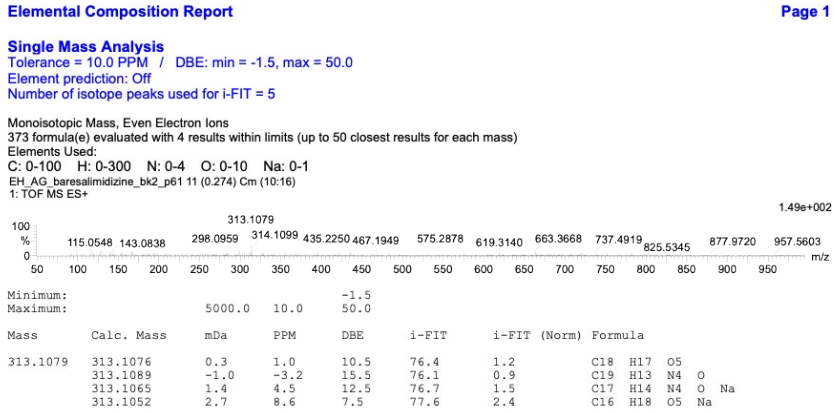
Mass Spectra

Analysis was performed using a syringe pump with a syringe filled with acetonitrile or sample diluted in acetonitrile at flow rate of 2 to 10 µL/min into a quadrupole time-of-flight mass spectrometer (Q-Tof Premier, Waters) with electrospray ionization (ESI) in positive mode. Data were collected and processed with Masslynx software (V4.1). The capillary voltage was set at 3.1 kV, the sample cone voltage was 30 V, and the extraction cone was 4.3 V. The source and desolvation temperature were maintained at 105 and 300 °C, respectively, with the desolvation gas flow set at 500 L/h. The Time-of-Flight mass spectrometer scan was 1 s long from 50 to 3000 m/z with a 0.1 s inter-scan delay in the centroid data format. A lock mass was used to correct instrument accuracy with a 0.1 µM solution of HP 1221 (Agilent part number G1969-85003).



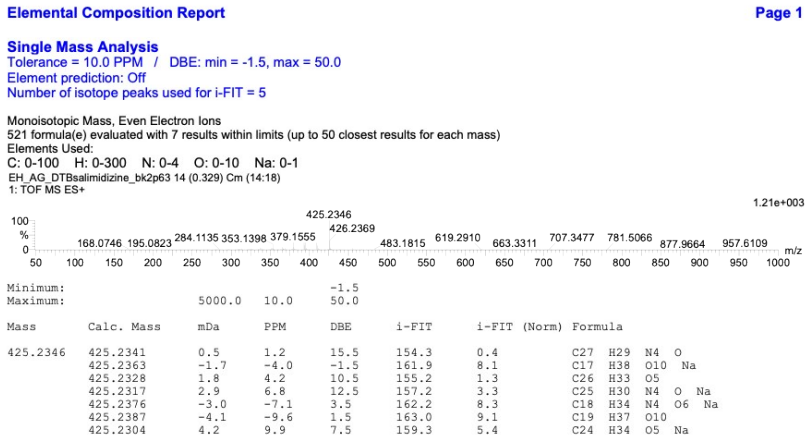
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
373 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-300 N: 0-4 O: 0-10 Na: 0-1
EH_AG_baresalimidizine_bk2_p61 11 (0.274) Cm (10:16)
1: TOF MS ES+

Minimum:				-1.5			
Maximum:		5000.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
313.1079	313.1076	0.3	1.0	10.5	76.4	1.2	C18 H17 O5
	313.1089	-1.0	-3.2	15.5	76.1	0.9	C19 H13 N4 O
	313.1065	1.4	4.5	12.5	76.7	1.5	C17 H14 N4 O Na
	313.1052	2.7	8.6	7.5	77.6	2.4	C16 H18 O5 Na

Figure S39. Mass Spectra of Salimidizine (L1)



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
521 formula(e) evaluated with 7 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-300 N: 0-4 O: 0-10 Na: 0-1
EH_AG_DTBsalimidizine_bk2p63 14 (0.329) Cm (14:18)
1: TOF MS ES+

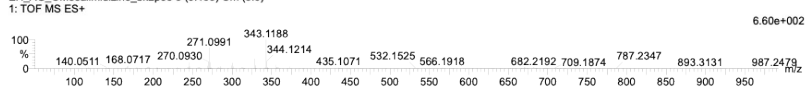
Minimum:				-1.5			
Maximum:		5000.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
425.2346	425.2341	0.5	1.2	15.5	154.3	0.4	C27 H29 N4 O
	425.2363	-1.7	-4.0	-1.5	161.9	8.1	C17 H38 O10 Na
	425.2328	1.8	4.2	10.5	155.2	1.3	C26 H33 O5
	425.2317	2.9	6.8	12.5	157.2	3.3	C25 H30 N4 O Na
	425.2376	-3.0	-7.1	3.5	162.2	8.3	C18 H34 N4 O6 Na
	425.2387	-4.1	-9.6	1.5	163.0	9.1	C19 H37 O10
	425.2304	4.2	9.9	7.5	159.3	5.4	C24 H34 O5 Na

Figure S40. Mass Spectra of DTB-Salimidizine (L2)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
418 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-300 N: 0-4 O: 0-10 Na: 0-1
EH_AG_OMesalimidizine_bk2p65 8 (0.183) Cm (8:9)
1: TOF MS ES+



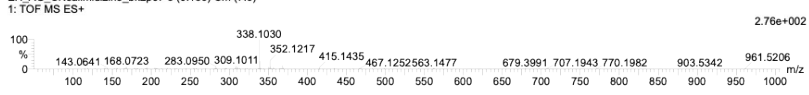
Minimum:				-1.5							
Maximum:		5000.0	10.0	50.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula				
343.1188	343.1182	0.6	1.7	10.5	96.6	1.3	C19	H19	O6		
	343.1195	-0.7	-2.0	15.5	96.2	0.8	C20	H15	N4	O2	
	343.1171	1.7	5.0	12.5	98.5	3.2	C18	H16	N4	O2	Na
	343.1211	-2.3	-6.7	16.5	96.8	1.5	C23	H16	N2	Na	
	343.1158	3.0	8.7	7.5	100.4	5.1	C17	H20	O6	Na	

Figure S41. Mass Spectra of OMe-Salimidizine (L3)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
560 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-300 N: 0-6 O: 0-10 Na: 0-1
EH_AG_CNsalimidizine_bk2p67 8 (0.183) Cm (7:9)
1: TOF MS ES+



Minimum:				-1.5							
Maximum:		5000.0	10.0	50.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula				
338.1030	338.1028	0.2	0.6	12.5	51.8	1.1	C19	H16	N	O5	
	338.1042	-1.2	-3.5	17.5	51.5	0.9	C20	H12	N5	O	
	338.1018	1.2	3.5	14.5	52.1	1.5	C18	H13	N5	O	Na
	338.1004	2.6	7.7	9.5	53.5	2.9	C17	H17	N	O5	Na
	338.1063	-3.3	-9.8	0.5	58.1	7.5	C10	H21	N	O10	Na

Figure S42. Mass Spectra of CN-Salimidizine (L4)

