Supplementary

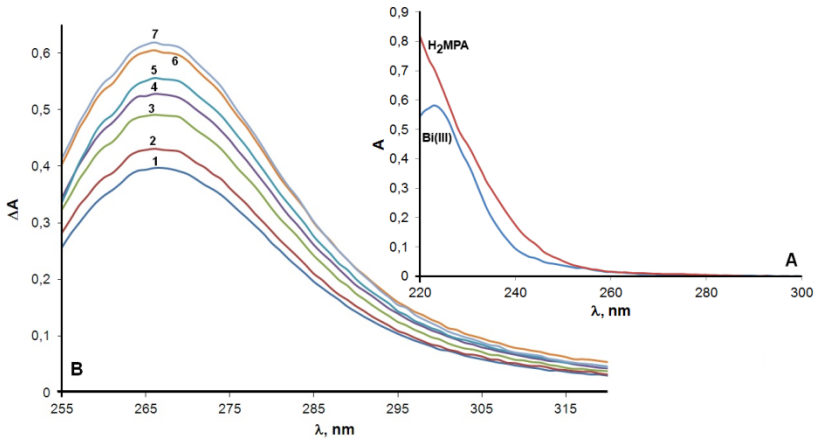

Figure S1. The UV-Vis spectra of Bi ($2.5\cdot10^{-4}$ M) and of H_2MPA ($3.0\cdot10^{-3}$ M) (A), ΔA versus λ (B) plots for Bi(III)-H_2MPA system: $C_{Bi}\cdot10^{-3}$ M: 1.5(1); 2.0 (2); 3.0 (3); 4.0 (4); 5.0 (5); 10.0 (6); 20.0 (7). C(H_2MPA) =$1.5\cdot10^{-4}$ M. 0.5 M HClO4. I = 0.5 ($HClO_4$). 298 K. l = 1 cm

Table S1. Absorbance data for Bi(III)-H_2MPA system in perchloric aqueous solutions. (C_{H2L} = $1.5\cdot10^{-4}$ M; λ = 267 nm; 298 K)

C_{Bi}, M	A in:					
	0.5 M $HClO_4$ + 0.5 M $NaClO_4$	0.5 M $HClO_4$	1 M $HClO_4$ + 1 M $NaClO_4$	0.5 M $HClO_4$ + 1.5 M $NaClO_4$	1 M $HClO_4$	2 M $HClO_4$
$1.5\cdot10^{-3}$	0.389	0.401	0.321	0.436	0.230	0.190
$2\cdot10^{-3}$	0.439	0.446	0.364	0.531	0.315	0.231
$3\cdot10^{-3}$	0.515	0.503	0.445	0.575	0.380	0.335
$4\cdot10^{-3}$	0.546	0.540	0.482	0.614	0.443	0.360
$5\cdot10^{-3}$	0.561	0.582	0.508	0.648	-	0.387
$6\cdot10^{-3}$	0.582	-	0.540	-	0.497	-
0.01	0.640	0.624	0.608	-	0.554	0.490
0.02	0.673	0.66	0.672	0.726	0.610	0.575

Table S2. Absorbance data for isomolar series for C_{Bi} =$2.5\cdot10^{-4}$ M (I = 0.5 ($HClO_4$), 298 K, *l* = 1 cm, λ = 267 nm) at different acidities

C(H_2MPA)$\cdot10^{-3}$, M	0.5M $HClO_4$	1.0M $HClO_4$	2.0M $HClO_4$
0.15	0.134	0.098	0.057
0.25	0.210	0.148	0.073
0.30	0.291	-	0.089
0.40	0.357	0.220	0.128
0.50	0.365	0.267	0.156
0.60	0.469	0.311	0.184
0.70	0.523	0.343	0.208
0.80	0.594	0.380	0.230
1.00	-	0.470	0.284
1.25	0.759	0.537	0.333

1.50	0.750	0.635	0.383
2.00	0.875	0.749	0.456
2.50	0.936	0.819	0.563
3.00	1.024	0.888	0.610
4.00	1.137	1.033	0.690
4.50	1.196	1.083	0.736

