Keys for the existence of stable dimers of bis-TTF-functionalized molecular clips presenting $[TTF]^{\cdot+}\cdots[TTF]^{\cdot+}$ long, multicenter bonds at room temperature

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Supporting Material

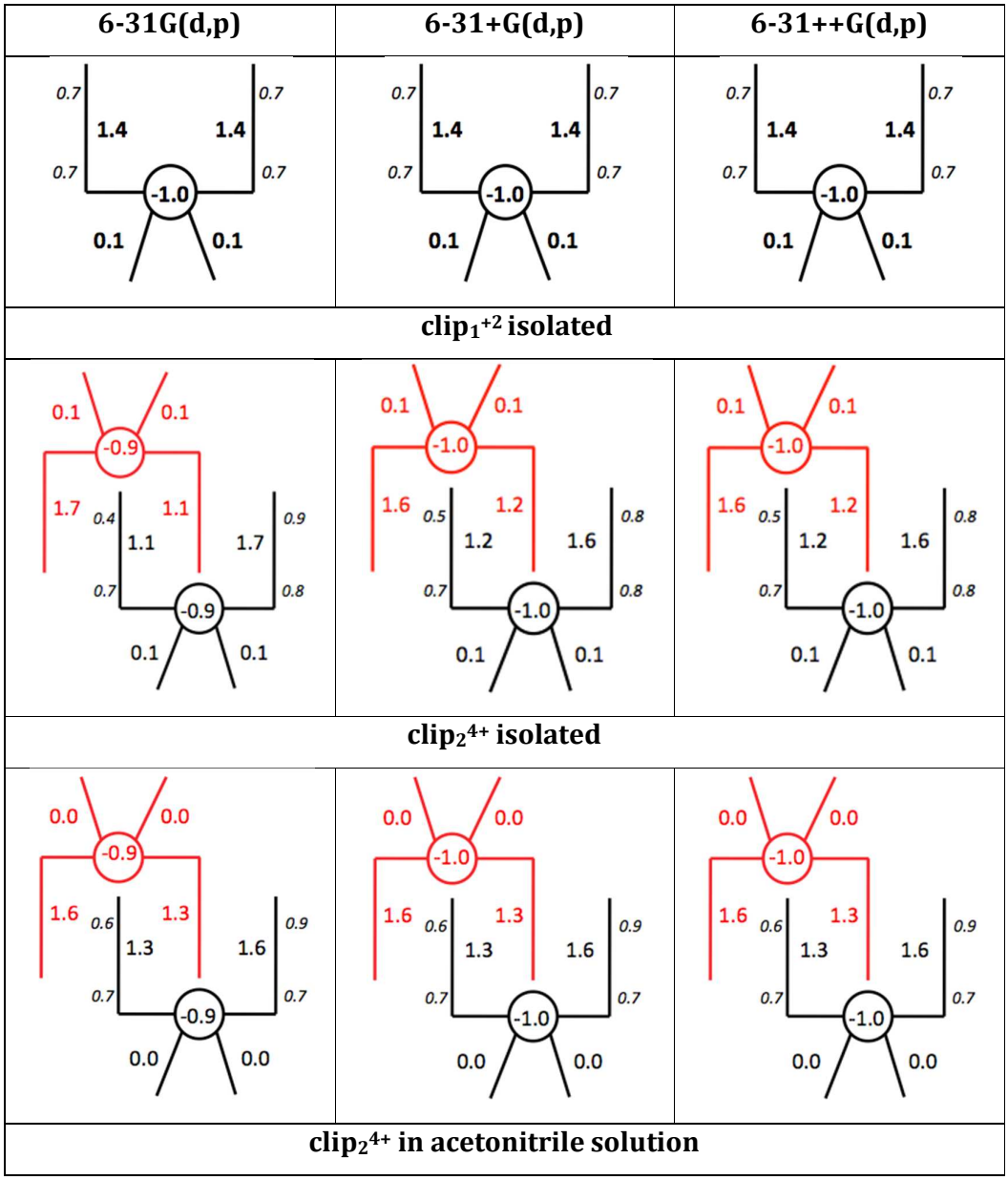


Figure S1. Representation of the net charge distribution on $clip_1^{2+}$ monomer and $clip_2^{4+}$ dimer studied in this work. The net atomic charge in the five groups defined in Figure 1 is given, indicating in italics the charge in the TTF_i and L_i-TTF_i parts of the L_i arms. The net charge in each group is computed by adding the NBO atomic charges for all atoms of the group. M06L/6-31G(d,p), M06L/6-31+G(d,p) and M06L/6-31++G(d,p) calculations are compared at M06L/6-31G(d,p) optimum geometries.

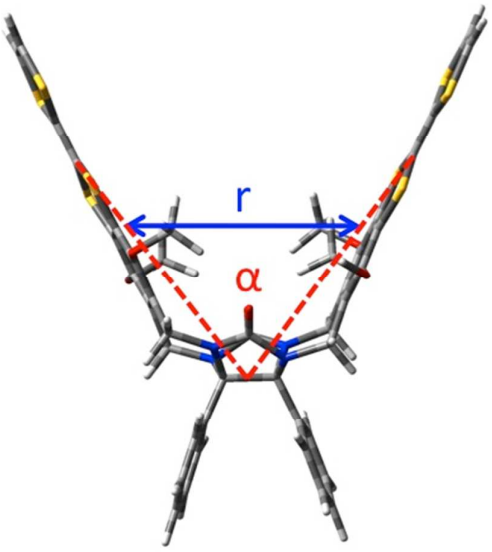


Figure S2. Geometrical parameters used to define the separation between the two arms of the V-shaped $clip_1^{n+}$ (n = 0-4) monomers: *r*, the distance between the C=C bonds of the TTF groups attached to the six-membered rings, and α, the $C_{central}$-dummy-$C_{central}$ angle (being dummy an atom of this class placed in the middle of the common C=C bond in the fused central five-membered rings and the C atom of each TTF group that forms part of the C=C bond that links the two six-membered rings in each TTF).

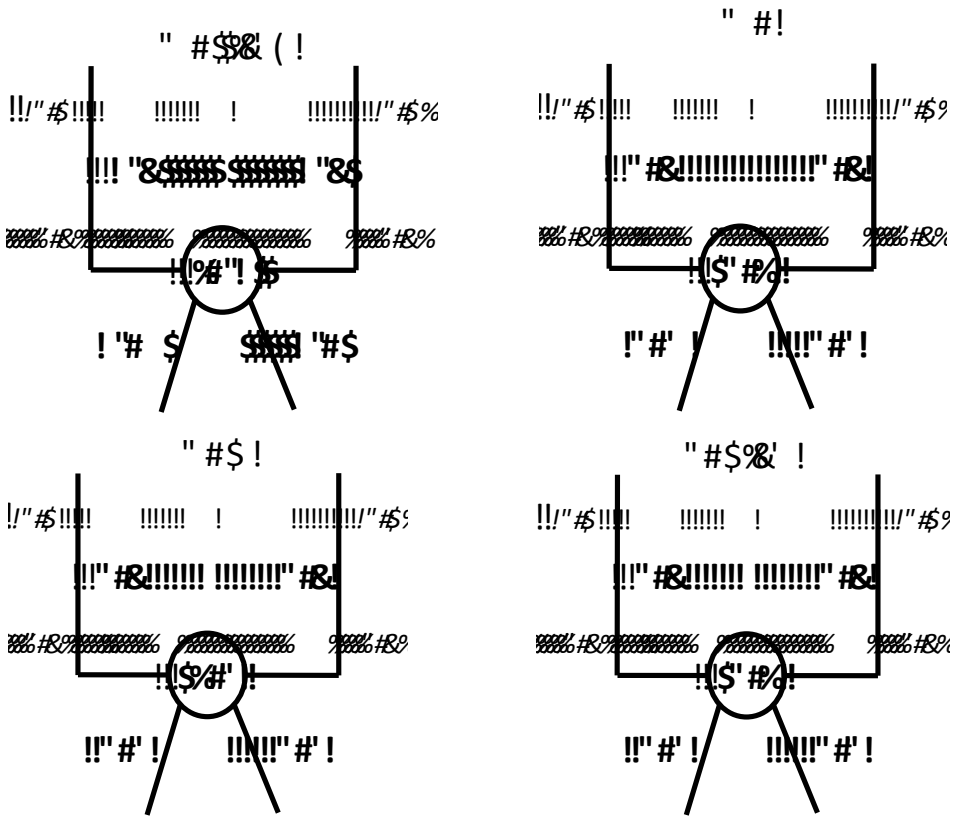


Figure S3. Charge distribution predicted by different population schemes on the five groups of $clip_1^0$ defined in Figure 1. The schemes tested are: Mulliken, Merz-Kolman (MK), Natural bond orbitals (NBO), and CHelpG.

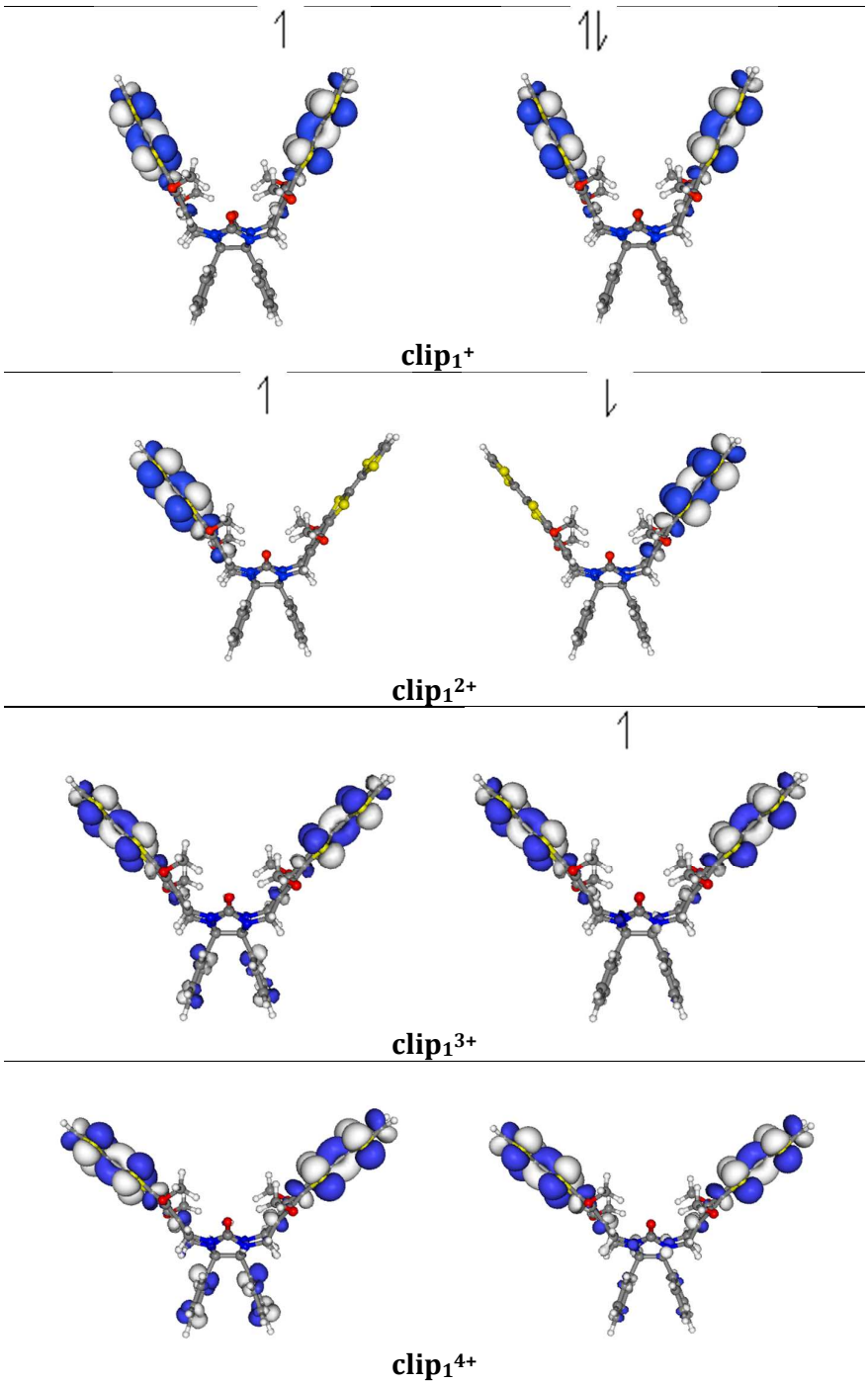


Figure S4. Shape and occupation of the two MOs of $clip_1^{n+}$ (n = 1 to 4) corresponding to the highest two MOs of $clip_1^{0}$ upon successive oxidations. The orbitals have been computed for each monomer ground state (M06L/6-31G(d,p) calculations) at its optimum geometry.

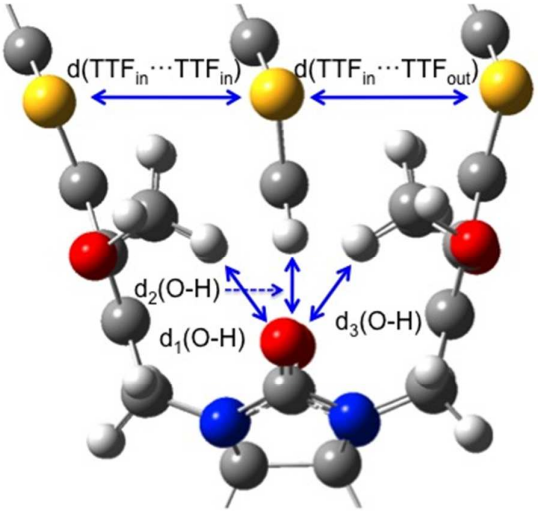


Figure S5. Intermolecular parameters used to determine the fragments relative disposition in the clip$_2^{n+}$ dimers.

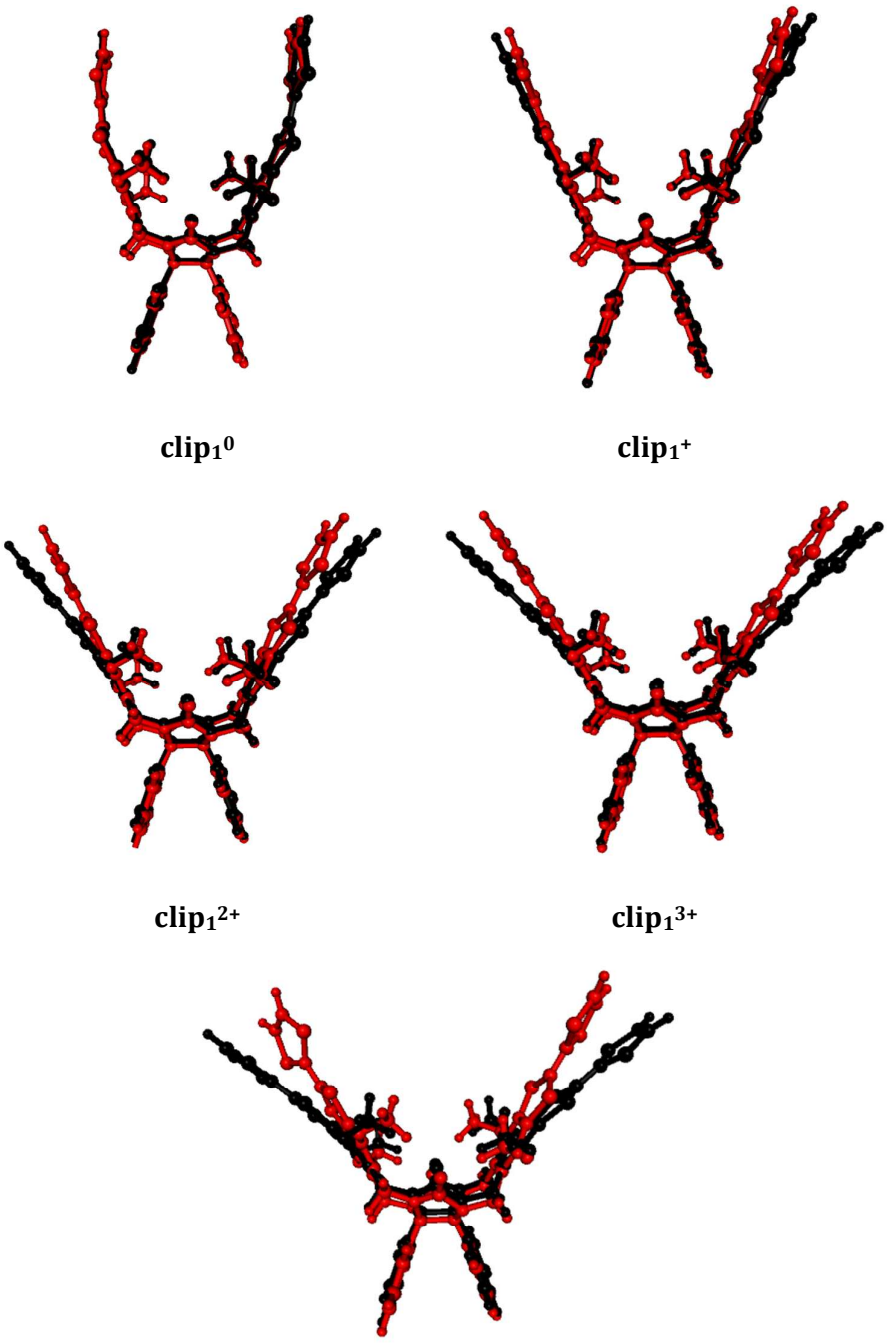
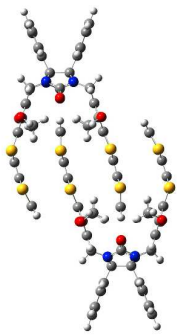
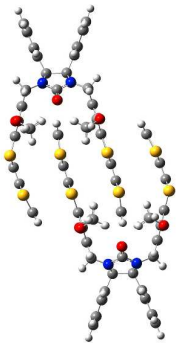
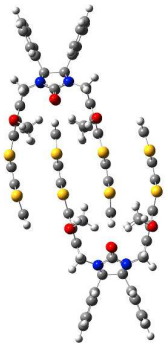
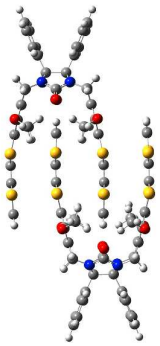
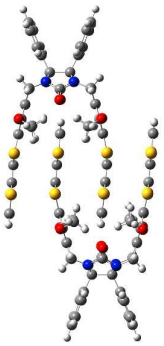


Figure S6. Comparison between isolated and solvated optimum structures of $clip_1^{n+}$ (n = 0 to 4) monomers obtained at M06L/6-31G(d,p) level. A PCM model has been used to describe the acetonitrile solution. The optimum structure in solution is superimposed (red) over the optimum isolated one (black).

				
Closed-shell singlet	Doublet	Closed-shell singlet	Doublet	Closed-shell singlet
$clip_2^{0}$	**$clip_2^{+}$**	**$clip_2^{2+}$**	**$clip_2^{3+}$**	**$clip_2^{4+}$**

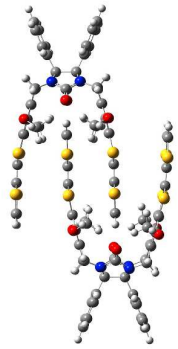
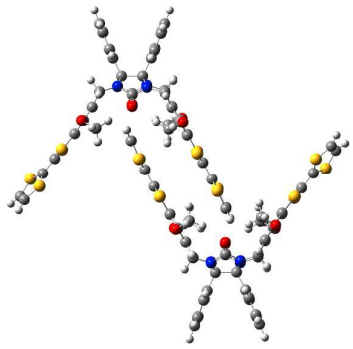
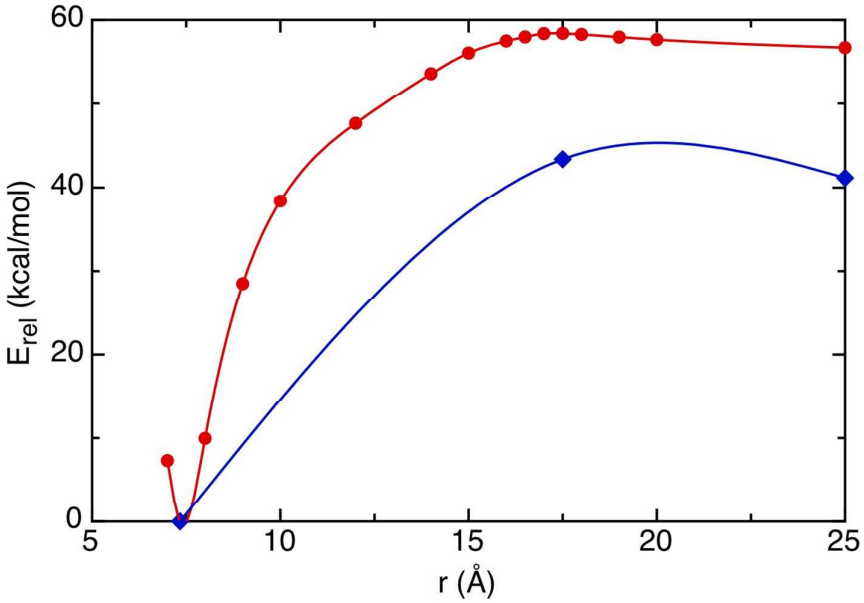
	
Closed-shell singlet	Closed-shell singlet
$clip_2^{6+}$	**$clip_2^{8+}$**

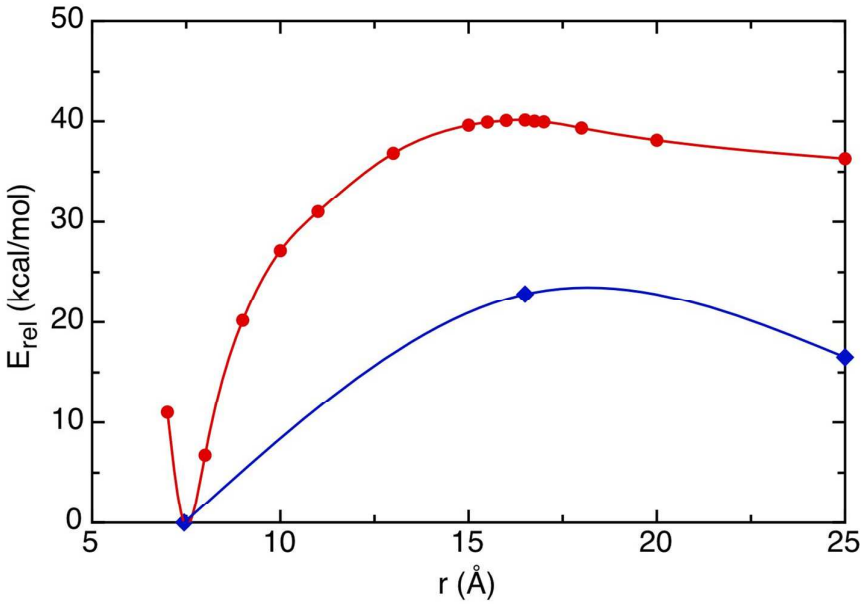
Figure S7. Optimum geometries of $clip_2^{n+}$ dimers (n = 0, 1, 2, 3, 4, 6, 8) in their ground electronic state (indicated under each geometry), in acetonitrile solution. M06L/6-31G(d,p) calculations in PCM continuous model.

clip$_2^{4+}$ in acetonitrile



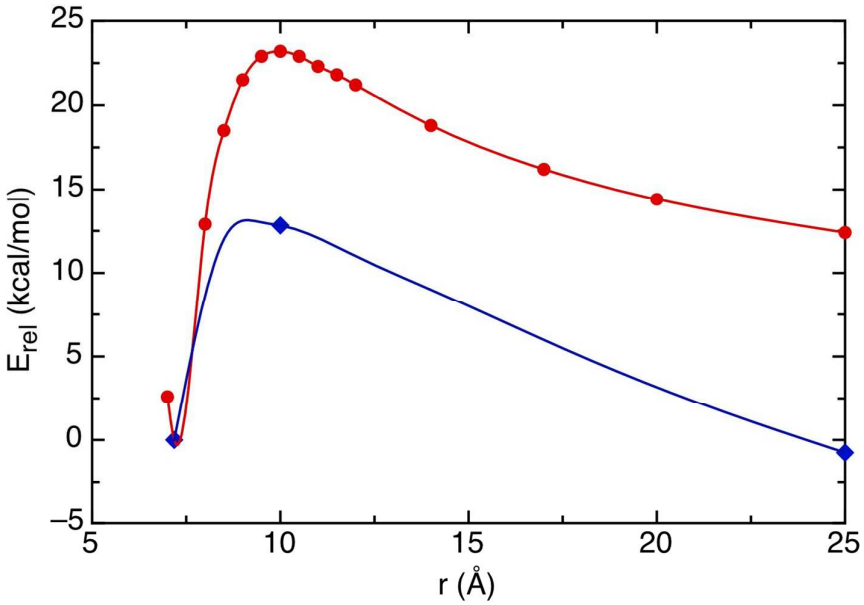
Estimated barrier = +43.4 kcal/mol
TΔS = +29.1 kcal/mol < Estimated barrier → **Dimer is stable at room T**

clip$_2^{6+}$ in acetonitrile



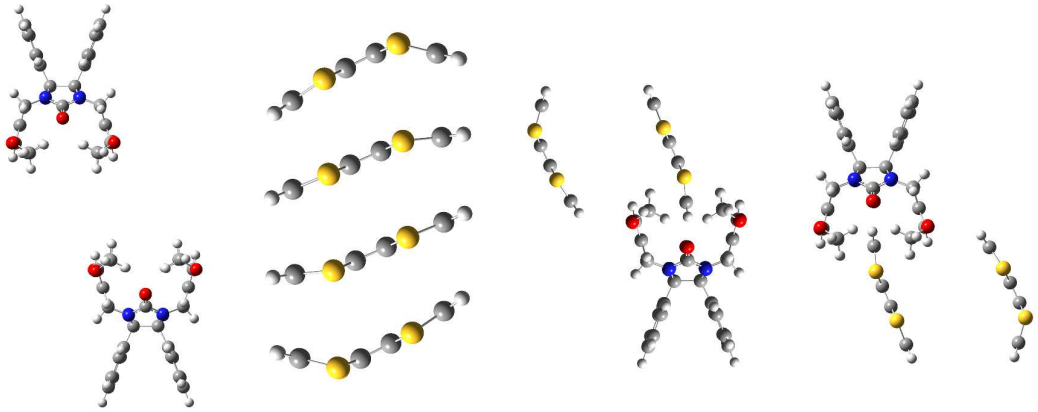
Estimated barrier = +22.7 kcal/mol
TΔS = +30.7 kcal/mol > Estimated barrier → **Dimer dissociates at room T**

clip$_2^{8+}$ in acetonitrile



Estimated barrier = +12.8 kcal/mol
TΔS =+25.5 kcal/mol > Estimated barrier → Dimer dissociates at room T

Figure S8. *Red lines with circles*: Scan of the potential energy surface in solution for the clip$_2^{4+}$, clip$_2^{6+}$, and clip$_2^{8+}$ dimers (top, center and bottom curves, respectively) as a function of the monomers separation (during this scan, the monomers geometries was frozen at their optimum in the dimer minimum energy structure); *Blue lines with rombus*: Curve obtained after reoptimizing the geometry of the highest energy point in the scan and the minimum of dimer and monomers.