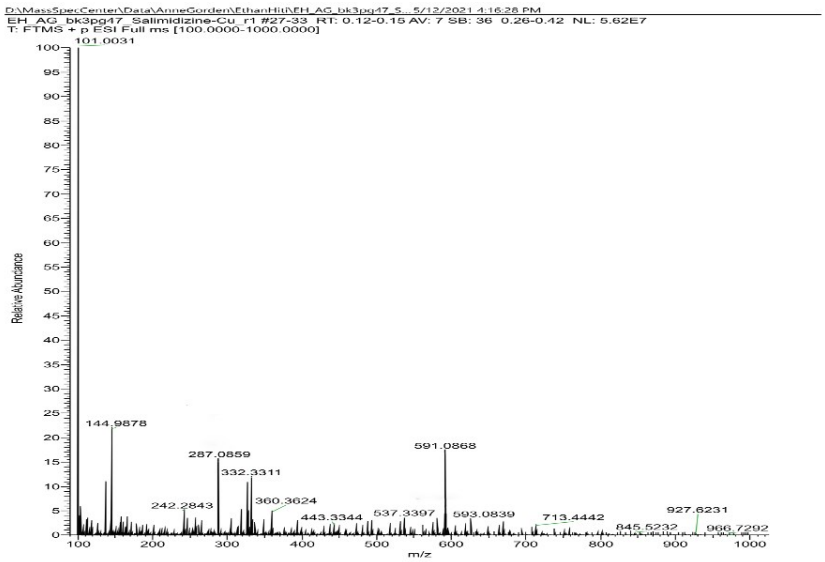


Figure S43. Mass spectra of Salimidizine (L1)-Cu complex

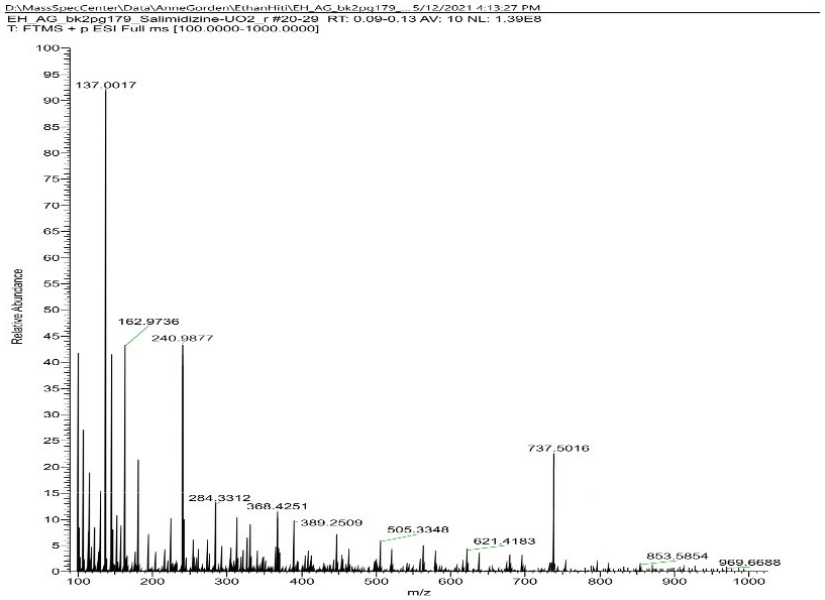


Figure S44. Mass spectra of Salimidizine (L1)-UO_2 complex

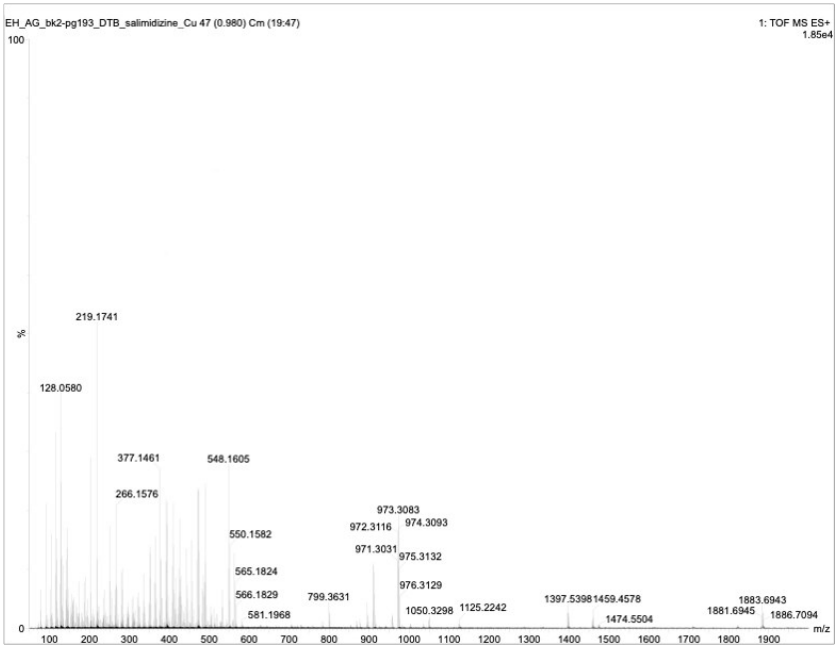


Figure S45. Mass spectra of DTB salimidizine (L2)-Cu complex

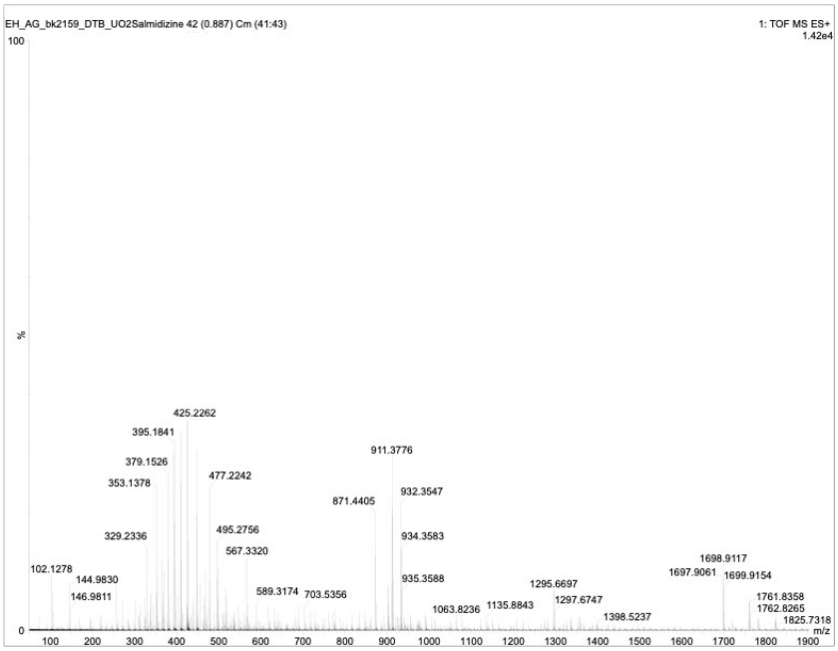


Figure S46. Mass spectra of DTB salimidizine (L2)-UO2 complex

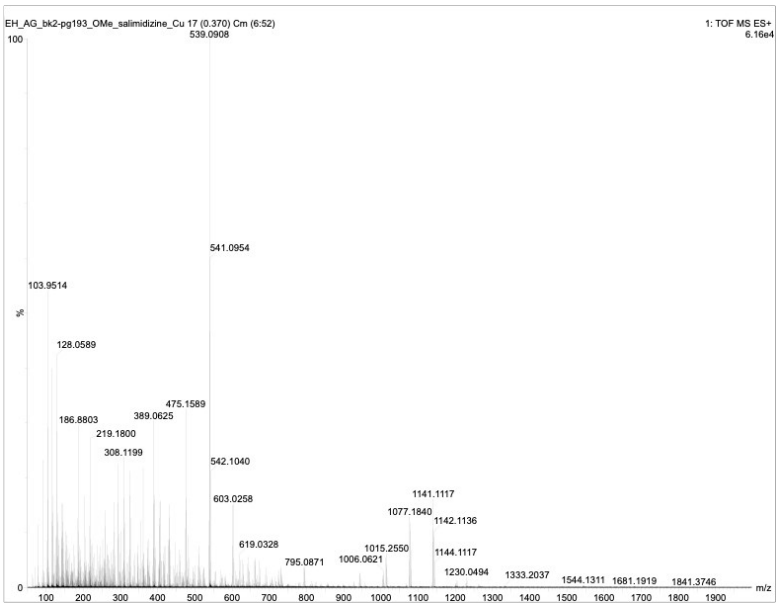


Figure S47. Mass spectra of OMe Salimidizine (L3)-Cu Complex

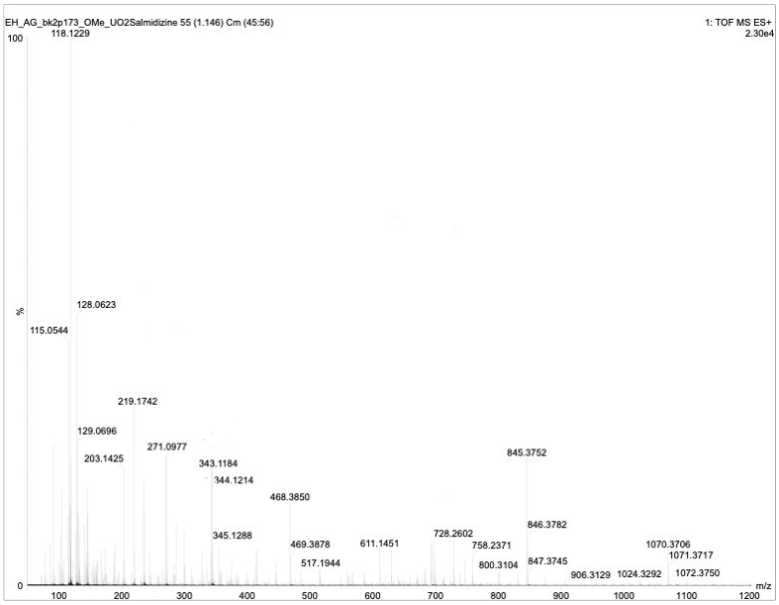


Figure S48.Mass spectra of OMe Salimidizine (L3)-UO2 Complex

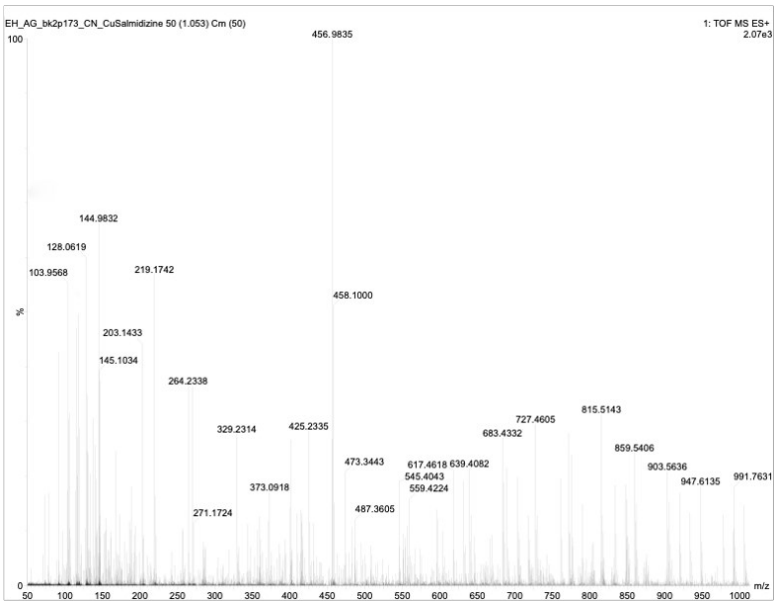


Figure S49. Mass spectra of CN-Salimidizine (L4)- Cu complex

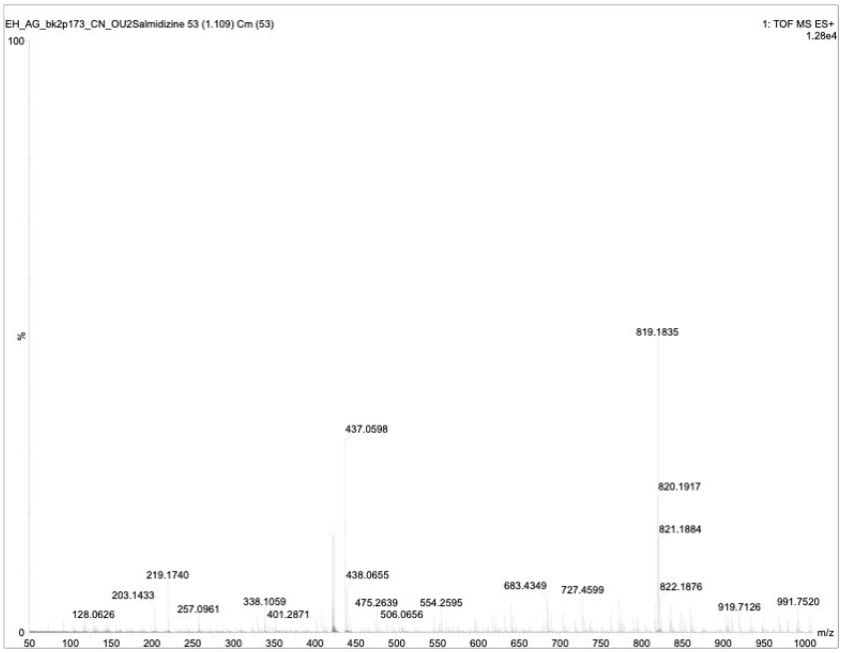


Figure S50. Mass spectra of CN-Salimidizine (L4)- UO2 complex

Computational Details (Table S1)

B3LYP/cc-pVDZ(-PP) Cartesian coordinates (in Å) of the optimal geometries for the ground and pertinent excited electronic state of the investigated uranyl and copper complexes.

$L_1Cu^{2+}(AcO)$							
Ground State				**Excited State**			
C	5.942091	-2.399390	0.000228	C	5.993400	-2.400341	0.004794
C	5.552291	-1.075670	0.000218	C	5.571285	-1.113640	-0.305673
C	4.981401	-3.434910	0.000108	C	5.048269	-3.359241	0.371211
C	4.176431	-0.696130	0.000078	C	4.182433	-0.740403	-0.257984
C	3.199051	-1.751660	0.000018	C	3.207124	-1.763420	0.065838
C	3.641861	-3.102570	0.000008	C	3.666026	-3.022558	0.400444
H	7.006511	-2.647610	0.000338	H	7.054083	-2.654147	-0.028358
H	6.281631	-0.264240	0.000288	H	6.273034	-0.325655	-0.582315
H	2.912391	-3.916330	-0.000112	H	2.959957	-3.797059	0.706179
H	5.290600	-4.480900	0.000078	H	5.354621	-4.372482	0.633624
C	1.786801	-1.456360	0.000048	C	1.754273	-1.467339	0.043146
N	1.210981	-0.242540	0.000058	N	1.195145	-0.260658	0.104400
N	0.817981	-2.433790	0.000108	N	0.805169	-2.436356	-0.015819
C	-0.177549	-0.430700	0.000058	C	-0.204811	-0.446049	0.082724
C	-0.435629	-1.845650	0.000068	C	-0.460167	-1.833504	0.000964
C	-1.212049	0.476940	0.000038	C	-1.250102	0.475355	0.107105
C	-1.698709	-2.382040	0.000048	C	-1.739831	-2.365196	-0.059829
C	-2.794659	-1.468950	-0.000002	C	-2.828495	-1.455347	-0.035591
C	-2.545609	-0.031620	0.000008	C	-2.576830	-0.019181	0.047368
N	-3.564129	0.848260	-0.000022	N	-3.596715	0.876876	0.072147
N	-4.044619	-1.964670	-0.000022	N	-4.086180	-1.955392	-0.092660
C	-4.807909	0.347780	-0.000052	C	-4.846648	0.371343	0.016958
C	-5.052499	-1.079140	-0.000042	C	-5.094640	-1.055574	-0.067222
C	-5.925569	1.242910	-0.000082	C	-5.961642	1.258538	0.040795
C	-6.403969	-1.550450	-0.000082	C	-6.441373	-1.512788	-0.124032
C	-7.205719	0.751030	-0.000102	C	-7.255538	0.775580	-0.015712
C	-7.447029	-0.659590	-0.000102	C	-7.497232	-0.619766	-0.098870
H	-1.047789	1.553040	0.000068	H	-1.088344	1.549433	0.177057
H	-1.905199	-3.452730	0.000038	H	-1.950590	-3.433203	-0.125937
H	-5.711569	2.313180	-0.000082	H	-5.746205	2.327091	0.105229
H	-8.055719	1.437020	-0.000122	H	-8.099177	1.469794	0.003622
H	-8.476889	-1.023760	-0.000122	H	-8.524981	-0.988353	-0.142936
H	-6.560179	-2.630710	-0.000082	H	-6.599552	-2.591421	-0.187342
O	3.902781	0.576380	-0.000012	O	3.879294	0.484778	-0.486618
H	0.999741	-3.426850	-0.000102	H	0.982011	-3.421232	-0.155750
Cu	2.224141	1.435370	-0.000232	Cu	2.198700	1.412708	-0.069877
C	1.322201	5.205280	0.000818	C	1.525467	5.203537	0.224477
C	1.691961	3.750090	-0.000212	C	1.793888	3.734978	0.106009
H	2.219371	5.835850	-0.008362	H	2.346810	5.786474	-0.209025
H	0.714551	5.424670	0.892288	H	1.403926	5.460667	1.288314

