Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information: Janusene as a Silver Ion Scavenger : Insights from Computation

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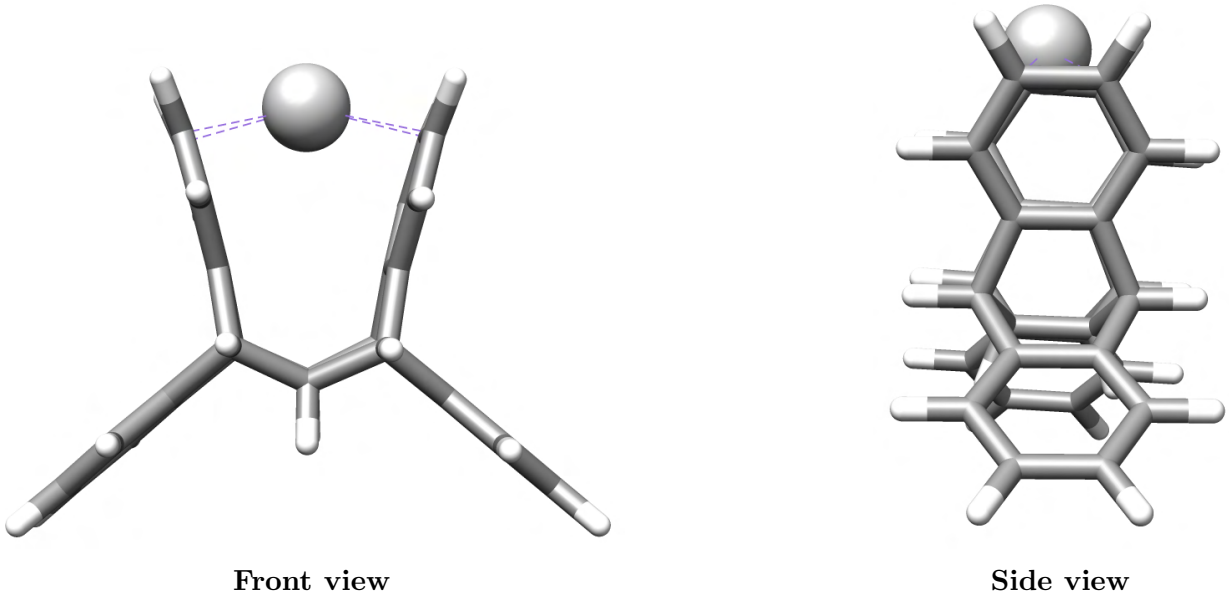
Contents

Supporting Information Available

In a nutshell, the first, second and third sections of the SI available includes the illustrations of all studied systems in different perspectives, the geometrical parameters of these systems and it's atomic charges. The fourth section brings the MEP isosurfaces of the studied systems, evidencing the modifications on the electronic density of janusene caused by Ag^+ ions. In the fifth section, QTAIM illustrations and the BCP parameters for the studied interactions are presented, evidencing the character of these interactions, as well as the effects caused by coordination of Ag^+ at positions C/E on the $[Ag_A \cdots Ag_B]^{2+}$ interaction. The sixth section, regarding the energy decomposition analysis, presents Table S15 containing all EDA terms for each fragmentation scheme employed, as well as the NOCVs deformation densities for the main fragmentations. Finally, the last two sections includes respectively the NCI analysis, with plots of s *vs.* ρ_b, and the Cartesian coordinates of the studied systems.

Systems Illustrations

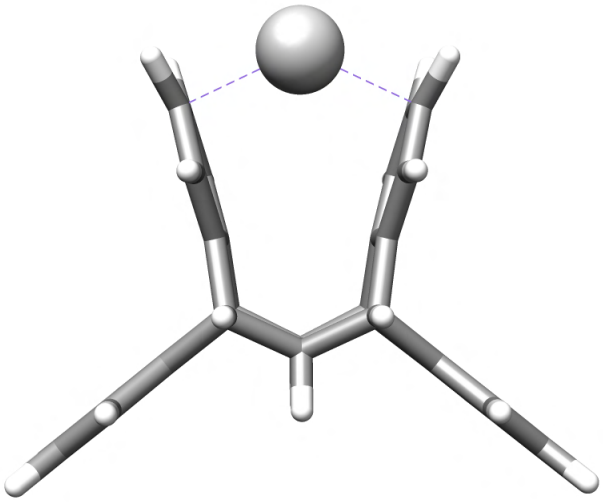
1Ag Systems



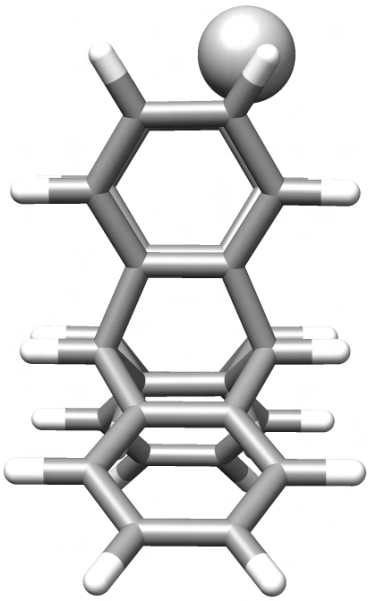
Front view **Side view**

Top view

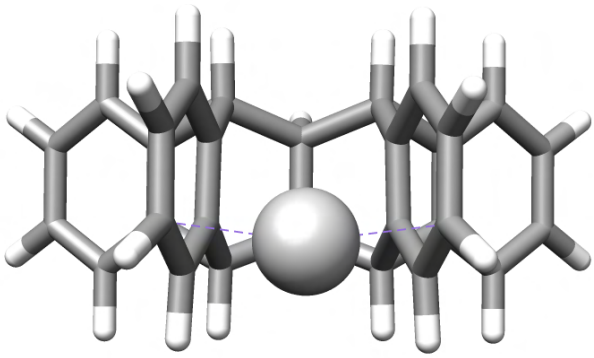
Figure S1: Illustration of system **1a**.



Front view

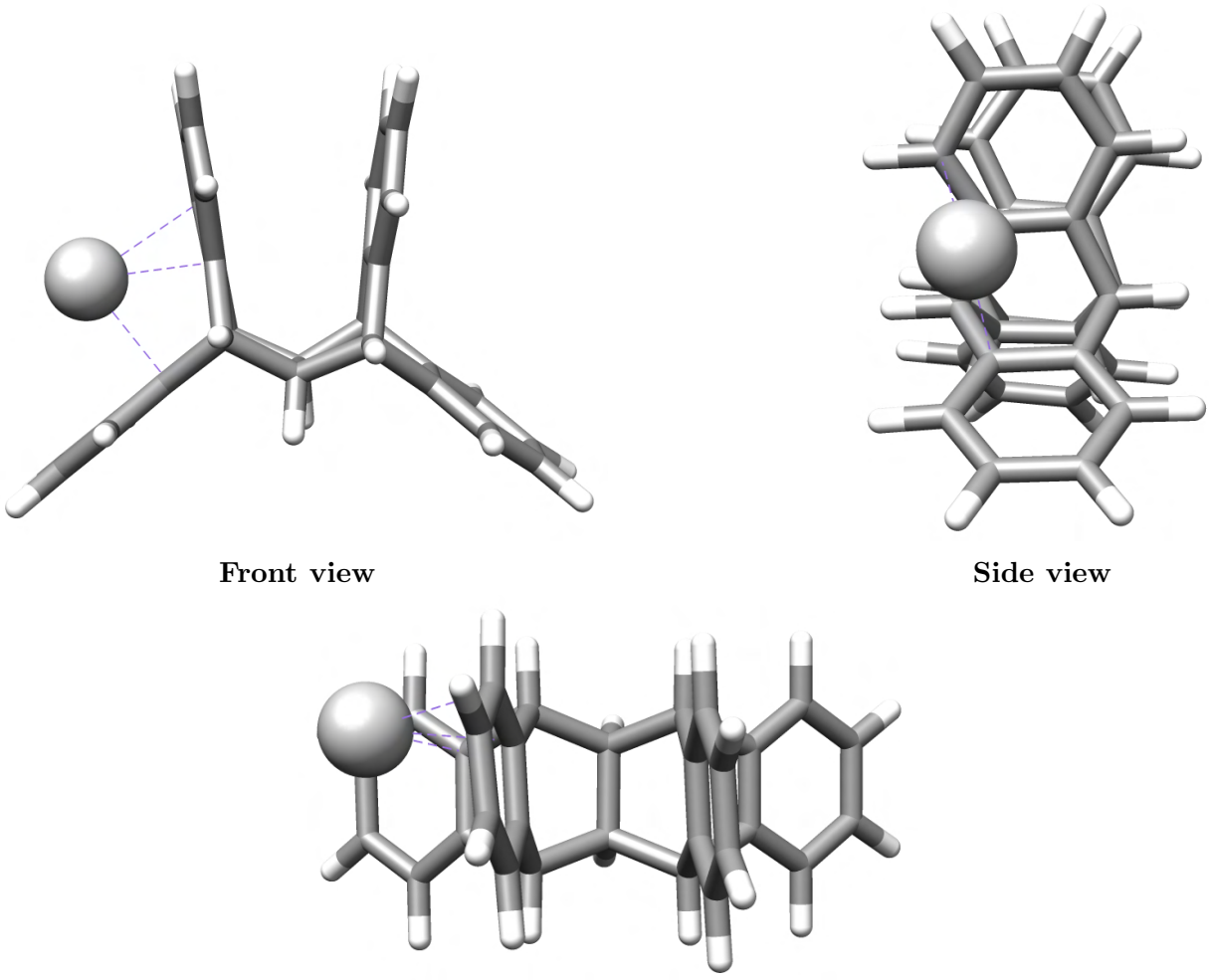


Side view



Top view

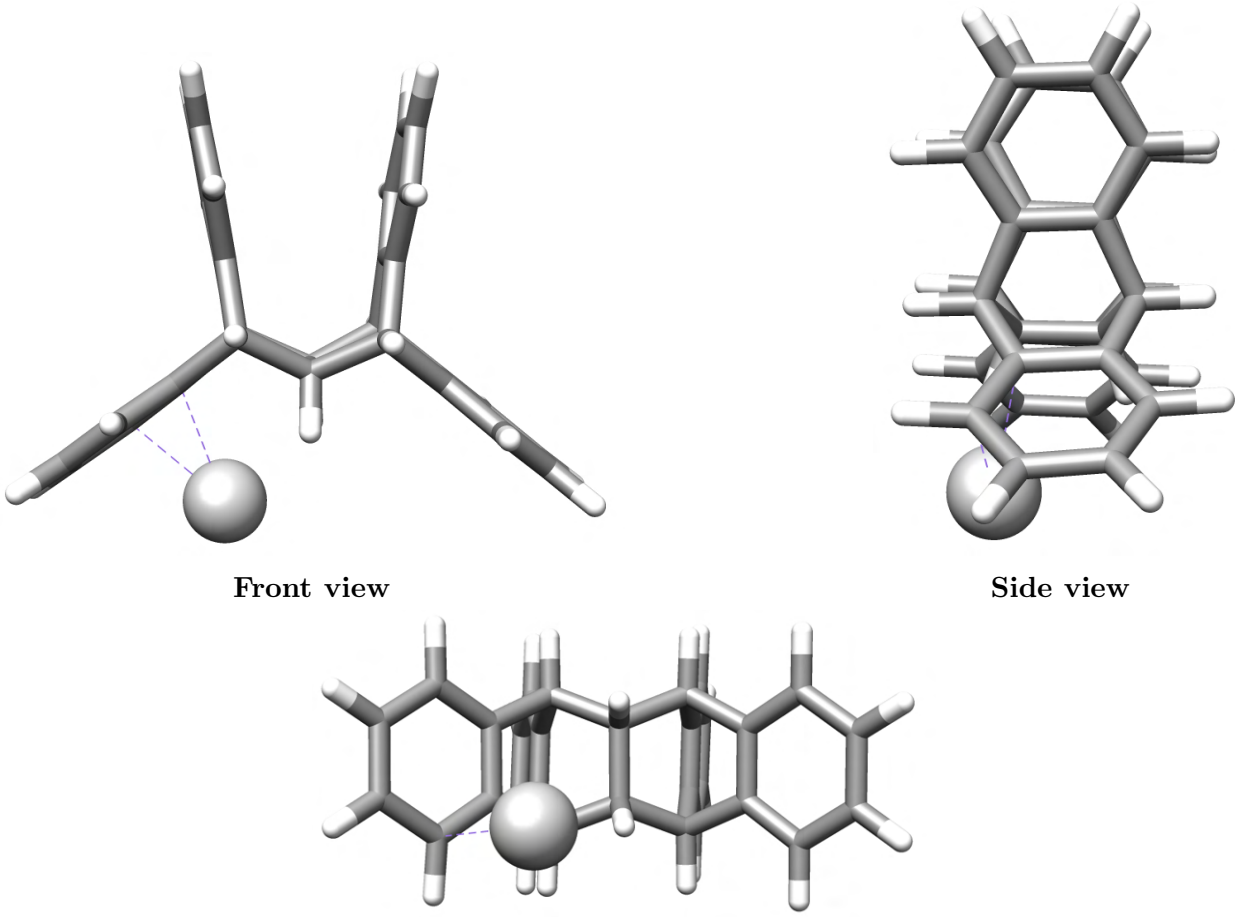
Figure S2: Illustration of system **1b**.



Front view **Side view**

Top view

Figure S3: Illustration of system **1c**.

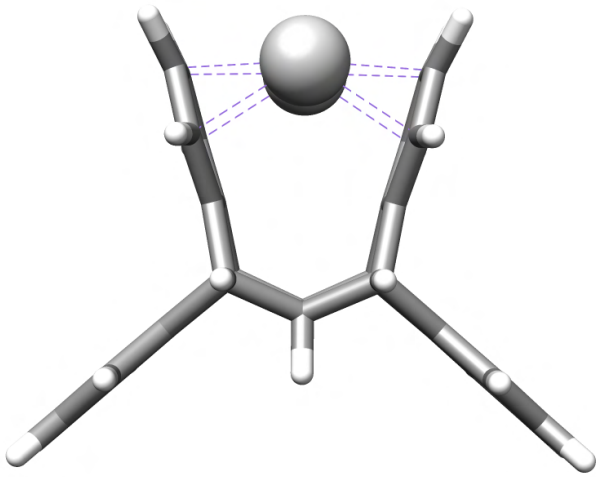


Front view **Side view**

Bottom view

Figure S4: Illustration of system **1d**.

2Ag Systems



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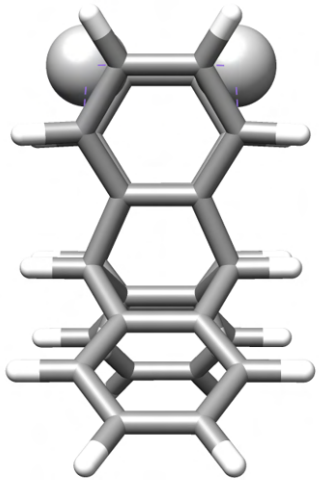

Side view

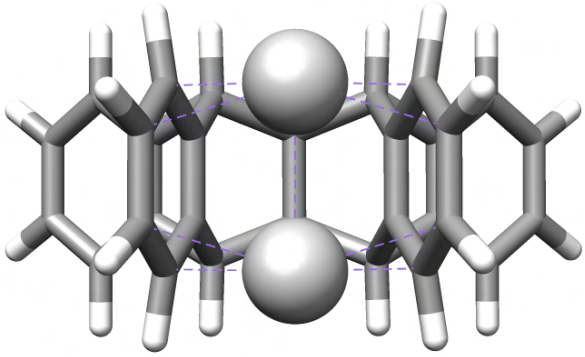

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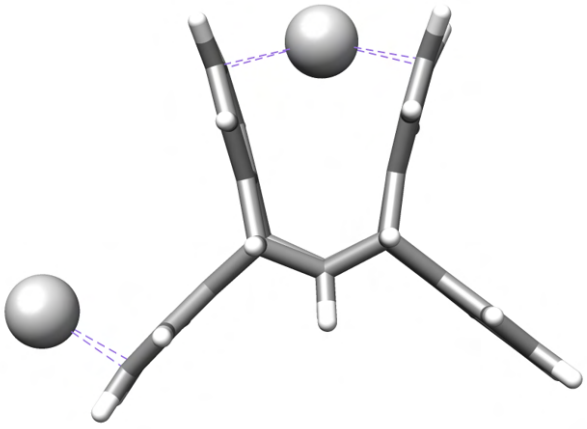
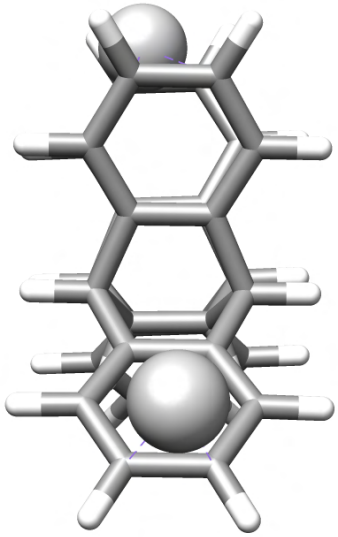
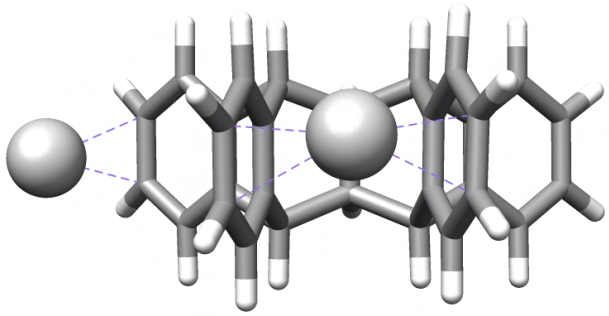
Figure S5: Illustration of system **2a**.



Front view

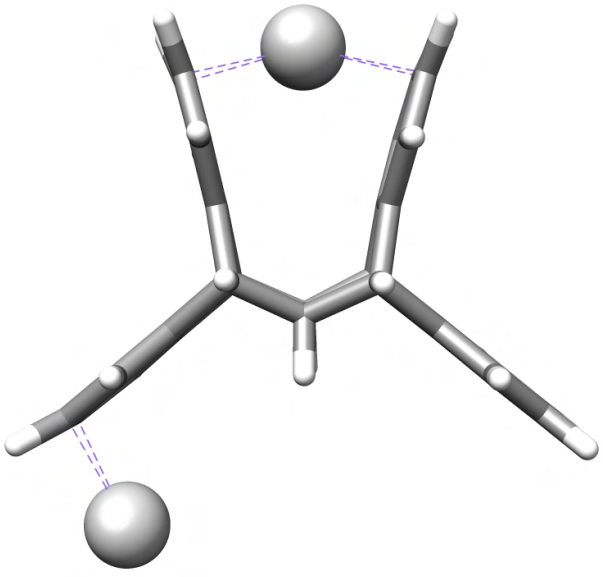


Side view



Top view

Figure S6: Illustration of system **2b**.



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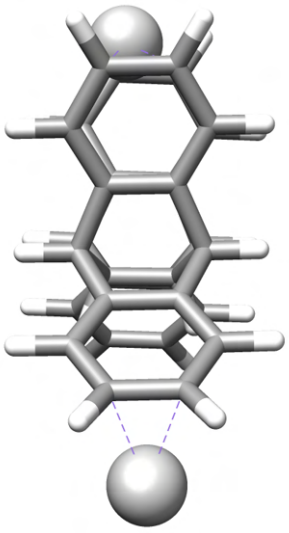
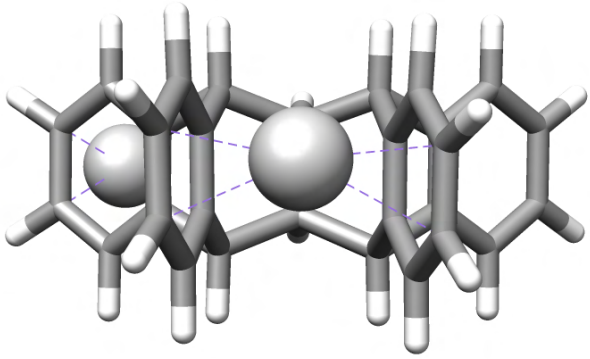
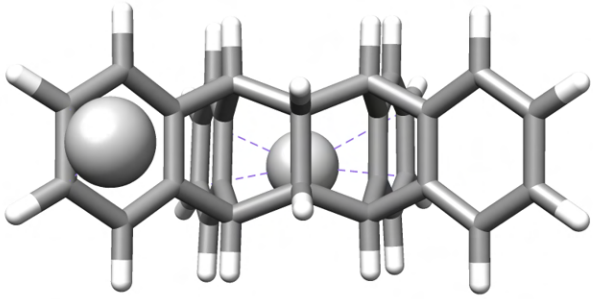


Side view

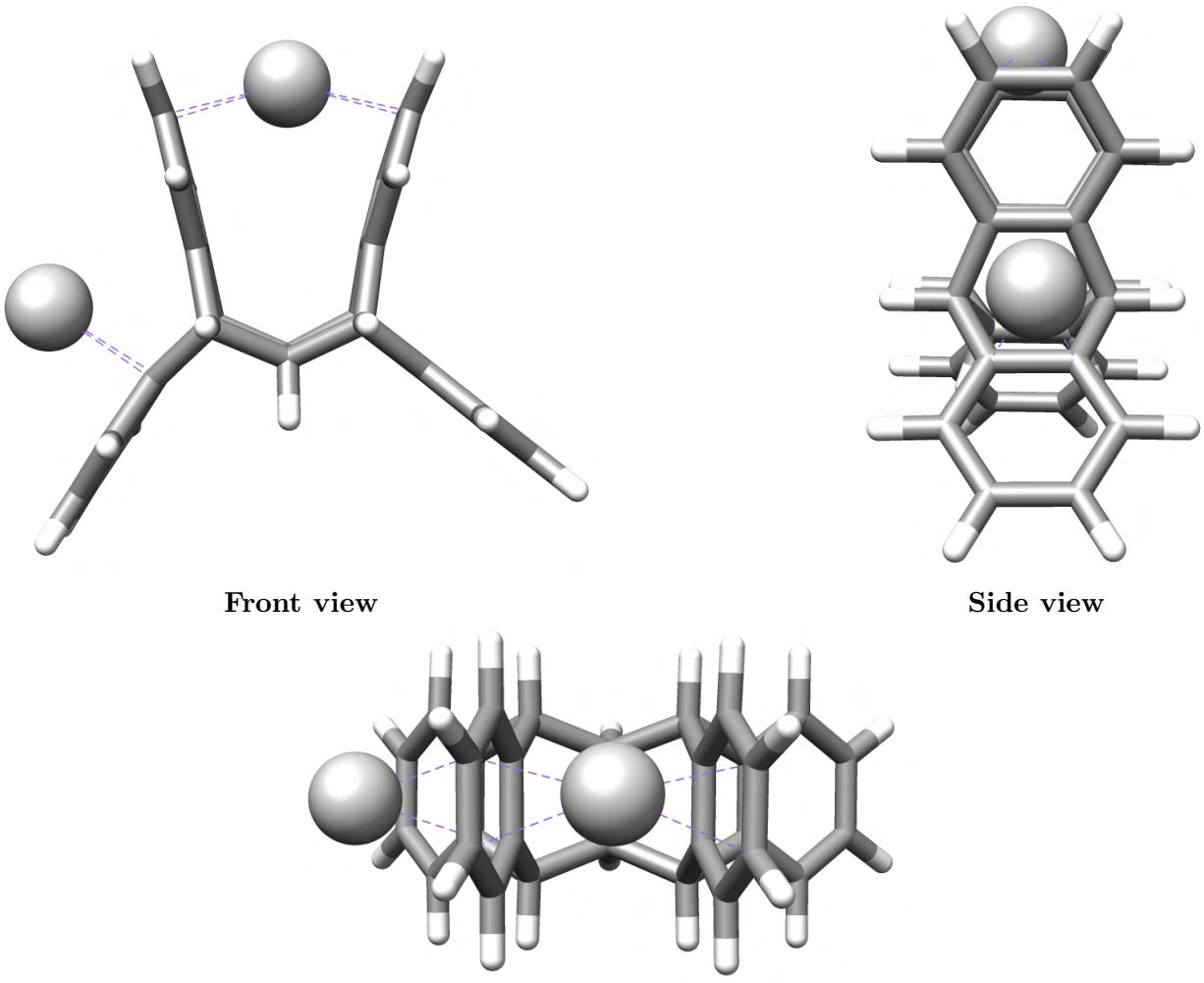


Top view



Bottom view

Figure S7: Illustration of system **2c**.



Front view **Side view**

Top view

Figure S8: Illustration of system **2d**.

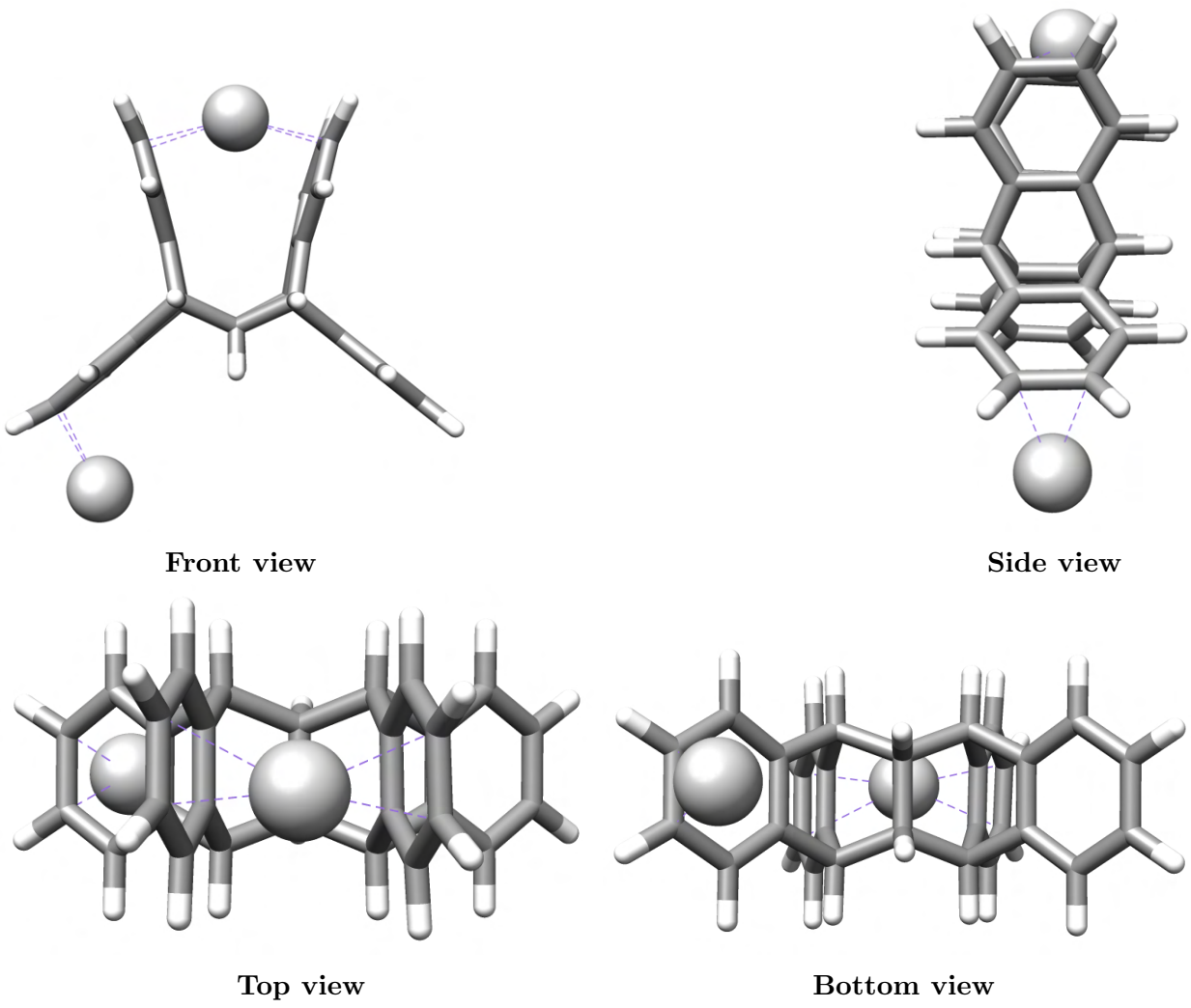
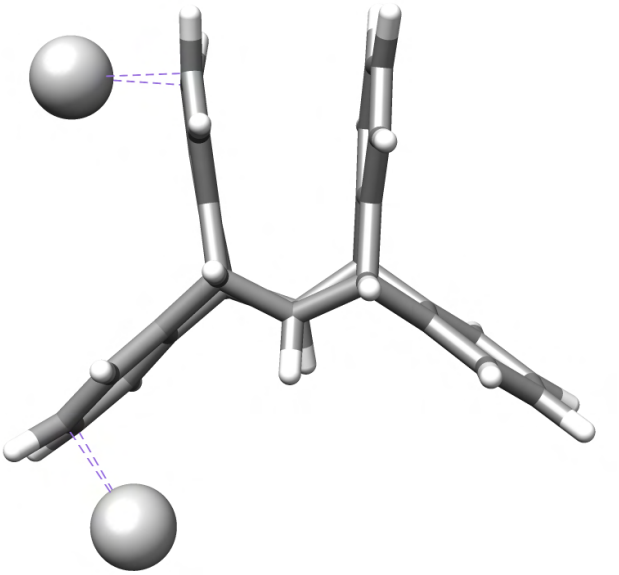
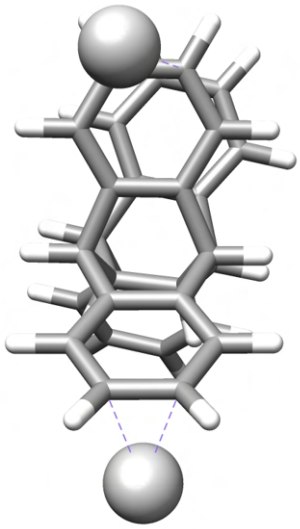


Figure S9: Illustration of system **2e**.



Front view



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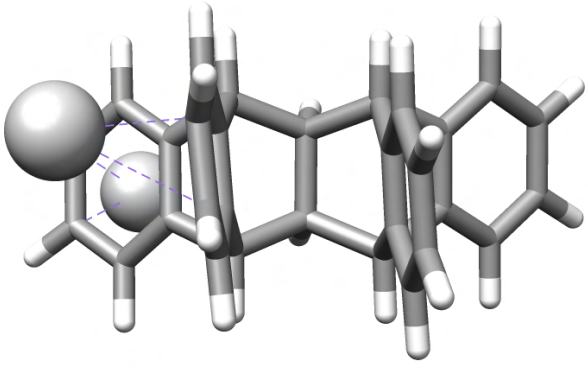

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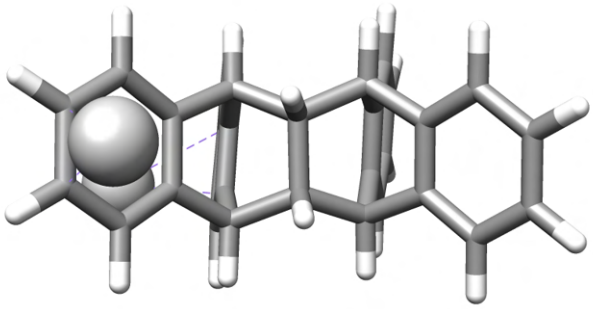
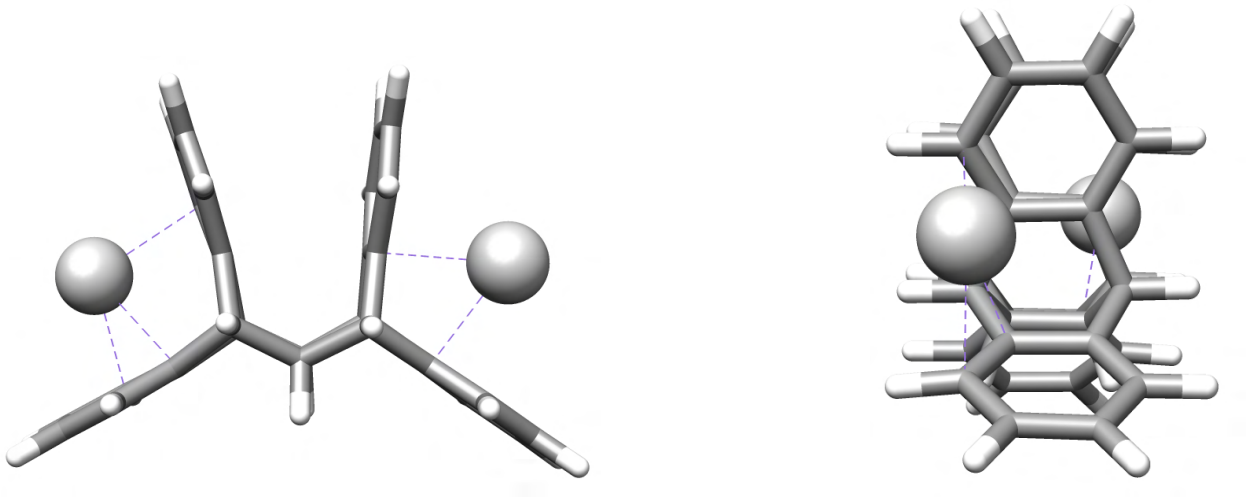


Bottom view

Figure S10: Illustration of system **2f**.



Front view **Side view**

Top view

Figure S11: Illustration of system **2g**.

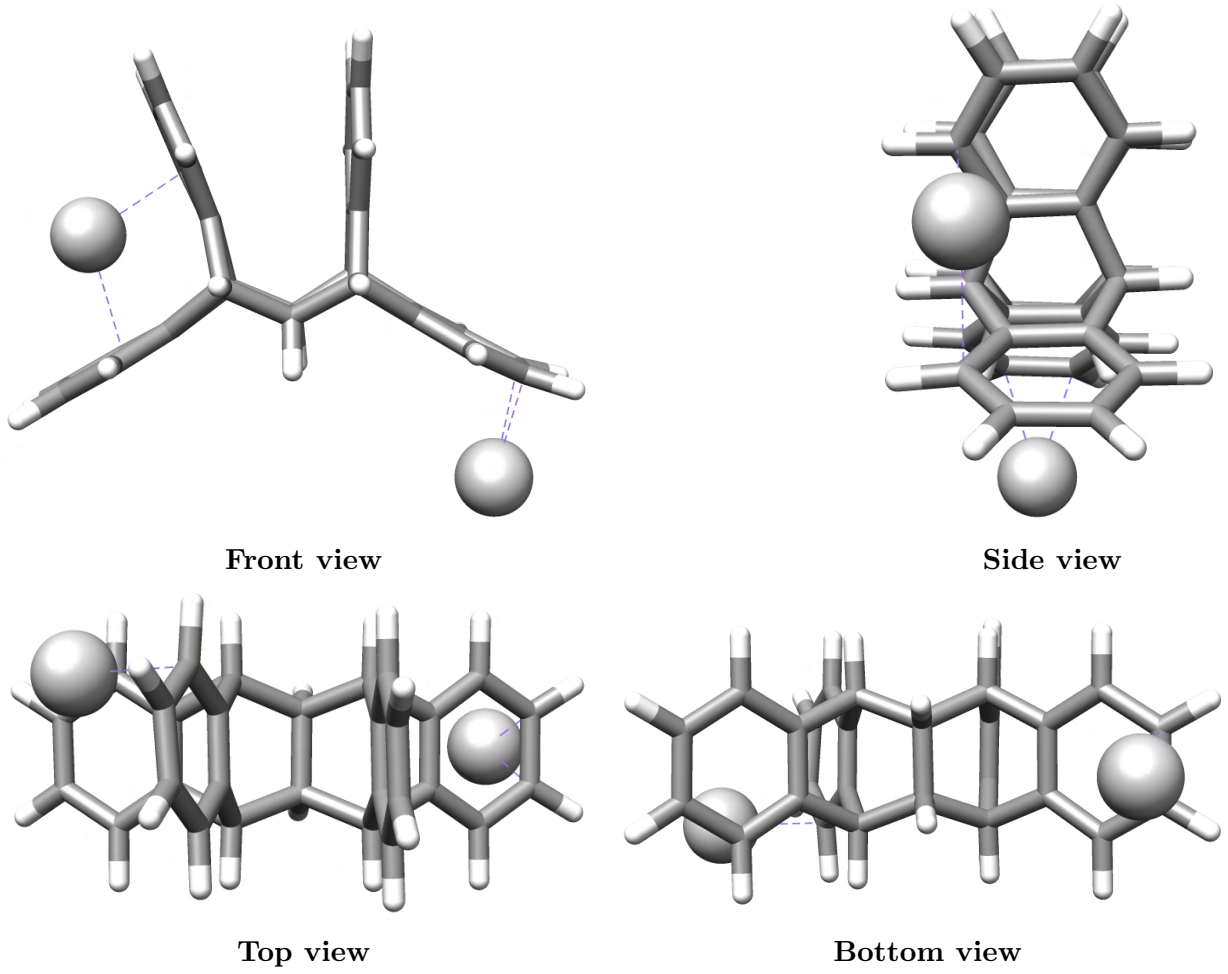
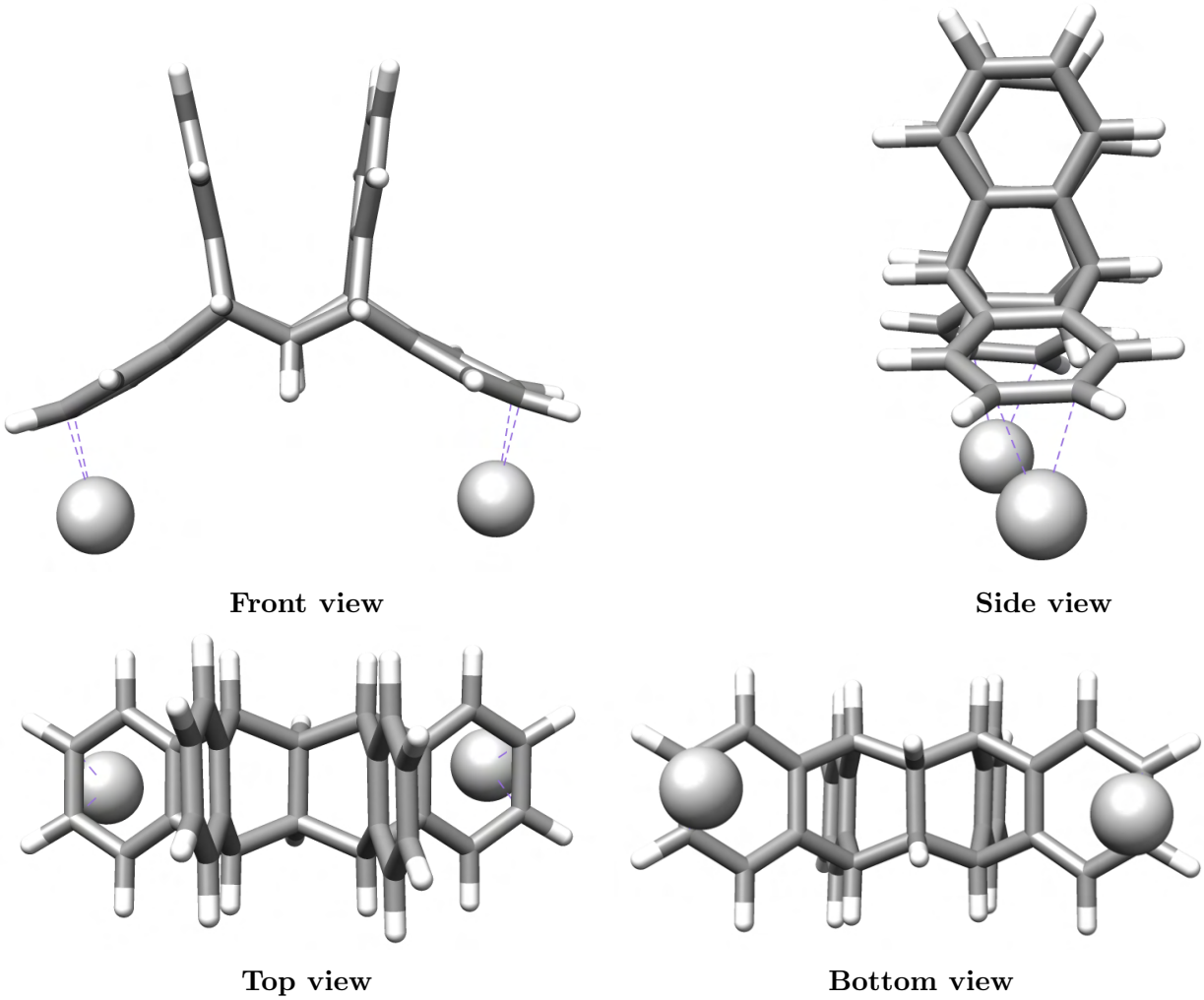


Figure S12: Illustration of system **2h**.

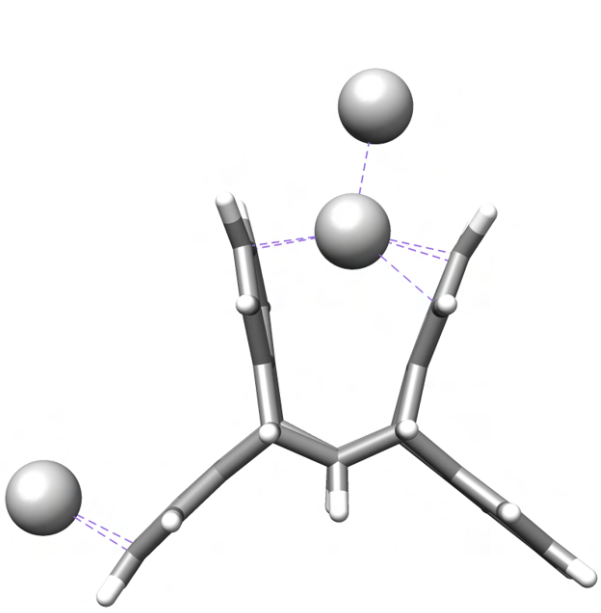


Front view **Side view**

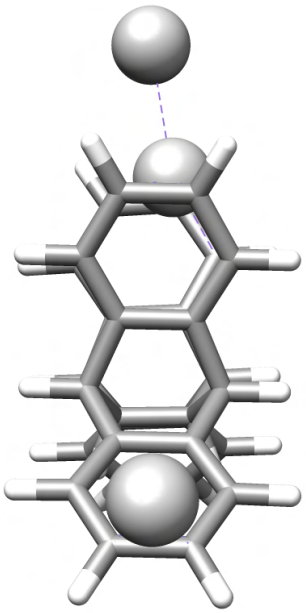
Top view **Bottom view**

Figure S13: Illustration of system **2i**.

3Ag Systems



Front view



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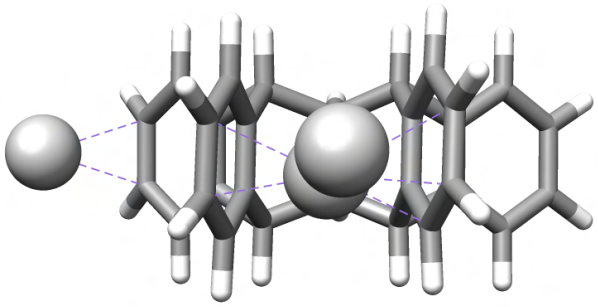
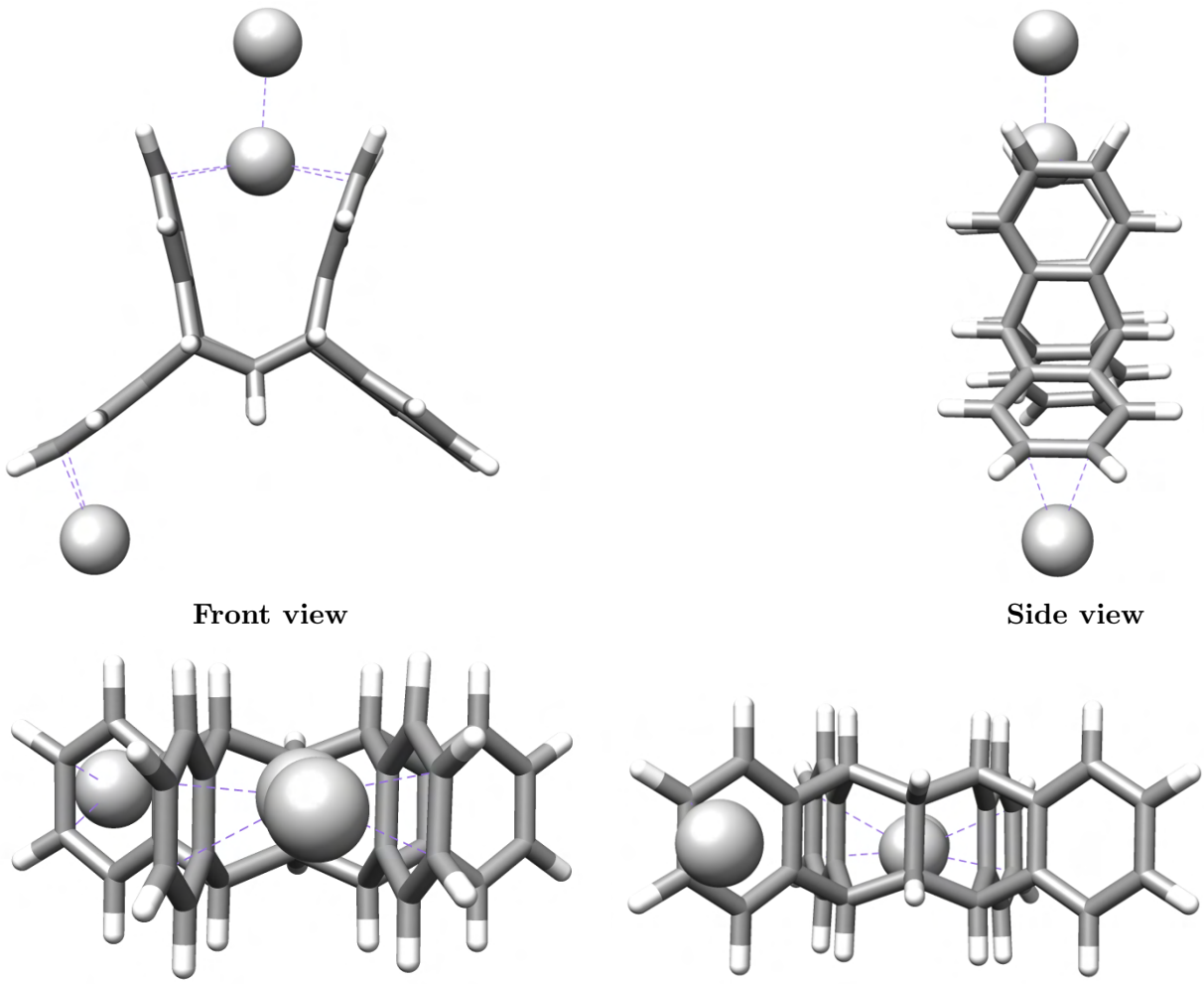


Top view

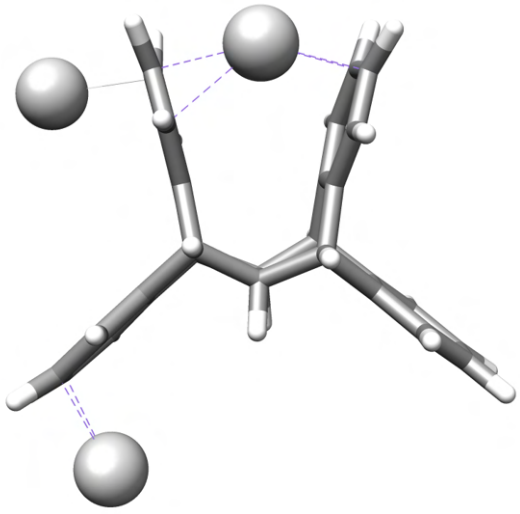
Figure S14: Illustration of system **3a**.



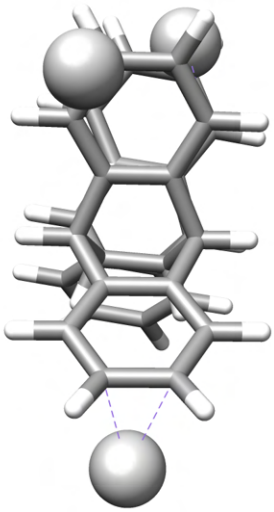
Front view **Side view**

Top view **Bottom view**

Figure S15: Illustration of system **3b**.



Front view



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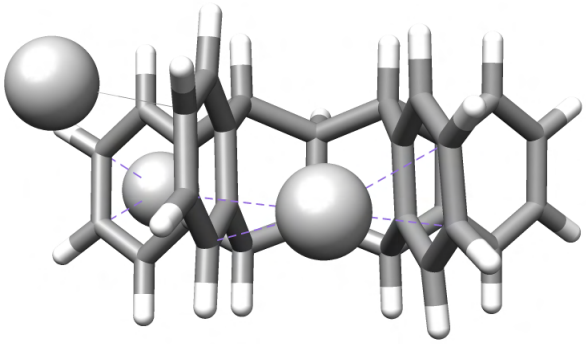
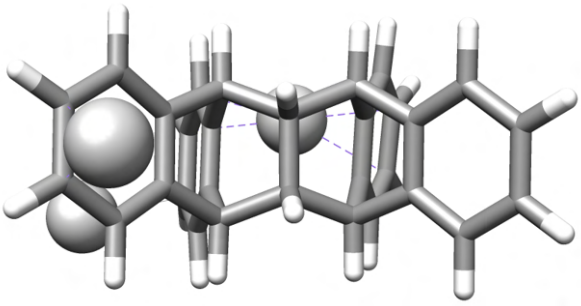
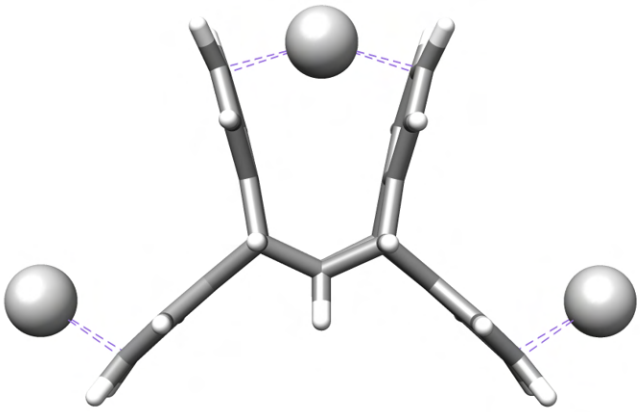


Top view

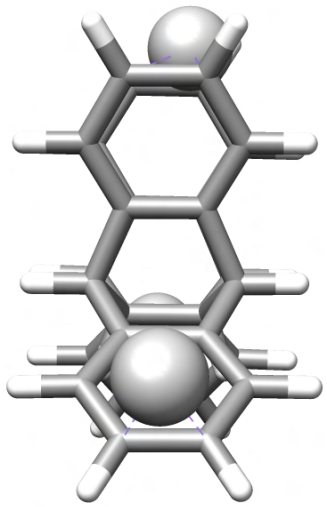


Bottom view

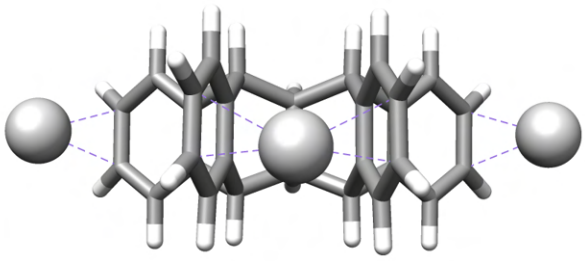
Figure S16: Illustration of system **3c**.



Front view

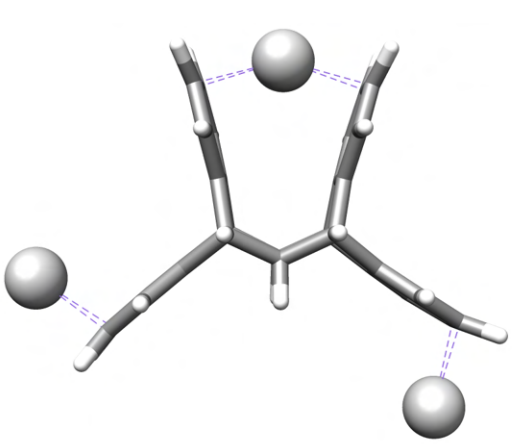


Side view

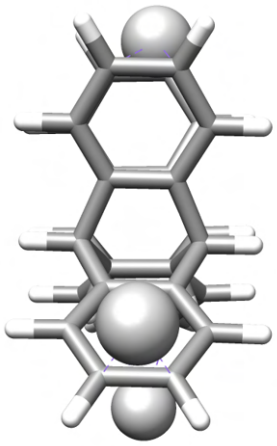


Top view

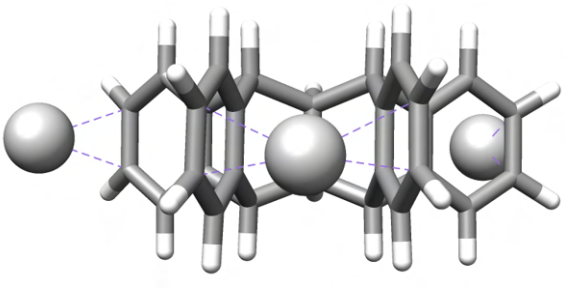
Figure S17: Illustration of system **3d**.