BR_1-BR_2 $2TTF_1$-$2TTF_2$ BR_1-$2TTF_2$ $2TTF_1$-BR_2

Figure S9. Structure of the four fragment-pairs whose energy is collected in Table 3 (see text for details).

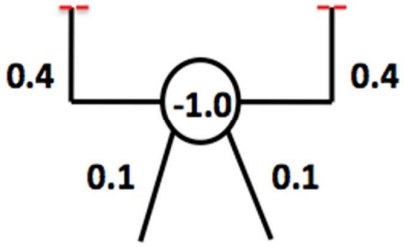


Figure S10. Charge distribution in the bridge fragment computed from Mulliken population analysis in the ground state.

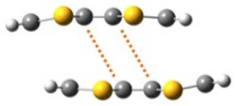
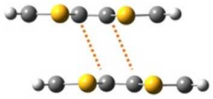
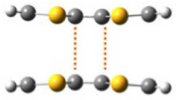
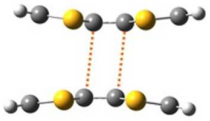
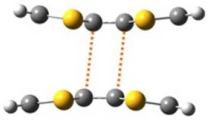
		
-10.7 (-9.4)	-28.3 (-20.4)	+39.1 (+38.1)
3.45	3.33	3.44
$[TTF]_2^0$	**$[TTF]_2^+$**	**$[TTF]_2^{2+}$**
		
+86.9 (+90.8)	+216.3 (+211.4)	
3.44 (frozen)	3.44 (frozen)	
$[TTF]_2^{3+}$	**$[TTF]_2^{4+}$**	

Figure S11. Optimum energy structures and their BSSE-uncorrected interaction energy computed at the M06L/6-31G(d,p) level and RASPT2/6-31G(d,p) level (in parenthesis) for isolated π-$[TTF]_2^{n+}$ (n = 0 to 4) dimers. The structures are fully characterized minima for the n = 0, 1, 2 dimers, while for the n = 3 and 4 dimers, where the dimers dissociate, they are the optimum ones at the frozen indicated C···C distance, dotted lines.

Table S1. Values of the shortest computed TTF···TTF distance (r), angle (α), and dipole moment (μ) of $clip_1^{2+}$ monomer, both isolated and in acetonitrile solution using the PCM model. M06L/6-31G(d,p), M06L/6-31+g(d,p) and M06L/6-31++G(d,p) calculations are compared.

	***r* (Å)**		***α* (º)**		**μ (Debye)**	
	isolated	solution	isolated	solution	isolated	solution
6-31G(d,p)	8.6	7.9	85.3	74.4	20.5	29.3
6-31+G(d,p)	8.6	7.8	84.8	73.2	20.5	30.2
6-31++G(d,p)	8.6	7.8	84.3	73.2	20.6	30.2

Table S2. Interaction and formation energy obtained at M06L/6-31G(d,p), M06L/6-31+G(d,p) and M06L/6-31++G(d,p) level, for the M06L/6-31G(d,p) optimum geometry of $clip_2^{4+}$ dimer both when isolated and in acetonitrile solution. Energy values in kcal/mol.

	6-31g(d,p)	*6-31+g(d,p)*	*6-31++g(d,p)*
		isolated	
$\mathbf{E_{int}}$	*+70.4*	*+57.2*	*+57.4*
$\mathbf{E_{for}}$	*+98.6*	*+91.2*	*+89.5*
		In acetonitrile solution	
$\mathbf{E_{for}}$	*-41.2*	*-48.0*	*-47.7*

Table S3. Values of the four energy components (in kcal/mol) of equation (2) computed for the M06L/6-31G(d,p) optimized $clip_2^{4+}$ dimer obtained at M06L/6-31G(d,p) and M06L/6-31+G(d,p) level. The following components were computed (see the main text for their definition): $2TTF_1$-$2TTF_2$, $2TTF_1$-BR_2, BR_1-$2TTF_2$, and BR_1-BR_2. The sum of these components (E_{sum}) is also given. The charge on both interacting fragments is indicated in each box as $fragment_1$/$fragment_2$. All energy data are BSSE-corrected.

	$E(BR_1\text{-}BR_2)$	$E(2TTF_1\text{-}2TTF_2)$	$E(2TTF_1\text{-}BR_2)$	$E(BR_1\text{-}2TTF_2)$	E_{sum}
	0/0	2+/2+	2+/0	0/2+	
6-31g**	**+0.01**	**+156.6**	**-36.6**	**-36.6**	**+83.5**
6-31+g**	**+0.02**	**+155.3**	**-35.3**	**-35.3**	**+84.8**

Table S4. Values of some relevant intermolecular parameters (defined in Figure S4) characteristic of each optimum ground state geometry of $clip_2^{n+}$ dimers. Two groups of values are collected: (1) when the $clip_2^{n+}$ dimers are isolated and (2) when they are in solution. In the second case, the solvent effects have been modeled using the continuous PCM model.

System	$d(TTF_{in}\cdots TTF_{in})$ (Å)	$d_2(TTF_{in}\cdots TTF_{out})$ (Å)	d_1(O-H) (Å)	d_2(O-H) (Å)	d_3(O-H) (Å)
Gas phase					
$clip_2^0$	3.63	3.64	2.28	2.36	2.25
$clip_2^+$	3.66	3.68	2.23	2.29	2.22
$clip_2^{2+}$	3.72	3.68	2.23	2.22	2.19
$clip_2^{3+}$	3.72	3.61	2.20	2.15	2.19
$clip_2^{4+}$	3.97	3.52	2.19	2.15	2.19
$clip_2^{6+}$	3.32	8.55	2.13	2.39	2.34
$clip_2^{8+}$	nam[a]	nam[a]	nam[a]	nam[a]	nam[a]
Acetonitrile solutions					
$clip_2^0$	3.97	3.86	2.27	2.34	2.27
$clip_2^+$	3.66	3.73	2.24	2.33	2.22
$clip_2^{2+}$	3.72	3.67	2.24	2.30	2.17
$clip_2^{3+}$	3.81	3.56	2.23	2.25	2.17
$clip_2^{4+}$	3.96	3.44	2.21	2.24	2.24
$clip_2^{6+}$	3.60	3.80	2.24	2.27	2.24
$clip_2^{8+}$	4.40	5.85	2.27	2.42	2.31

[a] Not a minimum

Table S5. Distribution of the 1+ net charge created when an isolated $clip_2^{n+}$ dimer is oxidized to $clip_2^{(n+1)+}$. All atomic charges have been computed at the M06L/6-31G(d,p) level on the ground state wavefunction. The groups are those defined in Figure 1. Distinction is made between inner and outer TTF groups, defined on the basis of their position within the TTF_4 stack, see Figure 7.

	$\mathbf{clip_2^0 \rightarrow clip_2^+}$	$\mathbf{clip_2^+ \rightarrow clip_2^{2+}}$	$\mathbf{clip_2^{2+} \rightarrow clip_2^{3+}}$	$\mathbf{clip_2^{3+} \rightarrow clip_2^{4+}}$
Inner TTF	+0.44	+0.20	+0.10	+0.10
Outer TTF	+0.22	+0.42	+0.50	+0.40
Total TTF	+0.66	+0.62	+0.60	+0.50
(L1–TTF1) +				
(L2–TTF2)	+0.22	+0.26	+0.30	+0.28
L3 + L4	+0.12	+0.08	+0.10	+0.22

Table S6. Distribution of the 1+ net charge created when an $clip_2^{n+}$ dimer dissolved in acetonitrile is oxidized to $clip_2^{(n+1)+}$. All atomic charges have been computed at the M06L/6-31G(d,p) level on the ground state wavefunction. The solvent is simulated using the continuous PCM model. The groups are those defined on Figure 1 (see Table S5 for a comparison with the isolated results).

	$\mathbf{clip_2^0 \rightarrow clip_2^+}$	$\mathbf{clip_2^+ \rightarrow clip_2^{2+}}$	$\mathbf{clip_2^{2+} \rightarrow clip_2^{3+}}$	$\mathbf{clip_2^{3+} \rightarrow clip_2^{4+}}$
Inner TTF	+0.64	+0.26	+0.14	+0.34
Outer TTF	+0.14	+0.50	+0.66	+0.52
Total TTF	+0.78	+0.76	+0.80	+0.86
(L1–TTF1) +				
(L2–TTF2)	+0.20	+0.20	+0.20	+0.16
L3 + L4	+0.04	+0.04	+0.00	+0.00

Table S7. Electron density (in atomic units) at the bond critical points of Figure 10.

	TTF_2^{2+}	$clip_2^{4+}$ external TTF···TTF	$clip_2^{4+}$ internal TTF···TTF
Density @ C-C bcp	0.006	0.006	0.002
Density @ S-S bcp	0.011	0.010	0.005

Table S8. Optimized cartesian coordinates (in Angstroms) of $clip_1^0$ at M06L/6-31G(d,p) level.

C	-0.168992	0.036057	0.114329
C	-0.106779	0.035626	1.505484
C	1.124927	0.027320	2.149376
C	2.309906	0.035352	1.409276
C	2.241013	0.026804	0.014539
C	1.007284	0.022816	-0.629503
H	-1.132011	0.042465	-0.388509
H	-1.020633	0.042369	2.092518
H	1.179748	0.039236	3.234786
H	3.159628	0.038281	-0.567409
H	0.966491	0.016331	-1.714971
C	3.643006	0.193734	2.110874
C	4.076656	1.699360	2.374794
C	2.951933	2.710177	2.283706
C	2.195572	3.033169	3.412135
C	2.586300	3.241951	1.044367
C	1.087087	3.867534	3.302375
H	2.473221	2.617817	4.378247
C	1.472042	4.065442	0.933184
H	3.172238	2.984634	0.166075
C	0.717796	4.378490	2.061659
H	0.507931	4.112850	4.187885
H	1.191015	4.463007	-0.038023
H	-0.152280	5.022970	1.974780
N	3.642465	-0.376797	3.445336
N	4.754491	-0.279211	1.307515
N	5.100235	1.917915	1.369298
N	4.628970	1.600153	3.711493
C	4.395130	0.393590	4.320787
C	5.612423	0.713685	0.908733
O	6.618537	0.570926	0.229123
O	4.744710	0.071481	5.447084
C	5.350850	2.688660	4.332936
C	5.955312	3.097377	1.434015
C	4.938594	-1.676161	0.981633
C	3.560708	-1.820961	3.629665
H	5.288835	3.952986	1.607400
H	6.403857	3.236047	0.448697
H	5.353425	2.503383	5.409095
H	4.780782	3.614669	4.162132
H	3.247739	-2.005454	4.658869
H	5.613590	-1.721745	0.124001
H	2.748088	-2.170774	2.978477
H	3.967290	-2.079104	0.656039
C	4.832023	-2.592523	3.354442
C	5.335735	-3.442101	4.349353
C	5.490777	-2.510093	2.111247
C	6.490696	-4.192561	4.110635
C	6.654770	-3.254251	1.889157
C	7.151372	-4.091992	2.888154
C	6.766892	2.853860	3.839464
C	7.807302	2.850022	4.773994
C	7.052231	3.059477	2.474393
C	9.121753	3.066383	4.359711
C	8.376684	3.275623	2.067742
C	9.406860	3.284548	3.013115

S	7.108788	-5.389457	5.242497
S	10.457025	3.210426	5.494344
S	8.531957	-5.154044	2.637315
S	11.073745	3.689837	2.619300
C	11.683702	3.261215	4.222535
C	8.602155	-5.649048	4.332921
C	12.995051	3.029609	4.468179
C	9.704971	-6.204891	4.887648
S	11.197311	-6.492019	3.981406
S	9.781657	-6.711993	6.581079
S	14.241570	3.101493	3.214702
S	13.612685	2.640032	6.080275
C	15.478147	2.373338	4.214493
C	15.194048	2.164971	5.506410
C	12.157152	-6.815894	5.406753
C	11.518887	-6.915234	6.579461
H	16.431420	2.155602	3.749459
H	15.885396	1.753426	6.230658
H	13.222256	-6.954495	5.270496
H	11.995379	-7.145035	7.524286
O	8.670711	3.587031	0.764327
O	7.560833	2.713495	6.118743
O	4.655449	-3.630450	5.525714
O	7.289654	-3.244328	0.670949
C	5.219467	-2.936049	6.647686
C	9.236556	2.506723	0.007841
C	7.695448	1.363810	6.580832
C	8.368711	-2.303646	0.604993
H	10.125731	2.098787	0.504420
H	9.532417	2.935771	-0.950334
H	8.495749	1.715929	-0.141623
H	7.562564	1.398090	7.662721
H	6.925492	0.721686	6.137121
H	8.693538	0.968898	6.351677
H	4.627282	-3.234901	7.513342
H	5.152956	-1.854865	6.497396
H	6.263741	-3.231053	6.810923
H	7.995599	-1.276413	0.689198
H	8.833732	-2.443131	-0.371390
H	9.110423	-2.501611	1.389100

Energy -5552.62688528 A.U.

Table S9. Optimized cartesian coordinates (in Angstroms) of $clip_1^+$ at M06L/6-31G(d,p) level.

C	-0.139494	0.176603	0.139243
C	-0.075698	0.136933	1.529773
C	1.156436	0.076068	2.170553
C	2.339147	0.065007	1.426616
C	2.268722	0.097296	0.031861
C	1.034276	0.149416	-0.608409
H	-1.102295	0.226245	-0.360599
H	-0.987900	0.155803	2.118416
H	1.210683	0.063433	3.256067
H	3.184500	0.098857	-0.554885
H	0.990887	0.175244	-1.693133
C	3.675980	0.165369	2.126439
C	4.167222	1.644844	2.410522
C	3.082808	2.698425	2.361498
C	2.347989	3.011011	3.507269
C	2.723655	3.276837	1.140949
C	1.265314	3.881965	3.432110
H	2.615844	2.557378	4.458997
C	1.636069	4.139076	1.065650
H	3.288932	3.024400	0.247489
C	0.902803	4.441661	2.210538
H	0.700840	4.118413	4.329071
H	1.359224	4.574223	0.109852
H	0.052866	5.114758	2.150997
N	3.669037	-0.427814	3.452408
N	4.774533	-0.341214	1.320888
N	5.187492	1.840515	1.395983
N	4.750337	1.494653	3.732989
C	4.481945	0.285096	4.321702
C	5.666815	0.624667	0.931591
O	6.679285	0.454109	0.266827
O	4.858374	-0.084785	5.425275
C	5.508290	2.550536	4.363012
C	6.063552	2.999275	1.454932
C	4.870679	-1.732108	0.945386
C	3.507871	-1.864407	3.612970
H	5.420480	3.866236	1.655291
H	6.494997	3.147025	0.463665
H	5.522620	2.351852	5.436426
H	4.962653	3.495064	4.217452
H	3.200905	-2.053866	4.642799
H	5.530385	-1.796152	0.077615
H	2.667515	-2.157879	2.969928
H	3.874042	-2.065178	0.618386
C	4.723947	-2.708553	3.297086
C	5.164526	-3.628217	4.257752
C	5.372463	-2.639760	2.043406
C	6.242475	-4.471185	3.967398
C	6.461606	-3.473310	1.772315
C	6.888741	-4.390185	2.735512
C	6.919987	2.701475	3.845100
C	7.975560	2.686590	4.761928
C	7.179267	2.931685	2.474989
C	9.278841	2.930626	4.321590
C	8.490682	3.164326	2.042298
C	9.534986	3.174258	2.973455

S	6.789107	-5.721155	5.063737
S	10.633944	3.033724	5.422319
S	8.175527	-5.535796	2.435245
S	11.184511	3.564346	2.544694
C	11.810576	3.402576	4.175550
C	8.076654	-6.285920	4.017118
C	13.141669	3.581464	4.460848
C	8.942154	-7.279940	4.403012
S	10.222611	-7.874791	3.362197
S	8.857547	-8.056979	5.973790
S	14.332123	3.958064	3.228057
S	13.789320	3.464956	6.088042
C	15.675989	4.022463	4.325250
C	15.429092	3.796981	5.625868
C	10.837545	-9.018880	4.513078
C	10.218107	-9.101521	5.701767
H	16.651458	4.242509	3.910084
H	16.176786	3.810921	6.408910
H	11.690118	-9.617171	4.218271
H	10.498880	-9.775724	6.501066
O	8.768853	3.495496	0.745554
O	7.776427	2.529362	6.107557
O	4.500949	-3.806460	5.439504
O	7.084023	-3.491802	0.552753
C	5.099421	-3.140801	6.564591
C	9.283888	2.416581	-0.053240
C	7.790294	1.159734	6.537565
C	8.179495	-2.569389	0.448963
H	10.179544	1.978843	0.406685
H	9.556829	2.860299	-1.010497
H	8.521230	1.644835	-0.191036
H	7.678095	1.184639	7.621261
H	6.958740	0.599681	6.094846
H	8.744749	0.681718	6.282218
H	4.501748	-3.424512	7.430358
H	5.077097	-2.056853	6.422204
H	6.132896	-3.478773	6.715791
H	7.829950	-1.533623	0.529950
H	8.616716	-2.732529	-0.535812
H	8.934581	-2.773695	1.218933

Energy -5552.43333577 A.U.

Table S10. Optimized cartesian coordinates (in Angstroms) of $clip_1^{2+}$ at M06L/6-31G(d,p) level.

C	-0.067745	-0.004283	0.111362
C	-0.028046	0.002703	1.503494
C	1.193376	0.000533	2.166943
C	2.388771	0.004332	1.442492
C	2.342844	-0.007822	0.046019
C	1.118935	-0.017345	-0.616069
H	-1.022404	-0.002141	-0.405685
H	-0.950780	0.011970	2.075311
H	1.225571	0.027182	3.253281
H	3.267537	0.009739	-0.526826
H	1.093293	-0.026696	-1.701342
C	3.706249	0.176882	2.160743
C	4.135327	1.678216	2.417886
C	3.016706	2.689384	2.327040
C	2.252521	3.003596	3.453625
C	2.655981	3.220502	1.085343
C	1.142741	3.835524	3.339814
H	2.517270	2.583360	4.421624
C	1.540031	4.041445	0.971442
H	3.239407	2.963461	0.204985
C	0.780656	4.349546	2.097978
H	0.556490	4.075563	4.221309
H	1.261312	4.439903	0.000674
H	-0.090157	4.991460	2.008487
N	3.708136	-0.385362	3.500816
N	4.845103	-0.310145	1.395499
N	5.173724	1.885009	1.422602
N	4.712739	1.578505	3.749545
C	4.490693	0.370149	4.360294
C	5.714158	0.678003	1.006228
O	6.755017	0.525955	0.381013
O	4.885808	0.032021	5.467953
C	5.372996	2.696655	4.374500
C	5.974492	3.092951	1.447240
C	4.980041	-1.698901	1.034613
C	3.559166	-1.813880	3.691652
H	5.273907	3.929134	1.576495
H	6.427692	3.219652	0.463057
H	5.375479	2.524331	5.452258
H	4.761505	3.595277	4.200626
H	3.244580	-1.987852	4.721680
H	5.660761	-1.759025	0.183589
H	2.723878	-2.130243	3.052335
H	4.000597	-2.056136	0.680881
C	4.771844	-2.671473	3.390592
C	5.141859	-3.631368	4.341546
C	5.450554	-2.610239	2.147383
C	6.159816	-4.539435	4.036861
C	6.503861	-3.491846	1.876573
C	6.839297	-4.468432	2.819400
C	6.777561	2.970820	3.883136
C	7.785635	3.146351	4.837536
C	7.054660	3.178012	2.507925
C	9.046917	3.585728	4.426552
C	8.333287	3.586237	2.106078
C	9.316260	3.809589	3.075290

S	6.585828	-5.857994	5.093353
S	10.318192	3.967619	5.554526
S	8.034455	-5.700587	2.517272
S	10.891533	4.450113	2.691576
C	11.441914	4.498593	4.339428
C	7.783593	-6.524609	4.026320
C	12.711291	4.972957	4.676365
C	8.482269	-7.689245	4.353777
S	9.664487	-8.404627	3.300615
S	8.214876	-8.548773	5.839939
S	13.852808	5.526250	3.488607
S	13.264287	5.075410	6.321193
C	15.080659	5.948603	4.628036
C	14.809930	5.740869	5.931414
C	10.021409	-9.738455	4.339489
C	9.354832	-9.803625	5.508700
H	16.005977	6.359165	4.242951
H	15.484905	5.960791	6.749526
H	10.759615	-10.455936	4.002504
H	9.477722	-10.581583	6.252184
O	8.636848	3.897047	0.814457
O	7.577951	3.022755	6.180267
O	4.468174	-3.811549	5.512670
O	7.160015	-3.528972	0.680845
C	4.981955	-3.049218	6.623979
C	9.146190	2.794158	0.037455
C	7.604732	1.668634	6.668197
C	8.201979	-2.545392	0.541014
H	10.081941	2.417325	0.469793
H	9.344228	3.198891	-0.953915
H	8.410152	1.986194	-0.016844
H	7.429318	1.737801	7.740879
H	6.818427	1.061690	6.205227
H	8.586280	1.214026	6.486353
H	4.347452	-3.300952	7.472357
H	4.934101	-1.976798	6.412552
H	6.016660	-3.340262	6.845157
H	7.800255	-1.527167	0.598405
H	8.635938	-2.712503	-0.443709
H	8.971750	-2.688910	1.309213

Energy -5552.15123593 A.U.

Table S11. Optimized cartesian coordinates (in Angstroms) of $clip_1^{3+}$ at M06L/6-31G(d,p) level.

C	0.026233	-0.031021	0.238312
C	0.089683	-0.008482	1.631175
C	1.321808	-0.014577	2.271633
C	2.505990	-0.027842	1.522691
C	2.435988	-0.053501	0.124921
C	1.201193	-0.058968	-0.513296
H	-0.937318	-0.028115	-0.261492
H	-0.823151	0.013470	2.217545
H	1.373479	0.022758	3.356793
H	3.350021	-0.048296	-0.464646
H	1.152953	-0.077235	-1.597283
C	3.840027	0.130864	2.216648
C	4.288787	1.625379	2.446455
C	3.175883	2.643535	2.336201
C	2.408417	2.978734	3.457717
C	2.826359	3.162515	1.082395
C	1.307300	3.816767	3.326690
H	2.663433	2.568103	4.432256
C	1.718966	3.990433	0.952237
H	3.412332	2.890290	0.208467
C	0.956665	4.318645	2.073189
H	0.716048	4.072806	4.199827
H	1.447333	4.380060	-0.023677
H	0.092205	4.966969	1.971576
N	3.858413	-0.416590	3.561931
N	4.959432	-0.385755	1.443930
N	5.330235	1.802613	1.449345
N	4.871220	1.545716	3.776302
C	4.657797	0.342194	4.404045
C	5.849626	0.581713	1.042298
O	6.886406	0.402798	0.420331
O	5.073429	0.013457	5.505341
C	5.514611	2.678750	4.387291
C	6.128010	3.009796	1.441499
C	5.049018	-1.776690	1.081727
C	3.668939	-1.835295	3.770407
H	5.424166	3.849542	1.536499
H	6.583223	3.109393	0.455387
H	5.519263	2.520779	5.466917
H	4.889194	3.567649	4.207088
H	3.363992	-1.990745	4.805979
H	5.714729	-1.858852	0.221097
H	2.809203	-2.131033	3.151905
H	4.055228	-2.104355	0.736450
C	4.832194	-2.750636	3.443212
C	5.139176	-3.756108	4.371091
C	5.490425	-2.718460	2.182391
C	6.056118	-4.749653	4.012711
C	6.462345	-3.677713	1.866841
C	6.714497	-4.710833	2.776170
C	6.910799	2.991600	3.893878
C	7.884814	3.280650	4.858150
C	7.194934	3.161371	2.510382
C	9.106048	3.821795	4.444361
C	8.448260	3.644975	2.105652

C	9.381625	4.007658	3.082928
S	6.366516	-6.135997	5.008668
S	10.307624	4.387628	5.560212
S	7.760012	-6.049002	2.416153
S	10.883753	4.789426	2.700973
C	11.379240	4.989876	4.344822
C	7.453980	-6.887961	3.896054
C	12.580580	5.653761	4.681287
C	8.032828	-8.148036	4.171286
S	9.084802	-8.956440	3.065351
S	7.718508	-9.011186	5.633886
S	13.654538	6.300563	3.492965
S	13.076157	5.907694	6.317073
C	14.787627	6.939890	4.615700
C	14.518519	6.757930	5.928682
C	9.326242	-10.348222	4.046941
C	8.690266	-10.372823	5.240179
H	15.655580	7.457055	4.221952
H	15.138940	7.105112	6.747226
H	9.969491	-11.133240	3.665410
H	8.746651	-11.181449	5.960238
O	8.765543	3.923327	0.815157
O	7.669122	3.198482	6.198161
O	4.488459	-3.917052	5.552417
O	7.089443	-3.747754	0.662674
C	4.979169	-3.105067	6.644791
C	9.201697	2.788819	0.030627
C	7.742713	1.867124	6.750768
C	8.180549	-2.819491	0.484667
H	10.168915	2.424852	0.395538
H	9.312077	3.161421	-0.986011
H	8.463160	1.982073	0.065737
H	7.527627	1.978405	7.811988
H	7.002915	1.201724	6.291860
H	8.750490	1.456770	6.619145
H	4.317469	-3.314200	7.483116
H	4.950287	-2.042081	6.387075
H	6.003541	-3.396420	6.903845
H	7.842144	-1.781326	0.577701
H	8.553187	-2.995643	-0.522806
H	8.974478	-3.022772	1.212427

Energy -5551.76933742 A.U.