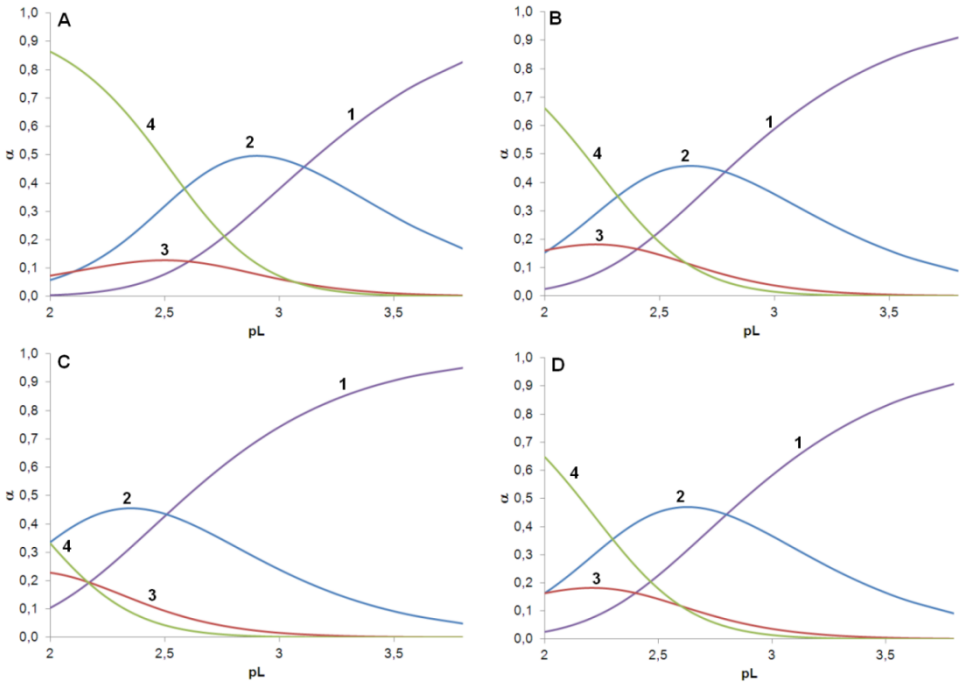

Figure S2. Distribution diagrams obtained from experimental conditional stability constants at different acidities ($HClO_4$): 0.5 M (A), 1.0 M (B), 2.0 M (C) and from «true» stability constant obtained excluding protonation of ligand; 1 – [M], 2 – [M(HL)], 3 – $[M(HL)_2]$, 4 – $[M(HL)_3]$

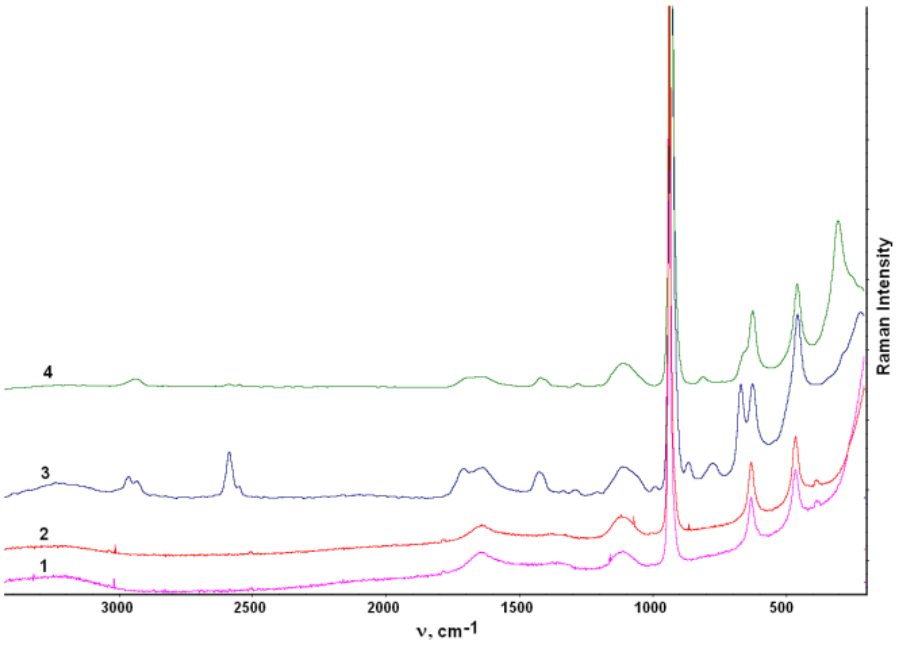

Figure S3. Raman spectra of aqueous solutions: 1 – $HClO_4$; 2 – Bi(III)/$HClO_4$; 3 – H_2MPA/$HClO_4$; 4 – Bi(III)/$HClO_4$/H_2MPA at $C_{Bi(III)}$ = 0.1 M, C_{H2MPA} = 0.3 M, C_{HClO4} = 0.8 M

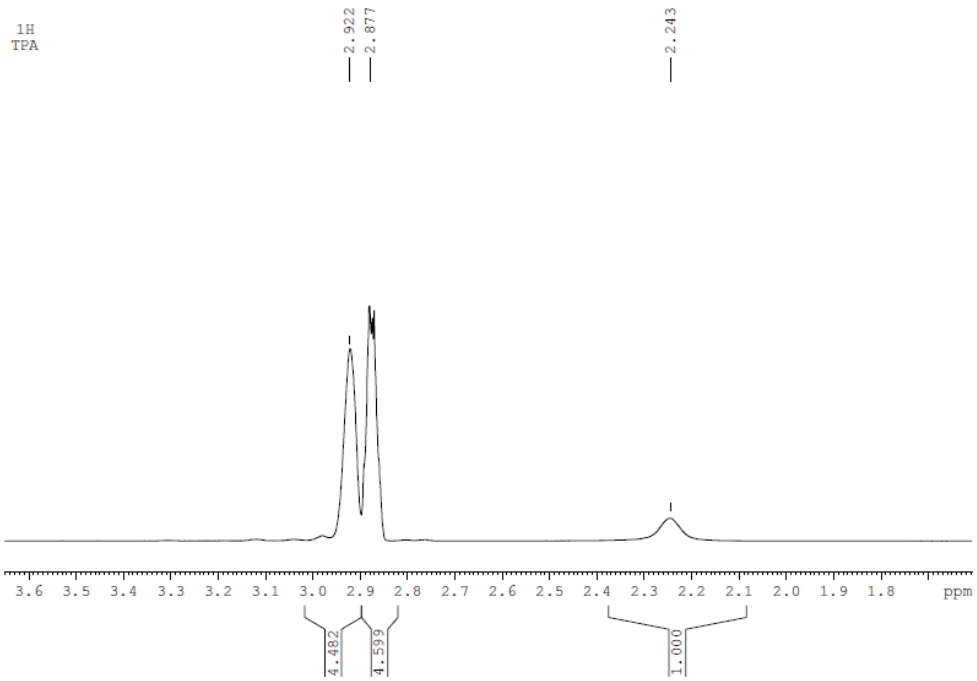

Figure S4. ^{1}H-NMR spectrum of H_2MPA in aqueous perchloric solution at C_{H2MPA} = 0.3 M and C_{HClO4} = 0.8 M