H	0.697001	5.422160	-0.878942	H	0.575940	5.442106	-0.277165
O	2.900071	3.365030	-0.002272	O	2.895494	3.282595	-0.349185
O	0.781011	2.849270	0.001568	O	0.920847	2.874908	0.468705
$L_1Cu^{2+}(AcO)(W)$							
Ground State				**Excited State**			
C	-5.394811	-3.203752	-0.068122	C	-5.466654	-3.166207	-0.012159
C	-5.152433	-1.849497	-0.170893	C	-5.180929	-1.841719	-0.323732
C	-4.331481	-4.119269	0.102071	C	-4.430093	-4.022399	0.359549
C	-3.829005	-1.314540	-0.106381	C	-3.839660	-1.324653	-0.271992
C	-2.747669	-2.251165	0.038908	C	-2.768481	-2.242566	0.054244
C	-3.038950	-3.638365	0.150172	C	-3.091125	-3.543086	0.390801
H	-6.423166	-3.571453	-0.113597	H	-6.495340	-3.528767	-0.048860
H	-5.963501	-1.130662	-0.296657	H	-5.961486	-1.133440	-0.604926
H	-2.227040	-4.354224	0.302640	H	-2.307348	-4.238338	0.698672
H	-4.527656	-5.187874	0.198709	H	-4.630996	-5.061410	0.622987
C	-1.380335	-1.798092	0.045078	C	-1.355957	-1.792672	0.026802
N	-0.941144	-0.527953	0.084022	N	-0.927679	-0.534839	0.089868
N	-0.313492	-2.666577	0.002447	N	-0.313669	-2.659563	-0.044846
C	0.460862	-0.568792	0.052780	C	0.487227	-0.576905	0.056475
C	0.868944	-1.947926	-0.004689	C	0.883213	-1.930541	-0.031925
C	1.399890	0.438404	0.055662	C	1.437524	0.442557	0.071996
C	2.180290	-2.348305	-0.057989	C	2.209214	-2.331119	-0.099624
C	3.176336	-1.327382	-0.054589	C	3.202331	-1.318260	-0.074736
C	2.778900	0.074045	0.003779	C	2.808152	0.084110	0.010040
N	3.698678	1.056386	0.011153	N	3.731479	1.078357	0.035576
N	4.470378	-1.688558	-0.105281	N	4.503965	-1.689254	-0.133759
C	4.987699	0.690432	-0.040062	C	5.025962	0.701944	-0.023354
C	5.379874	-0.702016	-0.099370	C	5.416160	-0.692894	-0.109601
C	6.004914	1.697998	-0.035909	C	6.045543	1.697384	-0.000660
C	6.772462	-1.027868	-0.152051	C	6.802493	-1.012287	-0.168673
C	7.328916	1.344029	-0.087524	C	7.380878	1.346961	-0.059889
C	7.716185	-0.032345	-0.146142	C	7.762037	-0.017380	-0.144424
H	1.127657	1.490701	0.106090	H	1.175096	1.497054	0.132929
H	2.495106	-3.391294	-0.104420	H	2.524384	-3.372734	-0.171741
H	5.680541	2.739160	0.008830	H	5.723821	2.738794	0.064158
H	8.102126	2.115509	-0.084546	H	8.150438	2.122423	-0.042152
H	8.777988	-0.285584	-0.186678	H	8.821704	-0.279925	-0.190637
H	7.040742	-2.084933	-0.196360	H	7.068568	-2.069345	-0.233289
O	-3.691732	-0.026406	-0.192668	O	-3.658344	-0.076460	-0.500333
H	-0.393278	-3.666990	-0.110063	H	-0.391855	-3.655455	-0.196468
Cu	-2.142818	1.057305	0.075016	Cu	-2.105586	1.061632	-0.003671
O	-0.844718	2.304377	0.949531	O	-0.948918	2.256791	1.066788
H	-1.394228	3.237666	0.918241	H	-1.538126	3.134415	1.162847
H	-0.635106	2.096140	1.872422	H	-0.564883	1.970221	1.907516
C	-4.159367	4.754154	-0.730664	C	-4.171763	4.717098	-0.718750
C	-3.123312	3.813244	-0.153972	C	-3.191971	3.761891	-0.074879

H	-4.121690	4.712376	-1.829933	H	-3.894247	4.865359	-1.773998
H	-3.986703	5.780006	-0.382632	H	-4.171488	5.678926	-0.191790
H	-5.163318	4.416439	-0.429588	H	-5.179619	4.274777	-0.708525
O	-2.268557	4.266757	0.654102	O	-2.510830	4.140239	0.907456
O	-3.199386	2.594288	-0.540323	O	-3.133148	2.588389	-0.609060
$L_1UO_2^{2+}$(AcO)							
Ground State				**Excited State**			
C	4.544877	3.984935	-0.003402	C	-4.831834	3.890710	-0.088207
C	4.366077	2.699401	-0.493735	C	-4.611812	2.618782	0.421394
C	3.468760	4.696165	0.555993	C	-3.761341	4.603957	-0.631784
C	3.103003	2.067001	-0.441600	C	-3.302421	2.019187	0.395413
C	1.998909	2.795265	0.104019	C	-2.186489	2.798335	-0.110354
C	2.216805	4.101872	0.600268	C	-2.449890	4.041243	-0.641540
H	5.535449	4.443923	-0.047028	H	-5.832477	4.324780	-0.072254
H	5.193435	2.136326	-0.928188	H	-5.417439	2.016810	0.843437
H	1.391345	4.645178	1.067326	H	-1.640896	4.623184	-1.086934
H	3.616048	5.698416	0.960646	H	-3.913320	5.601115	-1.046555
C	0.654894	2.234403	0.112100	C	-0.794453	2.269093	-0.069695
N	0.304414	0.945980	0.036950	N	-0.421989	1.000398	-0.199861
N	-0.460293	3.036758	0.187336	N	0.280911	3.087248	0.070925
C	-1.092362	0.900455	0.037931	C	0.987510	0.985695	-0.145773
C	-1.596846	2.243890	0.134557	C	1.446456	2.307694	0.033336
C	-1.950062	-0.174137	-0.031706	C	1.881700	-0.081877	-0.228860
C	-2.935474	2.545036	0.155090	C	2.792375	2.631170	0.140293
C	-3.850120	1.452419	0.080535	C	3.729897	1.568317	0.063002
C	-3.352236	0.084642	-0.011520	C	3.267309	0.193835	-0.121451
N	-4.197706	-0.960099	-0.081025	N	4.138146	-0.842272	-0.202555
N	-5.168721	1.716894	0.098561	N	5.047219	1.865093	0.162059
C	-5.509720	-0.689297	-0.062421	C	5.450508	-0.537922	-0.102107
C	-6.003276	0.669802	0.028895	C	5.908992	0.825319	0.082920
C	-6.451081	-1.766142	-0.134288	C	6.417751	-1.580093	-0.178798
C	-7.417091	0.894030	0.044646	C	7.307334	1.068074	0.181654
C	-7.797516	-1.508316	-0.116324	C	7.769069	-1.304282	-0.078417
C	-8.285028	-0.165278	-0.025960	C	8.216991	0.028675	0.103006
H	-1.614538	-1.209510	-0.109692	H	1.578146	-1.120331	-0.381965
H	-3.331899	3.558505	0.222961	H	3.164429	3.646850	0.278591
H	-6.051482	-2.779395	-0.202669	H	6.045012	-2.596847	-0.318408
H	-8.512927	-2.331791	-0.171376	H	8.498016	-2.115997	-0.138671
H	-9.363124	0.009804	-0.013800	H	9.287503	0.233324	0.180775
H	-7.762290	1.927082	0.113975	H	7.625293	2.103398	0.320824
O	2.954695	0.847320	-0.927701	O	-3.156408	0.811140	0.790719
H	-0.440883	4.045960	0.131062	H	0.238569	4.076144	0.277041
U	1.956854	-0.966379	-0.129624	U	-1.825032	-1.039369	0.084815
O	2.534189	-0.521772	1.502393	O	-2.484705	-0.777294	-1.549689
O	1.304075	-1.402793	-1.734778	O	-1.216661	-1.222008	1.744978
C	2.333134	-5.146308	0.754614	C	-1.945651	-5.278686	-0.369022

C	2.218654	-3.674516	0.475241	C	-1.927209	-3.785838	-0.236825
H	1.936187	-5.695184	-0.115641	H	-1.377726	-5.706930	0.473464
H	1.729167	-5.415368	1.631488	H	-1.440534	-5.578353	-1.297663
H	3.384470	-5.429013	0.894611	H	-2.974843	-5.657078	-0.336599
O	1.128946	-3.055287	0.731992	O	-0.886614	-3.119239	-0.571768
O	3.194444	-3.035807	-0.044230	O	-2.935056	-3.153810	0.233115

$L_1UO_2^{2+}$(AcO)(W)

Ground State				**Excited State**			
C	4.156296	4.431063	-0.087906	C	4.288344	4.463747	-0.035373
C	4.086260	3.099635	-0.471907	C	4.207573	3.152249	-0.481563
C	3.010374	5.109403	0.363084	C	3.142400	5.089946	0.459952
C	2.866507	2.386829	-0.417123	C	2.966446	2.421222	-0.439149
C	1.692807	3.078732	0.018230	C	1.769028	3.109141	0.010737
C	1.799949	4.434150	0.407874	C	1.895854	4.397385	0.481930
H	5.115084	4.953321	-0.130948	H	5.239845	4.996838	-0.061869
H	4.968392	2.561484	-0.822053	H	5.077580	2.615871	-0.862295
H	0.919765	4.956021	0.792058	H	1.024101	4.914402	0.887276
H	3.071423	6.150119	0.684284	H	3.185803	6.116330	0.826226
C	0.392311	2.423208	0.026294	C	0.435769	2.444684	-0.024471
N	0.135417	1.111425	0.044246	N	0.178178	1.155312	0.159430
N	-0.777700	3.147664	0.008075	N	-0.705297	3.158807	-0.214844
C	-1.255404	0.966496	0.020957	C	-1.226969	1.013784	0.090696
C	-1.854118	2.274215	-0.006757	C	-1.797201	2.281935	-0.153942
C	-2.034893	-0.168833	0.029504	C	-2.029068	-0.120240	0.215188
C	-3.210355	2.481022	-0.040998	C	-3.163589	2.484363	-0.288299
C	-4.045406	1.324272	-0.040644	C	-4.008684	1.351302	-0.165953
C	-3.451594	-0.007461	-0.000665	C	-3.431868	0.034014	0.088019
N	-4.221688	-1.111455	0.009061	N	-4.213117	-1.068774	0.216409
N	-5.379177	1.495353	-0.073087	N	-5.346515	1.529635	-0.289068
C	-5.549260	-0.933693	-0.023887	C	-5.544587	-0.883082	0.093727
C	-6.137469	0.389536	-0.066293	C	-6.116235	0.425434	-0.162914
C	-6.412087	-2.076766	-0.017272	C	-6.420950	-1.999340	0.217995
C	-7.563293	0.513193	-0.100582	C	-7.529763	0.541297	-0.282015
C	-7.773113	-1.914832	-0.051046	C	-7.789731	-1.845977	0.096469
C	-8.354138	-0.607112	-0.093113	C	-8.347979	-0.566973	-0.155327
H	-1.622061	-1.178110	0.059964	H	-1.630432	-1.116882	0.409944
H	-3.676797	3.466244	-0.067348	H	-3.617538	3.457347	-0.479668
H	-5.941866	-3.061150	0.014060	H	-5.963915	-2.972138	0.410703
H	-8.428316	-2.788718	-0.046624	H	-8.447383	-2.713167	0.193939
H	-9.441665	-0.508544	-0.119722	H	-9.431308	-0.459108	-0.249413
H	-7.980540	1.521210	-0.132509	H	-7.933655	1.537202	-0.475679
O	2.820573	1.125206	-0.800455	O	2.951392	1.186561	-0.765308
H	-0.826748	4.148301	-0.126655	H	-0.745365	4.134867	-0.474652
U	1.898699	-0.724840	0.009307	U	1.794508	-0.762587	0.077209
O	2.350459	-0.232474	1.672913	O	2.401458	-0.312398	1.701358