Front view



Side view



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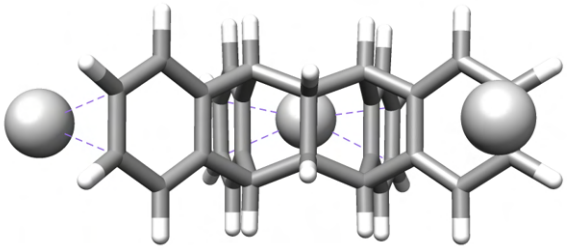
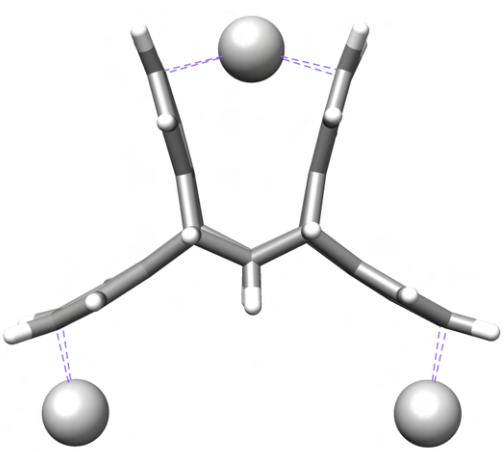
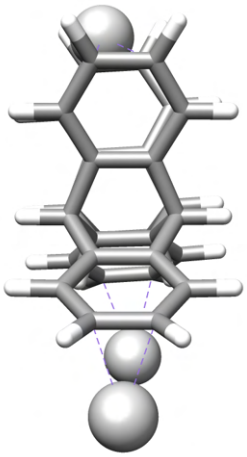


Bottom view

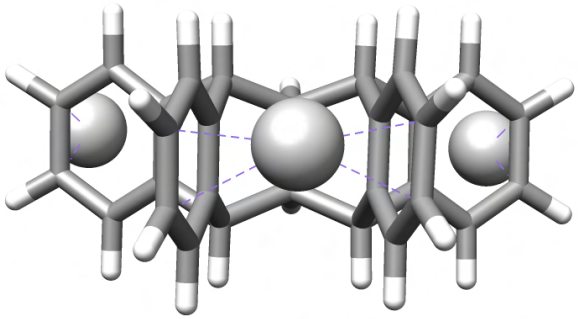
Figure S18: Illustration of system **3e**.



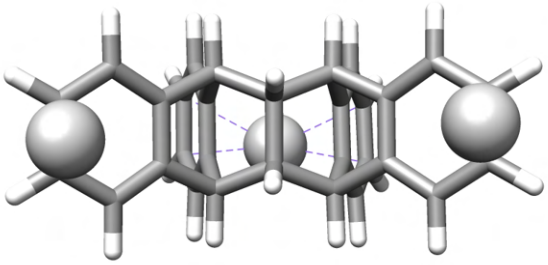
Front view



Side view

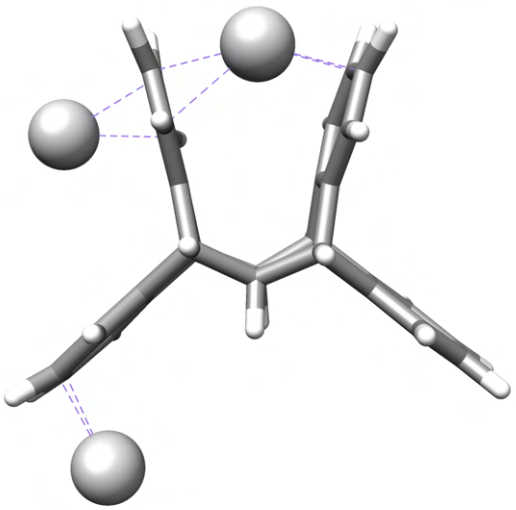


Top view

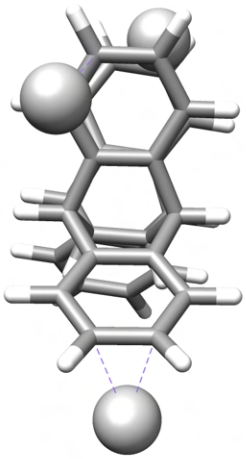


Bottom view

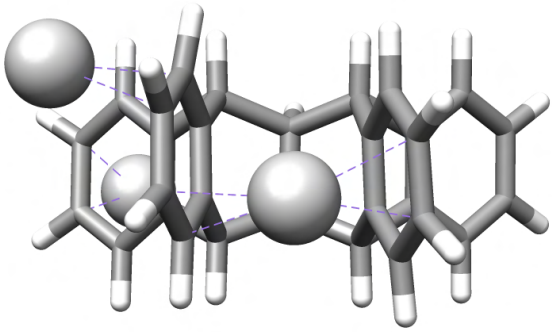
Figure S19: Illustration of system **3f**.



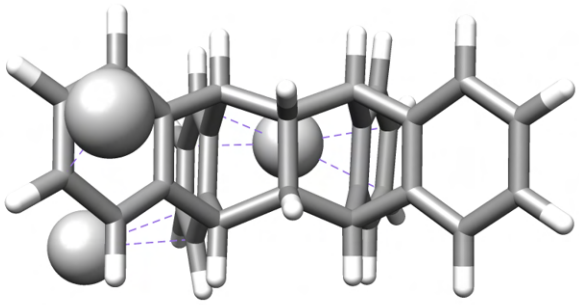
Front view



Side view

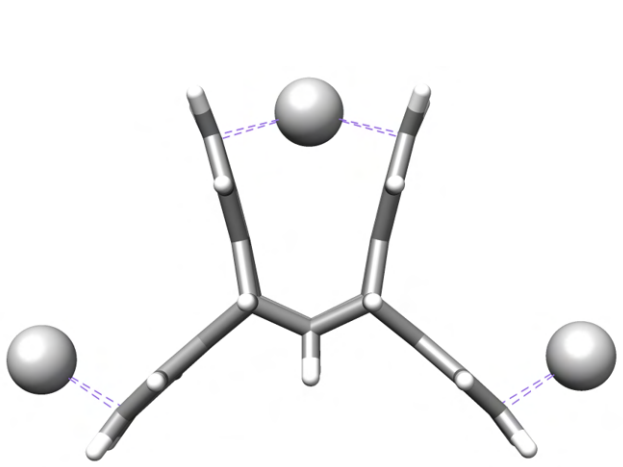


Top view

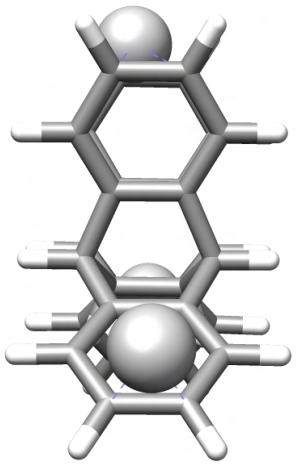


Bottom view

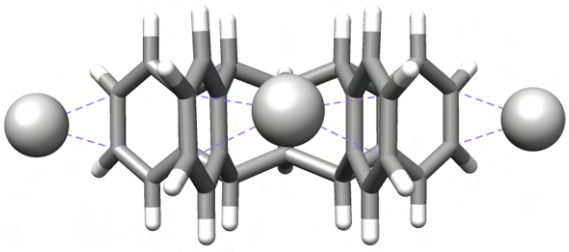
Figure S20: Illustration of system **3g**.



Front view

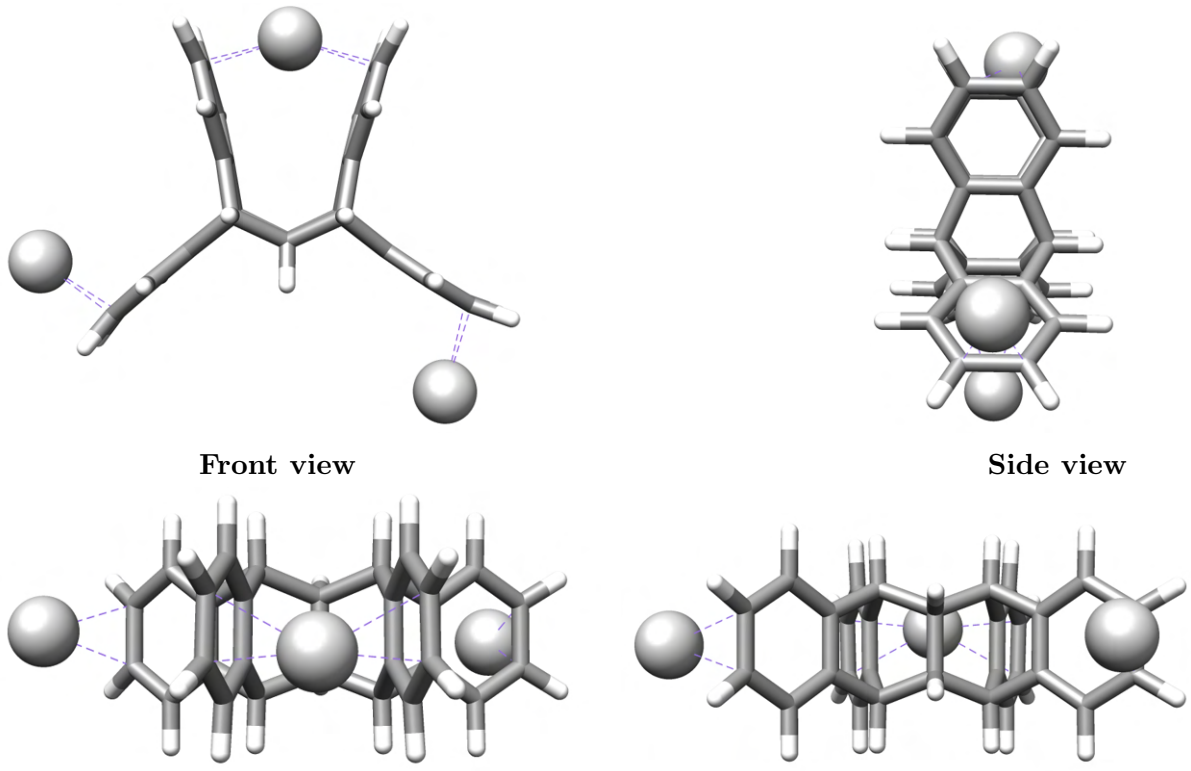


Side view



Top view

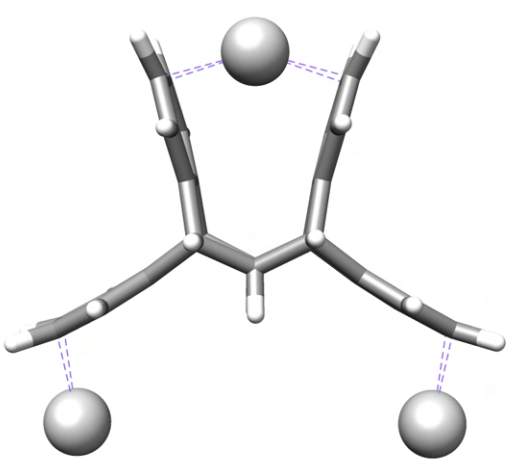
Figure S21: Illustration of system **3h**.



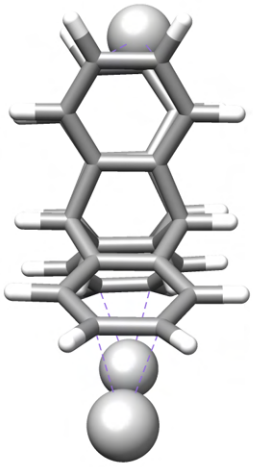
Front view **Side view**

Top view **Bottom view**

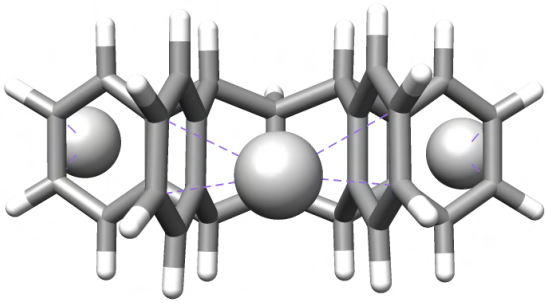
Figure S22: Illustration of system **3i**.



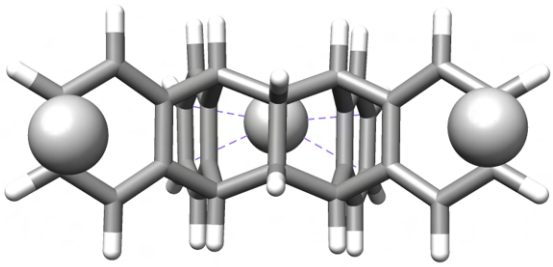
Front view



Side view



Top view



Bottom view

Figure S23: Illustration of system **3j**.

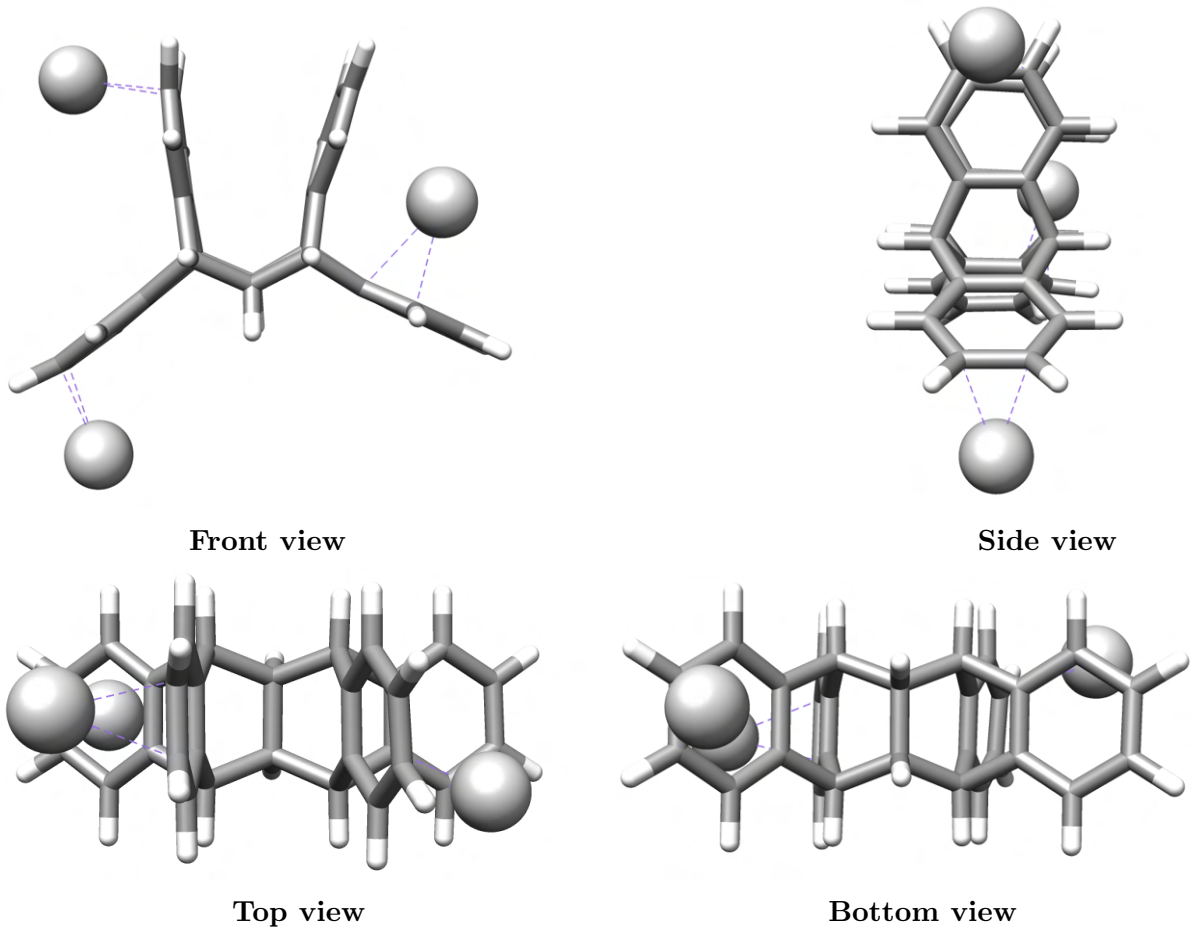
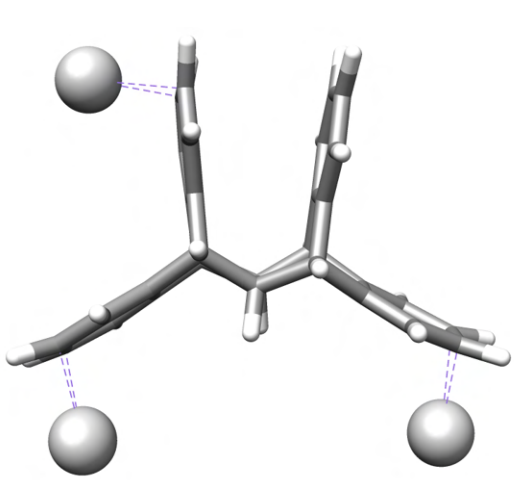
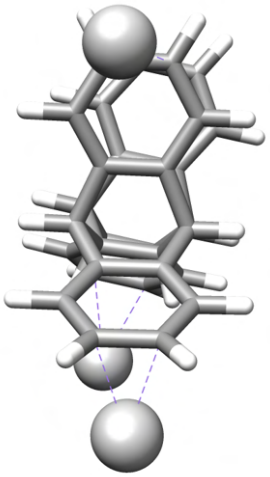


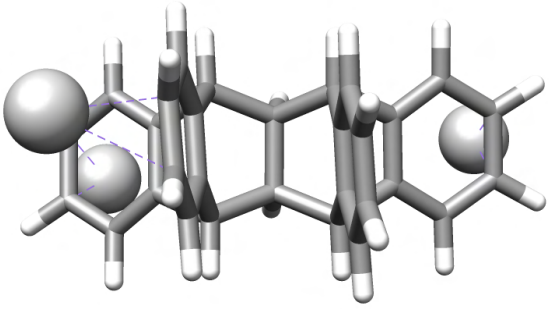
Figure S24: Illustration of system **3k**.



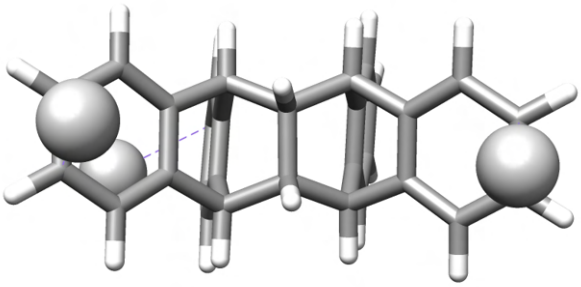
Front view



Side view



Top view



Bottom view

Figure S25: Illustration of system **3l**.

4Ag Systems

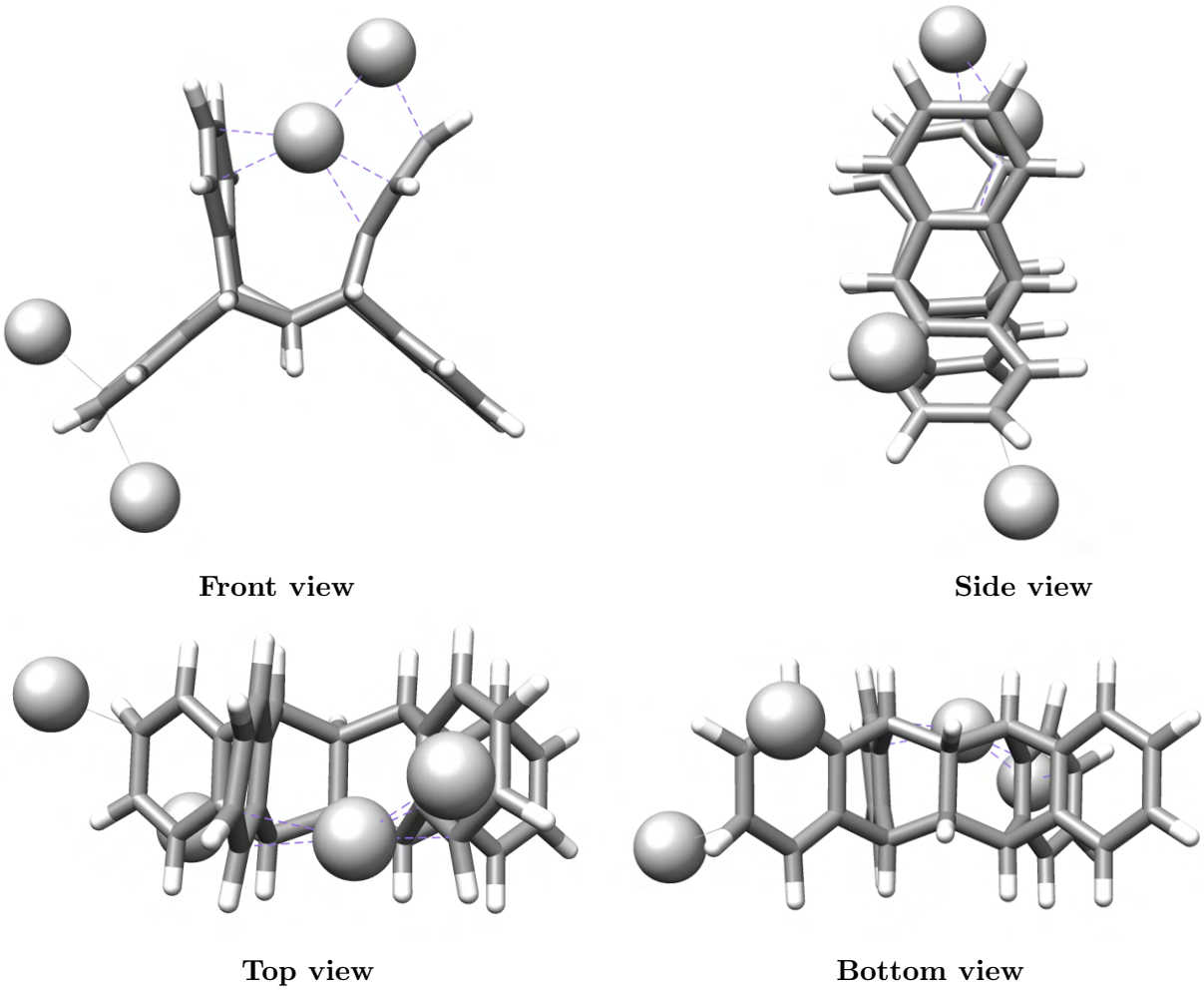
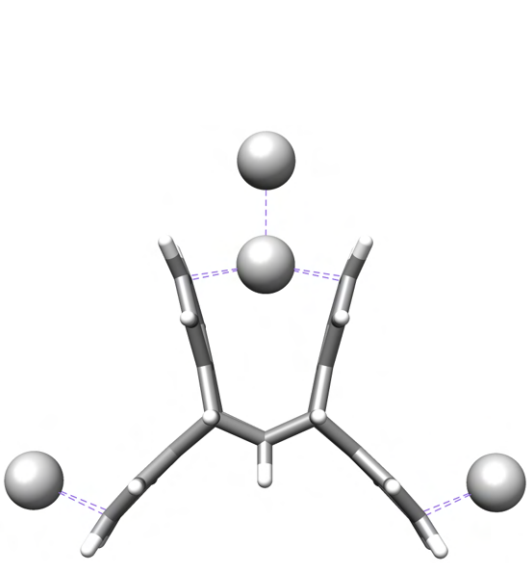
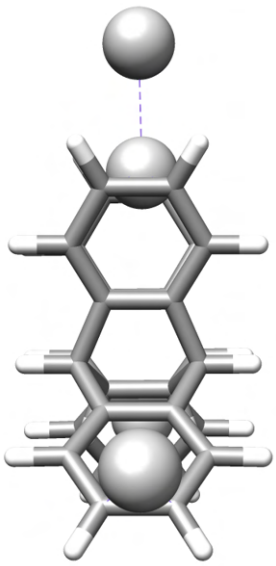


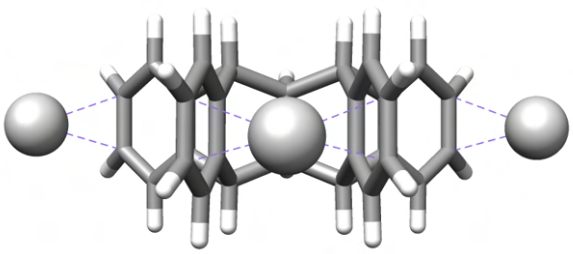
Figure S26: Illustration of system **4a**.



Front view



Side view



Top view

Figure S27: Illustration of system **4b**.

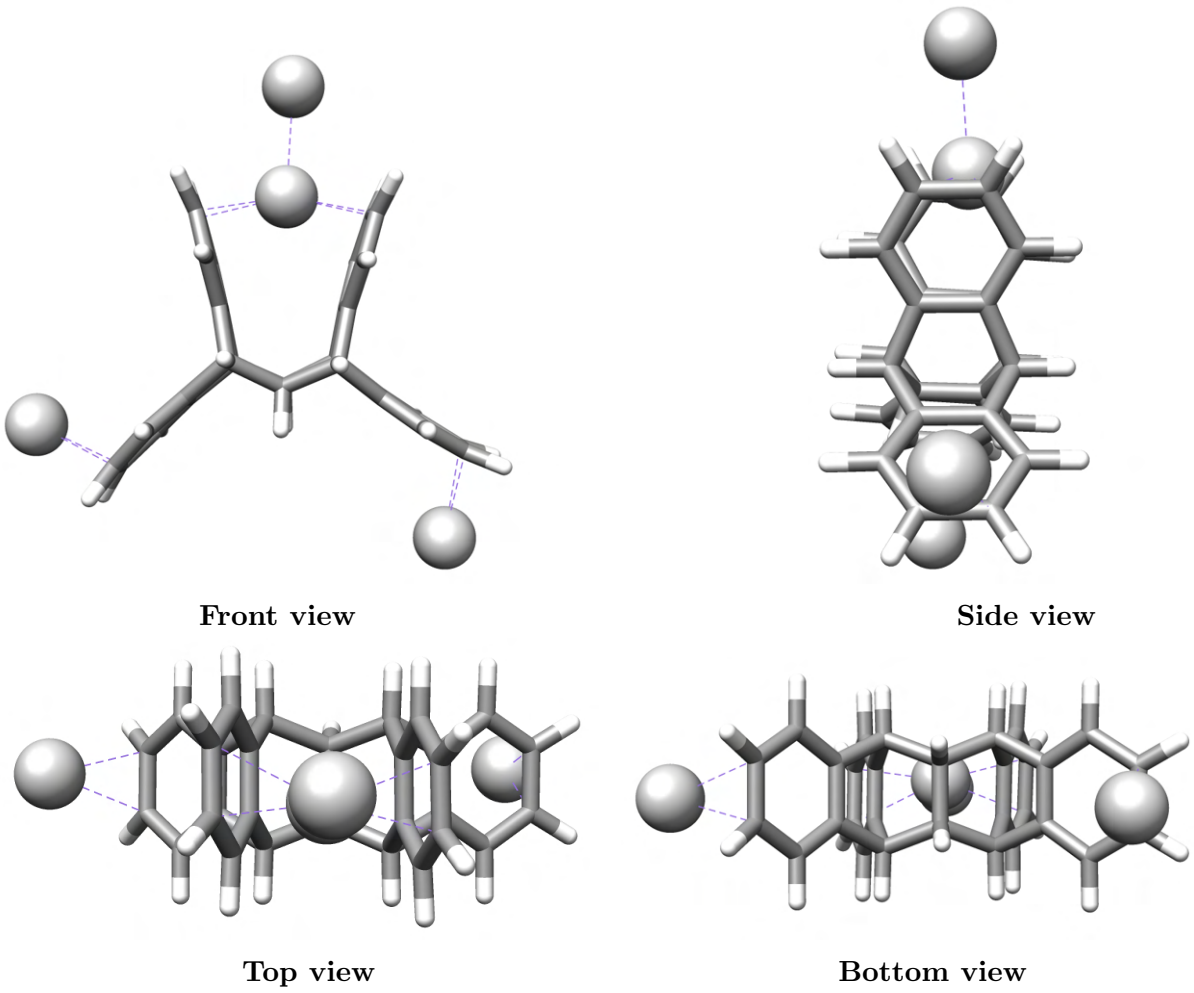


Figure S28: Illustration of system **4c**.

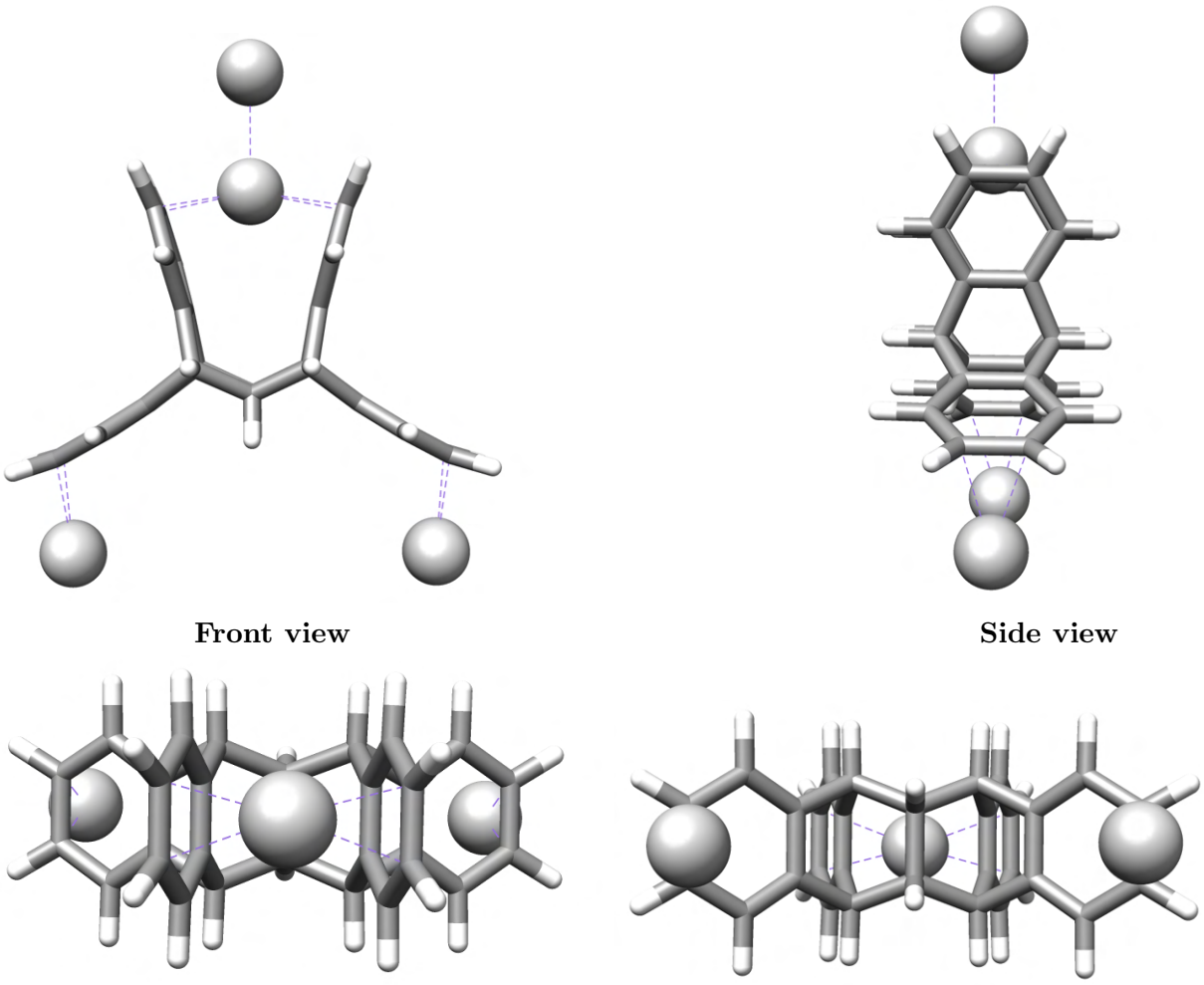
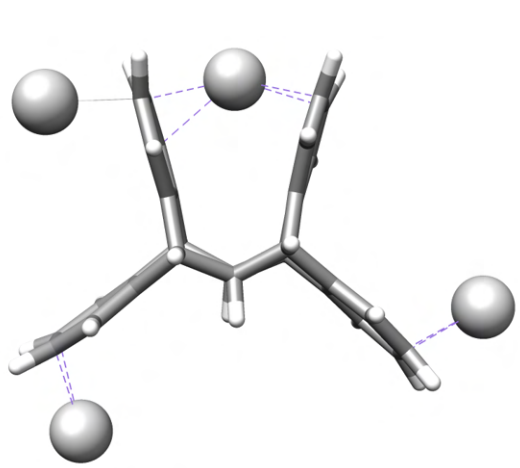
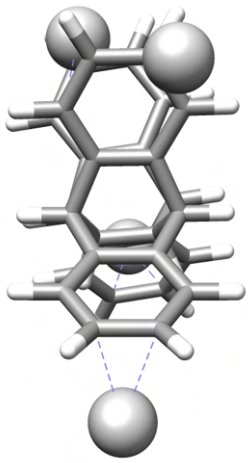


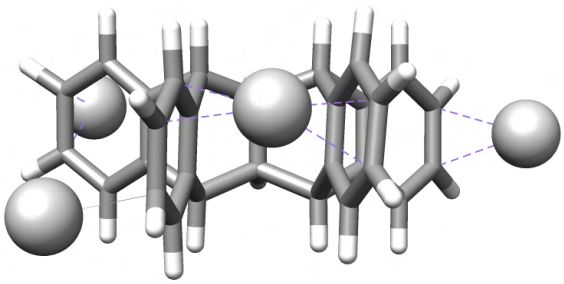
Figure S29: Illustration of system **4d**.



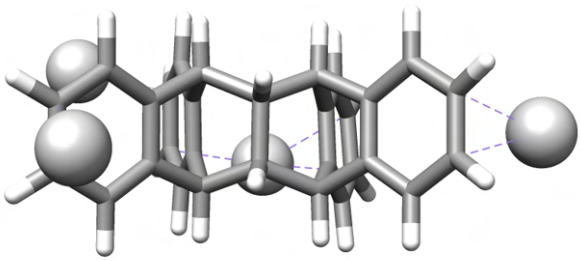
Front view



Side view

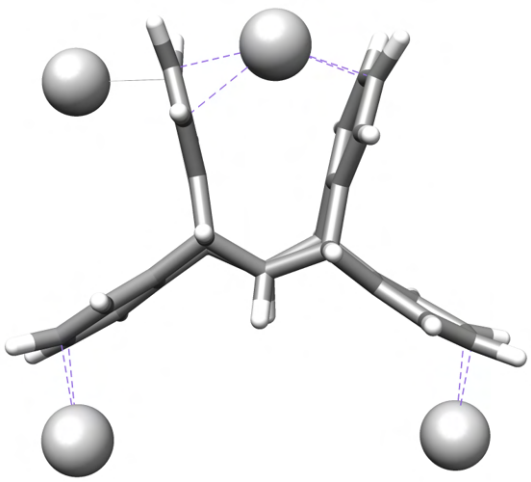


Top view

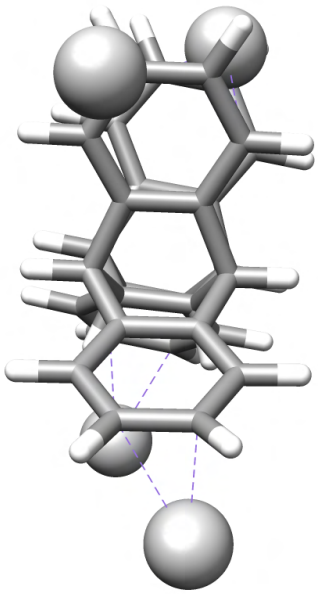


Bottom view

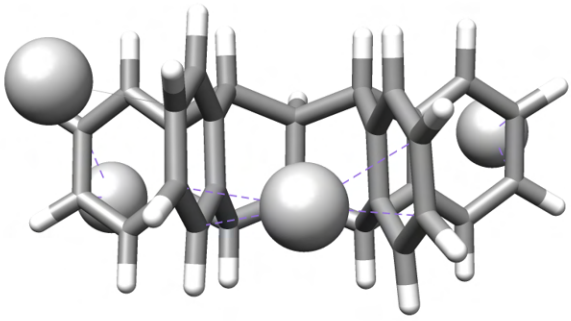
Figure S30: Illustration of system **4e**.



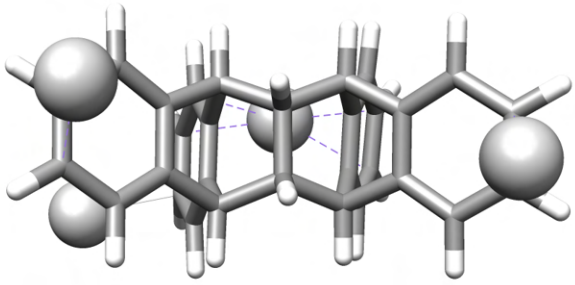
Front view



Side view

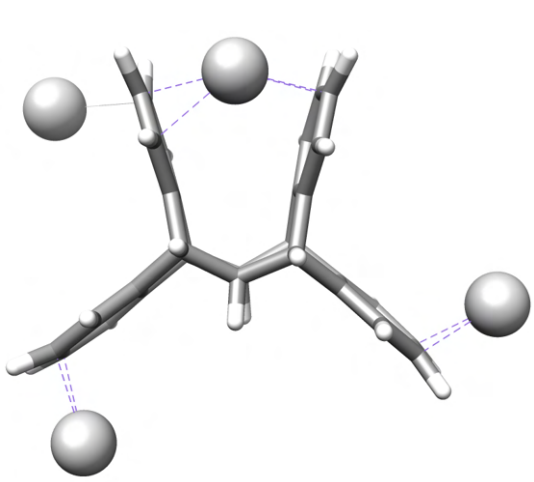


Top view

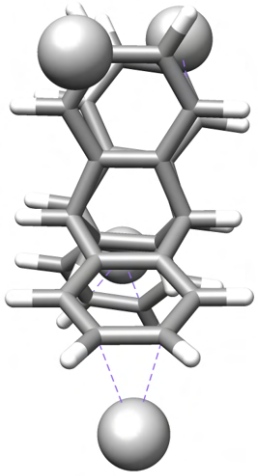


Bottom view

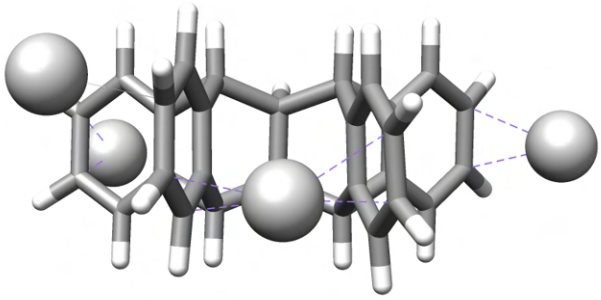
Figure S31: Illustration of system **4f**.



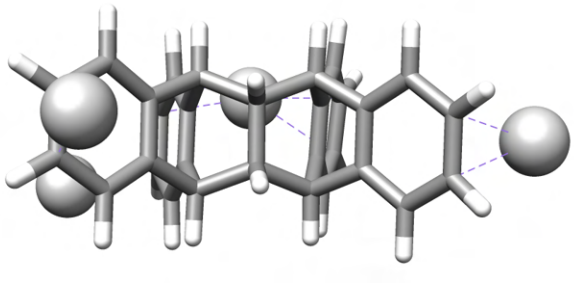
Front view



Side view

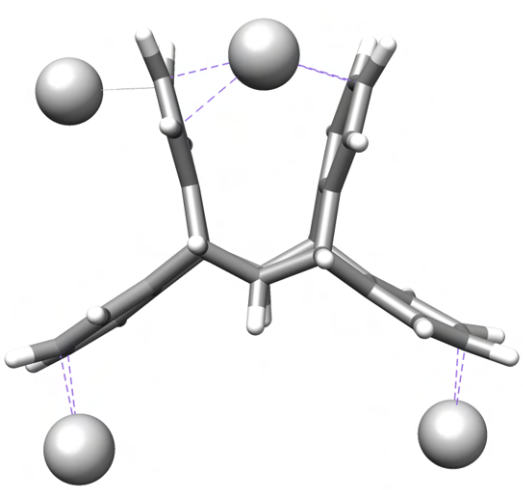


Top view

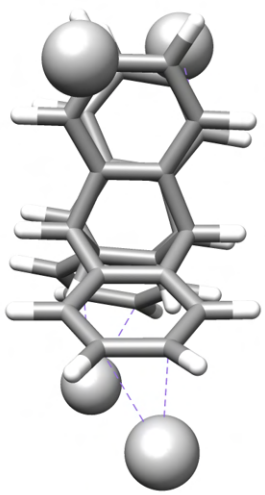


Bottom view

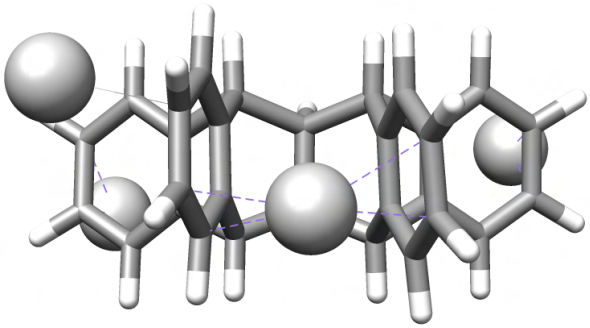
Figure S32: Illustration of system **4g**.



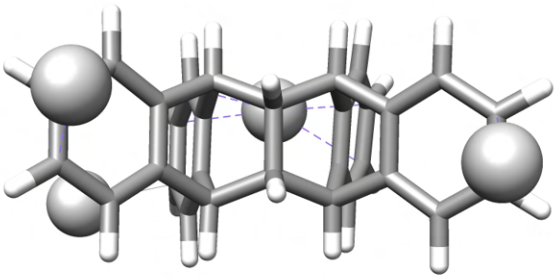
Front view



Side view

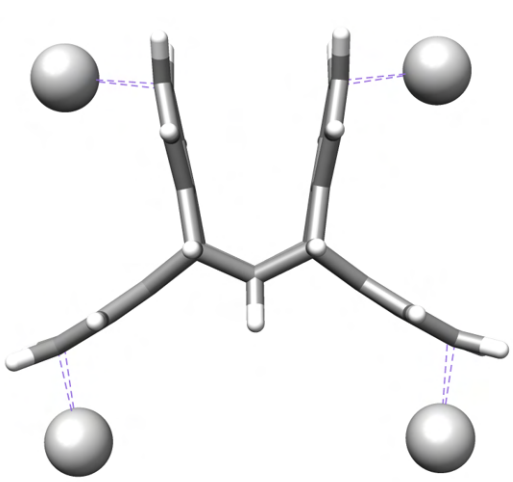


Top view

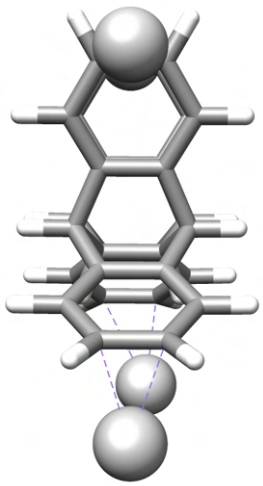


Bottom view

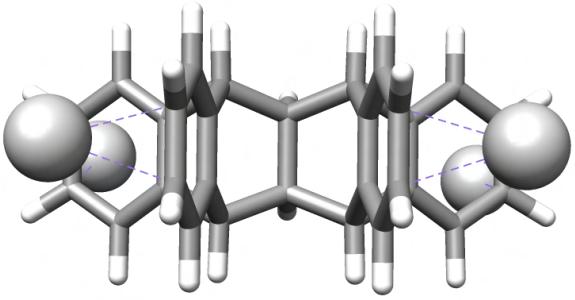
Figure S33: Illustration of system **4h**.



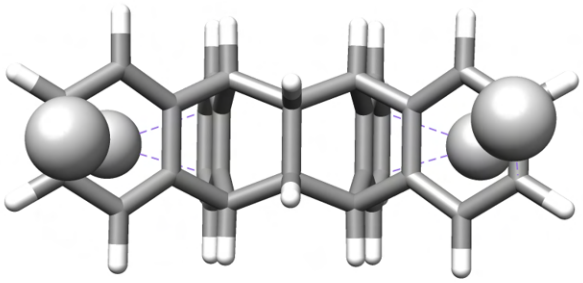
Front view



Side view



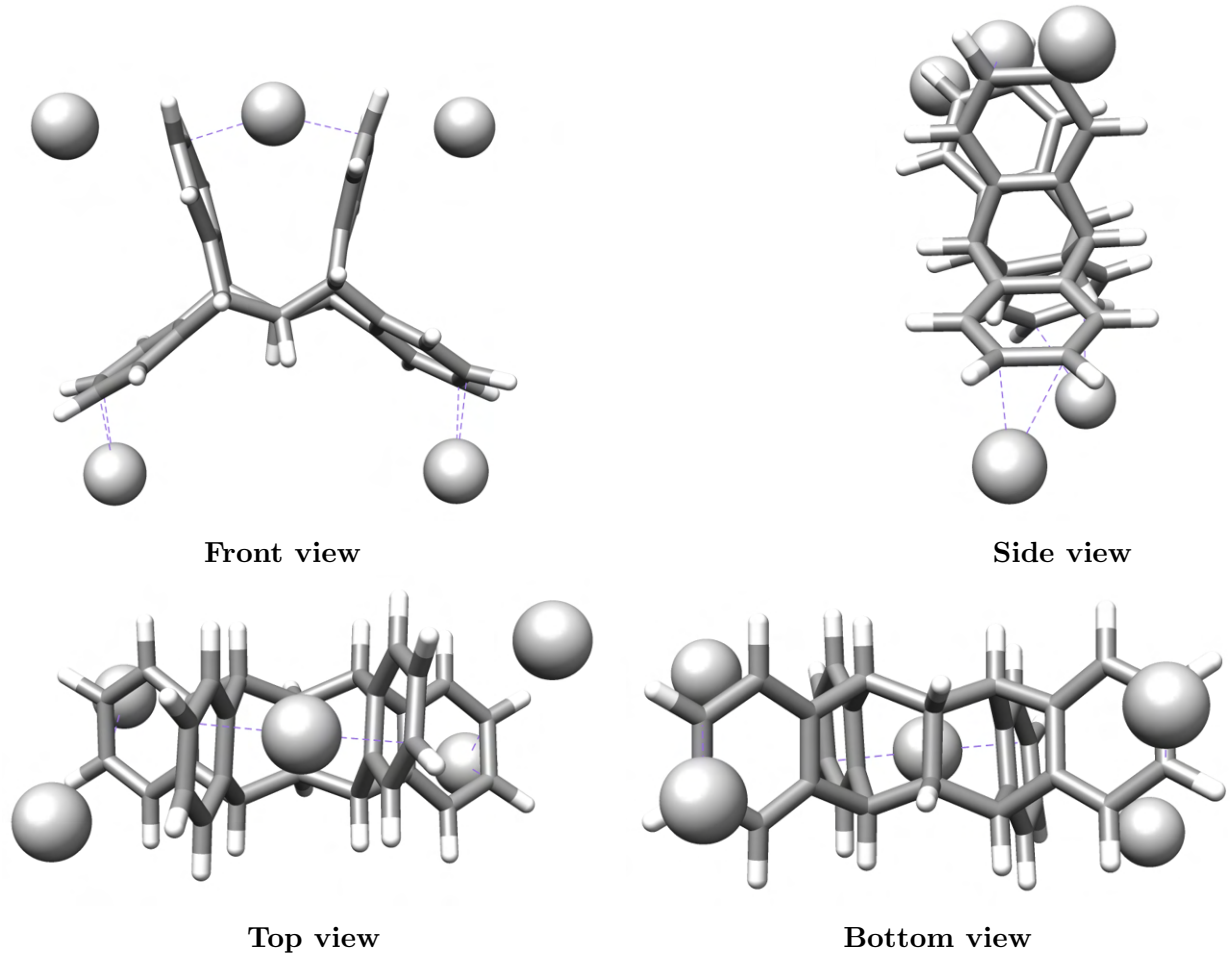
Top view



Bottom view

Figure S34: Illustration of system **4i**.

5Ag System



Front view **Side view**

Top view **Bottom view**

Figure S35: Illustration of system **5**.

Geometrical Parameters

Table S1: Geometric parameters for the janusene-Ag^{+} systems. Atoms labeled according to the Figure 2.

1a		1b		1c		1d	
F-F$^{'}$	3.764	F-F$^{'}$	3.766	F-F$^{'}$	3.355	F-F$^{'}$	3.443
A-F$_{\beta 1}$	2.405	B-F$_{\beta 1}$	2.306	C-F$_{\beta 1}$	3.795	D-L$_{\beta 1}$	2.971
A-F$_{\beta 2}$	2.333	B-F$_{\beta 2}$	2.447	C-F$_{\beta 2}$	3.357	D-L$_{\beta 2}$	3.516
A-F$^{'}_{\beta 1}$	2.532	B-F$^{'}_{\beta 1}$	2.286	C-L$_{\beta 1}$	3.846	D-C*	3.013
A-F$^{'}_{\beta 2}$	2.292	B-F$^{'}_{\beta 2}$	2.597	C-L$_{\beta 2}$	3.460	D-C$^{*'}$	3.511
A-C*	4.987	B-C*	4.869				
A-C$^{*'}$	4.895	B-C$^{*'}$	5.006				

Table S2: Geometric parameters for the [janusene-Ag_2]$^{2+}$ systems. Atoms labeled according to the Figure 2.

2a		2b		2c		2d		2e	
F-F$^{'}$	3.942	F-F$^{'}$	3.775	F-F$^{'}$	3.761	F-F$^{'}$	3.761	F-F$^{'}$	3.767
A-B	2.806	A-F$_{\beta 1}$	2.614	A-F$_{\beta 1}$	2.438	B-F$_{\beta 1}$	2.434	B-F$_{\beta 1}$	2.309
A-F$_{\beta 1}$	2.403	A-F$_{\beta 2}$	2.302	A-F$_{\beta 2}$	2.327	B-F$_{\beta 2}$	2.358	B-F$_{\beta 2}$	2.585
A-F$_{\beta 2}$	3.128	A-F$^{'}_{\beta 1}$	2.470	A-F$^{'}_{\beta 1}$	2.569	B-F$^{'}_{\beta 1}$	2.446	B-F$^{'}_{\beta 1}$	2.332
A-F$^{'}_{\beta 1}$	2.407	A-F$^{'}_{\beta 2}$	2.307	A-F$^{'}_{\beta 2}$	2.290	B-F$^{'}_{\beta 2}$	2.320	B-F$^{'}_{\beta 2}$	2.418
A-F$^{'}_{\beta 2}$	3.136	A-C*	5.035	A-C*	5.034	B-C*	5.019	B-C*	4.932
A-C*	4.448	A-C$^{*'}$	4.895	A-C$^{*'}$	4.914	B-C$^{*'}$	4.957	B-C$^{*'}$	5.041
A-C$^{*'}$	4.917	C-F$_{\beta 1}$	6.375	D-L$_{\beta 1}$	2.355	C-F$_{\beta 1}$	4.065	D-L$_{\beta 1}$	2.357
B-F$_{\beta 1}$	3.131	C-F$_{\beta 2}$	6.395	D-L$_{\beta 2}$	2.350	C-F$_{\beta 2}$	4.061	D-L$_{\beta 2}$	2.347
B-F$_{\beta 2}$	2.405	C-L$_{\beta 1}$	2.328	D-C*	5.066	C-L$_{\beta 1}$	3.417	D-C*	5.064
B-F$^{'}_{\beta 1}$	3.117	C-L$_{\beta 2}$	2.386	D-C$^{*'}$	5.108	C-L$_{\beta 2}$	3.434	D-C$^{*'}$	5.093
B-F$^{'}_{\beta 2}$	2.393								
B-C*	4.922								
B-C$^{*'}$	4.458								

2f		2g		2h		2i	
F-F$^{'}$	3.271	F-F$^{'}$	3.484	F-F$^{'}$	3.458	F-F$^{'}$	3.428
C-F$_{\beta 1}$	2.662	C-F$_{\beta 1}$	3.885	C-F$_{\beta 1}$	3.675	D-L$_{\beta 1}$	2.327
C-F$_{\beta 2}$	2.250	C-F$_{\beta 2}$	3.283	C-F$_{\beta 2}$	3.03	D-L$_{\beta 2}$	2.351
C-L$_{\beta 1}$	6.586	C-L$_{\beta 1}$	3.689	C-L$_{\beta 1}$	3.792	D-C*	5.378
C-L$_{\beta 2}$	6.496	C-L$_{\beta 2}$	3.071	C-L$_{\beta 2}$	3.197	D-C$^{*'}$	5.464
D-L$_{\beta 1}$	2.371	E-F$^{'}_{\beta 1}$	3.433	F-L$^{'}_{\beta 1}$	2.338	F-L$^{'}_{\beta 1}$	2.355
D-L$_{\beta 2}$	2.349	E-F$^{'}_{\beta 2}$	3.885	F-L$^{'}_{\beta 2}$	2.352	F-L$^{'}_{\beta 2}$	2.326
D-C*	4.882	E-L$^{'}_{\beta 1}$	3.399	F-C*	5.291	F-C*	5.465
D-C$^{*'}$	5.042	E-L$^{'}_{\beta 2}$	3.842	F-C$^{*'}$	5.247	F-C$^{*'}$	5.376

Table S3: Geometric parameters for the [janusene-Ag_3]$^{3+}$ systems. Atoms labeled according to the Figure 2.

