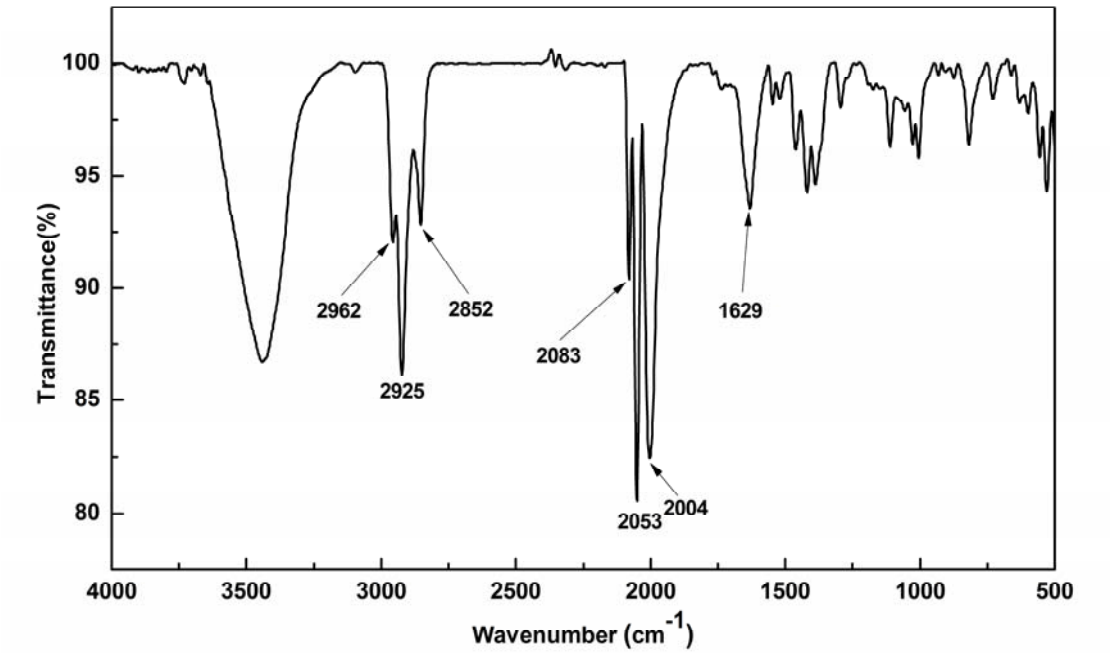
DFT-optimized IR spectrum of compound **9a** at the level of B3LYP/LanL2DZ/6-31G.



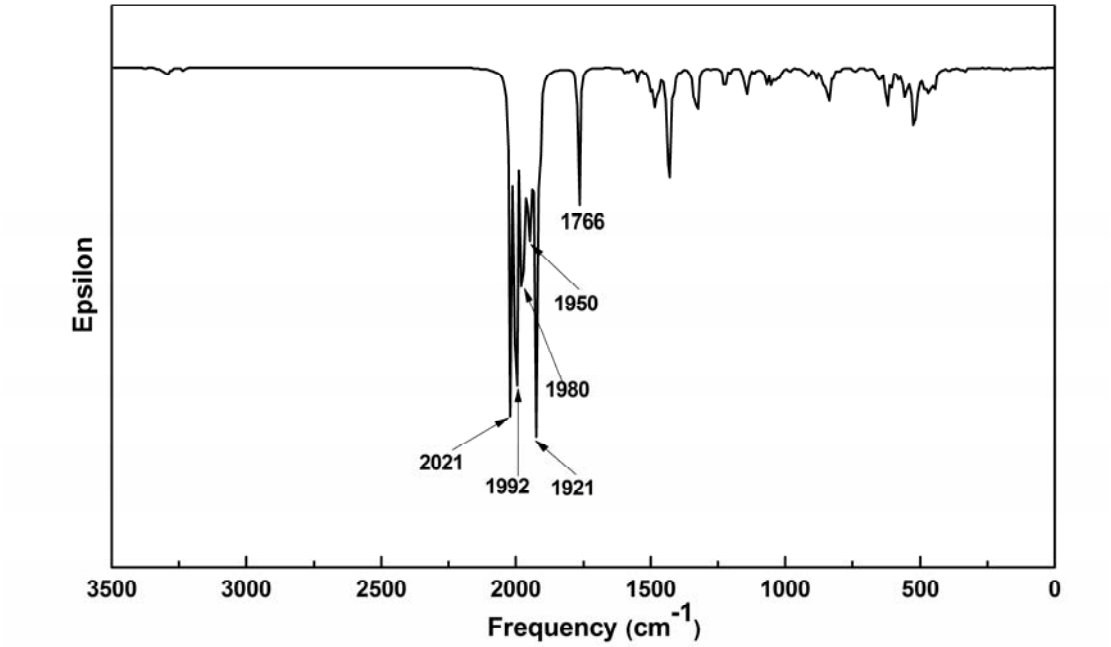
FT-IR spectrum of compound **9c**.



