Electronic Supplementary Information (ESI) for:

Unravelling the 6sp←6s Absorption Spectra of Bi(III) Complexes

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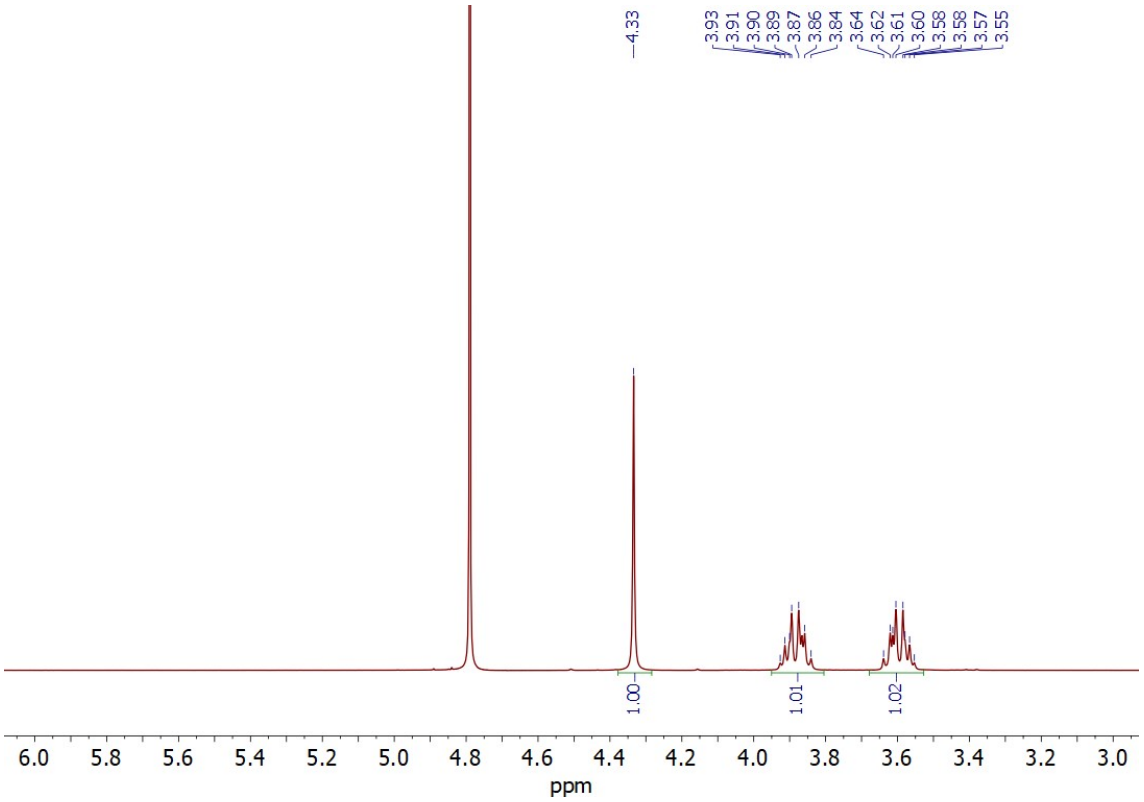

Figure S1. ^{1}H-NMR spectrum of compound **[Bi(NOTA)]** (400 MHz, D_2O, 298 K)