3a		3b		3c		3d		3e		3f	
F-F$'$	3.837	F-F$'$	3.828	F-F$'$	3.789	F-F$'$	3.762	F-F$'$	3.752	F-F$'$	3.745
A-B	2.731	A-B	2.736	A-F$_{\beta1}$	2.333	A-F$_{\beta1}$	2.310	A-F$_{\beta1}$	2.337	A-F$_{\beta1}$	2.610
A-F$_{\beta1}$	2.329	A-F$_{\beta1}$	2.618	A-F$_{\beta2}$	2.919	A-F$_{\beta2}$	2.568	A-F$_{\beta2}$	2.460	A-F$_{\beta2}$	2.309
A-F$_{\beta2}$	2.451	A-F$_{\beta2}$	2.298	A-F$'_{\beta1}$	2.295	A-F$'_{\beta1}$	2.312	A-F$'_{\beta1}$	2.314	A-F$'_{\beta1}$	2.451
A-F$'_{\beta1}$	2.284	A-F$'_{\beta1}$	2.452	A-F$'_{\beta2}$	2.435	A-F$'_{\beta2}$	2.510	A-F$'_{\beta2}$	2.549	A-F$'_{\beta2}$	2.335
A-F$'_{\beta2}$	2.654	A-F$'_{\beta2}$	2.318	A-C*	4.890	A-C*	4.955	A-C*	4.984	A-C*	5.104
A-C*	4.76 0	A-C*	4.888	A-C*$'$	5.115	A-C*$'$	5.090	A-C*$'$	5.091	A-C*$'$	4.981
A-C*$'$	4.897	A-C*$'$	4.761	C-F$_{\beta1}$	2.970	C-F$_{\beta1}$	6.377	C-F$_{\beta1}$	6.334	D-L$_{\beta1}$	2.363
B-F$_{\beta1}$	4.163	B-F$_{\beta1}$	4.165	C-F$_{\beta2}$	2.297	C-F$_{\beta2}$	6.372	C-F$_{\beta2}$	6.362	D-L$_{\beta2}$	2.361
B-F$_{\beta2}$	4.060	B-F$_{\beta2}$	3.957	C-L$_{\beta1}$	6.328	C-L$_{\beta1}$	2.393	C-L$_{\beta1}$	2.373	D-C*	5.575
B-F$'_{\beta1}$	3.467	B-F$'_{\beta1}$	3.868	C-L$_{\beta2}$	6.070	C-L$_{\beta2}$	2.344	C-L$_{\beta2}$	2.373	D-C*$'$	5.539
B-F$'_{\beta2}$	3.784	B-F$'_{\beta2}$	3.833	D-L$_{\beta1}$	2.443	E-F$'_{\beta1}$	6.407	F-L$'_{\beta1}$	2.361	F-L$'_{\beta1}$	2.355
B-C*	7.475	B-C*	7.562	D-L$_{\beta2}$	2.334	E-F$'_{\beta2}$	6.412	F-L$'_{\beta2}$	2.367	F-L$'_{\beta2}$	2.365
B-C*$'$	7.480	B-C*$'$	7.494	D-C*	5.119	E-L$'_{\beta1}$	2.402	F-C*	5.441	F-C*	5.523
C-F$_{\beta1}$	6.717	D-L$_{\beta1}$	2.375	D-C*$'$	5.174	E-L$'_{\beta2}$	2.340	F-C*$'$	5.460	F-C*$'$	5.574
C-F$_{\beta2}$	6.748	D-L$_{\beta2}$	2.369								
C-L$_{\beta1}$	2.377	D-C*	5.365								
C-L$_{\beta2}$	2.368	D-C*$'$	5.326								

3g		3h		3i		3j		3k		3l	
F-F$'$	3.777	F-F$'$	3.758	F-F$'$	3.759	F-F$'$	3.739	F-F$'$	3.546	F-F$'$	3.317
B-F$_{\beta1}$	2.311	B-F$_{\beta1}$	2.490	B-F$_{\beta1}$	2.312	B-F$_{\beta1}$	2.329	C-F$_{\beta1}$	2.454	C-F$_{\beta1}$	2.619
B-F$_{\beta2}$	2.791	B-F$_{\beta2}$	2.320	B-F$_{\beta2}$	2.575	B-F$_{\beta2}$	2.480	C-F$_{\beta2}$	2.325	C-F$_{\beta2}$	2.272
B-F$'_{\beta1}$	2.313	B-F$'_{\beta1}$	2.526	B-F$'_{\beta1}$	2.308	B-F$'_{\beta1}$	2.306	C-L$_{\beta1}$	6.529	C-L$_{\beta1}$	6.345
B-F$'_{\beta2}$	2.410	B-F$'_{\beta2}$	2.315	B-F$'_{\beta2}$	2.577	B-F$'_{\beta2}$	2.589	C-L$_{\beta2}$	6.494	C-L$_{\beta2}$	6.268
B-C*	4.914	B-C*	5.083	B-C*	4.955	B-C*	4.987	D-L$_{\beta1}$	2.364	D-L$_{\beta1}$	2.356
B-C*$'$	5.099	B-C*$'$	4.969	B-C*$'$	5.113	B-C*$'$	5.116	D-L$_{\beta2}$	2.380	D-L$_{\beta2}$	2.381
C-F$_{\beta1}$	3.297	C-F$_{\beta1}$	6.391	C-F$_{\beta1}$	6.336	D-L$_{\beta1}$	2.378	D-C*	5.287	D-C*	5.348
C-F$_{\beta2}$	2.505	C-F$_{\beta2}$	6.379	C-F$_{\beta2}$	6.347	D-L$_{\beta2}$	2.344	D-C*$'$	5.324	D-C*$'$	5.499
C-L$_{\beta1}$	5.685	C-L$_{\beta1}$	2.353	C-L$_{\beta1}$	2.388	D-C*	5.582	E-F$'_{\beta1}$	3.277	F-L$'_{\beta1}$	2.343
C-L$_{\beta2}$	5.283	C-L$_{\beta2}$	2.387	C-L$_{\beta2}$	2.358	D-C*$'$	5.531	E-F$'_{\beta2}$	3.864	F-L$'_{\beta2}$	2.358
D-L$_{\beta1}$	2.351	E-F$'_{\beta1}$	6.405	F-L$'_{\beta1}$	2.337	F-L$'_{\beta1}$	2.349	E-L$'_{\beta1}$	3.026	F-C*	5.659
D-L$_{\beta2}$	2.424	E-F$'_{\beta2}$	6.392	F-L$'_{\beta2}$	2.396	F-L$'_{\beta2}$	2.365	E-L$'_{\beta2}$	3.652	F-C*$'$	5.549
D-C*	5.111	E-L$'_{\beta1}$	2.365	F-C*	5.427	F-C*	5.529				
D-C*$'$	5.240	E-L$'_{\beta2}$	2.370	F-C*$'$	5.449	F-C*$'$	5.559				

Table S4: Geometric parameters for the [janusene-Ag_4]$^{4+}$ and [janusene-Ag_5]$^{5+}$ systems. Atoms labeled according to the Figure 2.

4a		4b		4c		4d		4e	
F-F$'$	4.073	F-F$'$	3.823	F-F$'$	3.827	F-F$'$	3.792	F-F$'$	3.803
A-B	2.853	A-B	2.813	A-B	2.817	A-B	2.822	A-F$_{\beta1}$	2.961
A-F$_{\beta1}$	2.330	A-F$_{\beta1}$	2.349	A-F$_{\beta1}$	2.297	A-F$_{\beta1}$	2.411	A-F$_{\beta2}$	2.362
A-F$_{\beta2}$	2.816	A-F$_{\beta2}$	2.387	A-F$_{\beta2}$	2.570	A-F$_{\beta2}$	2.334	A-F$'_{\beta1}$	2.501
A-F$'_{\beta1}$	2.846	A-F$'_{\beta1}$	2.332	A-F$'_{\beta1}$	2.351	A-F$'_{\beta1}$	2.401	A-F$'_{\beta2}$	2.306
A-F$'_{\beta2}$	3.552	A-F$'_{\beta2}$	2.403	A-F$'_{\beta2}$	2.380	A-F$'_{\beta2}$	2.336	A-C*	5.172
A-C*	4.180	A-C*	4.755	A-C*	4.770	A-C*	4.839	A-C*$'$	4.922
A-C*$'$	4.667	A-C*$'$	4.791	A-C*$'$	4.855	A-C*$'$	4.799	C-F$_{\beta1}$	2.321
B-F$_{\beta1}$	4.388	B-F$_{\beta1}$	3.967	B-F$_{\beta1}$	4.029	B-F$_{\beta1}$	4.041	C-F$_{\beta2}$	2.990
B-F$_{\beta2}$	4.202	B-F$_{\beta2}$	3.965	B-F$_{\beta2}$	4.148	B-F$_{\beta2}$	3.978	C-L$_{\beta1}$	5.982
B-F$'_{\beta1}$	2.335	B-F$'_{\beta1}$	3.944	B-F$'_{\beta1}$	3.949	B-F$'_{\beta1}$	4.010	C-L$_{\beta2}$	6.243
B-F$'_{\beta2}$	2.697	B-F$'_{\beta2}$	3.974	B-F$'_{\beta2}$	3.840	B-F$'_{\beta2}$	3.958	D-L$_{\beta1}$	2.430
B-C*	6.485	B-C*	7.555	B-C*	7.585	B-C*	7.634	D-L$_{\beta2}$	2.385
B-C*$'$	6.551	B-C*$'$	7.567	B-C*$'$	7.588	B-C*$'$	7.601	D-C*	5.568
C-F$_{\beta1}$	6.716	C-F$_{\beta1}$	6.756	C-F$_{\beta1}$	6.727	D-L$_{\beta1}$	2.402	D-C*$'$	5.444
C-F$_{\beta2}$	6.517	C-F$_{\beta2}$	6.774	C-F$_{\beta2}$	6.671	D-L$_{\beta2}$	2.378	E-F$'_{\beta1}$	6.599
C-L$_{\beta1}$	3.098	C-L$_{\beta1}$	2.387	C-L$_{\beta1}$	2.452	D-C*	5.695	E-F$'_{\beta2}$	6.503
C-L$_{\beta2}$	2.365	C-L$_{\beta2}$	2.410	C-L$_{\beta2}$	2.363	D-C*$'$	5.686	E-L$'_{\beta1}$	2.420
D-L$_{\beta1}$	2.362	E-F$'_{\beta1}$	6.765	F-L$'_{\beta1}$	2.433	F-L$'_{\beta1}$	2.373	E-L$'_{\beta2}$	2.378
D-L$_{\beta2}$	3.077	E-F$'_{\beta2}$	6.788	F-L$'_{\beta2}$	2.364	F-L$'_{\beta2}$	2.425		
D-C*	5.146	E-L$'_{\beta1}$	2.375	F-C*	5.643	F-C*	5.686		
D-C*$'$	5.449	E-L$'_{\beta2}$	2.430	F-C*$'$	5.564	F-C*$'$	5.714		

4f		4g		4h		4i		5	
F-F$'$	3.779	F-F$'$	3.907	F-F$'$	3.780	F-F$'$	3.565	F-F$'$	3.958
A-F$_{\beta1}$	2.364	B-F$_{\beta1}$	2.361	B-F$_{\beta1}$	2.357	C-F$_{\beta1}$	2.425	A-F$_{\beta1}$	2.739
A-F$_{\beta2}$	2.972	B-F$_{\beta2}$	2.994	B-F$_{\beta2}$	2.957	C-F$_{\beta2}$	2.378	A-F$_{\beta2}$	2.338
A-F$'_{\beta1}$	2.310	B-F$'_{\beta1}$	2.296	B-F$'_{\beta1}$	2.303	C-L$_{\beta1}$	6.176	A-F$'_{\beta1}$	2.339
A-F$'_{\beta2}$	2.473	B-F$'_{\beta2}$	2.554	B-F$'_{\beta2}$	2.450	C-L$_{\beta2}$	6.159	A-F$'_{\beta2}$	2.778
A-C*	4.963	B-C*	4.862	B-C*	4.936	D-L$_{\beta1}$	2.398	A-C*	5.053
A-C*$'$	5.204	B-C*$'$	5.144	B-C*$'$	5.186	D-L$_{\beta2}$	2.380	A-C*$'$	5.064
C-F$_{\beta1}$	2.976	C-F$_{\beta1}$	2.968	C-F$_{\beta1}$	2.991	D-C*	5.629	C-F$_{\beta1}$	2.694
C-F$_{\beta2}$	2.321	C-F$_{\beta2}$	2.319	C-F$_{\beta2}$	2.322	D-C*$'$	5.622	C-F$_{\beta2}$	3.350
C-L$_{\beta1}$	6.178	C-L$_{\beta1}$	6.257	C-L$_{\beta1}$	6.204	E-F$'_{\beta1}$	2.409	C-L$_{\beta1}$	6.445
C-L$_{\beta2}$	5.928	C-L$_{\beta2}$	6.000	C-L$_{\beta2}$	5.946	E-F$'_{\beta2}$	2.389	C-L$_{\beta2}$	6.671
D-L$_{\beta1}$	2.309	D-L$_{\beta1}$	2.384	D-L$_{\beta1}$	2.315	E-L$'_{\beta1}$	6.160	D-L$_{\beta1}$	2.655
D-L$_{\beta2}$	2.649	D-L$_{\beta2}$	2.427	D-L$_{\beta2}$	2.654	E-L$'_{\beta2}$	6.157	D-L$_{\beta2}$	2.352
D-C*	5.495	D-C*	5.447	D-C*	5.502	F-L$'_{\beta1}$	2.315	D-C*	6.001
D-C*$'$	5.768	D-C*$'$	5.563	D-C*$'$	5.765	F-L$'_{\beta2}$	2.577	D-C*$'$	5.679
F-L$'_{\beta1}$	2.426	E-F$'_{\beta1}$	6.523	F-L$'_{\beta1}$	2.440	F-C*	5.614	E-F$'_{\beta1}$	3.434
F-L$'_{\beta2}$	2.355	E-F$'_{\beta2}$	6.618	F-L$'_{\beta2}$	2.358	F-C*$'$	5.730	E-F$'_{\beta2}$	2.775
F-C*	5.814	E-L$'_{\beta1}$	2.379	F-C*	5.837			E-L$'_{\beta1}$	6.855
F-C*$'$	5.668	E-L$'_{\beta2}$	2.413	F-C*$'$	5.694			E-L$'_{\beta2}$	6.623
								F-L$'_{\beta1}$	2.438
								F-L$'_{\beta2}$	2.433
								F-C*	5.664
								F-C*$'$	5.853

Atomic Charges

Table S5: Atomic charges from Natural Population Analysis (NPA) for the janusene-Ag^+ systems. Values in a.u.

Fragment	1a	1b	1c	1d
Janusene	0.168	0.169	0.112	0.163
Ag^+	0.832	0.831	0.888	0.837

Table S6: Atomic charges from Natural Population Analysis (NPA) for the [janusene-Ag_2]$^{2+}$ systems. Values in a.u.

2a		2b		2c		2d		2e	
Janusene	0.326	Janusene	0.291	Janusene	0.287	Janusene	0.216	Janusene	0.288
A	0.837	A	0.847	A	0.849	B	0.854	B	0.848
B	0.837	C	0.862	D	0.864	C	0.930	D	0.864
2f		2g		2h		2i			
Janusene	0.341	Janusene	0.198	Janusene	0.282	Janusene	0.351		
C	0.804	C	0.880	C	0.867	D	0.825		
D	0.855	E	0.922	F	0.851	F	0.824		

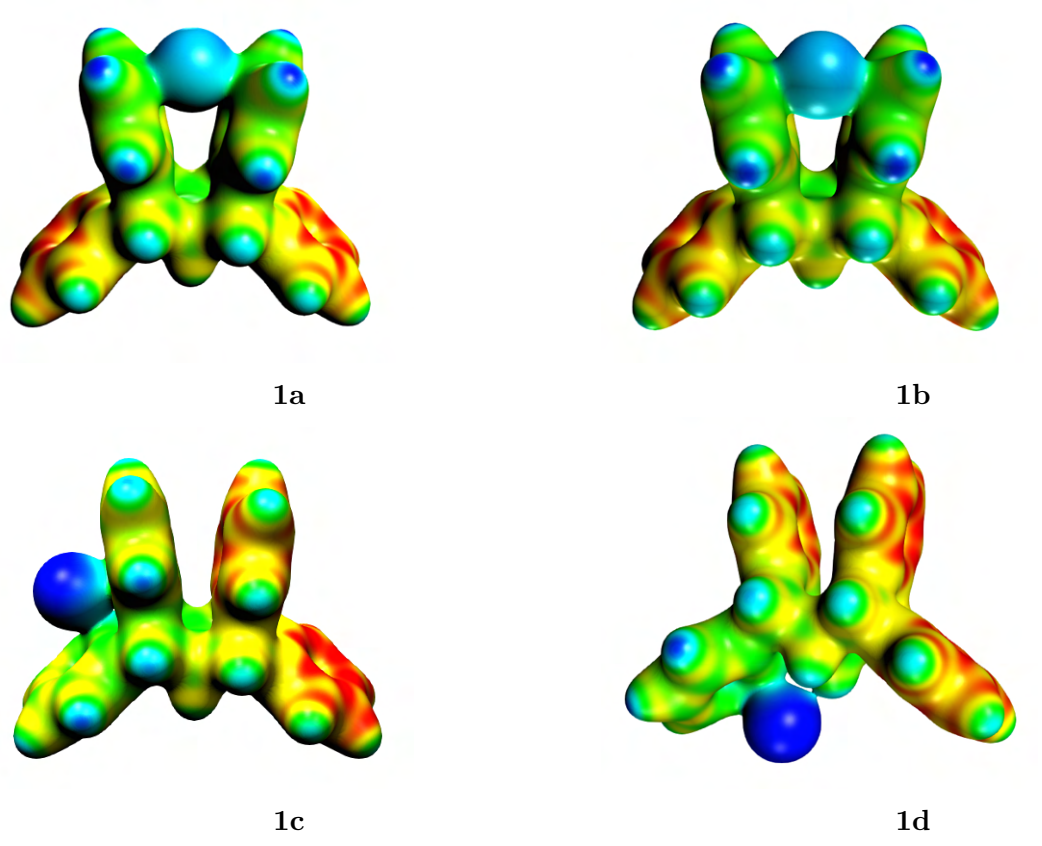
Table S7: Atomic charges from Natural Population Analysis (NPA) for the [janusene-Ag_3]$^{3+}$ systems. Values in a.u.

3a		3b		3c		3d		3e		3f	
Janusene	0.794	Janusene	0.784	Janusene	0.346	Janusene	0.356	Janusene	0.364	Janusene	0.383
A	0.648	A	0.660	A	0.871	A	0.865	A	0.865	A	0.866
B	0.667	B	0.666	C	0.888	C	0.890	C	0.890	D	0.875
C	0.891	D	0.890	D	0.895	E	0.889	F	0.881	F	0.876
3g		3h		3i		3j		3k		3l	
Janusene	0.342	Janusene	0.355	Janusene	0.365	Janusene	0.382	Janusene	0.324	Janusene	0.402
B	0.871	B	0.865	B	0.864	B	0.866	C	0.891	C	0.857
C	0.889	C	0.890	C	0.890	D	0.876	D	0.891	D	0.879
D	0.898	E	0.890	F	0.881	F	0.876	E	0.894	F	0.862

Table S8: Atomic charges from Natural Population Analysis (NPA) for the $[janusene\text{-}Ag_4]^{4+}$ and $[janusene\text{-}Ag_5]^{5+}$ systems. Values in a.u.

4a		4b		4c		4d		4e	
Janusene	0.525	Janusene	0.653	Janusene	0.660	Janusene	0.664	Janusene	0.363
A	0.787	A	0.677	A	0.671	A	0.673	A	0.887
B	0.828	B	0.842	B	0.845	B	0.850	C	0.924
C	0.931	C	0.914	C	0.913	D	0.907	D	0.914
D	0.929	E	0.914	F	0.911	F	0.906	E	0.912
4f		4g		4h		4i		5	
Janusene	0.386	Janusene	0.364	Janusene	0.388	Janusene	0.380	Janusene	0.355
A	0.888	B	0.888	B	0.888	C	0.912	A	0.891
C	0.922	C	0.922	C	0.922	D	0.901	C	0.954
D	0.904	D	0.914	D	0.903	E	0.912	D	0.920
F	0.900	E	0.912	F	0.899	F	0.895	E	0.956
								F	0.924

Molecular Electrostatic Potential (MEP)



1a **1b**

1c **1d**

Figure S36: Electrostatic potential surfaces mapped as an electron density surface of 0.030 [0.140(red) - 0.360(blue)] for the $[janusene{-}Ag]^+$. In all cases, arbitrary units (a.u.) are used.

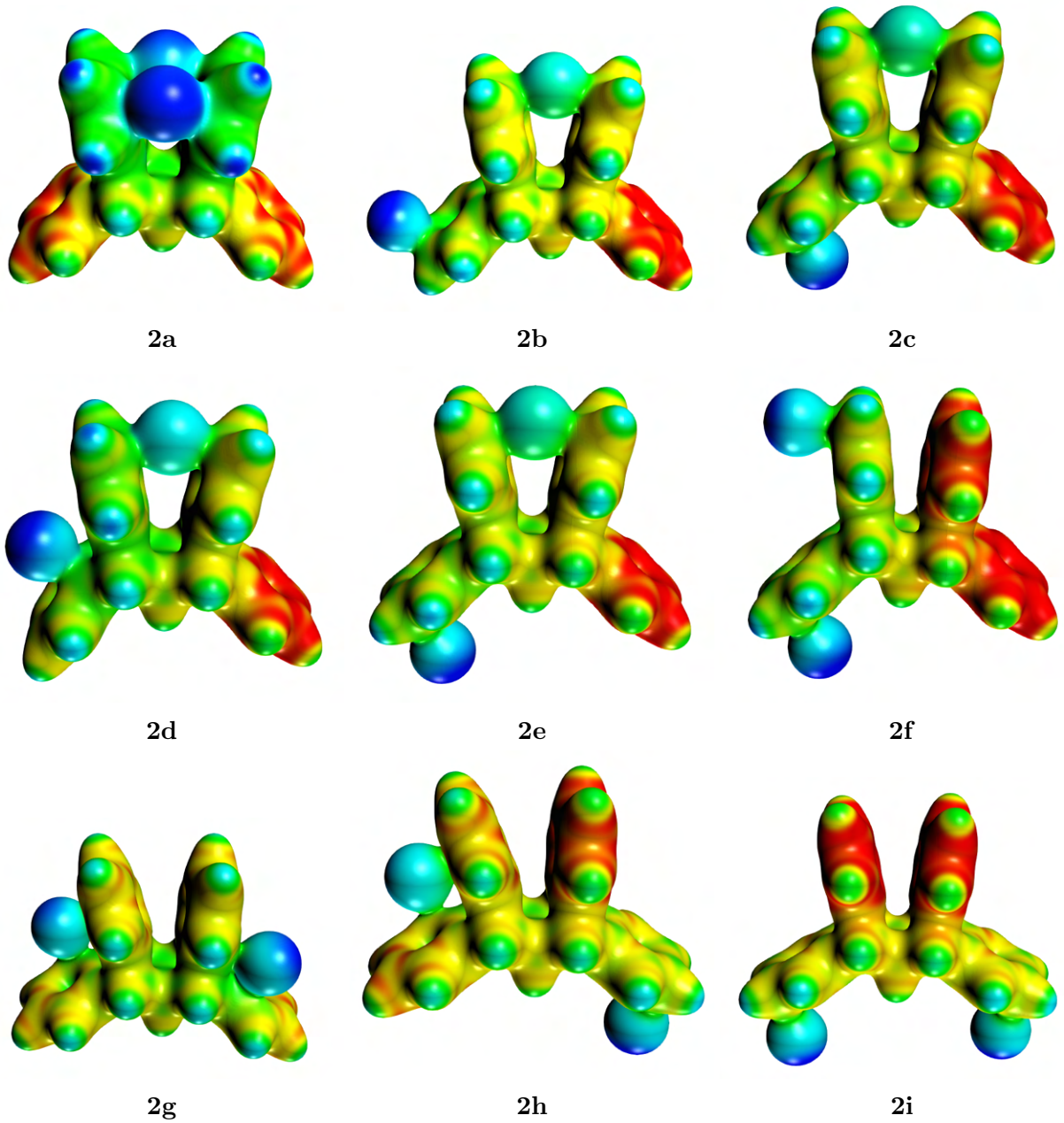


Figure S37: Electrostatic potential surfaces mapped as an electron density surface of 0.030 [0.240(red) - 0.490(blue)] for the [janusene−Ag_2]$^{2+}$. In all cases, arbitrary units (a.u.) are used.

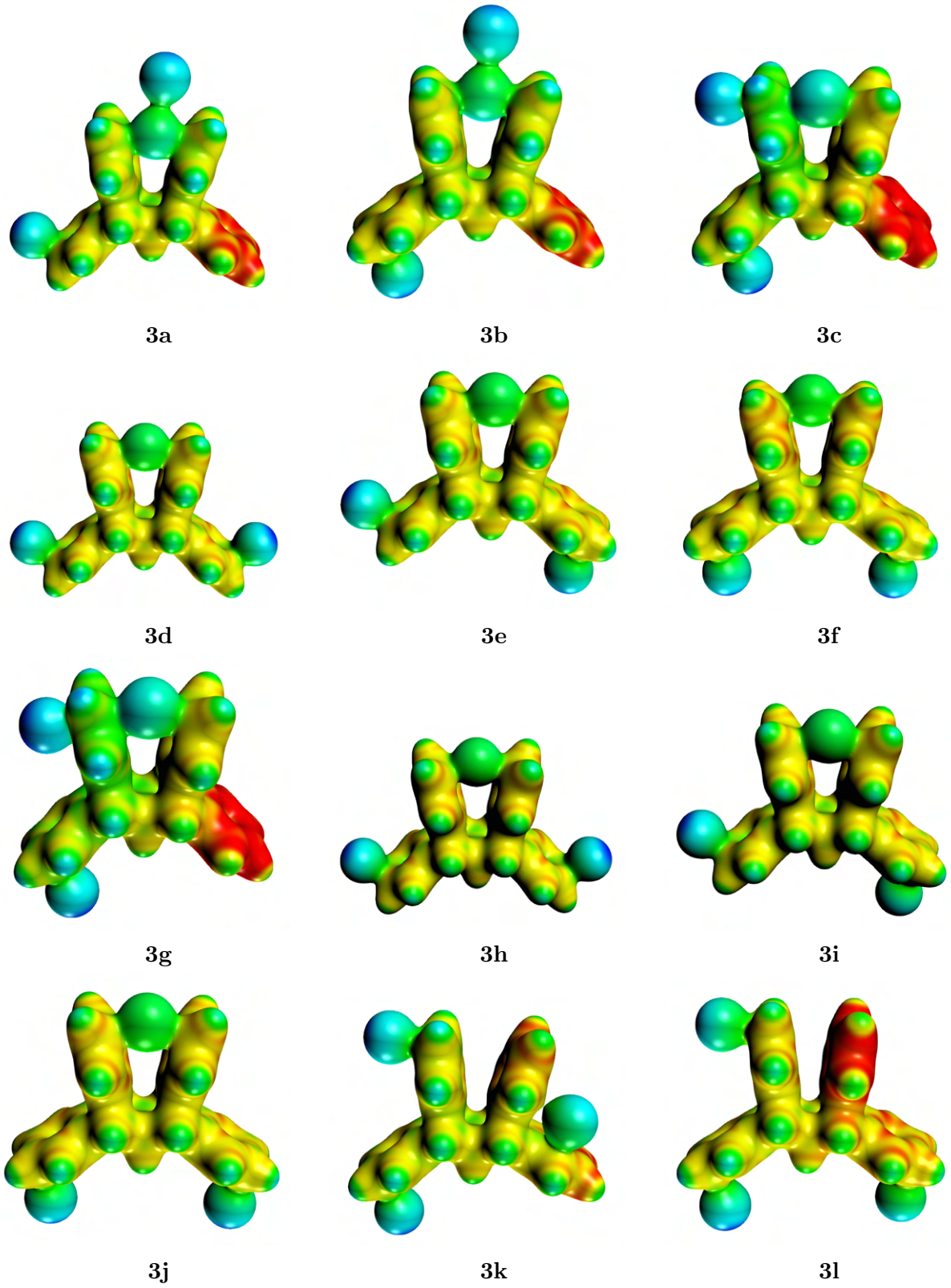


Figure S38: Electrostatic potential surfaces mapped as an electron density surface of 0.030 [0.330(red) - 0.610(blue)] for the [janusene−Ag_3]$^{3+}$. In all cases, arbitrary units (a.u.) are used.

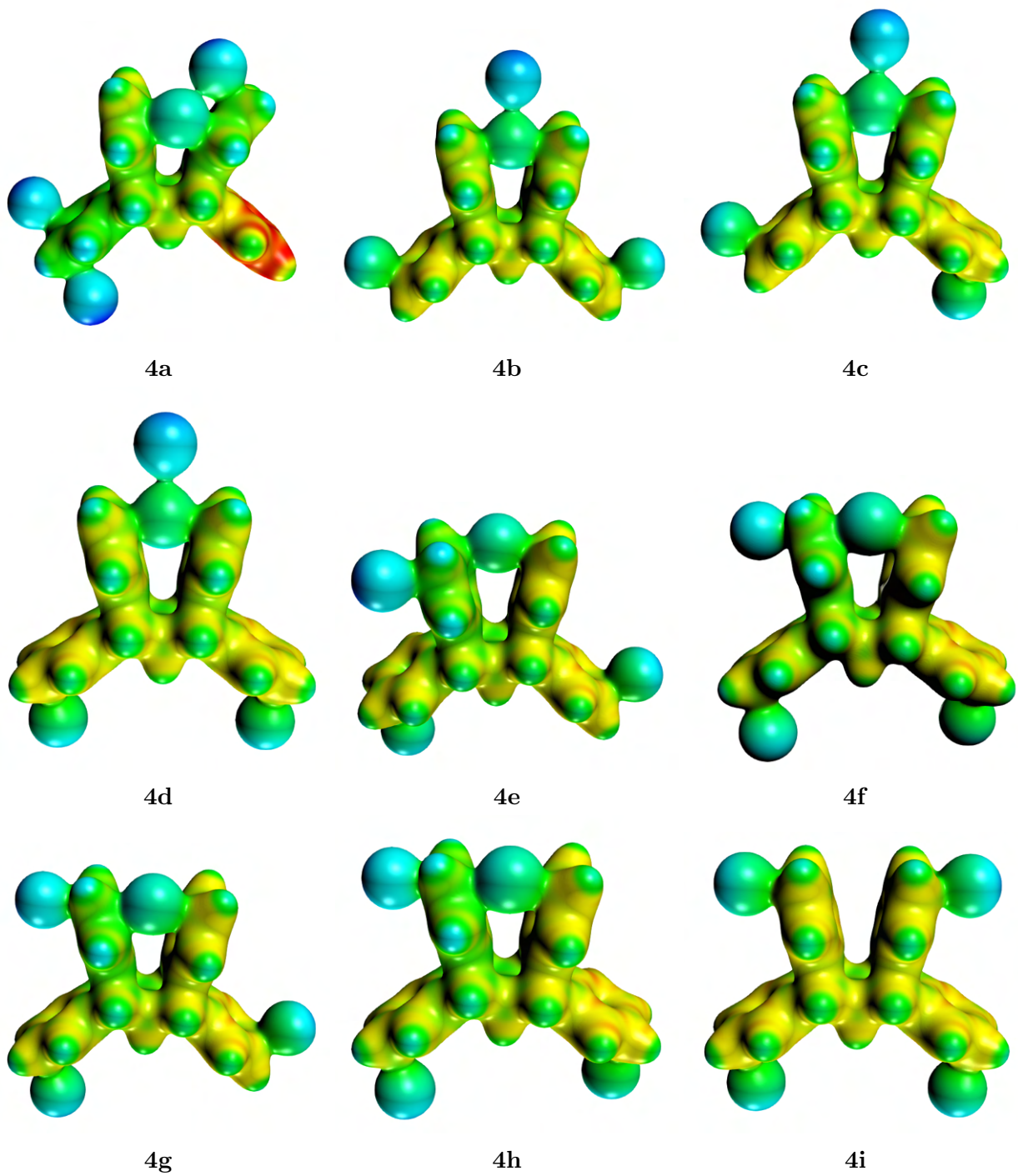


Figure S39: Electrostatic potential surfaces mapped as an electron density surface of 0.030 [0.390(red) - 0.710(blue)] for the [janusene$-Ag_2]^{4+}$. In all cases, arbitrary units (a.u.) are used.

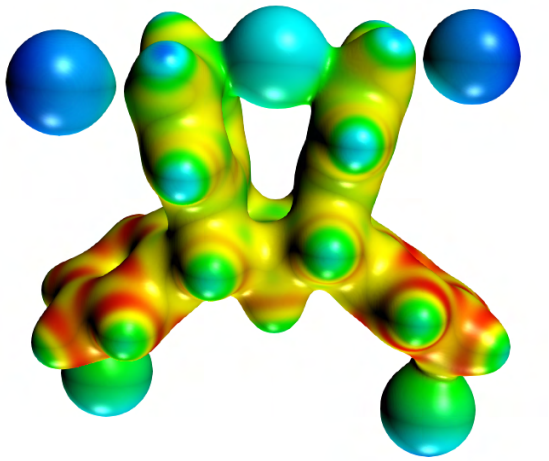


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Figure S40: Electrostatic potential surfaces mapped as an electron density surface of 0.030 [0.510(red) - 0.750(blue)] for the [janusene−Ag_5]$^{5+}$. In all cases, arbitrary units (a.u.) are used.

Quantum Theory of Atoms and Molecules (QTAIM)

1Ag Systems

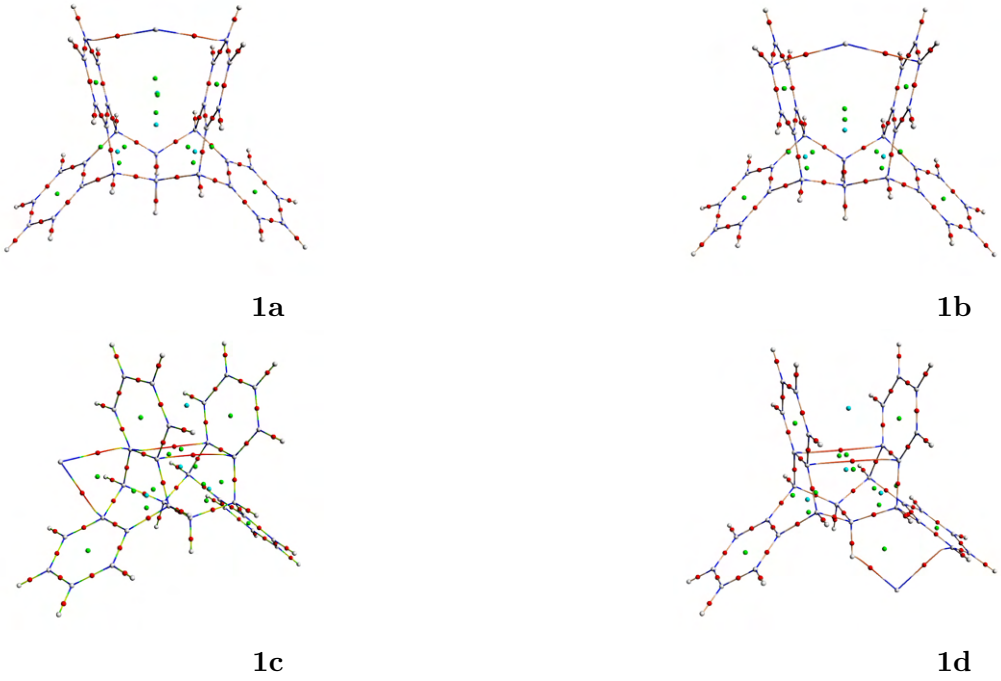


Figure S41: Topological map containing the QTAIM critical points. BCP(red), RCP(green), CCP(light blue) and NCP (white).

Table S9: Electron density (ρ_b), Laplacian of ρ_b ($\nabla^2\rho_b$) and the -G_b/V_b parameter at the BCP for the [janusene−Ag]$^+$ systems.

1a				**1b**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
A$\cdots$F$_{\beta 2}$	0.060	0.152	0.790	B$\cdots$F$_{\beta 1}$	0.062	0.150	0.772
A$\cdots$F$'_{\beta 2}$	0.063	0.146	0.761	B$\cdots$F$'_{\beta 1}$	0.064	0.144	0.754
1c				**1d**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
C$\cdots$F$_{ipso2}$	0.045	0.114	0.831	D$\cdots$L$_{\alpha 2}$	0.058	0.144	0.792
C$\cdots$L$_{ipso2}$	0.043	0.108	0.846	D$\cdots$H$_{C^{*\prime}}$	0.030	0.080	0.920
F$_{ipso1}\cdots$F$'_{ipso1}$	0.012	0.037	1.195	F$_{ipso1}\cdots$F$'_{ipso1}$	0.010	0.034	1.245
F$_{ipso2}\cdots$F$'_{ipso2}$	0.012	0.035	1.199	F$_{ipso2}\cdots$F$'_{ipso2}$	0.010	0.034	1.242

2Ag Systems

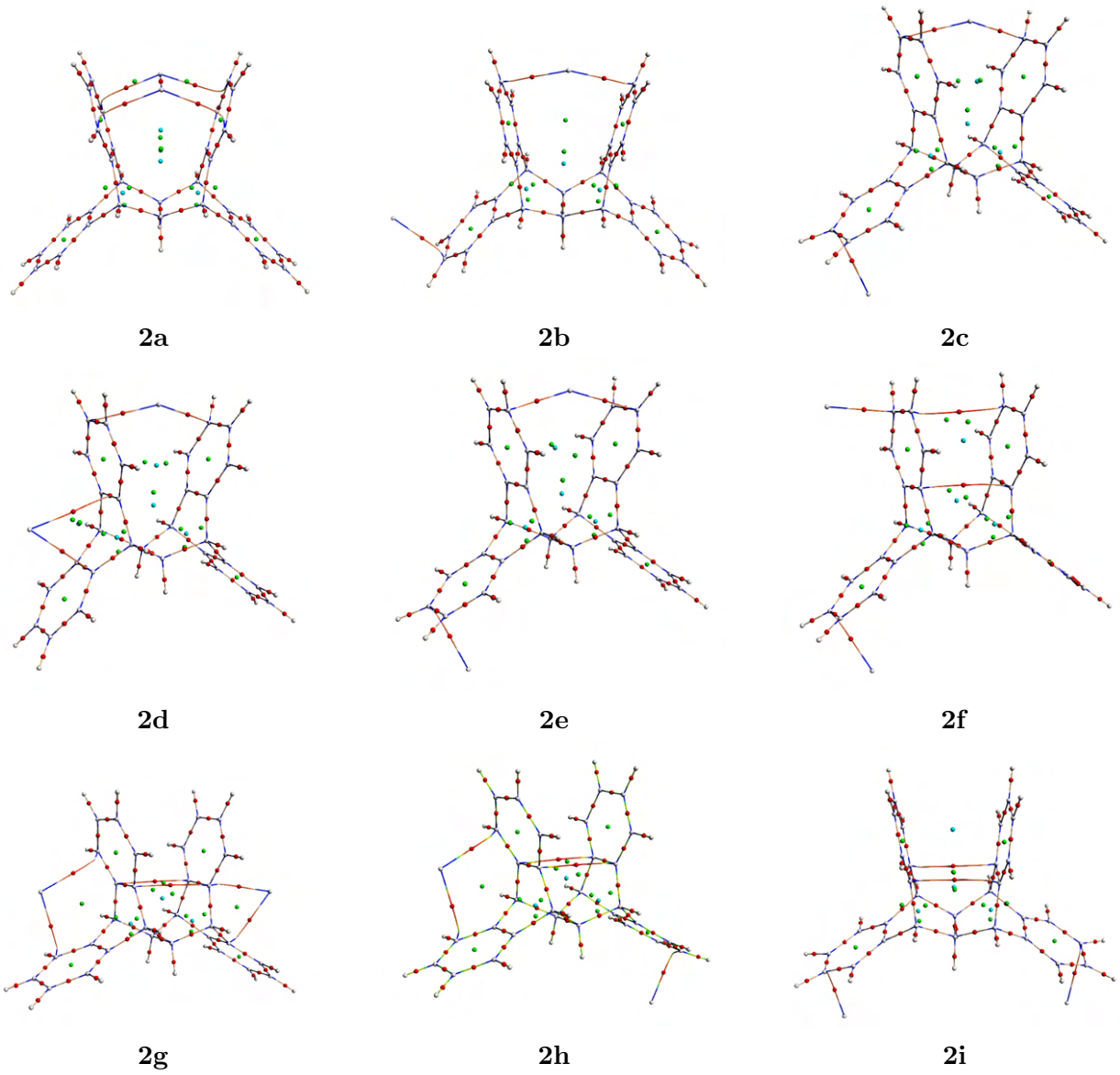


Figure S42: Topological map containing the QTAIM critical points. BCP(red), RCP(green), CCP(light blue) and NCP (white).

Table S10: Electron density (ρ_b), Laplacian of ρ_b ($\nabla^2\rho_b$) and the -G_b/V_b parameter at the BCP for the [janusene$-Ag_2]^{2+}$ systems.

2a				**2b**				**2c**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
A$\cdots$B	0.033	0.090	0.909	A$\cdots$F$_{\beta 2}$	0.062	0.141	0.763	A$\cdots$F$_{\beta 2}$	0.060	0.149	0.785
A$\cdots$F$_{\alpha 1}$	0.056	0.153	0.819	A$\cdots$F$'_{\beta 2}$	0.062	0.148	0.771	A$\cdots$F$'_{\beta 2}$	0.064	0.145	0.759
A$\cdots$F$'_{\alpha 1}$	0.056	0.152	0.820	C$\cdots$L$_{\beta 1}$	0.061	0.152	0.786	D$\cdots$L$_{\beta 2}$	0.060	0.160	0.806
B$\cdots$F$_{\alpha 2}$	0.056	0.152	0.822								
B$\cdots$F$'_{\beta 2}$	0.056	0.153	0.818								
2d				**2e**				**2f**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
B$\cdots$F$_{\beta 2}$	0.057	0.146	0.802	B$\cdots$F$_{\beta 1}$	0.061	0.140	0.767	C$\cdots$F$_{\beta 2}$	0.069	0.138	0.772
B$\cdots$F$'_{\beta 2}$	0.061	0.148	0.779	B$\cdots$F$'_{\beta 1}$	0.060	0.150	0.788	D$\cdots$L$_{\beta 2}$	0.059	0.155	0.800
C$\cdots$L$_{ipso1}$	0.054	0.144	0.819	D$\cdots$L$_{\beta 2}$	0.060	0.159	0.804	F$_{\beta 1}\cdots$F$'_{\beta 2}$	0.006	0.016	1.352
C$\cdots$F$^{BCP}_{ipso1\cdot ipso2}$	0.019	0.055	1.048					F$_{ipso1}\cdots$F$'_{ipso}$	0.012	0.038	1.171
2g				**2h**				**2i**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
C$\cdots$F$_{\alpha 2}$	0.033	0.083	0.897	C$\cdots$F$_{\alpha 2}$	0.046	0.109	0.821	D$\cdots$L$_{\beta 1}$	0.062	0.158	0.791
C$\cdots$L$_{\alpha 2}$	0.046	0.114	0.829	C$\cdots$L$_{\alpha 2}$	0.036	0.090	0.882	F$\cdots$L$'_{\beta 2}$	0.062	0.157	0.788
E$\cdots$F$'_{ipso1}$	0.041	0.104	0.858	F$\cdots$L$'_{\beta 1}$	0.060	0.160	0.798	F$_{ipso1}\cdots$F$'_{ipso1}$	0.011	0.036	1.226
E$\cdots$L$'_{ipso1}$	0.043	0.109	0.848	F$_{ipso1}\cdots$F$'_{ipso1}$	0.012	0.038	1.202	F$_{ipso2}\cdots$F$'_{ipso2}$	0.011	0.036	1.225
F$_{ipso1}\cdots$F$'_{ipso1}$	0.011	0.036	1.217	F$_{ipso2}\cdots$F$'_{ipso2}$	0.012	0.037	1.191				
F$_{ipso2}\cdots$F$'_{ipso2}$	0.012	0.036	1.200								

3Ag Systems

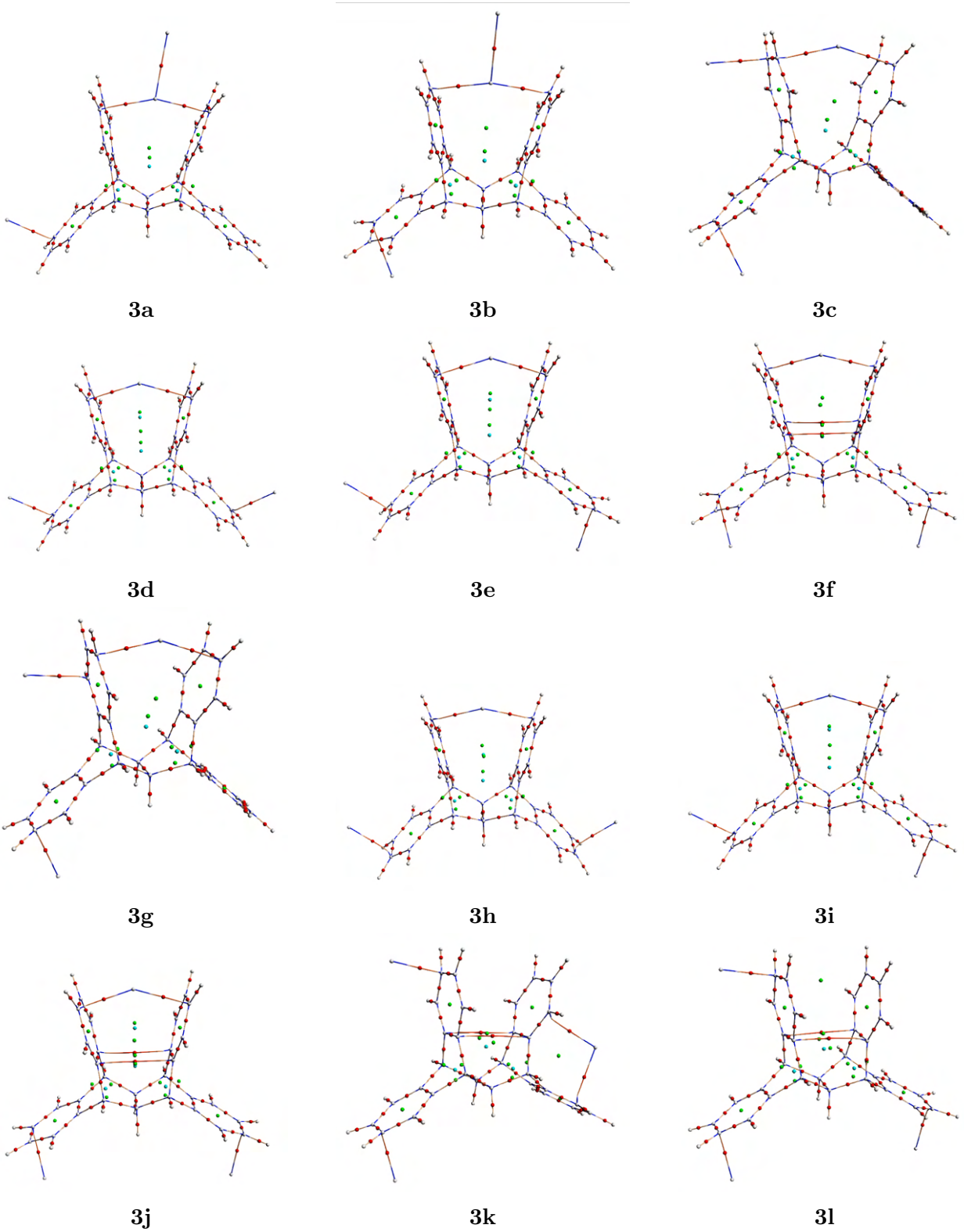


Figure S43: Topological map containing the QTAIM critical points. BCP(red), RCP(green), CCP(light blue) and NCP (white).

Table S11: Electron density (ρ_b), Laplacian of ρ_b ($\nabla^2\rho_b$) and the -G_b/V_b parameter at the BCP for the [janusene−Ag_3]$^{3+}$ systems.

3a				**3b**				**3c**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
A$\cdots$B	0.041	0.094	0.830	A$\cdots$B	0.040	0.093	0.830	A$\cdots$F$_{\beta1}$	0.057	0.135	0.781
A$\cdots$F$_{\beta1}$	0.060	0.140	0.772	A$\cdots$F$_{\beta2}$	0.063	0.133	0.744	A$\cdots$F$'_{\beta1}$	0.064	0.152	0.769
A$\cdots$F$'_{\beta1}$	0.065	0.136	0.736	A$\cdots$F$'_{\beta2}$	0.061	0.140	0.762	C$\cdots$F$_{\beta2}$	0.062	0.131	0.747
C$\cdots$L$_{\beta2}$	0.057	0.155	0.815	D$\cdots$L$_{\beta2}$	0.057	0.156	0.816	D$\cdots$L$_{\beta2}$	0.059	0.144	0.783
3d				**3e**				**3f**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
A$\cdots$F$_{\beta1}$	0.061	0.141	0.768	A$\cdots$F$_{\beta1}$	0.058	0.144	0.788	A$\cdots$F$_{\beta2}$	0.061	0.139	0.764
A$\cdots$F$'_{\beta1}$	0.061	0.144	0.774	A$\cdots$F$'_{\beta1}$	0.060	0.140	0.769	A$\cdots$F$'_{\beta2}$	0.059	0.146	0.787
C$\cdots$L$_{\beta2}$	0.059	0.150	0.796	C$\cdots$L$_{\beta1}$	0.057	0.158	0.821	D$\cdots$L$_{\beta2}$	0.058	0.159	0.815
E$\cdots$L$'_{\beta2}$	0.059	0.149	0.793	F$\cdots$L$'_{\beta1}$	0.058	0.158	0.813	F$\cdots$L$'_{\beta1}$	0.058	0.157	0.808
3g				**3h**				**3i**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
A$\cdots$F$_{\beta1}$	0.060	0.138	0.770	B$\cdots$F$_{\beta2}$	0.060	0.144	0.777	B$\cdots$F$_{\beta1}$	0.060	0.140	0.770
A$\cdots$F$'_{\beta1}$	0.062	0.153	0.778	B$\cdots$F$'_{\beta2}$	0.060	0.142	0.773	B$\cdots$F$'_{\beta1}$	0.061	0.140	0.766
C$\cdots$F$_{\alpha2}$	0.059	0.136	0.770	C$\cdots$L$_{\beta1}$	0.058	0.152	0.802	C$\cdots$L$_{\beta2}$	0.058	0.151	0.805
D$\cdots$L$_{\beta1}$	0.057	0.145	0.796	E$\cdots$L$'_{\beta1}$	0.058	0.158	0.816	F$\cdots$L$'_{\beta1}$	0.059	0.150	0.791
3j				**3k**				**3l**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
B$\cdots$F$_{\beta1}$	0.059	0.144	0.783	C$\cdots$F$_{\beta2}$	0.060	0.142	0.778	C$\cdots$F$_{\beta2}$	0.065	0.137	0.738
B$\cdots$F$'_{\beta1}$	0.061	0.140	0.766	D$\cdots$L$_{\beta1}$	0.057	0.153	0.810	D$\cdots$L$_{\beta1}$	0.058	0.153	0.805
D$\cdots$L$_{\beta2}$	0.059	0.153	0.799	E$\cdots$F$'_{\alpha1}$	0.030	0.076	0.917	F$\cdots$L$'_{\beta1}$	0.060	0.159	0.802
F$\cdots$L$'_{\beta1}$	0.059	0.157	0.806	E$\cdots$L$'_{\alpha1}$	0.046	0.112	0.824	F$_{ipso1}\cdots$F$'_{ipso1}$	0.012	0.038	1.187
				F$_{ipso1}\cdots$F$'_{ipso1}$	0.010	0.033	1.247	F$_{ipso2}\cdots$F$'_{ipso2}$	0.012	0.037	1.204
				F$_{ipso2}\cdots$F$'_{ipso2}$	0.010	0.034	1.243				

4Ag Systems

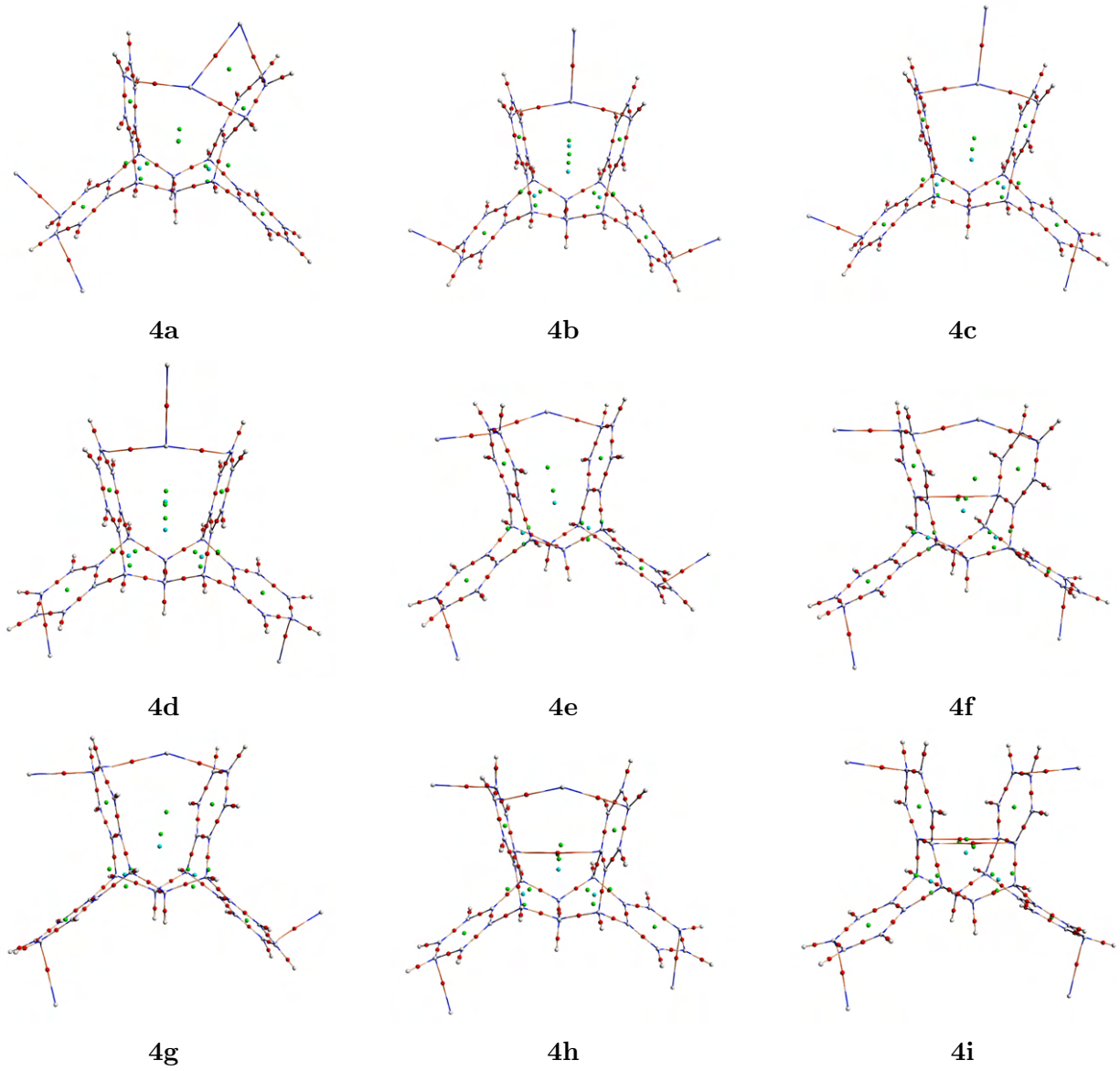
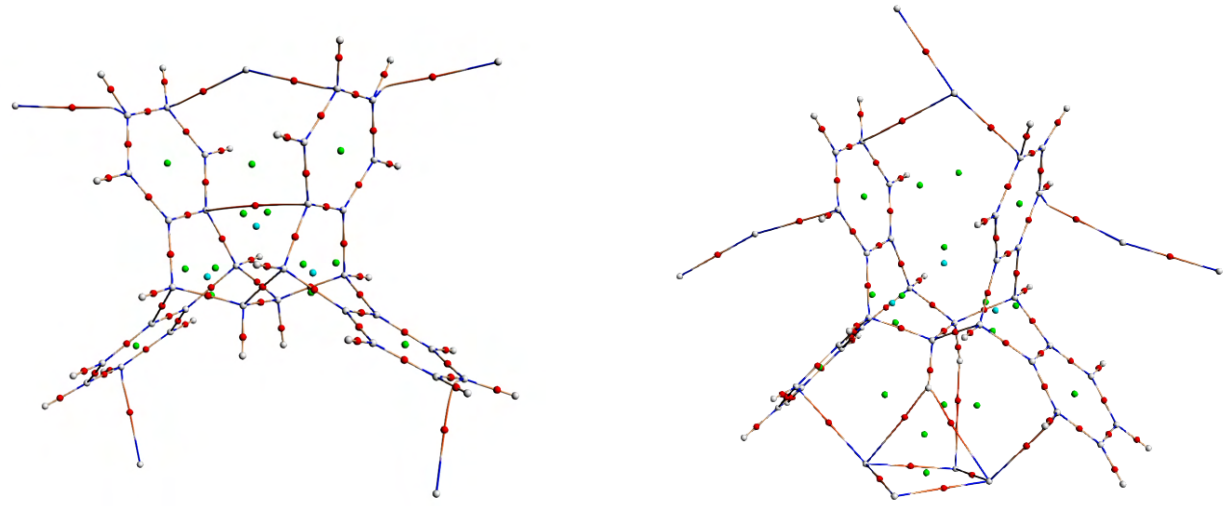


Figure S44: Topological map containing the QTAIM critical points. BCP(red), RCP(green), CCP(light blue) and NCP (white).