O	1.326782	-1.264606	-1.596828	O	1.266758	-1.170907	-1.579046
O	0.501475	-2.491257	0.981619	O	0.615876	-2.451873	0.936463
H	1.036749	-3.349673	0.673275	H	1.362134	-3.666133	0.437151
H	0.474411	-2.540659	1.949705	H	0.471018	-2.538428	1.891773
C	4.302001	-4.657024	-0.449192	C	4.244165	-4.755596	-0.703216
C	3.123817	-3.814775	-0.024955	C	3.166491	-3.834219	-0.214290
H	4.570883	-4.396782	-1.485506	H	4.225571	-4.745781	-1.805948
H	4.059114	-5.724562	-0.385954	H	4.070045	-5.782420	-0.359156
H	5.172329	-4.420115	0.181145	H	5.225810	-4.386408	-0.379093
O	2.022373	-4.348820	0.229193	O	2.037423	-4.389624	0.096722
O	3.330387	-2.536996	0.056917	O	3.370030	-2.597969	-0.140833

.

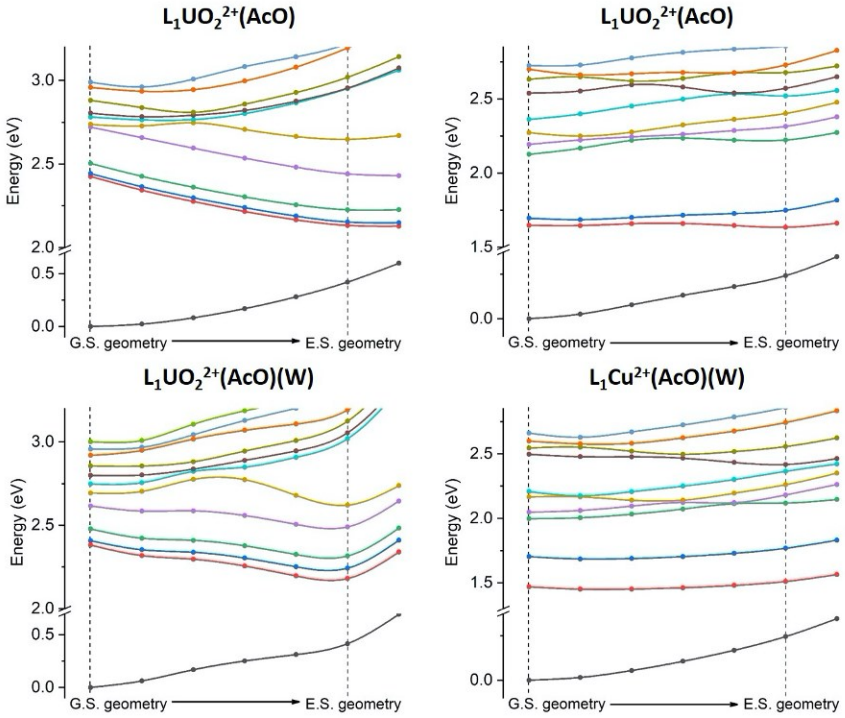


*Figure S*51. *Potential energy profiles for the investigated copper and uranyl complexes*

Crystallographic Tables (Table S2)

Salimidizine (**L1**)

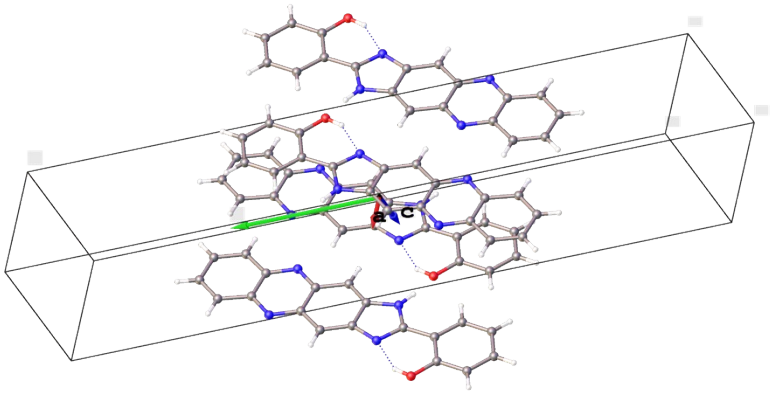


Table 1 Crystal data and structure refinement for Hiti070117_0m.

Identification code	Hiti070117_0m
Empirical formula	$C_{19}H_{12}N_4O$
Formula weight	312.33
Temperature/K	?
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	6.6597(6)
b/Å	30.064(3)
c/Å	7.2617(6)
α/°	90
β/°	108.293(2)
γ/°	90
Volume/Å^3	1380.5(2)
Z	4
ρ_{calc}g/cm^3	1.5027
μ/mm^{-1}	0.098
F(000)	648.3
Crystal size/mm^3	0.2 × 0.15 × 0.05
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.42 to 54.96
Index ranges	$-8 \le h \le 8$, $-39 \le k \le 39$, $-9 \le l \le 9$
Reflections collected	13927
Independent reflections	3173 [R_{int} = 0.0386, R_{sigma} = 0.0348]
Data/restraints/parameters	3173/0/218
Goodness-of-fit on F^2	1.067
Final R indexes [I>=2σ (I)]	R_1 = 0.0582, wR_2 = 0.1239
Final R indexes [all data]	R_1 = 0.0784, wR_2 = 0.1332
Largest diff. peak/hole / e Å^{-3}	0.41/-0.33

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Hiti070117_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N2	-4687(3)	-1097.8(6)	395(2)	21.2(4)
C10	-2987(3)	-829.6(6)	990(3)	18.3(4)
N3	-604(3)	-1402.1(5)	500(2)	20.2(4)
C17	-898(3)	-984.0(6)	1035(3)	18.3(4)
C16	-2314(3)	-1665.5(6)	-96(3)	20.2(4)
C6	1733(3)	848.2(6)	3842(3)	18.1(4)
C8	-1524(3)	-125.1(6)	2144(3)	18.7(4)
C11	-4373(3)	-1512.7(7)	-140(3)	20.5(4)
C18	868(3)	-694.0(6)	1630(3)	19.0(4)
C19	544(3)	-270.5(6)	2168(3)	17.9(4)
C9	-3263(3)	-391.2(6)	1575(3)	19.9(4)
C15	-2101(3)	-2106.6(7)	-730(3)	24.8(5)
C1	3918(3)	919.4(6)	4238(3)	18.8(4)
C12	-6124(3)	-1811.5(7)	-771(3)	26.4(5)
C2	4797(3)	1329.3(7)	4971(3)	23.6(4)
C5	486(3)	1196.8(7)	4146(3)	23.6(4)
C7	834(3)	416.4(6)	3138(3)	17.4(4)
C3	3531(3)	1665.0(7)	5267(3)	26.4(5)
C4	1360(4)	1600.1(7)	4840(3)	28.2(5)
C14	-3809(3)	-2377.0(7)	-1358(3)	28.2(5)
C13	-5840(3)	-2227.5(7)	-1369(3)	29.0(5)
O1	5211(2)	598.2(5)	3953(2)	25.8(3)
N1	-1249(2)	309.8(5)	2782(2)	20.3(4)
N4	1956(2)	81.6(5)	2797(2)	19.0(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for Hiti070117_0m. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N2	18.6(8)	22.6(9)	23.0(8)	-0.1(7)	7.5(7)	1.7(7)
C10	15.9(9)	22.2(10)	16.9(9)	0.1(8)	5.3(7)	3.4(7)
N3	19.4(8)	20.4(9)	21.7(8)	1.0(7)	7.6(7)	0.8(6)
C17	19.7(10)	18.7(10)	17.3(9)	3.0(8)	7.1(7)	1.3(7)
C16	22.2(10)	20.7(10)	18.5(9)	0.0(8)	7.4(8)	3.2(8)
C6	21.0(10)	16.8(9)	18.1(9)	0.2(8)	8.7(7)	2.5(7)
C8	20.7(10)	19.3(10)	18.3(9)	4.3(8)	9.2(8)	3.2(7)
C11	21.2(10)	22.8(11)	17.9(9)	0.5(8)	6.8(7)	3.4(8)
C18	14.2(9)	21.6(10)	21.9(9)	2.5(8)	6.8(7)	1.0(8)
C19	16.7(9)	20.2(10)	17.6(9)	1.5(8)	6.4(7)	3.6(7)
C9	15.6(9)	22.2(10)	23.5(9)	4.9(8)	8.6(8)	1.7(8)
C15	25.9(11)	22.6(11)	27.2(10)	3.0(9)	10.2(9)	2.9(8)
C1	20.6(10)	19.0(10)	17.6(9)	3.5(8)	7.3(7)	3.5(7)
C12	19.5(10)	28.6(12)	30.9(11)	-1.8(9)	7.5(8)	3.0(9)
C2	20.9(10)	25.7(11)	24.6(10)	-1.4(8)	7.6(8)	1.8(8)
C5	22.5(10)	23.4(11)	27.8(10)	4.4(8)	12.2(8)	1.4(8)
C7	17.5(9)	19.2(10)	16.5(9)	2.9(8)	6.9(7)	3.2(7)
C3	34.8(12)	18.3(10)	27.0(10)	-3.8(9)	11.0(9)	-2.4(8)
C4	33.8(12)	22.1(11)	31.8(11)	5.8(9)	14.7(9)	-1.9(9)

C14	34.6(12)	17.8(11)	32.1(11)	-0.2(9)	10.5(9)	0.5(9)
C13	27.0(12)	24.6(11)	34.2(11)	-8.2(9)	8.1(9)	0.9(9)
O1	17.1(7)	22.0(8)	39.8(8)	1.5(6)	10.9(6)	-3.9(6)
N1	17.1(8)	18.7(9)	27.4(8)	4.7(7)	10.4(7)	-0.1(7)
N4	18.6(8)	16.8(8)	21.9(8)	1.9(7)	6.8(6)	0.8(6)

Table 4 Bond Lengths for Hiti070117_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N2	C10	1.346(2)	C8	N1	1.380(2)
N2	C11	1.343(3)	C11	C12	1.429(3)
C10	C17	1.457(3)	C18	C19	1.368(3)
C10	C9	1.415(3)	C19	N4	1.394(2)
N3	C17	1.348(2)	C15	C14	1.356(3)
N3	C16	1.342(2)	C1	C2	1.396(3)
C17	C18	1.418(3)	C1	O1	1.352(2)
C16	C11	1.437(3)	C12	C13	1.356(3)
C16	C15	1.426(3)	C2	C3	1.375(3)
C6	C1	1.408(3)	C5	C4	1.371(3)
C6	C5	1.397(3)	C7	N1	1.367(2)
C6	C7	1.453(3)	C7	N4	1.322(2)
C8	C19	1.440(3)	C3	C4	1.394(3)
C8	C9	1.361(3)	C14	C13	1.423(3)

Table 5 Bond Angles for Hiti070117_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	N2	C10	117.24(17)	C18	C19	C8	120.99(17)
C17	C10	N2	121.17(17)	N4	C19	C8	108.50(16)
C9	C10	N2	118.62(17)	N4	C19	C18	130.52(17)
C9	C10	C17	120.21(17)	C8	C9	C10	117.41(17)
C16	N3	C17	117.24(17)	C14	C15	C16	120.5(2)
N3	C17	C10	120.95(17)	C2	C1	C6	119.67(18)
C18	C17	C10	120.38(17)	O1	C1	C6	121.80(17)
C18	C17	N3	118.67(17)	O1	C1	C2	118.53(17)
C11	C16	N3	121.73(18)	C13	C12	C11	120.1(2)
C15	C16	N3	119.49(18)	C3	C2	C1	120.22(19)
C15	C16	C11	118.77(18)	C4	C5	C6	121.15(19)
C5	C6	C1	118.74(18)	N1	C7	C6	123.86(17)
C7	C6	C1	119.51(17)	N4	C7	C6	123.47(17)
C7	C6	C5	121.75(17)	N4	C7	N1	112.66(17)
C9	C8	C19	123.03(18)	C4	C3	C2	120.4(2)
N1	C8	C19	104.96(16)	C3	C4	C5	119.75(19)
N1	C8	C9	132.01(18)	C13	C14	C15	120.6(2)
C16	C11	N2	121.66(18)	C14	C13	C12	121.1(2)

C12	C11	N2	119.44(18)	C7	N1	C8	107.78(16)
C12	C11	C16	118.90(18)	C7	N4	C19	106.10(16)
C19	C18	C17	117.97(17)				

Table 6 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for Hiti070117_0m.