Table S12. Optimized cartesian coordinates (in Angstroms) of $clip_1^{4+}$ at M06L/6-31G(d,p) level.

C	0.116731	-0.101564	0.344077
C	0.200096	-0.040537	1.737732
C	1.440951	-0.030727	2.359172
C	2.615189	-0.067279	1.590732
C	2.525202	-0.127968	0.192335
C	1.281560	-0.148142	-0.426489
H	-0.854294	-0.112233	-0.140802
H	-0.704887	-0.004076	2.335015
H	1.507579	0.030771	3.442529
H	3.429721	-0.137060	-0.411342
H	1.215136	-0.193288	-1.508425
C	3.959799	0.093283	2.264481
C	4.410002	1.589969	2.484856
C	3.298480	2.607036	2.349762
C	2.531964	2.977408	3.464424
C	2.951590	3.092398	1.078845
C	1.436029	3.816864	3.309609
H	2.782681	2.591294	4.449848
C	1.850582	3.923231	0.925772
H	3.537805	2.796856	0.212508
C	1.089495	4.286943	2.040092
H	0.844120	4.100003	4.173568
H	1.580784	4.289764	-0.059309
H	0.228893	4.937212	1.920091
N	4.002785	-0.452631	3.608717
N	5.070930	-0.429526	1.487075
N	5.464790	1.753875	1.500766
N	4.987019	1.523744	3.816465
C	4.801206	0.313918	4.447910
C	5.981742	0.528220	1.097758
O	7.024166	0.339864	0.493778
O	5.233539	-0.010884	5.540874
C	5.631267	2.663059	4.413277
C	6.241222	2.972190	1.456403
C	5.152206	-1.822895	1.135760
C	3.770969	-1.860538	3.835741
H	5.525437	3.805023	1.525990
H	6.694851	3.052223	0.467772
H	5.643372	2.512563	5.493440
H	4.992377	3.544512	4.233571
H	3.474733	-1.996121	4.876575
H	5.823536	-1.913927	0.280935
H	2.892278	-2.137975	3.234444
H	4.156757	-2.137591	0.778127
C	4.895168	-2.818381	3.494091
C	5.145009	-3.856257	4.406482
C	5.551724	-2.795595	2.228351
C	5.969755	-4.913008	4.004950
C	6.448090	-3.815870	1.876362
C	6.614528	-4.895340	2.754725
C	7.016183	3.021417	3.912747
C	7.957056	3.409357	4.878096
C	7.299624	3.176542	2.524115
C	9.136160	4.034704	4.451739
C	8.528490	3.714589	2.107164
C	9.416705	4.185172	3.081136

S	6.174449	-6.351285	4.946261
S	10.267533	4.751247	5.543766
S	7.520472	-6.307685	2.343904
S	10.843817	5.080747	2.689546
C	11.292731	5.394072	4.320854
C	7.161962	-7.160940	3.793792
C	12.437460	6.188362	4.642286
C	7.622753	-8.497867	4.012759
S	8.629185	-9.330759	2.896095
S	7.187772	-9.408029	5.404438
S	13.458860	6.870004	3.439188
S	12.884530	6.562645	6.259228
C	14.518777	7.655271	4.528854
C	14.250433	7.509851	5.852207
C	8.717972	-10.788177	3.788811
C	8.043218	-10.823009	4.966743
H	15.343886	8.227574	4.116280
H	14.828098	7.948105	6.660240
H	9.300183	-11.606209	3.375976
H	8.003364	-11.673958	5.639686
O	8.842939	3.968555	0.815940
O	7.740092	3.361512	6.214608
O	4.505377	-3.994283	5.590942
O	7.059347	-3.908841	0.671146
C	5.021072	-3.190298	6.683894
C	9.301644	2.827741	0.044844
C	7.840676	2.053838	6.827665
C	8.192344	-3.031017	0.466086
H	10.287664	2.509303	0.398784
H	9.375139	3.181272	-0.981373
H	8.592352	1.997434	0.115540
H	7.591789	2.206026	7.875797
H	7.137323	1.344296	6.378684
H	8.864365	1.675380	6.739395
H	4.330056	-3.347244	7.509356
H	5.058312	-2.132007	6.408677
H	6.020267	-3.538720	6.965511
H	7.910580	-1.979057	0.583528
H	8.519146	-3.213980	-0.555463
H	8.996019	-3.285668	1.164916

Energy -5551.30713916 A.U.

Table S13. Optimized cartesian coordinates (in Angstroms) of $clip_2^0$ at M06L/6-31G(d,p) level.

C	2.769739	-2.266668	5.050493
C	2.283980	-0.962227	5.076679
C	2.876331	0.018480	4.288951
C	3.959841	-0.294331	3.464739
C	4.448185	-1.602183	3.449860
C	3.855615	-2.582921	4.239090
H	2.305984	-3.033764	5.664124
H	1.439736	-0.706791	5.710581
H	2.495238	1.036708	4.303463
H	5.289848	-1.846835	2.806715
H	4.242949	-3.597630	4.217740
C	4.518443	0.751186	2.521197
C	3.776994	0.851042	1.100890
C	2.689027	-0.177381	0.865861
C	1.365338	0.094246	1.217668
C	3.015779	-1.443869	0.375512
C	0.386512	-0.886432	1.089239
H	1.109691	1.079161	1.600047
C	2.038033	-2.425224	0.251646
H	4.044967	-1.658477	0.098360
C	0.721658	-2.150222	0.612252
H	-0.639640	-0.661951	1.365842
H	2.306079	-3.407639	-0.126709
H	-0.041740	-2.916693	0.514863
N	4.350123	2.092729	3.049151
N	5.892987	0.471274	2.141030
N	4.879633	0.689051	0.170298
N	3.251728	2.206052	1.116982
C	3.731335	2.947968	2.173783
C	6.102825	0.605187	0.786584
O	7.190933	0.594101	0.222307
O	3.580355	4.154940	2.324218
C	2.791227	2.866869	-0.096171
C	4.752047	0.990711	-1.245979
C	6.998412	0.626843	3.080901
C	5.092846	2.569078	4.205421
H	3.800969	0.555051	-1.582543
H	5.554551	0.465855	-1.767357
H	2.169884	3.709593	0.211144
H	2.142621	2.152289	-0.620933
H	4.548725	3.420464	4.618948
H	7.845573	0.067436	2.679976
H	5.067716	1.766347	4.955234
H	6.690984	0.135903	4.014250
C	6.509935	2.978667	3.891726
C	6.915268	4.294466	4.150420
C	7.417265	2.055785	3.338266
C	8.208736	4.696971	3.810989
C	8.727379	2.458151	3.035644
C	9.110552	3.785278	3.255252
C	3.891051	3.361493	-1.005407
C	3.957041	4.723173	-1.329629
C	4.817824	2.463367	-1.567724
C	4.959092	5.190190	-2.191118
C	5.793890	2.929757	-2.455932
C	5.873283	4.296371	-2.753337

S	8.836807	6.321335	4.115476
S	5.044267	6.856403	-2.729729
S	10.738440	4.408293	2.946973
S	7.001095	4.940606	-3.930361
C	6.374770	6.591963	-3.863332
C	10.176351	6.080581	2.991510
C	6.878417	7.588909	-4.628976
C	10.649717	7.056601	2.179943
S	11.959556	6.794697	1.022457
S	10.005567	8.702977	2.188873
S	8.211904	7.358603	-5.766755
S	6.260793	9.244610	-4.592322
C	8.549431	9.072496	-5.923040
C	7.667248	9.926606	-5.387280
C	11.811585	8.368040	0.277335
C	10.931788	9.228022	0.803626
H	9.443789	9.353925	-6.471539
H	7.732577	11.009611	-5.435595
H	12.427946	8.566053	-0.591732
H	10.737223	10.224997	0.425997
O	6.586799	2.039342	-3.135303
O	2.964634	5.574919	-0.915708
O	6.082933	5.154527	4.821177
O	9.651525	1.533044	2.622196
C	5.503312	6.198166	4.028521
C	7.952542	1.983192	-2.707107
C	3.346128	6.530616	0.081207
C	10.065231	1.635815	1.253954
H	8.434262	2.967482	-2.761318
H	8.452503	1.298243	-3.392862
H	8.013923	1.594354	-1.684338
H	2.484364	7.186332	0.211471
H	3.573500	6.024105	1.025005
H	4.209569	7.126288	-0.238566
H	5.009827	6.869353	4.732788
H	4.764728	5.782202	3.335329
H	6.270395	6.757805	3.479548
H	9.239400	1.366263	0.588964
H	10.879867	0.920423	1.135163
H	10.435375	2.641147	1.019039
H	12.830261	17.343348	-4.973133
C	13.098152	16.361049	-5.351898
C	12.120286	15.379841	-5.475984
C	14.414445	16.086047	-5.712804
C	12.446841	14.113477	-5.966795
H	11.091178	15.594430	-5.198525
C	14.749365	14.822424	-6.190388
H	15.177944	16.852395	-5.615244
C	11.358797	13.085086	-6.201656
C	13.770432	13.841876	-6.318979
H	15.775447	14.597950	-6.467262
C	10.616957	13.184947	-7.621765
N	11.884071	11.730089	-6.217919
N	10.256403	13.247026	-5.270743
H	14.025931	12.857066	-6.701729
C	11.175127	14.230550	-8.565473
N	9.242492	13.464627	-7.241205
N	10.785280	11.843444	-8.149856
C	11.404305	10.988211	-7.274666

C	12.345121	11.069287	-5.004962
C	9.033032	13.330693	-5.886709
C	10.384485	12.945282	-3.854526
C	10.686620	15.538334	-8.550455
C	12.258291	13.917821	-9.390175
C	8.136810	13.309008	-8.180743
C	10.042288	11.367049	-9.305933
O	11.555316	9.781245	-7.425190
H	12.993873	11.783916	-4.480445
H	12.966418	10.226627	-5.312546
C	11.245679	10.574565	-4.095314
O	7.945047	13.341561	-5.322186
H	9.582116	13.470038	-3.332836
H	11.335626	13.381044	-3.518262
C	10.318970	11.472619	-3.532794
C	11.278654	16.519084	-9.340075
H	9.845234	15.782918	-7.906920
C	12.850107	14.898539	-10.178294
H	12.639499	12.899638	-9.404831
H	7.289720	13.868303	-7.779526
H	8.443893	13.800001	-9.114181
C	7.718058	11.880021	-8.438030
H	10.586371	10.515715	-9.719624
H	10.067117	12.169784	-10.055753
C	8.625348	10.957293	-8.991827
C	11.179919	9.212869	-3.771053
C	9.343162	11.006132	-2.644349
C	12.364159	16.202906	-10.152006
H	10.891167	17.533733	-9.318647
H	13.694077	14.643161	-10.812582
C	6.408068	11.477499	-8.135096
C	8.220085	9.641489	-9.250526
C	10.178053	8.745740	-2.909390
O	12.172371	8.361294	-4.185227
C	9.263945	9.639521	-2.346971
O	8.550324	11.896349	-1.964652
H	12.827474	16.970006	-10.765965
C	6.024899	10.150413	-8.354909
O	5.484035	12.402492	-7.721095
C	6.926705	9.238863	-8.910902
O	9.052284	8.781570	-9.921662
S	10.093190	7.079620	-2.370504
C	11.790962	7.405444	-5.181992
S	8.136394	8.995324	-1.169683
C	7.184556	11.952643	-2.392811
S	4.396990	9.527307	-8.046854
C	5.070466	12.298984	-6.352880
S	6.298728	7.614503	-9.215650
C	9.632279	7.737906	-9.129328
C	8.762467	7.343912	-1.237086
H	10.927863	6.809430	-4.861949
H	12.652940	6.750051	-5.312481
H	11.563166	7.911795	-6.125783
H	6.684394	12.636695	-1.706306
H	7.123129	12.342555	-3.415160
H	6.703137	10.968147	-2.339678
C	4.959188	7.855054	-8.091609
H	4.257284	13.015862	-6.233134
H	5.896914	12.566272	-5.687752

H	4.698399	11.294132	-6.118999
H	10.371378	8.153805	-8.436644
H	10.125177	7.066559	-9.833856
H	8.865429	7.178497	-8.579813
C	8.258794	6.346780	-0.471696
C	4.486198	6.879067	-7.279782
S	8.876495	4.691141	-0.508911
S	6.925632	6.576740	0.666533
S	5.130522	5.232770	-7.288634
S	3.176650	7.140996	-6.121959
C	7.470378	4.008878	0.286333
C	6.588156	4.862785	0.822367
C	4.205359	4.708126	-5.902511
C	3.325560	5.568078	-5.376184
H	7.405274	2.925864	0.334557
H	5.694194	4.581015	1.371308
H	4.400574	3.711471	-5.524371
H	2.710116	5.370471	-4.506374

Energy -11105.3346673 A.U.

Table S14. Optimized cartesian coordinates (in Angstroms) of $clip_2^+$ at M06L/6-31G(d,p) level.

C	2.939646	-2.218281	5.186148
C	2.367294	-0.950267	5.125833
C	2.892954	0.011898	4.271369
C	3.992344	-0.286371	3.462252
C	4.560580	-1.560071	3.524648
C	4.038588	-2.519860	4.387012
H	2.532161	-2.968182	5.857435
H	1.511050	-0.708044	5.748089
H	2.448440	1.003172	4.225563
H	5.412263	-1.796241	2.891786
H	4.491817	-3.505679	4.432984
C	4.496733	0.744398	2.477047
C	3.718030	0.804650	1.073485
C	2.630464	-0.229002	0.882953
C	1.308545	0.055195	1.232240
C	2.957056	-1.510536	0.433052
C	0.327973	-0.926894	1.131640
H	1.053089	1.049156	1.590603
C	1.976763	-2.492492	0.336976
H	3.985725	-1.735962	0.162302
C	0.660507	-2.203103	0.687118
H	-0.697093	-0.693856	1.403815
H	2.242251	-3.486209	-0.011511
H	-0.104411	-2.969930	0.610065
N	4.323443	2.098639	2.981217
N	5.870884	0.497031	2.064501
N	4.802185	0.635238	0.117010
N	3.194163	2.163131	1.066661
C	3.708940	2.930965	2.085687
C	6.040908	0.626724	0.707886
O	7.116385	0.681369	0.118289
O	3.594589	4.149037	2.187252
C	2.693797	2.792897	-0.144754
C	4.638769	0.918551	-1.298601
C	6.995583	0.684683	2.974192
C	5.088978	2.611288	4.107065
H	3.677886	0.484467	-1.604932
H	5.423014	0.384976	-1.838149
H	2.058952	3.628057	0.155100
H	2.053025	2.057674	-0.648441
H	4.539635	3.456040	4.526774
H	7.840665	0.123499	2.571647
H	5.105721	1.821055	4.868828
H	6.715250	0.215842	3.926279
C	6.486882	3.045830	3.740613
C	6.871343	4.375592	3.956157
C	7.397690	2.126132	3.185219
C	8.146342	4.794076	3.561662
C	8.692125	2.541486	2.839403
C	9.051007	3.884248	3.008559
C	3.774853	3.291008	-1.075823
C	3.834693	4.652783	-1.400898
C	4.701220	2.389581	-1.637416
C	4.847043	5.116776	-2.253956
C	5.675269	2.850555	-2.530659
C	5.760051	4.220712	-2.815206

S	8.733084	6.441997	3.785287
S	4.968807	6.788386	-2.766255
S	10.649776	4.520640	2.620886
S	6.907554	4.872371	-3.965211
C	6.338042	6.526304	-3.832398
C	10.112887	6.193013	2.721327
C	6.937683	7.553715	-4.505865
C	10.679195	7.197530	2.000074
S	12.030340	6.938330	0.895822
S	10.110352	8.864229	2.083838
S	8.330027	7.320950	-5.549926
S	6.398901	9.219294	-4.375642
C	8.641680	9.021516	-5.766705
C	7.763387	9.885924	-5.228702
C	11.995720	8.558869	0.246306
C	11.128912	9.428072	0.782795
H	9.526406	9.295677	-6.336925
H	7.824535	10.969408	-5.297402
H	12.685218	8.785376	-0.558656
H	11.014895	10.461160	0.474943
O	6.452390	1.966205	-3.228339
O	2.836071	5.500517	-1.005892
O	6.052776	5.235193	4.638779
O	9.628098	1.626159	2.440586
C	5.407624	6.249662	3.859550
C	7.827228	1.881755	-2.829031
C	3.181832	6.475792	-0.013029
C	10.017111	1.670737	1.062417
H	8.323622	2.859499	-2.882726
H	8.300741	1.202326	-3.537394
H	7.900777	1.476129	-1.815321
H	2.310043	7.122566	0.083701
H	3.390973	5.985451	0.942113
H	4.043513	7.080514	-0.322383
H	4.970156	6.944891	4.576368
H	4.621297	5.807963	3.239623
H	6.126501	6.792893	3.232956
H	9.192533	1.335659	0.427118
H	10.858222	0.983730	0.968927
H	10.345658	2.675129	0.766912
H	12.888864	17.424270	-5.084403
C	13.155104	16.431124	-5.433943
C	12.175520	15.448566	-5.531084
C	14.471601	16.143069	-5.784324
C	12.503047	14.167709	-5.982264
H	11.146704	15.672996	-5.260075
C	14.805004	14.867622	-6.230358
H	15.235985	16.910329	-5.706355
C	11.416394	13.133169	-6.173246
C	13.825151	13.884915	-6.331968
H	15.830209	14.635601	-6.502882
C	10.637912	13.192682	-7.576852
N	11.941534	11.775130	-6.166231
N	10.331845	13.301557	-5.216995
H	14.081397	12.891553	-6.691427
C	11.141938	14.223430	-8.562289
N	9.263498	13.439437	-7.164720
N	10.811961	11.838382	-8.080611
C	11.427299	11.006745	-7.185097

C	12.442351	11.145891	-4.954695
C	9.093253	13.309262	-5.808115
C	10.495099	13.018159	-3.801413
C	10.573419	15.496992	-8.624746
C	12.241046	13.925198	-9.371821
C	8.139265	13.250558	-8.074768
C	10.047481	11.325052	-9.206808
O	11.542693	9.788740	-7.286607
H	13.082174	11.881835	-4.450876
H	13.078190	10.311417	-5.254388
C	11.361552	10.646596	-4.023940
O	8.017762	13.253438	-5.218659
H	9.710124	13.550854	-3.262072
H	11.455466	13.453095	-3.494667
C	10.433923	11.547031	-3.462859
C	11.094792	16.456655	-9.487632
H	9.722011	15.733144	-7.991512
C	12.766018	14.887205	-10.226889
H	12.685806	12.934036	-9.325937
H	7.293577	13.811166	-7.672688
H	8.419585	13.719409	-9.026852
C	7.738245	11.808763	-8.285791
H	10.597648	10.480619	-9.626079
H	10.030550	12.115140	-9.968725
C	8.649764	10.889595	-8.840885
C	11.302939	9.284767	-3.698947
C	9.459756	11.085044	-2.570255
C	12.193320	16.155060	-10.287327
H	10.641339	17.442367	-9.533629
H	13.621973	14.644965	-10.849536
C	6.443948	11.392589	-7.940542
C	8.266302	9.559524	-9.056456
C	10.290473	8.819672	-2.846607
O	12.302901	8.438094	-4.092868
C	9.376361	9.714805	-2.285644
O	8.681054	11.968852	-1.873656
H	12.600260	16.904853	-10.959062
C	6.086033	10.049584	-8.109733
O	5.507000	12.307210	-7.542382
C	6.991417	9.140226	-8.662441
O	9.085931	8.700565	-9.738610
S	10.169789	7.147748	-2.335083
C	11.959556	7.462635	-5.086438
S	8.229527	9.061888	-1.135656
C	7.305931	12.049706	-2.272545
S	4.487473	9.412372	-7.722552
C	5.117867	12.262928	-6.164208
S	6.405524	7.492031	-8.886371
C	9.731138	7.686244	-8.959271
C	8.800344	7.408467	-1.268852
H	11.095989	6.859197	-4.779811
H	12.830853	6.814677	-5.179561
H	11.754399	7.952728	-6.042561
H	6.832254	12.732563	-1.567606
H	7.231304	12.449979	-3.288315
H	6.810459	11.071824	-2.213200
C	5.025298	7.740303	-7.822751
H	4.275366	12.948319	-6.071377
H	5.941711	12.600074	-5.529074

H	4.791258	11.258081	-5.868097
H	10.515770	8.128366	-8.337480
H	10.170992	6.992529	-9.676096
H	9.012021	7.141098	-8.334613
C	8.201405	6.380490	-0.595642
C	4.459406	6.735573	-7.101470
S	8.740610	4.715133	-0.727053
S	6.809350	6.612201	0.449034
S	5.029022	5.069130	-7.185096
S	3.108045	6.994206	-5.997334
C	7.376425	4.047577	0.125797
C	6.498093	4.911410	0.664694
C	4.010620	4.504869	-5.884119
C	3.143402	5.373720	-5.347719
H	7.315208	2.963984	0.193076
H	5.613987	4.636795	1.235631
H	4.125198	3.471885	-5.576097
H	2.453920	5.146917	-4.542828

Energy -11105.1587215 A.U.

Table S15. Optimized cartesian coordinates (in Angstroms) of $clip_2^{2+}$ at M06L/6-31G(d,p) level.