Table S12: Electron density (ρ_b), Laplacian of ρ_b ($\nabla^2\rho_b$) and the -G_b/V_b parameter at the BCP for the [janusene$-Ag_4]^{4+}$ systems.

4a				**4b**				**4c**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
A$\cdots$B	0.031	0.075	0.892	A$\cdots$B	0.034	0.078	0.854	A$\cdots$B	0.034	0.077	0.856
A$\cdots$F$_{\beta1}$	0.059	0.148	0.787	A$\cdots$F$_{\beta1}$	0.060	0.145	0.782	A$\cdots$F$_{\beta1}$	0.064	0.134	0.743
A$\cdots$F$'_{\alpha1}$	0.069	0.142	0.728	A$\cdots$F$'_{\beta1}$	0.061	0.144	0.772	A$\cdots$F$'_{\beta1}$	0.059	0.146	0.785
B$\cdots$F$'_{\beta1}$	0.058	0.119	0.746	C$\cdots$L$_{\beta1}$	0.054	0.146	0.821	C$\cdots$L$_{\beta2}$	0.056	0.139	0.800
C$\cdots$L$_{\beta2}$	0.054	0.119	0.778	E$\cdots$L$'_{\beta1}$	0.055	0.142	0.810	F$\cdots$L$'_{\beta2}$	0.056	0.142	0.804
D$\cdots$L$_{\beta1}$	0.054	0.120	0.775								
4d				**4e**				**4f**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
A$\cdots$B	0.034	0.076	0.857	A$\cdots$F$_{\beta2}$	0.054	0.130	0.795	A$\cdots$F$_{\beta1}$	0.054	0.129	0.795
A$\cdots$F$_{\beta2}$	0.060	0.142	0.771	A$\cdots$F$'_{\beta2}$	0.062	0.145	0.769	A$\cdots$F$'_{\beta1}$	0.061	0.146	0.773
A$\cdots$F$'_{\beta2}$	0.060	0.144	0.774	C$\cdots$F$_{\beta1}$	0.058	0.127	0.758	C$\cdots$F$_{\beta2}$	0.059	0.127	0.757
D$\cdots$L$_{\beta2}$	0.055	0.148	0.818	D$\cdots$L$_{\beta2}$	0.054	0.142	0.816	D$\cdots$L$_{\beta1}$	0.060	0.133	0.758
F$\cdots$L$'_{\beta2}$	0.055	0.143	0.810	E$\cdots$L$'_{\beta2}$	0.055	0.144	0.812	F$\cdots$L$'_{\beta2}$	0.057	0.144	0.799
4g				**4h**				**4i**			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b	BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
B$\cdots$F$_{\beta1}$	0.054	0.134	0.798	B$\cdots$F$_{\beta1}$	0.054	0.131	0.792	C$\cdots$F$_{\beta2}$	0.055	0.143	0.812
B$\cdots$F$'_{\beta1}$	0.062	0.143	0.762	B$\cdots$F$'_{\beta1}$	0.062	0.145	0.768	D$\cdots$L$_{\beta2}$	0.055	0.149	0.818
C$\cdots$F$_{\beta2}$	0.059	0.127	0.757	C$\cdots$F$_{\beta2}$	0.058	0.127	0.758	E$\cdots$F$'_{\beta2}$	0.054	0.146	0.821
D$\cdots$L$_{\beta1}$	0.054	0.142	0.817	D$\cdots$L$_{\beta1}$	0.060	0.131	0.760	F$\cdots$L$'_{\beta1}$	0.060	0.135	0.764
E$\cdots$L$'_{\beta1}$	0.055	0.146	0.815	F$\cdots$L$'_{\beta2}$	0.056	0.142	0.799				

5Ag System



5 **5^0**

Figure S45: Topological map containing the QTAIM critical points. BCP(red), RCP(green), CCP(light blue) and NCP (white).

Table S13: Electron density (ρ_b), Laplacian of ρ_b ($\nabla^2\rho_b$) and the -G_b/V_b parameter at BCP for the [janusene$-Ag_5]^{5+}$ system.

5			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
$A\cdots F_{\beta 2}$	0.056	0.131	0.782
$A\cdots F'_{\beta 1}$	0.056	0.130	0.780
$C\cdots F_{\beta 1}$	0.028	0.073	0.930
$D\cdots L_{\beta 2}$	0.055	0.127	0.782
$E\cdots F'_{\beta 2}$	0.025	0.067	0.971
$F\cdots L'_{\beta 2}$	0.050	0.140	0.846
$F_{ipso2}\cdots F'_{ipso1}$	0.008	0.025	1.309

Table S14: Electron density (ρ_b), Laplacian of ρ_b ($\nabla^2\rho_b$) and the -G_b/V_b parameter at the BCP for systems **5** and $\mathbf{5}^0$.

$\mathbf{5}^0$			
BCP	ρ_b	$\nabla^2\rho_b$	-G_b/V_b
$A\cdots F_{\beta 2}$	0.018	0.050	1.057
$A\cdots F'_{\beta 1}$	0.062	0.173	0.810
$A\cdots Cl_1$	0.085	0.253	0.776
$C\cdots F_{\alpha 1}$	0.059	0.153	0.796
$C\cdots Cl_2$	0.089	0.263	0.766
$D\cdots L_{\alpha 1}$	0.045	0.119	0.850
$D\cdots Cl_3$	0.052	0.164	0.871
$D\cdots Cl_5$	0.054	0.173	0.863
$D\cdots H_{C^*}$	0.014	0.041	1.116
$E\cdots F'_{\alpha 2}$	0.059	0.166	0.817
$E\cdots Cl_4$	0.090	0.265	0.780
$F\cdots L'_{\alpha 1}$	0.039	0.109	0.884
$F\cdots Cl_3$	0.056	0.176	0.858
$F\cdots Cl_5$	0.056	0.177	0.859
$F\cdots H_{C^*}$	0.015	0.041	1.107
$Cl_5\cdots H_{C^{*\prime}}$	0.012	0.034	1.171

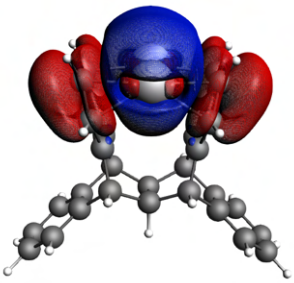
EDA/ETS-NOCV

Energy Decomposition

Table S15: Energy decomposition analysis ($kcal \cdot mol^{-1}$) for complexes **2a - 5** in different fragmentation schemes. Values in parenthesis and brackets represent the percentage contribution of each term for stabilizing and destabilizing contributions, respectively.

2a	Frag.(1)	Frag.(2)	ΔE_{int}	ΔE_{ele}	ΔE_{orb}	ΔE_{disp}	ΔE_{Pauli}
2a(i)	Janus	AB^{2+}	-204.24	-182.31 (45)	-202.95 (50)	-21.08 (5)	202.10 [100]
2a(ii)	Janus$\cdots B^{1+}$	A^{1+}	-8.71	-11.04 (9)	-96.17 (81)	-12.16 (10)	110.65 [100]
2a(iii)	Janus$\cdots A^{1+}$	B^{1+}	-8.65	-10.86 (9)	-96.08 (81)	-12.17 (10)	110.47 [100]
3a	Frag.(1)	Frag.(2)	ΔE_{int}	ΔE_{ele}	ΔE_{orb}	ΔE_{disp}	ΔE_{Pauli}
3a(i)	Janus	ABC^{3+}	-217.21	-154.51 (41)	-203.17 (54)	-21.12 (5)	161.60 [100]
3a(ii)	Janus$\cdots C^{1+}$	AB^{2+}	-86.59	-5.75 (3)	-170.31 (89)	-15.75 (8)	105.22 [100]
3a(iii)	Janus$\cdots BC^{2+}$	A^{1+}	14.47	13.29 [9]	-116.20 (90)	-12.57 (10)	129.95 [91]
3a(iv)	Janus$\cdots AC^{2+}$	B^{1+}	60.64	101.43 [87]	-49.71 (89)	-6.20 (11)	15.11 [13]
3a(v)	Janus$\cdots AB^{2+}$	C^{1+}	36.96	54.63 [53]	-60.41 (92)	-5.41 (8)	48.15 [47]
3b	Frag.(1)	Frag.(2)	ΔE_{int}	ΔE_{ele}	ΔE_{orb}	ΔE_{disp}	ΔE_{Pauli}
3b(i)	Janus	ABD^{3+}	-209.87	-152.39 (41)	-196.53 (53)	-21.19 (6)	160.23 [100]
3b(ii)	Janus$\cdots D^{1+}$	AB^{2+}	-86.81	-6.54 (3)	-167.88 (88)	-15.72 (9)	103.33 [100]
3b(iii)	Janus$\cdots BD^{2+}$	A^{1+}	13.17	13.41 [9]	-116.03 (90)	-12.75 (10)	128.53 [91]
3b(iv)	Janus$\cdots AD^{2+}$	B^{1+}	60.93	100.81 [87]	-48.36 (89)	-6.02 (11)	14.50 [13]
3b(v)	Janus$\cdots AB^{2+}$	D^{1+}	37.05	54.68 [53]	-60.39 (92)	-5.49 (8)	48.25 [47]
4a	Frag.(1)	Frag.(2)	ΔE_{int}	ΔE_{ele}	ΔE_{orb}	ΔE_{disp}	ΔE_{Pauli}
4a(i)	Janus	$ABCD^{4+}$	-241.39	-212.11 (46)	-223.27 (48)	-27.97 (6)	221.95 [100]
4a(ii)	Janus$\cdots CD^{2+}$	AB^{2+}	6.72	79.23 [36]	-195.57 (92)	-17.56 (8)	140.62 [64]
4a(iii)	Janus$\cdots BCD^{3+}$	A^{1+}	78.78	78.66 [40]	-104.38 (89)	-13.43 (11)	117.93 [60]
4a(iv)	Janus$\cdots ACD^{3+}$	B^{1+}	94.01	120.30 [72]	-66.03 (89)	-7.91 (11)	47.65 [28]
4a(v)	Janus$\cdots ABD^{3+}$	C^{1+}	108.35	128.70 [81]	-44.00 (88)	-5.77 (12)	29.42 [19]
4a(vi)	Janus$\cdots ABC^{3+}$	D^{1+}	108.29	128.81 [81]	-44.03 (88)	-5.82 (12)	29.34 [19]
4b	Frag.(1)	Frag.(2)	ΔE_{int}	ΔE_{ele}	ΔE_{orb}	ΔE_{disp}	ΔE_{Pauli}
4b(i)	Janus	$ABCE^{4+}$	-230.18	-201.91 (46)	-213.98 (48)	-26.01 (6)	211.72 [100]
4b(ii)	Janus$\cdots CE^{2+}$	AB^{2+}	15.98	79.18 [42]	-156.24 (91)	-15.70 (9)	108.74 [58]
4b(iii)	Janus$\cdots BCE^{3+}$	A^{1+}	66.55	63.24 [32]	-116.12 (90)	-12.83 (10)	132.26 [68]
4b(iv)	Janus$\cdots ACE^{3+}$	B^{1+}	109.98	142.58 [93]	-37.30 (86)	-5.95 (14)	10.66 [7]
4b(v)	Janus$\cdots ABE^{3+}$	C^{1+}	79.32	101.13 [71]	-58.25 (92)	-5.20 (8)	41.65 [29]
4b(vi)	Janus$\cdots ABC^{3+}$	E^{1+}	79.39	101.34 [71]	-58.02 (92)	-5.19 (8)	41.26 [29]
4c	Frag.(1)	Frag.(2)	ΔE_{int}	ΔE_{ele}	ΔE_{orb}	ΔE_{disp}	ΔE_{Pauli}
4c(i)	Janus	$ABCF^{4+}$	-226.47	-198.54 (46)	-209.67 (48)	-25.93 (6)	207.67 [100]
4c(ii)	Janus$\cdots CF^{2+}$	AB^{2+}	14.82	80.58 [44]	-154.66 (91)	-15.59 (9)	104.48 [56]
4c(iii)	Janus$\cdots BCF^{3+}$	A^{1+}	65.98	66.04 [34]	-114.72 (90)	-12.83 (10)	127.50 [66]
4c(iv)	Janus$\cdots ACF^{3+}$	B^{1+}	109.47	142.04 [93]	-37.05 (86)	-5.88 (14)	10.36 [7]
4c(v)	Janus$\cdots ABF^{3+}$	C^{1+}	80.18	102.08 [71]	-57.68 (92)	-5.25 (8)	41.03 [29]
4c(vi)	Janus$\cdots ABC^{3+}$	F^{1+}	80.46	102.56 [71]	-58.94 (92)	-5.16 (8)	42.00 [29]
4d	Frag.(1)	Frag.(2)	ΔE_{int}	ΔE_{ele}	ΔE_{orb}	ΔE_{disp}	ΔE_{Pauli}
4d(i)	Janus	$ABDF^{4+}$	-225.32	-201.27 (46)	-211.55 (48)	-25.55 (6)	213.06 [100]
4d(ii)	Janus$\cdots DF^{2+}$	AB^{2+}	13.62	77.70 [42]	-156.23 (91)	-15.49 (9)	107.65 [58]
4d(iii)	Janus$\cdots BDF^{3+}$	A^{1+}	65.07	62.65 [32]	-115.94 (90)	-12.78 (10)	131.14 [68]
4d(iv)	Janus$\cdots ADF^{3+}$	B^{1+}	108.42	140.76 [93]	-36.66 (86)	-5.83 (14)	10.15 [7]
4d(v)	Janus$\cdots ABF^{3+}$	D^{1+}	81.77	103.58 [71]	-58.79 (92)	-5.07 (8)	42.05 [29]
4d(vi)	Janus$\cdots ABD^{3+}$	F^{1+}	81.72	102.98 [70]	-59.41 (92)	-5.09 (8)	43.24 [30]
5	Frag.(1)	Frag.(2)	ΔE_{int}	ΔE_{ele}	ΔE_{orb}	ΔE_{disp}	ΔE_{Pauli}
5(i)	Janus	$ACDEF^{5+}$	-202.19	-194.35 (50)	-167.00 (42)	-30.97 (8)	190.14 [100]
5(ii)	Janus$\cdots CDEF^{4+}$	A^{1+}	134.64	152.28 [66]	-82.59 (87)	-11.98 (13)	76.93 [34]
5(iii)	Janus$\cdots ADEF^{4+}$	C^{1+}	144.40	166.88 [96]	-24.32 (82)	-5.46 (18)	7.31 [4]
5(iv)	Janus$\cdots ACEF^{4+}$	D^{1+}	117.64	137.72 [79]	-52.03 (91)	-4.92 (9)	36.87 [21]
5(v)	Janus$\cdots ACDF^{4+}$	E^{1+}	143.78	167.20 [95]	-27.02 (83)	-5.62 (17)	9.21 [5]
5(vi)	Janus$\cdots ACDE^{4+}$	F^{1+}	117.88	139.54 [81]	-50.26 (91)	-5.03 (9)	33.61 [19]

NOCV Deformation Densities



$\Delta q_{orb,1} = 0.66$ a.u
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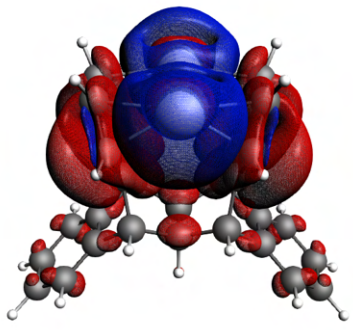

$\Delta q_{orb,2} = 0.53$ a.u
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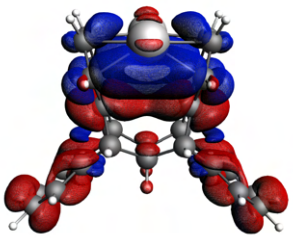

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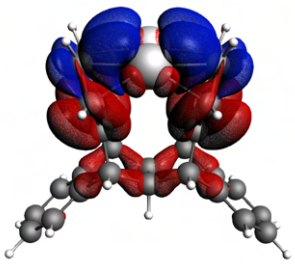
$\Delta E_{orb,3} = -16.50$ kcal.mol^{-1}



$\Delta q_{orb,4} = 0.37$ a.u
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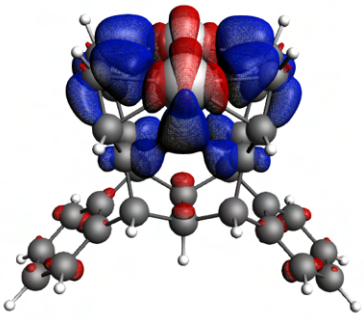
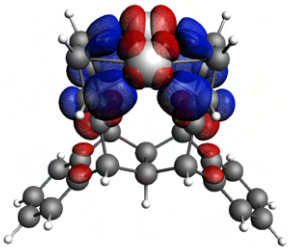


$\Delta q_{orb,5} = 0.32$ a.u
$\Delta E_{orb,5} = -10.18$ kcal.mol^{-1}



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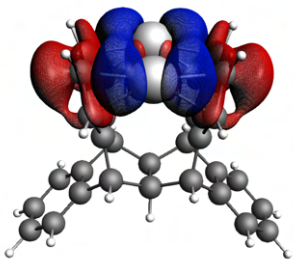
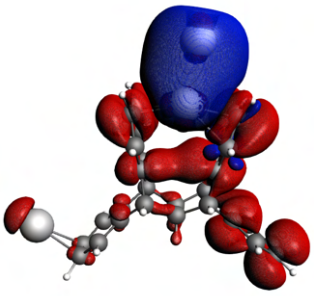
$\Delta E_{orb,6} = -10.67$ kcal.mol^{-1}

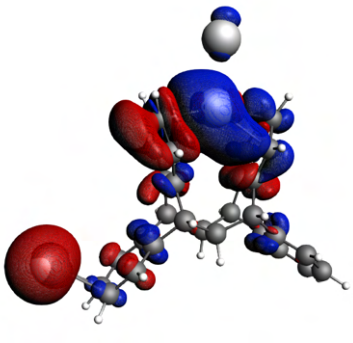


$\Delta q_{orb,7} = 0.23$ a.u
$\Delta E_{orb,7} = -12.06$ kcal.mol^{-1}

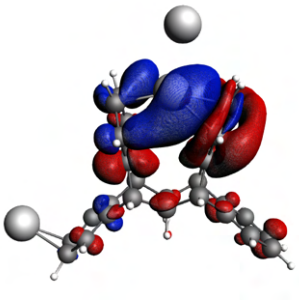
Figure S46: Density flow channels for fragmentation **2a(i)** contributing with more than 10 $kcal.mol^{-1}$ with their respective energies $\Delta E_{Orb,k}$ and charge transfer estimation Δq_k values. Red and blue regions indicate electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to 3×10^{-4} a.u.



$\Delta q_{orb,1} = 1.13$ a.u
$\Delta E_{orb,1} = -66.30$ kcal.mol^{-1}



$\Delta q_{orb,2} = 0.49$ a.u
$\Delta E_{orb,2} = -24.27$ kcal.mol^{-1}



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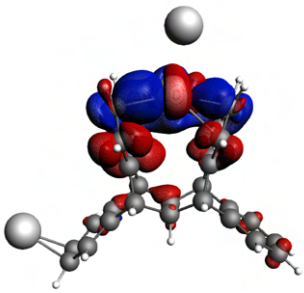
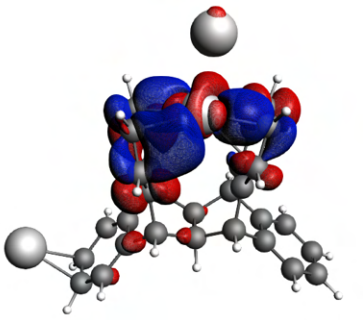
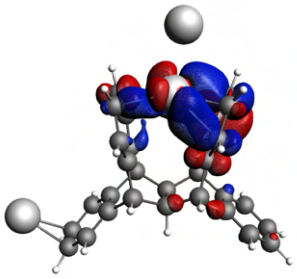
$\Delta E_{orb,3} = -17.69$ kcal.mol^{-1}



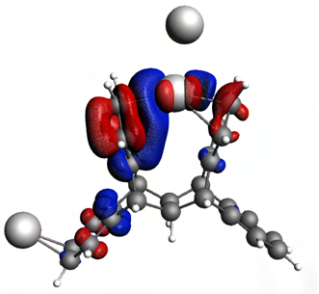
$\Delta q_{orb,4} = 0.29$ a.u
$\Delta E_{orb,4} = -11.38$ kcal.mol^{-1}



$\Delta q_{orb,5} = 0.24$ a.u
$\Delta E_{orb,5} = -8.96$ kcal.mol^{-1}

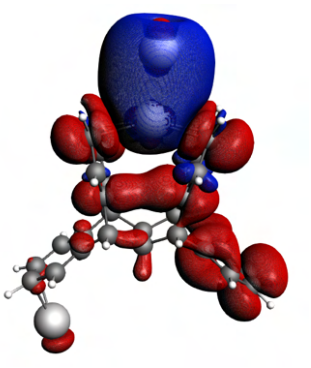


$\Delta q_{orb,6} = 0.21$ a.u
$\Delta E_{orb,6} = -7.20$ kcal.mol^{-1}

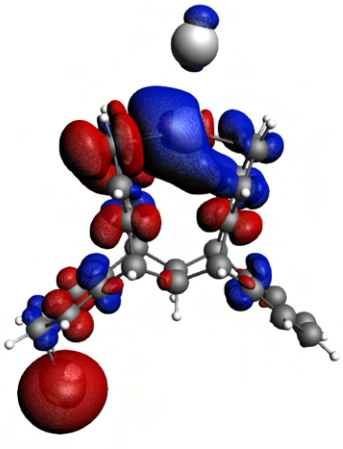


$\Delta q_{orb,7} = 0.16$ a.u
$\Delta E_{orb,7} = -5.15$ kcal.mol^{-1}

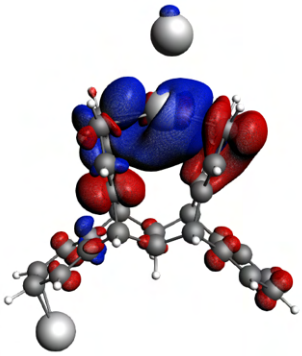
Figure S47: Density flow channels for fragmentation **3a(ii)** contributing with more than 5 $kcal.mol^{-1}$ with their respective energies $\Delta E_{Orb,k}$ and charge transfer estimation Δq_k values. Red and blue regions indicate electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to 3×10^{-4} a.u.



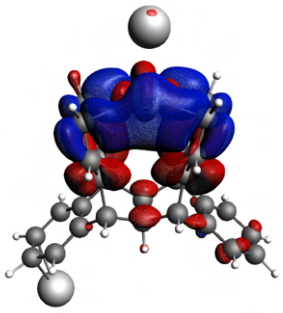
$\Delta q_{orb,1} = 1.12$ a.u
$\Delta E_{orb,1} = -64.87$ kcal.mol^{-1}



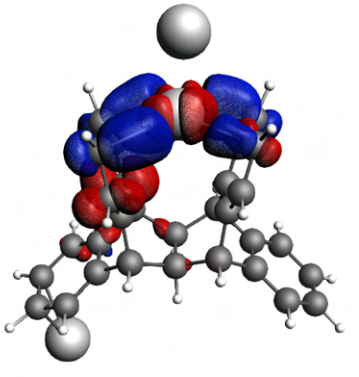
$\Delta q_{orb,2} = 0.47$ a.u
$\Delta E_{orb,2} = -22.39$ kcal.mol^{-1}



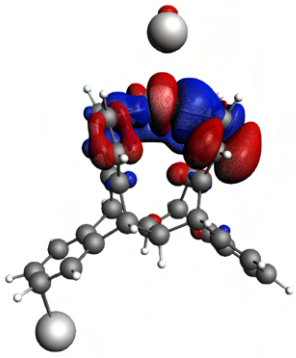
$\Delta q_{orb,3} = 0.34$ a.u
$\Delta E_{orb,3} = -16.70$ kcal.mol^{-1}



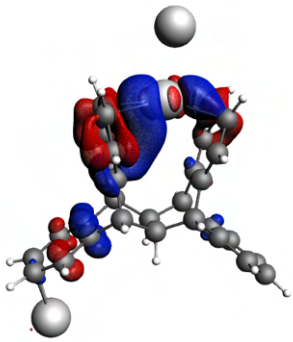
$\Delta q_{orb,4} = 0.29$ a.u
$\Delta E_{orb,4} = -12.73$ kcal.mol^{-1}



$\Delta q_{orb,5} = 0.23$ a.u
$\Delta E_{orb,5} = -7.56$ kcal.mol^{-1}

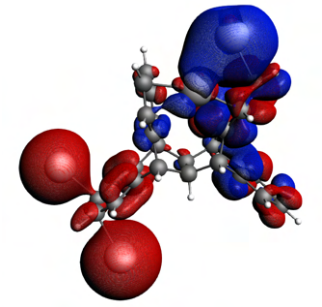


$\Delta q_{orb,6} = 0.23$ a.u
$\Delta E_{orb,6} = -9.04$ kcal.mol^{-1}

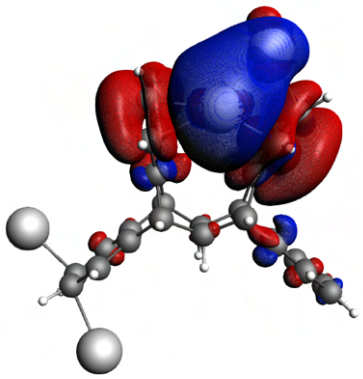


$\Delta q_{orb,7} = 0.16$ a.u
$\Delta E_{orb,7} = -5.17$ kcal.mol^{-1}

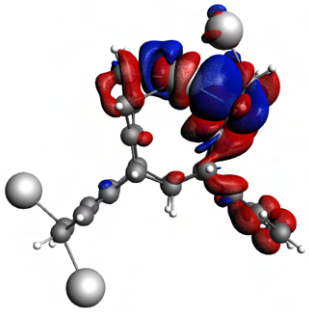
Figure S48: Density flow channels for fragmentation **3b(ii)** contributing with more than 5 $kcal.mol^{-1}$ with their respective energies $\Delta E_{Orb,k}$ and charge transfer estimation Δq_k values. Red and blue regions indicate electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to 3×10^{-4} a.u.



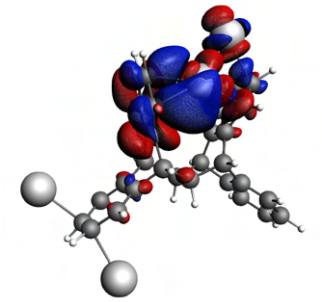
$\Delta q_{orb,1} = 1.13$ a.u
$\Delta E_{orb,1} = -61.83$ kcal.mol^{-1}



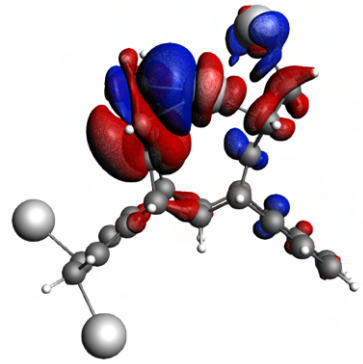
$\Delta q_{orb,2} = 0.72$ a.u
$\Delta E_{orb,2} = -41.63$ kcal.mol^{-1}



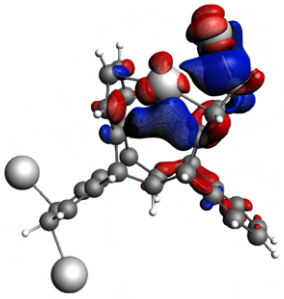
$\Delta q_{orb,3} = 0.36$ a.u
$\Delta E_{orb,3} = -17.42$ kcal.mol^{-1}



$\Delta q_{orb,4} = 0.31$ a.u
$\Delta E_{orb,4} = -12.25$ kcal.mol^{-1}

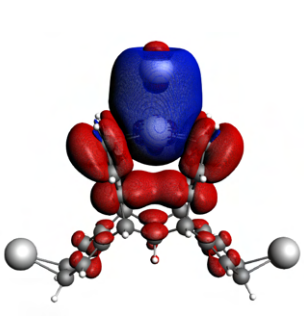


$\Delta q_{orb,5} = 0.29$ a.u
$\Delta E_{orb,5} = -13.35$ kcal.mol^{-1}

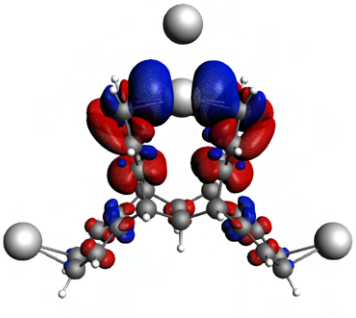


$\Delta q_{orb,6} = 0.24$ a.u
$\Delta E_{orb,6} = -7.27$ kcal.mol^{-1}

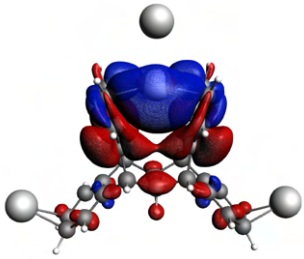
Figure S49: Density flow channels for fragmentation **4a(ii)** contributing with more than 5 $kcal.mol^{-1}$ with their respective energies $\Delta E_{Orb,k}$ and charge transfer estimation Δq_k values. Red and blue regions indicate electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to 3×10^{-4} a.u.



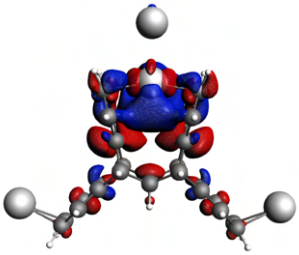
$\Delta q_{orb,1} = 0.95$ a.u
$\Delta E_{orb,1} = -55.16$ kcal.mol^{-1}



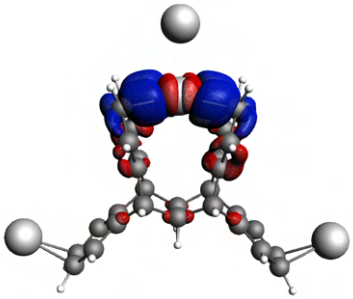
$\Delta q_{orb,2} = 0.35$ a.u
$\Delta E_{orb,2} = -18.68$ kcal.mol^{-1}



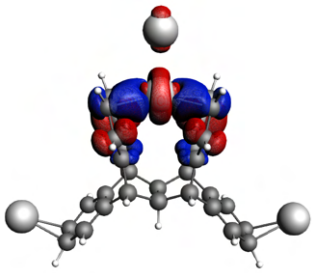
$\Delta q_{orb,3} = 0.33$ a.u
$\Delta E_{orb,3} = -15.20$ kcal.mol^{-1}



$\Delta q_{orb,4} = 0.31$ a.u
$\Delta E_{orb,4} = -13.00$ kcal.mol^{-1}

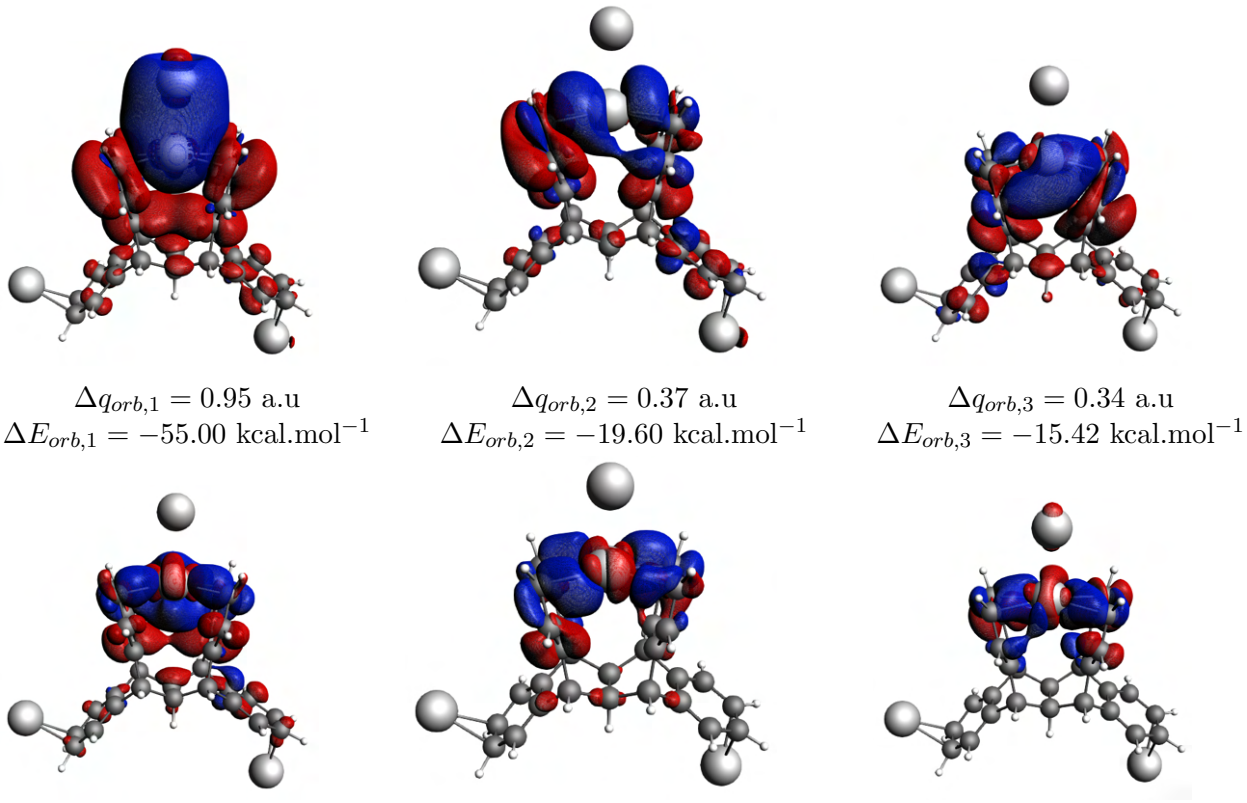


$\Delta q_{orb,5} = 0.27$ a.u
$\Delta E_{orb,5} = -9.66$ kcal.mol^{-1}



$\Delta q_{orb,6} = 0.22$ a.u
$\Delta E_{orb,6} = -7.74$ kcal.mol^{-1}

Figure S50: Density flow channels for fragmentation **4b(ii)** contributing with more than 5 $kcal.mol^{-1}$ with their respective energies $\Delta E_{Orb,k}$ and charge transfer estimation Δq_k values. Red and blue regions indicate electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to 3×10^{-4} a.u.



$\Delta q_{orb,1} = 0.95$ a.u
$\Delta E_{orb,1} = -55.00$ kcal.mol^{-1}

$\Delta q_{orb,2} = 0.37$ a.u
$\Delta E_{orb,2} = -19.60$ kcal.mol^{-1}

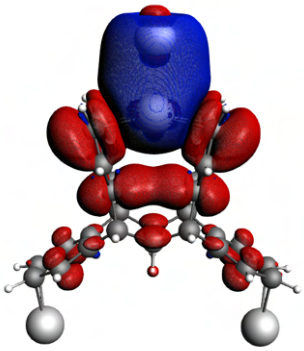
$\Delta q_{orb,3} = 0.34$ a.u
$\Delta E_{orb,3} = -15.42$ kcal.mol^{-1}

$\Delta q_{orb,4} = 0.30$ a.u
$\Delta E_{orb,4} = -12.08$ kcal.mol^{-1}

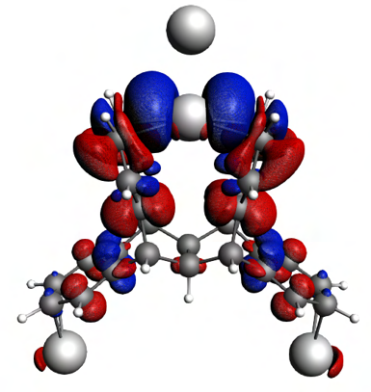
$\Delta q_{orb,5} = 0.26$ a.u
$\Delta E_{orb,5} = -9.18$ kcal.mol^{-1}

$\Delta q_{orb,6} = 0.21$ a.u
$\Delta E_{orb,6} = -7.63$ kcal.mol^{-1}

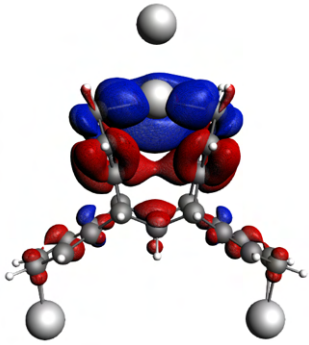
Figure S51: Density flow channels for fragmentation **4c(ii)** contributing with more than 5 $kcal.mol^{-1}$ with their respective energies $\Delta E_{Orb,k}$ and charge transfer estimation Δq_k values. Red and blue regions indicate electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to 3×10^{-4} a.u.



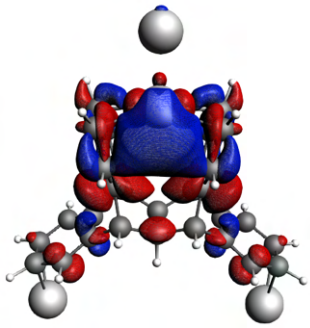
$\Delta q_{orb,1} = 0.95$ a.u
$\Delta E_{orb,1} = -55.26$ kcal.mol^{-1}



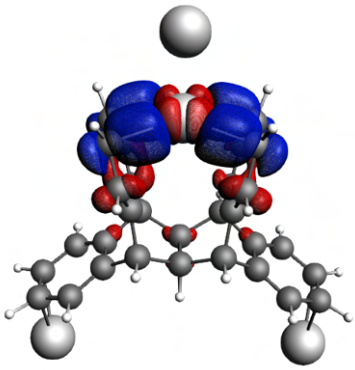
$\Delta q_{orb,2} = 0.37$ a.u
$\Delta E_{orb,2} = -19.18$ kcal.mol^{-1}



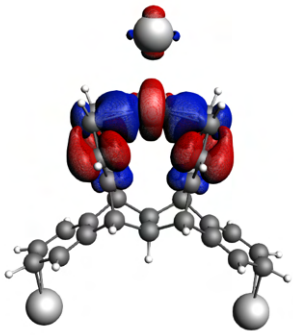
$\Delta q_{orb,3} = 0.33$ a.u
$\Delta E_{orb,3} = -15.03$ kcal.mol^{-1}



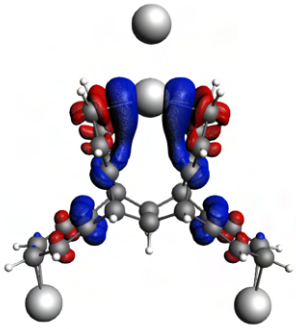
$\Delta q_{orb,4} = 0.32$ a.u
$\Delta E_{orb,4} = -12.78$ kcal.mol^{-1}



$\Delta q_{orb,5} = 0.27$ a.u
$\Delta E_{orb,5} = -9.52$ kcal.mol^{-1}

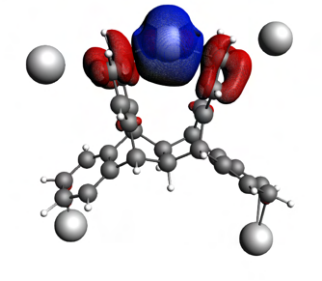


$\Delta q_{orb,6} = 0.22$ a.u
$\Delta E_{orb,6} = -7.93$ kcal.mol^{-1}

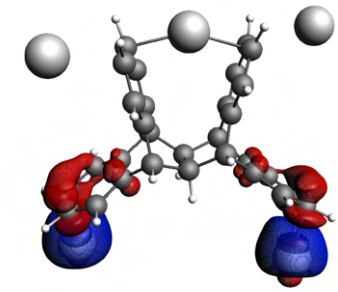


$\Delta q_{orb,7} = 0.16$ a.u
$\Delta E_{orb,7} = -5.02$ kcal.mol^{-1}

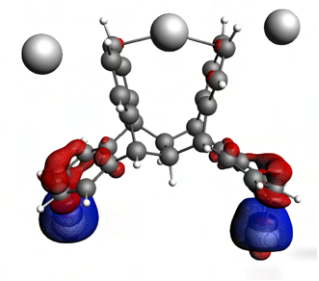
Figure S52: Density flow channels for fragmentation **4d(ii)** contributing with more than 5 $kcal.mol^{-1}$ with their respective energies $\Delta E_{Orb,k}$ and charge transfer estimation Δq_k values. Red and blue regions indicate electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to 3×10^{-4} a.u.



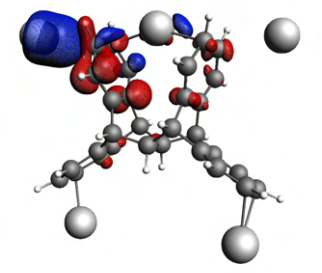
$\Delta q_{orb,1} = 0.53$ a.u
$\Delta E_{orb,1} = -24.57$ kcal.mol^{-1}



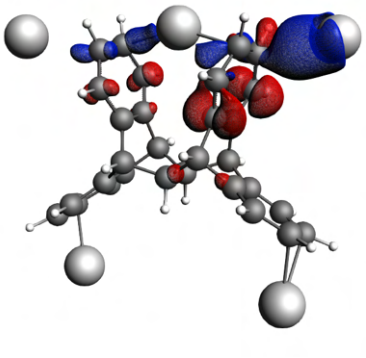
$\Delta q_{orb,2} = 0.49$ a.u
$\Delta E_{orb,2} = -19.32$ kcal.mol^{-1}



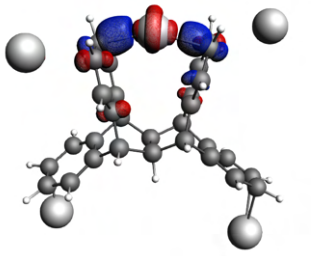
$\Delta q_{orb,3} = 0.47$ a.u
$\Delta E_{orb,3} = -18.91$ kcal.mol^{-1}



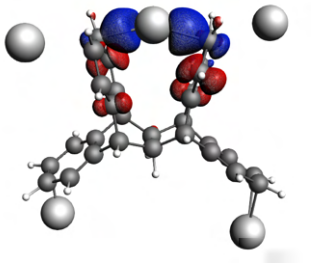
$\Delta q_{orb,4} = 0.41$ a.u
$\Delta E_{orb,4} = -12.70$ kcal.mol^{-1}



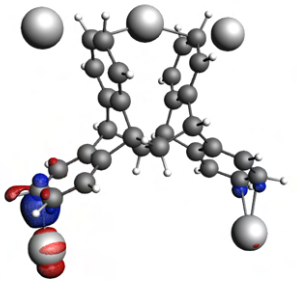
$\Delta q_{orb,5} = 0.39$ a.u
$\Delta E_{orb,5} = -10.85$ kcal.mol^{-1}



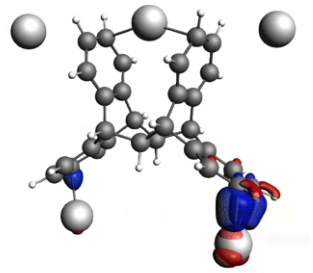
$\Delta q_{orb,6} = 0.28$ a.u
$\Delta E_{orb,6} = -9.48$ kcal.mol^{-1}



$\Delta q_{orb,7} = 0.26$ a.u
$\Delta E_{orb,7} = -9.89$ kcal.mol^{-1}

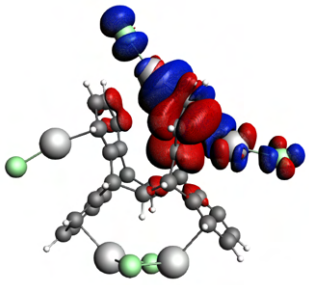


$\Delta q_{orb,8} = 0.21$ a.u
$\Delta E_{orb,8} = -5.63$ kcal.mol^{-1}

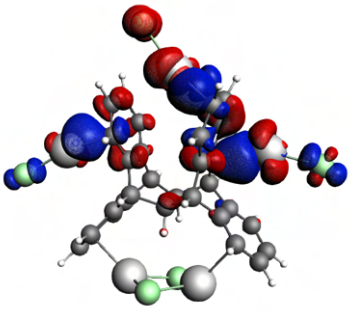


$\Delta q_{orb,9} = 0.21$ a.u
$\Delta E_{orb,9} = -5.34$ kcal.mol^{-1}

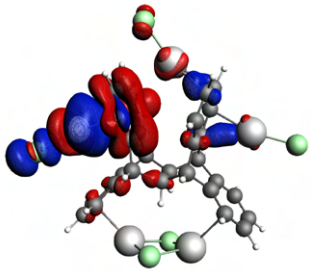
Figure S53: Most relevant density flow channels for fragmentation **5(i)** with their respective energies $\Delta E_{Orb,k}$ and charge transfer estimation Δq_k values. Red and blue regions indicate electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to 3×10^{-4} a.u.



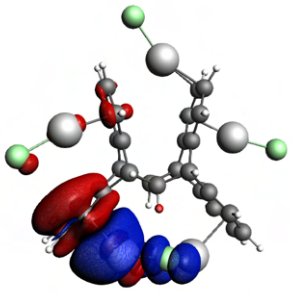
$\Delta q_{orb,1} = 0.44$ a.u
$\Delta E_{orb,1} = -15.63$ kcal.mol^{-1}



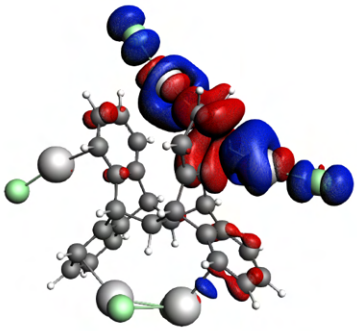
$\Delta q_{orb,2} = 0.40$ a.u
$\Delta E_{orb,2} = -12.91$ kcal.mol^{-1}



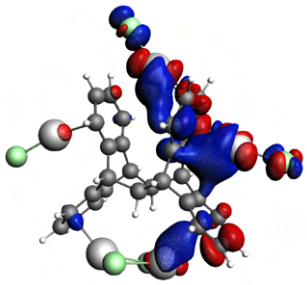
$\Delta q_{orb,3} = 0.36$ a.u
$\Delta E_{orb,3} = -12.84$ kcal.mol^{-1}



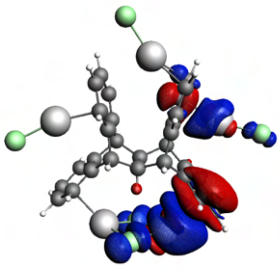
$\Delta q_{orb,4} = 0.33$ a.u
$\Delta E_{orb,4} = -9.90$ kcal.mol^{-1}



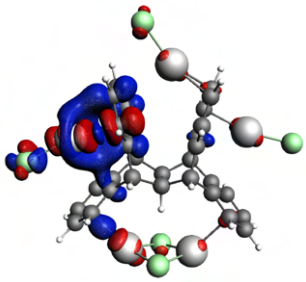
$\Delta q_{orb,5} = 0.32$ a.u
$\Delta E_{orb,5} = -11.50$ kcal.mol^{-1}



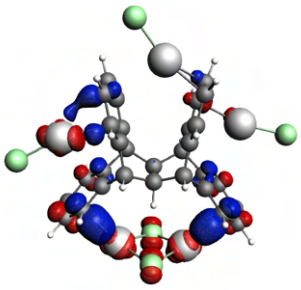
$\Delta q_{orb,6} = 0.30$ a.u
$\Delta E_{orb,6} = -8.67$ kcal.mol^{-1}



$\Delta q_{orb,7} = 0.29$ a.u
$\Delta E_{orb,7} = -8.29$ kcal.mol^{-1}



$\Delta q_{orb,8} = 0.27$ a.u
$\Delta E_{orb,8} = -6.38$ kcal.mol^{-1}



$\Delta q_{orb,9} = 0.24$ a.u
$\Delta E_{orb,9} = -5.02$ kcal.mol^{-1}

Figure S54: Most relevant density flow channels for fragmentation $\mathbf{5^0(i)}$ with their respective energies $\Delta E_{Orb,k}$ and charge transfer estimation Δq_k values. Red and blue regions indicate electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to 3×10^{-4} a.u.