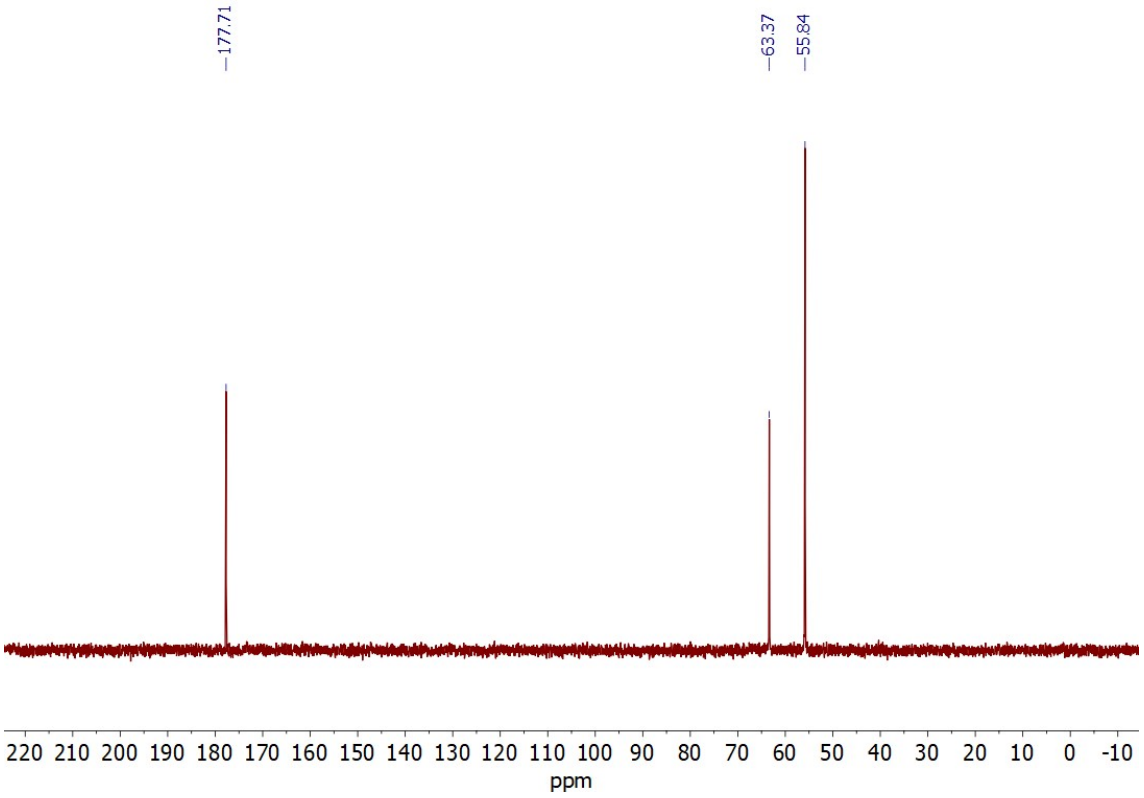

Figure S2. ^{13}C{^{1}H}-NMR spectrum of compound **[Bi(NOTA)]** (101 MHz, D_2O, 298 K)

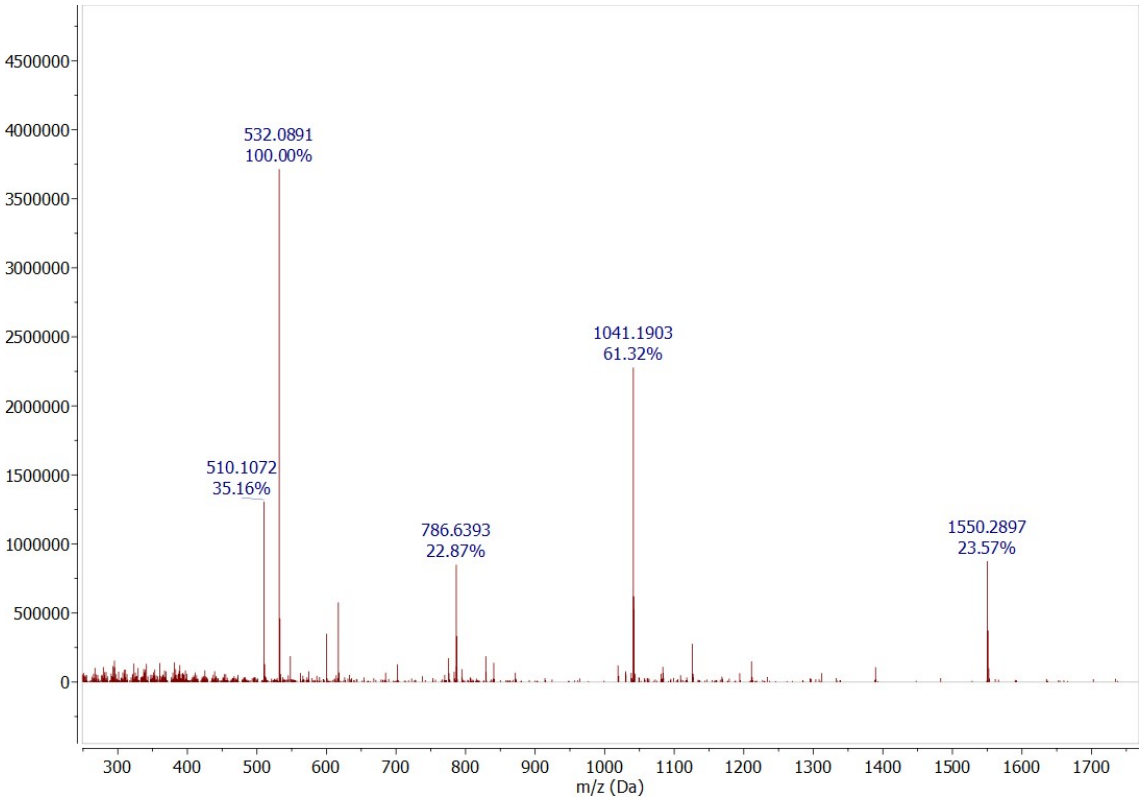

Figure S3. Experimental high resolution mass spectrum (ESI^+) of compound **[Bi(NOTA)]**.