C	3.304156	-2.448879	5.015020
C	2.725860	-1.189100	5.147317
C	3.147859	-0.138424	4.339256
C	4.153954	-0.341049	3.391820
C	4.732447	-1.606574	3.264942
C	4.310253	-2.655171	4.074525
H	2.973492	-3.268032	5.646044
H	1.943748	-1.023542	5.881729
H	2.688458	0.842618	4.432062
H	5.507728	-1.769893	2.520327
H	4.765262	-3.635110	3.968940
C	4.534007	0.757661	2.429526
C	3.695722	0.796566	1.058984
C	2.576541	-0.211384	0.951185
C	1.314598	0.088239	1.470939
C	2.820035	-1.487036	0.436890
C	0.312562	-0.875952	1.480532
H	1.123968	1.076858	1.881772
C	1.817397	-2.451020	0.450453
H	3.804769	-1.725380	0.042343
C	0.563642	-2.148425	0.974693
H	-0.664221	-0.634468	1.888602
H	2.016659	-3.441458	0.052886
H	-0.217204	-2.902667	0.987368
N	4.306530	2.090572	2.975301
N	5.900968	0.617193	1.944984
N	4.732360	0.596045	0.052254
N	3.204762	2.168061	1.045491
C	3.708937	2.928076	2.067889
C	5.997374	0.689826	0.583955
O	7.039719	0.791436	-0.060530
O	3.612998	4.149805	2.166028
C	2.613345	2.771128	-0.134096
C	4.499770	0.881434	-1.354992
C	7.055195	0.799194	2.810020
C	5.126521	2.625251	4.054034
H	3.520958	0.455766	-1.609656
H	5.249308	0.340878	-1.935166
H	1.987528	3.604777	0.188104
H	1.950752	2.020751	-0.584503
H	4.570214	3.435552	4.527887
H	7.898623	0.268306	2.365501
H	5.233519	1.825483	4.797294
H	6.825215	0.305410	3.762776
C	6.481028	3.131186	3.610900
C	6.811160	4.479757	3.802490
C	7.414722	2.250783	3.025540
C	8.049450	4.950389	3.342670
C	8.676707	2.713612	2.631437
C	8.973647	4.077346	2.762490
C	3.638344	3.258986	-1.132185
C	3.675643	4.616791	-1.475090
C	4.553150	2.352185	-1.707708
C	4.675628	5.076740	-2.345112
C	5.508731	2.807863	-2.625535
C	5.584348	4.179250	-2.912315

S	8.552419	6.624913	3.503417
S	4.812083	6.751004	-2.843795
S	10.507195	4.775461	2.272180
S	6.736855	4.839846	-4.051722
C	6.219017	6.497754	-3.852273
C	9.985649	6.428658	2.517984
C	6.897544	7.542597	-4.433221
C	10.632850	7.494750	1.943143
S	12.047936	7.305409	0.923418
S	10.084029	9.150199	2.136563
S	8.341982	7.312382	-5.397299
S	6.418637	9.214851	-4.229943
C	8.674186	9.007253	-5.593670
C	7.795770	9.876936	-5.057185
C	12.124255	8.981328	0.464226
C	11.232868	9.819001	1.017301
H	9.574562	9.275104	-6.145158
H	7.870002	10.962484	-5.108011
H	12.903172	9.272999	-0.230255
H	11.184165	10.885326	0.831009
O	6.273234	1.931399	-3.340413
O	2.680358	5.462340	-1.075659
O	6.003936	5.307034	4.527883
O	9.643106	1.837347	2.229218
C	5.262078	6.300865	3.807523
C	7.663687	1.845164	-2.989054
C	3.016198	6.427783	-0.068465
C	9.970935	1.822532	0.834695
H	8.141681	2.834346	-2.988974
H	8.125787	1.228899	-3.759449
H	7.772902	1.373243	-2.009719
H	2.142893	7.071913	0.027332
H	3.218912	5.927204	0.882863
H	3.877790	7.038188	-0.369193
H	4.913503	7.013864	4.554279
H	4.413693	5.840007	3.296116
H	5.895949	6.829495	3.082456
H	9.119833	1.462281	0.249379
H	10.807408	1.131653	0.735443
H	10.286778	2.813081	0.482112
H	12.922022	17.434251	-5.149770
C	13.192381	16.436425	-5.481491
C	12.218059	15.446943	-5.558030
C	14.509460	16.148769	-5.830513
C	12.552745	14.159932	-5.986862
H	11.188665	15.672318	-5.289599
C	14.849200	14.867980	-6.256420
H	15.269570	16.921396	-5.768534
C	11.473086	13.117416	-6.153315
C	13.874948	13.877930	-6.338093
H	15.874461	14.638128	-6.529502
C	10.682069	13.136890	-7.552314
N	12.000059	11.758293	-6.113856
N	10.390724	13.290194	-5.191016
H	14.137123	12.881448	-6.684608
C	11.167625	14.141223	-8.569256
N	9.306119	13.376242	-7.131549
N	10.853025	11.765486	-8.017195
C	11.457011	10.960862	-7.092491

C	12.518517	11.168597	-4.891069
C	9.150564	13.258078	-5.773929
C	10.572236	13.057370	-3.769504
C	10.591799	15.410291	-8.656561
C	12.262810	13.827370	-9.378744
C	8.176627	13.156535	-8.026481
C	10.084455	11.218123	-9.123320
O	11.532890	9.734567	-7.137547
H	13.151229	11.926221	-4.411993
H	13.164531	10.334033	-5.167724
C	11.447844	10.684303	-3.939549
O	8.078855	13.172247	-5.177166
H	9.794267	13.604012	-3.234085
H	11.534283	13.505943	-3.490034
C	10.523341	11.595604	-3.386826
C	11.103473	16.351464	-9.545227
H	9.744781	15.659748	-8.022242
C	12.777075	14.771559	-10.259855
H	12.715370	12.840845	-9.311898
H	7.330288	13.727663	-7.641393
H	8.448479	13.592098	-8.995997
C	7.783117	11.704377	-8.184043
H	10.638117	10.371719	-9.533438
H	10.047184	11.989854	-9.902324
C	8.695777	10.776491	-8.726170
C	11.391118	9.326204	-3.596911
C	9.555648	11.152522	-2.477193
C	12.197935	16.035203	-10.345050
H	10.646331	17.333948	-9.611361
H	13.629893	14.519490	-10.882458
C	6.500038	11.289445	-7.799037
C	8.326092	9.436341	-8.896275
C	10.374842	8.878559	-2.738768
O	12.384792	8.470422	-3.975122
C	9.467381	9.784657	-2.183115
O	8.786736	12.038540	-1.777194
H	12.597495	16.770957	-11.035900
C	6.161247	9.932134	-7.907071
O	5.553888	12.203048	-7.436353
C	7.064690	9.016761	-8.453843
O	9.125429	8.568064	-9.582882
S	10.220020	7.209168	-2.232130
C	12.056304	7.478854	-4.960465
S	8.295529	9.140026	-1.054737
C	7.415106	12.162556	-2.184460
S	4.599168	9.288828	-7.427600
C	5.166582	12.240933	-6.056984
S	6.513013	7.355465	-8.589366
C	9.832468	7.585896	-8.814171
C	8.806059	7.478151	-1.239195
H	11.161935	6.908430	-4.676989
H	12.909910	6.802958	-4.994818
H	11.909463	7.951637	-5.934604
H	6.948277	12.823293	-1.454931
H	7.357047	12.602396	-3.184038
H	6.902013	11.191272	-2.165814
C	5.077399	7.616397	-7.623356
H	4.300602	12.900344	-6.011415
H	5.979442	12.645615	-5.449053

H	4.874217	11.248759	-5.689036
H	10.631053	8.060390	-8.237301
H	10.253190	6.888458	-9.537909
H	9.157246	7.036093	-8.144835
C	8.124539	6.436398	-0.656659
C	4.395011	6.583954	-7.028881
S	8.596400	4.764391	-0.874024
S	6.693928	6.666907	0.326053
S	4.886333	4.907908	-7.196544
S	2.988359	6.839283	-6.011886
C	7.233643	4.102620	-0.024770
C	6.364060	4.971902	0.526250
C	3.717826	4.297639	-6.063617
C	2.855004	5.173954	-5.525674
H	7.163024	3.017134	0.023576
H	5.474436	4.701096	1.093161
H	3.730266	3.233723	-5.858970
H	2.068544	4.921464	-4.824422

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Table S16. Optimized cartesian coordinates (in Angstroms) of $clip_2^{3+}$ at M06L/6-31G(d,p) level.

C	3.497050	-2.405452	5.011710
C	2.889292	-1.159444	5.144786
C	3.259943	-0.109280	4.311505
C	4.245461	-0.298957	3.339163
C	4.854724	-1.550511	3.212190
C	4.481420	-2.598803	4.045561
H	3.205307	-3.224532	5.661394
H	2.123848	-1.005008	5.898512
H	2.775296	0.859583	4.405214
H	5.612416	-1.706133	2.447894
H	4.958322	-3.568084	3.940154
C	4.561808	0.794938	2.352390
C	3.680034	0.807592	1.008030
C	2.569182	-0.209375	0.942147
C	1.304653	0.096789	1.452324
C	2.829620	-1.503450	0.483187
C	0.316170	-0.880312	1.506854
H	1.099857	1.098121	1.824020
C	1.841483	-2.479990	0.544746
H	3.816703	-1.748392	0.098283
C	0.584850	-2.170789	1.059106
H	-0.662924	-0.635063	1.906479
H	2.054066	-3.484989	0.193837
H	-0.184493	-2.934748	1.110526
N	4.328457	2.132007	2.891967
N	5.917406	0.691988	1.821869
N	4.690895	0.612953	-0.028989
N	3.185014	2.180560	0.987134
C	3.712957	2.954378	1.984410
C	5.965022	0.771486	0.459754
O	6.978603	0.937285	-0.219858
O	3.629700	4.180478	2.062389
C	2.546581	2.760355	-0.179432
C	4.401827	0.863498	-1.431478
C	7.093110	0.893735	2.649077
C	5.164845	2.682203	3.947890
H	3.414824	0.430030	-1.635151
H	5.126411	0.312551	-2.033500
H	1.922324	3.592827	0.149385
H	1.875970	1.997136	-0.595056
H	4.608637	3.479010	4.443859
H	7.933433	0.376874	2.183104
H	5.313149	1.883535	4.684968
H	6.902288	0.400776	3.610692
C	6.496324	3.216179	3.464604
C	6.804016	4.570267	3.651369
C	7.431130	2.353007	2.851199
C	8.023185	5.060075	3.156320
C	8.675807	2.833445	2.424340
C	8.949833	4.203880	2.551266
C	3.532910	3.240016	-1.221695
C	3.548658	4.593670	-1.585884
C	4.435250	2.328369	-1.812427
C	4.535111	5.045822	-2.475213
C	5.366744	2.774022	-2.760671
C	5.437238	4.144895	-3.049250

S	8.494689	6.738313	3.297801
S	4.697471	6.724527	-2.957310
S	10.450784	4.931324	2.023915
S	6.610453	4.812043	-4.166258
C	6.156923	6.472287	-3.881448
C	9.969807	6.561580	2.393370
C	6.929455	7.523153	-4.330627
C	10.712268	7.660144	1.978922
S	12.200075	7.508989	1.084022
S	10.206457	9.299660	2.283930
S	8.424421	7.288141	-5.205125
S	6.503411	9.194879	-4.054876
C	8.770279	8.978815	-5.394742
C	7.890578	9.853538	-4.864626
C	12.453845	9.212268	0.910818
C	11.541972	10.033271	1.464826
H	9.681866	9.237464	-5.934758
H	7.969068	10.940547	-4.909380
H	13.345253	9.534915	0.386472
H	11.588033	11.115526	1.448184
O	6.108180	1.904724	-3.502628
O	2.560284	5.441766	-1.182481
O	6.018518	5.382461	4.409194
O	9.647666	1.976428	2.007298
C	5.199300	6.348707	3.733523
C	7.501857	1.760536	-3.176328
C	2.889172	6.397120	-0.161799
C	9.945767	1.941881	0.605518
H	7.967820	2.737925	-2.988053
H	7.968224	1.307160	-4.050387
H	7.619412	1.122417	-2.299320
H	2.011160	7.033189	-0.058966
H	3.095903	5.885766	0.782557
H	3.745212	7.018919	-0.457340
H	4.869428	7.046888	4.501670
H	4.342326	5.857664	3.267326
H	5.772939	6.900075	2.974536
H	9.068087	1.617156	0.038426
H	10.748935	1.214987	0.494513
H	10.299509	2.916171	0.241902
H	12.965010	17.446074	-5.368935
C	13.224999	16.432600	-5.657722
C	12.250189	15.440893	-5.651033
C	14.529936	16.127043	-6.036229
C	12.572848	14.134618	-6.028963
H	11.229040	15.682196	-5.364899
C	14.858678	14.826030	-6.406524
H	15.289672	16.902336	-6.042154
C	11.487262	13.093375	-6.133141
C	13.883689	13.833631	-6.407604
H	15.874648	14.583568	-6.701816
C	10.660182	13.067929	-7.512779
N	12.006443	11.731183	-6.058525
N	10.427535	13.289220	-5.146729
H	14.136154	12.823233	-6.719644
C	11.093238	14.056519	-8.564748
N	9.289621	13.281522	-7.056928
N	10.840983	11.685889	-7.948065
C	11.453217	10.909014	-7.005935

C	12.579242	11.190448	-4.839169
C	9.175179	13.202632	-5.694360
C	10.653074	13.108784	-3.724396
C	10.492972	15.314521	-8.657212
C	12.174293	13.746973	-9.395218
C	8.143792	13.033233	-7.918643
C	10.056229	11.101727	-9.021586
O	11.516194	9.679049	-7.015004
H	13.223973	11.969769	-4.413686
H	13.223518	10.351836	-5.107749
C	11.548171	10.735571	-3.829466
O	8.121209	13.096289	-5.066239
H	9.890402	13.670466	-3.182623
H	11.620261	13.572629	-3.492105
C	10.628637	11.659699	-3.285480
C	10.970059	16.250840	-9.569832
H	9.657759	15.562967	-8.006717
C	12.654127	14.687353	-10.299484
H	12.646524	12.769896	-9.324559
H	7.297121	13.600410	-7.528989
H	8.385831	13.449576	-8.904243
C	7.769635	11.571107	-8.034295
H	10.613477	10.258536	-9.433012
H	9.979427	11.856183	-9.814272
C	8.686452	10.643085	-8.574655
C	11.518974	9.390058	-3.434615
C	9.686755	11.241116	-2.335462
C	12.053645	15.940955	-10.387037
H	10.496324	17.224896	-9.639908
H	13.497035	14.440952	-10.937345
C	6.499746	11.152132	-7.613715
C	8.337636	9.292410	-8.703522
C	10.515491	8.963357	-2.552108
O	12.511730	8.527314	-3.791477
C	9.610698	9.879930	-2.008369
O	8.927463	12.133124	-1.637502
H	12.427896	16.674081	-11.094337
C	6.182565	9.785210	-7.678802
O	5.543284	12.056123	-7.269166
C	7.090891	8.868267	-8.218818
O	9.118615	8.420628	-9.398220
S	10.339589	7.297160	-2.035065
C	12.203251	7.534255	-4.783658
S	8.422773	9.244003	-0.888303
C	7.554552	12.282760	-2.037512
S	4.645949	9.134017	-7.154183
C	5.184721	12.156487	-5.884031
S	6.563397	7.202013	-8.294927
C	9.889563	7.469279	-8.649780
C	8.869634	7.575416	-1.136693
H	11.309046	6.957588	-4.509773
H	13.061336	6.864149	-4.805948
H	12.065325	8.007581	-5.758307
H	7.098503	12.930907	-1.290510
H	7.496890	12.742102	-3.027247
H	7.032049	11.315670	-2.035795
C	5.074213	7.472840	-7.438976
H	4.326420	12.825802	-5.850436
H	6.014775	12.576679	-5.310870

H	4.890188	11.182711	-5.469019
H	10.699442	7.973307	-8.116578
H	10.293091	6.773843	-9.384439
H	9.261748	6.911213	-7.940959
C	8.088438	6.531520	-0.686317
C	4.281925	6.422738	-6.991193
S	8.489522	4.859934	-0.996648
S	6.612093	6.770059	0.216790
S	4.703455	4.752424	-7.254588
S	2.811809	6.672436	-6.089221
C	7.110668	4.204679	-0.172072
C	6.248470	5.079968	0.384408
C	3.337863	4.108989	-6.408833
C	2.471107	4.989295	-5.873807
H	7.022943	3.118255	-0.147339
H	5.343347	4.814783	0.932593
H	3.236851	3.031322	-6.365074
H	1.568768	4.725387	-5.335476

Energy -11104.5650436 A.U.

Table S17. Optimized cartesian coordinates (in Angstroms) of $clip_2^{4+}$ at M06L/6-31G(d,p) level.

C	3.453209	-2.355921	5.098147
C	2.846596	-1.103873	5.204002
C	3.224736	-0.067605	4.354142
C	4.215437	-0.277207	3.392953
C	4.821413	-1.535988	3.291161
C	4.441577	-2.569583	4.141915
H	3.154813	-3.160921	5.761876
H	2.076717	-0.935217	5.949936
H	2.741364	0.903402	4.430277
H	5.582430	-1.708384	2.533921
H	4.917317	-3.541114	4.056590
C	4.546904	0.797536	2.392301
C	3.673718	0.803764	1.040534
C	2.570012	-0.218296	0.970851
C	1.293886	0.087898	1.451868
C	2.850705	-1.521108	0.549981
C	0.311923	-0.898456	1.512374
H	1.071951	1.094384	1.799011
C	1.869543	-2.506683	0.619392
H	3.845314	-1.767981	0.185835
C	0.600486	-2.197087	1.103203
H	-0.676112	-0.652265	1.888172
H	2.098120	-3.517873	0.298214
H	-0.162096	-2.966961	1.160767
N	4.326519	2.147171	2.908868
N	5.906682	0.677298	1.871832
N	4.696182	0.617148	0.011180
N	3.180155	2.177998	1.006744
C	3.737120	2.963102	1.978566
C	5.962731	0.784465	0.511203
O	6.980948	0.980318	-0.154834
O	3.701142	4.194278	2.017566
C	2.546017	2.747915	-0.166651
C	4.415393	0.843928	-1.395815
C	7.078258	0.884944	2.703380
C	5.158950	2.702013	3.964361
H	3.434534	0.397059	-1.600824
H	5.147663	0.290534	-1.986089
H	1.917854	3.581687	0.151418
H	1.876318	1.980570	-0.576515
H	4.606017	3.504784	4.454143
H	7.918560	0.351471	2.256642
H	5.303932	1.909754	4.708724
H	6.877171	0.414997	3.674405
C	6.491477	3.224550	3.473703
C	6.797200	4.582199	3.633296
C	7.423366	2.346203	2.873877
C	8.016391	5.056846	3.121355
C	8.668086	2.811501	2.428866
C	8.941828	4.185302	2.527168
C	3.525732	3.217822	-1.220164
C	3.515621	4.562556	-1.618821
C	4.431353	2.302370	-1.804528
C	4.472176	4.999940	-2.546461
C	5.336067	2.733893	-2.785809
C	5.372486	4.095702	-3.118522

S	8.492997	6.729528	3.229596
S	4.593176	6.664875	-3.088584
S	10.440054	4.902717	1.993021
S	6.498697	4.749316	-4.292485
C	6.061383	6.410879	-3.996468
C	9.986673	6.528751	2.378484
C	6.864915	7.463237	-4.400816
C	10.792611	7.622143	2.035821
S	12.312261	7.443471	1.219465
S	10.354095	9.258294	2.405830
S	8.377802	7.227469	-5.239641
S	6.474858	9.130570	-4.065875
C	8.759654	8.914536	-5.373093
C	7.885069	9.790479	-4.831495
C	12.706955	9.122845	1.238765
C	11.803681	9.960203	1.789345
H	9.682104	9.175681	-5.897222
H	7.980356	10.878651	-4.850773
H	13.664119	9.421224	0.827022
H	11.924693	11.032819	1.885001
O	6.088213	1.862892	-3.512482
O	2.534157	5.416610	-1.217301
O	6.024752	5.405592	4.385580
O	9.636388	1.945726	2.035619
C	5.197983	6.372989	3.718138
C	7.479225	1.735681	-3.165073
C	2.874357	6.377696	-0.204164
C	9.961961	1.882817	0.639495
H	7.963319	2.721620	-3.104056
H	7.935294	1.166611	-3.973600
H	7.583922	1.207921	-2.215419
H	1.997570	7.013883	-0.094346
H	3.093765	5.870893	0.739570
H	3.726668	6.997779	-0.516263
H	4.872147	7.066005	4.492090
H	4.341213	5.880430	3.254549
H	5.766673	6.928775	2.957939
H	9.097292	1.536840	0.067125
H	10.776195	1.164510	0.561504
H	10.310640	2.853152	0.259344
H	12.971958	17.462150	-5.396092
C	13.225771	16.450230	-5.695010
C	12.251977	15.455745	-5.665035
C	14.519724	16.148411	-6.111065
C	12.566529	14.150859	-6.056101
H	11.237910	15.696516	-5.353861
C	14.840426	14.848521	-6.494132
H	15.277511	16.924831	-6.136960
C	11.478401	13.114377	-6.151732
C	13.866818	13.852976	-6.471811
H	15.848341	14.608970	-6.817734
C	10.637665	13.097668	-7.524614
N	11.987675	11.746067	-6.086469
N	10.426441	13.299578	-5.153288
H	14.114804	12.844812	-6.795026
C	11.054277	14.095360	-8.572260
N	9.269328	13.295596	-7.050184
N	10.816984	11.717476	-7.971311
C	11.408536	10.931100	-7.022722

C	12.582395	11.201001	-4.880368
C	9.172445	13.178540	-5.688632
C	10.668389	13.115874	-3.734581
C	10.455419	15.354271	-8.641581
C	12.127525	13.794386	-9.420505
C	8.116217	13.052114	-7.902257
C	10.022594	11.144706	-9.042892
O	11.429904	9.698604	-7.018283
H	13.235567	11.978548	-4.464382
H	13.223488	10.363873	-5.161303
C	11.574146	10.745374	-3.847481
O	8.130050	13.010941	-5.052756
H	9.913106	13.675815	-3.180800
H	11.637528	13.581062	-3.512962
C	10.656856	11.667610	-3.292379
C	10.926187	16.301736	-9.548314
H	9.627668	15.598313	-7.980128
C	12.599187	14.744862	-10.320539
H	12.600424	12.816595	-9.366394
H	7.271087	13.615293	-7.503924
H	8.346588	13.472522	-8.888727
C	7.748399	11.588782	-8.018603
H	10.577837	10.314652	-9.482473
H	9.924748	11.912857	-9.820046
C	8.666015	10.669588	-8.577014
C	11.574198	9.405778	-3.431588
C	9.741926	11.252644	-2.313773
C	12.001386	16.000112	-10.383595
H	10.455146	17.278092	-9.600485
H	13.433065	14.503990	-10.971788
C	6.487064	11.163367	-7.578808
C	8.331441	9.315554	-8.705853
C	10.603796	8.983960	-2.511334
O	12.559900	8.542922	-3.801484
C	9.700482	9.897330	-1.958613
O	8.979113	12.138106	-1.615163
H	12.368122	16.742505	-11.084789
C	6.183907	9.791904	-7.641932
O	5.528017	12.058332	-7.233755
C	7.095914	8.882720	-8.199334
O	9.097791	8.456090	-9.424299
S	10.476817	7.328322	-1.945690
C	12.235567	7.558715	-4.798432
S	8.564243	9.262562	-0.783224
C	7.598387	12.262983	-1.999584
S	4.664047	9.122594	-7.108414
C	5.160669	12.170345	-5.850626
S	6.581819	7.218550	-8.271544
C	9.901249	7.499044	-8.715604
C	9.001423	7.596377	-1.055059
H	11.357301	6.967583	-4.502196
H	13.101000	6.900593	-4.855284
H	12.061777	8.042627	-5.762295
H	7.140469	12.906880	-1.250420
H	7.521489	12.715739	-2.990817
H	7.094544	11.285261	-1.985997
C	5.082331	7.477392	-7.446624
H	4.299909	12.836463	-5.829804
H	5.986570	12.597147	-5.277021

H	4.865975	11.198958	-5.429166
H	10.735434	7.999171	-8.218890
H	10.264956	6.804218	-9.470855
H	9.303521	6.942740	-7.978766
C	8.194736	6.546365	-0.651107
C	4.247866	6.411949	-7.083484
S	8.572251	4.882188	-1.013838
S	6.693652	6.778493	0.208420
S	4.642600	4.759479	-7.428855
S	2.736960	6.642707	-6.264176
C	7.163618	4.219784	-0.250170
C	6.299871	5.091578	0.314850
C	3.178636	4.104706	-6.794047
C	2.299100	4.974108	-6.254908
H	7.058067	3.132742	-0.262356
H	5.380373	4.823261	0.840214
H	3.030363	3.033937	-6.871152
H	1.336433	4.707910	-5.833884

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Table S18. Optimized cartesian coordinates (in Angstroms) of $clip_2^{6+}$ at M06L/6-31G(d,p) level.