Atom	*x*	*y*	*z*	U(eq)
H18	2206(3)	-788.7(6)	1654(3)	22.8(5)
H9	-4582(3)	-288.7(6)	1571(3)	23.8(5)
H15	-778(3)	-2209.7(7)	-714(3)	29.8(5)
H12	-7459(3)	-1720.8(7)	-771(3)	31.7(6)
H2	6244(3)	1375.4(7)	5259(3)	28.3(5)
H5	-961(3)	1154.5(7)	3872(3)	28.3(5)
H3	4127(3)	1937.2(7)	5756(3)	31.7(6)
H4	507(4)	1829.7(7)	5026(3)	33.9(6)
H14	-3652(3)	-2662.7(7)	-1785(3)	33.8(6)
H13	-6993(3)	-2418.3(7)	-1794(3)	34.8(6)
H1	4528(8)	370(3)	3580(40)	38.7(5)
H1a	-2216(2)	482.9(5)	2929(2)	24.3(4)

3,5-Ditertbutylsalimidizine (**L2**)

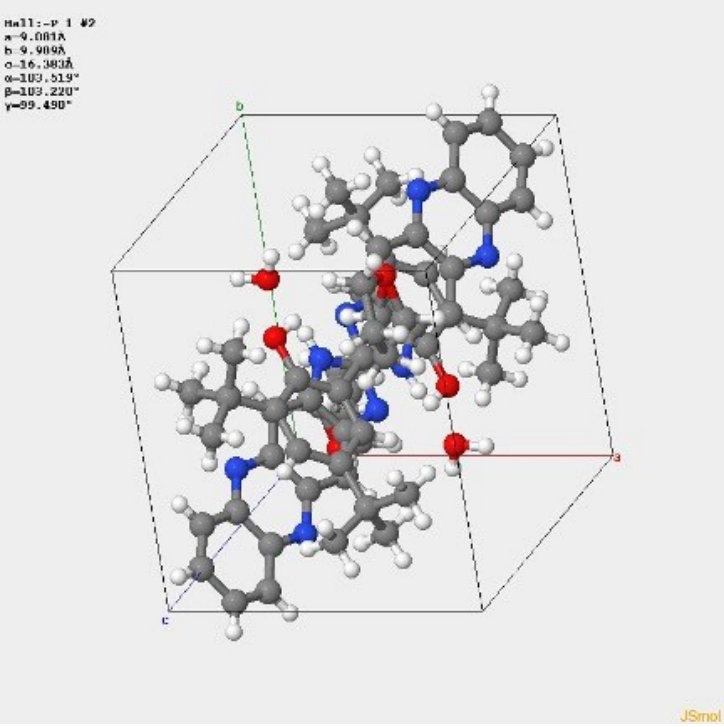


Table 1. Sample and crystal data for bam126.

Identification code	bam126
Chemical formula	$C_{31}H_{38}N_4O_3$

Formula weight	514.65 g/mol	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal size	0.070 x 0.100 x 0.110 mm	
Crystal habit	clear orange fragment	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.0812(5) Å	α = 103.5190(10)°
	b = 9.9887(5) Å	β = 103.2200(10)°
	c = 16.3825(9) Å	γ = 99.4900(10)°
Volume	1368.65(13) $Å^3$	
Z	2	
Density (calculated)	1.249 g/cm^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	552	

Table 2. Data collection and structure refinement for bam126.

Diffractometer	Bruker APEX κ-geometry diffractometer
Radiation source	microfocus sealed tube (Mo Kα, λ = 0.71073 Å)
Theta range for data collection	2.15 to 28.70°
Index ranges	-12<=h<=12, -13<=k<=13, -22<=l<=21
Reflections collected	29332
Independent reflections	7073 [R(int) = 0.0336]
Coverage of independent reflections	99.8%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9940 and 0.9910
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2017/1 (Sheldrick, 2017)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	7073 / 0 / 367
Goodness-of-fit on F^2	1.054
Final R indices	5267 data; I>2σ(I) R1 = 0.0489, wR2 = 0.1266
	all data R1 = 0.0686, wR2 = 0.1411
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0633P)^2+0.5063P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.430 and -0.278 $eÅ^{-3}$
R.M.S. deviation from mean	0.046 $eÅ^{-3}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O1	0.34101(13)	0.66604(11)	0.70893(7)	0.0339(3)
C1	0.93468(19)	0.11217(17)	0.30393(11)	0.0344(3)
C2	0.85053(18)	0.10680(15)	0.36212(10)	0.0307(3)
N4	0.74673(14)	0.98087(12)	0.45223(7)	0.0245(2)
C3	0.83540(16)	0.98850(14)	0.39737(9)	0.0236(3)

	x/a	y/b	z/c	U(eq)
C6	0.63185(16)	0.85007(14)	0.53489(9)	0.0242(3)
C5	0.73100(15)	0.86455(13)	0.48070(8)	0.0214(3)
C7	0.62149(16)	0.73358(14)	0.56571(8)	0.0220(3)
C9	0.57047(16)	0.57551(14)	0.63241(8)	0.0226(3)
N8	0.53665(14)	0.69534(12)	0.62050(8)	0.0250(2)
C10	0.50930(15)	0.50455(14)	0.69007(8)	0.0220(3)
C11	0.56507(16)	0.39073(14)	0.71131(9)	0.0230(3)
C12	0.51321(16)	0.32659(14)	0.76927(9)	0.0227(3)
C13	0.40122(16)	0.37994(14)	0.80517(9)	0.0240(3)
C14	0.34085(16)	0.49268(14)	0.78676(9)	0.0240(3)
C15	0.39694(16)	0.55582(14)	0.72802(9)	0.0243(3)
C16	0.58506(16)	0.20978(15)	0.79721(9)	0.0249(3)
C17	0.59430(18)	0.09827(15)	0.71767(10)	0.0303(3)
C18	0.4912(2)	0.13341(18)	0.84657(12)	0.0388(4)
C19	0.75054(19)	0.27792(18)	0.85711(11)	0.0366(4)
C20	0.22113(17)	0.54906(15)	0.83004(9)	0.0279(3)
O1W	0.78603(14)	0.28539(12)	0.56158(8)	0.0352(3)
C21	0.2867(2)	0.70581(17)	0.88291(11)	0.0397(4)
C22	0.06869(18)	0.53274(17)	0.76012(11)	0.0337(3)
C24	0.01139(19)	0.00352(17)	0.27773(11)	0.0345(3)
C25	0.00306(18)	0.89135(16)	0.31172(10)	0.0308(3)
C26	0.91450(16)	0.87970(14)	0.37200(9)	0.0236(3)
N27	0.90728(13)	0.76758(12)	0.40436(8)	0.0241(2)
C28	0.81548(15)	0.75623(13)	0.45748(8)	0.0209(3)
C29	0.80315(16)	0.63686(14)	0.49070(9)	0.0227(3)
C30	0.70846(15)	0.62896(13)	0.54418(8)	0.0212(3)
N31	0.67212(13)	0.53086(12)	0.58780(7)	0.0230(2)
C23	0.1820(2)	0.46741(18)	0.89382(11)	0.0360(4)
O1S	0.8159(2)	0.93674(15)	0.89744(10)	0.0624(4)
C2S	0.7876(4)	0.7114(2)	0.91845(17)	0.0725(7)
C3S	0.8043(3)	0.8172(2)	0.00370(14)	0.0601(6)
C4S	0.7824(3)	0.9488(3)	0.97859(16)	0.0676(6)
C1SA	0.7518(10)	0.7981(5)	0.8515(3)	0.0555(16)
C1SB	0.838(2)	0.7940(9)	0.8649(7)	0.064(3)

Table 4. Bond lengths (Å) for bam126.

O1-C15	1.3566(16)	O1-H1	0.82
C1-C2	1.356(2)	C1-C24	1.420(2)
C1-H1A	0.93	C2-C3	1.4320(18)
C2-H2	0.93	N4-C3	1.3434(18)
N4-C5	1.3480(16)	C3-C26	1.4327(19)
C6-C7	1.3704(18)	C6-C5	1.4152(19)
C6-H6	0.93	C5-C28	1.4555(17)
C7-N8	1.3873(17)	C7-C30	1.4378(18)
C9-N8	1.3298(17)	C9-N31	1.3701(17)
C9-C10	1.4583(18)	C10-C11	1.4015(18)
C10-C15	1.4155(18)	C11-C12	1.3868(18)
C11-H11	0.93	C12-C13	1.4036(18)

C12-C16	1.5364(18)	C13-C14	1.3952(18)
C13-H13	0.93	C14-C15	1.4091(19)
C14-C20	1.5393(18)	C16-C17	1.532(2)
C16-C18	1.534(2)	C16-C19	1.536(2)
C17-H17A	0.96	C17-H17B	0.96
C17-H17C	0.96	C18-H18A	0.96
C18-H18B	0.96	C18-H18C	0.96
C19-H19A	0.96	C19-H19B	0.96
C19-H19C	0.96	C20-C23	1.535(2)
C20-C22	1.539(2)	C20-C21	1.542(2)
O1W-H1W	0.89(2)	O1W-H2W	0.84(2)
C21-H21A	0.96	C21-H21B	0.96
C21-H21C	0.96	C22-H22A	0.96
C22-H22B	0.96	C22-H22C	0.96
C24-C25	1.362(2)	C24-H24	0.93
C25-C26	1.4219(19)	C25-H25	0.93
C26-N27	1.3449(16)	N27-C28	1.3461(17)
C28-C29	1.4205(17)	C29-C30	1.3667(18)
C29-H29	0.93	C30-N31	1.3815(16)
N31-H31	0.86	C23-H23A	0.96
C23-H23B	0.96	C23-H23C	0.96
O1S-C1SA	1.367(5)	O1S-C4S	1.413(3)
O1S-C1SB	1.466(8)	C2S-C1SB	1.436(10)
C2S-C3S	1.500(3)	C2S-C1SA	1.560(6)
C2S-H2SA	0.97	C2S-H2SB	0.97
C3S-C4S	1.496(3)	C3S-H3SA	0.97
C3S-H3SB	0.97	C4S-H4SC	0.97
C4S-H4SD	0.97	C1SA-H1SA	0.97
C1SA-H1SB	0.97	C1SB-H1SC	0.97
C1SB-H1SD	0.97		

Table 5. Bond angles (°) for bam126.