Non-Covalent Interactions Index (NCI)

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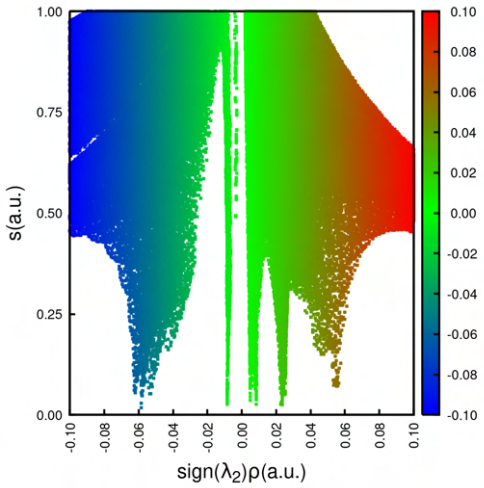
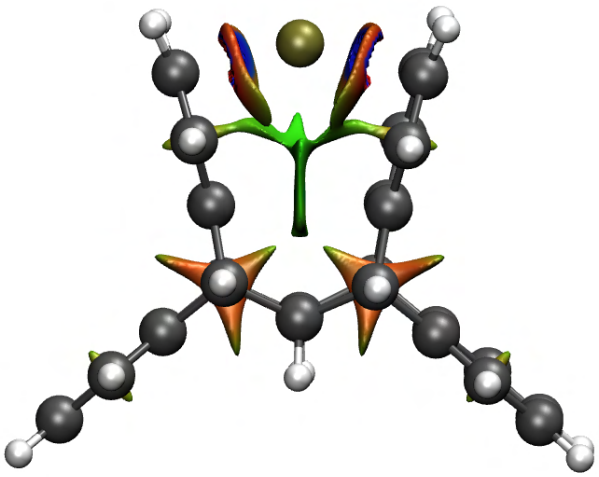
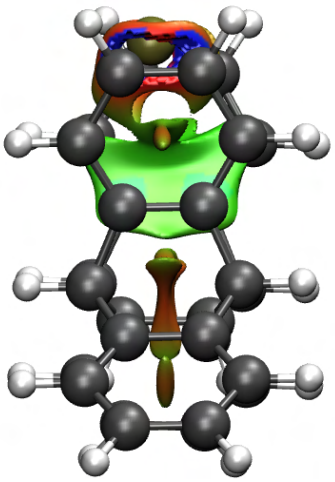


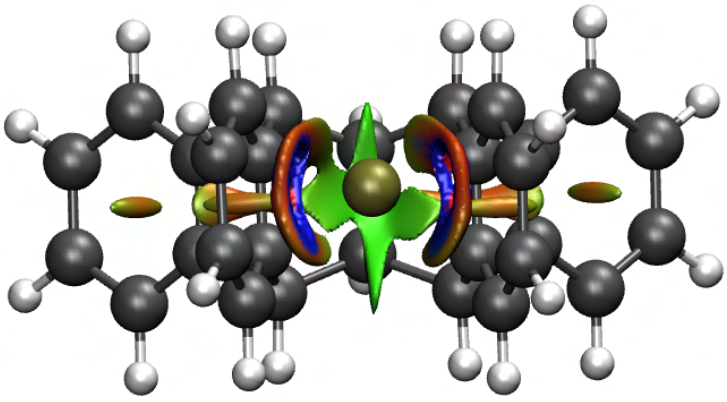
Plot of the RDG x sign(λ_2)ρ



Front view

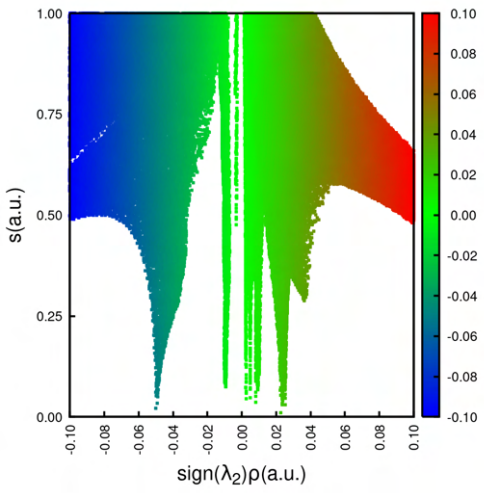


Side view

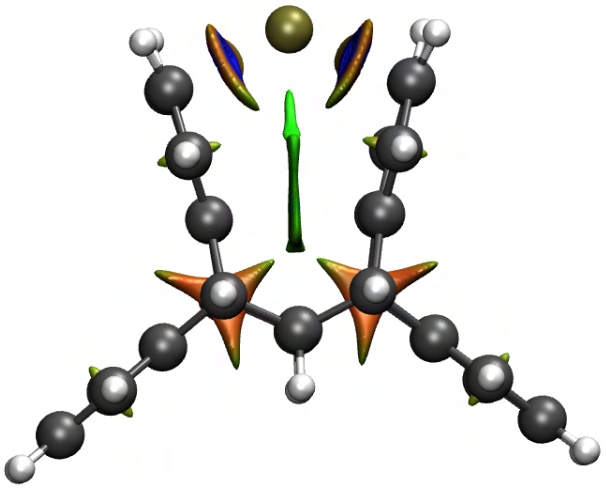


Top view

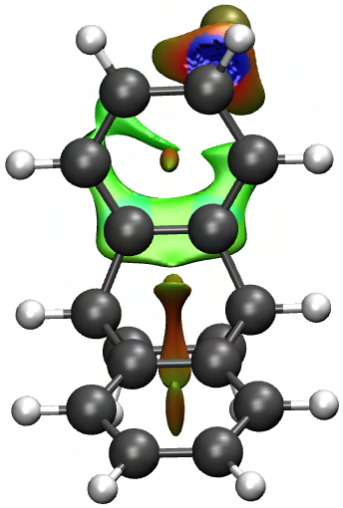
Figure S55: NCI images of system 1a.



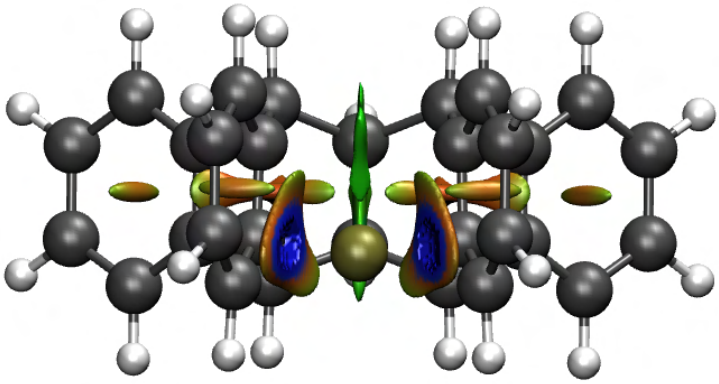
Plot of the RDG x sign(λ_2)ρ



Front view

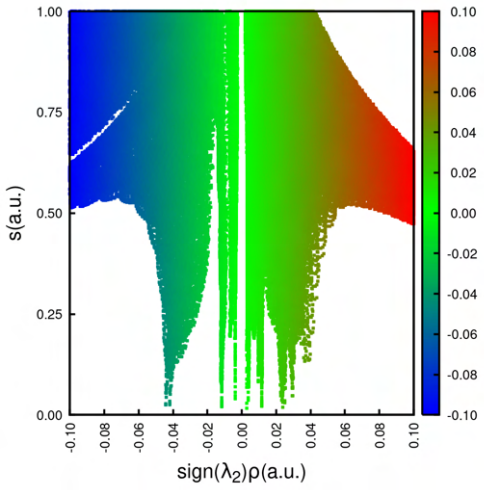


Side view

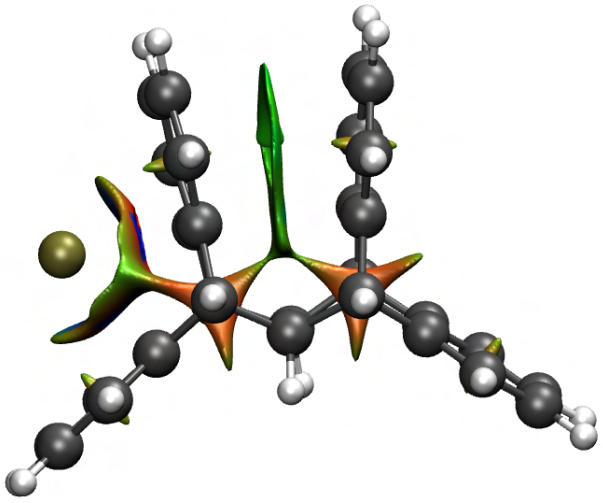


Top view

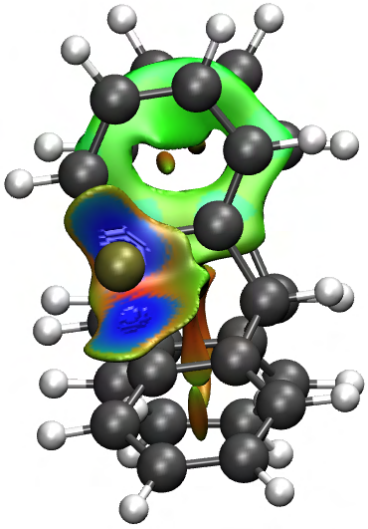
Figure S56: NCI images of system 1b.



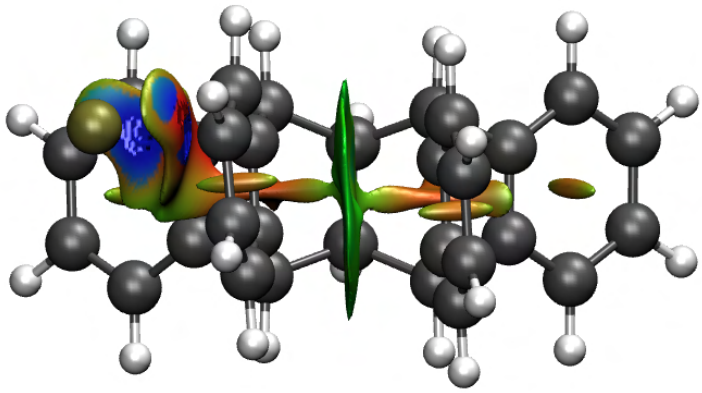
Plot of the RDG x sign(λ_2)ρ



Front view

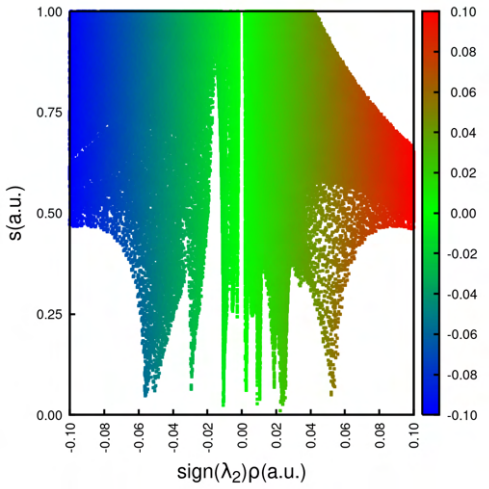


Side view

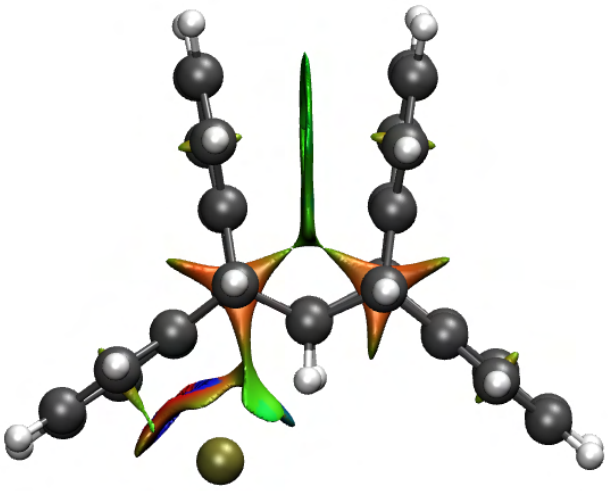


Top view

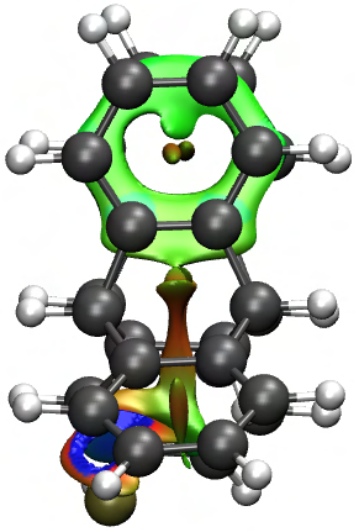
Figure S57: NCI images of system 1c.



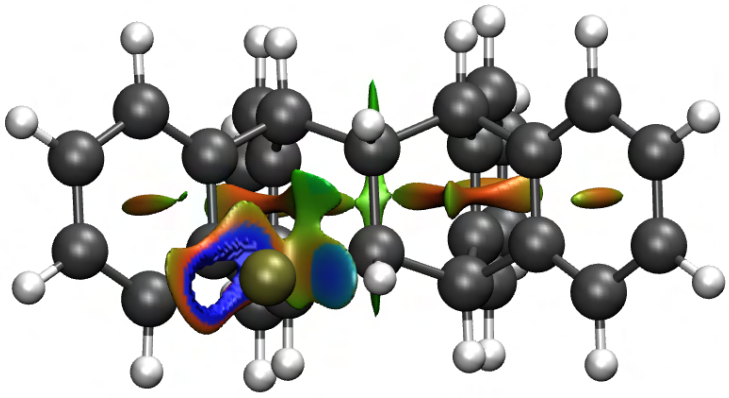
Plot of the RDG x sign(λ_2)ρ



Front view



Side view



Bottom view

Figure S58: NCI images of system 1d.

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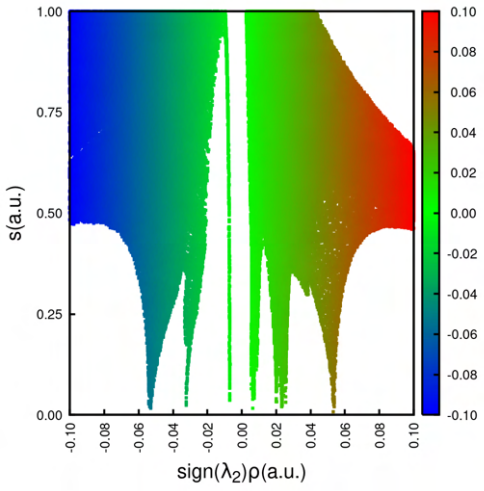
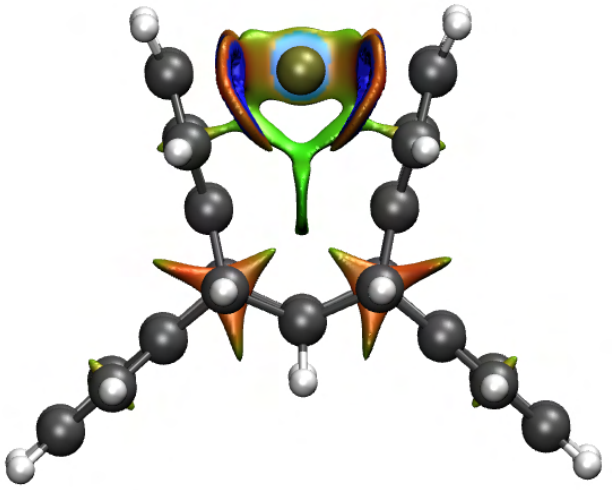
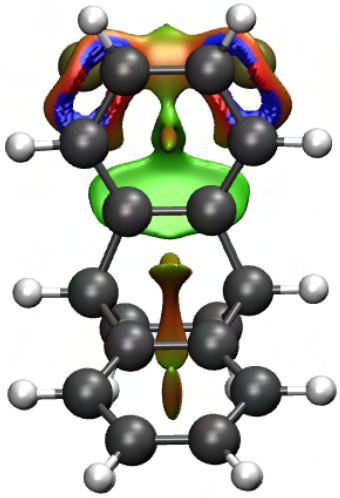


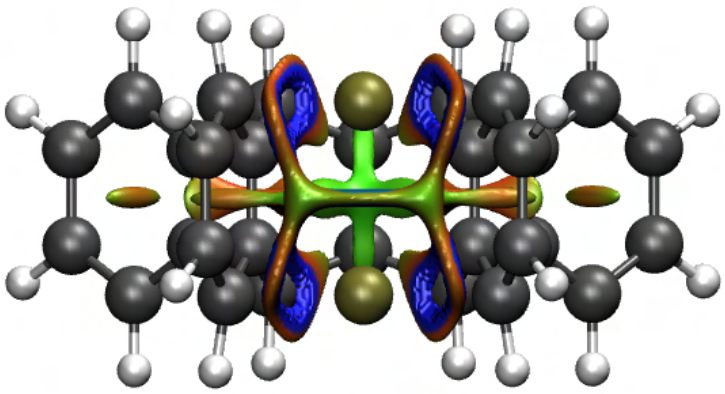
Plot of the RDG x sign(λ_2)ρ



Front view

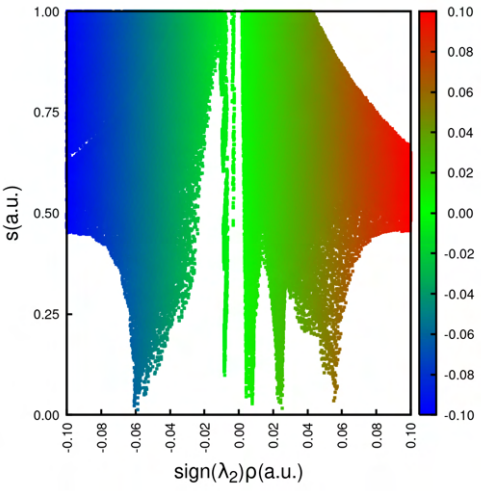


Side view

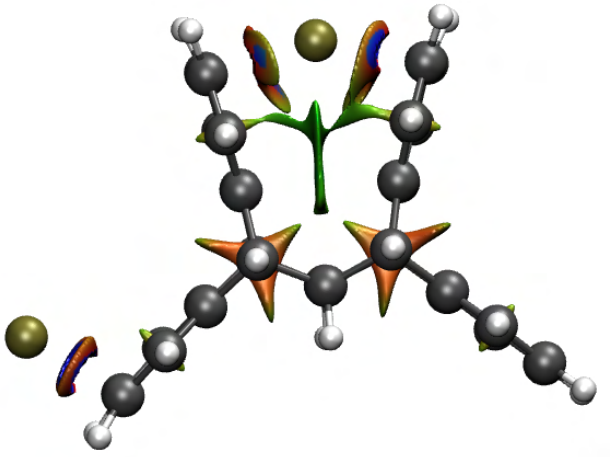


Top view

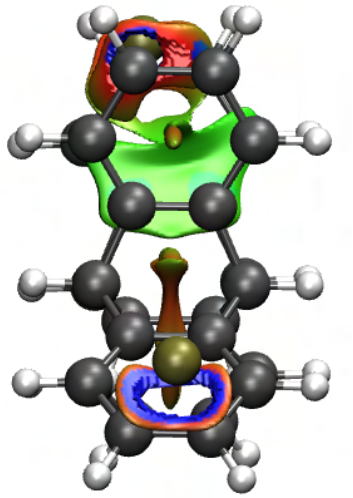
Figure S59: NCI images of system 2a.



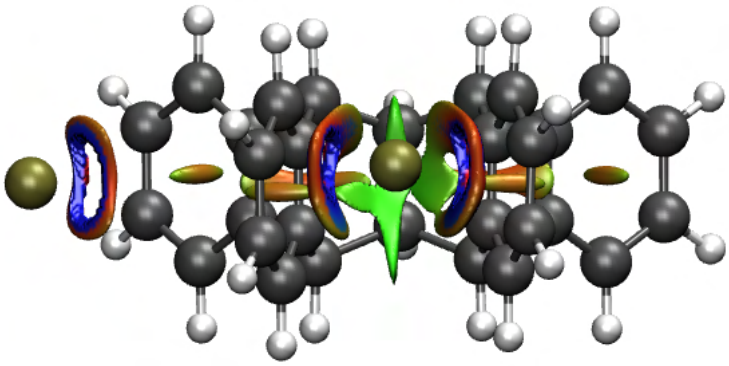
Plot of the RDG x sign(λ_2)ρ



Front view

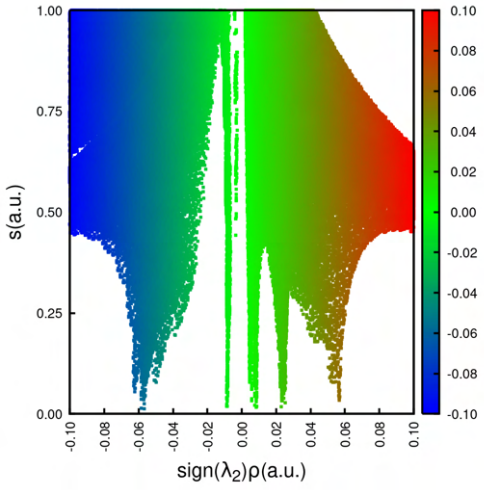


Side view

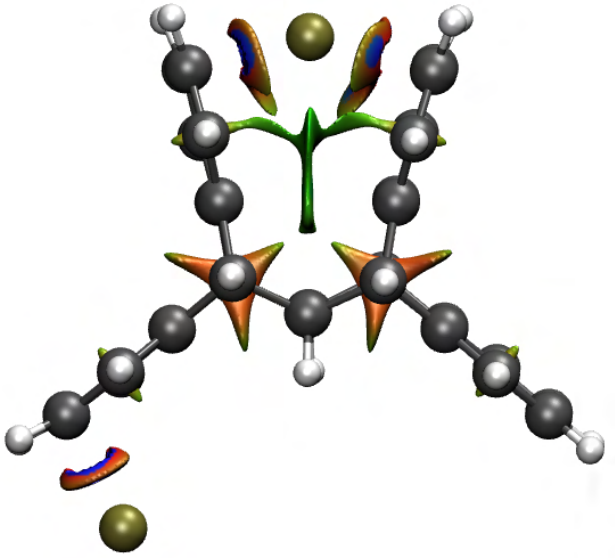


Top view

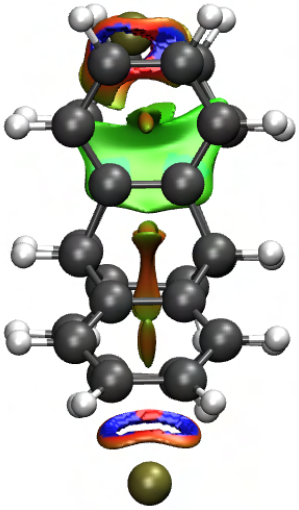
Figure S60: NCI images of system 2b.



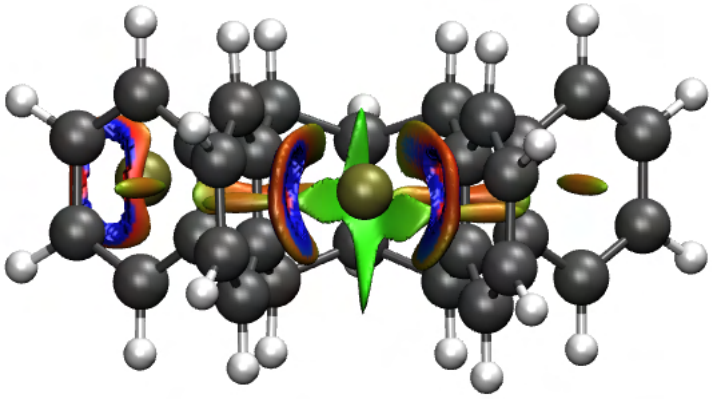
Plot of the RDG x sign(λ_2)ρ



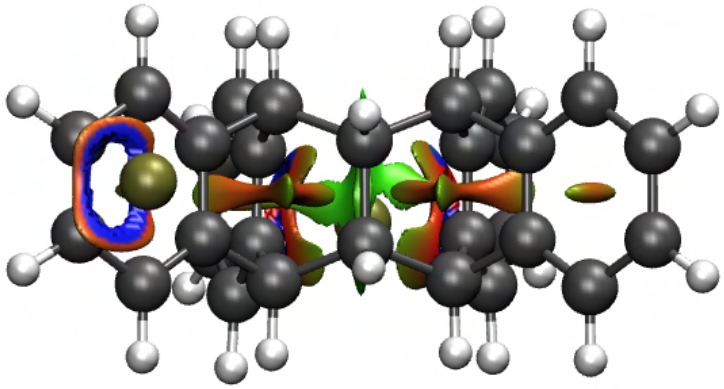
Front view



Side view

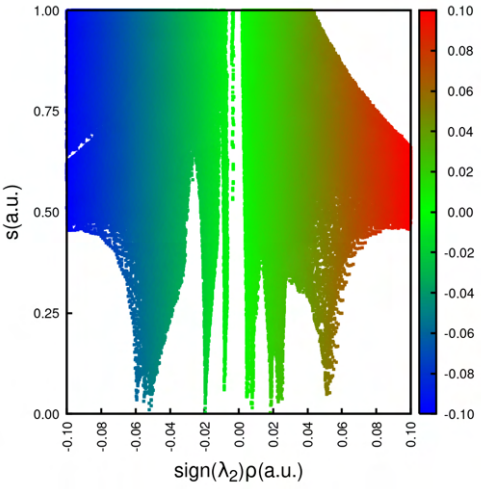


Top view

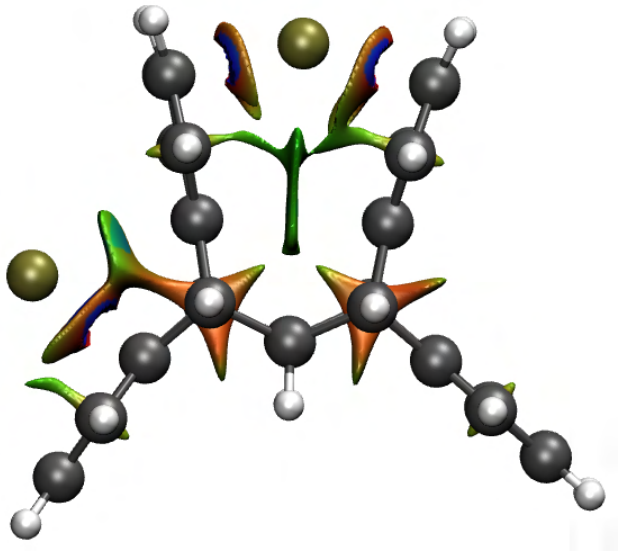


Bottom view

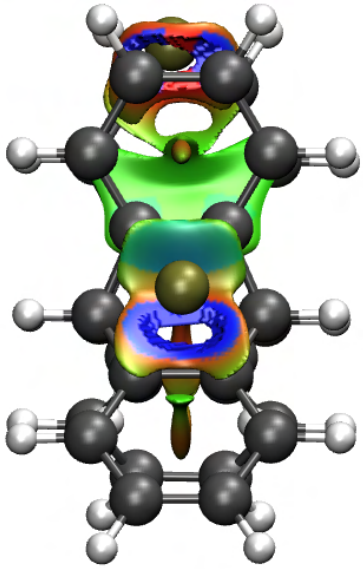
Figure S61: NCI images of system 2c.



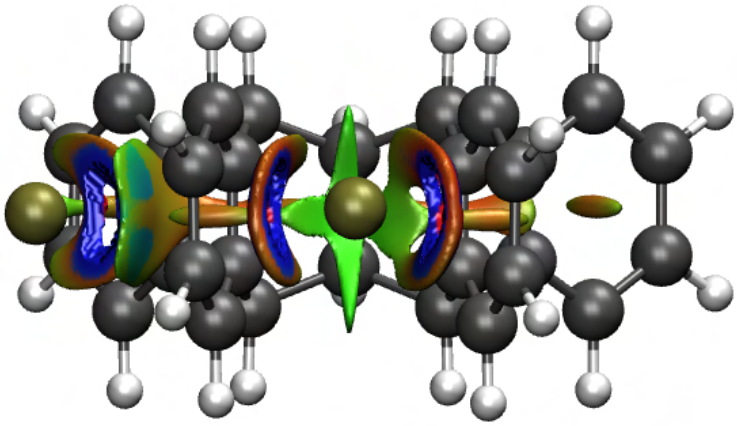
Plot of the RDG x sign(λ_2)ρ



Front view

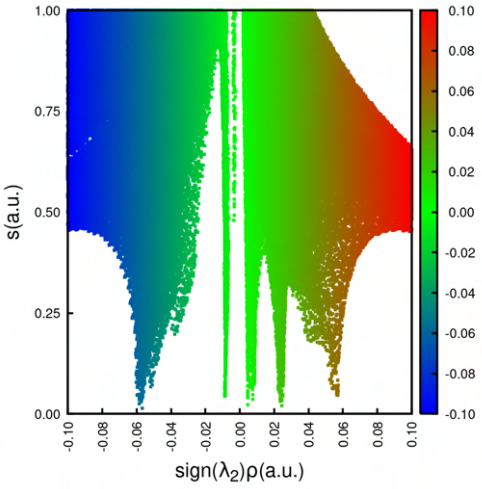


Side view

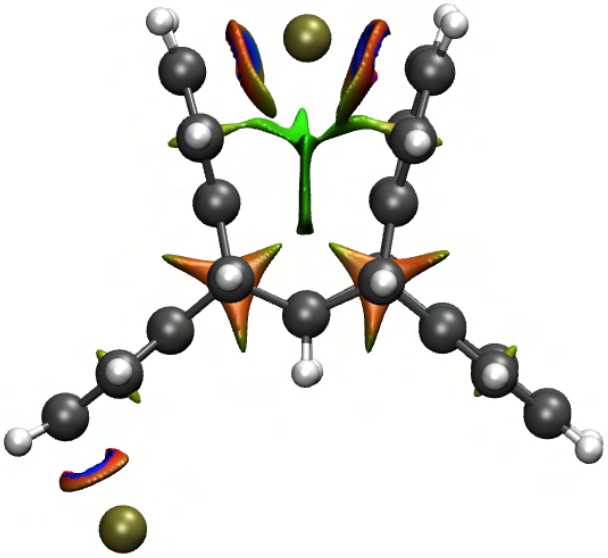


Top view

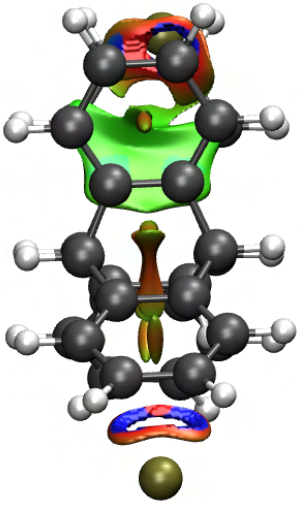
Figure S62: NCI images of system 2d.



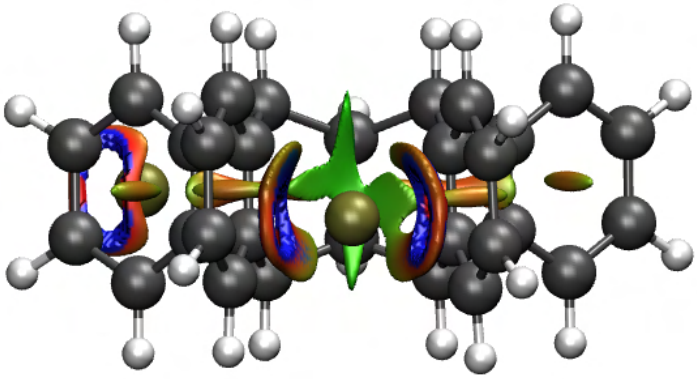
Plot of the RDG x sign(λ_2)ρ



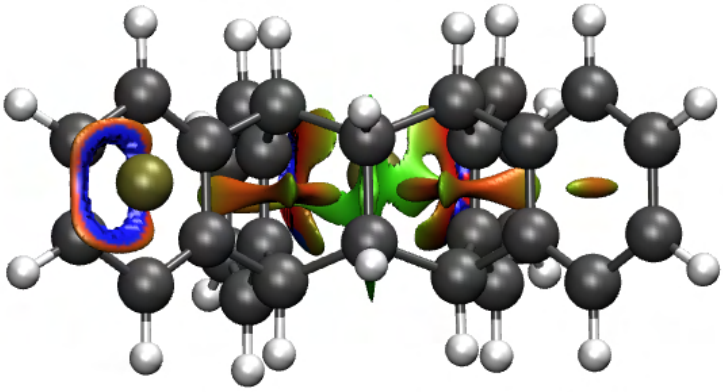
Front view



Side view

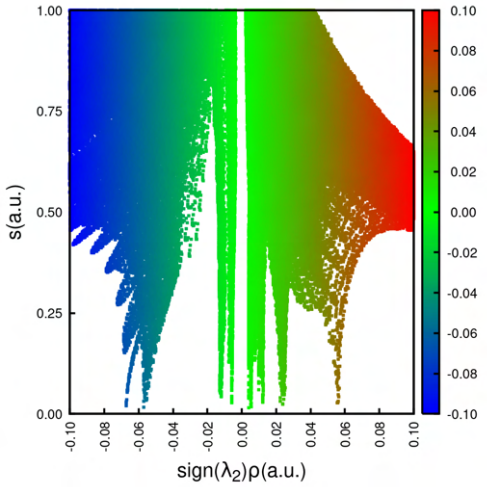


Top view

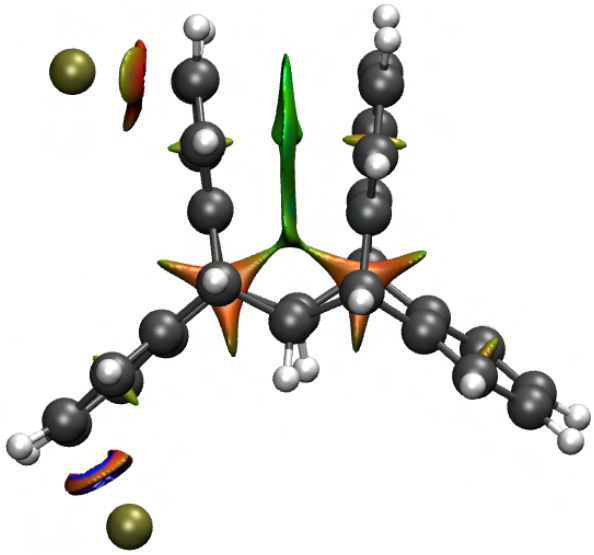


Bottom view

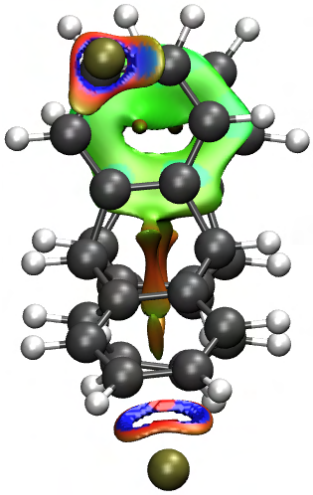
Figure S63: NCI images of system 2e.



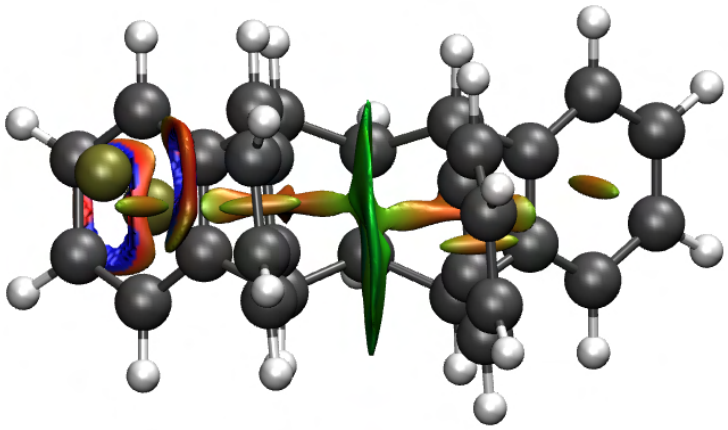
Plot of the RDG x sign(λ_2)ρ



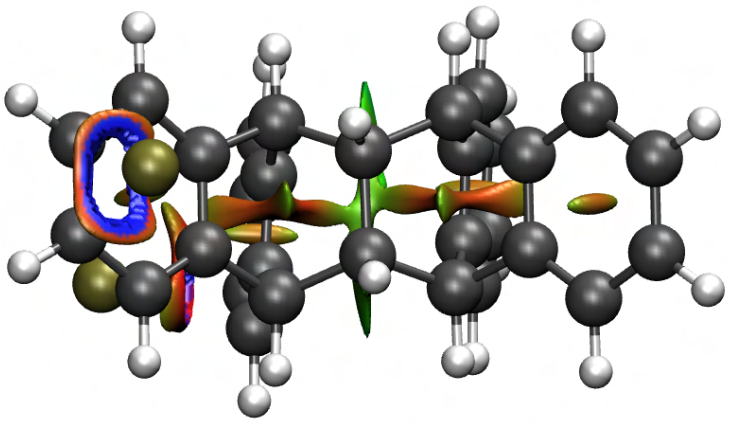
Front view



Side view

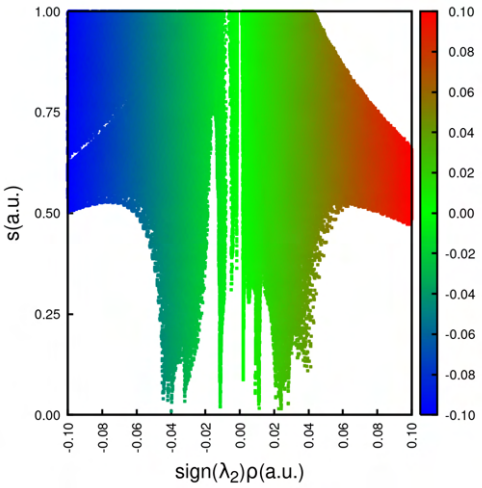


Top view

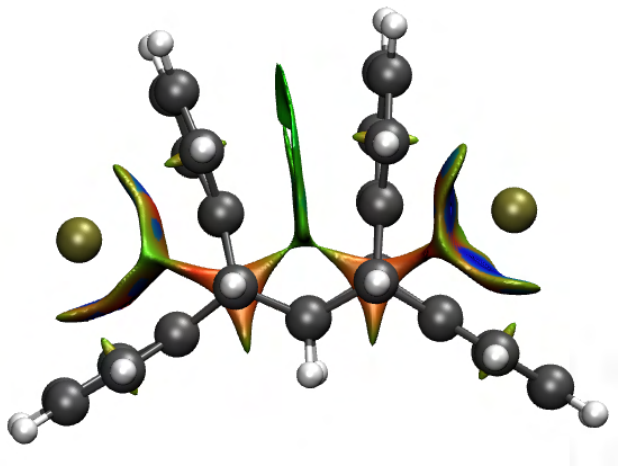


Bottom view

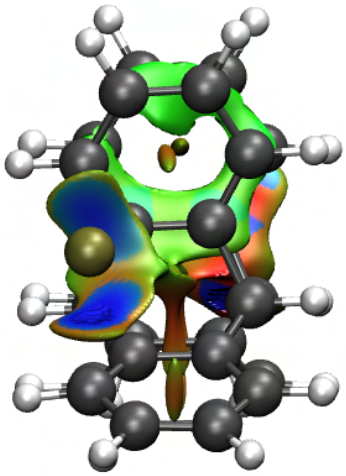
Figure S64: NCI images of system 2f.



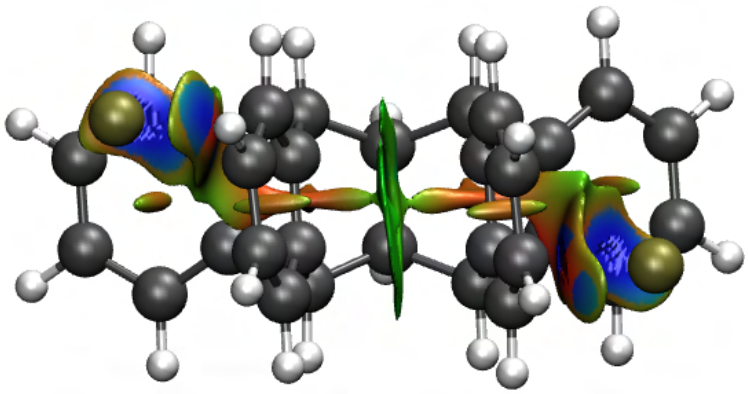
Plot of the RDG x sign(λ_2)ρ



Front view

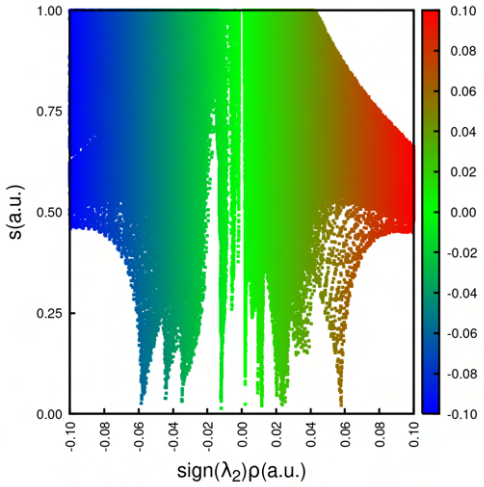


Side view

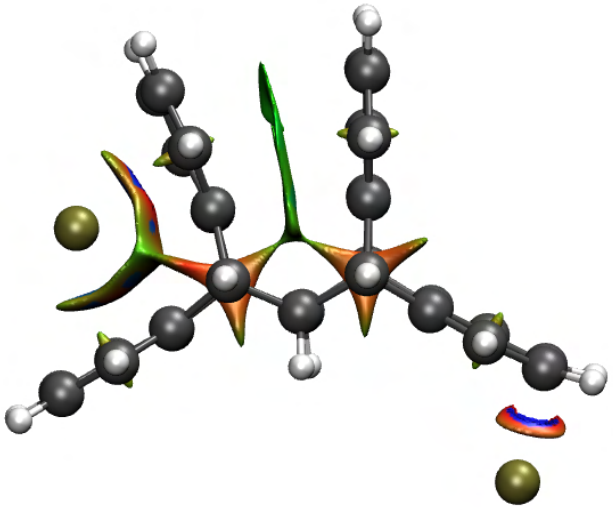


Top view

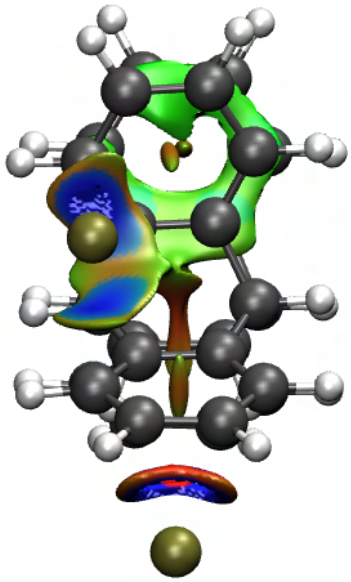
Figure S65: NCI images of system 2g.



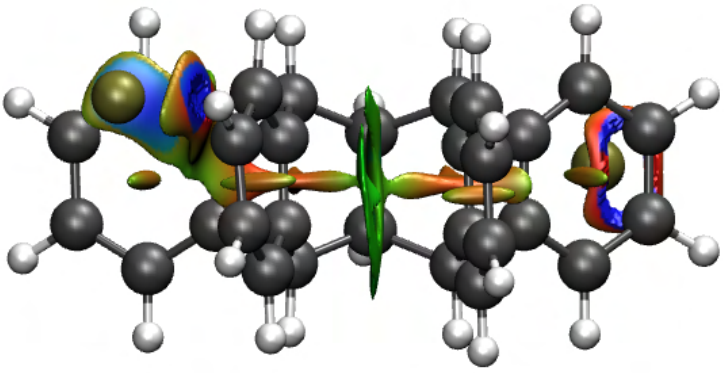
Plot of the RDG x sign(λ_2)ρ



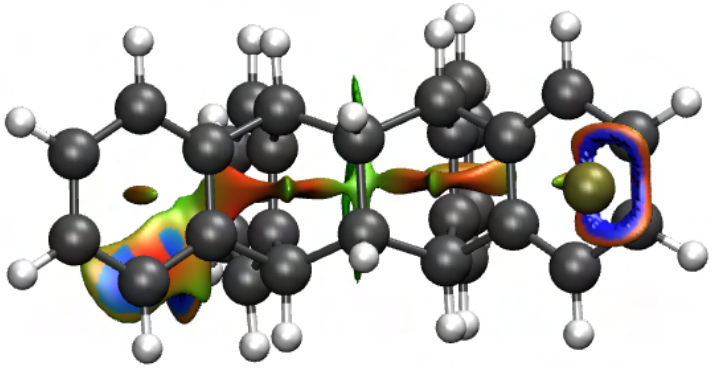
Front view



Side view

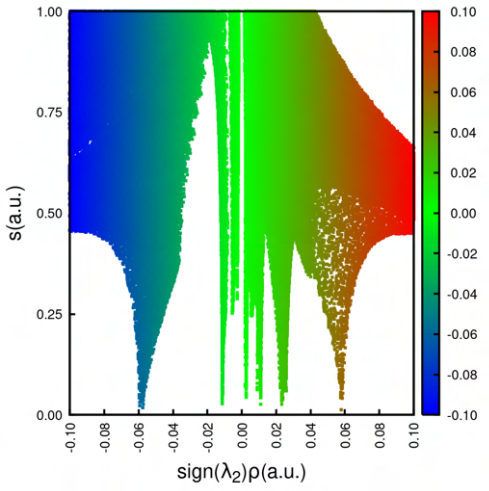


Top view

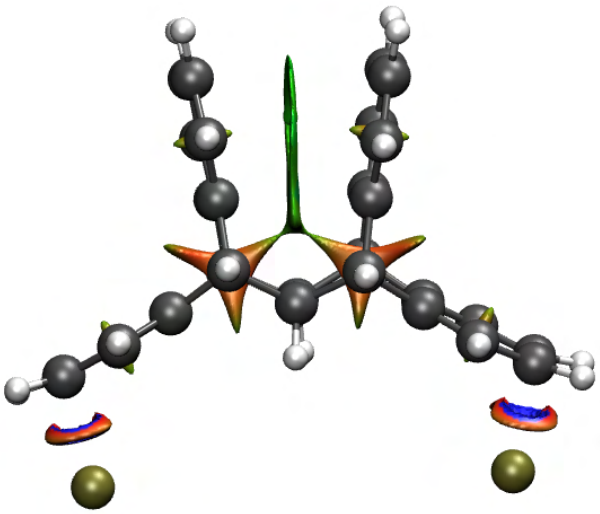


Bottom view

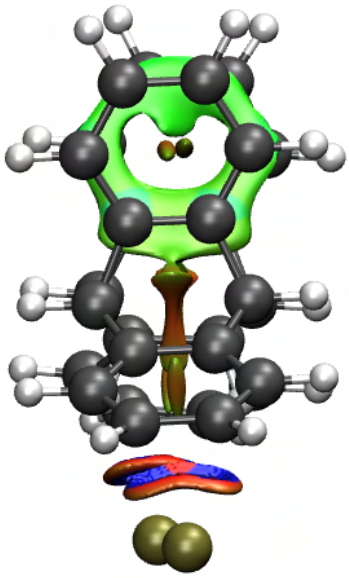
Figure S66: NCI images of system 2h.



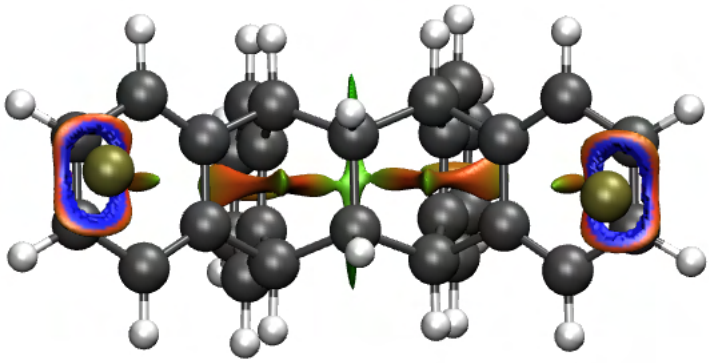
Plot of the RDG x sign(λ_2)ρ



Front view



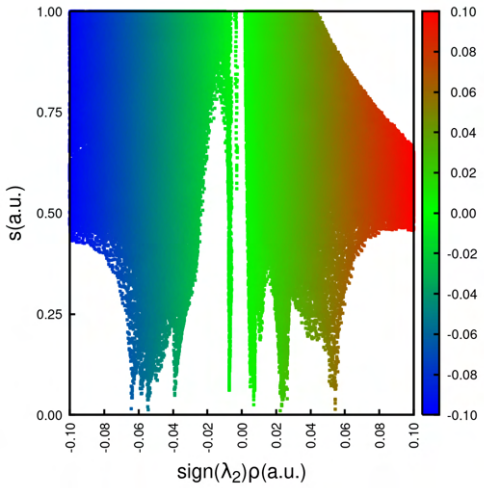
Side view



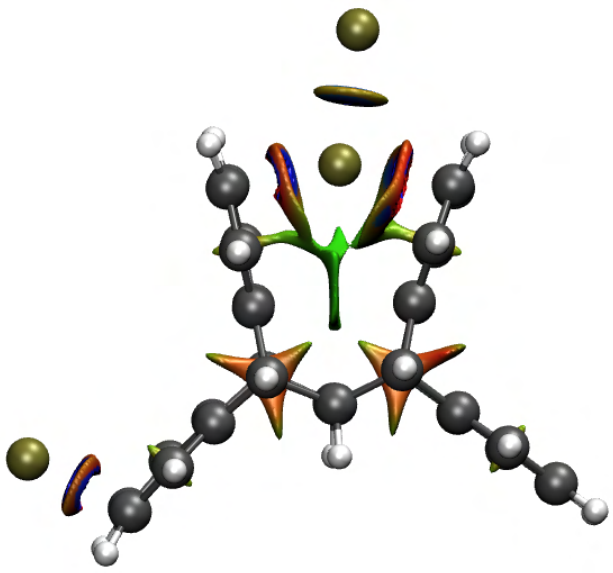
Bottom view

Figure S67: NCI images of system 2i.

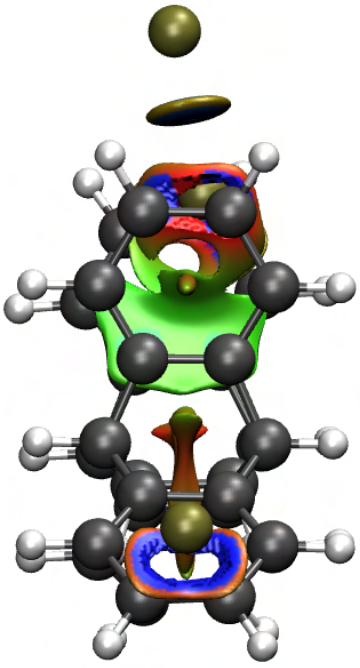
3Ag Systems



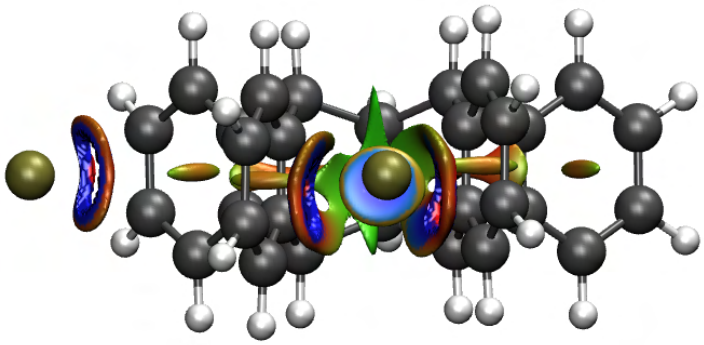
Plot of the RDG x sign(λ_2)ρ



Front view

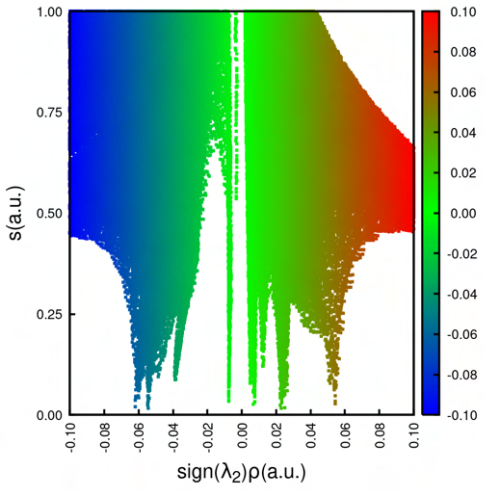


Side view

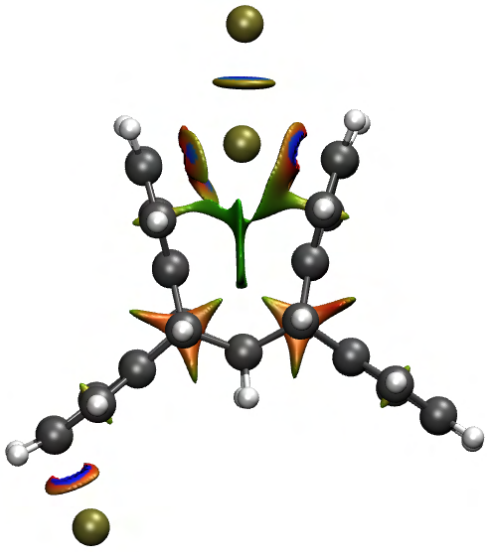


Top view

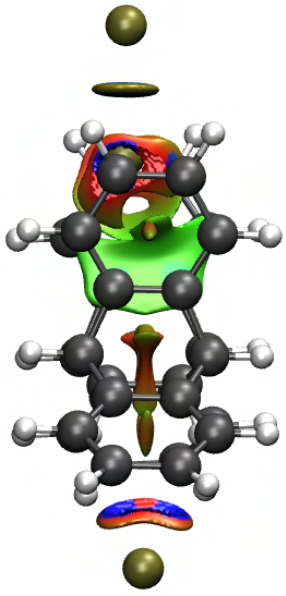
Figure S68: NCI images of system 3a.