C	2.987768	-2.636811	5.475201
C	2.533705	-1.326827	5.654007
C	3.248338	-0.249105	5.102150
C	4.422135	-0.485582	4.378673
C	4.871731	-1.798768	4.192760
C	4.156258	-2.874315	4.747696
H	2.434549	-3.466250	5.902792
H	1.628943	-1.138326	6.222794
H	2.885247	0.767685	5.228213
H	5.772995	-1.982917	3.613657
H	4.514507	-3.889227	4.609235
C	5.066344	0.631725	3.614859
C	4.448042	0.839428	2.146614
C	3.354029	-0.126717	1.807758
C	2.031388	0.161328	2.161767
C	3.681484	-1.398844	1.322145
C	1.034723	-0.819663	2.018708
H	1.778791	1.142256	2.556395
C	2.683807	-2.378331	1.183125
H	4.709891	-1.626153	1.055162
C	1.362682	-2.088596	1.533414
H	0.009397	-0.589034	2.287741
H	2.942421	-3.360582	0.800605
H	0.593506	-2.845407	1.427514
N	4.899020	1.962257	4.209492
N	6.489392	0.436192	3.324820
N	5.639393	0.729405	1.293189
N	4.026556	2.246115	2.185652
C	4.559478	2.929001	3.272866
C	6.822408	0.778137	2.020048
O	7.963508	1.042863	1.587362
O	4.681088	4.165876	3.400693
C	3.515494	2.887320	0.976270
C	5.532262	0.995965	-0.139549
C	7.450845	0.270437	4.404220
C	5.406622	2.245753	5.544136
H	4.582838	0.543635	-0.462757
H	6.336094	0.473797	-0.663152
H	2.870693	3.723033	1.258632
H	2.880730	2.138859	0.479135
H	4.886882	3.122095	5.937430
H	8.345036	-0.213322	4.005054
H	5.119642	1.388707	6.173768
H	6.994988	-0.428872	5.122890
C	6.912579	2.434041	5.705316
C	7.313878	3.420914	6.625624
C	7.855795	1.517537	5.183430
C	8.630543	3.392423	7.088834
C	9.205525	1.577907	5.578786
C	9.558937	2.488045	6.575646
C	4.571722	3.361101	-0.010663
C	4.462374	4.670381	-0.516089
C	5.530113	2.464842	-0.534900
C	5.315570	5.041114	-1.557588
C	6.395494	2.868413	-1.569263
C	6.255486	4.165031	-2.068289

S	9.159308	4.437972	8.443001
S	5.194719	6.675947	-2.299322
S	11.185222	2.465499	7.325234
S	7.280181	4.724791	-3.437307
C	6.520094	6.352065	-3.469972
C	10.788107	3.716601	8.533767
C	6.893107	7.294695	-4.398692
C	11.683791	4.065780	9.543574
S	13.281540	3.304148	9.704397
S	11.287207	5.263230	10.797016
S	8.180265	6.999300	-5.602278
S	6.134767	8.909827	-4.476452
C	8.158657	8.674659	-6.251007
C	7.243482	9.526510	-5.748915
C	13.725137	4.196276	11.184014
C	12.828748	5.076887	11.675245
H	8.879515	8.916398	-7.033256
H	7.107568	10.559068	-6.066181
H	14.695716	3.981953	11.619335
H	12.966903	5.680798	12.566276
O	7.282799	2.044521	-2.233444
O	3.484740	5.578698	-0.158187
O	6.451391	4.328618	7.208069
O	10.173359	0.694749	5.139814
C	6.006648	5.446824	6.303992
C	8.530308	1.621865	-1.514972
C	3.600721	6.237845	1.184273
C	10.666276	0.956800	3.741340
H	9.261306	2.439612	-1.552841
H	8.897892	0.775652	-2.095457
H	8.320069	1.332742	-0.478670
H	2.608466	6.651012	1.366337
H	3.879890	5.515304	1.960197
H	4.335087	7.050902	1.122432
H	5.247999	5.968830	6.887474
H	5.587899	5.049484	5.369994
H	6.858987	6.105170	6.100645
H	9.826048	0.991119	3.035218
H	11.325127	0.114045	3.533536
H	11.226418	1.899312	3.726799
H	12.261712	17.296994	-6.034552
C	12.520227	16.311021	-6.407339
C	11.524254	15.326561	-6.526080
C	13.839271	16.020589	-6.763788
C	11.851277	14.049920	-7.000229
H	10.497005	15.554633	-6.254732
C	14.166759	14.746708	-7.236728
H	14.607347	16.780585	-6.672675
C	10.755606	13.078667	-7.319242
C	13.171665	13.761631	-7.361600
H	15.190762	14.515431	-7.510315
C	10.119382	13.277530	-8.779967
N	11.176406	11.670559	-7.351362
N	9.573309	13.195756	-6.455498
H	13.423985	12.777200	-7.747017
C	10.819272	14.319048	-9.599300
N	8.717747	13.574570	-8.471256
N	10.191255	11.917542	-9.329126
C	10.570452	10.972067	-8.391956

C	11.691433	11.040627	-6.135442
C	8.382964	13.219524	-7.167173
C	9.688390	12.944687	-5.021349
C	10.466865	15.667230	-9.458954
C	11.953027	13.971404	-10.341121
C	7.746372	13.745739	-9.543752
C	9.635541	11.619716	-10.640796
O	10.421525	9.733589	-8.483391
H	12.329833	11.793558	-5.650382
H	12.334181	10.201390	-6.411535
C	10.639446	10.576706	-5.138834
O	7.237076	12.999420	-6.724014
H	8.889491	13.475110	-4.498258
H	10.642238	13.394527	-4.707308
C	9.685845	11.478733	-4.615323
C	11.241859	16.664812	-10.075732
H	9.595872	15.938874	-8.869697
C	12.724202	14.971036	-10.960585
H	12.240906	12.926837	-10.429982
H	6.895273	14.312500	-9.160080
H	8.235806	14.371642	-10.306371
C	7.243215	12.487423	-10.243095
H	10.104698	10.710701	-11.022891
H	9.940652	12.446604	-11.301962
C	8.119061	11.496798	-10.748851
C	10.746736	9.270339	-4.624831
C	8.821279	11.084059	-3.576883
C	12.368461	16.316215	-10.824830
H	10.960052	17.707675	-9.971030
H	13.595791	14.695005	-11.544019
C	5.880269	12.481856	-10.594900
C	7.638213	10.491141	-11.608355
C	9.892749	8.907513	-3.581033
O	11.722587	8.357632	-4.974987
C	8.956025	9.788459	-3.072638
O	7.939804	11.916551	-2.915065
H	12.964434	17.086820	-11.301976
C	5.447035	11.542882	-11.532035
O	4.974625	13.437591	-10.179916
C	6.307960	10.565215	-12.027277
O	8.433964	9.519599	-12.182562
S	10.008852	7.274437	-2.834439
C	11.607989	7.684631	-6.311005
S	7.931374	9.235324	-1.700006
C	6.689855	12.338019	-3.629104
S	3.798432	11.619025	-12.227273
C	4.522361	13.293468	-8.750085
S	5.675386	9.484630	-13.308030
C	8.879193	8.424258	-11.253148
C	8.684658	7.604686	-1.663909
H	10.885850	6.861761	-6.236814
H	12.604984	7.284387	-6.496298
H	11.311710	8.396833	-7.089463
H	6.318662	13.176633	-3.039839
H	6.895870	12.640474	-4.662745
H	5.962649	11.516474	-3.598447
C	4.081445	10.283189	-13.375770
H	3.957115	14.205836	-8.559660
H	5.386729	13.206931	-8.079040

H	3.874591	12.413357	-8.666658
H	9.356313	8.841277	-10.355975
H	9.592044	7.851600	-11.847072
H	8.015046	7.805607	-10.985062
C	8.309125	6.662798	-0.734895
C	3.125534	9.923478	-14.324747
S	9.067773	5.047194	-0.655935
S	7.019860	6.956637	0.466797
S	3.382925	8.599843	-15.484091
S	1.581099	10.788652	-14.496671
C	7.957010	4.428128	0.612832
C	7.040717	5.279543	1.113901
C	1.822952	8.826783	-16.319627
C	1.012358	9.808390	-15.873709
H	8.091578	3.394447	0.929236
H	6.319880	5.037398	1.894937
H	1.605702	8.163740	-17.150531
H	0.041708	10.056826	-16.291026

Energy -11103.1281596 A.U.

Table S19. Optimized cartesian coordinates (in Angstroms) of $clip_1^0$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	-0.175608	0.028114	0.163758
C	-0.099777	0.036502	1.555046
C	1.138878	0.027130	2.187047
C	2.316179	0.026403	1.433827
C	2.234313	0.010046	0.039663
C	0.993629	0.005978	-0.592235
H	-1.143431	0.035624	-0.329311
H	-1.007445	0.049512	2.151102
H	1.201292	0.045437	3.271976
H	3.144855	0.017219	-0.554360
H	0.942391	-0.005791	-1.676896
C	3.655438	0.188333	2.121468
C	4.094019	1.693840	2.374610
C	2.976015	2.709851	2.269231
C	2.212373	3.043976	3.389905
C	2.622136	3.231486	1.021690
C	1.106700	3.880674	3.264155
H	2.477191	2.636982	4.362866
C	1.510386	4.057104	0.894652
H	3.212675	2.967241	0.148566
C	0.747875	4.381360	2.015412
H	0.521099	4.133986	4.142754
H	1.238459	4.447509	-0.081836
H	-0.120196	5.026452	1.916128
N	3.670557	-0.377352	3.458269
N	4.761711	-0.293674	1.314024
N	5.126038	1.898508	1.374369
N	4.646015	1.604252	3.713475
C	4.415110	0.401734	4.327713
C	5.621443	0.692760	0.908978
O	6.623177	0.542771	0.219052
O	4.765271	0.086370	5.459059
C	5.358464	2.702866	4.326629
C	5.974362	3.081309	1.421998
C	4.927227	-1.692285	0.988020
C	3.571439	-1.817302	3.651790
H	5.306353	3.938052	1.579123
H	6.424665	3.207259	0.435991
H	5.356247	2.531402	5.404610
H	4.785826	3.624060	4.144126
H	3.265587	-1.992846	4.684449
H	5.591006	-1.747851	0.122958
H	2.748721	-2.162689	3.012186
H	3.949844	-2.086540	0.672995
C	4.830360	-2.606281	3.364225
C	5.326682	-3.470721	4.350394
C	5.479607	-2.532304	2.114648
C	6.467246	-4.238702	4.101627
C	6.626754	-3.299613	1.881172
C	7.118427	-4.146838	2.874129
C	6.776232	2.873586	3.836435
C	7.812434	2.900705	4.776066
C	7.066412	3.066516	2.469768
C	9.125888	3.129360	4.366466
C	8.389897	3.302597	2.070033
C	9.414878	3.335811	3.019609

S	7.073710	-5.449869	5.227475
S	10.454691	3.308328	5.507067
S	8.477147	-5.236169	2.608301
S	11.078811	3.762208	2.627764
C	11.688396	3.363061	4.240281
C	8.555616	-5.734726	4.304119
C	13.001422	3.146058	4.494018
C	9.658057	-6.301853	4.849888
S	11.139812	-6.602216	3.931808
S	9.746688	-6.803737	6.543536
S	14.251608	3.214300	3.245098
S	13.615801	2.774179	6.110681
C	15.497206	2.515539	4.258679
C	15.209863	2.316717	5.550696
C	12.109468	-6.952293	5.346637
C	11.481450	-7.043051	6.524790
H	16.454611	2.308411	3.797755
H	15.901196	1.923458	6.284877
H	13.169673	-7.110991	5.196069
H	11.959842	-7.286122	7.465177
O	8.692836	3.609484	0.766218
O	7.564963	2.784177	6.123476
O	4.653835	-3.658562	5.532521
O	7.252560	-3.305379	0.657099
C	5.225196	-2.954738	6.647632
C	9.246342	2.515690	0.015862
C	7.692775	1.437479	6.603767
C	8.337301	-2.368704	0.575135
H	10.136411	2.108576	0.510503
H	9.534760	2.928279	-0.951136
H	8.498972	1.727563	-0.113960
H	7.548556	1.482233	7.683410
H	6.927774	0.793321	6.155195
H	8.691658	1.038708	6.388027
H	4.637171	-3.241022	7.519656
H	5.162333	-1.875236	6.484349
H	6.269413	-3.250663	6.806388
H	7.967609	-1.341018	0.664891
H	8.791103	-2.511120	-0.405634
H	9.085617	-2.567727	1.351848

Energy -5552.64749626 A.U.

Table S20. Optimized cartesian coordinates (in Angstroms) of clip$_1^+$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	-0.182832	0.176169	0.120757
C	-0.116736	0.127314	1.511716
C	1.117239	0.070381	2.150401
C	2.299115	0.074517	1.404367
C	2.226996	0.113276	0.009907
C	0.990731	0.159959	-0.628684
H	-1.146732	0.223435	-0.377524
H	-1.028003	0.135010	2.102237
H	1.172438	0.046689	3.235578
H	3.140807	0.123630	-0.579088
H	0.946585	0.192022	-1.713177
C	3.635918	0.183519	2.105410
C	4.110115	1.667566	2.402112
C	3.014730	2.711062	2.344767
C	2.263178	3.011231	3.483010
C	2.666462	3.293240	1.122473
C	1.173024	3.872899	3.398735
H	2.523538	2.557354	4.436250
C	1.571305	4.146024	1.037587
H	3.247183	3.055496	0.235127
C	0.819985	4.435681	2.175073
H	0.595576	4.098656	4.290142
H	1.303840	4.584512	0.080515
H	-0.035769	5.100900	2.108175
N	3.629766	-0.419489	3.425990
N	4.738082	-0.303492	1.294168
N	5.136350	1.880556	1.398211
N	4.676415	1.518639	3.731172
C	4.404271	0.308956	4.313968
C	5.612980	0.676754	0.906536
O	6.613985	0.526140	0.216582
O	4.747460	-0.051824	5.433424
C	5.437193	2.570973	4.365951
C	6.005889	3.045410	1.472297
C	4.861801	-1.694588	0.923864
C	3.492474	-1.860527	3.578608
H	5.359935	3.906147	1.686727
H	6.434500	3.209134	0.482520
H	5.444599	2.369258	5.438549
H	4.900517	3.519687	4.219479
H	3.175880	-2.058428	4.603789
H	5.522005	-1.746013	0.055946
H	2.667516	-2.169430	2.923848
H	3.873298	-2.051721	0.599791
C	4.732761	-2.673243	3.274797
C	5.198860	-3.574939	4.239890
C	5.387120	-2.584327	2.025710
C	6.313903	-4.374096	3.964195
C	6.508111	-3.378078	1.766849
C	6.965919	-4.271569	2.737598
C	6.853072	2.707563	3.856072
C	7.907319	2.646611	4.771522
C	7.120529	2.959575	2.491672
C	9.217591	2.860573	4.337410
C	8.436952	3.178919	2.067641
C	9.482084	3.135570	2.997242

S	6.905013	-5.594413	5.070794
S	10.575310	2.885822	5.439982
S	8.305534	-5.360692	2.454656
S	11.143960	3.493585	2.582999
C	11.771135	3.193698	4.194388
C	8.239727	-6.092675	4.048372
C	13.117375	3.206970	4.465327
C	9.173321	-7.009370	4.464938
S	10.501924	-7.531049	3.447723
S	9.139859	-7.746401	6.056355
S	14.328807	3.509750	3.235547
S	13.764827	2.912438	6.068101
C	15.686372	3.300267	4.298306
C	15.429366	3.028274	5.587928
C	11.214314	-8.569832	4.642633
C	10.593485	-8.669589	5.828984
H	16.675008	3.406302	3.870914
H	16.180535	2.882410	6.353166
H	12.120127	-9.096356	4.370872
H	10.926802	-9.285422	6.654171
O	8.720513	3.539976	0.777416
O	7.701027	2.458237	6.114120
O	4.528367	-3.774984	5.417033
O	7.142407	-3.372515	0.551070
C	5.112922	-3.111476	6.552466
C	9.239116	2.477140	-0.043096
C	7.733752	1.075432	6.507282
C	8.229176	-2.433378	0.479330
H	10.125135	2.020381	0.414488
H	9.525221	2.940475	-0.986964
H	8.471540	1.715835	-0.206174
H	7.629799	1.066705	7.591870
H	6.904293	0.523987	6.051407
H	8.689102	0.613960	6.230320
H	4.524478	-3.419878	7.415988
H	5.062721	-2.027406	6.422396
H	6.154291	-3.423492	6.698014
H	7.859930	-1.406514	0.576586
H	8.683445	-2.570410	-0.501437
H	8.975080	-2.639516	1.256132

Energy -5552.48444349 A.U.

Table S21. Optimized cartesian coordinates (in Angstroms) of $clip_1^{2+}$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	-0.199755	0.119984	-0.043770
C	-0.186007	0.076202	1.348989
C	1.023302	0.052499	2.035194
C	2.231982	0.085054	1.334097
C	2.212670	0.117107	-0.062388
C	1.001293	0.129870	-0.748053
H	-1.144674	0.141168	-0.578743
H	-1.119339	0.062664	1.903990
H	1.037010	0.033023	3.121767
H	3.147890	0.148533	-0.616268
H	0.998076	0.156942	-1.833523
C	3.538289	0.235004	2.082289
C	3.957730	1.730733	2.391436
C	2.832363	2.739623	2.321036
C	2.053955	3.010486	3.448524
C	2.488059	3.319353	1.096345
C	0.942512	3.843286	3.351895
H	2.310540	2.557954	4.403405
C	1.370919	4.141675	0.998845
H	3.088759	3.104356	0.216557
C	0.594580	4.404437	2.126055
H	0.345150	4.047583	4.235258
H	1.106659	4.578392	0.040167
H	-0.277233	5.047304	2.049546
N	3.508150	-0.365579	3.403612
N	4.684065	-0.219489	1.311398
N	4.995310	1.978448	1.407636
N	4.510487	1.592377	3.728025
C	4.250966	0.378244	4.307678
C	5.532521	0.790041	0.939922
O	6.558500	0.672511	0.281529
O	4.581178	0.023569	5.432472
C	5.213400	2.672075	4.381000
C	5.813104	3.177711	1.493187
C	4.861320	-1.605752	0.947387
C	3.401149	-1.808588	3.549662
H	5.128969	4.012039	1.693325
H	6.253130	3.358908	0.511609
H	5.210036	2.467822	5.453069
H	4.641371	3.598917	4.228643
H	3.046659	-2.020702	4.559274
H	5.548272	-1.640321	0.099741
H	2.614076	-2.138749	2.859774
H	3.894975	-1.995330	0.594972
C	4.673267	-2.588779	3.293475
C	5.118356	-3.479304	4.276107
C	5.374241	-2.480609	2.068033
C	6.261520	-4.251733	4.036624
C	6.523280	-3.243517	1.846934
C	6.959735	-4.130229	2.835741
C	6.630741	2.877431	3.896569
C	7.664280	2.879262	4.835928
C	6.910718	3.146265	2.534488
C	8.965899	3.182374	4.425910
C	8.216916	3.446053	2.133757
C	9.239554	3.473278	3.089573

S	6.844313	-5.453108	5.156122
S	10.297872	3.292442	5.543383
S	8.334624	-5.179891	2.618565
S	10.879635	3.926978	2.714980
C	11.467142	3.744686	4.340367
C	8.190195	-5.939756	4.173637
C	12.806475	3.965423	4.663927
C	9.103307	-6.900588	4.611917
S	10.443996	-7.425478	3.645635
S	8.983978	-7.657915	6.168257
S	13.990253	4.421071	3.479213
S	13.418161	3.809004	6.280870
C	15.308185	4.500527	4.588501
C	15.044368	4.217322	5.879546
C	11.053842	-8.542499	4.808818
C	10.381336	-8.651209	5.971899
H	16.279604	4.772628	4.195951
H	15.771579	4.227414	6.681269
H	11.943091	-9.102367	4.549723
H	10.648996	-9.308876	6.788791
O	8.512664	3.820536	0.853629
O	7.451039	2.678403	6.172017
O	4.413027	-3.700279	5.424772
O	7.204751	-3.226154	0.661169
C	4.931876	-3.021227	6.585229
C	9.069821	2.773325	0.034760
C	7.493938	1.292755	6.562325
C	8.247058	-2.233533	0.606764
H	9.968740	2.348448	0.497549
H	9.342295	3.246443	-0.907744
H	8.328991	1.986113	-0.128195
H	7.368635	1.282470	7.644215
H	6.681535	0.730533	6.089774
H	8.460547	0.846596	6.302372
H	4.312546	-3.343920	7.420932
H	4.862162	-1.939352	6.449272
H	5.972855	-3.308447	6.777327
H	7.825166	-1.224806	0.669248
H	8.739393	-2.368989	-0.355271
H	8.973970	-2.387805	1.412582

Energy -5552.31109616 A.U.

Table S22. Optimized cartesian coordinates (in Angstroms) of $clip_1^{3+}$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	-0.180012	0.072533	0.130500
C	-0.121469	0.063857	1.522501
C	1.109105	0.041572	2.169570
C	2.294454	0.042994	1.429140
C	2.230608	0.043731	0.033619
C	0.997610	0.053396	-0.612392
H	-1.141631	0.091784	-0.373854
H	-1.035994	0.075266	2.107665
H	1.156523	0.049990	3.255383
H	3.147040	0.055566	-0.551365
H	0.959156	0.055695	-1.697434
C	3.624554	0.196503	2.132941
C	4.067266	1.695025	2.395423
C	2.959025	2.718946	2.281632
C	2.180772	3.048647	3.393757
C	2.628212	3.250617	1.031840
C	1.083720	3.894566	3.256956
H	2.423851	2.631353	4.368007
C	1.524821	4.085435	0.894737
H	3.226711	2.987352	0.163860
C	0.748865	4.407613	2.006655
H	0.486276	4.145061	4.128069
H	1.270463	4.484486	-0.082742
H	-0.112418	5.060165	1.899019
N	3.629056	-0.373893	3.467898
N	4.742172	-0.293695	1.343719
N	5.116134	1.893188	1.412189
N	4.615104	1.597335	3.736798
C	4.375455	0.393085	4.346355
C	5.618411	0.687005	0.953702
O	6.634143	0.531809	0.287839
O	4.724040	0.066909	5.473812
C	5.295081	2.703583	4.364167
C	5.936314	3.088657	1.448983
C	4.867946	-1.685819	0.987823
C	3.491405	-1.805216	3.657922
H	5.254130	3.938003	1.584270
H	6.397193	3.213399	0.468228
H	5.282113	2.533858	5.441965
H	4.713146	3.618438	4.179379
H	3.182967	-1.980178	4.689499
H	5.530527	-1.750909	0.123218
H	2.661701	-2.134454	3.019148
H	3.882365	-2.049844	0.662341
C	4.719999	-2.638070	3.357310
C	5.147147	-3.551646	4.325270
C	5.376504	-2.576144	2.098719
C	6.215010	-4.408042	4.030486
C	6.460096	-3.412811	1.826635
C	6.867231	-4.337455	2.794706
C	6.712804	2.927769	3.890070
C	7.718159	3.039209	4.852657
C	7.010926	3.134204	2.515771
C	9.007146	3.406647	4.452003
C	8.306574	3.483756	2.124413
C	9.296419	3.635641	3.102534

S	6.749799	-5.654178	5.109267
S	10.292097	3.691742	5.577134
S	8.121482	-5.499288	2.518972
S	10.902595	4.179791	2.747294
C	11.437316	4.173853	4.384411
C	7.964154	-6.264216	4.052722
C	12.749695	4.570436	4.735115
C	8.778515	-7.362495	4.421252
S	9.956380	-8.038478	3.365635
S	8.657829	-8.122369	5.959253
S	13.903763	5.088935	3.567335
S	13.306450	4.586328	6.363593
C	15.156856	5.392702	4.694791
C	14.877987	5.160016	5.998589
C	10.482054	-9.251790	4.456677
C	9.875090	-9.292310	5.665903
H	16.102944	5.755671	4.314023
H	15.567577	5.306586	6.820193
H	11.265837	-9.921726	4.126802
H	10.096768	-9.999416	6.455120
O	8.628732	3.794860	0.837211
O	7.490542	2.910476	6.190978
O	4.496541	-3.726738	5.509707
O	7.092784	-3.443893	0.618858
C	5.066843	-2.996816	6.617574
C	9.148545	2.687923	0.069508
C	7.519572	1.548490	6.667178
C	8.167035	-2.488064	0.496971
H	10.053104	2.281433	0.536771
H	9.399686	3.098057	-0.907286
H	8.392278	1.903664	-0.024708
H	7.340932	1.606747	7.739671
H	6.733603	0.952758	6.191384
H	8.500139	1.096963	6.482061
H	4.478283	-3.276458	7.489599
H	4.998985	-1.921312	6.435284
H	6.112491	-3.285112	6.777272
H	7.783968	-1.464284	0.563414
H	8.604743	-2.657571	-0.485316
H	8.923924	-2.658596	1.270279

Energy -5552.11141898 A.U.

Table S23. Optimized cartesian coordinates (in Angstroms) of $clip_1^{4+}$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	-2.214582	7.222409	-1.300763
C	-2.193991	6.840578	0.039411
C	-1.775942	5.563280	0.395534
C	-1.369264	4.656204	-0.587770
C	-1.395148	5.042298	-1.930090
C	-1.818086	6.320102	-2.284231
H	-2.539498	8.220979	-1.577208
H	-2.503237	7.539456	0.810775
H	-1.745623	5.268969	1.441374
H	-1.070422	4.348587	-2.701556
H	-1.832812	6.610227	-3.330118
C	-0.781487	3.322153	-0.191141
C	0.772692	3.326253	0.072199
C	1.358492	4.670660	0.435588
C	1.381892	5.087596	1.768909
C	1.766165	5.555084	-0.567551
C	1.803512	6.373063	2.094675
H	1.057146	4.411125	2.555608
C	2.182444	6.840654	-0.239741
H	1.738897	5.236564	-1.606442
C	2.200643	7.253023	1.091412
H	1.816796	6.686508	3.133863
H	2.492183	7.522001	-1.026422
H	2.524293	8.257928	1.345443
N	-1.308963	2.810780	1.059727
N	-0.872332	2.322829	-1.246721
N	1.301017	2.780013	-1.163421
N	0.863708	2.356722	1.155503
C	-0.346390	2.069003	1.732026
C	0.338832	2.015085	-1.810742
O	0.538443	1.231480	-2.729153
O	-0.544424	1.319005	2.678381
C	2.134053	1.870071	1.634280
C	2.705895	2.428163	-1.258232
C	-2.140485	1.807929	-1.700930
C	-2.714816	2.467106	1.166646
H	3.270925	3.246519	-0.794733
H	2.988857	2.413379	-2.311147
H	1.982665	1.469647	2.638009
H	2.821916	2.722944	1.734762
H	-3.001443	2.496878	2.218218
H	-1.989020	1.371558	-2.689598
H	-3.276379	3.267453	0.668611
H	-2.835737	2.650968	-1.830339
C	-3.104530	1.131936	0.573049
C	-3.858287	0.260578	1.362730
C	-2.789178	0.799005	-0.776649
C	-4.301409	-0.942622	0.799180
C	-3.192124	-0.424681	-1.312626
C	-3.957101	-1.288991	-0.518410
C	2.789633	0.833041	0.748102
C	3.197413	-0.369165	1.327608
C	3.097321	1.116451	-0.614021
C	3.965258	-1.258171	0.564302
C	3.846887	0.216079	-1.374640
C	4.293250	-0.966197	-0.770626

S	-5.314921	-2.062510	1.628234
S	4.602174	-2.726904	1.198354
S	-4.613549	-2.766343	-1.110995
S	5.338537	-2.094602	-1.550000
C	5.440005	-3.158385	-0.221731
C	-5.433302	-3.163849	0.330794
C	6.213413	-4.371248	-0.297540
C	-6.202539	-4.375288	0.447854
S	-5.907289	-5.740506	-0.529641
S	-7.466961	-4.544009	1.577650
S	6.497141	-5.176345	-1.771942
S	6.912327	-5.093741	1.077796
C	7.438396	-6.427667	-1.103809
C	7.622001	-6.397791	0.243059
C	-7.138123	-6.704097	0.147428
C	-7.863977	-6.144614	1.151536
H	7.829925	-7.184242	-1.772213
H	8.187068	-7.123451	0.815074
H	-7.273440	-7.706114	-0.240486
H	-8.673195	-6.628242	1.684414
O	4.268595	0.487870	-2.637664
O	2.985674	-0.696317	2.629916
O	-4.288646	0.577558	2.612400
O	-2.980465	-0.796041	-2.602841
C	-3.429035	0.137833	3.689558
C	3.416720	-0.019925	-3.690855
C	1.666541	-1.214685	2.915090
C	-1.659872	-1.319345	-2.870810
H	3.340092	-1.111374	-3.636035
H	3.904938	0.262765	-4.621518
H	2.421830	0.426840	-3.620993
H	1.674084	-1.463884	3.974409
H	0.897902	-0.461401	2.715950
H	1.474087	-2.116395	2.325011
H	-3.922054	0.460534	4.604465
H	-2.440549	0.594431	3.597401
H	-3.335487	-0.953578	3.691363
H	-0.893838	-0.559206	-2.688399
H	-1.663412	-1.595436	-3.923399
H	-1.468329	-2.205043	-2.256872

Energy -5551.90099141 A.U.