C15-O1-H1	109.5	C2-C1-C24	121.44(13)
C2-C1-H1A	119.3	C24-C1-H1A	119.3
C1-C2-C3	119.97(14)	C1-C2-H2	120.0
C3-C2-H2	120.0	C3-N4-C5	117.43(11)
N4-C3-C2	119.74(12)	N4-C3-C26	121.57(12)
C2-C3-C26	118.69(13)	C7-C6-C5	117.91(12)
C7-C6-H6	121.0	C5-C6-H6	121.0
N4-C5-C6	118.72(12)	N4-C5-C28	121.05(12)
C6-C5-C28	120.22(11)	C6-C7-N8	129.68(12)
C6-C7-C30	121.43(12)	N8-C7-C30	108.88(11)
N8-C9-N31	112.78(11)	N8-C9-C10	122.56(12)
N31-C9-C10	124.61(12)	C9-N8-C7	105.82(11)
C11-C10-C15	119.74(12)	C11-C10-C9	120.97(12)
C15-C10-C9	119.23(12)	C12-C11-C10	121.57(12)
C12-C11-H11	119.2	C10-C11-H11	119.2
C11-C12-C13	117.01(12)	C11-C12-C16	120.72(12)
C13-C12-C16	122.13(12)	C14-C13-C12	124.31(12)

C14-C13-H13	117.8	C12-C13-H13	117.8
C13-C14-C15	117.11(12)	C13-C14-C20	121.94(12)
C15-C14-C20	120.93(12)	O1-C15-C14	118.61(12)
O1-C15-C10	121.12(12)	C14-C15-C10	120.27(12)
C17-C16-C18	107.66(12)	C17-C16-C19	108.64(12)
C18-C16-C19	108.89(13)	C17-C16-C12	110.99(11)
C18-C16-C12	112.26(11)	C19-C16-C12	108.33(12)
C16-C17-H17A	109.5	C16-C17-H17B	109.5
H17A-C17-H17B	109.5	C16-C17-H17C	109.5
H17A-C17-H17C	109.5	H17B-C17-H17C	109.5
C16-C18-H18A	109.5	C16-C18-H18B	109.5
H18A-C18-H18B	109.5	C16-C18-H18C	109.5
H18A-C18-H18C	109.5	H18B-C18-H18C	109.5
C16-C19-H19A	109.5	C16-C19-H19B	109.5
H19A-C19-H19B	109.5	C16-C19-H19C	109.5
H19A-C19-H19C	109.5	H19B-C19-H19C	109.5
C23-C20-C22	107.45(13)	C23-C20-C14	111.61(12)
C22-C20-C14	110.20(12)	C23-C20-C21	107.23(13)
C22-C20-C21	110.11(13)	C14-C20-C21	110.16(12)
H1W-O1W-H2W	103.6(18)	C20-C21-H21A	109.5
C20-C21-H21B	109.5	H21A-C21-H21B	109.5
C20-C21-H21C	109.5	H21A-C21-H21C	109.5
H21B-C21-H21C	109.5	C20-C22-H22A	109.5
C20-C22-H22B	109.5	H22A-C22-H22B	109.5
C20-C22-H22C	109.5	H22A-C22-H22C	109.5
H22B-C22-H22C	109.5	C25-C24-C1	120.19(14)
C25-C24-H24	119.9	C1-C24-H24	119.9
C24-C25-C26	120.56(14)	C24-C25-H25	119.7
C26-C25-H25	119.7	N27-C26-C25	119.51(12)
N27-C26-C3	121.37(12)	C25-C26-C3	119.11(12)
C26-N27-C28	117.78(11)	N27-C28-C29	118.73(11)
N27-C28-C5	120.60(11)	C29-C28-C5	120.66(12)
C30-C29-C28	116.97(12)	C30-C29-H29	121.5
C28-C29-H29	121.5	C29-C30-N31	132.04(12)
C29-C30-C7	122.77(12)	N31-C30-C7	105.18(11)
C9-N31-C30	107.33(11)	C9-N31-H31	126.3
C30-N31-H31	126.3	C20-C23-H23A	109.5
C20-C23-H23B	109.5	H23A-C23-H23B	109.5
C20-C23-H23C	109.5	H23A-C23-H23C	109.5
H23B-C23-H23C	109.5	C1SA-O1S-C4S	104.2(3)
C4S-O1S-C1SB	108.6(4)	C1SB-C2S-C3S	104.9(4)
C3S-C2S-C1SA	102.4(3)	C3S-C2S-H2SA	111.3
C1SA-C2S-H2SA	111.3	C3S-C2S-H2SB	111.3
C1SA-C2S-H2SB	111.3	H2SA-C2S-H2SB	109.2
C4S-C3S-C2S	103.83(18)	C4S-C3S-H3SA	111.0
C2S-C3S-H3SA	111.0	C4S-C3S-H3SB	111.0
C2S-C3S-H3SB	111.0	H3SA-C3S-H3SB	109.0
O1S-C4S-C3S	107.13(17)	O1S-C4S-H4SC	110.3
C3S-C4S-H4SC	110.3	O1S-C4S-H4SD	110.3

C3S-C4S-H4SD	110.3	H4SC-C4S-H4SD	108.5
O1S-C1SA-C2S	105.8(3)	O1S-C1SA-H1SA	110.6
C2S-C1SA-H1SA	110.6	O1S-C1SA-H1SB	110.6
C2S-C1SA-H1SB	110.6	H1SA-C1SA-H1SB	108.7
C2S-C1SB-O1S	107.3(6)	C2S-C1SB-H1SC	110.3
O1S-C1SB-H1SC	110.3	C2S-C1SB-H1SD	110.3
O1S-C1SB-H1SD	110.3	H1SC-C1SB-H1SD	108.5

Table 6. Torsion angles (°) for bam126.

C24-C1-C2-C3	-1.1(2)	C5-N4-C3-C2	177.27(12)
C5-N4-C3-C26	-1.93(19)	C1-C2-C3-N4	-177.29(14)
C1-C2-C3-C26	1.9(2)	C3-N4-C5-C6	-176.74(12)
C3-N4-C5-C28	4.08(19)	C7-C6-C5-N4	-177.76(12)
C7-C6-C5-C28	1.4(2)	C5-C6-C7-N8	178.66(13)
C5-C6-C7-C30	0.1(2)	N31-C9-N8-C7	-0.63(16)
C10-C9-N8-C7	176.98(12)	C6-C7-N8-C9	-178.17(14)
C30-C7-N8-C9	0.49(15)	N8-C9-C10-C11	-170.37(13)
N31-C9-C10-C11	6.9(2)	N8-C9-C10-C15	6.8(2)
N31-C9-C10-C15	-175.87(13)	C15-C10-C11-C12	-0.2(2)
C9-C10-C11-C12	176.93(13)	C10-C11-C12-C13	0.6(2)
C10-C11-C12-C16	-175.16(12)	C11-C12-C13-C14	-0.5(2)
C16-C12-C13-C14	175.14(13)	C12-C13-C14-C15	0.1(2)
C12-C13-C14-C20	-178.39(13)	C13-C14-C15-O1	-179.78(13)
C20-C14-C15-O1	-1.2(2)	C13-C14-C15-C10	0.2(2)
C20-C14-C15-C10	178.75(13)	C11-C10-C15-O1	179.83(13)
C9-C10-C15-O1	2.6(2)	C11-C10-C15-C14	-0.2(2)
C9-C10-C15-C14	-177.38(13)	C11-C12-C16-C17	-48.24(17)
C13-C12-C16-C17	136.27(14)	C11-C12-C16-C18	-168.78(13)
C13-C12-C16-C18	15.72(19)	C11-C12-C16-C19	70.95(16)
C13-C12-C16-C19	-104.54(15)	C13-C14-C20-C23	0.6(2)
C15-C14-C20-C23	-177.90(13)	C13-C14-C20-C22	-118.73(15)
C15-C14-C20-C22	62.80(17)	C13-C14-C20-C21	119.57(15)
C15-C14-C20-C21	-58.90(18)	C2-C1-C24-C25	-0.7(3)
C1-C24-C25-C26	1.6(2)	C24-C25-C26-N27	179.64(14)
C24-C25-C26-C3	-0.7(2)	N4-C3-C26-N27	-2.2(2)
C2-C3-C26-N27	178.59(13)	N4-C3-C26-C25	178.16(13)
C2-C3-C26-C25	-1.0(2)	C25-C26-N27-C28	-176.42(13)
C3-C26-N27-C28	3.94(19)	C26-N27-C28-C29	178.49(12)
C26-N27-C28-C5	-1.76(19)	N4-C5-C28-N27	-2.35(19)
C6-C5-C28-N27	178.48(12)	N4-C5-C28-C29	177.39(12)
C6-C5-C28-C29	-1.77(19)	N27-C28-C29-C30	-179.80(12)
C5-C28-C29-C30	0.44(19)	C28-C29-C30-N31	-179.01(13)
C28-C29-C30-C7	1.2(2)	C6-C7-C30-C29	-1.5(2)
N8-C7-C30-C29	179.69(13)	C6-C7-C30-N31	178.61(13)
N8-C7-C30-N31	-0.18(14)	N8-C9-N31-C30	0.53(16)
C10-C9-N31-C30	-177.03(12)	C29-C30-N31-C9	179.96(14)
C7-C30-N31-C9	-0.19(14)	C1SB-C2S-C3S-C4S	28.9(9)
C1SA-C2S-C3S-C4S	-1.6(4)	C1SA-O1S-C4S-C3S	40.0(5)
C1SB-O1S-C4S-C3S	7.3(9)	C2S-C3S-C4S-O1S	-22.3(3)
C4S-O1S-C1SA-C2S	-40.3(6)	C3S-C2S-C1SA-O1S	25.8(6)
C3S-C2S-C1SB-O1S	-25.1(13)	C4S-O1S-C1SB-C2S	11.4(14)

Table 7. Anisotropic atomic displacement parameters (Å²) for bam126.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0427(6)	0.0322(6)	0.0458(6)	0.0235(5)	0.0261(5)	0.0234(5)
C1	0.0407(9)	0.0292(8)	0.0391(8)	0.0206(6)	0.0117(7)	0.0073(6)
C2	0.0386(8)	0.0237(7)	0.0347(8)	0.0145(6)	0.0112(6)	0.0107(6)
N4	0.0296(6)	0.0193(5)	0.0262(6)	0.0089(4)	0.0071(5)	0.0072(5)
C3	0.0257(7)	0.0194(6)	0.0244(6)	0.0078(5)	0.0036(5)	0.0046(5)
C6	0.0302(7)	0.0200(6)	0.0269(7)	0.0083(5)	0.0108(5)	0.0113(5)
C5	0.0243(6)	0.0171(6)	0.0221(6)	0.0061(5)	0.0045(5)	0.0051(5)
C7	0.0254(6)	0.0203(6)	0.0216(6)	0.0062(5)	0.0076(5)	0.0071(5)
C9	0.0257(6)	0.0220(6)	0.0221(6)	0.0075(5)	0.0074(5)	0.0081(5)
N8	0.0318(6)	0.0229(6)	0.0269(6)	0.0113(5)	0.0130(5)	0.0114(5)
C10	0.0253(6)	0.0221(6)	0.0221(6)	0.0087(5)	0.0092(5)	0.0082(5)
C11	0.0255(6)	0.0238(6)	0.0238(6)	0.0085(5)	0.0098(5)	0.0099(5)
C12	0.0247(6)	0.0226(6)	0.0229(6)	0.0080(5)	0.0071(5)	0.0080(5)
C13	0.0284(7)	0.0242(6)	0.0234(6)	0.0096(5)	0.0107(5)	0.0080(5)
C14	0.0260(7)	0.0235(6)	0.0252(6)	0.0067(5)	0.0104(5)	0.0082(5)
C15	0.0283(7)	0.0225(6)	0.0265(7)	0.0095(5)	0.0098(5)	0.0111(5)
C16	0.0284(7)	0.0258(7)	0.0271(7)	0.0131(5)	0.0107(5)	0.0118(5)
C17	0.0342(8)	0.0268(7)	0.0336(8)	0.0097(6)	0.0109(6)	0.0132(6)
C18	0.0467(9)	0.0404(9)	0.0493(10)	0.0297(8)	0.0266(8)	0.0217(7)
C19	0.0344(8)	0.0365(8)	0.0366(8)	0.0117(7)	0.0014(7)	0.0117(7)
C20	0.0327(7)	0.0263(7)	0.0308(7)	0.0088(6)	0.0163(6)	0.0121(6)
O1W	0.0326(6)	0.0281(6)	0.0454(7)	0.0060(5)	0.0107(5)	0.0149(5)
C21	0.0486(10)	0.0315(8)	0.0396(9)	0.0018(7)	0.0208(8)	0.0105(7)
C22	0.0330(8)	0.0331(8)	0.0422(9)	0.0132(7)	0.0166(7)	0.0152(6)
C24	0.0375(8)	0.0353(8)	0.0393(8)	0.0207(7)	0.0170(7)	0.0080(7)
C25	0.0319(7)	0.0302(7)	0.0383(8)	0.0166(6)	0.0160(6)	0.0102(6)
C26	0.0239(6)	0.0216(6)	0.0259(7)	0.0096(5)	0.0057(5)	0.0049(5)
N27	0.0260(6)	0.0218(5)	0.0287(6)	0.0115(5)	0.0096(5)	0.0076(4)
C28	0.0216(6)	0.0183(6)	0.0229(6)	0.0067(5)	0.0053(5)	0.0052(5)
C29	0.0262(6)	0.0184(6)	0.0272(7)	0.0091(5)	0.0089(5)	0.0091(5)
C30	0.0243(6)	0.0178(6)	0.0224(6)	0.0077(5)	0.0053(5)	0.0061(5)
N31	0.0279(6)	0.0203(5)	0.0270(6)	0.0112(4)	0.0117(5)	0.0106(4)
C23	0.0420(9)	0.0414(9)	0.0379(8)	0.0165(7)	0.0252(7)	0.0184(7)
O1S	0.0827(11)	0.0466(8)	0.0621(9)	0.0276(7)	0.0173(8)	0.0124(8)
C2S	0.115(2)	0.0395(11)	0.0775(16)	0.0226(11)	0.0474(15)	0.0201(12)
C3S	0.0792(15)	0.0646(14)	0.0561(12)	0.0323(11)	0.0308(11)	0.0314(12)
C4S	0.0937(18)	0.0544(13)	0.0657(14)	0.0187(11)	0.0272(13)	0.0376(13)
C1SA	0.070(3)	0.047(2)	0.0398(18)	0.0138(14)	0.009(2)	-0.005(2)
C1SB	0.096(9)	0.047(4)	0.047(4)	0.008(3)	0.020(5)	0.022(5)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²) for bam126.