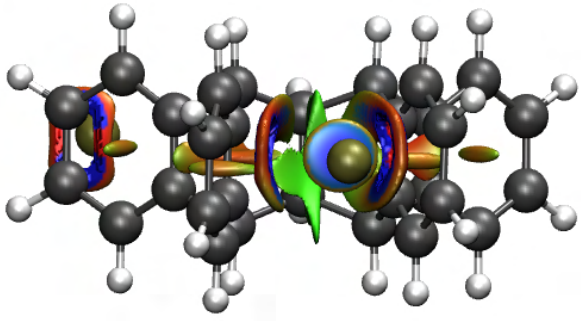
Plot of the RDG x sign(λ_2)ρ



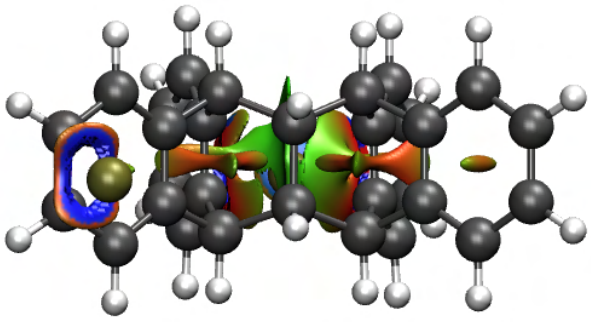
Front view



Side view

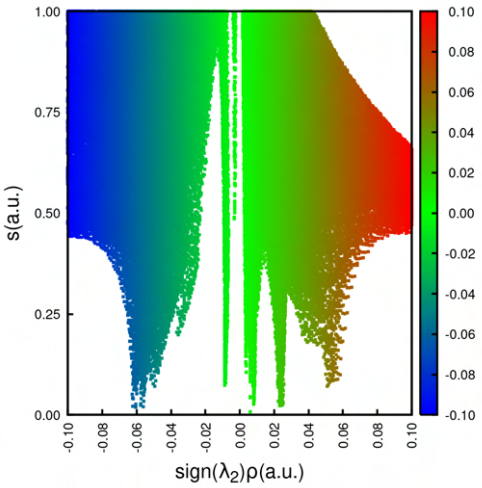


Top view

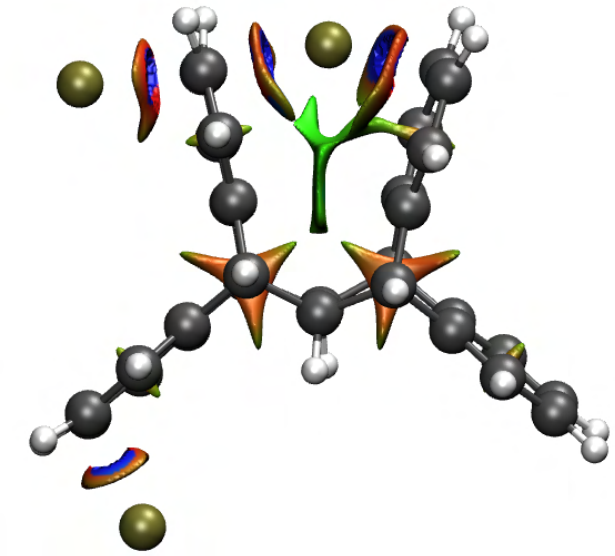


Bottom view

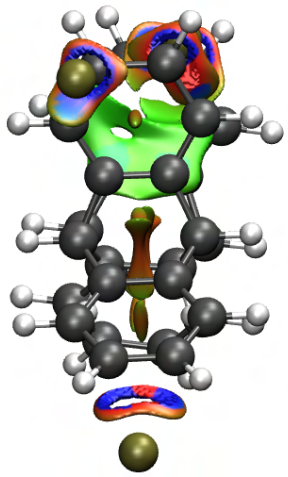
Figure S69: NCI images of system 3b.



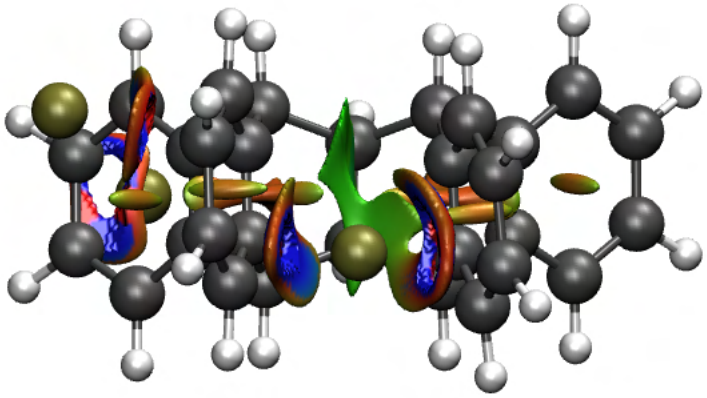
Plot of the RDG x sign(λ_2)ρ



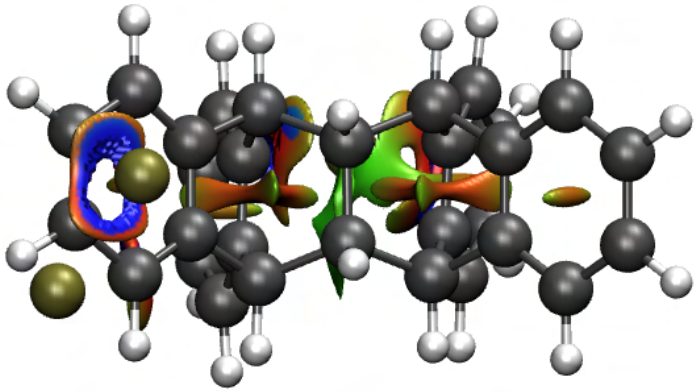
Front view



Side view

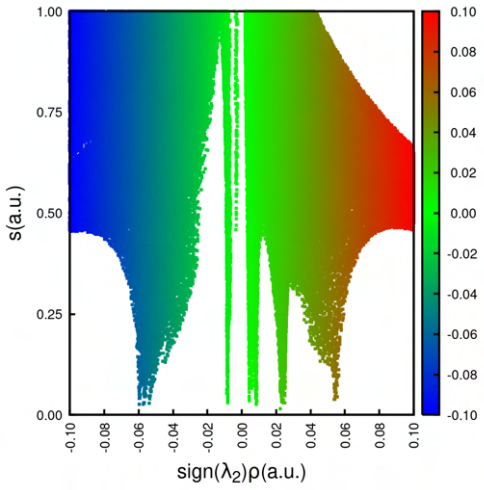


Top view

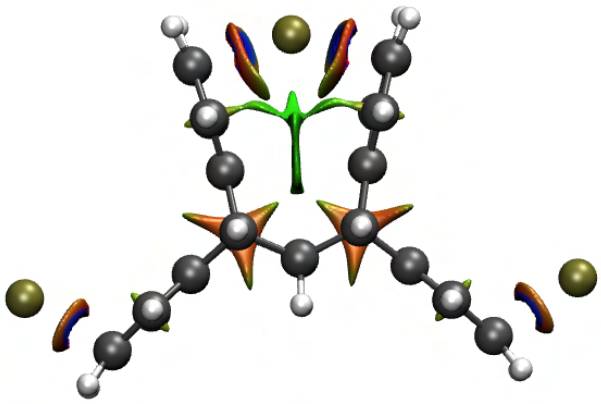


Bottom view

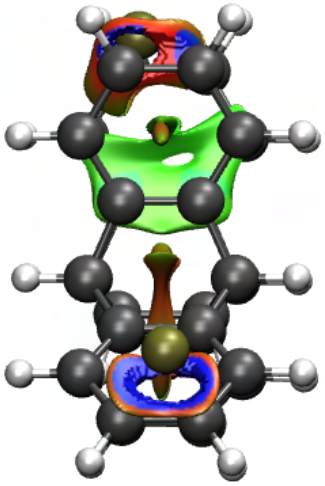
Figure S70: NCI images of system 3c.



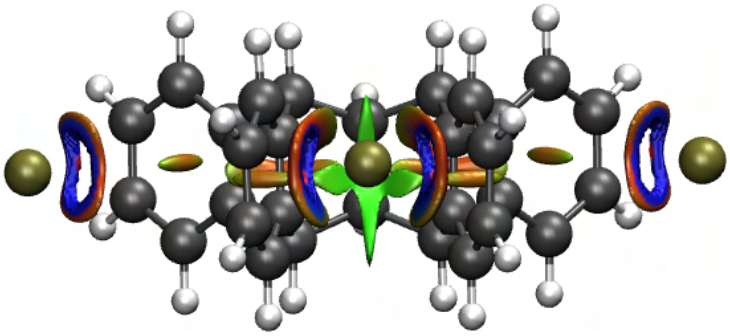
Plot of the RDG x sign(λ_2)ρ



Front view

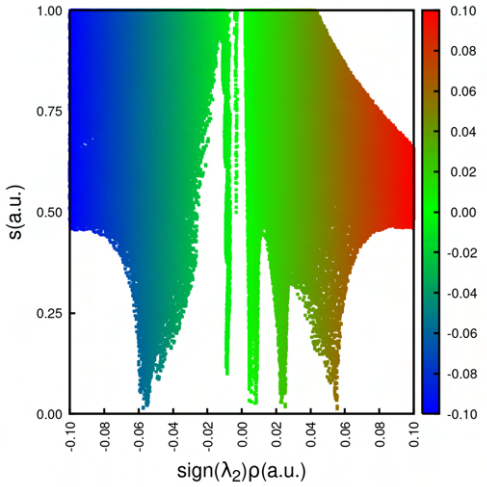


Side view

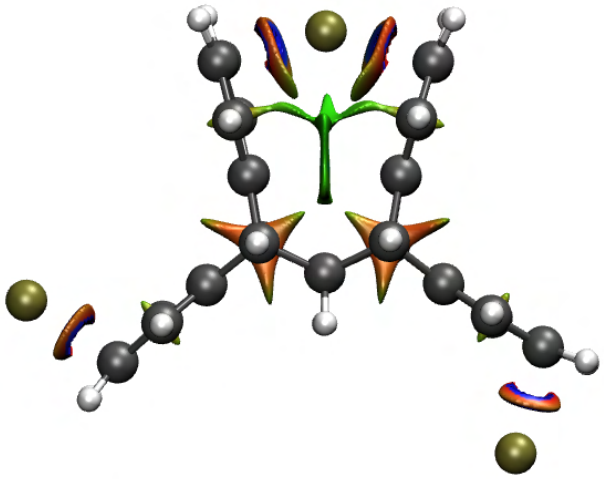


Top view

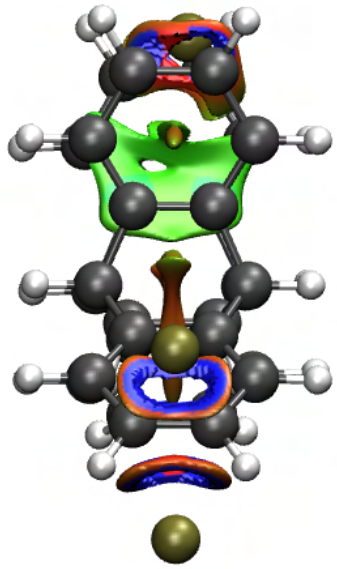
Figure S71: NCI images of system 3d.



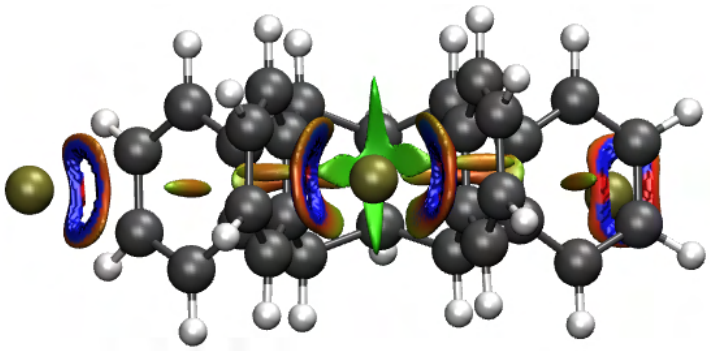
Plot of the RDG x sign(λ_2)ρ



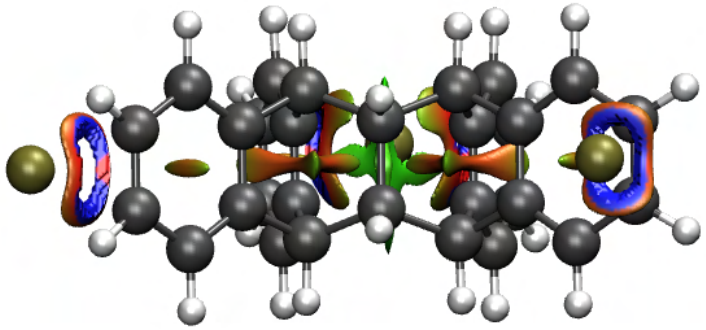
Front view



Side view

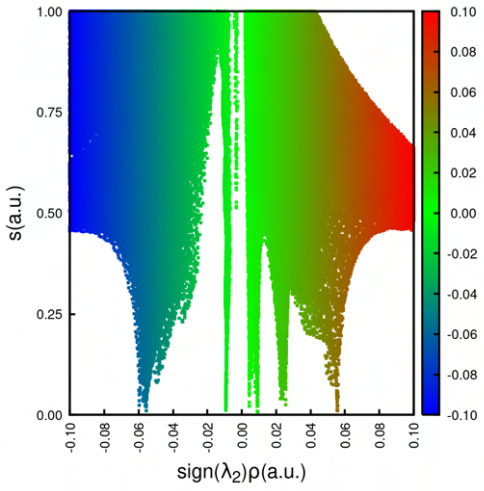


Top view

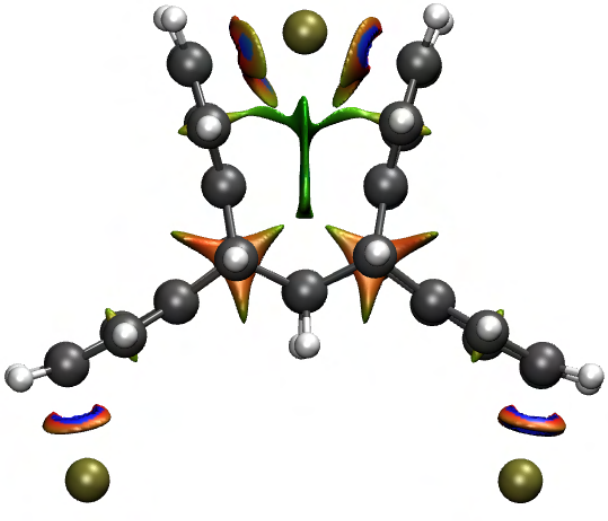


Bottom view

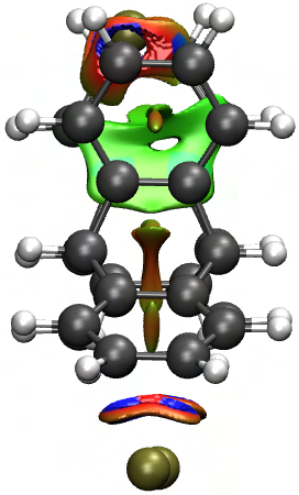
Figure S72: NCI images of system 3e.



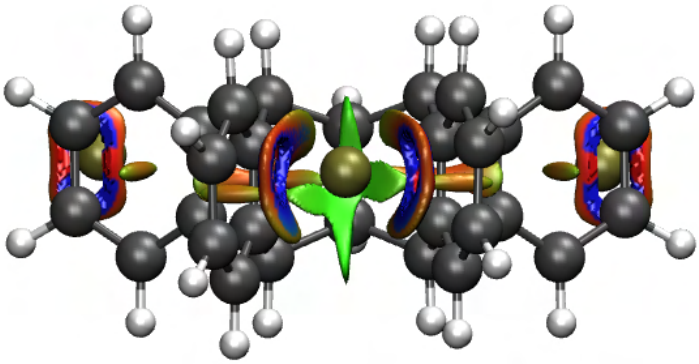
Plot of the RDG x sign(λ_2)ρ



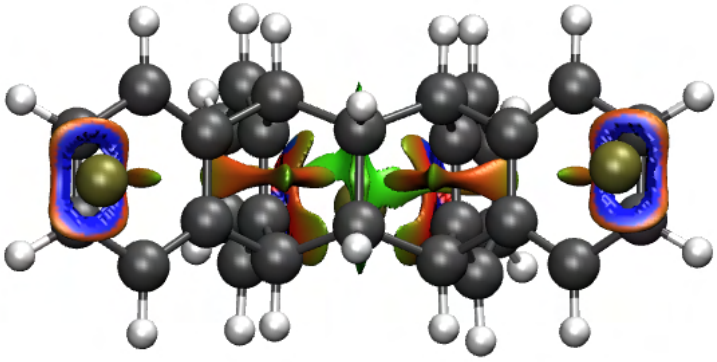
Front view



Side view

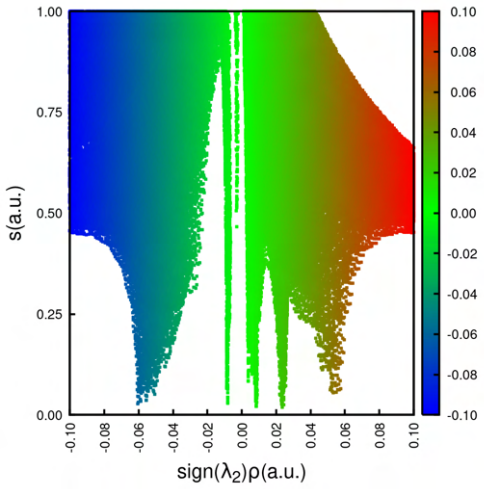


Top view

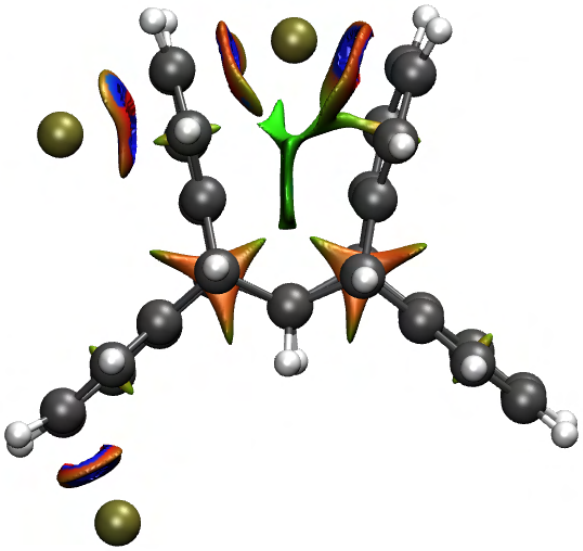


Bottom view

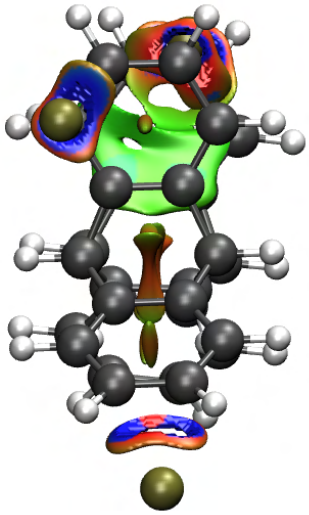
Figure S73: NCI images of system 3f.



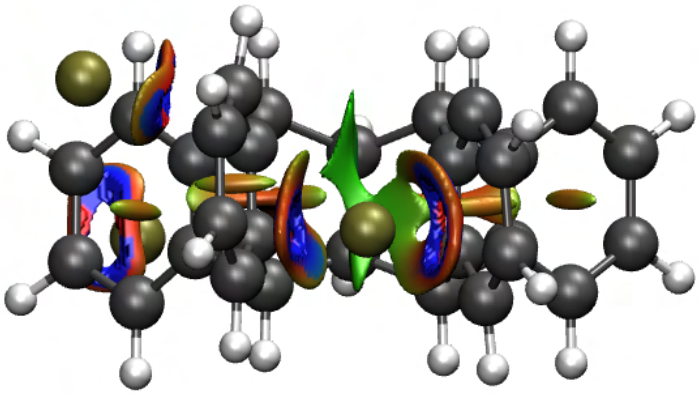
Plot of the RDG x sign(λ_2)ρ



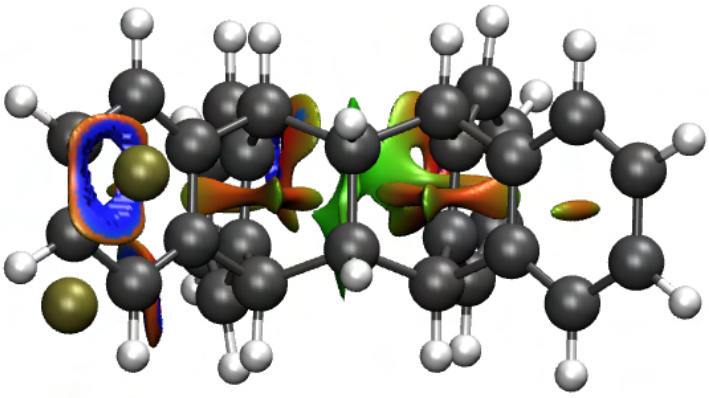
Front view



Side view

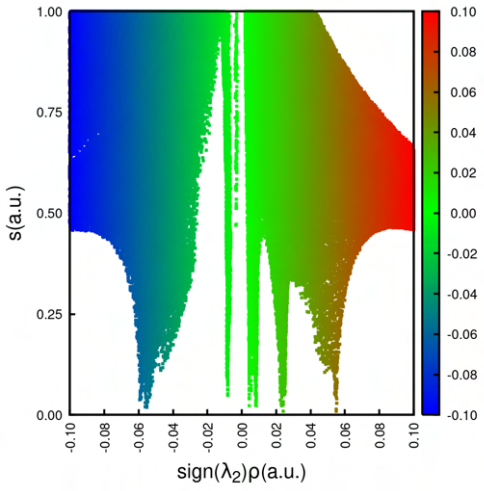


Top view

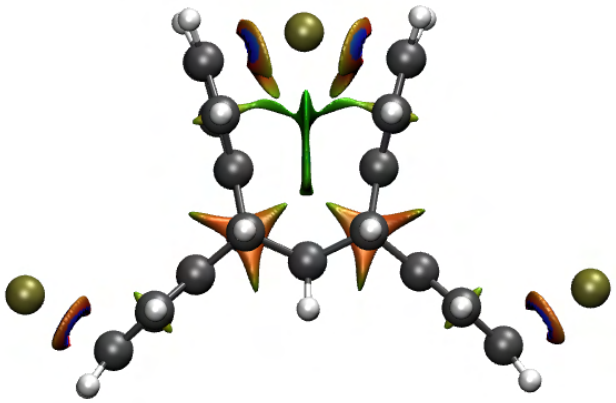


Bottom view

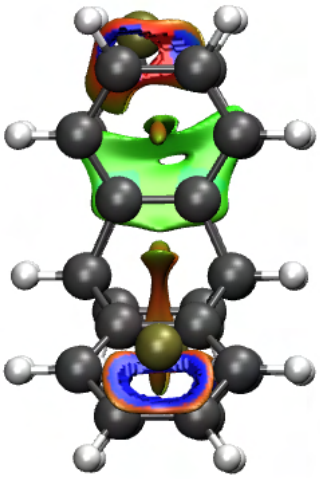
Figure S74: NCI images of system 3g.



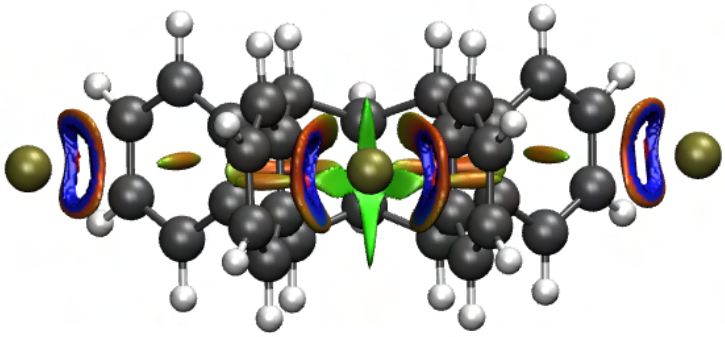
Plot of the RDG x sign(λ_2)ρ



Front view

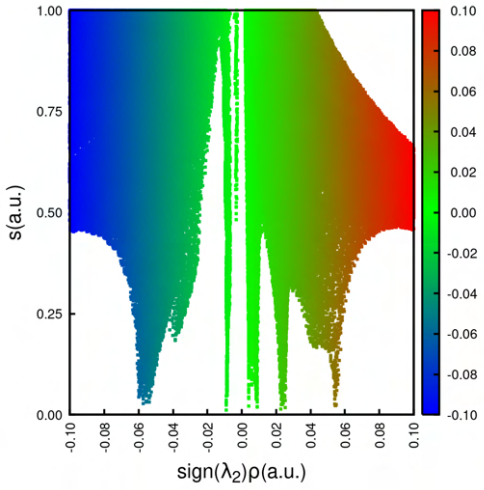


Side view

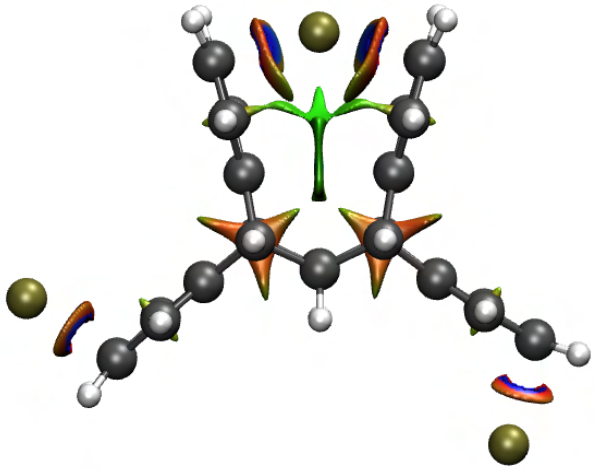


Top view

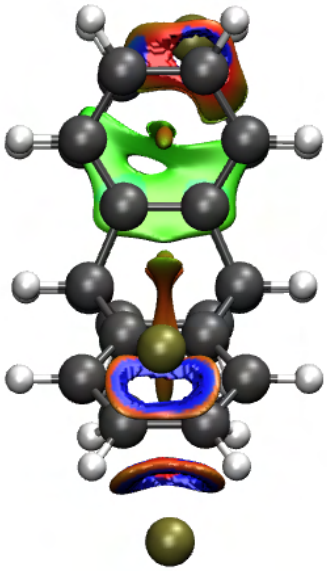
Figure S75: NCI images of system 3h.



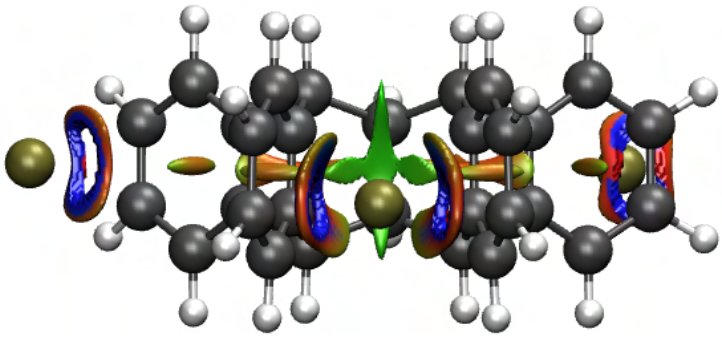
Plot of the RDG x sign(λ_2)ρ



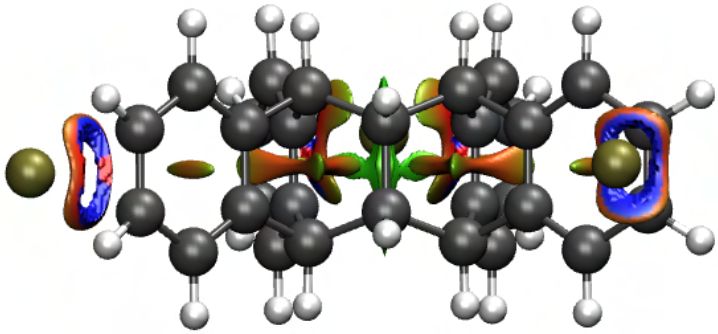
Front view



Side view

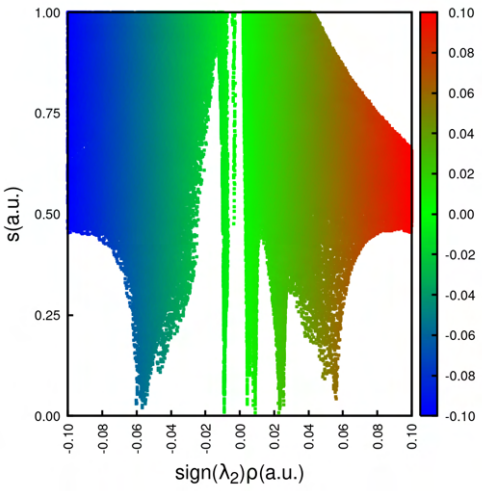


Top view

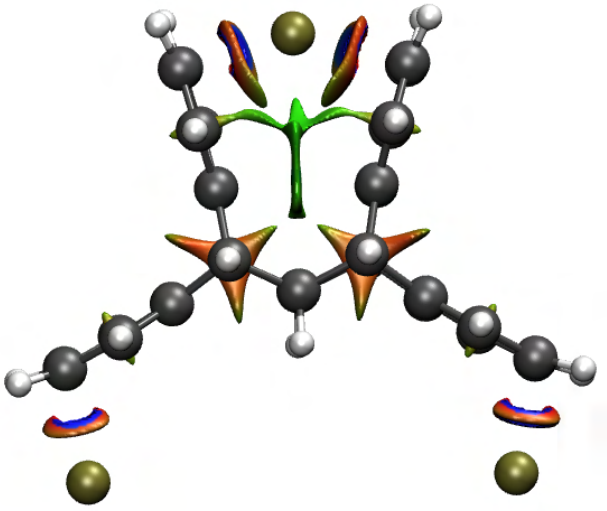


Bottom view

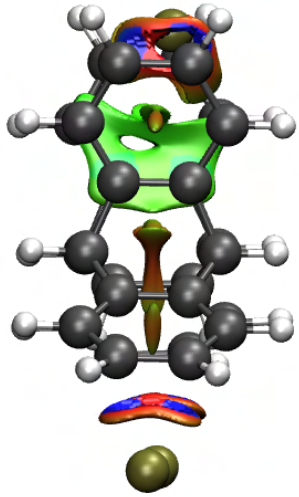
Figure S76: NCI images of system 3i.



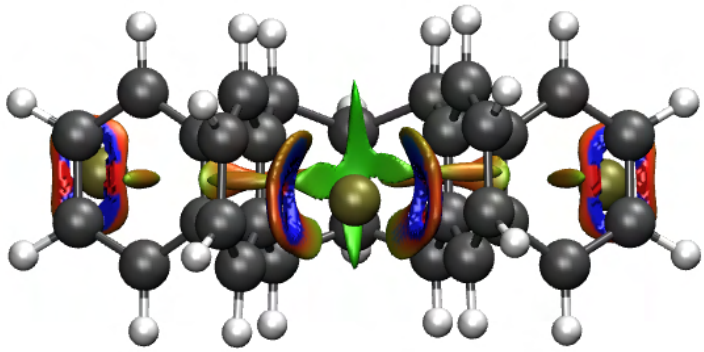
Plot of the RDG x sign(λ_2)ρ



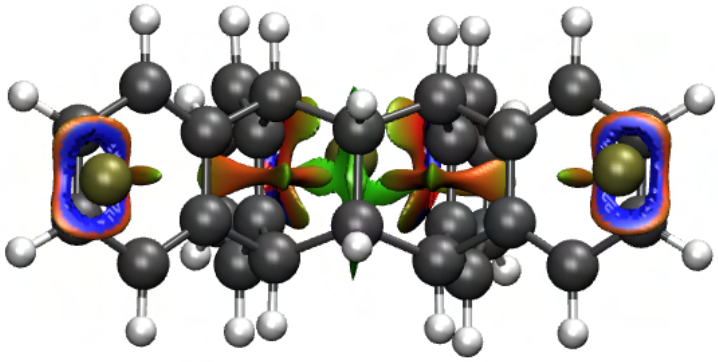
Front view



Side view

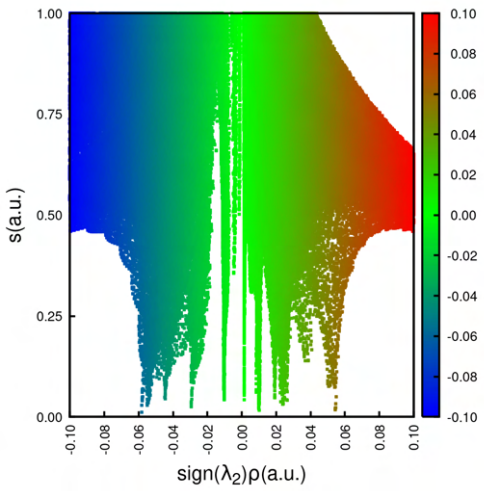


Top view

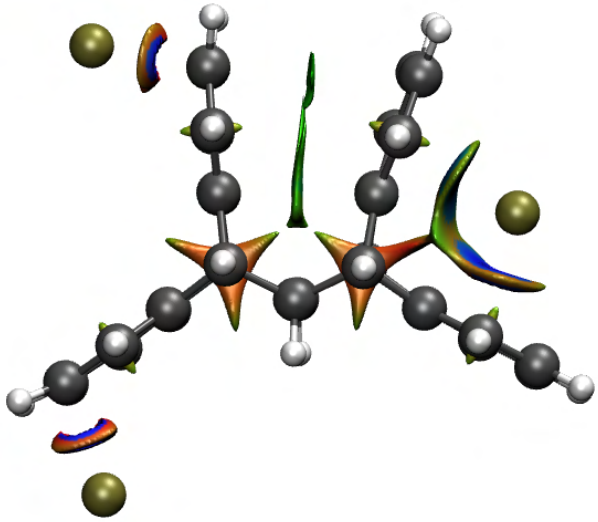


Bottom view

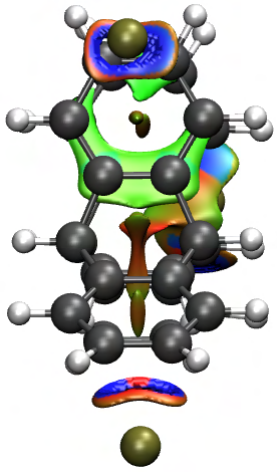
Figure S77: NCI images of system 3j.



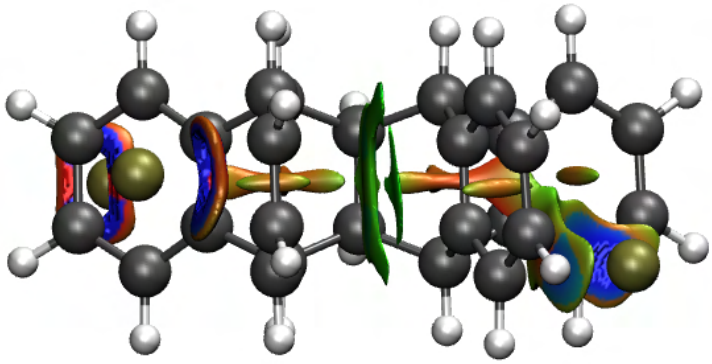
Plot of the RDG x sign(λ_2)ρ



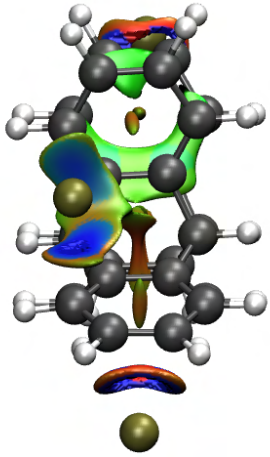
Front view



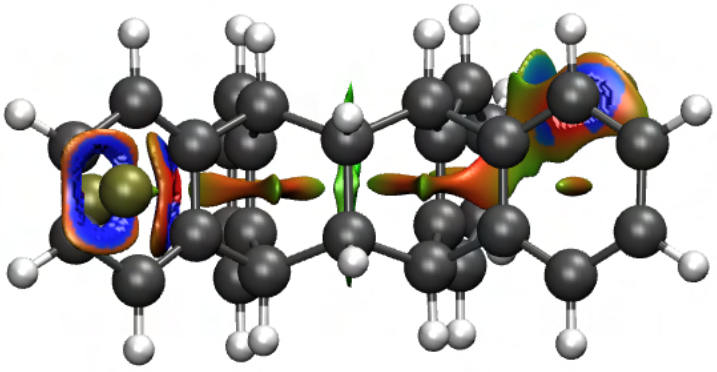
Side view



Top view

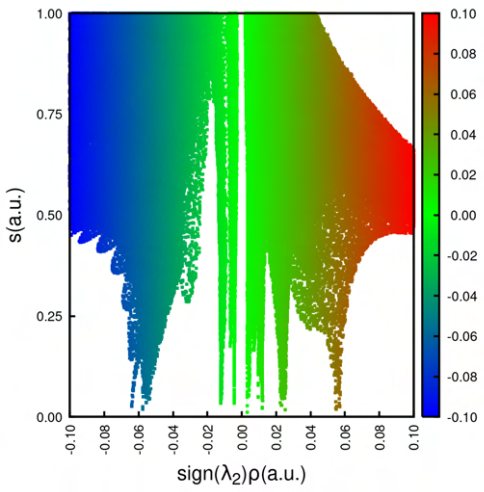


Side view B

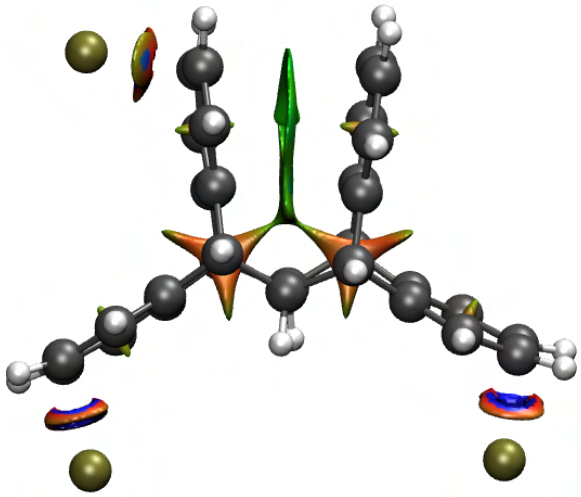


Bottom view

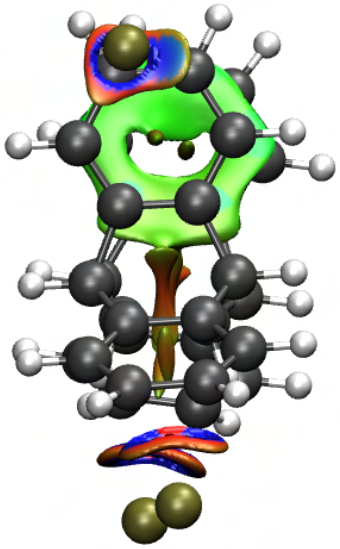
Figure S78: NCI images of system 3k.



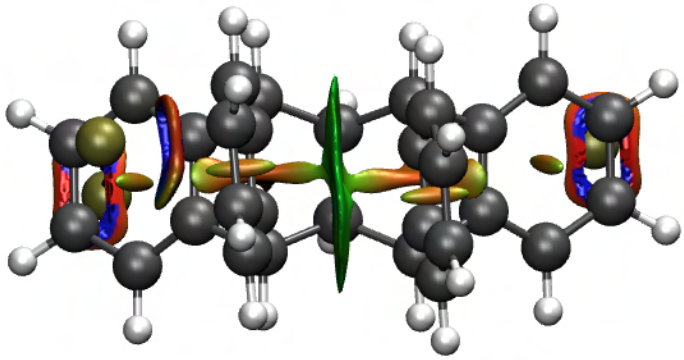
Plot of the RDG x sign(λ_2)ρ



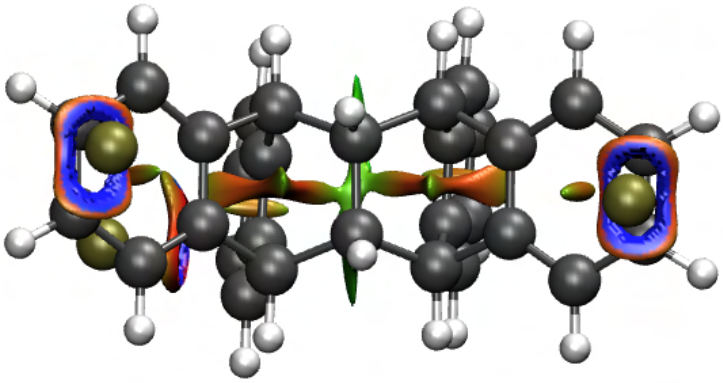
Front view



Side view



Top view



Bottom view

Figure S79: NCI images of system 3l.

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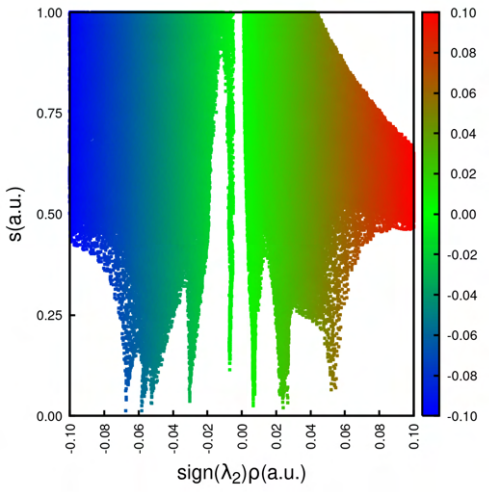
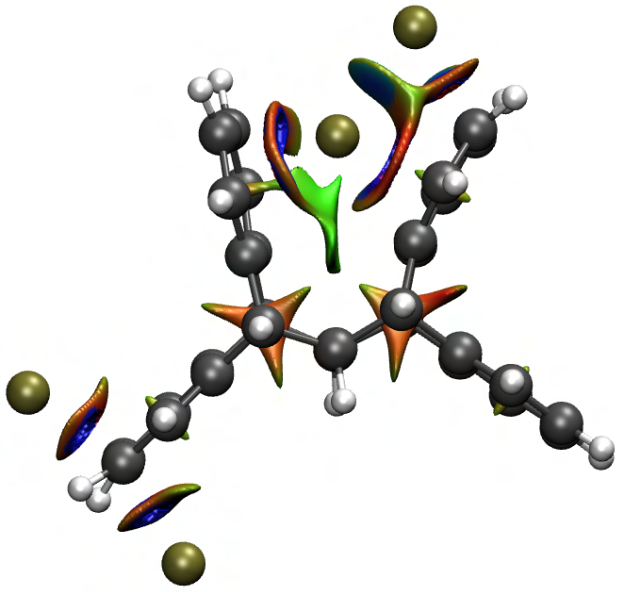
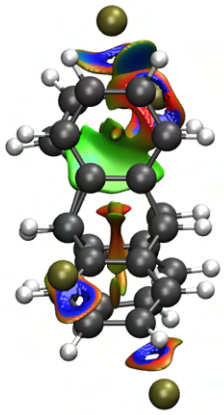


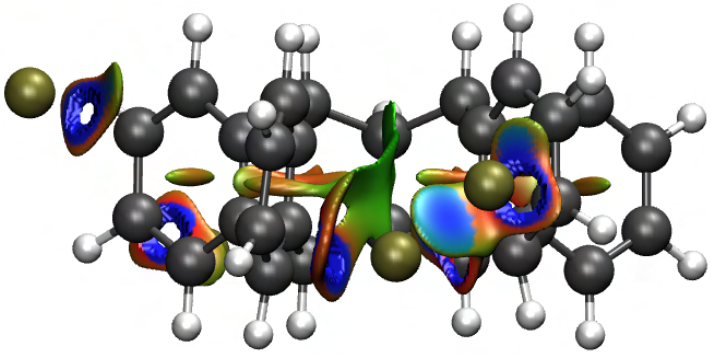
Plot of the RDG x sign(λ_2)ρ



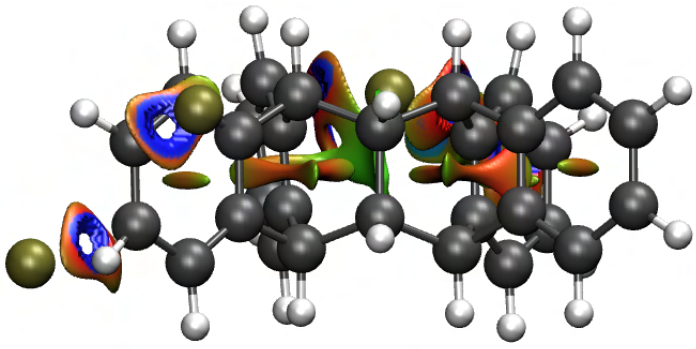
Front view



Side view

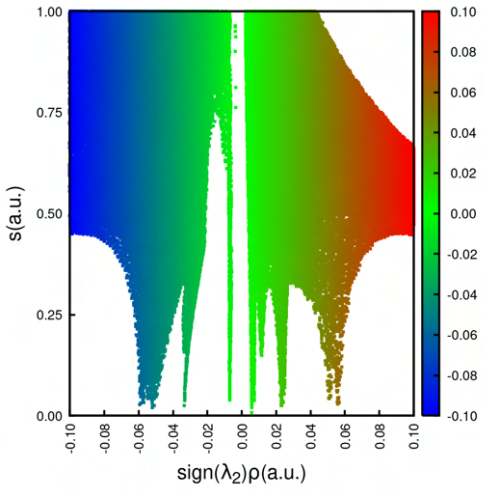


Top view

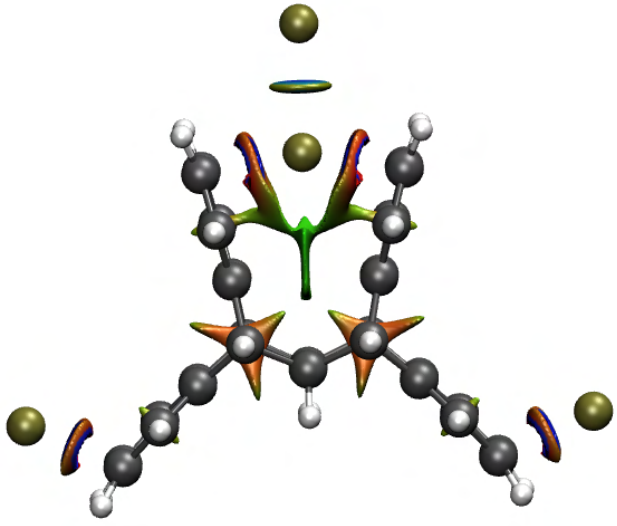


Bottom view

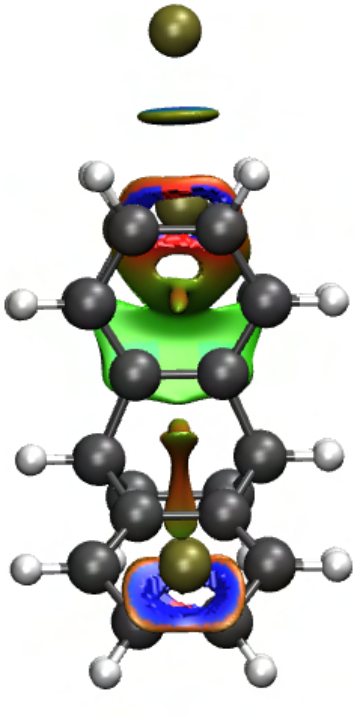
Figure S80: NCI images of system 4a.



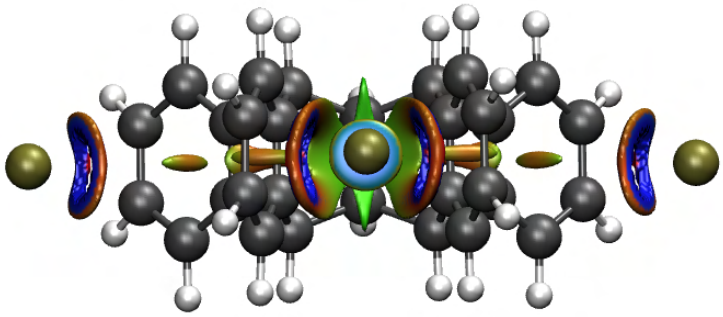
Plot of the RDG x sign(λ_2)ρ



Front view

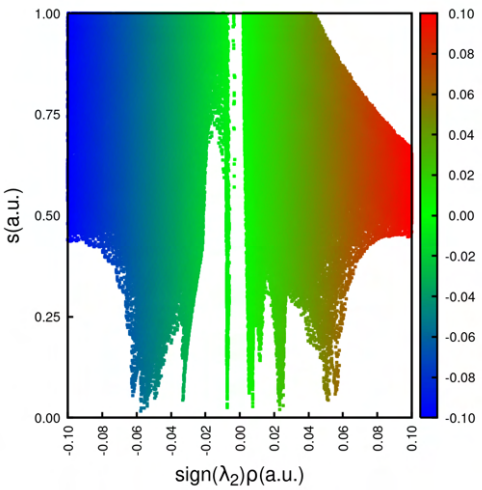


Side view

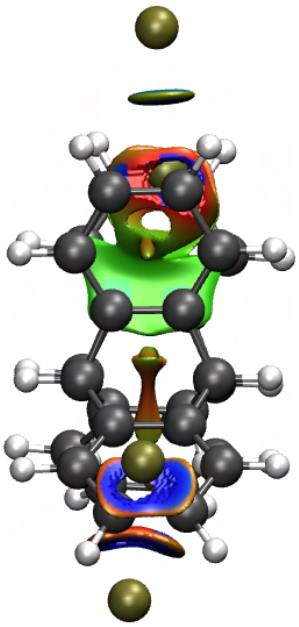


Top view

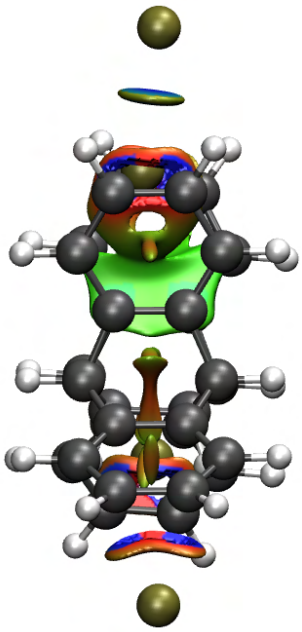
Figure S81: NCI images of system 4b.



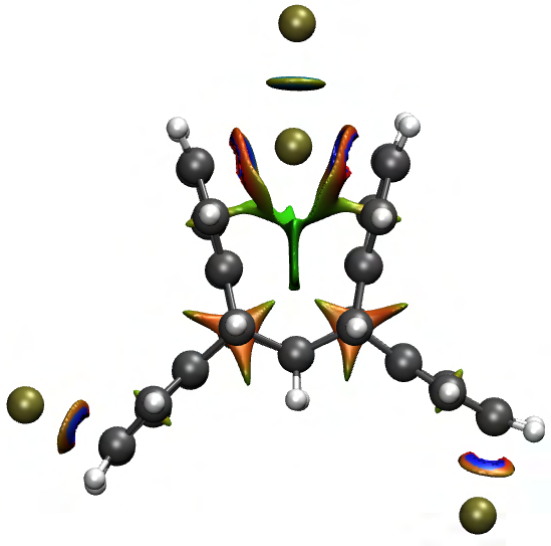
Plot of the RDG x sign(λ_2)ρ



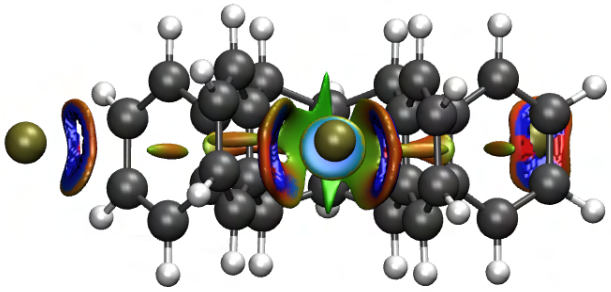
Side view



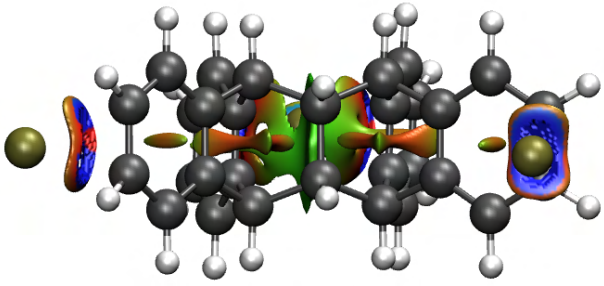
Side view B



Front view

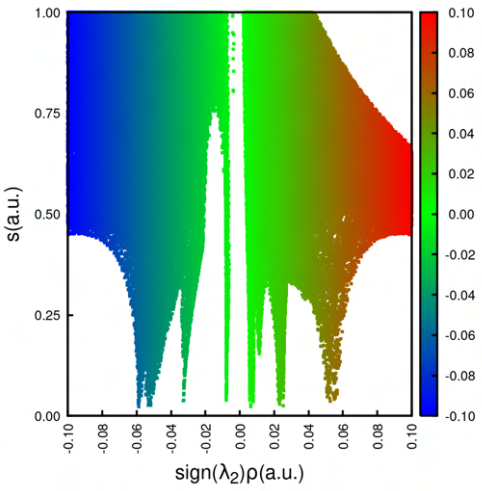


Top view

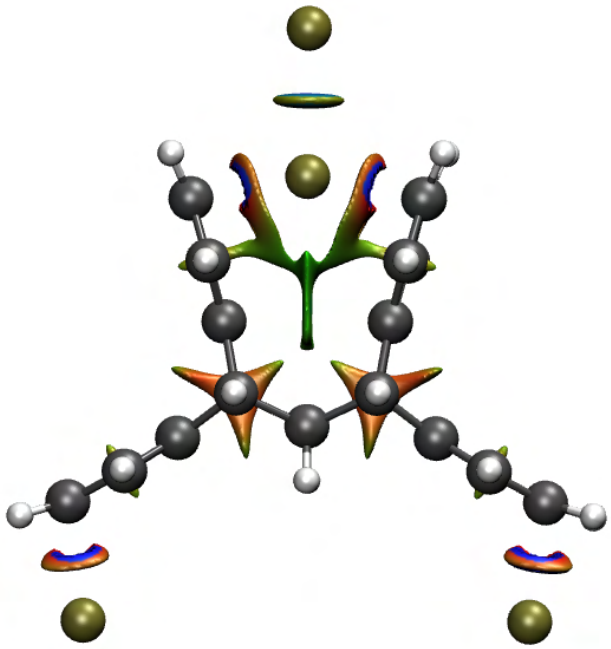


Bottom view

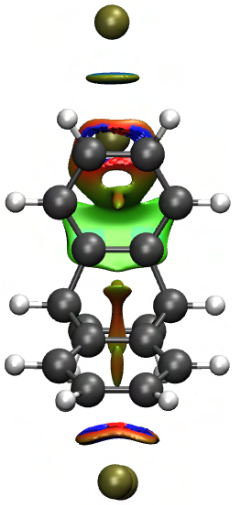
Figure S82: NCI images of system 4c.