Table S24. Optimized cartesian coordinates (in Angstroms) of $clip_2^0$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	2.850705	-2.207863	5.128454
C	2.364418	-0.902730	5.148770
C	2.926913	0.064755	4.322202
C	3.981276	-0.263590	3.466251
C	4.470259	-1.571899	3.455572
C	3.907408	-2.538925	4.283622
H	2.410791	-2.963450	5.772804
H	1.543173	-0.636240	5.807608
H	2.542157	1.081502	4.333440
H	5.289273	-1.830059	2.788946
H	4.294829	-3.553448	4.266252
C	4.512344	0.764731	2.489295
C	3.751578	0.829966	1.078902
C	2.675738	-0.216746	0.877731
C	1.361096	0.032495	1.278434
C	3.010201	-1.479298	0.381448
C	0.397647	-0.968416	1.192123
H	1.098834	1.012512	1.668667
C	2.046814	-2.479815	0.296835
H	4.032161	-1.679254	0.069446
C	0.739654	-2.228374	0.706973
H	-0.620956	-0.763103	1.508169
H	2.319800	-3.458328	-0.087399
H	-0.011653	-3.010017	0.642460
N	4.344272	2.117410	2.989314
N	5.884845	0.493543	2.093780
N	4.845056	0.671667	0.135179
N	3.213343	2.181270	1.076321
C	3.701963	2.946141	2.109066
C	6.074055	0.606537	0.736456
O	7.159322	0.597655	0.160568
O	3.544205	4.157529	2.239894
C	2.718020	2.807950	-0.139934
C	4.688162	0.939474	-1.283912
C	6.997668	0.670685	3.016407
C	5.091867	2.619972	4.128070
H	3.737828	0.486908	-1.596720
H	5.485759	0.412483	-1.809849
H	2.082830	3.643025	0.158361
H	2.076155	2.072559	-0.641726
H	4.543947	3.471730	4.534619
H	7.842763	0.105795	2.620241
H	5.086504	1.832772	4.893433
H	6.705631	0.199848	3.964022
C	6.502859	3.034487	3.791127
C	6.909010	4.351004	4.041134
C	7.410444	2.107688	3.243283
C	8.203278	4.751555	3.702690
C	8.718923	2.510264	2.937145
C	9.103788	3.837373	3.153144
C	3.794263	3.303050	-1.078053
C	3.832456	4.657852	-1.434753
C	4.725518	2.406364	-1.637175
C	4.805673	5.118298	-2.330751
C	5.674641	2.868023	-2.556185
C	5.720264	4.225884	-2.890522

S	8.837621	6.365229	4.046825
S	4.832422	6.767171	-2.940403
S	10.748950	4.434435	2.891909
S	6.790451	4.852497	-4.134093
C	6.250029	6.526715	-3.968043
C	10.242577	6.121460	3.006281
C	6.863461	7.549202	-4.611417
C	10.827289	7.124453	2.308272
S	12.205700	6.873918	1.231338
S	10.275464	8.799856	2.400036
S	8.267027	7.318146	-5.660126
S	6.321938	9.226562	-4.497514
C	8.634191	9.028344	-5.785805
C	7.757793	9.890605	-5.254789
C	12.132343	8.478642	0.534175
C	11.260556	9.346354	1.060333
H	9.548148	9.303198	-6.305642
H	7.848179	10.972868	-5.282196
H	12.804856	8.694329	-0.287048
H	11.124288	10.368466	0.727984
O	6.479365	1.982447	-3.230318
O	2.843557	5.513007	-1.016245
O	6.086484	5.216717	4.718931
O	9.650817	1.587058	2.533477
C	5.481632	6.242200	3.918388
C	7.845502	1.950655	-2.794408
C	3.243904	6.485546	-0.040305
C	10.049522	1.676093	1.157699
H	8.313045	2.939540	-2.873400
H	8.358652	1.256439	-3.460097
H	7.905949	1.589359	-1.762131
H	2.387202	7.145904	0.096059
H	3.489860	5.994118	0.906291
H	4.100654	7.074250	-0.389036
H	4.938295	6.884504	4.611938
H	4.784464	5.799651	3.199646
H	6.239067	6.837967	3.395080
H	9.201349	1.453825	0.503857
H	10.826105	0.923389	1.021453
H	10.463478	2.663987	0.923711
H	12.815119	17.394925	-5.013491
C	13.088390	16.416340	-5.397334
C	12.125206	15.415631	-5.481913
C	14.395714	16.164998	-5.807024
C	12.460026	14.152984	-5.977724
H	11.103127	15.615512	-5.170250
C	14.738083	14.904943	-6.291659
H	15.146865	16.946793	-5.742544
C	11.384382	13.106102	-6.179003
C	13.774832	13.903839	-6.377943
H	15.756816	14.699693	-6.607322
C	10.623712	13.171290	-7.589443
N	11.922848	11.754877	-6.176421
N	10.290784	13.264165	-5.235399
H	14.037383	12.923746	-6.767789
C	11.154924	14.199504	-8.566428
N	9.251166	13.442523	-7.194071
N	10.791783	11.818580	-8.089347
C	11.434335	10.989958	-7.209194

C	12.417951	11.128131	-4.960098
C	9.061836	13.329232	-5.836771
C	10.447656	12.996563	-3.816283
C	10.665876	15.507788	-8.556114
C	12.209521	13.871050	-9.422051
C	8.138456	13.265177	-8.116820
C	10.044521	11.316012	-9.228293
O	11.592341	9.778616	-7.340084
H	13.059783	11.863463	-4.458178
H	13.053141	10.293038	-5.258350
C	11.341598	10.633006	-4.022090
O	7.976526	13.337852	-5.260951
H	9.650026	13.523557	-3.290398
H	11.397966	13.449206	-3.503507
C	10.410352	11.529701	-3.462949
C	11.228920	16.474695	-9.384175
H	9.846677	15.766029	-7.889750
C	12.772216	14.838414	-10.248619
H	12.594298	12.854305	-9.433044
H	7.293263	13.830011	-7.720790
H	8.430565	13.736008	-9.064415
C	7.725809	11.828134	-8.343753
H	10.592548	10.464265	-9.634725
H	10.049992	12.103206	-9.993666
C	8.633498	10.901440	-8.891583
C	11.303337	9.278203	-3.665398
C	9.461220	11.068081	-2.543955
C	12.285884	16.143537	-10.228642
H	10.841449	17.489204	-9.367092
H	13.593653	14.571844	-10.907183
C	6.417305	11.425458	-8.037779
C	8.227425	9.584927	-9.141689
C	10.330101	8.817795	-2.769386
O	12.292186	8.422966	-4.083909
C	9.415547	9.710227	-2.209607
O	8.656471	11.953681	-1.869868
H	12.725953	16.899035	-10.872989
C	6.032542	10.098328	-8.253796
O	5.485320	12.348611	-7.634196
C	6.933168	9.184277	-8.803386
O	9.050093	8.719246	-9.819411
S	10.303235	7.168914	-2.159748
C	11.891775	7.450557	-5.059957
S	8.345321	9.083672	-0.966045
C	7.290341	11.985343	-2.305839
S	4.387458	9.500979	-7.992563
C	5.086262	12.259361	-6.258521
S	6.299072	7.570559	-9.147722
C	9.655077	7.694032	-9.018612
C	8.885631	7.409410	-1.132136
H	11.035256	6.861575	-4.711117
H	12.748584	6.790414	-5.196688
H	11.645504	7.942120	-6.006394
H	6.777039	12.679370	-1.640074
H	7.229904	12.346750	-3.338082
H	6.822997	10.996353	-2.227036
C	4.893990	7.814025	-8.107273
H	4.309450	13.011856	-6.122426
H	5.934207	12.481777	-5.604440

H	4.672518	11.271339	-6.024741
H	10.351808	8.136894	-8.299637
H	10.198938	7.051918	-9.711924
H	8.897655	7.098002	-8.495590
C	8.272175	6.386902	-0.488812
C	4.309305	6.810766	-7.409618
S	8.813775	4.709582	-0.602788
S	6.868552	6.617838	0.559861
S	4.861235	5.135420	-7.501916
S	2.930711	7.060817	-6.332826
C	7.378081	4.045458	0.154642
C	6.501578	4.907609	0.685656
C	3.876055	4.588421	-6.162475
C	3.004167	5.455903	-5.636127
H	7.287937	2.963184	0.182017
H	5.587792	4.632571	1.205705
H	4.012385	3.566223	-5.830435
H	2.331722	5.239980	-4.814908

Energy -11105.3680503 A.U.

Table S25. Optimized cartesian coordinates (in Angstroms) of $clip_2^+$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	2.885673	-2.245920	5.121913
C	2.383216	-0.946977	5.147684
C	2.931229	0.029694	4.322362
C	3.986805	-0.284223	3.462595
C	4.492858	-1.585908	3.446744
C	3.944659	-2.561752	4.274156
H	2.456627	-3.008659	5.765118
H	1.560517	-0.692730	5.809426
H	2.534007	1.041603	4.336613
H	5.312345	-1.832932	2.776515
H	4.344622	-3.571266	4.253218
C	4.498425	0.751267	2.484779
C	3.725101	0.808767	1.078883
C	2.641715	-0.231318	0.892890
C	1.330635	0.031979	1.295971
C	2.966271	-1.500737	0.407937
C	0.359695	-0.962629	1.221712
H	1.076513	1.017179	1.678318
C	1.995433	-2.495006	0.336767
H	3.985966	-1.710128	0.094804
C	0.691461	-2.229623	0.748193
H	-0.656438	-0.746986	1.538584
H	2.259866	-3.479349	-0.038289
H	-0.065642	-3.006393	0.693706
N	4.322624	2.103275	2.987638
N	5.872201	0.500612	2.076821
N	4.810557	0.640202	0.126062
N	3.196361	2.164417	1.070830
C	3.694546	2.930962	2.096762
C	6.045668	0.616063	0.719534
O	7.124874	0.645275	0.132208
O	3.556824	4.146690	2.210957
C	2.696548	2.789884	-0.143515
C	4.648586	0.919619	-1.290675
C	6.991544	0.681205	2.991651
C	5.081485	2.613032	4.117705
H	3.689396	0.486807	-1.601480
H	5.434029	0.384858	-1.826465
H	2.056285	3.621413	0.153349
H	2.061413	2.053258	-0.650712
H	4.530696	3.458068	4.534477
H	7.836519	0.118700	2.591592
H	5.093787	1.824720	4.881138
H	6.707776	0.210436	3.941438
C	6.484265	3.042759	3.762494
C	6.876047	4.368144	3.991459
C	7.396585	2.121602	3.211108
C	8.155031	4.784198	3.611900
C	8.696409	2.535350	2.882940
C	9.060367	3.874553	3.062076
C	3.780465	3.290373	-1.070395
C	3.839128	4.651874	-1.395170
C	4.710349	2.390270	-1.629028
C	4.850915	5.115122	-2.249519
C	5.687059	2.850846	-2.518677
C	5.767230	4.220305	-2.806996

S	8.752311	6.426725	3.866128
S	4.972203	6.785836	-2.765109
S	10.672672	4.505009	2.707422
S	6.915538	4.873773	-3.954938
C	6.339750	6.523409	-3.829250
C	10.134806	6.181333	2.799136
C	6.940682	7.552570	-4.505597
C	10.687899	7.180808	2.065247
S	12.041882	6.924988	0.961436
S	10.108556	8.846301	2.134827
S	8.336581	7.316483	-5.540591
S	6.403239	9.216165	-4.374624
C	8.634523	9.014430	-5.781938
C	7.754713	9.880266	-5.246683
C	11.985064	8.537853	0.287064
C	11.112742	9.404263	0.816580
H	9.514105	9.291442	-6.358380
H	7.813602	10.962982	-5.326805
H	12.669673	8.760878	-0.522546
H	10.988124	10.432812	0.498758
O	6.475439	1.966343	-3.204352
O	2.843732	5.501406	-0.994892
O	6.060292	5.233195	4.675278
O	9.639160	1.621982	2.487190
C	5.409663	6.236618	3.881142
C	7.851075	1.903391	-2.798842
C	3.200477	6.479902	-0.006974
C	10.014975	1.670810	1.102300
H	8.348094	2.875834	-2.902101
H	8.327260	1.188995	-3.469387
H	7.923440	1.551146	-1.765615
H	2.323316	7.114325	0.115132
H	3.442693	5.990100	0.940172
H	4.044363	7.098640	-0.334335
H	4.952091	6.930202	4.586484
H	4.640167	5.779946	3.251923
H	6.130238	6.784827	3.261847
H	9.176384	1.358991	0.474802
H	10.842110	0.969985	0.991171
H	10.356986	2.671958	0.813244
H	12.875684	17.415554	-5.061847
C	13.140175	16.431249	-5.436960
C	12.169401	15.436918	-5.508158
C	14.444153	16.165975	-5.848435
C	12.494032	14.167540	-5.993166
H	11.149698	15.646230	-5.195000
C	14.775990	14.899027	-6.322027
H	15.201204	16.942796	-5.793935
C	11.410727	13.127372	-6.179170
C	13.805122	13.904353	-6.396295
H	15.792128	14.683472	-6.638946
C	10.637442	13.184788	-7.585091
N	11.939578	11.771760	-6.171081
N	10.325233	13.295861	-5.226385
H	14.059306	12.919185	-6.778684
C	11.149013	14.220290	-8.562920
N	9.263634	13.435360	-7.177180
N	10.813355	11.832786	-8.087913
C	11.441484	11.005164	-7.197017

C	12.439490	11.146384	-4.956729
C	9.090135	13.319940	-5.819892
C	10.487191	13.016450	-3.809646
C	10.642942	15.521968	-8.547038
C	12.204527	13.906385	-9.422768
C	8.144344	13.254601	-8.092040
C	10.054602	11.322921	-9.218000
O	11.579306	9.789449	-7.311235
H	13.074555	11.883094	-4.449567
H	13.079840	10.314914	-5.253578
C	11.355629	10.645799	-4.029840
O	8.010916	13.290671	-5.232597
H	9.701681	13.551127	-3.273872
H	11.446329	13.449354	-3.498808
C	10.425582	11.545790	-3.471294
C	11.191054	16.497812	-9.374508
H	9.823498	15.768980	-7.876755
C	12.752453	14.883057	-10.248149
H	12.601767	12.894483	-9.437037
H	7.299298	13.817033	-7.692030
H	8.428092	13.725357	-9.041840
C	7.739452	11.814154	-8.311463
H	10.605497	10.477925	-9.634709
H	10.042248	12.111205	-9.981462
C	8.651859	10.893069	-8.862823
C	11.297148	9.284308	-3.705010
C	9.448882	11.085100	-2.581688
C	12.249973	16.181989	-10.222353
H	10.791077	17.507320	-9.353547
H	13.575099	14.628815	-10.909958
C	6.439659	11.400296	-7.983325
C	8.260200	9.567646	-9.091791
C	10.285276	8.820920	-2.850842
O	12.292791	8.434911	-4.104945
C	9.368832	9.715625	-2.293407
O	8.660361	11.969512	-1.896057
H	12.678948	16.944727	-10.865607
C	6.075821	10.061066	-8.162460
O	5.496820	12.313568	-7.587569
C	6.981234	9.151493	-8.712276
O	9.076070	8.702679	-9.775580
S	10.164002	7.150131	-2.335502
C	11.936562	7.456386	-5.093028
S	8.220507	9.061992	-1.145572
C	7.284739	12.032308	-2.301639
S	4.463558	9.430507	-7.807797
C	5.121015	12.264625	-6.202682
S	6.384044	7.508946	-8.966581
C	9.726659	7.699200	-8.981480
C	8.796418	7.412400	-1.271357
H	11.091766	6.838427	-4.766539
H	12.813373	6.821229	-5.213810
H	11.695894	7.946102	-6.040610
H	6.808462	12.746717	-1.631173
H	7.212390	12.384465	-3.334897
H	6.787798	11.059832	-2.198325
C	5.001517	7.754214	-7.899603
H	4.293964	12.965535	-6.091459
H	5.959649	12.576283	-5.575161

H	4.778899	11.263478	-5.913750
H	10.496068	8.155831	-8.352122
H	10.184367	7.005739	-9.686857
H	9.006050	7.150848	-8.362352
C	8.195577	6.383161	-0.595063
C	4.448476	6.754661	-7.165782
S	8.733183	4.719622	-0.726134
S	6.799682	6.619068	0.439999
S	5.027877	5.089192	-7.235490
S	3.094472	7.010343	-6.061973
C	7.381830	4.055358	0.145974
C	6.501964	4.921084	0.681319
C	4.023665	4.531084	-5.917337
C	3.151338	5.397430	-5.387726
H	7.323031	2.972634	0.226017
H	5.622471	4.643912	1.257813
H	4.148336	3.502515	-5.599601
H	2.466722	5.174322	-4.578145

Energy -11105.2161268 A.U.

Table S26. Optimized cartesian coordinates (in Angstroms) of $clip_2^{2+}$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	3.283105	-2.443511	4.997355
C	2.706765	-1.181394	5.123128
C	3.136101	-0.133068	4.314678
C	4.146360	-0.340185	3.372752
C	4.724690	-1.606460	3.253631
C	4.295552	-2.653008	4.063432
H	2.946150	-3.261211	5.627649
H	1.919894	-1.011634	5.851923
H	2.680088	0.849757	4.402433
H	5.504691	-1.771362	2.514777
H	4.749989	-3.633902	3.961576
C	4.537451	0.759336	2.411099
C	3.705404	0.795385	1.037591
C	2.595415	-0.226727	0.925810
C	1.328158	0.057335	1.441084
C	2.853619	-1.496362	0.403867
C	0.335811	-0.917920	1.441672
H	1.125006	1.042782	1.852692
C	1.860680	-2.471375	0.407460
H	3.841075	-1.719810	0.008221
C	0.601497	-2.185680	0.929731
H	-0.645164	-0.687344	1.846547
H	2.072345	-3.456547	0.002561
H	-0.172117	-2.947981	0.934122
N	4.301620	2.087134	2.956656
N	5.903526	0.607766	1.936846
N	4.743936	0.598166	0.036459
N	3.195419	2.157190	1.027297
C	3.673518	2.916851	2.061889
C	6.007622	0.660279	0.573644
O	7.057116	0.715539	-0.063604
O	3.528201	4.130858	2.185746
C	2.609217	2.760004	-0.157246
C	4.514871	0.885509	-1.372144
C	7.054264	0.801503	2.803889
C	5.113873	2.628456	4.036981
H	3.541009	0.455867	-1.636199
H	5.271404	0.350255	-1.947428
H	1.977457	3.588394	0.165641
H	1.954188	2.010506	-0.618357
H	4.550731	3.440851	4.498822
H	7.899600	0.275862	2.357368
H	5.217583	1.836347	4.788577
H	6.831184	0.307765	3.758173
C	6.470959	3.134142	3.601555
C	6.802853	4.481440	3.797392
C	7.407919	2.254948	3.020193
C	8.043119	4.955169	3.348618
C	8.671680	2.721856	2.636160
C	8.970334	4.084127	2.772145
C	3.639025	3.257379	-1.144695
C	3.673042	4.616503	-1.479560
C	4.561340	2.357007	-1.718917
C	4.675430	5.084747	-2.343368
C	5.519623	2.819692	-2.628283
C	5.590041	4.192361	-2.910016

S	8.545501	6.630176	3.520092
S	4.819908	6.762252	-2.822199
S	10.509260	4.783251	2.293510
S	6.753512	4.862516	-4.028122
C	6.221195	6.513550	-3.834902
C	9.982083	6.439284	2.532638
C	6.898638	7.560984	-4.419222
C	10.618634	7.505034	1.950906
S	12.034276	7.323065	0.928739
S	10.057553	9.158703	2.135993
S	8.346225	7.323910	-5.373007
S	6.425445	9.231638	-4.210569
C	8.680901	9.015445	-5.571520
C	7.803512	9.888456	-5.036663
C	12.084230	8.994910	0.445672
C	11.188065	9.827793	0.995878
H	9.581301	9.284156	-6.120910
H	7.885810	10.972475	-5.089934
H	12.845847	9.284912	-0.267931
H	11.116160	10.888520	0.788000
O	6.299662	1.947662	-3.333454
O	2.676321	5.457472	-1.071736
O	5.985921	5.312683	4.513958
O	9.642921	1.848004	2.229695
C	5.254313	6.296750	3.764223
C	7.689651	1.887582	-2.970376
C	3.020805	6.428167	-0.070497
C	9.955765	1.848640	0.828206
H	8.157749	2.879787	-2.988087
H	8.166588	1.260960	-3.722717
H	7.797850	1.439682	-1.980031
H	2.150788	7.075674	0.028827
H	3.229996	5.932084	0.881237
H	3.880680	7.036787	-0.375699
H	4.843134	6.989209	4.497991
H	4.450180	5.818120	3.200933
H	5.909683	6.853260	3.082857
H	9.091878	1.512290	0.248657
H	10.778883	1.145593	0.706477
H	10.283316	2.838247	0.487792
H	12.963739	17.424872	-5.228112
C	13.223950	16.421865	-5.553052
C	12.244030	15.435012	-5.595911
C	14.532901	16.124316	-5.925641
C	12.564683	14.141521	-6.015505
H	11.221677	15.666341	-5.307488
C	14.859327	14.834574	-6.336948
H	15.297441	16.894889	-5.890444
C	11.474858	13.101854	-6.156569
C	13.879048	13.847588	-6.385257
H	15.878657	14.594579	-6.624136
C	10.675158	13.117175	-7.549898
N	11.999033	11.745090	-6.114245
N	10.406012	13.298689	-5.187876
H	14.129552	12.844252	-6.719533
C	11.158299	14.128257	-8.565677
N	9.306007	13.362083	-7.122708
N	10.853073	11.752286	-8.020340
C	11.481930	10.950128	-7.107272

C	12.525845	11.159398	-4.891766
C	9.160668	13.286859	-5.760123
C	10.596771	13.063838	-3.765750
C	10.589976	15.401850	-8.634361
C	12.245803	13.816929	-9.386270
C	8.169412	13.143153	-8.007290
C	10.072146	11.201562	-9.116209
O	11.600127	9.729202	-7.180164
H	13.166324	11.912848	-4.417856
H	13.164902	10.321431	-5.172467
C	11.458769	10.685248	-3.932959
O	8.091062	13.257358	-5.154963
H	9.824506	13.616448	-3.228995
H	11.562515	13.504126	-3.488633
C	10.539919	11.603241	-3.381726
C	11.105707	16.352937	-9.510862
H	9.746681	15.646942	-7.993990
C	12.765471	14.771038	-10.254557
H	12.689284	12.825607	-9.336283
H	7.328030	13.712074	-7.608934
H	8.427822	13.582004	-8.978879
C	7.774248	11.691778	-8.166982
H	10.623629	10.353224	-9.524859
H	10.027336	11.967887	-9.900014
C	8.684544	10.762284	-8.709997
C	11.397207	9.329484	-3.586544
C	9.569896	11.168092	-2.472073
C	12.197678	16.041805	-10.317286
H	10.654899	17.339684	-9.559871
H	13.614712	14.520703	-10.883196
C	6.490517	11.277705	-7.784520
C	8.308293	9.423556	-8.878411
C	10.381941	8.889488	-2.723300
O	12.380861	8.466063	-3.976946
C	9.477388	9.801358	-2.171184
O	8.795710	12.062945	-1.788457
H	12.602639	16.785932	-10.996634
C	6.146226	9.922813	-7.891055
O	5.544249	12.193146	-7.413230
C	7.047385	9.004820	-8.434974
O	9.107017	8.548408	-9.563405
S	10.215782	7.222798	-2.218104
C	12.024444	7.471357	-4.951237
S	8.296324	9.161917	-1.052553
C	7.416187	12.147149	-2.183237
S	4.578842	9.286748	-7.413509
C	5.187684	12.223131	-6.022032
S	6.489683	7.343393	-8.570953
C	9.812610	7.575411	-8.775745
C	8.808409	7.501807	-1.223432
H	11.145959	6.893547	-4.639797
H	12.879804	6.800410	-5.016567
H	11.839706	7.942148	-5.919703
H	6.940169	12.811043	-1.463072
H	7.339221	12.565328	-3.190263
H	6.923171	11.167506	-2.141909
C	5.056619	7.608811	-7.595462
H	4.348319	12.913196	-5.944827
H	6.027620	12.588308	-5.426604

H	4.867317	11.237436	-5.663893
H	10.592806	8.062642	-8.185423
H	10.256975	6.879994	-9.486925
H	9.132425	7.020406	-8.117951
C	8.121559	6.462670	-0.635874
C	4.383448	6.584765	-6.982520
S	8.583943	4.790178	-0.853483
S	6.683855	6.705703	0.329773
S	4.876417	4.906005	-7.128816
S	2.983444	6.850451	-5.956025
C	7.210489	4.139538	-0.016575
C	6.341240	5.015188	0.527185
C	3.747365	4.317409	-5.941684
C	2.887467	5.199058	-5.410282
H	7.127266	3.055900	0.031411
H	5.444138	4.746373	1.081965
H	3.786190	3.263015	-5.696448
H	2.129117	4.962278	-4.673863

Energy -11105.0526623 A.U.