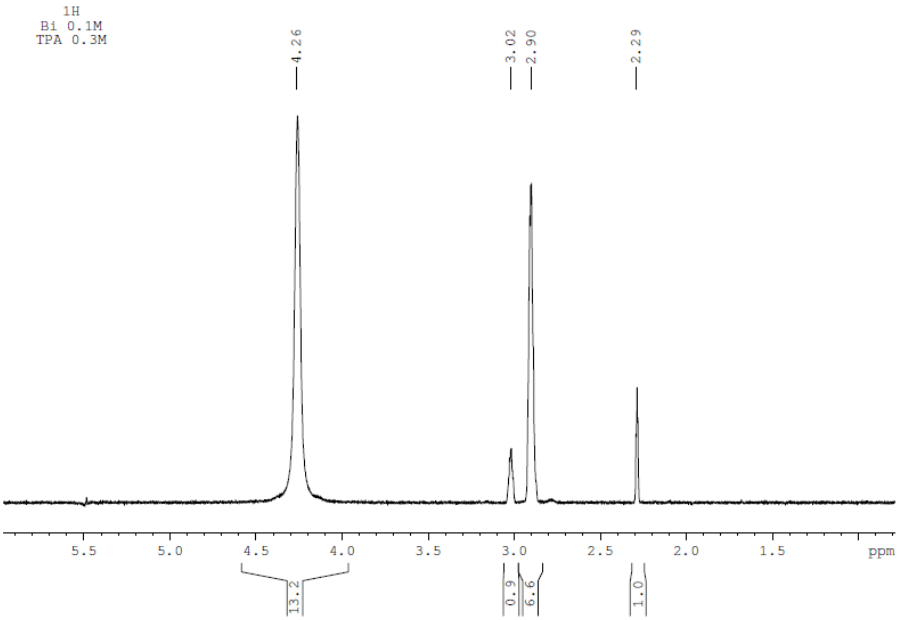

Figure S5. ^{1}H-NMR spectrum of Bi-H_2MPA system in aqueous perchloric solution at C_{Bi} = 0.1 M, C_{H2MPA} = 0.3 M and C_{HClO4} = 0.8 M

Table S3. Free Gibbs energies for the thermodynamic cycle (Def2-TZVPP)

Name	DFT	E, a.u.	ZPE, a.u.	E(SMD), a.u.
$Bi(HMPA)(H_2O)_3*H_2O^{2+}$	M06	-1185.86438	0.182145	-1186.132349
H_2MPA		-666.5386745	0.090247	-666.547042
$Bi(H_2O)_6^{3+}$		-672.2114887	0.14852	-672.8580632
$Bi(HMPA)_2(H_2O)_2^{+}$		-1699.297751	0.216948	-1699.376401
$Bi(HMPA)_3$		-2212.611974	0.249362	-2212.633585

$H_5O_2^+$		-153.1876838	0.058614	-153.3037497
$H_7O_3^+$		-229.6506778	0.08316	-229.7528162
$Bi(HMPA)_2^+$		-1546.404442	0.167313	-1546.482211
$Bi(HMPA)(H_2O)_3*H_2O^{2+}$	PBE0	-1185.389495	0.182601	-1185.656379
H_2MPA		-666.2818727	0.090695	-666.2906751
$Bi(H_2O)_6^{3+}$		-671.8964779	0.147221	-672.5459324
$H_5O_2^+$		-153.0999499	0.058187	-153.216463
$Bi(HMPA)(H_2O)_3^{2+}$		-1108.970613	0.15784	-1109.250898
$H_7O_3^+$		-229.5209997	0.083421	-229.6240611
$Bi(HMPA)(H_2O)_3*H_2O^{2+}$	M11	-1185.781204	0.182377	-1186.049083
H_2MPA		-666.5881588	0.090645	-666.598183
$Bi(H_2O)_6^{3+}$		-672.1034781	0.149347	-672.7559622
$H_5O_2^+$		-153.2163793	0.055949	-153.3329846
$Bi(HMPA)(H_2O)_3*H_2O^{2+}$	M06L	-1186.178309	0.182143	-1186.444925
H_2MPA		-666.6695429	0.090589	-666.6776181
$Bi(H_2O)_6^{3+}$		-672.441899	0.14832	-673.0889467
$H_5O_2^+$		-153.2315955	0.0589	-153.3475307
$Bi(HMPA)(H_2O)_3*H_2O^{2+}$	M11L	-1186.21161	0.184411	-1186.478167
H_2MPA		-666.6307722	0.090289	-666.6384018
$Bi(H_2O)_6^{3+}$		-672.4945767	0.152096	-673.1517915
$H_5O_2^+$		-153.2191984	0.059409	-153.3359381

Table S4. Percentage composition of $Bi(H_2O)_3(HMPA)^{2+}\cdot H_2O$ and $Bi(HMPA)_3$ molecular orbitals

Compounds	MO	Energy, eV	Bi	ΣS
$Bi(H_2O)_3(HMPA)^{2+}\cdot H_2O$	HOMO	-7.769	-	47.66 ($3p_x$) 15.20 ($3p_y$) 10.54 ($3p_z$)
	LUMO	-2.076	43.28 ($6p_x$) 12.63 ($6p_z$)	-
$Bi(H_2O)_3(HMPA)_2^+$	HOMO-1	-6.904	-	59.56 ($3p_y$)
	HOMO	-6.819	-	13.58 ($3p_x$) 34.74 ($3p_y$) 20.46 ($3p_z$)
	LUMO+1	-1.148	17.46 ($6p_z$)	-
	LUMO+2	-1.075	4.69 ($6p_x$) 17.66 ($6p_y$)	-
$Bi(HMPA)_3$	HOMO-1	-6.476	-	36.92 ($3p_x$) 26.66 ($3p_y$) 9.04 ($3p_z$)
	HOMO	-6.223	-	21.96 ($3p_x$) 20.49 ($3p_y$) 25.80 ($3p_z$)
	LUMO	-0.770	32.20 ($6p_y$)	-
	LUMO+1	-0.754	35.60 ($6p_x$)	
	LUMO+2	-0.487	30.47 ($6p_z$)	-