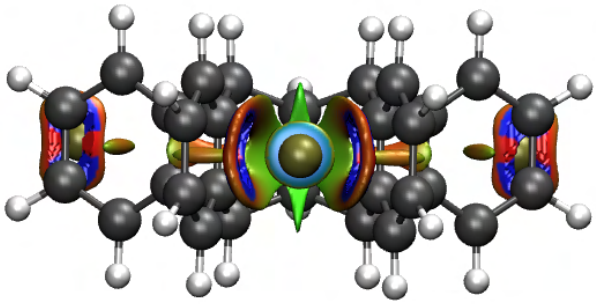
Plot of the RDG x sign(λ_2)ρ



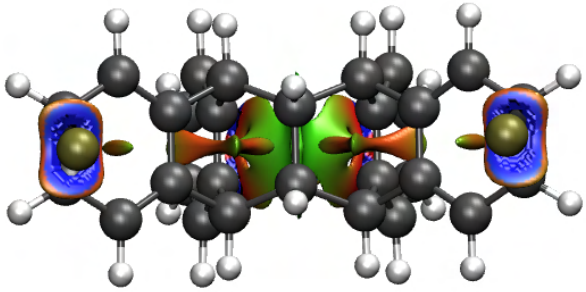
Front view



Side view

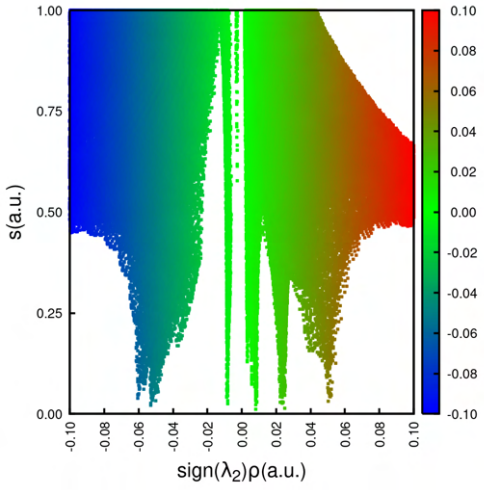


Top view

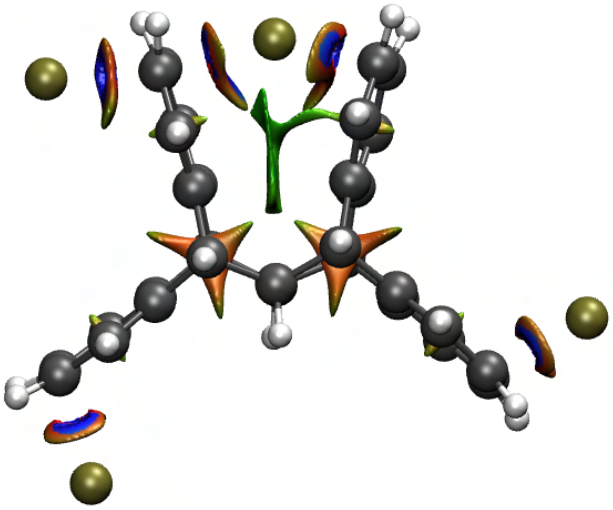


Bottom view

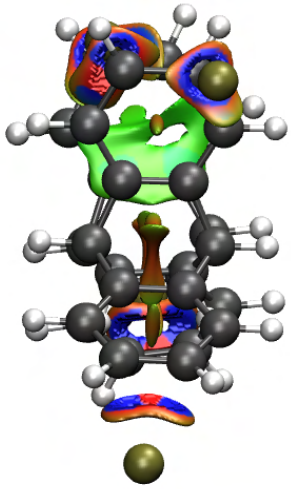
Figure S83: NCI images of system 4d.



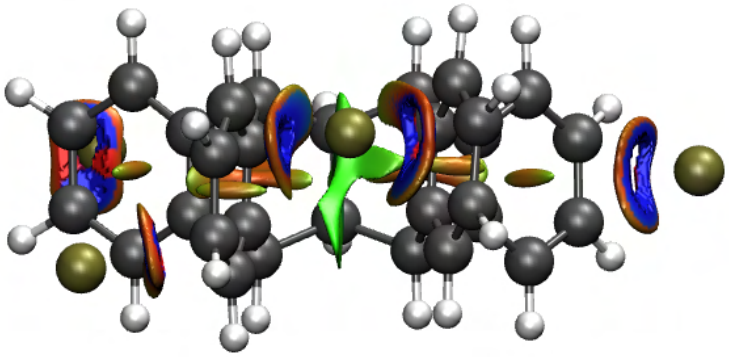
Plot of the RDG x sign(λ_2)ρ



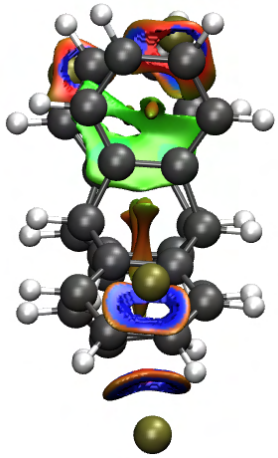
Front view



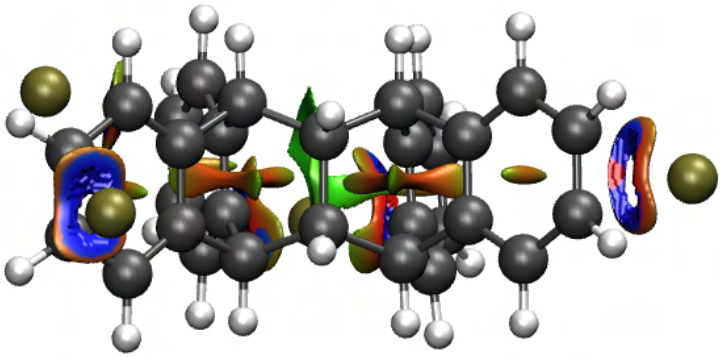
Side view



Top view

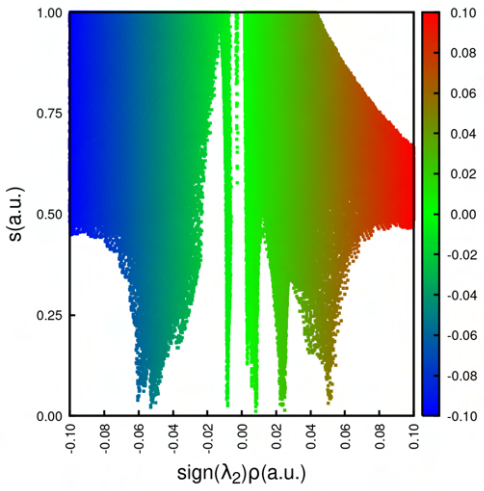


Side view B

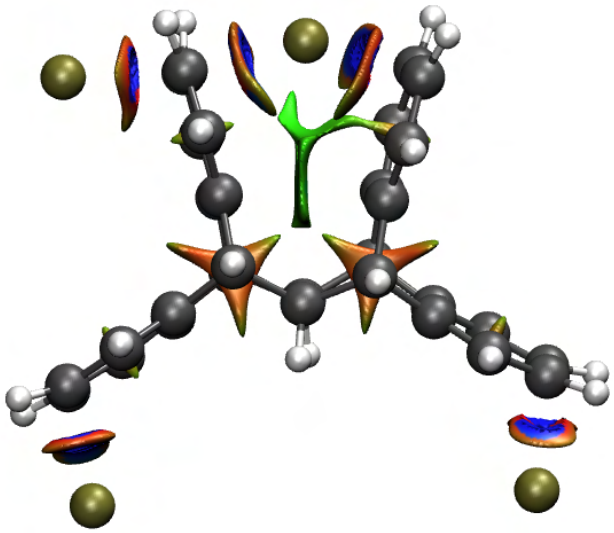


Bottom view

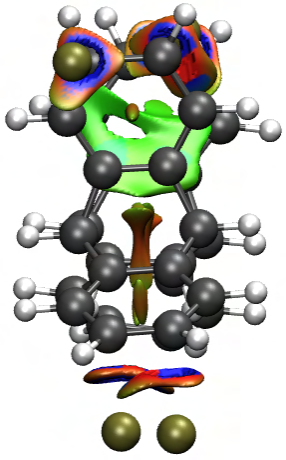
Figure S84: NCI images of system 4e.



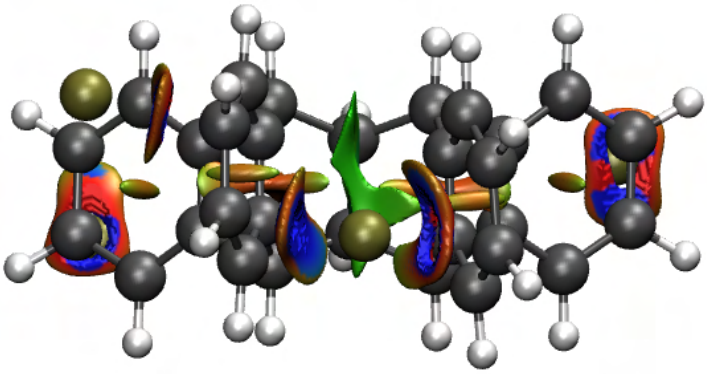
Plot of the RDG x sign(λ_2)ρ



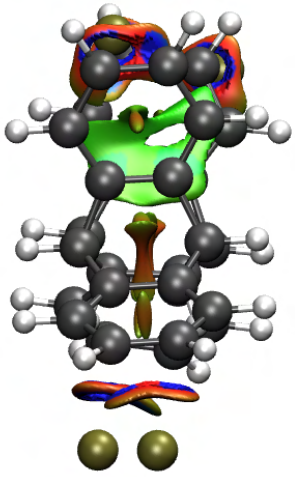
Front view



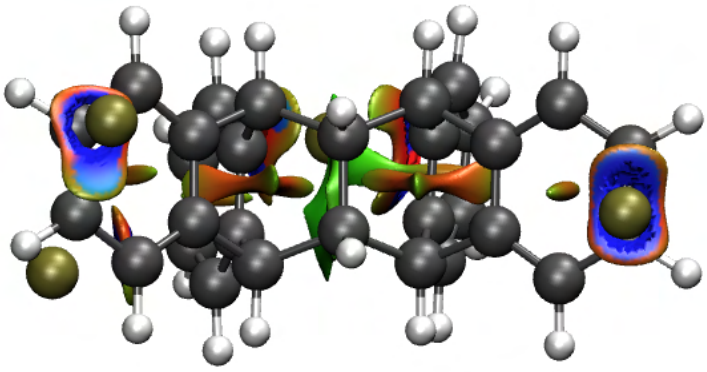
Side view



Top view

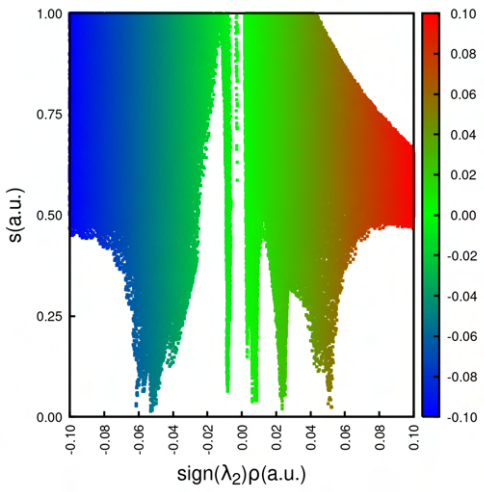


Side view B

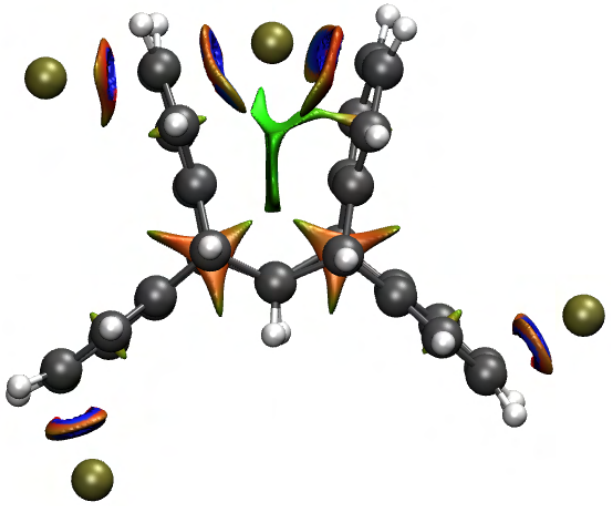


Bottom view

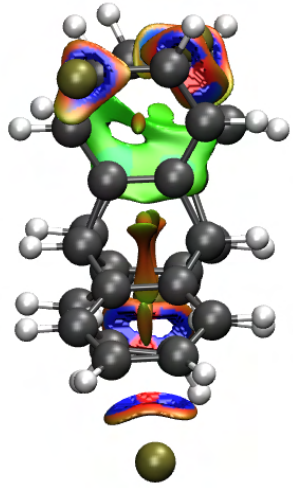
Figure S85: NCI images of system 4f.



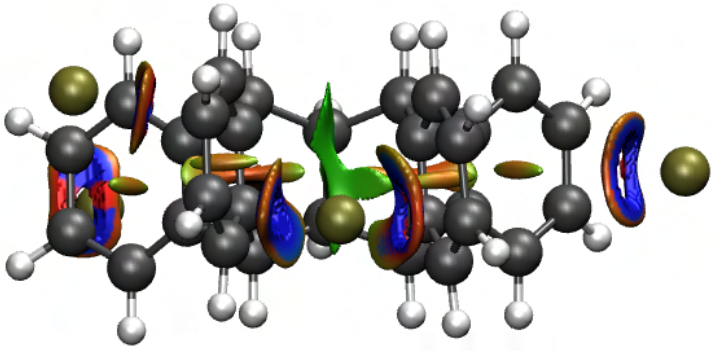
Plot of the RDG x sign(λ_2)ρ



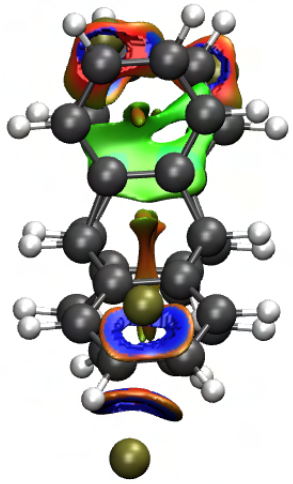
Front view



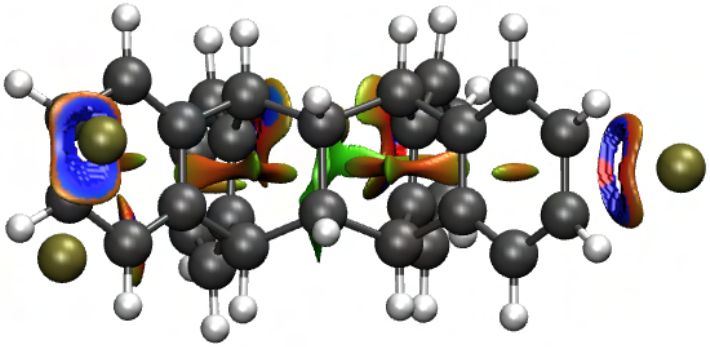
Side view



Top view

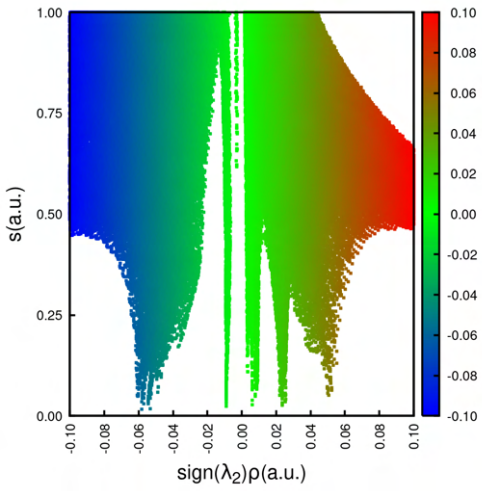


Side view B

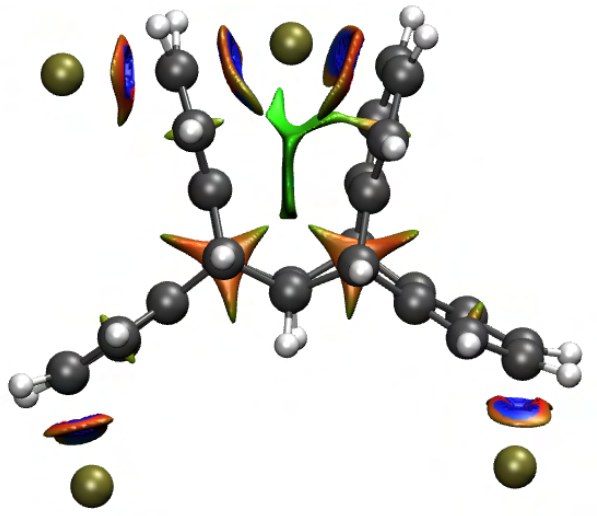


Bottom view

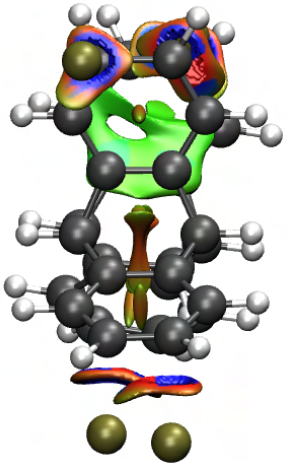
Figure S86: NCI images of system 4g.



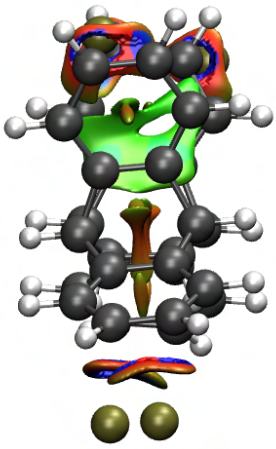
Plot of the RDG x sign(λ_2)ρ



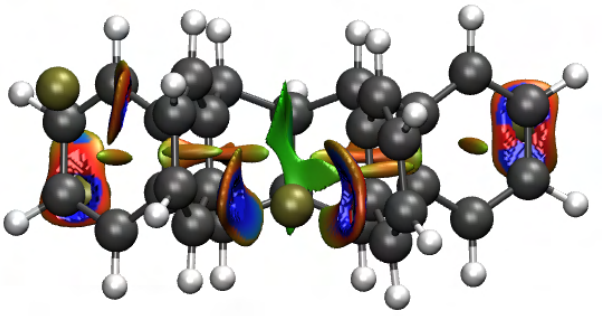
Front view



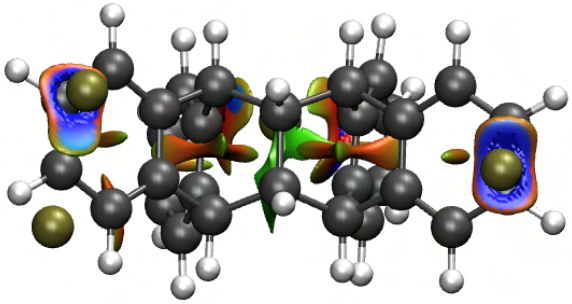
Side view



Side view B

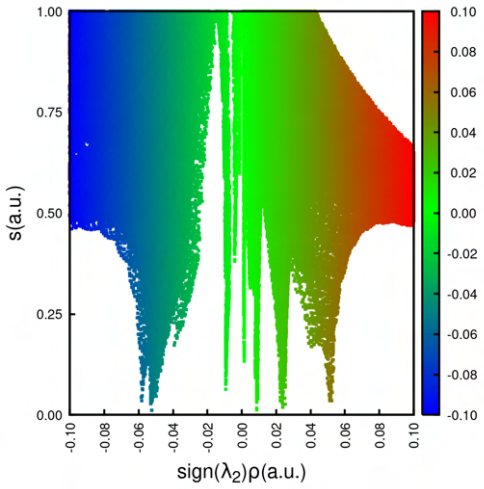


Top view

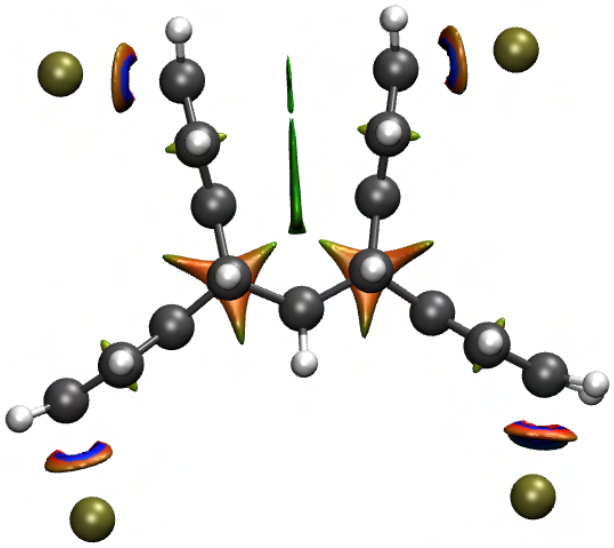


Bottom view

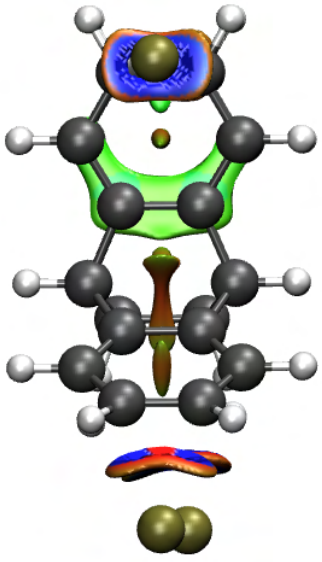
Figure S87: NCI images of system 4h.



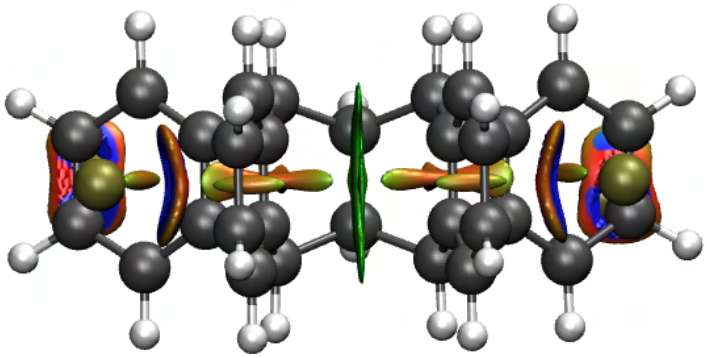
Plot of the RDG x sign(λ_2)ρ



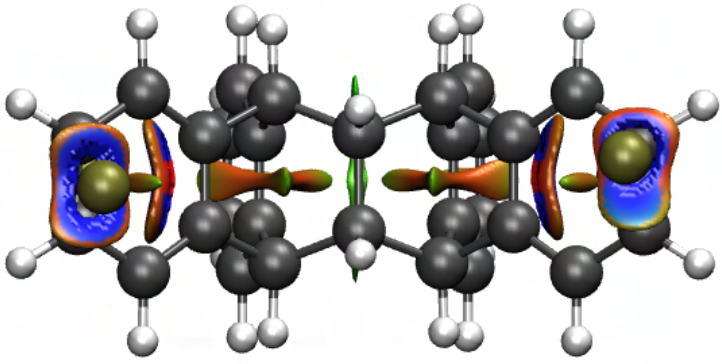
Front view



Side view



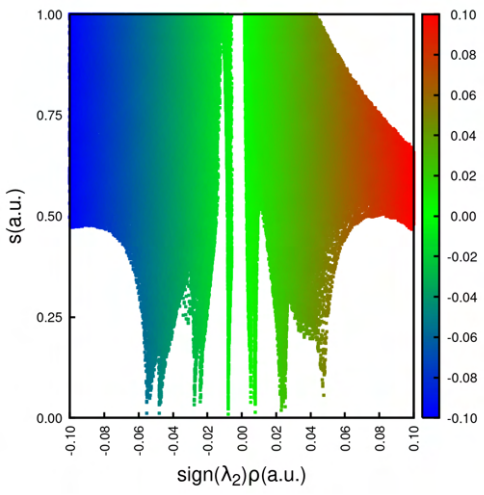
Top view



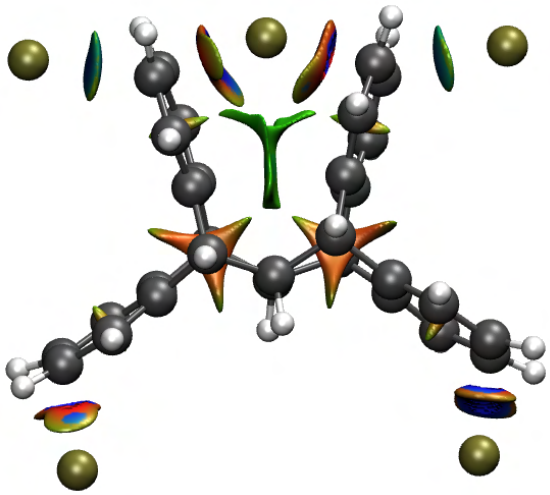
Bottom view

Figure S88: NCI images of system 4i.

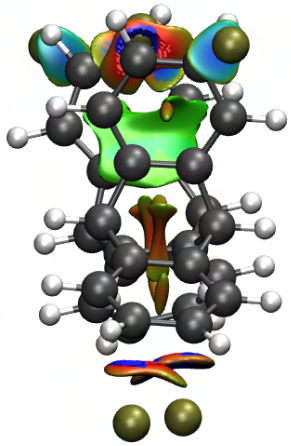
5Ag System



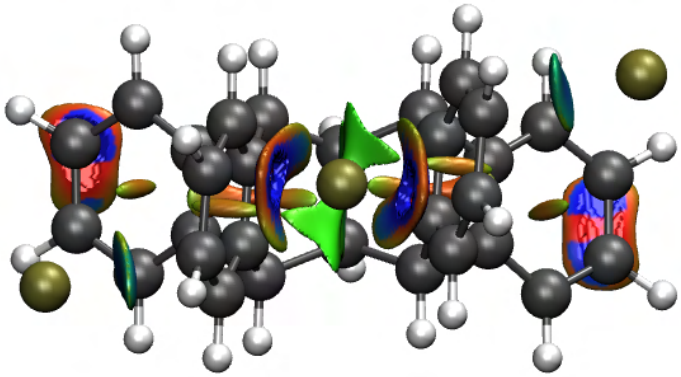
Plot of the RDG x sign(λ_2)ρ



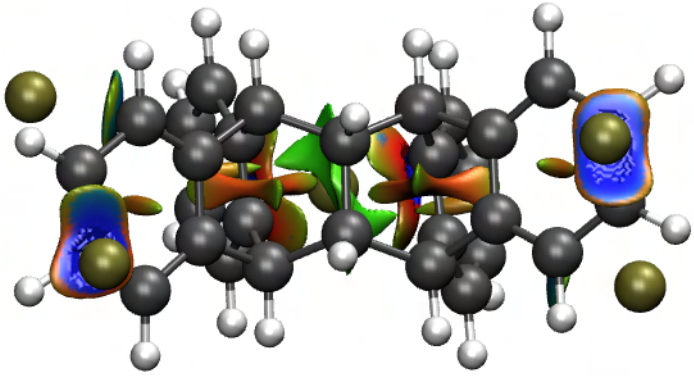
Front view



Side view



Top view



Bottom view

Figure S89: NCI images of system 5.

Cartesian Coordinates

Table S16: Cartesian coordinates of janusene-Ag^+ **1a** and **1b**

1a	x	y	z
C	1.126983	-0.291195	-0.879128
C	0.552396	-1.639732	-1.423039
C	0.718206	-1.747502	1.172691
C	0.664308	0.920979	1.318893
C	0.384004	1.030733	-1.266581
C	1.603487	-2.770771	0.472739
C	2.455289	-3.681001	1.086940
C	3.229050	-4.533429	0.290747
C	3.148368	-4.468061	-1.100476
C	2.291840	-3.549957	-1.718891
C	1.521827	-2.705036	-0.928385
C	-0.674554	-2.007874	0.652498
C	-1.779992	-2.364980	1.413700
C	-2.987567	-2.720139	0.773744
C	-3.071507	-2.693699	-0.643979
C	-1.942315	-2.302704	-1.405697
C	-0.760476	-1.967137	-0.759764
C	-0.765673	1.119000	0.888214
C	-1.850997	1.333894	1.730159
C	-3.110338	1.636709	1.184270
C	-3.274789	1.701542	-0.224327
C	-2.160404	1.457466	-1.074100
C	-0.918930	1.174585	-0.516474
C	1.279544	2.132401	-0.714816
C	1.435534	2.068964	0.680088
C	2.246066	2.984801	1.340248
C	2.903386	3.972049	0.596958
C	2.748126	4.035127	-0.788058
C	1.933635	3.111356	-1.453213
H	-1.712997	-2.408818	2.500115
H	-3.818525	-3.114842	1.357625
H	-3.954144	-3.094033	-1.142947
H	-1.999172	-2.302360	-2.493621
H	-1.723956	1.300391	2.811502
H	-3.944007	1.894616	1.836027
H	-4.204814	2.085943	-0.645304
H	-2.277987	1.541835	-2.154047
H	2.368848	2.936415	2.422227
H	3.538124	4.696697	1.104539
H	3.261882	4.808991	-1.356295
H	2.126285	-0.202120	-1.320264
H	0.249746	1.108185	-2.351716
H	0.771801	0.904224	2.409511
H	0.474517	-1.623957	-2.516186
H	0.774912	-1.825822	2.264520
C	1.263732	-0.369373	0.673657
H	2.327137	-0.362733	0.938943
H	1.814914	3.160368	-2.535639
H	2.230138	-3.499687	-2.806006
H	3.753474	-5.137074	-1.710377
H	3.896673	-5.253338	0.761574
H	2.521000	-3.731588	2.173794
Ag	-3.677748	-0.541300	0.022953

1b	x	y	z
C	1.102737	-0.294798	-0.880431
C	0.478275	-1.622361	-1.421105
C	0.696405	-1.761294	1.169155
C	0.528858	0.913808	1.289266
C	0.423481	1.045092	-1.308113
C	1.574645	-2.768870	0.439190
C	2.446254	-3.679629	1.024273
C	3.195206	-4.530002	0.202669
C	3.069311	-4.463301	-1.185123
C	2.192710	-3.545112	-1.774525
C	1.448129	-2.701871	-0.958549
C	-0.701896	-2.035288	0.677304
C	-1.776660	-2.447795	1.453090
C	-3.010909	-2.769096	0.829531
C	-3.136879	-2.644181	-0.579867
C	-2.035467	-2.219682	-1.350284
C	-0.825446	-1.936909	-0.729086
C	-0.869076	1.120548	0.755889
C	-2.011881	1.352839	1.513574
C	-3.239902	1.661183	0.860620
C	-3.284064	1.719835	-0.556970
C	-2.122830	1.474392	-1.304906
C	-0.925753	1.192227	-0.654575
C	1.289541	2.133851	-0.687096
C	1.343146	2.066055	0.715290
C	2.109041	2.974727	1.435612
C	2.824652	3.959911	0.745281
C	2.771625	4.027131	-0.647021
C	2.001157	3.111045	-1.372537
H	-1.670932	-2.563321	2.531357
H	-3.807643	-3.239448	1.406523
H	-4.053664	-2.969087	-1.070590
H	-2.130332	-2.149959	-2.433253
H	-1.966615	1.349926	2.602476
H	-4.091387	2.012618	1.445254
H	-4.206204	2.017128	-1.054249
H	-2.155220	1.537032	-2.392015
H	2.153174	2.921829	2.523467
H	3.424938	4.679265	1.300159
H	3.330476	4.798960	-1.174069
H	2.115947	-0.256802	-1.296734
H	0.368600	1.129766	-2.399544
H	0.556713	0.889870	2.384935
H	0.373423	-1.596623	-2.511866
H	0.779659	-1.849394	2.258555
C	1.194958	-0.363347	0.676147
H	2.248871	-0.310056	0.972524
H	1.961342	3.164237	-2.460610
H	2.096697	-3.492846	-2.859102
H	3.654482	-5.131581	-1.814987
H	3.878383	-5.249787	0.650802
H	2.546110	-3.732268	2.108529
Ag	-3.669618	-0.570091	0.606237

Table S17: Cartesian coordinates of janusene-Ag^+ **1c** and **1d**

1c	x	y	z
C	1.172076	-0.263076	-0.858943
C	0.607338	-1.600615	-1.429057
C	0.670372	-1.711791	1.172644
C	0.732035	0.934905	1.351870
C	0.349927	1.018991	-1.216252
C	1.545275	-2.766156	0.517783
C	2.369418	-3.688686	1.150517
C	3.127219	-4.586572	0.383922
C	3.064848	-4.564874	-1.007685
C	2.257786	-3.621355	-1.666756
C	1.503719	-2.712293	-0.900583
C	-0.722756	-1.892613	0.599555
C	-1.903721	-2.092161	1.302656
C	-3.098428	-2.338242	0.611478
C	-3.120274	-2.400794	-0.779125
C	-1.943410	-2.172331	-1.513673
C	-0.747416	-1.895831	-0.816748
C	-0.723575	1.057245	0.978622
C	-1.792978	1.185019	1.855381
C	-3.089468	1.301386	1.343409
C	-3.305581	1.280514	-0.035088
C	-2.227349	1.160633	-0.918398
C	-0.934100	1.059166	-0.412434
C	1.222714	2.153916	-0.705892
C	1.449716	2.092639	0.679426
C	2.254480	3.039622	1.301840
C	2.831626	4.057415	0.533407
C	2.605110	4.118325	-0.841691
C	1.800169	3.160732	-1.470078
H	-1.902192	-2.057620	2.391270
H	-4.019069	-2.489938	1.172001
H	-4.053176	-2.596192	-1.304396
H	-1.968466	-2.110551	-2.602389
H	-1.621037	1.203395	2.931889
H	-3.932921	1.416937	2.022578
H	-4.316990	1.376870	-0.427148
H	-2.396316	1.170139	-1.995622
H	2.427801	2.996086	2.377309
H	3.456554	4.808837	1.013685
H	3.053201	4.917594	-1.430099
H	2.166379	-0.136422	-1.303573
H	0.169986	1.087233	-2.296072
H	0.889266	0.921981	2.436848
H	0.573117	-1.580270	-2.525017
H	0.677911	-1.787636	2.265570
C	1.307646	-0.358757	0.692434
H	2.369542	-0.408186	0.961332
H	1.623130	3.209876	-2.544725
H	2.264155	-3.548445	-2.755072
H	3.659882	-5.264194	-1.592351
H	3.767851	-5.311401	0.883437
H	2.421883	-3.719262	2.238594
Ag	-0.381928	-4.304679	-1.166808

1d	x	y	z
C	1.127860	-0.306120	-0.920230
C	0.534840	-1.645980	-1.458830
C	0.701660	-1.764770	1.133330
C	0.689370	0.898440	1.293570
C	0.350300	1.003980	-1.287240
C	1.575580	-2.790440	0.432230
C	2.419280	-3.711170	1.042500
C	3.178360	-4.575950	0.244650
C	3.095090	-4.507190	-1.146530
C	2.251940	-3.573700	-1.760690
C	1.492260	-2.719330	-0.969550
C	-0.707830	-1.946270	0.611660
C	-1.842900	-2.187920	1.377410
C	-3.064080	-2.411790	0.736550
C	-3.145290	-2.388380	-0.657520
C	-2.007190	-2.132760	-1.427120
C	-0.793270	-1.907650	-0.789970
C	-0.757750	1.083620	0.886490
C	-1.832990	1.239600	1.752260
C	-3.112750	1.409110	1.217800
C	-3.303050	1.425160	-0.164910
C	-2.217180	1.280860	-1.032930
C	-0.943640	1.111690	-0.503590
C	1.221280	2.127660	-0.763360
C	1.433660	2.042740	0.638590
C	2.232590	3.021890	1.291970
C	2.767530	4.095420	0.533750
C	2.515020	4.176430	-0.830830
C	1.752300	3.191360	-1.481140
H	-1.778800	-2.214020	2.465240
H	-3.955530	-2.615460	1.327810
H	-4.100140	-2.573630	-1.147210
H	-2.069430	-2.112950	-2.515240
H	-1.682740	1.217840	2.831510
H	-3.965820	1.526800	1.883900
H	-4.304530	1.555460	-0.571710
H	-2.368230	1.295680	-2.111920
H	2.286290	3.040520	2.382520
H	3.340320	4.871530	1.037980
H	2.907020	5.016380	-1.401830
H	2.124210	-0.211350	-1.373970
H	0.191530	1.075720	-2.369020
H	0.819330	0.882540	2.382370
H	0.458310	-1.623970	-2.552250
H	0.757560	-1.840590	2.225890
C	1.265000	-0.398280	0.636050
H	2.353710	-0.425380	0.909520
H	1.564530	3.270530	-2.551790
H	2.183260	-3.525640	-2.847750
H	3.683090	-5.189340	-1.758900
H	3.829220	-5.312800	0.713130
H	2.476760	-3.771890	2.129790
Ag	3.749980	1.301380	0.783730

Table S18: Cartesian coordinates of [janusene-Ag_2]$^{2+}$ **2a** and **2b**

2a	x	y	z
C	1.138469	-0.261030	-0.838800
C	0.531695	-1.592482	-1.400383
C	0.737689	-1.752054	1.195858
C	0.663105	0.938802	1.365341
C	0.461720	1.096956	-1.231562
C	1.617254	-2.760955	0.458375
C	2.482443	-3.677068	1.045233
C	3.243858	-4.510190	0.217230
C	3.133163	-4.425102	-1.171587
C	2.258970	-3.504955	-1.761720
C	1.506047	-2.675281	-0.938874
C	-0.649327	-2.029834	0.686613
C	-1.737143	-2.486862	1.457922
C	-2.978516	-2.788786	0.834434
C	-3.092156	-2.698470	-0.588586
C	-1.961412	-2.310077	-1.357130
C	-0.760915	-1.942512	-0.717074
C	-0.737948	1.202578	0.887876
C	-1.848983	1.495770	1.704728
C	-3.106725	1.802200	1.117283
C	-3.217037	1.887983	-0.306095
C	-2.066491	1.665899	-1.111600
C	-0.846658	1.287782	-0.516298
C	1.377954	2.162907	-0.632237
C	1.485891	2.078108	0.765340
C	2.301893	2.957552	1.467396
C	3.017751	3.926508	0.754786
C	2.910706	4.010619	-0.634363
C	2.085305	3.127601	-1.340195
H	-1.593333	-2.717270	2.515916
H	-3.774966	-3.274694	1.399369
H	-3.972706	-3.117407	-1.077182
H	-1.989679	-2.405381	-2.444957
H	-1.717131	1.598501	2.784274
H	-3.928841	2.166020	1.734832
H	-4.119867	2.317611	-0.742124
H	-2.101611	1.896419	-2.178694
H	2.390173	2.893996	2.551562
H	3.661259	4.622098	1.290686
H	3.471386	4.771274	-1.174980
H	2.143100	-0.207709	-1.272997
H	0.364413	1.194976	-2.318431
H	0.734810	0.904099	2.458065
H	0.434083	-1.558062	-2.491084
H	0.813100	-1.851442	2.284337
C	1.259893	-0.355358	0.711870
H	2.320070	-0.343137	0.988461
H	2.006191	3.195242	-2.424819
H	2.177290	-3.440197	-2.846327
H	3.729536	-5.081550	-1.802970
H	3.926008	-5.232621	0.662116
H	2.573535	-3.745334	2.128873
Ag	-3.078832	-0.539281	1.674804
Ag	-3.310577	-0.362267	-1.106605

2b	x	y	z
C	1.090590	-0.334490	-0.846870
C	0.417940	-1.664530	-1.350270
C	0.663290	-1.743770	1.246090
C	0.589780	0.927020	1.310510
C	0.441940	1.017090	-1.289260
C	1.509620	-2.783330	0.535500
C	2.394300	-3.665250	1.136770
C	3.187040	-4.514140	0.326940
C	3.046430	-4.474070	-1.096530
C	2.119940	-3.586920	-1.686280
C	1.373800	-2.743160	-0.876420
C	-0.752000	-1.975880	0.774250
C	-1.841570	-2.275510	1.586010
C	-3.083890	-2.563730	1.000820
C	-3.229360	-2.530370	-0.409560
C	-2.111540	-2.205230	-1.226200
C	-0.885270	-1.932710	-0.628770
C	-0.812740	1.162510	0.799460
C	-1.930360	1.433140	1.580550
C	-3.137410	1.819940	0.964450
C	-3.213670	1.915150	-0.451140
C	-2.072410	1.602560	-1.237460
C	-0.888820	1.232360	-0.610680
C	1.356790	2.086620	-0.703130
C	1.427660	2.045460	0.699460
C	2.217970	2.953840	1.393290
C	2.938910	3.913210	0.672840
C	2.869630	3.953410	-0.720130
C	2.076770	3.035850	-1.418910
H	-1.731920	-2.308270	2.669350
H	-3.924790	-2.869540	1.622160
H	-4.146060	-2.903080	-0.870550
H	-2.215790	-2.210810	-2.311020
H	-1.869580	1.396760	2.667670
H	-3.984100	2.137190	1.572280
H	-4.093460	2.358360	-0.919110
H	-2.120160	1.707050	-2.321020
H	2.270550	2.928310	2.481620
H	3.553570	4.637140	1.205290
H	3.430550	4.708490	-1.268430
H	2.095500	-0.329450	-1.285280
H	0.371540	1.083210	-2.380900
H	0.639060	0.921450	2.405270
H	0.301670	-1.662720	-2.439490
H	0.757570	-1.805830	2.335600
C	1.211360	-0.373730	0.708360
H	2.270940	-0.348220	0.988440
H	2.020150	3.073050	-2.506710
H	2.034860	-3.539740	-2.771290
H	3.762360	-5.006880	-1.724820
H	4.024510	-5.056300	0.771660
H	2.524500	-3.677950	2.218290
Ag	1.885070	-6.365640	-0.220030
Ag	-3.752190	-0.305930	-0.123830

Table S19: Cartesian coordinates of [janusene-Ag_2]$^{2+}$ **2c** and **2d**

2c	x	y	z
C	1.097291	-0.252611	-0.901569
C	0.528197	-1.604339	-1.458304
C	0.729497	-1.743781	1.138469
C	0.644166	0.917981	1.320863
C	0.328617	1.062284	-1.260480
C	1.620886	-2.738131	0.418801
C	2.482672	-3.645185	1.016230
C	3.234840	-4.524523	0.203739
C	3.133238	-4.440280	-1.221227
C	2.280210	-3.478142	-1.810067
C	1.519438	-2.654562	-0.994407
C	-0.670065	-2.011288	0.628997
C	-1.767104	-2.360674	1.405711
C	-2.984918	-2.694244	0.777555
C	-3.085887	-2.664942	-0.637559
C	-1.964090	-2.281654	-1.414249
C	-0.773785	-1.958068	-0.777607
C	-0.795584	1.104527	0.910147
C	-1.867443	1.312154	1.771861
C	-3.129900	1.636326	1.248942
C	-3.312732	1.732363	-0.155489
C	-2.212579	1.490501	-1.027049
C	-0.967069	1.181963	-0.489675
C	1.222105	2.164914	-0.703814
C	1.396090	2.083588	0.688270
C	2.195719	3.004777	1.354340
C	2.824150	4.015707	0.617356
C	2.651624	4.096133	-0.764842
C	1.847677	3.167045	-1.435959
H	-1.689631	-2.407935	2.491032
H	-3.815919	-3.073756	1.371770
H	-3.977031	-3.059457	-1.127112
H	-2.037277	-2.273966	-2.501080
H	-1.725163	1.267442	2.851034
H	-3.953393	1.886865	1.916533
H	-4.240879	2.143852	-0.555408
H	-2.343232	1.608266	-2.102489
H	2.326560	2.948959	2.435012
H	3.444439	4.749617	1.129160
H	3.137624	4.892866	-1.325680
H	2.087154	-0.137478	-1.359493
H	0.181125	1.152907	-2.342656
H	0.766704	0.885595	2.409353
H	0.435800	-1.575710	-2.549271
H	0.801264	-1.835104	2.227653
C	1.256832	-0.350309	0.647908
H	2.323199	-0.327012	0.904474
H	1.709449	3.236802	-2.514885
H	2.192414	-3.428227	-2.894629
H	3.573565	-5.224040	-1.840834
H	3.753526	-5.370687	0.658590
H	2.550834	-3.722315	2.100522
Ag	5.129956	-3.372906	-0.589733
Ag	-3.730221	-0.515047	-0.011298

2d	x	y	z
C	0.998670	-0.388830	-0.896770
C	0.344690	-1.711030	-1.447320
C	0.607300	-1.877910	1.151520
C	0.601400	0.793150	1.330270
C	0.304910	0.965050	-1.254420
C	1.488630	-2.869850	0.404060
C	2.559740	-3.603540	0.952080
C	3.481020	-4.216180	0.098980
C	3.347610	-4.116980	-1.291080
C	2.287330	-3.407110	-1.859900
C	1.349850	-2.772850	-1.023090
C	-0.811030	-2.085850	0.678450
C	-1.909230	-2.380920	1.481300
C	-3.163820	-2.629320	0.882770
C	-3.305180	-2.557640	-0.526580
C	-2.187280	-2.230100	-1.332630
C	-0.951820	-2.004550	-0.733000
C	-0.825900	1.049730	0.910920
C	-1.888970	1.319550	1.765640
C	-3.128330	1.729380	1.232060
C	-3.292570	1.838290	-0.175500
C	-2.208100	1.524860	-1.036290
C	-0.986290	1.145360	-0.491330
C	1.247850	2.021050	-0.686200
C	1.408130	1.927860	0.706140
C	2.244800	2.808470	1.381330
C	2.921880	3.792420	0.651470
C	2.763520	3.884200	-0.731690
C	1.923190	2.995100	-1.411850
H	-1.805600	-2.439800	2.564200
H	-3.999220	-2.969580	1.495190
H	-4.239460	-2.868490	-0.996280
H	-2.298220	-2.177710	-2.415270
H	-1.758560	1.270330	2.846160
H	-3.928430	2.056950	1.895350
H	-4.198960	2.287850	-0.582650
H	-2.325780	1.643290	-2.113070
H	2.368120	2.742180	2.462150
H	3.573800	4.494000	1.169240
H	3.292360	4.657160	-1.286890
H	1.989490	-0.339500	-1.363580
H	0.170070	1.068100	-2.337050
H	0.716630	0.751830	2.419210
H	0.223540	-1.670490	-2.535090
H	0.704670	-1.977590	2.237930
C	1.168410	-0.494040	0.652810
H	2.237140	-0.507260	0.897520
H	1.798960	3.071840	-2.491880
H	2.206420	-3.305150	-2.941730
H	4.083460	-4.591320	-1.938410
H	4.319350	-4.766810	0.522630
H	2.689300	-3.650380	2.032980
Ag	-3.830800	-0.383650	0.219310
Ag	0.122770	-4.721490	-0.266910

Table S20: Cartesian coordinates of [janusene-Ag_2]$^{2+}$ **2e** and **2f**

2e	x	y	z
C	1.081630	-0.259740	-0.890980
C	0.520390	-1.606950	-1.460130
C	0.634690	-1.738360	1.142060
C	0.565250	0.935080	1.304630
C	0.326660	1.049960	-1.286530
C	1.546920	-2.738700	0.456290
C	2.387230	-3.645320	1.083900
C	3.158200	-4.533710	0.299290
C	3.097570	-4.458910	-1.128370
C	2.267550	-3.495400	-1.747750
C	1.487940	-2.662900	-0.959730
C	-0.746410	-2.012350	0.584030
C	-1.863300	-2.397730	1.317190
C	-3.065410	-2.727470	0.634670
C	-3.115990	-2.649260	-0.780450
C	-1.980980	-2.248220	-1.503000
C	-0.806730	-1.945310	-0.822650
C	-0.859890	1.131220	0.848790
C	-1.950670	1.380570	1.670790
C	-3.208830	1.682350	1.090390
C	-3.344320	1.699350	-0.323380
C	-2.225450	1.432940	-1.142220
C	-0.992410	1.171560	-0.558430
C	1.204690	2.157420	-0.715340
C	1.343120	2.087790	0.681240
C	2.129100	3.012290	1.359250
C	2.777830	4.015620	0.629860
C	2.640060	4.084700	-0.756930
C	1.851970	3.151050	-1.440230
H	-1.815630	-2.492330	2.401520
H	-3.890100	-3.186120	1.182960
H	-4.016030	-2.965840	-1.306040
H	-2.019330	-2.202880	-2.590500
H	-1.840750	1.393400	2.754540
H	-4.031090	2.026120	1.718380
H	-4.282430	2.024450	-0.772390
H	-2.328940	1.481990	-2.225440
H	2.230750	2.966860	2.443440
H	3.385270	4.753800	1.150770
H	3.139880	4.876960	-1.311710
H	2.087250	-0.151980	-1.314940
H	0.211580	1.128730	-2.373380
H	0.656180	0.914530	2.396410
H	0.464360	-1.581800	-2.553580
H	0.669610	-1.826090	2.233310
C	1.185010	-0.347850	0.663700
H	2.241930	-0.331870	0.956810
H	1.739670	3.212530	-2.522510
H	2.211040	-3.452220	-2.834650
H	3.549180	-5.250150	-1.729980
H	3.659730	-5.378910	0.774550
H	2.423770	-3.716270	2.170200
Ag	-3.742990	-0.521680	0.546800
Ag	5.075680	-3.389420	-0.445750

2f	x	y	z
C	1.188590	-0.246650	-0.873060
C	0.702830	-1.623210	-1.461590
C	0.662000	-1.708640	1.145780
C	0.736890	0.935520	1.347750
C	0.310190	1.006060	-1.216810
C	1.588410	-2.735940	0.530880
C	2.404400	-3.616820	1.225730
C	3.272690	-4.469680	0.508650
C	3.327050	-4.394070	-0.919140
C	2.506840	-3.469180	-1.606140
C	1.637150	-2.663450	-0.886020
C	-0.697360	-1.903690	0.510220
C	-1.899350	-2.080240	1.191320
C	-3.085340	-2.241140	0.469950
C	-3.057010	-2.293060	-0.957160
C	-1.816420	-2.132250	-1.640000
C	-0.664300	-1.919710	-0.903210
C	-0.726130	1.017270	1.000310
C	-1.781620	1.108540	1.902840
C	-3.089860	1.172160	1.418950
C	-3.329430	1.142320	0.041700
C	-2.262860	1.071300	-0.865780
C	-0.959810	1.014710	-0.386200
C	1.164040	2.162320	-0.722150
C	1.420230	2.104910	0.659020
C	2.212740	3.070150	1.269710
C	2.747420	4.103070	0.491350
C	2.492420	4.160290	-0.879770
C	1.701060	3.184050	-1.496330
H	-1.929000	-2.038750	2.278450
H	-4.042700	-2.264180	0.988380
H	-3.989880	-2.174210	-1.514890
H	-1.800250	-2.097930	-2.728680
H	-1.586860	1.142670	2.974870
H	-3.924060	1.264540	2.112610
H	-4.350250	1.216450	-0.331010
H	-2.456080	1.088340	-1.938740
H	2.402910	3.034550	2.342420
H	3.357770	4.872610	0.961030
H	2.904630	4.974640	-1.473330
H	2.175980	-0.060990	-1.311480
H	0.108190	1.067380	-2.292610
H	0.916070	0.925350	2.428890
H	0.716040	-1.608270	-2.556420
H	0.623780	-1.775040	2.238120
C	1.315490	-0.350430	0.676220
H	2.374280	-0.409670	0.959200
H	1.498690	3.234900	-2.566110
H	2.541220	-3.422470	-2.693990
H	3.867520	-5.159370	-1.479720
H	3.779430	-5.286800	1.025330
H	2.361830	-3.679850	2.312360
Ag	-3.166940	-4.539340	-0.872030
Ag	5.189660	-3.216970	-0.094850

Table S21: Cartesian coordinates of [janusene-Ag_2]$^{2+}$ **2g** and **2h**

2g	x	y	z
C	1.246280	-0.217980	-0.844060
C	0.623130	-1.543270	-1.370690
C	0.795370	-1.625020	1.223130
C	0.761450	0.998730	1.347800
C	0.459730	1.078010	-1.238010
C	1.602180	-2.724000	0.538580
C	2.295280	-3.760390	1.156280
C	2.820290	-4.807670	0.385100
C	2.656440	-4.821230	-0.998740
C	1.990700	-3.752160	-1.647720
C	1.489380	-2.689870	-0.864830
C	-0.622250	-1.837350	0.708110
C	-1.735220	-2.195080	1.463790
C	-2.911070	-2.613100	0.824540
C	-2.975650	-2.681930	-0.566100
C	-1.868140	-2.284950	-1.347380
C	-0.705760	-1.832300	-0.697880
C	-0.689330	1.132120	0.922270
C	-1.803900	1.262590	1.772070
C	-3.087120	1.351130	1.203080
C	-3.246120	1.296230	-0.179880
C	-2.132460	1.188830	-1.026400
C	-0.854950	1.125680	-0.483780
C	1.309240	2.221990	-0.707340
C	1.449890	2.195880	0.702170
C	2.169010	3.211860	1.364760
C	2.761410	4.234220	0.599790
C	2.654350	4.225600	-0.789120
C	1.928150	3.221360	-1.447790
H	-1.680860	-2.196590	2.552470
H	-3.771610	-2.911980	1.420140
H	-3.888140	-3.016590	-1.056580
H	-1.954740	-2.225840	-2.434860
H	-1.679480	1.216540	2.855210
H	-3.957190	1.445270	1.850140
H	-4.244270	1.355530	-0.610110
H	-2.270770	1.173010	-2.107340
H	2.328500	3.163090	2.443150
H	3.327230	5.018290	1.099630
H	3.132620	5.011490	-1.371000
H	2.239980	-0.134150	-1.298940
H	0.317490	1.141210	-2.322490
H	0.878840	0.990430	2.438070
H	0.544700	-1.534690	-2.464770
H	0.852720	-1.695300	2.315010
C	1.387960	-0.278410	0.708370
H	2.450440	-0.274070	0.978650
H	1.839900	3.237300	-2.533810
H	1.996860	-3.684740	-2.738430
H	3.073740	-5.631890	-1.593760
H	3.349920	-5.623800	0.873040
H	2.399910	-3.782200	2.240900
Ag	-0.359090	-4.455310	-1.452760
Ag	-0.503350	3.608880	1.321440