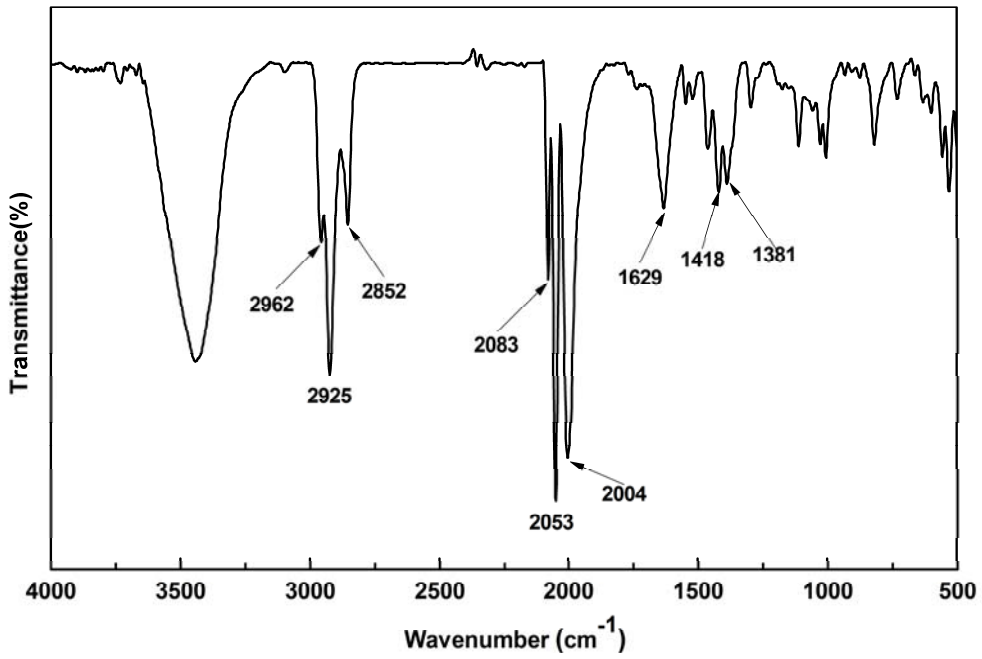
DFT-optimized IR spectrum of compound **9c** at the level of B3LYP/LanL2DZ/6-31G.



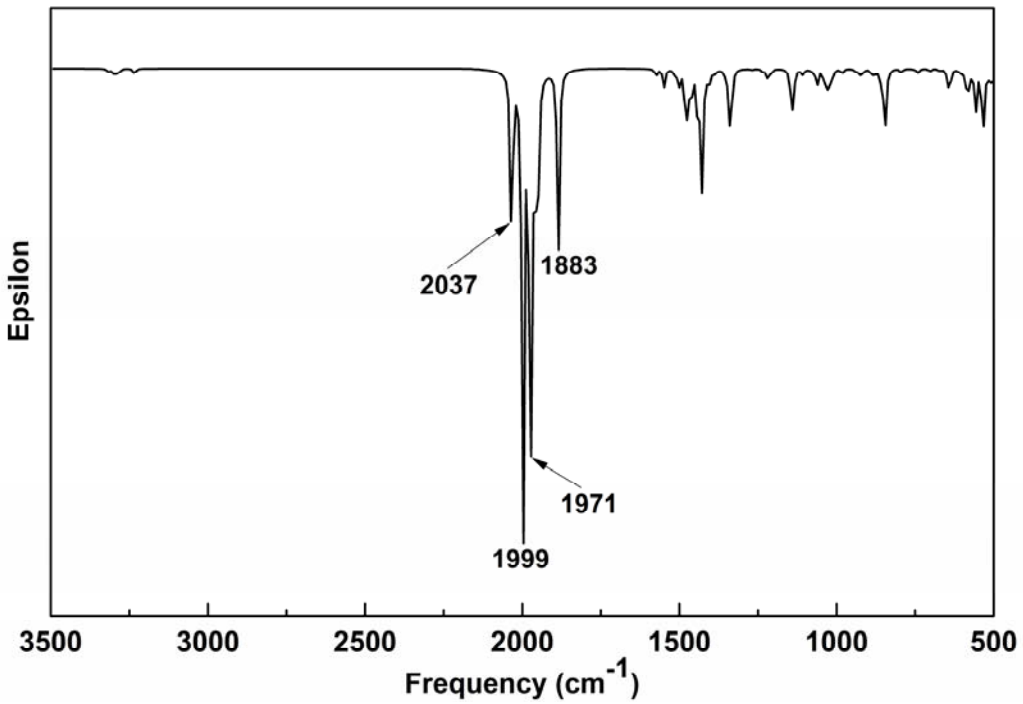
FT-IR spectrum of compound **10a**.



DFT-optimized IR spectrum of compound **10a** at the level of B3LYP/LanL2DZ/6-31G



FT-IR spectrum of compound **10b**.



DFT-optimized IR spectrum of compound **10b** at the level of B3LYP/LanL2DZ/6-31G.