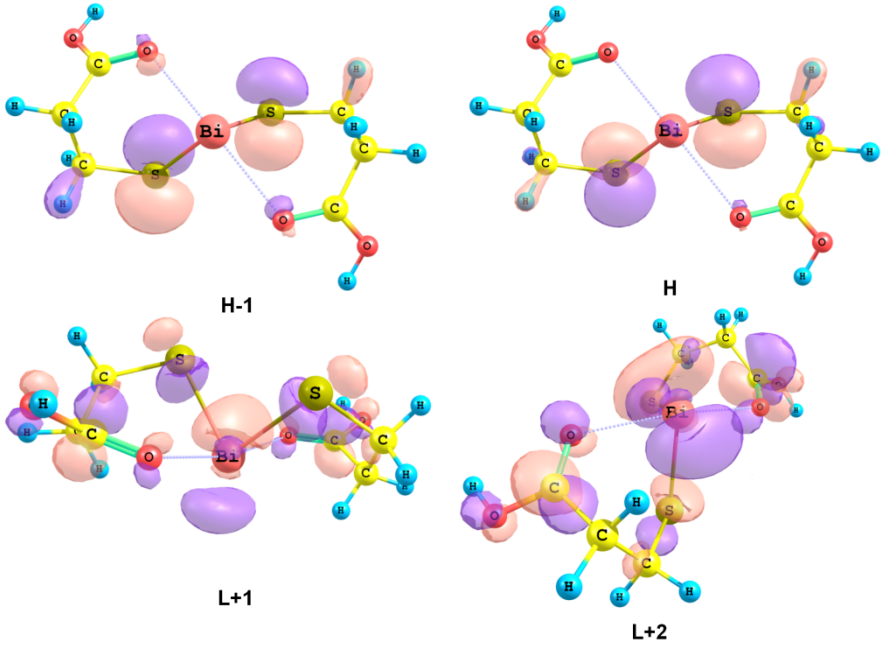

Fig. S6. Rendered MO of $Bi(HMPA)_2$

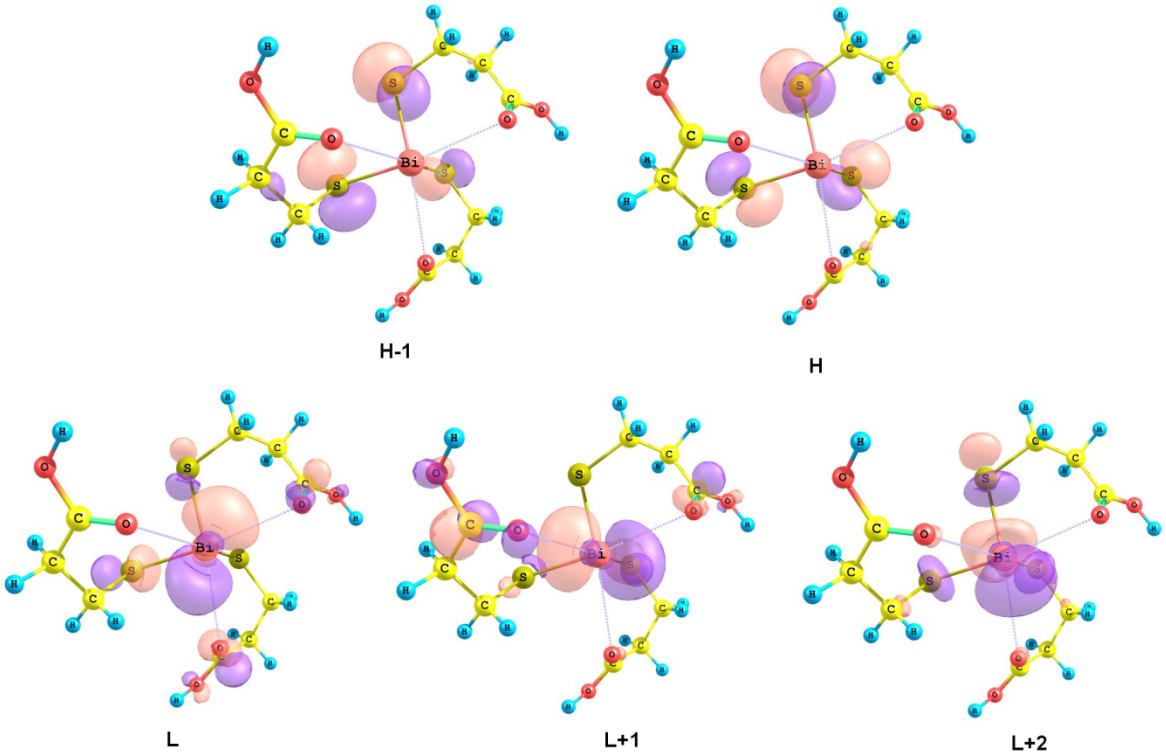

Fig. S7. Rendered MO of $Bi(HMPA)_3$

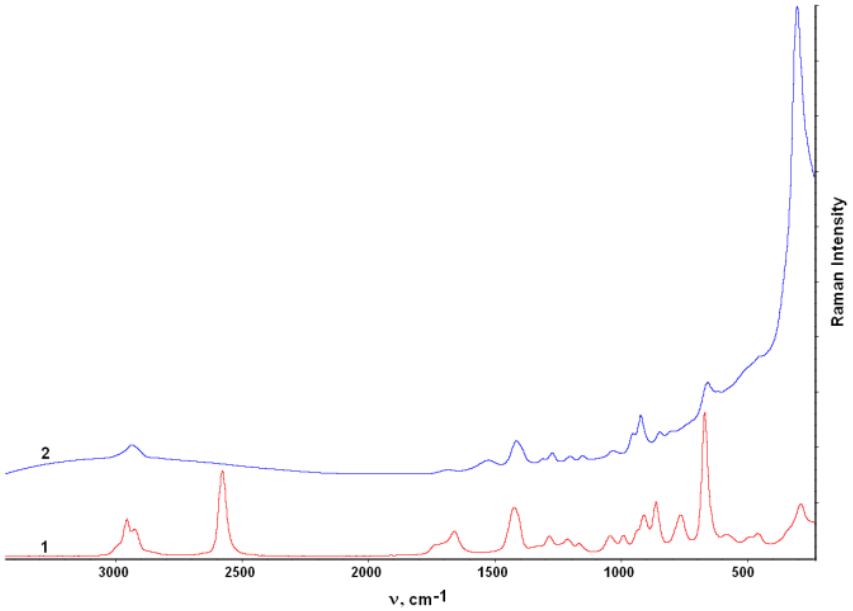

Figure S8. Raman spectra of solid $H[Bi(MPA)_2]$ and of H_2MPA

Cartesian coordinates for optimized:
$Bi(HMPA)(H_2O)_3*H_2O^{2+}$ (M06)
symmetry c1

Bi	-1.030000179	-0.280482026	0.388739906
O	-1.301267647	-1.999406477	2.203496242
O	1.406539848	-0.797261205	0.470907754
H	-1.515237661	-2.937165176	2.163466588
H	1.888327487	-1.530428238	0.074780246
H	-1.075296179	-1.799318412	3.117720667
H	2.049463233	-0.264361432	0.950294940
O	-0.687013657	1.475085431	-1.146672724
H	-0.090657762	2.205142506	-0.957481795
H	-0.898526073	1.476240115	-2.129382596
S	-0.372455545	1.229779478	2.231311171
C	-1.709891087	2.491425720	2.124293769
C	-3.077627137	2.025700389	2.563478001
C	-3.770638498	1.105624156	1.620926525
O	-5.045280283	1.031040940	1.813926866
O	-3.222329597	0.453082122	0.720919404
H	-1.730154528	2.923411551	1.124154374
H	-1.357583007	3.270896385	2.799418864
H	-3.736438595	2.884514483	2.720376404
H	-3.037192529	1.521661271	3.535818846
H	-5.474027798	0.412014784	1.202423646
O	-1.282079961	1.388426366	-3.665301372
H	-0.658139721	1.212168306	-4.372523905
H	-2.003497637	1.880538196	-4.062685268

$Bi(HMPA)(H_2O)_3*H_2O^{2+}$ (M06/SMD)

symmetry c1

Bi	-0.949477657	-0.397075430	0.486401649
O	-0.683682248	-2.222540003	2.133122717
O	1.430078187	-0.541025063	0.354275668