Table S27. Optimized cartesian coordinates (in Angstroms) of $clip_2^{3+}$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	3.396049	-2.387432	4.968147
C	2.822998	-1.125958	5.112564
C	3.228898	-0.075852	4.294355
C	4.213203	-0.280817	3.324804
C	4.790638	-1.545991	3.188861
C	4.383425	-2.594475	4.006993
H	3.076097	-3.206891	5.604876
H	2.056094	-0.958130	5.862622
H	2.773671	0.905920	4.396208
H	5.551181	-1.709441	2.429691
H	4.835610	-3.574767	3.891229
C	4.570830	0.816026	2.347848
C	3.714074	0.830270	0.988887
C	2.610772	-0.201448	0.907194
C	1.355625	0.071792	1.457009
C	2.868036	-1.470620	0.383516
C	0.376430	-0.915785	1.494714
H	1.152480	1.057384	1.868300
C	1.887696	-2.457356	0.422935
H	3.846025	-1.685584	-0.039306
C	0.642282	-2.183818	0.983419
H	-0.594655	-0.694573	1.927481
H	2.098793	-3.442207	0.017118
H	-0.120997	-2.955584	1.017838
N	4.329577	2.146228	2.886015
N	5.929898	0.679997	1.849226
N	4.736215	0.632915	-0.028774
N	3.194771	2.188755	0.971775
C	3.674693	2.960624	1.995792
C	6.008220	0.716264	0.483898
O	7.045965	0.779717	-0.171794
O	3.515419	4.173754	2.114844
C	2.573807	2.768343	-0.207117
C	4.474692	0.892522	-1.436842
C	7.094046	0.889515	2.692387
C	5.153721	2.703492	3.948672
H	3.500831	0.447125	-1.673188
H	5.225068	0.356916	-2.019767
H	1.942467	3.596268	0.117952
H	1.913609	2.006552	-0.640044
H	4.590743	3.511537	4.418142
H	7.936578	0.370525	2.233379
H	5.282274	1.917674	4.702879
H	6.896508	0.401380	3.654994
C	6.498874	3.221999	3.486698
C	6.818975	4.572674	3.673918
C	7.435729	2.348910	2.892292
C	8.045817	5.056117	3.192768
C	8.688287	2.822679	2.482640
C	8.971444	4.192025	2.601475
C	3.573208	3.258526	-1.230583
C	3.583451	4.612344	-1.588250
C	4.494835	2.358739	-1.809552
C	4.571733	5.077660	-2.470016
C	5.433694	2.816504	-2.742267
C	5.488597	4.187294	-3.037149

S	8.523301	6.735434	3.321976
S	4.721482	6.757092	-2.942169
S	10.477358	4.908911	2.068811
S	6.655745	4.865882	-4.146900
C	6.157653	6.516052	-3.899909
C	9.987059	6.548562	2.395408
C	6.901978	7.571862	-4.387170
C	10.705245	7.642491	1.934060
S	12.170150	7.489060	1.002915
S	10.190087	9.282497	2.218449
S	8.393468	7.335614	-5.263506
S	6.472376	9.238838	-4.103908
C	8.744940	9.024802	-5.433761
C	7.865170	9.897704	-4.899856
C	12.391907	9.189560	0.775959
C	11.487002	10.012140	1.337998
H	9.657698	9.288202	-5.965431
H	7.952087	10.982338	-4.935259
H	13.250306	9.508677	0.198616
H	11.506748	11.093010	1.279417
O	6.216792	1.946919	-3.444039
O	2.592198	5.453437	-1.172049
O	6.018725	5.396000	4.412354
O	9.661850	1.956958	2.075068
C	5.225447	6.354704	3.690996
C	7.611704	1.900080	-3.094377
C	2.943259	6.419562	-0.167413
C	9.957995	1.929236	0.669279
H	8.065758	2.899028	-3.097952
H	8.090559	1.295505	-3.863045
H	7.735365	1.437017	-2.113422
H	2.077771	7.072622	-0.066815
H	3.149435	5.919204	0.782589
H	3.806722	7.023520	-0.472190
H	4.810015	7.023497	4.443415
H	4.425140	5.848425	3.147087
H	5.836357	6.943669	2.995586
H	9.083210	1.593472	0.106050
H	10.770116	1.213355	0.552367
H	10.295576	2.907389	0.306297
H	12.966725	17.401649	-5.305560
C	13.222610	16.392041	-5.612675
C	12.242537	15.404579	-5.620502
C	14.526292	16.086588	-5.996874
C	12.557646	14.102882	-6.018485
H	11.224072	15.642978	-5.324019
C	14.847506	14.788529	-6.385427
H	15.290890	16.857845	-5.989316
C	11.466441	13.060811	-6.125848
C	13.866919	13.800999	-6.400053
H	15.862747	14.542616	-6.681793
C	10.647195	13.048210	-7.507993
N	11.991618	11.705422	-6.063222
N	10.410914	13.270837	-5.145034
H	14.113134	12.791663	-6.719113
C	11.106789	14.046694	-8.546173
N	9.282090	13.286968	-7.064499
N	10.829196	11.677026	-7.958597
C	11.471399	10.893107	-7.038740

C	12.554045	11.152108	-4.842063
C	9.157668	13.244335	-5.698368
C	10.628756	13.073588	-3.721262
C	10.526406	15.314151	-8.626597
C	12.187944	13.732169	-9.373955
C	8.136185	13.045903	-7.929576
C	10.040040	11.101845	-9.034823
O	11.590922	9.670979	-7.095007
H	13.204160	11.919300	-4.404540
H	13.190009	10.310325	-5.118373
C	11.516208	10.697821	-3.841687
O	8.096278	13.223826	-5.077882
H	9.859736	13.630144	-3.183987
H	11.593599	13.532380	-3.472063
C	10.598758	11.622065	-3.295972
C	11.026283	16.257551	-9.520400
H	9.687517	15.561318	-7.981167
C	12.691787	14.679032	-10.259267
H	12.639871	12.745157	-9.314991
H	7.294513	13.613272	-7.530043
H	8.376146	13.469512	-8.912371
C	7.751414	11.587850	-8.059764
H	10.593755	10.252929	-9.438865
H	9.973188	11.854510	-9.830029
C	8.662678	10.655276	-8.599353
C	11.476745	9.350884	-3.459050
C	9.650685	11.201533	-2.355730
C	12.113734	15.944615	-10.332171
H	10.567188	17.239891	-9.578222
H	13.537047	14.427352	-10.892650
C	6.476285	11.174457	-7.652006
C	8.300132	9.309624	-8.736674
C	10.475489	8.922955	-2.574113
O	12.456314	8.483070	-3.845886
C	9.573773	9.840210	-2.025590
O	8.873385	12.101717	-1.685186
H	12.507260	16.683372	-11.023865
C	6.146553	9.811129	-7.721623
O	5.525654	12.087320	-7.297874
C	7.049034	8.889635	-8.259764
O	9.088690	8.432920	-9.424606
S	10.302567	7.259124	-2.060413
C	12.096932	7.483483	-4.815530
S	8.392875	9.205105	-0.902799
C	7.491287	12.172233	-2.076181
S	4.608119	9.168490	-7.186566
C	5.184145	12.167787	-5.903951
S	6.513432	7.223797	-8.330070
C	9.827869	7.472175	-8.650653
C	8.862986	7.541030	-1.120012
H	11.210668	6.917274	-4.504140
H	12.945549	6.803244	-4.868233
H	11.923374	7.948695	-5.788532
H	7.012180	12.835622	-1.357901
H	7.406925	12.583854	-3.085307
H	7.007344	11.188462	-2.026005
C	5.044998	7.500549	-7.434954
H	4.344216	12.858297	-5.844615
H	6.030172	12.555863	-5.331984

H	4.868829	11.195692	-5.505766
H	10.619839	7.970826	-8.086827
H	10.256649	6.777413	-9.371321
H	9.175082	6.913823	-7.968560
C	8.105093	6.496907	-0.629161
C	4.285208	6.455475	-6.928681
S	8.507263	4.827246	-0.941054
S	6.627636	6.742384	0.266274
S	4.729154	4.785080	-7.151763
S	2.837985	6.707849	-5.991534
C	7.118077	4.177815	-0.133989
C	6.254476	5.055129	0.418397
C	3.421389	4.147604	-6.216829
C	2.555237	5.029283	-5.683706
H	7.022790	3.094072	-0.112876
H	5.345480	4.791374	0.956714
H	3.362706	3.072308	-6.105357
H	1.696079	4.769524	-5.078287

Energy -11104.8762874 A.U.

Table S28. Optimized cartesian coordinates (in Angstroms) of $clip_2^{4+}$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	3.444185	-2.343738	4.990351
C	2.881164	-1.078562	5.141306
C	3.274272	-0.034501	4.309434
C	4.235643	-0.249725	3.319089
C	4.804886	-1.518064	3.177957
C	4.409933	-2.560391	4.009605
H	3.133802	-3.158491	5.637739
H	2.132089	-0.903056	5.907411
H	2.827289	0.950328	4.417790
H	5.548398	-1.689231	2.403710
H	4.855189	-3.543261	3.889479
C	4.574826	0.839202	2.327880
C	3.693610	0.852566	0.984786
C	2.580813	-0.168546	0.932990
C	1.341099	0.120961	1.508828
C	2.818016	-1.445739	0.419631
C	0.357274	-0.859695	1.583927
H	1.155135	1.112633	1.913583
C	1.832636	-2.425248	0.495836
H	3.784911	-1.673479	-0.021832
C	0.603066	-2.135996	1.083150
H	-0.601300	-0.626676	2.037848
H	2.027621	-3.416796	0.098598
H	-0.163334	-2.902556	1.147768
N	4.350239	2.173985	2.861652
N	5.925009	0.699189	1.803390
N	4.696646	0.645082	-0.050328
N	3.190440	2.218460	0.964665
C	3.711114	2.994934	1.965153
C	5.976592	0.750224	0.437271
O	6.999663	0.842792	-0.238009
O	3.601275	4.215403	2.065703
C	2.540958	2.786318	-0.203470
C	4.405144	0.878744	-1.456032
C	7.106003	0.907244	2.622188
C	5.201255	2.730180	3.902159
H	3.427938	0.426245	-1.663753
H	5.143429	0.334301	-2.046258
H	1.924301	3.623655	0.126213
H	1.860869	2.024072	-0.603898
H	4.652653	3.536102	4.389631
H	7.937844	0.382564	2.150513
H	5.355948	1.942462	4.648801
H	6.927035	0.427753	3.592380
C	6.530167	3.249868	3.398222
C	6.834376	4.609945	3.541346
C	7.455273	2.367067	2.799944
C	8.056282	5.085603	3.030753
C	8.695934	2.832241	2.351501
C	8.974748	4.204766	2.445101
C	3.506371	3.250092	-1.271259
C	3.495504	4.592717	-1.667282
C	4.409734	2.336651	-1.861619
C	4.454695	5.035943	-2.589914
C	5.310118	2.769943	-2.843303
C	5.351794	4.133879	-3.170175

S	8.546334	6.759844	3.101293
S	4.606136	6.708563	-3.079643
S	10.469053	4.902412	1.876328
S	6.501500	4.799505	-4.305723
C	6.063514	6.453253	-3.994657
C	10.032175	6.535811	2.243173
C	6.880931	7.505449	-4.383530
C	10.841293	7.619390	1.871143
S	12.323326	7.417839	0.999450
S	10.426166	9.260839	2.230692
S	8.392523	7.253878	-5.209328
S	6.509366	9.166158	-4.024792
C	8.798880	8.932405	-5.315127
C	7.932390	9.813788	-4.767646
C	12.705231	9.094611	0.935185
C	11.829263	9.947142	1.508109
H	9.728028	9.186768	-5.824279
H	8.047188	10.897383	-4.766050
H	13.621013	9.381866	0.434003
H	11.935173	11.024002	1.539038
O	6.072461	1.890934	-3.553256
O	2.523270	5.450438	-1.243973
O	6.019387	5.419516	4.270569
O	9.661441	1.963434	1.940843
C	5.313936	6.465876	3.585055
C	7.472666	1.824815	-3.222801
C	2.898154	6.400245	-0.231174
C	9.945421	1.914459	0.531829
H	7.934301	2.820614	-3.216344
H	7.935452	1.231351	-4.009418
H	7.605561	1.345106	-2.251487
H	2.047041	7.070232	-0.121006
H	3.098993	5.885718	0.712271
H	3.771590	6.989811	-0.537736
H	4.720953	6.965519	4.348878
H	4.652949	6.044860	2.823904
H	5.993946	7.200702	3.139336
H	9.057607	1.597039	-0.020543
H	10.737881	1.177116	0.417321
H	10.307626	2.878999	0.156169
H	12.986825	17.422820	-5.414882
C	13.233494	16.406415	-5.706345
C	12.254845	15.418779	-5.658384
C	14.523915	16.092548	-6.126725
C	12.557805	14.109103	-6.038947
H	11.245617	15.664486	-5.336939
C	14.833555	14.786131	-6.496197
H	15.287014	16.864254	-6.164731
C	11.462557	13.069083	-6.101282
C	13.854048	13.798354	-6.456569
H	15.838314	14.534081	-6.821775
C	10.605220	13.044575	-7.460535
N	11.985137	11.712497	-6.038938
N	10.434083	13.284189	-5.092572
H	14.090186	12.783342	-6.765210
C	11.019833	14.042930	-8.516575
N	9.250589	13.266742	-6.977785
N	10.788034	11.672856	-7.911191
C	11.444784	10.894145	-6.996774

C	12.594852	11.173676	-4.835135
C	9.166260	13.220033	-5.608916
C	10.693739	13.099225	-3.674543
C	10.421288	15.302825	-8.585191
C	12.076743	13.735843	-9.377643
C	8.084659	13.016990	-7.810704
C	9.977632	11.091719	-8.966745
O	11.557415	9.670673	-7.044471
H	13.258465	11.947213	-4.429837
H	13.224449	10.331616	-5.125410
C	11.599404	10.727588	-3.788281
O	8.124760	13.164618	-4.957948
H	9.937956	13.655915	-3.119051
H	11.662520	13.565819	-3.457554
C	10.688122	11.652550	-3.229018
C	10.881241	16.246596	-9.499750
H	9.601069	15.544678	-7.914144
C	12.539812	14.682792	-10.284826
H	12.542063	12.754662	-9.326344
H	7.248212	13.575798	-7.389281
H	8.291819	13.440307	-8.800916
C	7.711817	11.555262	-7.928301
H	10.527612	10.250262	-9.390835
H	9.878942	11.845655	-9.757122
C	8.618125	10.630557	-8.492678
C	11.594140	9.389645	-3.375407
C	9.775385	11.240677	-2.249862
C	11.944957	15.941242	-10.345109
H	10.409265	17.223311	-9.547868
H	13.366256	14.436965	-10.944792
C	6.452211	11.134885	-7.483997
C	8.268131	9.281744	-8.620754
C	10.622982	8.968355	-2.454852
O	12.565826	8.520254	-3.773845
C	9.725450	9.883809	-1.896343
O	9.003978	12.137593	-1.571752
H	12.307002	16.680532	-11.053216
C	6.135046	9.767034	-7.544874
O	5.505478	12.039767	-7.111257
C	7.032266	8.853644	-8.109250
O	9.037377	8.414400	-9.336016
S	10.463359	7.307288	-1.931790
C	12.192225	7.526917	-4.745786
S	8.561512	9.242229	-0.759745
C	7.613196	12.201058	-1.936657
S	4.624685	9.108325	-6.971105
C	5.189429	12.124137	-5.711019
S	6.513554	7.188919	-8.158598
C	9.826526	7.463478	-8.598447
C	8.996398	7.581991	-1.039539
H	11.303283	6.967741	-4.428511
H	13.033707	6.838686	-4.805098
H	12.016704	7.997071	-5.715925
H	7.144843	12.858382	-1.206187
H	7.507622	12.614154	-2.942294
H	7.134674	11.214859	-1.879624
C	5.032806	7.459140	-7.303749
H	4.385179	12.853594	-5.634182
H	6.061673	12.467308	-5.150532

H	4.832174	11.166030	-5.314629
H	10.615068	7.976592	-8.043751
H	10.257758	6.797889	-9.344149
H	9.209660	6.868944	-7.913328
C	8.176807	6.531369	-0.650821
C	4.205121	6.397926	-6.907696
S	8.540898	4.875835	-1.043484
S	6.678320	6.770830	0.200774
S	4.592027	4.743745	-7.240354
S	2.734496	6.638335	-6.026318
C	7.123987	4.218818	-0.300538
C	6.265049	5.091857	0.271694
C	3.190380	4.091519	-6.484652
C	2.332095	4.968181	-5.921448
H	7.003847	3.136779	-0.329931
H	5.341563	4.825660	0.785368
H	3.071277	3.015562	-6.488705
H	1.418746	4.703670	-5.403579

Energy -11104.6877775 A.U.

Table S29. Optimized cartesian coordinates (in Angstroms) of $clip_2^{6+}$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	3.397485	-2.484969	5.012042
C	2.817697	-1.228034	5.170889
C	3.220718	-0.166212	4.366925
C	4.209193	-0.355979	3.397817
C	4.792599	-1.616872	3.246081
C	4.387878	-2.676655	4.050755
H	3.078502	-3.315629	5.638528
H	2.046121	-1.072781	5.922183
H	2.757977	0.813481	4.479449
H	5.554722	-1.769667	2.482920
H	4.844666	-3.655861	3.923227
C	4.555776	0.751862	2.434339
C	3.689838	0.788677	1.081814
C	2.577966	-0.229088	0.992176
C	1.325794	0.053407	1.544748
C	2.824347	-1.497426	0.460520
C	0.336814	-0.924457	1.574253
H	1.131943	1.039353	1.965755
C	1.834345	-2.474416	0.493065
H	3.802123	-1.720866	0.035360
C	0.591085	-2.191409	1.054167
H	-0.634259	-0.696380	2.009085
H	2.036264	-3.460685	0.080172
H	-0.181290	-2.957550	1.083124
N	4.324270	2.078646	2.987314
N	5.914725	0.634753	1.920358
N	4.707861	0.606002	0.055196
N	3.191604	2.158238	1.077875
C	3.738701	2.921706	2.073411
C	5.976911	0.744668	0.558282
O	7.001423	0.912103	-0.101235
O	3.691014	4.146963	2.157125
C	2.566405	2.746918	-0.092444
C	4.425684	0.847645	-1.349999
C	7.082943	0.829047	2.757167
C	5.146893	2.608352	4.060272
H	3.442706	0.406005	-1.562104
H	5.159878	0.297321	-1.943046
H	1.944227	3.581460	0.238606
H	1.892253	1.990634	-0.517896
H	4.583823	3.397317	4.563343
H	7.925893	0.311298	2.292944
H	5.292238	1.799118	4.788485
H	6.889553	0.329654	3.716764
C	6.483087	3.148186	3.600793
C	6.785590	4.495412	3.828187
C	7.425691	2.285404	2.980306
C	8.020090	4.984426	3.362183
C	8.680961	2.758922	2.586839
C	8.956406	4.126813	2.752820
C	3.553618	3.223375	-1.133815
C	3.566251	4.577386	-1.490550
C	4.450424	2.309775	-1.734804
C	4.546144	5.024048	-2.391536
C	5.375985	2.745563	-2.690647
C	5.443328	4.118509	-2.978582

S	8.518350	6.631410	3.536050
S	4.734260	6.695008	-2.848810
S	10.455336	4.855716	2.286065
S	6.621280	4.798462	-4.066758
C	6.155890	6.440251	-3.797804
C	10.018277	6.446923	2.736191
C	6.911863	7.506497	-4.300984
C	10.811870	7.580183	2.373549
S	12.253533	7.443219	1.464027
S	10.329400	9.181372	2.733174
S	8.358421	7.264739	-5.231507
S	6.467726	9.167148	-4.056974
C	8.685452	8.943419	-5.463373
C	7.811704	9.824036	-4.918187
C	12.536693	9.119391	1.337584
C	11.632854	9.937252	1.936023
H	9.581504	9.211453	-6.030633
H	7.898690	10.913246	-4.973588
H	13.416974	9.447344	0.793698
H	11.677004	11.021604	1.944857
O	6.112876	1.861862	-3.413848
O	2.594297	5.424195	-1.059640
O	5.985832	5.276640	4.592246
O	9.659472	1.920387	2.162690
C	5.237683	6.329388	3.955085
C	7.514705	1.741992	-3.111187
C	2.951028	6.391683	-0.058859
C	9.955921	1.911117	0.754759
H	8.039926	2.699236	-3.234897
H	7.907383	1.032677	-3.839890
H	7.648586	1.358704	-2.096224
H	2.060189	7.003154	0.086369
H	3.218065	5.886946	0.875193
H	3.770284	7.040796	-0.396568
H	4.723144	6.844028	4.766227
H	4.515017	5.904160	3.253969
H	5.894998	7.046703	3.445423
H	9.093894	1.540515	0.192298
H	10.801446	1.233023	0.639689
H	10.253617	2.907595	0.398520
H	13.004513	17.456804	-5.392317
C	13.257263	16.443734	-5.698483
C	12.273308	15.460522	-5.706454
C	14.560264	16.131995	-6.080666
C	12.584377	14.157313	-6.103505
H	11.252911	15.705253	-5.412977
C	14.876844	14.832685	-6.469381
H	15.329534	16.901795	-6.073121
C	11.489608	13.123023	-6.211663
C	13.892329	13.849251	-6.485559
H	15.893295	14.582139	-6.765888
C	10.652892	13.123277	-7.585413
N	12.002764	11.760232	-6.162534
N	10.441540	13.315941	-5.216078
H	14.135881	12.837987	-6.808618
C	11.089121	14.133664	-8.617720
N	9.289696	13.334239	-7.117886
N	10.830768	11.754278	-8.047955
C	11.424681	10.955084	-7.108784

C	12.582634	11.200047	-4.954627
C	9.185920	13.225582	-5.754206
C	10.681774	13.116043	-3.797762
C	10.493916	15.395660	-8.681778
C	12.170874	13.838611	-9.452199
C	8.136138	13.108590	-7.970629
C	10.038331	11.192072	-9.123295
O	11.452794	9.726405	-7.127813
H	13.234461	11.968914	-4.518628
H	13.222599	10.362841	-5.242211
C	11.557755	10.737346	-3.945523
O	8.136964	13.094348	-5.126188
H	9.928564	13.679269	-3.241780
H	11.656161	13.567966	-3.567137
C	10.650373	11.663224	-3.378254
C	10.980044	16.352945	-9.568095
H	9.656171	15.630877	-8.026573
C	12.660194	14.799482	-10.330013
H	12.637176	12.855219	-9.402858
H	7.296936	13.675906	-7.561233
H	8.365942	13.541002	-8.954122
C	7.750503	11.651708	-8.120050
H	10.593649	10.356851	-9.556950
H	9.950220	11.960024	-9.904171
C	8.669105	10.726437	-8.683184
C	11.526536	9.386611	-3.576798
C	9.712562	11.248003	-2.426042
C	12.067289	16.059138	-10.387573
H	10.510282	17.333375	-9.613329
H	13.507743	14.563091	-10.970006
C	6.471661	11.240399	-7.728702
C	8.317271	9.385391	-8.862260
C	10.532452	8.962040	-2.680163
O	12.498992	8.524912	-3.973812
C	9.640951	9.882502	-2.109152
O	8.960349	12.137729	-1.725238
H	12.451607	16.810955	-11.074079
C	6.142422	9.878221	-7.854533
O	5.524897	12.131114	-7.343511
C	7.054605	8.963957	-8.410643
O	9.096990	8.520541	-9.557530
S	10.326793	7.302438	-2.200266
C	12.153572	7.512646	-4.935918
S	8.460831	9.230823	-1.006531
C	7.576623	12.275653	-2.095317
S	4.611558	9.217852	-7.388507
C	5.192017	12.179352	-5.943875
S	6.509334	7.323612	-8.522623
C	9.843707	7.544804	-8.805631
C	8.905807	7.582081	-1.259615
H	11.286676	6.921119	-4.611546
H	13.021892	6.855793	-4.988968
H	11.959530	7.969671	-5.909938
H	7.128649	12.901398	-1.323219
H	7.494437	12.752550	-3.075788
H	7.063735	11.302829	-2.103632
C	5.002984	7.593508	-7.758552
H	4.374241	12.895338	-5.863675
H	6.056231	12.518329	-5.366405

H	4.843320	11.204240	-5.575118
H	10.672282	8.028967	-8.281363
H	10.211341	6.826449	-9.538346
H	9.200377	7.020036	-8.084326
C	8.142158	6.517329	-0.761347
C	4.153647	6.512707	-7.364084
S	8.589059	4.861937	-1.028564
S	6.692073	6.741634	0.165581
S	4.575371	4.875644	-7.625907
S	2.688251	6.758073	-6.517377
C	7.248684	4.188180	-0.179521
C	6.371360	5.059606	0.374646
C	3.213921	4.218389	-6.838165
C	2.324963	5.104340	-6.319319
H	7.169337	3.097762	-0.136660
H	5.473977	4.775966	0.930349
H	3.122414	3.138002	-6.792067
H	1.413032	4.842323	-5.792011

Energy -11104.2491392 A.U.