	x/a	y/b	z/c	U(eq)
H1	0.3883	0.6985	0.6782	0.051
H1W	0.887(2)	0.289(2)	0.5765(12)	0.041

	x/a	y/b	z/c	U(eq)
H1A	0.9423	1.1887	0.2807	0.041
H2	0.8027	1.1799	0.3791	0.037
H2W	0.748(2)	0.203(2)	0.5273(12)	0.037
H6	0.5755	0.9175	0.5491	0.029
H11	0.6386	0.3574	0.6859	0.028
H13	0.3649	0.3373	0.8438	0.029
H17A	0.4913	0.0530	0.6805	0.045
H17B	0.6437	0.0288	0.7369	0.045
H17C	0.6537	0.1431	0.6858	0.045
H18A	0.3851	0.0976	0.8116	0.058
H18B	0.4948	0.1986	0.9007	0.058
H18C	0.5347	0.0563	0.8583	0.058
H19A	0.7974	0.2063	0.8751	0.055
H19B	0.7462	0.3471	0.9077	0.055
H19C	0.8114	0.3229	0.8260	0.055
H21A	0.3050	0.7613	0.8441	0.06
H21B	0.3827	0.7151	0.9256	0.06
H21C	0.2133	0.7386	0.9119	0.06
H22A	0.0901	0.5790	0.7175	0.051
H22B	-0.0021	0.5750	0.7873	0.051
H22C	0.0229	0.4341	0.7319	0.051
H24	1.0675	1.0090	0.2372	0.041
H25	1.0557	0.8218	0.2954	0.037
H29	0.8571	0.5672	0.4767	0.027
H31	0.7069	0.4557	0.5871	0.028
H23A	0.1406	0.3690	0.8630	0.054
H23B	0.1063	0.5043	0.9190	0.054
H23C	0.2745	0.4778	0.9393	0.054
H2SA	0.7030	0.6301	0.9065	0.087
H2SB	0.8829	0.6797	0.9179	0.087
H3SA	0.7259	0.7861	1.0309	0.072
H3SB	0.9064	0.8325	1.0437	0.072
H4SC	0.6763	0.9582	0.9734	0.081
H4SD	0.8519	1.0314	1.0226	0.081
H1SA	0.7977	0.7701	0.8041	0.067
H1SB	0.6405	0.7833	0.8272	0.067
H1SC	0.7782	0.7524	0.8043	0.077
H1SD	0.9472	0.7976	0.8686	0.077

Table 9. Hydrogen bond distances (Å) and angles (°) for bam126.

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
O1-H1···N8	0.82	1.81	2.5583(15)	150.2
O1W-H1W···N27	0.89(2)	2.02(2)	2.8742(16)	162.0(18)
C2-H2···O1	0.93	2.64	3.3375(17)	131.9
O1W-H2W···N4	0.84(2)	2.27(2)	3.0644(16)	156.8(17)
N31-H31···O1W	0.86	1.95	2.7953(15)	168.4

UO_2[L1](OAc)(DMSO)

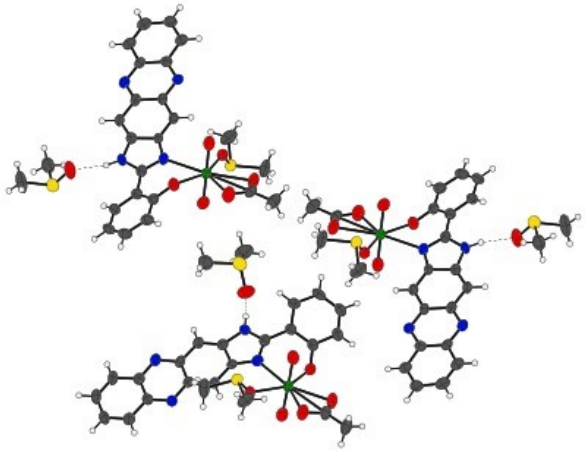


Table 1 Crystal data and structure refinement for bam115bJN091119.

Identification code	bam115bJN091119
Empirical formula	$C_{25}H_{26}N_4O_7S_2U$
Formula weight	796.65
Temperature/K	273.(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.585(5)
b/Å	20.419(11)

c/Å	16.091(9)
α/°	90
β/°	101.633(8)
γ/°	90
Volume/Å^3	2763.(3)
Z	4
ρ_{calc}g/cm^3	1.915
μ/mm^{-1}	6.077
F(000)	1536.0
Crystal size/mm^3	0.100 × 0.100 × 0.100
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.26 to 53.14
Index ranges	-10 ≤ h ≤ 10, -25 ≤ k ≤ 25, -20 ≤ l ≤ 20
Reflections collected	33110
Independent reflections	5707 [R_{int} = 0.0639, R_{sigma} = 0.0441]
Data/restraints/parameters	5707/11/357
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0450, wR_2 = 0.1157
Final R indexes [all data]	R_1 = 0.0602, wR_2 = 0.1281
Largest diff. peak/hole / e Å^{-3}	3.75/-1.15

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for bam115bJN091119. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	5964.3(3)	2095.5(2)	6340.5(2)	28.97(11)
S1S	3327(3)	5481.4(11)	8541.1(14)	48.9(5)
S1	4087(2)	2546.0(8)	4221.5(12)	34.2(4)
N1	5311(7)	4237(3)	7257(4)	32.1(13)
O1	6239(6)	2271(2)	7719(3)	35.9(11)
C1	5278(9)	2571(3)	8144(4)	32.2(15)
N2	7220(7)	5690(3)	5277(4)	33.1(13)
O2	8035(7)	2151(2)	6421(3)	39.3(12)
C2	4843(10)	2262(4)	8842(5)	37.8(16)
N3	8000(7)	4521(3)	4478(4)	29.9(12)
O3	3872(8)	2066(2)	6237(4)	42.5(13)
C3	3955(10)	2585(4)	9327(5)	42.6(18)
O4	6245(8)	989(3)	6907(4)	52.5(16)
N4	5838(7)	3327(3)	6622(4)	32.2(13)
C4	3396(10)	3210(4)	9117(5)	42.5(18)

C5	3776(9)	3528(4)	8424(5)	35.4(16)
O5	5879(7)	1063(2)	5534(3)	46.4(14)
C6	4733(8)	3214(3)	7933(4)	32.0(15)
O6	5544(6)	2470(2)	4943(3)	32.3(10)
C7	5292(8)	3576(3)	7256(4)	30.8(15)
C8	5942(8)	4451(3)	6568(4)	30.2(14)
C9	6264(9)	5051(3)	6310(4)	32.3(15)
C10	6933(9)	5090(3)	5567(4)	29.8(14)
C19	6262(8)	3842(3)	6184(4)	24.4(12)
C18	6965(9)	3881(3)	5477(4)	30.6(14)
C17	7305(8)	4501(3)	5156(4)	27.3(13)
C16	8314(8)	5120(3)	4207(4)	31.6(15)
C15	9089(8)	5176(4)	3495(5)	35.8(16)
C14	9409(9)	5778(4)	3206(5)	38.0(17)
C11	7914(8)	5706(3)	4593(4)	30.4(14)
C12	8239(9)	6320(4)	4252(5)	38.0(17)
C20	6123(10)	723(4)	6191(6)	44(2)
C1S	3325(13)	6130(5)	7820(6)	61(2)
O1S	4765(9)	5086(3)	8480(4)	64.7(19)
C21	6212(12)	-6(4)	6148(7)	58(2)
C22	4758(13)	3130(5)	3565(6)	58(3)
C23	4134(11)	1826(4)	3606(6)	54(2)
C2S	3900(15)	5933(6)	9491(6)	77(4)
C13	8940(9)	6351(4)	3581(5)	40.6(18)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for bam115bJN091119. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+...]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
U1	35.45(18)	25.03(15)	26.53(16)	-0.96(10)	6.49(11)	0.39(9)
S1S	50.8(13)	53.2(12)	44.3(12)	-4.3(10)	13.7(10)	-6.5(9)
S1	36.3(10)	30.1(8)	34.9(9)	1.5(7)	4.5(8)	-0.3(7)
N1	44(4)	28(3)	27(3)	3(2)	15(3)	-3(2)
O1	45(3)	33(2)	30(3)	5(2)	8(2)	1(2)
C1	35(4)	34(3)	26(3)	-4(3)	3(3)	-1(3)
N2	38(3)	28(3)	32(3)	-2(2)	4(3)	0(2)