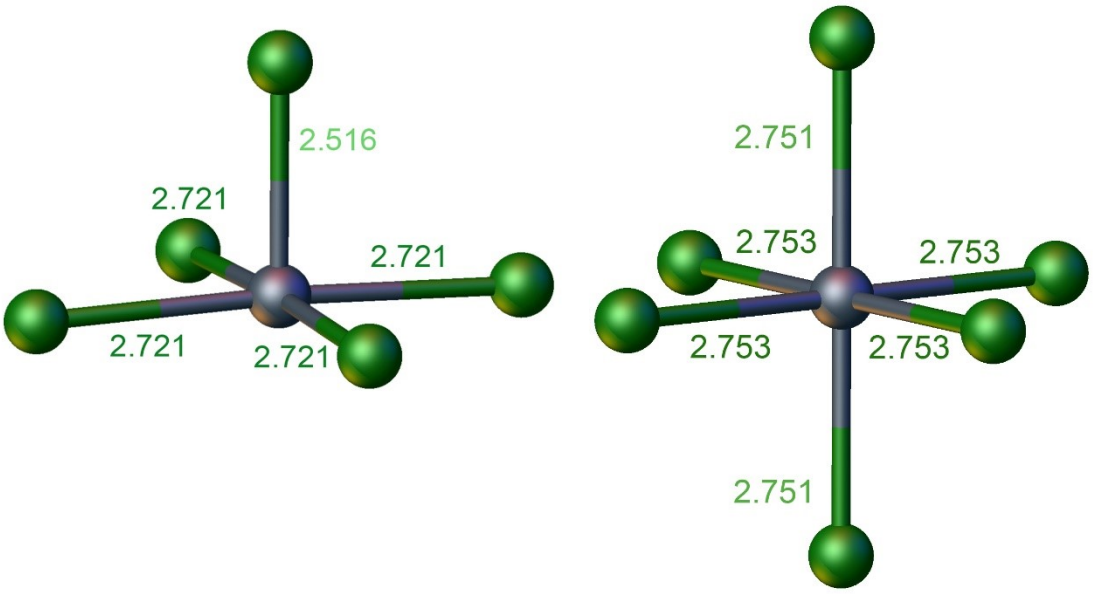

Figure S4. Optimised geometries of $[BiCl_5]^{2-}$ and $[BiCl_6]^{3-}$ obtained with DFT calculations. The numbers correspond to bond distances in Å.

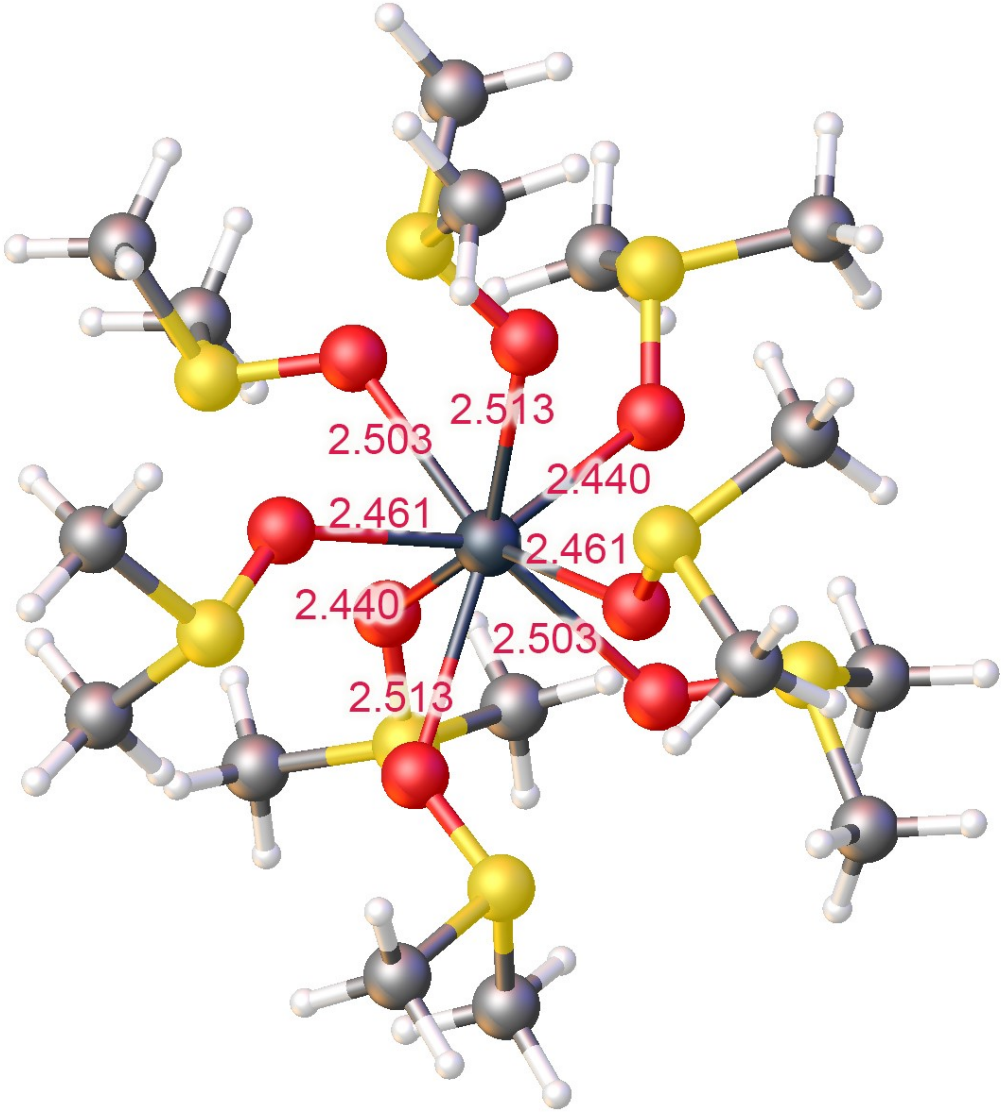

Figure S5. Optimised geometry of the $[Bi(DMSO)_8]^{3+}$ system obtained with DFT calculations. The numbers correspond to bond distances in Å.