H	-0.795624068	-3.155654992	1.918319386
H	1.872780181	-1.250796463	-0.125002800
H	-1.082866729	-2.081976625	2.998796336
H	2.021280999	-0.213592805	1.042039371
O	-0.510822264	1.541735904	-0.781363789
H	0.385930648	1.865082751	-0.922288979
H	-0.980057798	1.495270886	-1.656551384
S	-0.622371661	0.920189141	2.574667486
C	-1.639209935	2.401338309	2.198089718
C	-3.129991954	2.182279676	2.283466430
C	-3.721136602	1.375428924	1.182455593
O	-5.022241388	1.495123234	1.102118120
O	-3.104323469	0.661589348	0.395716658
H	-1.340731148	2.808825895	1.233671511
H	-1.334853198	3.121254135	2.956948465
H	-3.653170995	3.141629108	2.303227200
H	-3.402647722	1.685134347	3.220532786
H	-5.397143937	0.930420854	0.405095174
O	-1.943869916	1.075738278	-2.916974992
H	-1.499038397	0.834443077	-3.734074826
H	-2.627813442	1.705506748	-3.160280942

$Bi(HMPA)_2(H_2O)_2^{+}$ (M06)

symmetry c2

Bi	0.000000000	0.000000000	0.366294963
S	-1.098019881	-1.312007566	-1.509603186
C	-2.746981763	-1.749403408	-0.833628466
C	-3.317472039	-0.828116558	0.245283961
C	3.167465112	-0.610440230	-0.114501456
O	4.197279503	-1.116192556	-0.746389664
O	2.165197198	-1.269040318	0.123942538
H	-2.799560443	-1.000759033	1.190978081
H	-2.720039185	-2.761886328	-0.435183316
H	-4.372237926	-1.063598914	0.389418969
H	-3.403635312	-1.749019078	-1.704063210
H	4.006464308	-2.030502871	-0.999088348
O	-0.426701185	-2.612727661	1.462845907
H	-0.139941793	-3.080593602	2.248896073
H	-0.203269017	-3.179108357	0.719766985