Table S30. Optimized cartesian coordinates (in Angstroms) of $clip_2^{8+}$ in acetonitrile at M06L/6-31G(d,p) level. PCM solvation model was used.

C	2.937131	-2.008283	5.453614
C	2.500539	-0.685659	5.471729
C	3.138722	0.270285	4.688530
C	4.220595	-0.090638	3.881129
C	4.656735	-1.417801	3.867023
C	4.016430	-2.371838	4.651866
H	2.437059	-2.754713	6.063323
H	1.659095	-0.396777	6.093679
H	2.787862	1.299422	4.694564
H	5.488300	-1.704704	3.228038
H	4.360716	-3.401214	4.634037
C	4.829945	0.924595	2.943696
C	4.124724	1.055149	1.520426
C	3.044932	0.038228	1.234043
C	1.716911	0.300961	1.579656
C	3.385656	-1.213317	0.712947
C	0.742731	-0.678066	1.408705
H	1.450783	1.269731	1.994952
C	2.410416	-2.191175	0.546491
H	4.418455	-1.427500	0.449079
C	1.088229	-1.926375	0.896421
H	-0.286386	-0.465143	1.680662
H	2.685754	-3.161815	0.145566
H	0.328309	-2.690882	0.767722
N	4.737104	2.283058	3.449698
N	6.205954	0.614091	2.586816
N	5.254840	0.941439	0.611990
N	3.630162	2.424164	1.534436
C	4.176950	3.163078	2.561005
C	6.460239	0.826528	1.251087
O	7.571639	0.870810	0.725416
O	4.148545	4.385574	2.675251
C	3.096889	3.038962	0.336147
C	5.095118	1.132775	-0.810403
C	7.259346	0.603400	3.578893
C	5.377845	2.679729	4.679451
H	4.158984	0.639387	-1.106254
H	5.896498	0.601317	-1.324402
H	2.483292	3.888619	0.637058
H	2.416204	2.310616	-0.124238
H	4.871403	3.570106	5.054084
H	8.094265	0.028904	3.175975
H	5.197970	1.887075	5.419170
H	6.885421	0.038068	4.442784
C	6.867344	2.929408	4.595813
C	7.361230	4.094373	5.187387
C	7.758628	1.949113	4.066875
C	8.748588	4.271713	5.270685
C	9.141454	2.146328	4.135612
C	9.627844	3.308100	4.752499
C	4.105320	3.487618	-0.702043
C	3.997970	4.789762	-1.200210
C	5.051904	2.575627	-1.255386
C	4.879800	5.195635	-2.213664
C	5.889277	2.968244	-2.299779
C	5.818511	4.294320	-2.748018

S	9.475621	5.578697	6.126641
S	4.877512	6.774453	-2.909232
S	11.305879	3.597097	5.021435
S	6.826400	4.904751	-4.000457
C	6.148713	6.471662	-4.011715
C	11.078220	5.046487	5.890286
C	6.650085	7.487532	-4.897056
C	12.193833	5.780016	6.430123
S	13.719541	5.063547	6.689232
S	12.074557	7.421573	6.873111
S	7.949779	7.199374	-5.968375
S	6.013334	9.070038	-4.945470
C	8.049812	8.795114	-6.560272
C	7.134014	9.677993	-6.078162
C	14.459653	6.459900	7.319015
C	13.679645	7.570275	7.416484
H	8.851875	9.023447	-7.261679
H	7.076255	10.739142	-6.316523
H	15.498955	6.396844	7.617222
H	14.002301	8.530078	7.801009
O	6.677551	2.110099	-2.996796
O	3.011615	5.641354	-0.819842
O	6.574477	5.006395	5.816599
O	10.055359	1.208680	3.770541
C	6.025598	6.040289	4.970629
C	7.980322	1.806850	-2.454727
C	3.338211	6.541817	0.261145
C	10.436868	1.213868	2.377565
H	8.649457	2.667615	-2.560105
H	8.361506	0.985616	-3.058528
H	7.911243	1.498602	-1.407159
H	2.416013	7.073370	0.487443
H	3.676550	5.979079	1.135839
H	4.100530	7.265045	-0.052246
H	5.439230	6.677112	5.629664
H	5.381139	5.607387	4.198130
H	6.827667	6.627256	4.510586
H	9.577795	0.978176	1.742019
H	11.196592	0.441380	2.279489
H	10.863219	2.183351	2.095135
H	12.253703	17.139990	-5.000781
C	12.555506	16.189621	-5.430161
C	11.603939	15.197525	-5.642951
C	13.887490	15.965192	-5.770973
C	11.978360	13.971966	-6.201445
H	10.562941	15.380432	-5.387825
C	14.266638	14.742472	-6.320112
H	14.629013	16.741068	-5.607405
C	10.925756	12.940397	-6.533863
C	13.316569	13.749254	-6.536470
H	15.303628	14.560772	-6.585014
C	10.242319	13.089070	-7.966312
N	11.454400	11.584500	-6.575464
N	9.778086	13.005015	-5.641462
H	13.610586	12.800530	-6.978616
C	10.830455	14.156413	-8.858686
N	8.849710	13.333425	-7.627471
N	10.394725	11.751080	-8.513675
C	10.957566	10.861456	-7.637531

C	11.988783	10.958494	-5.384441
C	8.579179	13.069647	-6.303058
C	9.914018	12.774568	-4.221705
C	10.355975	15.469056	-8.797016
C	11.928716	13.859117	-9.669927
C	7.822599	13.337086	-8.646535
C	9.801000	11.369109	-9.771691
O	11.028473	9.643769	-7.788417
H	12.637617	11.697168	-4.895708
H	12.636349	10.137572	-5.694035
C	10.977616	10.454565	-4.375307
O	7.463015	12.946856	-5.802698
H	9.083321	13.263219	-3.711502
H	10.824831	13.291441	-3.889830
C	9.995933	11.322331	-3.812699
C	10.976304	16.471713	-9.536053
H	9.511577	15.707547	-8.154925
C	12.545227	14.863028	-10.409579
H	12.310909	12.842060	-9.712490
H	6.957502	13.869607	-8.250152
H	8.199450	13.943752	-9.480758
C	7.384454	11.992617	-9.195100
H	10.350486	10.510482	-10.159325
H	9.969677	12.190659	-10.481589
C	8.321280	11.062307	-9.734307
C	11.116344	9.145487	-3.907244
C	9.157732	10.880718	-2.786101
C	12.071870	16.171173	-10.341989
H	10.602877	17.489534	-9.479508
H	13.398985	14.622210	-11.035160
C	6.011787	11.750249	-9.302988
C	7.883444	9.898598	-10.370977
C	10.232170	8.690952	-2.917844
O	12.142917	8.333253	-4.265689
C	9.260978	9.546843	-2.367480
O	8.338145	11.703317	-2.082468
H	12.556077	16.955470	-10.915759
C	5.581589	10.589171	-9.961120
O	5.055813	12.641082	-8.931010
C	6.505667	9.674528	-10.489919
O	8.716986	9.031126	-11.004159
S	10.293929	7.097699	-2.267912
C	11.942246	7.503643	-5.432155
S	8.268007	8.861233	-1.135754
C	7.022810	11.941574	-2.626061
S	3.922553	10.267825	-10.299670
C	4.664054	12.588375	-7.540823
S	5.839476	8.344892	-11.360779
C	9.274087	7.993279	-10.170147
C	9.005014	7.319400	-1.170429
H	11.222070	6.706935	-5.217131
H	12.913324	7.059826	-5.642359
H	11.607898	8.105203	-6.282022
H	6.580814	12.708649	-1.993405
H	7.085734	12.295137	-3.659766
H	6.413953	11.032323	-2.566546
C	4.215752	8.831041	-11.170095
H	3.877564	13.331804	-7.430448
H	5.509799	12.832061	-6.891316

H	4.271616	11.597290	-7.289261
H	9.909748	8.424923	-9.389654
H	9.872601	7.372254	-10.833342
H	8.477093	7.389372	-9.722649
C	8.561161	6.254079	-0.314034
C	3.135930	8.073465	-11.747835
S	9.281852	4.704094	-0.325137
S	7.260693	6.437404	0.775829
S	3.385417	6.941913	-12.999524
S	1.517914	8.254288	-11.241824
C	8.208718	4.002560	0.801922
C	7.253766	4.821565	1.316594
C	1.752337	6.490626	-13.152250
C	0.868705	7.118343	-12.330872
H	8.302534	2.936753	1.006436
H	6.469687	4.533121	2.013175
H	1.497360	5.743729	-13.893921
H	-0.200464	6.946809	-12.311292

Energy -11103.8006947 A.U.

Table S31. Optimized cartesian coordinates (in Angstroms) of $clip_1^{2+}$ at M06L/6-31+G(d,p) level.

C	-0.047846	-0.011168	0.050486
C	-0.026809	-0.014351	1.443958
C	1.186485	-0.010470	2.124364
C	2.392121	0.007021	1.416636
C	2.364875	0.004216	0.019159
C	1.149759	-0.009563	-0.660701
H	-0.995312	-0.012830	-0.479730
H	-0.957288	-0.015726	2.003569
H	1.202433	0.007953	3.211519
H	3.296537	0.031350	-0.542350
H	1.139596	-0.010538	-1.746407
C	3.700092	0.180035	2.153249
C	4.123958	1.679769	2.421069
C	3.001342	2.688785	2.348823
C	2.240843	2.983477	3.483621
C	2.636444	3.243140	1.118172
C	1.131099	3.819400	3.389545
H	2.508254	2.547126	4.443969
C	1.521847	4.070139	1.023353
H	3.216234	3.002801	0.230292
C	0.766147	4.359187	2.158456
H	0.547845	4.042953	4.277544
H	1.240668	4.486561	0.060676
H	-0.103494	5.004650	2.084033
N	3.687651	-0.387583	3.491139
N	4.849664	-0.300856	1.398290
N	5.156358	1.899161	1.422290
N	4.708915	1.568602	3.749714
C	4.472485	0.361002	4.355215
C	5.707596	0.695793	1.008869
O	6.753000	0.554496	0.385859
O	4.860144	0.014496	5.464560
C	5.375967	2.681732	4.379491
C	5.956091	3.109273	1.455233
C	4.995476	-1.689899	1.038110
C	3.543881	-1.819113	3.674039
H	5.256482	3.943546	1.600668
H	6.400536	3.247269	0.468539
H	5.382166	2.501973	5.455978
H	4.766666	3.583853	4.214992
H	3.214385	-1.997432	4.698679
H	5.681758	-1.745585	0.191310
H	2.720513	-2.138800	3.021009
H	4.020628	-2.053548	0.677541
C	4.767811	-2.666445	3.389582
C	5.133718	-3.624009	4.344613
C	5.463208	-2.597106	2.155570
C	6.164337	-4.522923	4.053312
C	6.527850	-3.469531	1.898169
C	6.859843	-4.444517	2.844694
C	6.779157	2.953706	3.881890
C	7.797122	3.111791	4.829268
C	7.045685	3.178368	2.506825
C	9.057503	3.550740	4.412975
C	8.322692	3.585671	2.098769
C	9.315963	3.791861	3.061847

S	6.585743	-5.841596	5.111932
S	10.340081	3.913722	5.534555
S	8.067033	-5.668029	2.555652
S	10.889549	4.434416	2.673909
C	11.452430	4.459546	4.317138
C	7.800778	-6.496688	4.058509
C	12.725287	4.930014	4.649307
C	8.501875	-7.658981	4.391912
S	9.699038	-8.365518	3.350070
S	8.220465	-8.521701	5.873230
S	13.856292	5.493711	3.457068
S	13.289680	5.015717	6.290794
C	15.093086	5.904460	4.590765
C	14.832674	5.683734	5.895007
C	10.048521	-9.700897	4.389442
C	9.368129	-9.771770	5.551331
H	16.016375	6.318353	4.203558
H	15.515643	5.895522	6.708981
H	10.793294	-10.415681	4.060263
H	9.486325	-10.552124	6.293494
O	8.610640	3.919430	0.808764
O	7.599434	2.975767	6.172801
O	4.439840	-3.814526	5.502834
O	7.195614	-3.503938	0.708289
C	4.930162	-3.063763	6.633206
C	9.126825	2.838798	0.004266
C	7.607614	1.616667	6.649649
C	8.224217	-2.505824	0.564941
H	10.070211	2.464939	0.422325
H	9.311025	3.267405	-0.979654
H	8.399215	2.023981	-0.059798
H	7.429439	1.679504	7.722241
H	6.815060	1.024468	6.178857
H	8.584689	1.153732	6.464858
H	4.277432	-3.324616	7.464852
H	4.886253	-1.989589	6.430397
H	5.960277	-3.357707	6.871373
H	7.808164	-1.493618	0.622260
H	8.657510	-2.668324	-0.420800
H	8.995836	-2.640110	1.332883

Energy -5552.18961780 A.U.

Table S32. Optimized cartesian coordinates (in Angstroms) of $clip_1^{2+}$ at M06L/6-31++G(d,p) level.

C	-0.035881	-0.007406	0.011069
C	-0.027059	-0.015670	1.404707
C	1.180202	-0.010689	2.095970
C	2.391901	0.012335	1.398881
C	2.376937	0.014606	0.001218
C	1.167948	0.000225	-0.689468
H	-0.978615	-0.009905	-0.527553
H	-0.962508	-0.021855	1.956066
H	1.186708	0.003828	3.183290
H	3.313259	0.045623	-0.552282
H	1.167532	0.003218	-1.775253
C	3.693669	0.183728	2.146811
C	4.114817	1.681747	2.422752
C	2.989833	2.688718	2.361755
C	2.233520	2.973148	3.501897
C	2.619518	3.252676	1.137076
C	1.122324	3.808388	3.419166
H	2.505445	2.529738	4.457716
C	1.503654	4.079330	1.053658
H	3.196129	3.020212	0.244971
C	0.752138	4.358235	2.194090
H	0.542290	4.023866	4.311329
H	1.218228	4.503418	0.095549
H	-0.118493	5.003342	2.128429
N	3.672184	-0.388071	3.482730
N	4.849846	-0.292935	1.398588
N	5.143897	1.909026	1.422407
N	4.704117	1.561844	3.749105
C	4.460634	0.353518	4.350410
C	5.702548	0.708295	1.009889
O	6.750168	0.573062	0.389328
O	4.845970	0.000149	5.458362
C	5.373827	2.671080	4.383308
C	5.940672	3.121159	1.460421
C	5.000729	-1.680901	1.035639
C	3.528219	-1.820596	3.659137
H	5.239623	3.952414	1.615673
H	6.380433	3.267912	0.472877
H	5.384411	2.484569	5.458644
H	4.764103	3.574385	4.226631
H	3.190830	-2.003276	4.680447
H	5.693064	-1.733132	0.193514
H	2.710872	-2.138758	2.997883
H	4.028970	-2.045594	0.667718
C	4.756425	-2.663924	3.382429
C	5.119475	-3.619720	4.340019
C	5.462442	-2.589162	2.154802
C	6.158771	-4.511512	4.057858
C	6.534644	-3.454756	1.906422
C	6.864610	-4.428015	2.855599
C	6.775106	2.945985	3.881436
C	7.798731	3.092203	4.824581
C	7.034915	3.183047	2.507143
C	9.057959	3.532247	4.405686
C	8.310267	3.591778	2.096016
C	9.309172	3.786446	3.055572

S	6.580221	-5.827221	5.120263
S	10.349080	3.878165	5.522825
S	8.083100	-5.642671	2.577517
S	10.881833	4.429078	2.664709
C	11.456316	4.431692	4.304216
C	7.811237	-6.471989	4.078959
C	12.733408	4.893133	4.632634
C	8.518812	-7.628244	4.419575
S	9.730489	-8.326495	3.388821
S	8.231294	-8.491721	5.899235
S	13.856917	5.467716	3.438555
S	13.311134	4.956049	6.270487
C	15.104360	5.858862	4.567170
C	14.853659	5.622858	5.870662
C	10.080371	-9.658809	4.432084
C	9.390403	-9.733834	5.588065
H	16.026306	6.273905	4.177908
H	15.544402	5.821460	6.681409
H	10.833164	-10.368515	4.110065
H	9.507998	-10.512849	6.331752
O	8.591697	3.936137	0.807310
O	7.608778	2.940387	6.167644
O	4.416637	-3.812372	5.492450
O	7.214532	-3.482762	0.723158
C	4.912622	-3.078420	6.631365
C	9.113396	2.863856	-0.004892
C	7.618239	1.574970	6.625721
C	8.240357	-2.479724	0.595713
H	10.054125	2.485851	0.415658
H	9.303725	3.302105	-0.983446
H	8.386477	2.049461	-0.080805
H	7.452674	1.623144	7.701122
H	6.818150	0.991864	6.156199
H	8.591522	1.111589	6.422538
H	4.262011	-3.348191	7.461889
H	4.870863	-2.001772	6.441735
H	5.942961	-3.378272	6.862115
H	7.818120	-1.469634	0.645842
H	8.690342	-2.640064	-0.382923
H	8.999980	-2.609556	1.376385

Energy -5552.19121252 A.U.

Table S33. Optimized cartesian coordinates (in Angstroms) of $clip_1^{2+}$ in acetonitrile at M06L/6-31+G(d,p) level. PCM solvation model was used.

C	-0.137530	0.115943	-0.198643
C	-0.173351	0.041647	1.193566
C	1.011350	0.030056	1.924764
C	2.244394	0.099547	1.269742
C	2.274715	0.163669	-0.126020
C	1.089284	0.169171	-0.857076
H	-1.062261	0.127354	-0.767967
H	-1.126029	-0.005186	1.713159
H	0.984420	-0.015706	3.010578
H	3.228162	0.222491	-0.645578
H	1.126551	0.221255	-1.941053
C	3.525576	0.244214	2.062338
C	3.935735	1.732454	2.400328
C	2.801533	2.733670	2.379609
C	2.033356	2.948658	3.526594
C	2.441900	3.367797	1.186373
C	0.916790	3.780284	3.481259
H	2.300628	2.455954	4.458448
C	1.323347	4.195076	1.140670
H	3.033963	3.196972	0.290504
C	0.556838	4.401627	2.287275
H	0.326928	3.938242	4.379268
H	1.049555	4.677974	0.206967
H	-0.316451	5.045971	2.250163
N	3.460628	-0.371510	3.375252
N	4.696431	-0.195640	1.316838
N	4.958327	2.010939	1.409797
N	4.508779	1.560590	3.727193
C	4.211929	0.349689	4.292772
C	5.520326	0.831800	0.944451
O	6.553841	0.738588	0.290414
O	4.523676	-0.027520	5.417681
C	5.223306	2.626243	4.394297
C	5.770744	3.214700	1.518348
C	4.895651	-1.579800	0.949990
C	3.361498	-1.820086	3.496697
H	5.086271	4.036281	1.763938
H	6.187038	3.432878	0.533975
H	5.232755	2.400735	5.462063
H	4.653507	3.558732	4.268712
H	2.967099	-2.050591	4.487041
H	5.600255	-1.604274	0.116637
H	2.608420	-2.147401	2.768945
H	3.941257	-1.979389	0.576383
C	4.655708	-2.576047	3.283890
C	5.090747	-3.454000	4.282626
C	5.394056	-2.447965	2.082319
C	6.260609	-4.199355	4.081578
C	6.568016	-3.181897	1.899687
C	6.993877	-4.058832	2.902428
C	6.634459	2.834987	3.891629
C	7.687729	2.794312	4.808074
C	6.889919	3.147218	2.533612
C	8.983886	3.102571	4.382575
C	8.190410	3.448083	2.115625

C	9.233227	3.437821	3.050746
S	6.835192	-5.396535	5.210853
S	10.338439	3.168120	5.476561
S	8.394791	-5.080378	2.722027
S	10.867792	3.899388	2.662146
C	11.483718	3.661027	4.268367
C	8.213589	-5.855953	4.263518
C	12.830183	3.871465	4.571609
C	9.125331	-6.811003	4.719440
S	10.496220	-7.313465	3.785348
S	8.969688	-7.580527	6.265610
S	13.984456	4.372834	3.377022
S	13.477147	3.655133	6.166750
C	15.327460	4.412328	4.457513
C	15.093707	4.079723	5.743569
C	11.085632	-8.433059	4.956688
C	10.381461	-8.558497	6.100329
H	16.290207	4.699975	4.054021
H	15.840526	4.060076	6.527293
H	11.987631	-8.982525	4.718584
H	10.634151	-9.220613	6.918829
O	8.455452	3.863538	0.840576
O	7.499402	2.548459	6.141335
O	4.341414	-3.690042	5.400377
O	7.282743	-3.149969	0.733046
C	4.829061	-3.068517	6.606093
C	9.041172	2.863438	-0.017508
C	7.515185	1.148581	6.483497
C	8.305751	-2.135431	0.701124
H	9.953333	2.448336	0.427383
H	9.294883	3.378797	-0.942693
H	8.322274	2.061602	-0.204862
H	7.418623	1.104605	7.567278
H	6.674225	0.625850	6.015200
H	8.462183	0.688813	6.179294
H	4.157562	-3.393714	7.399206
H	4.803729	-1.981317	6.500993
H	5.848074	-3.400008	6.838341
H	7.859579	-1.136458	0.751737
H	8.822152	-2.261927	-0.249471
H	9.014931	-2.274346	1.525301

Energy -5552.35147700 A.U.

Table S34. Optimized cartesian coordinates (in Angstroms) of $clip_1^{2+}$ in acetonitrile at M06L/6-31++G(d,p) level. PCM solvation model was used.

C	-0.140487	0.109726	-0.196696
C	-0.175629	0.037915	1.195678
C	1.009374	0.029090	1.926471
C	2.242076	0.098699	1.270848
C	2.271754	0.160358	-0.125028
C	1.086051	0.163273	-0.855672
H	-1.065475	0.118685	-0.765729
H	-1.128093	-0.009560	1.715692
H	0.982766	-0.015325	3.012348
H	3.224908	0.218929	-0.645174
H	1.122884	0.213416	-1.939797
C	3.523746	0.244197	2.062701
C	3.933929	1.732717	2.400119
C	2.800630	2.735100	2.377581
C	2.034038	2.955387	3.524596
C	2.442162	3.367549	1.183098
C	0.920383	3.790907	3.478185
H	2.300603	2.464399	4.457559
C	1.326529	4.198632	1.136288
H	3.033308	3.193267	0.287302
C	0.561672	4.410756	2.283035
H	0.331909	3.953225	4.376372
H	1.053843	4.680527	0.201693
H	-0.309217	5.058377	2.245162
N	3.459622	-0.371497	3.375819
N	4.694078	-0.195745	1.316598
N	4.957423	2.010576	1.410133
N	4.505811	1.561741	3.727477
C	4.210550	0.350444	4.293034
C	5.518779	0.831257	0.944744
O	6.552324	0.737387	0.290878
O	4.523148	-0.026251	5.417852
C	5.221053	2.627057	4.394244
C	5.769986	3.214228	1.518369
C	4.893256	-1.579844	0.949720
C	3.360962	-1.820065	3.497780
H	5.085449	4.036030	1.763276
H	6.186653	3.432075	0.534061
H	5.230048	2.401983	5.462084
H	4.651986	3.559929	4.268003
H	2.967518	-2.050408	4.488569
H	5.597423	-1.604296	0.116003
H	2.607062	-2.147683	2.770923
H	3.938609	-1.979545	0.576813
C	4.654695	-2.576579	3.283603
C	5.090385	-3.455201	4.281380
C	5.392295	-2.448217	2.081556
C	6.259890	-4.200692	4.078950
C	6.566253	-3.181845	1.897881
C	6.992673	-4.059563	2.899678
C	6.632490	2.835184	3.892148
C	7.685238	2.794093	4.809137
C	6.888642	3.147452	2.534258
C	8.981634	3.102797	4.384624
C	8.189326	3.448390	2.117190

C	9.231492	3.438253	3.052998
S	6.834400	-5.398548	5.207457
S	10.335922	3.167918	5.478923
S	8.393979	-5.080393	2.718758
S	10.865898	3.900613	2.664920
C	11.481863	3.659442	4.270721
C	8.214344	-5.855114	4.260944
C	12.828534	3.868396	4.574025
C	9.127633	-6.808562	4.717079
S	10.499719	-7.308428	3.783377
S	8.972944	-7.578386	6.263183
S	13.982980	4.369847	3.379664
S	13.475527	3.650294	6.168881
C	15.326268	4.407204	4.459934
C	15.092429	4.073774	5.745766
C	11.091135	-8.426607	4.955056
C	10.386872	-8.553404	6.098496
H	16.289257	4.694321	4.056577
H	15.839440	4.052786	6.529299
H	11.994363	-8.974301	4.717385
H	10.640771	-9.214946	6.917112
O	8.456041	3.863168	0.842206
O	7.495826	2.546345	6.141945
O	4.343236	-3.691743	5.400590
O	7.280975	-3.147756	0.731256
C	4.832178	-3.066545	6.604119
C	9.040299	2.860890	-0.014571
C	7.519376	1.146057	6.481814
C	8.306888	-2.136061	0.704656
H	9.946952	2.439116	0.435364
H	9.302690	3.376021	-0.937525
H	8.317370	2.063887	-0.206988
H	7.422994	1.099101	7.565530
H	6.681500	0.619535	6.012180
H	8.468807	0.692100	6.176280
H	4.169797	-3.399915	7.401584
H	4.794801	-1.979584	6.500229
H	5.856479	-3.387255	6.828218
H	7.863295	-1.136138	0.759532
H	8.824198	-2.259421	-0.245914
H	9.014438	-2.280599	1.529330

Energy -5552.35310478 A.U.

Complete list of authors of reference 46:

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