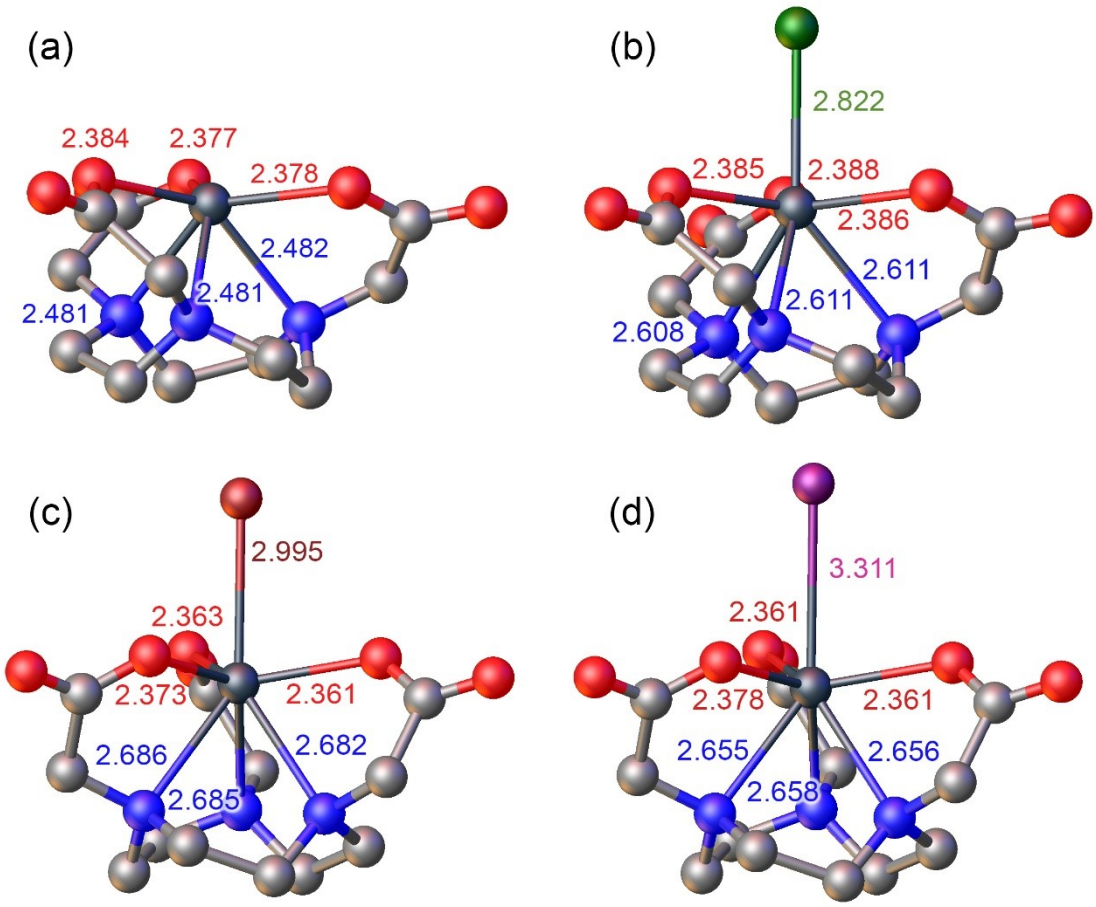

Figure S6. Optimised geometries of the [Bi(NOTA)] (a), $[Bi(NOTA)Cl]^-$ (b), $[Bi(NOTA)Br]^-$ (c) and $[Bi(NOTA)I]^-$ (d) obtained with DFT calculations. The numbers correspond to bond distances in Å.

Table S1. Cartesian coordinates obtained from geometry optimizations for the $[BiCl_6]^{3-}$ system.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	83	0.000403	-0.000553	0.000340
2	17	1.182712	1.342957	2.092362
3	17	-1.859783	2.012387	-0.240889
4	17	1.644416	1.313386	-1.774261
5	17	-1.181879	-1.344086	-2.091656
6	17	1.860604	-2.013502	0.241538
7	17	-1.643675	-1.314472	1.774897

E(RwB97XD) = -2976.7175547 Hartree
Zero-point correction = 0.004057
Thermal correction to Energy = 0.017444
Thermal correction to Enthalpy = 0.018388
Thermal correction to Gibbs Free Energy = -0.041233
Sum of electronic and zero-point Energies = -2976.713498
Sum of electronic and thermal Energies = -2976.700111
Sum of electronic and thermal Enthalpies = -2976.699167
Sum of electronic and thermal Free Energies = -2976.758788

Table S2. Cartesian coordinates obtained from geometry optimizations for the $[BiCl_5]^{2-}$ system (square pyramidal).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	83	0.058086	0.043159	-0.058510
2	17	1.180271	1.333395	2.058391
3	17	-1.832980	1.991411	-0.240596
4	17	1.559150	1.244134	-1.681972
5	17	-1.160292	-1.324173	-2.070876
6	17	1.852589	-1.982155	0.227849

E(RwB97XD) = -2516.3130116 Hartree
Zero-point correction = 0.003641
Thermal correction to Energy = 0.014646
Thermal correction to Enthalpy = 0.015590
Thermal correction to Gibbs Free Energy = -0.038143
Sum of electronic and zero-point Energies = -2516.309370
Sum of electronic and thermal Energies = -2516.298366
Sum of electronic and thermal Enthalpies = -2516.297422
Sum of electronic and thermal Free Energies = -2516.351155