$Bi(HMPA)_2(H_2O)_2^+$ (M06/SMD)

symmetry c1

Bi	-0.001872198	0.007141517	0.301751822
S	-1.118346617	-1.269729910	-1.610054679
S	1.135963509	1.319380649	-1.584599011
C	-2.737879883	-1.729151175	-0.879774924
C	2.782018032	1.723150663	-0.877045827
C	-3.285510963	-0.807422935	0.209745919
C	3.294793565	0.792919049	0.220549888
C	3.152454782	-0.640639654	-0.153859113
C	-3.172072811	0.632852899	-0.148644740
O	4.215206989	-1.155419745	-0.732566062
O	-4.263869596	1.150576139	-0.669449365
O	2.127510222	-1.286981208	0.019080131
O	-2.150559991	1.289963417	0.000922347
H	-2.736747141	-0.965260676	1.141080677
H	2.739577883	0.959992542	1.145885488
H	-2.673923252	-2.735479783	-0.470496450
H	2.767393354	2.738269915	-0.484734372
H	-4.328303575	-1.062955354	0.397253839
H	4.341750508	1.022829625	0.419229892
H	-3.427506795	-1.754186091	-1.723597109
H	3.466358059	1.707084621	-1.726252936
H	4.069164516	-2.077058157	-1.003004438
H	-4.141164912	2.083360992	-0.917160419
O	-0.414038836	-2.498631672	1.486345396
O	0.409150375	2.510396630	1.523227488
H	-0.089737600	-2.651522749	2.378074695
H	-0.067682647	2.711203839	2.333584640
H	-0.053208891	-3.210914225	0.951096767
H	0.161083915	3.196230836	0.897055154

$Bi(HMPA)_3$ (M06)

symmetry c3

Bi	0.000000000	0.000000000	-0.060948427
H	0.660853215	-3.629023098	0.821870325
S	-2.058471167	-0.834967459	1.325158611
C	-2.868042394	-1.845829523	0.020629951
C	-2.384476731	-3.288097973	0.008554065
C	-0.894683079	-3.287050664	-0.139352246
O	-0.264298048	-3.937208420	0.822083421
O	-0.319289926	-2.682906767	-1.018622296
H	-2.716949995	-1.380612420	-0.954643858
H	-3.936776133	-1.814591849	0.230508533
H	-2.825296293	-3.819290867	-0.839592831
H	-2.663532291	-3.800496619	0.927923175

$Bi(HMPA)_3$ (M06/SMD)

symmetry c1

Bi	0.157450423	0.158649420	-0.035292432
H	0.376336971	-4.628812667	-0.281851932
H	4.226285403	2.561082193	-0.640890540
H	-4.160739890	1.624459850	-1.108167022
S	-1.924614181	-0.449983921	1.379259440
S	1.788756234	-1.091507658	1.529426015
S	0.486030068	2.290324624	1.379876211
C	-2.785343228	-1.612781203	0.255749462
C	3.082682464	-1.564690464	0.320568996
C	-0.528610769	3.546085664	0.510523482
C	-2.320855323	-3.043509307	0.388584651
C	4.174021423	-0.530568716	0.185874783
C	-2.023886151	3.329855119	0.546431339
C	-0.973528319	-3.292853576	-0.202285510
C	3.728141740	0.730311865	-0.477194858
C	-2.532399229	2.372503623	-0.478615238
O	-0.470295265	-4.473279209	0.164753484
O	4.511413500	1.765387761	-0.165402505
O	-3.857311909	2.226517693	-0.411834036
O	-0.394088935	-2.547279257	-0.958558225
O	2.795121699	0.828576409	-1.241204598
O	-1.860234617	1.806683867	-1.312651706
H	-2.690800639	-1.268130763	-0.776041303
H	2.628595668	-1.792309357	-0.645148384
H	-0.179681705	3.652777995	-0.516565828
H	-3.841699145	-1.546213056	0.515572609
H	3.509658920	-2.495885505	0.691988964
H	-0.289825482	4.478008446	1.022903505
H	-3.007400576	-3.718938045	-0.136648321
H	4.993242282	-0.920214855	-0.431017950
H	-2.547843733	4.274773705	0.365865525
H	-2.319887701	-3.368869751	1.430591704
H	4.612746984	-0.289793078	1.155209473
H	-2.361436985	2.989622157	1.528792867

$Bi(MPA)_2$-polymer^{3-} (M06)

symmetry c2

Bi	0.000000000	0.000000000	-1.384520275
S	1.658993630	0.878197139	-3.254522979
C	1.716173936	2.601432239	-2.613425258
C	0.531856609	3.442129709	-3.048643637
C	0.841154870	-3.103217945	-2.448908973
O	1.806300739	-3.761433528	-2.819669736

O	0.869625236	-2.180605347	-1.555428074
H	0.418671991	3.404613726	-4.147721899
H	2.655649224	3.040112347	-2.995313876
H	0.704519215	4.509731842	-2.802706074
H	1.814434925	2.583551345	-1.512306908
Bi	6.618070264	1.077859745	-0.272214084
S	6.465281109	-0.978100086	-1.795679588
C	4.627912898	-1.159814220	-1.942231311
C	3.816051933	-1.111531693	-0.658515608
C	3.430053586	0.284742745	-0.211108422
O	2.281407548	0.528892298	0.153531001
O	4.351725601	1.196488852	-0.230326623
H	4.371618781	-1.597401679	0.167284782
H	4.492102005	-2.149282800	-2.410393833
H	2.884754705	-1.682619439	-0.819594482
H	4.238525651	-0.417900340	-2.660883648
O	8.940527650	0.684778356	-0.243964318
S	6.649599630	-0.147763422	2.026245128
C	9.826079725	0.311705772	0.606342323
C	9.403197669	-0.696232429	1.686805357
C	8.017027078	-1.300099853	1.602210315
O	10.993361916	0.685840133	0.623093293
H	7.919574253	-2.135543566	2.317922699
H	7.820306930	-1.722985498	0.598803447
H	10.168971765	-1.495502002	1.657341010
H	9.541956651	-0.194726351	2.662966300

$H_5O_2^+$ (M06)
symmetry c2

O	-1.182809413	0.144912166	-0.017541293
H	0.000000000	0.000000000	0.036588158
H	-1.710927303	-0.537649888	-0.445474910
H	-1.661263003	0.517503585	0.730188953