O2	51(3)	39(3)	25(3)	3(2)	-1(2)	-1(2)
C2	39(4)	42(4)	34(4)	-5(3)	8(3)	5(3)
N3	29(3)	30(3)	30(3)	-2(2)	4(2)	0(2)
O3	53(4)	37(3)	36(3)	-6(2)	7(3)	1(2)
C3	42(5)	52(5)	36(4)	-6(4)	14(4)	7(3)
O4	88(5)	30(3)	41(3)	4(3)	15(3)	8(2)
N4	37(3)	27(3)	33(3)	-1(2)	6(3)	-6(2)
C4	38(4)	59(5)	35(4)	-7(4)	18(3)	-5(4)
C5	31(4)	39(4)	37(4)	0(3)	10(3)	-4(3)
O5	72(4)	28(2)	37(3)	-2(2)	6(3)	-1(2)
C6	30(4)	38(4)	28(3)	-1(3)	5(3)	0(3)
O6	38(3)	31(2)	28(2)	-1(2)	5(2)	1.0(19)
C7	33(4)	34(3)	23(3)	0(3)	-2(3)	-1(3)
C8	30(4)	32(3)	28(3)	2(3)	2(3)	-1(3)
C9	45(4)	24(3)	29(4)	0(3)	10(3)	-4(3)
C10	37(4)	24(3)	25(3)	1(3)	-1(3)	1(2)
C19	24.4(15)	23.7(15)	24.1(15)	2.5(9)	2.4(10)	-2.7(9)
C18	40(4)	23(3)	30(3)	0(3)	9(3)	-1(3)
C17	30(4)	28(3)	22(3)	2(3)	0(3)	-3(2)
C16	29(4)	37(4)	29(4)	-2(3)	5(3)	2(3)
C15	31(4)	38(4)	36(4)	-4(3)	0(3)	1(3)
C14	43(4)	43(4)	29(4)	-5(3)	8(3)	7(3)
C11	28(4)	30(3)	30(4)	-4(3)	-2(3)	-2(3)
C12	42(4)	31(3)	38(4)	-5(3)	0(3)	8(3)
C20	55(5)	23(3)	55(5)	-7(3)	16(4)	2(3)
C1S	79(7)	57(5)	49(5)	2(5)	23(5)	-7(4)
O1S	77(5)	55(4)	64(4)	17(3)	20(4)	-20(3)
C21	72(7)	27(4)	72(6)	-4(4)	10(5)	8(4)
C22	71(6)	51(5)	42(5)	-20(5)	-13(4)	17(4)
C23	57(6)	37(4)	58(6)	8(4)	-14(5)	-20(4)
C2S	108(9)	75(7)	44(5)	37(6)	8(6)	-20(5)
C13	43(5)	41(4)	33(4)	-7(3)	-3(3)	13(3)

Table 4 Bond Lengths for bam115bJN091119.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
U1	O2	1.760(6)	N3	C17	1.346(9)
U1	O3	1.772(6)	C3	C4	1.380(12)
U1	O1	2.213(5)	O4	C20	1.259(10)
U1	O6	2.333(5)	N4	C7	1.308(9)

U1	O4	2.430(5)	N4	C19	1.356(9)
U1	O5	2.468(5)	C4	C5	1.385(11)
U1	N4	2.562(6)	C5	C6	1.404(10)
U1	C20	2.819(8)	O5	C20	1.248(10)
S1S	O1S	1.495(7)	C6	C7	1.476(10)
S1S	C1S	1.761(10)	C8	C9	1.340(10)
S1S	C2S	1.769(10)	C8	C19	1.438(9)
S1	O6	1.534(5)	C9	C10	1.429(10)
S1	C22	1.765(9)	C10	C17	1.439(9)
S1	C23	1.778(8)	C19	C18	1.393(9)
N1	C7	1.350(9)	C18	C17	1.419(9)
N1	C8	1.399(9)	C16	C11	1.422(10)
O1	C1	1.323(9)	C16	C15	1.441(10)
C1	C2	1.403(10)	C15	C14	1.362(10)
C1	C6	1.411(10)	C14	C13	1.412(11)
N2	C10	1.351(8)	C11	C12	1.420(9)
N2	C11	1.353(9)	C12	C13	1.340(11)
C2	C3	1.366(11)	C20	C21	1.491(11)
N3	C16	1.345(9)			

Table 5 Bond Angles for bam115bJN091119.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	U1	O3	178.0(2)	C7	N4	C19	106.3(6)
O2	U1	O1	90.8(2)	C7	N4	U1	123.6(5)
O3	U1	O1	90.0(2)	C19	N4	U1	130.1(4)
O2	U1	O6	90.4(2)	C3	C4	C5	120.1(7)
O3	U1	O6	87.9(2)	C4	C5	C6	119.9(7)
O1	U1	O6	151.37(17)	C20	O5	U1	92.8(5)
O2	U1	O4	90.6(2)	C5	C6	C1	119.5(6)
O3	U1	O4	91.5(2)	C5	C6	C7	120.1(6)
O1	U1	O4	77.99(19)	C1	C6	C7	120.1(6)
O6	U1	O4	130.60(18)	S1	O6	U1	135.0(3)
O2	U1	O5	90.9(2)	N4	C7	N1	112.6(6)
O3	U1	O5	90.0(2)	N4	C7	C6	127.1(6)
O1	U1	O5	130.64(17)	N1	C7	C6	120.4(6)
O6	U1	O5	77.93(17)	C9	C8	N1	131.8(6)
O4	U1	O5	52.67(19)	C9	C8	C19	126.0(7)
O2	U1	N4	90.1(2)	N1	C8	C19	102.1(6)
O3	U1	N4	88.4(2)	C8	C9	C10	116.9(6)
O1	U1	N4	70.34(19)	N2	C10	C9	118.2(6)
O6	U1	N4	81.05(18)	N2	C10	C17	121.7(6)

O4	U1	N4	148.3(2)	C9	C10	C17	120.1(6)
O5	U1	N4	158.96(19)	N4	C19	C18	132.4(6)
O2	U1	C20	90.3(2)	N4	C19	C8	110.6(6)
O3	U1	C20	91.3(2)	C18	C19	C8	116.9(6)
O1	U1	C20	104.4(2)	C19	C18	C17	120.2(6)
O6	U1	C20	104.2(2)	N3	C17	C18	118.6(6)
O4	U1	C20	26.4(2)	N3	C17	C10	121.6(6)
O5	U1	C20	26.2(2)	C18	C17	C10	119.8(6)
N4	U1	C20	174.8(2)	N3	C16	C11	122.8(6)
O1S	S1S	C1S	104.7(5)	N3	C16	C15	119.0(6)
O1S	S1S	C2S	104.4(5)	C11	C16	C15	118.2(6)
C1S	S1S	C2S	98.1(5)	C14	C15	C16	120.0(7)
O6	S1	C22	101.9(4)	C15	C14	C13	120.5(7)
O6	S1	C23	103.4(3)	N2	C11	C12	119.3(6)
C22	S1	C23	100.3(5)	N2	C11	C16	121.3(6)
C7	N1	C8	108.5(6)	C12	C11	C16	119.4(7)
C1	O1	U1	129.9(5)	C13	C12	C11	120.6(7)
O1	C1	C2	120.0(7)	O5	C20	O4	120.2(7)
O1	C1	C6	121.2(6)	O5	C20	C21	121.2(8)
C2	C1	C6	118.8(7)	O4	C20	C21	118.5(8)
C10	N2	C11	116.4(6)	O5	C20	U1	61.0(4)
C3	C2	C1	120.6(7)	O4	C20	U1	59.2(4)
C16	N3	C17	116.1(6)	C21	C20	U1	177.8(7)
C2	C3	C4	121.0(7)	C12	C13	C14	121.2(7)
C20	O4	U1	94.3(5)				

Table 6 Hydrogen Bonds for bam115bJN091119.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1	O1S	0.86	1.89	2.732(8)	167.2
C18	H18	O6	0.93	2.53	3.179(8)	126.9
C1S	H01C	O3[1]	0.96	2.37	3.265(11)	155.0
C22	H01F	O1[2]	0.96	2.48	3.161(11)	127.9
C23	H00E	O1[2]	0.96	2.52	3.191(10)	127.0
C2S	H01I	O3[1]	0.96	2.55	3.356(12)	141.3

[1]1/2-X,1/2+Y,3/2-Z; [2]-1/2+X,1/2-Y,-1/2+Z

Table 7 Torsion Angles for bam115bJN091119.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
U1	O1	C1	C2	128.9(6)	C7	N4	C19	C8	-0.6(8)
U1	O1	C1	C6	-54.1(9)	U1	N4	C19	C8	178.6(4)
O1	C1	C2	C3	174.7(7)	C9	C8	C19	N4	177.9(7)
C6	C1	C2	C3	-2.3(12)	N1	C8	C19	N4	0.2(7)
C1	C2	C3	C4	3.4(13)	C9	C8	C19	C18	-0.3(10)
C2	C3	C4	C5	-2.2(13)	N1	C8	C19	C18	-177.9(6)
C3	C4	C5	C6	-0.1(12)	N4	C19	C18	C17	-178.9(7)
C4	C5	C6	C1	1.1(11)	C8	C19	C18	C17	-1.2(10)
C4	C5	C6	C7	-173.0(7)	C16	N3	C17	C18	-179.2(6)
O1	C1	C6	C5	-176.9(7)	C16	N3	C17	C10	-0.4(9)
C2	C1	C6	C5	0.1(11)	C19	C18	C17	N3	179.3(6)
O1	C1	C6	C7	-2.9(10)	C19	C18	C17	C10	0.5(10)
C2	C1	C6	C7	174.1(7)	N2	C10	C17	N3	2.0(10)
C22	S1	O6	U1	159.1(5)	C9	C10	C17	N3	-177.1(6)
C23	S1	O6	U1	-97.1(5)	N2	C10	C17	C18	-179.2(7)
C19	N4	C7	N1	0.8(8)	C9	C10	C17	C18	1.7(10)
U1	N4	C7	N1	-178.5(4)	C17	N3	C16	C11	-1.4(10)
C19	N4	C7	C6	-177.7(7)	C17	N3	C16	C15	178.7(6)
U1	N4	C7	C6	3.0(10)	N3	C16	C15	C14	179.5(7)
C8	N1	C7	N4	-0.7(8)	C11	C16	C15	C14	-0.4(10)
C8	N1	C7	C6	178.0(6)	C16	C15	C14	C13	-2.1(11)
C5	C6	C7	N4	-161.8(7)	C10	N2	C11	C12	179.6(6)
C1	C6	C7	N4	24.2(11)	C10	N2	C11	C16	-0.1(10)
C5	C6	C7	N1	19.7(10)	N3	C16	C11	N2	1.7(11)
C1	C6	C7	N1	-154.3(7)	C15	C16	C11	N2	-178.3(6)
C7	N1	C8	C9	-177.2(8)	N3	C16	C11	C12	-178.0(6)
C7	N1	C8	C19	0.3(7)	C15	C16	C11	C12	2.0(10)
N1	C8	C9	C10	179.3(7)	N2	C11	C12	C13	179.3(7)
C19	C8	C9	C10	2.4(11)	C16	C11	C12	C13	-1.1(11)
C11	N2	C10	C9	177.4(6)	U1	O5	C20	O4	2.2(9)
C11	N2	C10	C17	-1.7(10)	U1	O5	C20	C21	179.8(8)
C8	C9	C10	N2	177.8(7)	U1	O4	C20	O5	-2.2(9)
C8	C9	C10	C17	-3.1(10)	U1	O4	C20	C21	-179.9(7)
C7	N4	C19	C18	177.1(7)	C11	C12	C13	C14	-1.5(11)
U1	N4	C19	C18	-3.7(11)	C15	C14	C13	C12	3.1(12)

Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for bam115bJN091119.

Atom	*x*	*y*	*z*	U(eq)

H1	4990.19	4485.27	7620.79	38
H2	5161.41	1832.58	8975.49	45
H3	3724.1	2382.12	9804.65	51
H4	2762.6	3418.34	9442.7	51
H5	3397.17	3948.18	8283.48	43
H9	6060.75	5424.51	6601.02	39
H18	7211.72	3500	5214.72	37
H15	9371.13	4800.87	3232.18	43
H14	9941.06	5812.17	2758	46
H12	7962.93	6704.89	4496.45	46
H01A	2999.64	5969.75	7250.75	91
H01B	4376.08	6311.15	7892.9	91
H01C	2598.86	6463.54	7923.65	91
H00A	5193.99	-177.18	5879.59	87
H00B	6507.82	-180.55	6712.13	87
H00D	6993.51	-128.49	5826.11	87
H01D	5734.2	2981.78	3424.69	87
H01E	4935.39	3540.96	3859.75	87
H01F	3970.43	3185.95	3054.55	87
H00E	3326.81	1852.38	3098.98	81
H00F	3942.45	1450.12	3930.13	81
H00G	5158.21	1786.21	3457.9	81
H01G	4825.36	6189.93	9463.74	115
H01H	4140.24	5637.04	9963.41	115
H01I	3047.22	6217.76	9563.15	115
H13	9121.69	6758.04	3357.57	49

References

1. Sheldrick, G. M., *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2008,** *A64*, 112.
2. Bruker Bruker AXS Inc.: Madison, Wisconsin, USA, 2001.
3. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H., OLEX2: A complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009,** *42*, 339-341.