Table S3. Cartesian coordinates obtained from geometry optimizations for the $[Bi(DMSO)_8]^{3+}$ system.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	83	0.000000	0.000000	0.030813
2	16	-3.273854	-0.840332	1.094145
3	8	-1.848688	-1.371028	1.014219
4	6	-3.748138	-1.053312	2.800399
5	1	-3.138625	-0.366043	3.382575
6	1	-3.576813	-2.083321	3.109018
7	1	-4.800463	-0.792605	2.908286
8	6	-4.277567	-2.117726	0.357691
9	1	-4.011747	-2.155261	-0.696420
10	1	-5.327047	-1.846281	0.467248
11	1	-4.078409	-3.073010	0.840446
12	16	3.273854	0.840332	1.094145
13	8	1.848688	1.371028	1.014219
14	6	4.277567	2.117726	0.357691
15	1	4.011747	2.155261	-0.696420
16	1	5.327047	1.846281	0.467248
17	1	4.078409	3.073010	0.840446
18	6	3.748138	1.053312	2.800399
19	1	3.138625	0.366043	3.382575
20	1	3.576813	2.083321	3.109018
21	1	4.800463	0.792605	2.908286
22	16	1.015347	3.144724	-1.488208
23	8	-0.138665	2.301013	-0.968672
24	6	1.123756	4.540820	-0.383882
25	1	1.452027	4.152552	0.576908
26	1	0.150121	5.019032	-0.293310
27	1	1.860379	5.239366	-0.779802
28	6	0.355383	3.976688	-2.922984
29	1	0.161440	3.218690	-3.678511
30	1	1.102402	4.678535	-3.292266
31	1	-0.562155	4.499385	-2.658272
32	16	0.776293	-2.661810	2.302225
33	8	1.135329	-1.279528	1.770704
34	6	-0.000000	-2.354986	3.878046
35	1	-0.930418	-1.836303	3.660836
36	1	0.651072	-1.741068	4.497668
37	1	-0.206073	-3.308877	4.362273
38	6	2.326946	-3.336308	2.868964
39	1	2.947990	-3.509972	1.993334
40	1	2.129044	-4.283981	3.369138
41	1	2.808775	-2.636712	3.549342
42	16	-1.015347	-3.144724	-1.488208

43	8	0.138665	-2.301013	-0.968672
44	6	-0.355383	-3.976688	-2.922984
45	1	-0.161440	-3.218690	-3.678511
46	1	-1.102402	-4.678535	-3.292266
47	1	0.562155	-4.499385	-2.658272
48	6	-1.123756	-4.540820	-0.383882
49	1	-1.452027	-4.152552	0.576908
50	1	-0.150121	-5.019032	-0.293310
51	1	-1.860379	-5.239366	-0.779802
52	16	-0.776293	2.661810	2.302225
53	8	-1.135329	1.279528	1.770704
54	6	-2.326946	3.336308	2.868964
55	1	-2.947990	3.509972	1.993334
56	1	-2.129044	4.283981	3.369138
57	1	-2.808775	2.636712	3.549342
58	6	0.000000	2.354986	3.878046
59	1	0.930418	1.836303	3.660836
60	1	-0.651072	1.741068	4.497668
61	1	0.206073	3.308877	4.362273
62	16	-2.201310	0.974980	-2.713650
63	8	-1.852331	0.007254	-1.590010
64	6	-3.407607	0.093823	-3.688477
65	1	-2.900722	-0.746300	-4.157204
66	1	-3.784769	0.764981	-4.459607
67	1	-4.217737	-0.252133	-3.049418
68	6	-3.272015	2.193606	-1.971478
69	1	-2.654036	2.761798	-1.280851
70	1	-4.083569	1.691728	-1.447651
71	1	-3.660949	2.843924	-2.754275
72	16	2.201310	-0.974980	-2.713650
73	6	3.272015	-2.193606	-1.971478
74	1	2.654036	-2.761798	-1.280851
75	1	4.083569	-1.691728	-1.447651
76	1	3.660949	-2.843924	-2.754275
77	6	3.407607	-0.093823	-3.688477
78	1	2.900722	0.746300	-4.157204
79	1	3.784769	-0.764981	-4.459607
80	1	4.217737	0.252133	-3.049418
81	8	1.852331	-0.007254	-1.590010

E(RwB97XD) = -4640.030995 Hartree
Zero-point correction = 0.652466
Thermal correction to Energy = 0.709983
Thermal correction to Enthalpy = 0.710927
Thermal correction to Gibbs Free Energy = 0.552671
Sum of electronic and zero-point Energies = -4639.378529
Sum of electronic and thermal Energies = -4639.321012
Sum of electronic and thermal Enthalpies = -4639.320068
Sum of electronic and thermal Free Energies = -4639.478324