$H_5O_2^+$ (M06/SMD)
symmetry c1

O	-1.175102955	0.163625827	-0.067633312
O	1.180898884	-0.179182516	-0.047664227
H	-0.004064368	-0.023457911	-0.003754388
H	-1.720704631	-0.561877822	-0.395006501
H	1.666708760	0.585227972	-0.381398152
H	-1.576231226	0.532205801	0.728637313
H	1.628495536	-0.516541351	0.737752926

H_2MPA (M06)

symmetry c1

S	-7.535523332	2.902229871	0.255709827
H	-7.505984344	1.996854343	-0.738098237
C	-5.865751678	3.559178120	-0.019882324
C	-4.783253831	2.530024533	0.202580070
C	-3.404433944	3.105753162	0.073715375
O	-2.466335537	2.152312086	0.194057932
O	-3.140072264	4.259830884	-0.105889163
H	-5.761883371	4.381828170	0.687390080
H	-5.795961724	3.997162488	-1.014618589
H	-4.873918280	1.697240277	-0.500243565
H	-4.872369920	2.077484582	1.193917427
H	-1.610707809	2.590343821	0.112273901

H_2MPA (M06/SMD)

symmetry c1

S	-7.538538656	2.874740614	0.217090285
H	-7.436037094	1.981320331	-0.777103829
C	-5.873757099	3.573638151	0.000897624
C	-4.788900489	2.547537737	0.221721634
C	-3.411093277	3.106132515	0.061497884
O	-2.478398289	2.150905369	0.192313545
O	-3.139558521	4.259488436	-0.156081492
H	-5.803974889	4.383135790	0.727531289
H	-5.798185896	4.023599167	-0.987930291
H	-4.894606643	1.705776372	-0.468476509
H	-4.858776937	2.109617968	1.221267561
H	-1.594368245	2.534349888	0.088185031

$Bi(H_2O)_6^{3+}$ (M06)

symmetry c1

Bi	0.286934782	0.186921476	-0.082449676
O	0.268052037	-1.731973892	1.302387658
O	1.535473488	1.155083545	1.796338410
O	-1.632009535	0.715514448	1.212223711
H	-0.175261408	-2.577368968	1.133934339
H	2.494464721	1.288763047	1.849005714
H	-2.185818097	1.502871193	1.097297442
H	0.803861690	-1.848909374	2.102607964
H	1.167896364	1.632916937	2.554434816
H	-1.967696083	0.246135932	1.990608142
O	-1.317602233	-1.100491663	-1.257419516
O	1.785433052	-1.016356507	-1.614567646
O	-0.604123274	2.014991375	-1.439163067
H	-2.272661791	-1.151930130	-1.101185959

H	2.265500373	-1.839122581	-1.437975316
H	-0.283824674	2.929818503	-1.469011228
H	-1.125582362	-1.652484959	-2.031171690
H	2.171346116	-0.665003701	-2.431694473
H	-1.228183822	1.934235665	-2.175529084

$Bi(H_2O)_6^{3+}$ (M06/SMD)

symmetry c1

Bi	-0.134185830	0.011101527	0.044169879
O	0.556571739	-2.031316323	1.108391069
O	1.465931849	1.236052542	1.286679657
O	-1.810188008	0.976766339	1.507971928
H	0.090649359	-2.863071337	0.961042737
H	2.414725576	1.067433282	1.336805353
H	-2.396218643	1.711060007	1.289294810
H	0.935384013	-2.051359639	1.995302550
H	1.206681719	1.801290357	2.024404804
H	-2.257437783	0.410476872	2.147629690
O	-1.564112561	-1.367381060	-1.290344421
O	1.646080353	-0.678578387	-1.321346530
O	-0.254223322	1.900094847	-1.349238756
H	-2.527979653	-1.352753288	-1.255455322
H	2.235527198	-1.408354570	-1.094280158
H	0.216172382	2.726020407	-1.179600856
H	-1.288970301	-1.915176088	-2.034735656
H	2.090695847	-0.095897890	-1.948712718
H	-0.625103933	1.923592402	-2.240722192

$Bi(HMPA)_2$ (M06)

Symmetry c2

Bi	0.000000000	0.000000000	-0.238040877
S	1.210121502	1.240825811	1.567262058
S	-1.210121502	-1.240825811	1.567262058
C	1.423711131	2.937369409	0.898923183
C	-1.423711131	-2.937369409	0.898923183
C	0.520525784	3.369372513	-0.254591138
C	-0.520525784	-3.369372513	-0.254591138
C	-0.924772235	3.107381484	0.013964530
C	0.924772235	-3.107381484	0.013964530
O	-1.586792396	4.145666305	0.451010784
O	1.586792396	-4.145666305	0.451010784
O	-1.457220054	2.015521394	-0.135537146
O	1.457220054	-2.015521394	-0.135537146
H	0.798469365	2.839139353	-1.169270367
H	-0.798469365	-2.839139353	-1.169270367
H	2.459738118	3.056421944	0.588170856

H	-2.459738118	-3.056421944	0.588170856
H	0.671183464	4.434041540	-0.433416983
H	-0.671183464	-4.434041540	-0.433416983
H	1.258712737	3.585354743	1.760294436
H	-1.258712737	-3.585354743	1.760294436
H	-2.503381090	3.896515468	0.639742707
H	2.503381090	-3.896515468	0.639742707