Table S4. Cartesian coordinates obtained from geometry optimizations for the [Bi(NOTA)] system (Δ(δδδ) isomer).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	83	-0.176402	0.034977	0.237585
2	6	-1.867712	-1.583581	-1.963286
3	6	-0.704752	-1.020511	-2.790003
4	1	-0.538578	-1.663370	-3.656005
5	1	-1.021338	-0.043392	-3.157970
6	6	0.979798	-1.499096	2.809082
7	6	1.709311	-2.197676	1.655008
8	1	2.652833	-2.603828	2.023425
9	1	1.084702	-3.037384	1.346518
10	6	0.197028	3.215974	-0.022612
11	6	1.645486	2.712786	-0.038328
12	1	2.267871	3.432769	-0.572353
13	1	1.982195	2.687949	0.999221
14	6	1.117239	-2.177058	-1.708165
15	1	1.462605	-2.660399	-2.625565
16	1	0.319934	-2.794911	-1.296704
17	6	2.270753	-2.106906	-0.721885
18	1	2.547587	-3.123494	-0.446684
19	1	3.152342	-1.677945	-1.188967
20	6	2.964596	-0.314316	0.813957
21	1	3.934370	-0.797910	0.956135
22	1	2.688195	0.143961	1.763271
23	6	3.097525	0.759633	-0.252109
24	1	3.777644	1.525946	0.116782
25	1	3.562835	0.358943	-1.147721
26	6	1.580270	1.414854	-2.074235
27	1	2.383857	1.980313	-2.552905
28	1	0.651732	1.956625	-2.251240
29	6	1.497534	0.037667	-2.710756
30	1	1.208398	0.160056	-3.753494
31	1	2.473966	-0.437429	-2.729380
32	7	0.536862	-0.853009	-2.019301
33	7	1.935450	-1.326471	0.491856
34	7	1.795289	1.366825	-0.611934
35	8	0.279358	-0.469386	2.498372
36	8	-1.791986	-1.421378	-0.692651
37	8	-2.794738	-2.111112	-2.557603
38	8	1.078892	-1.978234	3.927502
39	8	0.006029	4.418796	0.064758
40	8	-0.717151	2.316569	-0.064439

E(RwB97XD) = -1298.6400072 Hartree
Zero-point correction = 0.322329

Thermal correction to Energy = 0.342753
Thermal correction to Enthalpy = 0.343697
Thermal correction to Gibbs Free Energy = 0.272245
Sum of electronic and zero-point Energies = -1298.317678
Sum of electronic and thermal Energies = -1298.297254
Sum of electronic and thermal Enthalpies = -1298.296310
Sum of electronic and thermal Free Energies = -1298.367762

Table S5. Cartesian coordinates obtained from geometry optimizations for the [Bi(NOTA)] system (Λ(δδδ) isomer).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	83	0.020136	-0.006911	-0.450930
2	6	2.508205	-0.531080	1.485624
3	6	1.465127	-1.579680	1.897974
4	1	1.578755	-2.427178	1.219343
5	1	1.676518	-1.932324	2.907334
6	6	-1.647978	-2.485315	-1.577663
7	6	-2.708902	-1.495549	-1.074731
8	1	-2.879784	-0.775076	-1.877080
9	1	-3.647205	-2.020241	-0.895672
10	6	-1.069821	2.971304	-0.870757
11	6	-0.676392	2.901451	0.611815
12	1	0.395691	3.101125	0.666884
13	1	-1.189051	3.686803	1.166993
14	6	-0.900563	-2.159767	1.741816
15	1	-0.990336	-2.644507	2.716650
16	1	-0.537637	-2.899064	1.033186
17	6	-2.276311	-1.658438	1.320759
18	1	-2.905719	-2.525270	1.123049
19	1	-2.750639	-1.126311	2.140092
20	6	-3.048254	0.459723	0.348720
21	1	-4.062007	0.219655	0.676893
22	1	-3.119145	0.978471	-0.603282
23	6	-2.400428	1.361230	1.392583
24	1	-2.915085	2.321209	1.376536
25	1	-2.556503	0.955587	2.387853
26	6	-0.178940	1.362807	2.439416
27	1	-0.578784	1.976227	3.249940
28	1	0.843754	1.679660	2.254098
29	6	-0.206772	-0.096335	2.876627
30	1	0.514642	-0.221442	3.683268
31	1	-1.174966	-0.342379	3.302407
32	7	0.090254	-1.069627	1.791073
33	7	-2.268226	-0.770882	0.126481
34	7	-0.941552	1.578846	1.196990
35	8	-0.432047	-2.177158	-1.308140

36	8	2.109896	0.338398	0.631077
37	8	3.634315	-0.611315	1.950920
38	8	-2.012050	-3.456761	-2.221199
39	8	-1.361581	4.057060	-1.347750
40	8	-1.016269	1.860858	-1.509555

E(RwB97XD) = -1298.6457176 Hartree
Zero-point correction = 0.323202
Thermal correction to Energy = 0.343214
Thermal correction to Enthalpy = 0.344159
Thermal correction to Gibbs Free Energy = 0.274832
Sum of electronic and zero-point Energies = -1298.322516
Sum of electronic and thermal Energies = -1298.302503
Sum of electronic and thermal Enthalpies = -1298.301559
Sum of electronic and thermal Free Energies = -1298.370886

Table S6. Cartesian coordinates obtained from geometry optimizations for the $[Bi(NOTA)Cl]^-$ system.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	83	0.032615	-0.080781	-0.816010
2	6	-0.904607	-3.165239	-0.334453
3	6	-0.185439	-2.917894	0.994052
4	1	-0.561296	-3.632792	1.732072
5	1	0.869977	-3.143707	0.826951
6	6	-2.226560	2.268276	-0.995256
7	6	-2.637027	1.632758	0.335780
8	1	-3.208292	2.367457	0.911074
9	1	-3.311891	0.808288	0.095742
10	6	3.168153	0.716776	-0.408323
11	6	2.559041	1.502770	0.756027
12	1	3.343375	1.695625	1.494053
13	1	2.243210	2.467820	0.353878
14	6	-1.690313	-1.258837	1.864152
15	1	-1.972656	-1.860283	2.736460
16	1	-2.336380	-1.565363	1.041184
17	6	-1.949575	0.205842	2.177187
18	1	-3.018414	0.326609	2.361179
19	1	-1.463535	0.488906	3.107381
20	6	-0.669020	2.213338	1.586475
21	1	-1.217209	2.824135	2.313706
22	1	-0.444765	2.854651	0.733727
23	6	0.636048	1.757741	2.219276
24	1	1.225660	2.646426	2.450349

25	1	0.448866	1.279103	3.177253
26	6	1.826265	-0.380615	2.054666
27	1	2.460360	-0.134969	2.914899
28	1	2.437447	-0.958728	1.361424
29	6	0.669122	-1.242605	2.532951
30	1	1.083161	-2.166364	2.940447
31	1	0.157001	-0.765110	3.364408
32	7	-0.302745	-1.541460	1.467057
33	7	-1.508603	1.108325	1.099805
34	7	1.403373	0.842894	1.356922
35	8	-1.143942	1.840837	-1.532128
36	8	-1.048371	-2.156143	-1.112321
37	8	-1.271986	-4.304118	-0.594138
38	8	-2.961085	3.117398	-1.484647
39	8	4.348508	0.900026	-0.678799
40	8	2.384305	-0.067976	-1.050849
41	17	0.254840	-0.360014	-3.524474

E(RwB97XD) = -1759.0435515 Hartree
Zero-point correction = 0.321596
Thermal correction to Energy = 0.344491
Thermal correction to Enthalpy = 0.345435
Thermal correction to Gibbs Free Energy = 0.267393
Sum of electronic and zero-point Energies = -1758.721955
Sum of electronic and thermal Energies = -1758.699061
Sum of electronic and thermal Enthalpies = -1758.698117
Sum of electronic and thermal Free Energies = -1758.776159

Table S7. Cartesian coordinates obtained from geometry optimizations for the $[Bi(NOTA)Br]^-$ system.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	83	-0.031757	-0.075417	-0.799838
2	6	3.084434	0.761799	-0.766659
3	6	2.987451	-0.311486	0.326663
4	1	3.033431	-1.280374	-0.176092
5	1	3.854455	-0.239795	0.985535
6	6	-0.842941	-3.125963	-0.131564
7	6	-1.729218	-2.302473	0.813112
8	1	-2.594026	-1.976196	0.230987
9	1	-2.095008	-2.941197	1.618948
10	6	-2.278691	2.228701	-0.600252
11	6	-1.125636	2.774607	0.253344
12	1	-0.411780	3.233157	-0.434915
13	1	-1.499918	3.560084	0.912153
14	6	1.427536	-1.472212	1.794112
15	1	2.110698	-1.615535	2.636761

16	1	1.581991	-2.295142	1.100365
17	6	-0.001398	-1.500694	2.324617
18	1	-0.200525	-2.507231	2.694841
19	1	-0.092526	-0.846317	3.187539
20	6	-1.969616	-0.114862	1.856450
21	1	-2.431770	-0.455328	2.788075
22	1	-2.760834	0.009330	1.121253
23	6	-1.289721	1.224234	2.119449
24	1	-2.067195	1.956423	2.341877
25	1	-0.678824	1.162499	3.016081
26	6	0.891027	2.130504	1.456948
27	1	0.822894	2.877366	2.253821
28	1	1.391735	2.595189	0.611111
29	6	1.717968	0.956375	1.969203
30	1	2.738376	1.308543	2.125966
31	1	1.360402	0.647333	2.947813
32	7	1.730824	-0.226558	1.074953
33	7	-1.035362	-1.121235	1.331915
34	7	-0.445286	1.717316	1.004755
35	8	0.012268	-2.461206	-0.815602
36	8	1.975153	1.121446	-1.297149
37	8	4.190962	1.174617	-1.087450
38	8	-1.023588	-4.334148	-0.203941
39	8	-3.230883	2.959810	-0.837871
40	8	-2.131874	1.034063	-1.038687
41	35	-0.228162	-0.381867	-3.853486

E(RwB97XD) = -3873.0597367 Hartree
Zero-point correction = 0.322986
Thermal correction to Energy = 0.345592
Thermal correction to Enthalpy = 0.346536
Thermal correction to Gibbs Free Energy = 0.269221
Sum of electronic and zero-point Energies = -3872.736751
Sum of electronic and thermal Energies = -3872.714145
Sum of electronic and thermal Enthalpies = -3872.713201
Sum of electronic and thermal Free Energies = -3872.790515

Table S8. Cartesian coordinates obtained from geometry optimizations for the $[Bi(NOTA)I]^-$ system.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	83	-0.034768	-0.071167	-0.774920
2	6	3.074903	0.762115	-0.766173
3	6	2.981558	-0.314268	0.324368
4	1	3.023779	-1.282277	-0.180206
5	1	3.850084	-0.245550	0.981227
6	6	-0.840787	-3.121331	-0.128816