$Bi(HMPA)_2$ (M06/SMD)

symmetry c1

Bi	0.025402842	-0.008683603	-0.358234242
S	-1.400721872	-1.139145772	1.396265752
S	1.308327628	1.202446353	1.455996662
C	-1.500053549	-2.877344574	0.810878610
C	1.464894686	2.915810998	0.811201774
C	-0.481034955	-3.328254387	-0.228974316
C	0.485870417	3.326025964	-0.284900151
C	0.934245569	-3.050650632	0.142543914
C	-0.923854969	3.037990593	0.092556840
O	1.622403329	-4.099176770	0.517491570
O	-1.563837828	4.045500569	0.632702922
O	1.440022821	-1.931769412	0.102013646
O	-1.450145068	1.938877615	-0.052780186
H	-0.658992020	-2.821784884	-1.182040934
H	0.707049740	2.787081745	-1.209312420
H	-2.494146794	-3.041830004	0.399555506
H	2.477016211	3.055632097	0.438084229
H	-0.611955821	-4.396001609	-0.402919585
H	0.609746091	4.389011160	-0.490294321
H	-1.409748276	-3.484329312	1.711467944
H	1.337603158	3.554014499	1.686100005
H	2.546582583	-3.873261040	0.722361057
H	-2.464673926	3.799840406	0.905300685

$H_7O_3^+$ (M06/SMD)

symmetry c1

H	1.652539220	0.429491801	0.005268836
O	0.853347677	-0.110333896	-0.001859323
H	0.305293516	-0.068058366	0.871836238
H	0.298190598	-0.015180500	-0.858796419
O	-0.558286245	-0.036544220	2.063937521
O	-0.576893178	0.053315392	-2.064061289
H	-0.342958475	-0.647886017	2.774938660
H	-0.523235603	-0.694308419	-2.666306444
H	-0.707436039	0.820609143	2.474286957
H	-0.514909677	0.849757329	-2.599244737

$H_7O_3^+$ (M06)

symmetry cs

H	1.704704281	0.332417256	0.000000000
O	0.857779832	-0.123774519	0.000000000
H	0.333692856	-0.011637773	-0.878182041
H	0.333692856	-0.011637773	0.878182041
O	-0.400244612	0.055338733	-2.157062288
O	-0.400244612	0.055338733	2.157062288
H	-0.492342575	-0.685178585	-2.759191491
H	-0.492342575	-0.685178585	2.759191491
H	-0.779521827	0.827587380	-2.579286504
H	-0.779521827	0.827587380	2.579286504

$Bi(HMPA)_2^+$ (PBE0)

symmetry c1

Bi	-1.008715198	-0.342622977	0.479473127
O	-1.283139688	-2.025638714	2.233532815
O	1.440378902	-0.719692889	0.444188649
H	-1.441015415	-2.974975920	2.164482815
H	1.937030317	-1.414354656	-0.003915282
H	-1.081215323	-1.828076651	3.155812097
H	2.073426731	-0.208872900	0.962080532
O	-0.722797666	1.498993451	-1.121227507
H	0.015751919	2.117579009	-1.081524361
H	-1.076110626	1.535948517	-2.018421207
S	-0.373490575	1.167150256	2.295558589
C	-1.668284281	2.457080336	2.171648467
C	-3.076439661	2.019306120	2.520419077
C	-3.740057802	1.149131169	1.509793426
O	-5.027711379	1.149353992	1.578625319
O	-3.150843469	0.461091740	0.653850941
H	-1.625057838	2.928875740	1.190429145
H	-1.335891643	3.198728999	2.899691424
H	-3.714819781	2.896282958	2.662810791
H	-3.107609158	1.481501751	3.475484989
H	-5.436033433	0.554873842	0.928052685

$Bi(HMPA)_2^+$ (PBE0/SMD)

symmetry c1

Bi	-0.968711884	-0.387582486	0.470039287
O	-1.383901784	-1.936333348	2.254043109
O	1.401313158	-0.611102853	0.333307450
H	-1.547042236	-2.883068457	2.167919868
H	1.828091023	-1.332779093	-0.143992582
H	-1.153123194	-1.733715651	3.167787854

H	2.069925254	-0.129854924	0.834280803
O	-0.644356175	1.556720730	-0.913962851
H	0.243268357	1.909339586	-1.057506106
H	-1.105472037	1.593885527	-1.761640037
S	-0.402228995	1.107573869	2.365888783
C	-1.654842793	2.417332045	2.152116941
C	-3.075302124	2.022870423	2.492559893
C	-3.714759647	1.117206196	1.505141159
O	-5.011215152	1.013182421	1.631398344
O	-3.121979677	0.495228454	0.616645836
H	-1.587277317	2.821768890	1.142475104
H	-1.328938562	3.201603268	2.836223110
H	-3.704581287	2.915344564	2.560544610
H	-3.142463742	1.537018773	3.472372334
H	-5.399046249	0.407025240	0.975203623

$H_7O_3^+$ (PBE0/SMD)

symmetry c1

H	1.647395373	0.429008175	0.002910197
O	0.856589242	-0.123791925	-0.004367411
H	0.287504211	-0.017965978	-0.873370291
H	0.292412448	-0.059941211	0.875694355
O	-0.575059146	0.052296829	-2.009028617
O	-0.559882760	-0.036385958	2.013250286
H	-0.510171044	-0.694138144	-2.614458624
H	-0.334167460	-0.647811124	2.723543259
H	-0.512508511	0.855899185	-2.536731088
H	-0.706460558	0.823692397	2.422557933

$H_7O_3^+$ (PBE0)

symmetry cs

H	1.692095732	0.380537333	0.000000000
O	0.868034347	-0.116835871	0.000000000
H	0.324683222	-0.008348324	-0.883782183
H	0.324683222	-0.008348324	0.883782183
O	-0.464005346	0.036554511	-2.074615667
O	-0.464005346	0.036554511	2.074615667
H	-0.494209096	-0.702036661	-2.688370830
H	-0.494209096	-0.702036661	2.688370830
H	-0.703707923	0.832410866	-2.555603312
H	-0.703707923	0.832410866	2.555603312