7	6	-1.728678	-2.299145	0.815964
8	1	-2.592898	-1.970645	0.234381
9	1	-2.095106	-2.938284	1.620846
10	6	-2.279472	2.229240	-0.587331
11	6	-1.122225	2.775521	0.260537
12	1	-0.408738	3.229551	-0.430813
13	1	-1.491224	3.562447	0.920121
14	6	1.428190	-1.473659	1.800613
15	1	2.112362	-1.612001	2.642962
16	1	1.584237	-2.297798	1.109225
17	6	-0.000691	-1.501688	2.331338
18	1	-0.202191	-2.508077	2.700058
19	1	-0.091324	-0.847759	3.194414
20	6	-1.968383	-0.113623	1.866999
21	1	-2.425980	-0.455889	2.799803
22	1	-2.762447	0.010350	1.135152
23	6	-1.287320	1.225015	2.128674
24	1	-2.063611	1.958304	2.350290
25	1	-0.675389	1.163986	3.024670
26	6	0.893352	2.130286	1.466443
27	1	0.822203	2.872521	2.266886
28	1	1.393374	2.599975	0.623433
29	6	1.720219	0.954215	1.974010
30	1	2.741973	1.303560	2.126919
31	1	1.365652	0.643943	2.953194
32	7	1.727634	-0.228372	1.078153
33	7	-1.034310	-1.118977	1.338483
34	7	-0.442702	1.716697	1.012470
35	8	0.027539	-2.457534	-0.797047
36	8	1.961124	1.135314	-1.277763
37	8	4.180544	1.163869	-1.101989
38	8	-1.033574	-4.326418	-0.215178
39	8	-3.230252	2.961421	-0.825548
40	8	-2.135528	1.032199	-1.020223
41	53	-0.226056	-0.397907	-4.120488

E(RwB97XD) = -1594.6326966 Hartree
Zero-point correction = 0.322699
Thermal correction to Energy = 0.345423
Thermal correction to Enthalpy = 0.346367
Thermal correction to Gibbs Free Energy = 0.267722
Sum of electronic and zero-point Energies = -1594.309997
Sum of electronic and thermal Energies = -1594.287274
Sum of electronic and thermal Enthalpies = -1594.286330
Sum of electronic and thermal Free Energies = -1594.364974

Sample ORCA input file.

```
#
# NEVPT2_BiNOTA2
#
! RIJCOSX tightscf Normalprint dkh2 autoaux moread DKH-def2-
TZVPP
%moinp "NEVPT2_BiNOTA.gbw"
%basis
newgto Bi "SARC-DKH-TZVPP" end
newauxgto Bi "autoaux" end
end
%pal
  nprocs 24
end
% maxcore 55000
* xyz 0 1
 Bi                 0.00030100    0.00019100   -0.77704500
 C                 -1.70867900   -2.69600100   -0.61760700
 C                 -2.39542700   -1.73988100    0.36820100
 H                 -3.08204100   -1.12121500   -0.21276200
 H                 -2.98753500   -2.31090300    1.08317900
 C                 -1.48880700    2.82018200   -0.61948000
 C                 -0.31299100    2.94306400    0.36056800
 H                  0.56331600    3.22700900   -0.22552700
 H                 -0.50876600    3.74452400    1.07268500
 C                  3.19290500   -0.12774000   -0.61913400
 C                  2.70678900   -1.20302600    0.36328000
 H                  2.51259200   -2.10456800   -0.22133500
 H                  3.49681600   -1.43454400    1.07747500
 C                 -2.08843300    0.32297600    1.63617100
 H                 -2.69217300    0.04535400    2.50321000
 H                 -2.75512400    0.73128100    0.88169000
 C                 -1.07488700    1.37550100    2.06770200
 H                 -1.61800200    2.28835000    2.30931000
 H                 -0.58195800    1.07003300    2.98594000
 C                  1.32508700    1.65070600    1.62980800
 H                  1.38793700    2.31511600    2.49446800
 H                  2.01068500    2.02142900    0.87287200
 C                  1.72987200    0.24754800    2.06494000
 H                  2.79177800    0.26189000    2.30750800
 H                  1.21759400   -0.02311800    2.98351600
 C                  0.76786700   -1.96993400    1.63113100
 H                  1.31173600   -2.35747900    2.49549300
 H                  0.74487700   -2.74916600    0.87422200
 C                 -0.64877300   -1.61821000    2.06753000
 H                 -1.16706700   -2.54464700    2.31216300
 H                 -0.62592400   -1.03860100    2.98554700
 N                 -1.43501400   -0.86336100    1.05462400
 N                 -0.03033400    1.67620800    1.05152900
 N                  1.46828000   -0.81004100    1.05152600
 O                 -1.67406400    1.65240600   -1.11754600
 O                 -0.60739600   -2.27344000   -1.12110700
 O                 -2.25817500   -3.75262700   -0.88715800
 O                 -2.13259800    3.82159200   -0.88985700
 O                  4.38340800   -0.07522300   -0.88644800
 O                  2.27740200    0.61637500   -1.12129700
*
```

```
%cpcm smd true # turn on SMD
SMDsolvent "water" # specify the name of solvent from the list
end
%method
AngularGrid 7
AngularGridX 5
IntAccX 4.5
end
%rel
picturechange true
FiniteNuc true
end
%casscf
nel 2
norb 9
mult 3,1
nroots 6,10
trafostep ri
PTMethod sc_nevpt2
PTSettings
QDType QD_VanVleck
end
rel
DoSOC true
NInitStates 8
end
end
```

Table S9. Last orbital frozen during the NEVPT2 step and orbitals included in the active space.

	Last orbital frozen	Orbitals in the Active Space
Bi(III)	33	39-42
$[BiCl_6]^{3-}$	63	93-101
$[BiCl_5]^{2-}$	58	84-92
$[Bi(DMSO)_8]^{3+}$	97	207-210
[Bi(NOTA)]	54	120-128
$[Bi(NOTA)Cl]^{-}$	59	129-137
$[Bi(NOTA)Br]^{-}$	63	138-146
$[Bi(NOTA)I]^{-}$	72	147-155