2h	x	y	z
C	1.247150	-0.209120	-0.892950
C	0.603130	-1.522360	-1.423470
C	0.778470	-1.617750	1.168540
C	0.795920	1.011010	1.306130
C	0.464520	1.092540	-1.275370
C	1.564640	-2.729090	0.477650
C	2.216170	-3.794480	1.091640
C	2.704230	-4.854550	0.314530
C	2.543090	-4.851510	-1.070610
C	1.919470	-3.756360	-1.711960
C	1.455180	-2.684850	-0.926360
C	-0.641130	-1.825710	0.654580
C	-1.743860	-2.216670	1.408880
C	-2.907950	-2.667120	0.771990
C	-2.976240	-2.728590	-0.618670
C	-1.879370	-2.291650	-1.401880
C	-0.726520	-1.807230	-0.748290
C	-0.655990	1.124100	0.894500
C	-1.748680	1.177600	1.750990
C	-3.035960	1.228290	1.207330
C	-3.218890	1.229350	-0.176790
C	-2.117010	1.192610	-1.037970
C	-0.836140	1.142010	-0.497060
C	1.307420	2.234430	-0.749840
C	1.496920	2.182910	0.656560
C	2.205830	3.177890	1.312540
C	2.696210	4.281510	0.576740
C	2.506210	4.332530	-0.842140
C	1.828940	3.278870	-1.497940
H	-1.688990	-2.216090	2.497250
H	-3.759040	-2.989800	1.368660
H	-3.883510	-3.074810	-1.110910
H	-1.985510	-2.190800	-2.484670
H	-1.606250	1.174290	2.831530
H	-3.900600	1.274290	1.867370
H	-4.225280	1.276090	-0.589680
H	-2.262480	1.210330	-2.118090
H	2.331090	3.153650	2.394340
H	3.048530	5.169810	1.105220
H	2.721780	5.256410	-1.382370
H	2.239500	-0.143240	-1.356610
H	0.308940	1.159980	-2.358140
H	0.925560	1.002880	2.394090
H	0.519360	-1.507950	-2.517130
H	0.834830	-1.691360	2.260170
C	1.397760	-0.280700	0.658360
H	2.462330	-0.313020	0.921610
H	1.665850	3.331730	-2.573680
H	1.899150	-3.697670	-2.802730
H	2.926850	-5.676480	-1.668730
H	3.198150	-5.695490	0.798140
H	2.310530	-3.828660	2.176960
Ag	-0.591000	-4.389180	-1.502890
Ag	4.727600	3.688090	-0.408010

Table S22: Cartesian coordinates of [janusene-Ag_2]$^{2+}$ **2i** and [janusene-Ag_3]$^{3+}$ **3a**

2i	x	y	z
C	1.221540	-0.253750	-0.894360
C	0.625370	-1.576630	-1.473460
C	0.753000	-1.735490	1.122180
C	0.769000	0.891740	1.341900
C	0.405640	1.039440	-1.232030
C	1.567090	-2.806320	0.425140
C	2.232610	-3.856940	1.036420
C	2.800600	-4.877970	0.238330
C	2.747530	-4.776820	-1.190520
C	2.124440	-3.660740	-1.792890
C	1.510000	-2.709060	-0.993160
C	-0.651200	-1.927620	0.571880
C	-1.790380	-2.219110	1.312890
C	-2.996420	-2.447480	0.643900
C	-3.055780	-2.395920	-0.750220
C	-1.910610	-2.104880	-1.496040
C	-0.715730	-1.865010	-0.828260
C	-0.688120	1.048060	0.954610
C	-1.758470	1.179270	1.831100
C	-3.043110	1.350960	1.309120
C	-3.244500	1.393640	-0.072030
C	-2.164350	1.276560	-0.951640
C	-0.886400	1.103310	-0.433260
C	1.230440	2.186900	-0.686070
C	1.442730	2.096500	0.717840
C	2.103890	3.106590	1.400230
C	2.503530	4.268860	0.703730
C	2.285170	4.362950	-0.709790
C	1.674510	3.288770	-1.399520
H	-1.746560	-2.269360	2.400450
H	-3.894100	-2.677750	1.215070
H	-3.998630	-2.588350	-1.259220
H	-1.955520	-2.065650	-2.584150
H	-1.600190	1.145970	2.908780
H	-3.891400	1.455810	1.983270
H	-4.249340	1.530180	-0.467920
H	-2.324860	1.319260	-2.028470
H	2.243180	3.051920	2.479100
H	2.800880	5.158290	1.262750
H	2.403350	5.326880	-1.209730
H	2.213740	-0.127490	-1.348960
H	0.234240	1.130850	-2.310450
H	0.912400	0.856240	2.427610
H	0.564240	-1.537100	-2.566750
H	0.790360	-1.833240	2.212960
C	1.369810	-0.375320	0.652490
H	2.435630	-0.404950	0.917500
H	1.484830	3.374990	-2.468630
H	2.058560	-3.603150	-2.878600
H	3.014080	-5.641360	-1.801720
H	3.094700	-5.822680	0.700760
H	2.249670	-3.951020	2.121430
Ag	4.924800	-4.250000	-0.475700
Ag	4.551970	3.938390	-0.400710

3a	x	y	z
C	1.123645	-0.363078	-0.878091
C	0.468411	-1.685865	-1.423400
C	0.748986	-1.858389	1.167489
C	0.600680	0.817873	1.319813
C	0.458516	0.984025	-1.288983
C	1.613725	-2.851124	0.405489
C	2.538825	-3.720289	0.963641
C	3.361160	-4.492851	0.111256
C	3.199371	-4.406916	-1.304540
C	2.216496	-3.548810	-1.851609
C	1.452658	-2.766013	-0.999596
C	-0.666682	-2.093764	0.706271
C	-1.746309	-2.419460	1.517581
C	-3.018473	-2.633589	0.928858
C	-3.177007	-2.493429	-0.479795
C	-2.069049	-2.153807	-1.286606
C	-0.823386	-1.975812	-0.697023
C	-0.794243	1.104410	0.810771
C	-1.899489	1.426583	1.593857
C	-3.104456	1.861824	0.960020
C	-3.149587	1.989620	-0.465071
C	-2.034586	1.651046	-1.236968
C	-0.865288	1.215377	-0.609466
C	1.320418	2.076471	-0.664580
C	1.398601	1.985588	0.751488
C	2.134108	2.912527	1.478938
C	2.801139	3.928920	0.788136
C	2.718069	4.022810	-0.614025
C	1.967009	3.102112	-1.347087
H	-1.622583	-2.541087	2.593304
H	-3.833247	-3.039686	1.529488
H	-4.126168	-2.756982	-0.945639
H	-2.193901	-2.070006	-2.365616
H	-1.840383	1.408519	2.681864
H	-3.898512	2.301281	1.564624
H	-4.036700	2.411297	-0.935800
H	-2.067948	1.767416	-2.319408
H	2.196373	2.852390	2.564672
H	3.386805	4.662680	1.339918
H	3.246014	4.823537	-1.129521
H	2.127398	-0.329434	-1.318515
H	0.392032	1.082810	-2.377522
H	0.645878	0.779417	2.413529
H	0.339134	-1.645610	-2.510102
H	0.861407	-1.957812	2.252231
C	1.246629	-0.449243	0.673578
H	2.305259	-0.400470	0.954814
H	1.901947	3.181951	-2.431425
H	2.115597	-3.467969	-2.933367
H	3.945287	-4.856355	-1.964654
H	4.228024	-5.011419	0.527934
H	2.683637	-3.771494	2.042235
Ag	-6.213507	0.004670	0.529840
Ag	2.270208	-6.474459	-0.618648
Ag	-3.513183	-0.369390	0.705878

Table S23: Cartesian coordinates of [janusene-Ag_3]$^{3+}$ **3b** and **3c**

3b	x	y	z
C	1.190780	-0.293910	-0.868030
C	0.590910	-1.650030	-1.384620
C	0.869420	-1.751760	1.209850
C	0.624500	0.903940	1.311910
C	0.473330	1.023900	-1.298340
C	1.745920	-2.755980	0.474280
C	2.595360	-3.678900	1.064190
C	3.273190	-4.612260	0.245690
C	3.116720	-4.562600	-1.172200
C	2.284870	-3.578440	-1.756760
C	1.590640	-2.705940	-0.933410
C	-0.537800	-2.047410	0.752980
C	-1.604610	-2.393670	1.578250
C	-2.845990	-2.706620	1.006880
C	-3.016960	-2.646590	-0.406400
C	-1.916060	-2.286330	-1.238800
C	-0.691830	-1.985930	-0.652940
C	-0.782430	1.120540	0.803950
C	-1.901860	1.376620	1.591590
C	-3.113460	1.749580	0.976810
C	-3.196240	1.846700	-0.448460
C	-2.052300	1.565520	-1.241780
C	-0.862760	1.202920	-0.618650
C	1.295600	2.155640	-0.693080
C	1.364330	2.099560	0.724440
C	2.040170	3.081730	1.441140
C	2.670980	4.109200	0.736760
C	2.605200	4.163570	-0.667680
C	1.907620	3.190520	-1.389420
H	-1.474690	-2.454530	2.658100
H	-3.663820	-3.061080	1.633230
H	-3.916960	-3.064900	-0.860380
H	-2.035270	-2.292490	-2.322080
H	-1.839000	1.335170	2.678220
H	-3.960320	2.063950	1.585690
H	-4.083500	2.281090	-0.908750
H	-2.106620	1.676950	-2.324150
H	2.088730	3.047890	2.528890
H	3.216590	4.880720	1.278060
H	3.100220	4.977020	-1.196140
H	2.190810	-0.227110	-1.313170
H	0.401150	1.101830	-2.388480
H	0.672700	0.883540	2.405990
H	0.462120	-1.640300	-2.472210
H	0.980790	-1.823220	2.296910
C	1.320560	-0.343340	0.684590
H	2.376810	-0.248360	0.964820
H	1.853890	3.243790	-2.476200
H	2.155330	-3.556590	-2.838180
H	3.485050	-5.386990	-1.787780
H	3.763430	-5.472660	0.707870
H	2.702970	-3.734590	2.146810
Ag	-6.225760	-0.411040	0.199470
Ag	5.270630	-3.711720	-0.671480
Ag	-3.504800	-0.422860	-0.080400

3c	x	y	z
C	1.094900	-0.542822	-0.909805
C	0.465522	-1.836344	-1.546245
C	0.499239	-2.065135	1.056347
C	0.764316	0.593454	1.352814
C	0.397990	0.820594	-1.219556
C	1.350312	-3.113960	0.352666
C	2.127047	-4.080982	0.975428
C	2.890844	-4.964005	0.183210
C	2.895219	-4.826043	-1.236639
C	2.129992	-3.802171	-1.850440
C	1.349548	-2.974516	-1.057437
C	-0.878565	-2.187672	0.453830
C	-2.062943	-2.478273	1.156445
C	-3.277812	-2.657546	0.454608
C	-3.292553	-2.550056	-0.977280
C	-2.086106	-2.246909	-1.667923
C	-0.893540	-2.087809	-0.951999
C	-0.657197	0.929466	0.987314
C	-1.661618	1.282458	1.882048
C	-2.918330	1.719794	1.385913
C	-3.145732	1.744251	-0.020316
C	-2.112453	1.375591	-0.910969
C	-0.867865	1.005942	-0.410123
C	1.383537	1.843139	-0.659022
C	1.604096	1.699195	0.720937
C	2.495494	2.535027	1.386195
C	3.167453	3.523925	0.657113
C	2.946253	3.668253	-0.712899
C	2.051087	2.824053	-1.383582
H	-2.038475	-2.627314	2.236821
H	-4.170283	-3.008878	0.980748
H	-4.252653	-2.456033	-1.497635
H	-2.110402	-2.071330	-2.744459
H	-1.475124	1.290273	2.955786
H	-3.649562	2.165045	2.062065
H	-4.074330	2.163546	-0.407891
H	-2.278881	1.459169	-1.984671
H	2.663281	2.432949	2.458156
H	3.860924	4.190645	1.166870
H	3.467096	4.447833	-1.266387
H	2.097472	-0.467009	-1.346180
H	0.230492	0.952003	-2.294476
H	0.916665	0.522598	2.435308
H	0.440818	-1.764911	-2.638625
H	0.495075	-2.189416	2.144084
C	1.212208	-0.716077	0.633040
H	2.264407	-0.857301	0.907113
H	1.877444	2.945900	-2.452489
H	2.131835	-3.706095	-2.935786
H	3.328744	-5.615288	-1.857468
H	3.360946	-5.834324	0.645602
H	2.126475	-4.190121	2.059302
Ag	-3.159085	-4.739506	-1.659671
Ag	-3.656044	-0.415816	0.980188
Ag	4.968741	-3.960137	-0.618914

Table S24: Cartesian coordinates of [janusene-Ag_3]$^{3+}$ **3d** and **3e**

3d	x	y	z
C	1.034400	-0.289920	-0.883370
C	0.435420	-1.636330	-1.417500
C	0.667830	-1.755310	1.178250
C	0.549940	0.919340	1.316430
C	0.278420	1.026340	-1.276210
C	1.554030	-2.759820	0.454710
C	2.439850	-3.645880	1.049060
C	3.252910	-4.462520	0.231350
C	3.129640	-4.395370	-1.189620
C	2.191000	-3.511260	-1.775260
C	1.428180	-2.694010	-0.955820
C	-0.735460	-2.042770	0.686520
C	-1.807390	-2.453580	1.471950
C	-3.033100	-2.809980	0.846620
C	-3.155050	-2.721140	-0.564140
C	-2.064070	-2.291860	-1.339940
C	-0.862080	-1.973190	-0.716520
C	-0.884310	1.107630	0.871640
C	-1.973870	1.327900	1.706090
C	-3.243980	1.605000	1.134730
C	-3.390210	1.626120	-0.276780
C	-2.276590	1.389760	-1.105390
C	-1.032950	1.151780	-0.531010
C	1.164470	2.134350	-0.723480
C	1.316180	2.073170	0.684810
C	2.122900	2.981400	1.353830
C	2.831540	3.952410	0.612170
C	2.681140	4.014760	-0.806180
C	1.822270	3.102040	-1.466120
H	-1.705450	-2.552050	2.552500
H	-3.821030	-3.287940	1.431850
H	-4.071790	-3.056150	-1.048730
H	-2.158750	-2.245850	-2.424240
H	-1.857630	1.334840	2.789580
H	-4.065500	1.936460	1.772250
H	-4.346030	1.909990	-0.716800
H	-2.392620	1.431200	-2.187780
H	2.255260	2.926580	2.433700
H	3.607920	4.544810	1.100840
H	3.363550	4.631800	-1.396380
H	2.029360	-0.207370	-1.336500
H	0.152910	1.101520	-2.361620
H	0.652920	0.904610	2.406720
H	0.329860	-1.617650	-2.507410
H	0.756330	-1.836960	2.266870
C	1.182240	-0.362480	0.669410
H	2.246440	-0.329070	0.930980
H	1.729140	3.139820	-2.550850
H	2.115550	-3.448560	-2.860210
H	3.876890	-4.881630	-1.821590
H	4.079950	-5.018670	0.677860
H	2.552450	-3.687530	2.131760
Ag	2.059790	-6.382030	-0.555920
Ag	1.447290	5.824060	0.018830
Ag	-3.764920	-0.619650	0.790000

3e	x	y	z
C	1.116544	-0.367697	-0.894420
C	0.407262	-1.667355	-1.411755
C	0.676856	-1.796987	1.179344
C	0.664599	0.873680	1.288712
C	0.468889	0.993321	-1.309276
C	1.480664	-2.859027	0.443478
C	2.309336	-3.806655	1.024229
C	3.035243	-4.692670	0.193883
C	2.881999	-4.625798	-1.224040
C	2.004503	-3.674219	-1.794582
C	1.328306	-2.793123	-0.964971
C	-0.750728	-1.996996	0.716981
C	-1.829183	-2.332794	1.525210
C	-3.088473	-2.597498	0.929373
C	-3.237890	-2.490502	-0.477627
C	-2.133431	-2.137027	-1.280629
C	-0.899087	-1.910816	-0.684204
C	-0.748021	1.142108	0.803529
C	-1.842317	1.443426	1.607071
C	-3.068643	1.825175	0.998562
C	-3.168137	1.874099	-0.415948
C	-2.053884	1.552890	-1.211851
C	-0.853634	1.206291	-0.601492
C	1.379023	2.069356	-0.731038
C	1.484036	2.006213	0.682425
C	2.207689	2.957379	1.383905
C	2.787562	4.040034	0.680560
C	2.681195	4.103715	-0.742207
C	1.996949	3.083966	-1.444813
H	-1.711934	-2.433281	2.603831
H	-3.899998	-3.006804	1.533176
H	-4.180545	-2.775828	-0.945023
H	-2.250894	-2.079730	-2.362155
H	-1.757973	1.444564	2.693497
H	-3.877730	2.222333	1.614329
H	-4.084332	2.238055	-0.880301
H	-2.129399	1.618532	-2.296583
H	2.269799	2.928501	2.471088
H	3.141649	4.911247	1.237197
H	2.957190	5.022135	-1.266049
H	2.115584	-0.376098	-1.347141
H	0.376993	1.074170	-2.397657
H	0.734140	0.855535	2.381694
H	0.281749	-1.643725	-2.499541
H	0.781054	-1.880435	2.266482
C	1.252565	-0.433617	0.658738
H	2.315593	-0.442085	0.929013
H	1.896677	3.151751	-2.527395
H	1.904548	-3.616183	-2.877854
H	3.562144	-5.185826	-1.870024
H	3.831968	-5.303258	0.624994
H	2.443072	-3.850800	2.104536
Ag	1.680432	-6.525862	-0.464471
Ag	4.907704	3.501836	-0.208749
Ag	-3.730805	-0.366628	0.660713

Table S25: Cartesian coordinates of [janusene-Ag_3]$^{3+}$ **3f** and **3g**

3f	x	y	z
C	1.214398	-0.303160	-0.889220
C	0.563406	-1.639583	-1.383471
C	0.839763	-1.711980	1.207775
C	0.660825	0.935187	1.270340
C	0.511512	1.023627	-1.331155
C	1.660039	-2.777504	0.492463
C	2.403217	-3.776787	1.100427
C	2.946036	-4.813500	0.305080
C	2.788078	-4.779559	-1.114178
C	2.091145	-3.707991	-1.721116
C	1.505034	-2.742754	-0.918106
C	-0.580201	-1.984487	0.753557
C	-1.635670	-2.365980	1.575536
C	-2.859569	-2.743429	0.999483
C	-3.020338	-2.715720	-0.409294
C	-1.939690	-2.300152	-1.235801
C	-0.730697	-1.941918	-0.647307
C	-0.757360	1.103982	0.755421
C	-1.887348	1.307862	1.537394
C	-3.113765	1.623112	0.915224
C	-3.191487	1.714198	-0.498749
C	-2.035513	1.472570	-1.283551
C	-0.835488	1.173604	-0.652073
C	1.337988	2.160310	-0.744311
C	1.409348	2.118887	0.672691
C	2.024040	3.137509	1.383078
C	2.518662	4.264661	0.684466
C	2.449500	4.305062	-0.741769
C	1.884276	3.219707	-1.451633
H	-1.510635	-2.412943	2.656643
H	-3.664920	-3.124697	1.626584
H	-3.908070	-3.160345	-0.863720
H	-2.051612	-2.322896	-2.319540
H	-1.830525	1.270358	2.624472
H	-3.976276	1.896775	1.523077
H	-4.097618	2.097584	-0.969930
H	-2.091218	1.568027	-2.367393
H	2.054562	3.124620	2.471797
H	2.764012	5.172529	1.241625
H	2.647859	5.242023	-1.268123
H	2.215139	-0.275039	-1.338145
H	0.438083	1.089256	-2.421965
H	0.706925	0.929082	2.364608
H	0.433717	-1.641505	-2.471061
H	0.947028	-1.772163	2.296106
C	1.344458	-0.335573	0.664534
H	2.403419	-0.270408	0.944281
H	1.807402	3.269826	-2.537081
H	1.950999	-3.701790	-2.801357
H	3.026365	-5.665856	-1.707914
H	3.305538	-5.725019	0.789266
H	2.501273	-3.823865	2.184279
Ag	5.048740	-4.292386	-0.639665
Ag	4.709556	3.971454	-0.128173
Ag	-3.698772	-0.530343	-0.089819

3g	x	y	z
C	1.107416	-0.277822	-0.863286
C	0.606315	-1.660438	-1.433549
C	0.637603	-1.742119	1.177593
C	0.608718	0.942265	1.321011
C	0.297264	0.994118	-1.268147
C	1.593480	-2.738782	0.538748
C	2.450997	-3.596526	1.210242
C	3.303003	-4.446976	0.462566
C	3.306506	-4.377799	-0.961896
C	2.454614	-3.466886	-1.626244
C	1.591480	-2.678446	-0.877978
C	-0.718938	-2.029797	0.574266
C	-1.880828	-2.375156	1.279766
C	-3.074273	-2.704142	0.583568
C	-3.094185	-2.659567	-0.835479
C	-1.907737	-2.313106	-1.550885
C	-0.725571	-2.005822	-0.831972
C	-0.828099	1.120717	0.902758
C	-1.887704	1.424905	1.749933
C	-3.161826	1.723349	1.198773
C	-3.348545	1.659824	-0.210781
C	-2.259734	1.335474	-1.054031
C	-1.003808	1.102160	-0.501535
C	1.167794	2.132976	-0.744899
C	1.354114	2.091121	0.648562
C	2.134983	3.047978	1.285796
C	2.735393	4.051959	0.515087
C	2.551156	4.092170	-0.868849
C	1.765430	3.128127	-1.510866
H	-1.860719	-2.447968	2.367920
H	-3.923696	-3.129059	1.124920
H	-4.031009	-2.819308	-1.372532
H	-1.966260	-2.088963	-2.619770
H	-1.736940	1.502532	2.826425
H	-3.952082	2.126106	1.833687
H	-4.295768	1.980889	-0.644428
H	-2.399998	1.350830	-2.134664
H	2.273566	3.028320	2.366507
H	3.343453	4.812792	1.001609
H	3.014476	4.885518	-1.452942
H	2.107780	-0.141337	-1.289942
H	0.150848	1.049385	-2.352761
H	0.734555	0.946224	2.409208
H	0.588529	-1.649462	-2.528644
H	0.631029	-1.809131	2.270378
C	1.207468	-0.352712	0.689596
H	2.263068	-0.359349	0.986015
H	1.618102	3.168686	-2.589800
H	2.462773	-3.417032	-2.714801
H	3.848284	-5.128798	-1.541084
H	3.812256	-5.272304	0.967529
H	2.449372	-3.657447	2.298032
Ag	-3.703055	-0.492348	0.814610
Ag	-1.899762	-4.627896	-1.822596
Ag	5.297631	-3.322498	-0.070115

Table S26: Cartesian coordinates of [janusene-Ag_3]$^{3+}$ **3h** and **3i**

3h	x	y	z
C	0.943183	-0.298765	-0.801374
C	0.334481	-1.628138	-1.370901
C	0.530434	-1.799364	1.224777
C	0.441736	0.862805	1.419278
C	0.218619	1.042470	-1.173744
C	1.409648	-2.804175	0.493387
C	2.274377	-3.713802	1.081497
C	3.087883	-4.527571	0.256613
C	2.983515	-4.429804	-1.164055
C	2.067815	-3.521744	-1.742894
C	1.306835	-2.707921	-0.917554
C	-0.872078	-2.048116	0.712658
C	-1.965870	-2.421633	1.484749
C	-3.179711	-2.756095	0.852620
C	-3.285023	-2.695458	-0.561429
C	-2.167366	-2.283558	-1.333737
C	-0.975567	-1.967416	-0.692717
C	-0.982579	1.075492	0.955419
C	-2.087297	1.258463	1.779768
C	-3.332154	1.583574	1.209368
C	-3.458214	1.705856	-0.198760
C	-2.326699	1.487642	-1.029313
C	-1.102755	1.178924	-0.446607
C	1.112563	2.120846	-0.576895
C	1.234233	2.022755	0.832341
C	2.042719	2.900321	1.537518
C	2.780936	3.879057	0.832445
C	2.656111	3.979097	-0.586029
C	1.796828	3.097904	-1.283272
H	-1.885599	-2.493164	2.568847
H	-4.010045	-3.147439	1.440393
H	-4.170603	-3.095016	-1.058573
H	-2.242858	-2.260572	-2.420534
H	-1.992495	1.187556	2.862729
H	-4.180816	1.822332	1.850154
H	-4.378342	2.105044	-0.629460
H	-2.418569	1.610125	-2.108232
H	2.156979	2.816632	2.617672
H	3.568300	4.433394	1.348612
H	3.346852	4.612360	-1.147395
H	1.944632	-0.223376	-1.241552
H	0.113717	1.148646	-2.258786
H	0.525176	0.816693	2.510325
H	0.244454	-1.586352	-2.461630
H	0.603674	-1.902348	2.312715
C	1.071976	-0.406906	0.749729
H	2.132823	-0.391438	1.026666
H	1.723285	3.164595	-2.368131
H	2.006165	-3.438094	-2.827297
H	3.719451	-4.929779	-1.797564
H	3.912460	-5.089222	0.702351
H	2.373967	-3.777058	2.164496
Ag	-3.953750	-0.546933	0.002624
Ag	1.888548	-6.425654	-0.446577
Ag	1.440182	5.772805	0.372867

3i	x	y	z
C	1.071800	-0.350200	-0.886550
C	0.390230	-1.655640	-1.425010
C	0.631780	-1.806170	1.167960
C	0.627980	0.865060	1.314340
C	0.391930	1.001990	-1.279680
C	1.453200	-2.854780	0.432160
C	2.282310	-3.801410	1.014310
C	3.026170	-4.671830	0.185440
C	2.893080	-4.590890	-1.233780
C	2.016200	-3.638980	-1.806860
C	1.319430	-2.774520	-0.977250
C	-0.788910	-2.014310	0.684520
C	-1.875010	-2.373700	1.474540
C	-3.125340	-2.646890	0.856050
C	-3.253280	-2.532030	-0.552240
C	-2.145110	-2.159520	-1.332840
C	-0.921500	-1.920920	-0.716290
C	-0.793870	1.126200	0.853850
C	-1.875300	1.422460	1.676860
C	-3.117310	1.788610	1.089070
C	-3.242030	1.829100	-0.323900
C	-2.138880	1.520100	-1.138020
C	-0.922980	1.189920	-0.548780
C	1.296620	2.085710	-0.706790
C	1.427210	2.010250	0.703740
C	2.149650	2.965090	1.400810
C	2.704880	4.062010	0.695970
C	2.574520	4.134330	-0.724280
C	1.891840	3.112830	-1.422640
H	-1.769910	-2.491540	2.552930
H	-3.934850	-3.087450	1.441450
H	-4.192810	-2.804020	-1.032920
H	-2.245940	-2.094200	-2.415650
H	-1.769290	1.431250	2.761480
H	-3.917640	2.185320	1.716700
H	-4.172260	2.175570	-0.773440
H	-2.234250	1.582960	-2.221410
H	2.228180	2.929890	2.486860
H	3.047100	4.937580	1.253980
H	2.843700	5.054750	-1.247310
H	2.070330	-0.328680	-1.340140
H	0.281350	1.090490	-2.365840
H	0.715500	0.839060	2.405930
H	0.278230	-1.622850	-2.514070
H	0.722310	-1.899240	2.255640
C	1.210320	-0.435360	0.665790
H	2.273840	-0.450950	0.933910
H	1.774340	3.186710	-2.503140
H	1.931140	-3.569300	-2.890800
H	3.591480	-5.133140	-1.875950
H	3.816910	-5.286590	0.621310
H	2.400620	-3.855410	2.096010
Ag	-3.742370	-0.418340	0.834250
Ag	1.694700	-6.507440	-0.561930
Ag	4.820380	3.534530	-0.135080

Table S27: Cartesian coordinates of [janusene-Ag_3]$^{3+}$ **3j** and **3k**

3j	x	y	z
C	1.170760	-0.286310	-0.879720
C	0.525240	-1.610490	-1.408480
C	0.784660	-1.741750	1.182700
C	0.620030	0.914450	1.303030
C	0.454890	1.039710	-1.295970
C	1.610940	-2.789890	0.448870
C	2.353460	-3.800910	1.038730
C	2.899530	-4.819890	0.224840
C	2.746700	-4.757410	-1.193980
C	2.050670	-3.673290	-1.781740
C	1.461900	-2.724870	-0.961190
C	-0.631720	-2.008500	0.710570
C	-1.689800	-2.425770	1.507690
C	-2.924810	-2.768300	0.899060
C	-3.070580	-2.657190	-0.508020
C	-1.987810	-2.222030	-1.298650
C	-0.775820	-1.919120	-0.690360
C	-0.800090	1.101970	0.798550
C	-1.921610	1.336280	1.587420
C	-3.159320	1.650510	0.961710
C	-3.240290	1.699680	-0.453530
C	-2.099070	1.448920	-1.233510
C	-0.889370	1.169210	-0.606830
C	1.281870	2.170200	-0.697640
C	1.369220	2.104460	0.717610
C	1.994600	3.109610	1.437660
C	2.482640	4.248140	0.752210
C	2.395560	4.313220	-0.672140
C	1.821150	3.240510	-1.393580
H	-1.570880	-2.538440	2.584830
H	-3.708220	-3.244260	1.490950
H	-3.988550	-3.000350	-0.985180
H	-2.099450	-2.168420	-2.380850
H	-1.852600	1.338350	2.674990
H	-3.997350	2.003090	1.566230
H	-4.171750	2.004830	-0.929530
H	-2.162400	1.514100	-2.319010
H	2.038120	3.078660	2.525690
H	2.734130	5.146540	1.321900
H	2.588390	5.258940	-1.184840
H	2.172810	-0.241670	-1.324390
H	0.373500	1.121940	-2.385100
H	0.674290	0.891650	2.396790
H	0.403820	-1.586660	-2.496710
H	0.885030	-1.827020	2.270020
C	1.293800	-0.352310	0.673520
H	2.352050	-0.298770	0.958050
H	1.731140	3.309240	-2.476990
H	1.912720	-3.646170	-2.861960
H	2.979830	-5.634350	-1.803910
H	3.265550	-5.737690	0.691430
H	2.448140	-3.870150	2.121720
Ag	-3.688190	-0.577740	0.693750
Ag	4.998040	-4.276840	-0.753500
Ag	4.659750	3.967700	-0.074410

3k	x	y	z
C	1.279430	-0.343760	-0.925360
C	0.722360	-1.699660	-1.488170
C	0.840020	-1.815790	1.116020
C	0.694480	0.820190	1.268540
C	0.483390	0.935360	-1.322720
C	1.735890	-2.835090	0.431880
C	2.550060	-3.762200	1.064510
C	3.285170	-4.683880	0.281580
C	3.224300	-4.614990	-1.143300
C	2.431350	-3.625350	-1.768270
C	1.676590	-2.766690	-0.982880
C	-0.552640	-2.042360	0.568360
C	-1.696180	-2.274970	1.320380
C	-2.934970	-2.424410	0.666550
C	-2.997900	-2.384220	-0.759230
C	-1.813390	-2.186690	-1.510330
C	-0.613250	-1.994550	-0.844780
C	-0.740060	0.977560	0.796470
C	-1.831500	1.316000	1.614650
C	-3.064260	1.640850	1.008550
C	-3.190320	1.612770	-0.381580
C	-2.088650	1.300930	-1.190530
C	-0.858680	1.010710	-0.605720
C	1.266840	2.109010	-0.735840
C	1.359040	2.055650	0.667260
C	1.839590	3.166170	1.394720
C	2.272870	4.311320	0.680130
C	2.237230	4.323700	-0.714350
C	1.736950	3.223900	-1.425480
H	-1.654450	-2.299330	2.408580
H	-3.857540	-2.438070	1.249400
H	-3.967930	-2.305500	-1.257140
H	-1.868040	-2.129000	-2.596810
H	-1.754460	1.248970	2.702520
H	-3.919830	1.899970	1.630670
H	-4.142780	1.870360	-0.842080
H	-2.186240	1.338970	-2.275720
H	2.008970	3.098090	2.472300
H	2.671380	5.164810	1.226690
H	2.587830	5.201530	-1.254310
H	2.283120	-0.228520	-1.351340
H	0.377680	1.017160	-2.409970
H	0.776380	0.798010	2.362000
H	0.664500	-1.677950	-2.581470
H	0.877340	-1.897370	2.207580
C	1.379740	-0.422860	0.629550
H	2.432930	-0.384100	0.932360
H	1.678590	3.264900	-2.513060
H	2.378440	-3.585240	-2.855690
H	3.645370	-5.424460	-1.744340
H	3.745170	-5.549970	0.763920
H	2.588160	-3.829180	2.151220
Ag	-3.216400	-4.656320	-0.315150
Ag	-0.557250	3.681510	1.547480
Ag	5.335040	-3.760590	-0.440160

Table S28: Cartesian coordinates of [janusene-Ag_3]$^{3+}$ **3l** and [janusene-Ag_4]$^{4+}$ **4a**

3l	x	y	z
C	1.275940	-0.283060	-0.896320
C	0.737940	-1.640550	-1.474030
C	0.771040	-1.739250	1.131350
C	0.855390	0.892750	1.332200
C	0.414350	0.981450	-1.233200
C	1.629060	-2.813740	0.485340
C	2.332060	-3.807820	1.148290
C	3.012700	-4.792240	0.393440
C	3.025190	-4.713300	-1.033400
C	2.352540	-3.655700	-1.686820
C	1.635690	-2.739010	-0.931900
C	-0.613610	-1.925830	0.536010
C	-1.788620	-2.134690	1.250890
C	-2.995640	-2.303940	0.560050
C	-3.008460	-2.328630	-0.866750
C	-1.793530	-2.145070	-1.583210
C	-0.623370	-1.921760	-0.877930
C	-0.614810	1.003540	0.990390
C	-1.660460	1.120630	1.899810
C	-2.967670	1.227550	1.417910
C	-3.213860	1.221790	0.041790
C	-2.156530	1.124600	-0.871640
C	-0.855560	1.016150	-0.393140
C	1.226850	2.164030	-0.732330
C	1.488150	2.101500	0.662190
C	2.119340	3.150340	1.312210
C	2.430310	4.326040	0.588090
C	2.165920	4.388040	-0.815570
C	1.596340	3.274010	-1.475130
H	-1.787650	-2.117450	2.339440
H	-3.937060	-2.336610	1.108370
H	-3.959450	-2.221400	-1.397620
H	-1.809480	-2.110990	-2.671950
H	-1.464470	1.139370	2.971800
H	-3.795980	1.338280	2.115940
H	-4.233560	1.331250	-0.324770
H	-2.353720	1.156120	-1.943240
H	2.290780	3.121930	2.387560
H	2.673800	5.240920	1.134270
H	2.215860	5.348190	-1.334810
H	2.261900	-0.128410	-1.352100
H	0.207050	1.050350	-2.306910
H	1.037500	0.879040	2.412270
H	0.719050	-1.622880	-2.568760
H	0.764160	-1.811780	2.224000
C	1.425000	-0.390200	0.650250
H	2.487440	-0.458930	0.916400
H	1.369490	3.338650	-2.538530
H	2.346690	-3.611910	-2.775380
H	3.394940	-5.558910	-1.618260
H	3.361500	-5.702300	0.888230
H	2.311970	-3.880820	2.235070
Ag	-3.233120	-4.584280	-0.705140
Ag	5.177960	-4.098870	-0.223800
Ag	4.497740	4.218640	-0.498270

4a	x	y	z
C	1.014798	-0.396422	-0.894709
C	0.417613	-1.769378	-1.396728
C	0.787445	-1.874707	1.187793
C	0.391162	0.814801	1.263467
C	0.289630	0.902821	-1.350864
C	1.689906	-2.816366	0.411302
C	2.649055	-3.684637	0.956533
C	3.426944	-4.508503	0.105434
C	3.222301	-4.449973	-1.316326
C	2.249285	-3.566213	-1.845818
C	1.470454	-2.778076	-0.981949
C	-0.623681	-2.214690	0.768718
C	-1.665314	-2.598332	1.624629
C	-2.967900	-2.793719	1.080651
C	-3.185728	-2.587710	-0.305617
C	-2.117416	-2.259040	-1.151767
C	-0.839034	-2.097336	-0.615801
C	-1.004417	1.071470	0.720312
C	-2.096530	1.566070	1.471149
C	-3.208738	2.192439	0.775876
C	-3.215369	2.226496	-0.644338
C	-2.167908	1.643504	-1.367249
C	-1.055526	1.121384	-0.704117
C	1.112692	2.041827	-0.738067
C	1.159105	2.001970	0.668775
C	1.838184	2.982473	1.384871
C	2.481468	4.008025	0.676455
C	2.435539	4.048230	-0.719308
C	1.742552	3.066488	-1.439851
H	-1.478310	-2.805421	2.679501
H	-3.759252	-3.219594	1.700126
H	-4.176699	-2.764462	-0.722673
H	-2.290089	-2.152734	-2.222506
H	-1.977541	1.765729	2.540099
H	-3.806754	2.919494	1.341323
H	-3.972249	2.811252	-1.170831
H	-2.167094	1.718897	-2.454590
H	1.870988	2.964823	2.473988
H	3.012945	4.786221	1.222510
H	2.934254	4.855596	-1.253693
H	2.014094	-0.322839	-1.340311
H	0.240887	0.970595	-2.442713
H	0.421124	0.809661	2.358582
H	0.250949	-1.757223	-2.478837
H	0.939332	-1.948223	2.269719
C	1.139568	-0.426579	0.656840
H	2.186432	-0.261419	0.936959
H	1.699858	3.112222	-2.527764
H	2.155967	-3.453638	-2.927917
H	3.960236	-4.907882	-1.988253
H	3.999798	-5.341469	0.534856
H	2.751891	-3.780915	2.039075
Ag	-5.194306	0.967511	0.687128
Ag	1.908918	-6.332561	-1.885653
Ag	5.410971	-3.293017	0.510785
Ag	-2.934017	-0.520360	1.590203

Table S29: Cartesian coordinates of [janusene-Ag_4]$^{4+}$ **4b** and **4c**

4b	x	y	z
C	1.010855	-0.317665	-0.895695
C	0.407554	-1.675537	-1.410649
C	0.651533	-1.756275	1.191243
C	0.526421	0.943399	1.277890
C	0.305769	1.020457	-1.326317
C	1.548829	-2.762294	0.474082
C	2.477775	-3.598340	1.075229
C	3.340989	-4.366638	0.257882
C	3.205695	-4.323503	-1.159688
C	2.208486	-3.513776	-1.751031
C	1.414764	-2.720030	-0.936066
C	-0.748959	-2.059790	0.714706
C	-1.820239	-2.436013	1.516678
C	-3.056588	-2.776930	0.909331
C	-3.191619	-2.718839	-0.511853
C	-2.091525	-2.324512	-1.311376
C	-0.882910	-2.009639	-0.700771
C	-0.892282	1.159935	0.805137
C	-1.997736	1.388983	1.616188
C	-3.254300	1.672832	1.016556
C	-3.371474	1.705208	-0.407208
C	-2.237541	1.459165	-1.215729
C	-1.012087	1.200658	-0.612106
C	1.221093	2.108678	-0.770510
C	1.340166	2.067840	0.640846
C	2.193547	2.934351	1.307011
C	2.997414	3.822857	0.551964
C	2.876165	3.862482	-0.866858
C	1.952873	3.016769	-1.521808
H	-1.715055	-2.508208	2.598773
H	-3.851828	-3.216104	1.512543
H	-4.094851	-3.102752	-0.986622
H	-2.193369	-2.309982	-2.396071
H	-1.908275	1.392725	2.702294
H	-4.084901	2.010637	1.637426
H	-4.301934	2.039567	-0.866416
H	-2.328963	1.512098	-2.300277
H	2.309493	2.893246	2.389632
H	3.835541	4.327201	1.042093
H	3.605825	4.417967	-1.461786
H	2.009100	-0.265536	-1.345892
H	0.204401	1.082170	-2.414913
H	0.608483	0.941557	2.369933
H	0.297749	-1.672724	-2.500147
H	0.747203	-1.820337	2.280236
C	1.147852	-0.362044	0.657592
H	2.209500	-0.321689	0.927708
H	1.879823	3.039659	-2.608607
H	2.124816	-3.470532	-2.836469
H	3.974157	-4.771536	-1.795263
H	4.219132	-4.838561	0.707930
H	2.602479	-3.619997	2.157413
Ag	-6.400731	-0.666390	0.589139
Ag	2.441469	-6.478617	-0.397698
Ag	1.944871	5.898536	0.076572
Ag	-3.596785	-0.548762	0.395913

4c	x	y	z
C	1.112240	-0.383970	-0.888460
C	0.482350	-1.717540	-1.431730
C	0.645580	-1.820050	1.174030
C	0.731560	0.866250	1.309820
C	0.418360	0.965160	-1.283310
C	1.501110	-2.876120	0.480500
C	2.349450	-3.777620	1.106700
C	3.181550	-4.600350	0.316460
C	3.102160	-4.540090	-1.104480
C	2.187740	-3.653130	-1.725330
C	1.419240	-2.814460	-0.932410
C	-0.757960	-2.036460	0.649420
C	-1.878720	-2.346330	1.411570
C	-3.115790	-2.620620	0.753550
C	-3.184070	-2.585240	-0.671970
C	-2.042980	-2.255700	-1.422980
C	-0.843490	-1.992360	-0.767060
C	-0.693890	1.154890	0.897170
C	-1.740120	1.473710	1.755240
C	-2.996660	1.839190	1.210570
C	-3.178920	1.855200	-0.207120
C	-2.101990	1.515830	-1.065790
C	-0.869540	1.187130	-0.515390
C	1.349590	2.054150	-0.751570
C	1.528040	1.992940	0.653400
C	2.284980	2.946650	1.318020
C	2.821350	4.028820	0.585200
C	2.642960	4.092680	-0.826630
C	1.926260	3.070800	-1.497090
H	-1.818860	-2.426610	2.496880
H	-3.943200	-3.044420	1.325390
H	-4.101030	-2.889890	-1.175750
H	-2.097550	-2.242980	-2.510970
H	-1.596730	1.490460	2.835120
H	-3.774470	2.237500	1.862550
H	-4.094030	2.270010	-0.630460
H	-2.240500	1.568950	-2.145000
H	2.404780	2.918700	2.400370
H	3.215880	4.893560	1.124860
H	2.869750	5.019050	-1.363080
H	2.109050	-0.336890	-1.342580
H	0.273860	1.039310	-2.366140
H	0.856300	0.853970	2.397480
H	0.408500	-1.702660	-2.524010
H	0.700810	-1.894610	2.265110
C	1.253220	-0.461490	0.662210
H	2.315480	-0.509200	0.928690
H	1.769940	3.141960	-2.572830
H	2.145930	-3.598410	-2.812630
H	3.872510	-5.021550	-1.714090
H	3.987490	-5.162460	0.794260
H	2.426970	-3.819340	2.192540
Ag	-6.326900	-0.192810	0.596350
Ag	2.124100	-6.625220	-0.574660
Ag	4.944320	3.634850	-0.536370
Ag	-3.515100	-0.365510	0.590900

Table S30: Cartesian coordinates of [janusene-Ag_4]$^{4+}$ **4d** and **4e**

4d	x	y	z
C	1.217690	-0.291970	-0.869250
C	0.605620	-1.640850	-1.382130
C	0.864460	-1.726540	1.216000
C	0.744950	0.945640	1.315760
C	0.490010	1.034800	-1.282750
C	1.698300	-2.785370	0.497490
C	2.441400	-3.785530	1.106570
C	2.999750	-4.809150	0.306270
C	2.860650	-4.762340	-1.111080
C	2.162470	-3.691330	-1.719150
C	1.558940	-2.738180	-0.913000
C	-0.547610	-2.014920	0.749750
C	-1.611030	-2.394790	1.560200
C	-2.840760	-2.759310	0.964220
C	-2.986150	-2.716600	-0.455790
C	-1.892500	-2.311000	-1.268070
C	-0.688730	-1.969620	-0.664840
C	-0.687890	1.142060	0.865310
C	-1.780410	1.360180	1.696190
C	-3.038680	1.659720	1.122520
C	-3.180180	1.718160	-0.297550
C	-2.055980	1.475280	-1.131790
C	-0.826420	1.194560	-0.549590
C	1.345580	2.171580	-0.727700
C	1.481870	2.124680	0.682920
C	2.134730	3.138220	1.367930
C	2.602370	4.263580	0.646420
C	2.467080	4.307770	-0.771260
C	1.865910	3.229360	-1.458950
H	-1.499180	-2.457780	2.642060
H	-3.633680	-3.187740	1.577480
H	-3.875120	-3.141930	-0.923110
H	-1.999530	-2.315550	-2.352350
H	-1.674070	1.347410	2.780350
H	-3.864920	1.969990	1.762440
H	-4.103580	2.099130	-0.735280
H	-2.163090	1.555400	-2.213100
H	2.215600	3.125000	2.454330
H	2.870050	5.170930	1.196650
H	2.656080	5.241430	-1.308040
H	2.209260	-0.231150	-1.333470
H	0.371130	1.101510	-2.369260
H	0.839450	0.938820	2.406710
H	0.487020	-1.636520	-2.470700
H	0.963500	-1.793260	2.304510
C	1.371800	-0.343200	0.680760
H	2.435550	-0.305600	0.944540
H	1.741950	3.283270	-2.539950
H	2.035520	-3.678490	-2.801120
H	3.107330	-5.642130	-1.712870
H	3.363960	-5.720190	0.789420
H	2.528950	-3.843460	2.190950
Ag	-6.253750	-0.649920	0.482050
Ag	5.161820	-4.381150	-0.647890
Ag	4.813670	4.097160	-0.197200
Ag	-3.443910	-0.538180	0.256050

4e	x	y	z
C	1.137510	-0.206860	-0.860180
C	0.538170	-1.554030	-1.417050
C	0.856270	-1.740270	1.168600
C	0.432540	0.899160	1.323480
C	0.430650	1.128250	-1.276080
C	1.774630	-2.676740	0.384270
C	2.692970	-3.563500	0.926400
C	3.385850	-4.446630	0.065750
C	3.188260	-4.371500	-1.341800
C	2.301630	-3.407620	-1.882210
C	1.585320	-2.594910	-1.017550
C	-0.537850	-2.100710	0.713110
C	-1.569440	-2.586060	1.524950
C	-2.798370	-2.992110	0.942970
C	-2.976150	-2.887850	-0.477000
C	-1.923560	-2.385590	-1.278080
C	-0.714620	-1.981140	-0.679150
C	-0.956620	1.017010	0.726530
C	-2.149260	1.082480	1.440900
C	-3.349830	1.382800	0.764920
C	-3.342220	1.604310	-0.641010
C	-2.125400	1.483120	-1.362900
C	-0.953330	1.186420	-0.675520
C	1.217670	2.234870	-0.579680
C	1.196280	2.126640	0.832480
C	1.873890	3.038490	1.627030
C	2.633650	4.058580	1.009180
C	2.658620	4.167350	-0.410520
C	1.920190	3.254390	-1.202830
H	-1.455730	-2.604780	2.609880
H	-3.676720	-3.144570	1.584130
H	-3.867630	-3.313330	-0.947750
H	-2.028690	-2.380320	-2.364280
H	-2.159580	0.969180	2.524690
H	-4.265330	1.554600	1.332020
H	-4.230460	2.006500	-1.132790
H	-2.113300	1.677420	-2.435440
H	1.872150	2.953040	2.713090
H	3.325620	4.650340	1.613560
H	3.384110	4.827550	-0.893780
H	2.146850	-0.153560	-1.284530
H	0.425010	1.249520	-2.364370
H	0.415220	0.835350	2.416720
H	0.389360	-1.509470	-2.500870
H	0.985210	-1.845550	2.250790
C	1.233020	-0.294150	0.692150
H	2.274360	-0.151030	1.002670
H	1.954670	3.335820	-2.288730
H	2.147580	-3.362820	-2.959800
H	3.562780	-5.169960	-1.989320
H	3.932060	-5.290370	0.495890
H	2.840910	-3.635870	2.003420
Ag	-2.419580	-5.261140	1.254340
Ag	1.347130	5.999490	0.349410
Ag	5.408210	-3.582190	-0.968720
Ag	-3.757560	-0.663430	-0.604470

Table S31: Cartesian coordinates of [janusene-Ag_4]$^{4+}$ **4f** and **4g**

4f	x	y	z
C	-4.872250	-2.783730	0.105500
C	-3.544460	-3.147420	-0.260580
C	-2.856870	-4.147130	0.472310
C	-5.505780	-3.423230	1.195370
C	-4.849020	-4.458730	1.843140
C	-3.524840	-4.816350	1.484830
H	-5.468360	-2.152880	-0.559210
H	-6.532720	-3.161110	1.447670
H	-3.136280	-2.824160	-1.223280
H	-1.852340	-4.439420	0.168290
C	-5.476080	-5.422530	2.849520
C	-3.020470	-6.049720	2.232190
C	-3.098200	-5.661900	3.746660
C	-4.584060	-5.403560	4.131680
C	-5.363980	-6.768560	2.167870
H	-6.512130	-5.154870	3.082330
C	-4.029830	-7.129770	1.875280
H	-2.000520	-6.319330	1.937410
C	-2.453070	-6.669530	4.762260
H	-2.523890	-4.734150	3.853210
C	-4.990880	-6.380070	5.301530
H	-4.682480	-4.398220	4.557860
C	-4.082410	-5.958010	6.457470
C	-2.706180	-6.087920	6.151200
H	-1.385830	-6.805590	4.558750
C	-3.214160	-7.975330	4.757140
C	-4.587820	-7.816680	5.026750
H	-6.053020	-6.286360	5.550820
C	-4.491240	-5.525260	7.709300
C	-1.731570	-5.755170	7.085570
C	-3.506160	-5.253980	8.700160
C	-2.125360	-5.369090	8.378420
H	-5.547830	-5.460370	7.968430
H	-3.815700	-5.221700	9.752420
H	-0.671940	-5.851300	6.850390
H	-1.373180	-5.265900	9.162550
C	-2.660450	-9.248610	4.586380
C	-5.416650	-8.946120	5.168340
C	-3.478760	-10.400440	4.720180
C	-4.874400	-10.244280	5.014800
H	-5.485510	-11.123140	5.243340
H	-3.111290	-11.369630	4.357610
H	-6.459820	-8.830000	5.467080
H	-1.613930	-9.362210	4.299840
C	-3.754960	-8.308250	1.188750
C	-6.429880	-7.545770	1.728960
C	-4.821510	-9.110800	0.729610
C	-6.168140	-8.723440	0.981370
H	-4.619190	-9.963690	0.080430
H	-6.986470	-9.244450	0.480030
H	-7.460420	-7.232760	1.896290
H	-2.731420	-8.585400	0.937380
Ag	-5.740920	-10.049520	2.824470
Ag	-2.613600	-11.054880	6.771930
Ag	-3.159200	-2.976530	8.851320
Ag	-3.347280	-0.960550	0.600590

4g	x	y	z
C	1.093280	-0.207600	-0.842930
C	0.634460	-1.587090	-1.432870
C	0.648470	-1.706120	1.176160
C	0.558500	0.975030	1.360900
C	0.243210	1.053720	-1.228260
C	1.622110	-2.692650	0.527440
C	2.430870	-3.600050	1.193440
C	3.227370	-4.494120	0.435850
C	3.241280	-4.406030	-0.984770
C	2.456640	-3.429340	-1.641820
C	1.629790	-2.610320	-0.887390
C	-0.692420	-2.047790	0.559200
C	-1.819810	-2.530080	1.255670
C	-2.969680	-2.941920	0.540290
C	-2.975440	-2.873100	-0.893320
C	-1.827260	-2.391510	-1.573640
C	-0.696100	-2.000290	-0.848480
C	-0.886520	1.103870	0.943460
C	-1.964560	1.315310	1.798250
C	-3.260180	1.511690	1.247140
C	-3.439020	1.453590	-0.163700
C	-2.332530	1.244430	-1.009120
C	-1.061780	1.100830	-0.457340
C	1.078990	2.214320	-0.693680
C	1.271970	2.156090	0.708430
C	2.057380	3.096420	1.357020
C	2.709000	4.095010	0.592790
C	2.512600	4.153360	-0.816710
C	1.668180	3.213750	-1.452740
H	-1.780350	-2.666010	2.338010
H	-3.800310	-3.421530	1.066720
H	-3.931030	-2.944470	-1.429580
H	-1.850950	-2.283840	-2.659050
H	-1.821160	1.387490	2.876640
H	-4.078560	1.852890	1.885060
H	-4.417980	1.671330	-0.591650
H	-2.474370	1.256850	-2.089640
H	2.224420	3.048560	2.432640
H	3.496260	4.694380	1.058440
H	3.137980	4.809520	-1.427580
H	2.091330	-0.034640	-1.261940
H	0.093200	1.119900	-2.311230
H	0.685830	0.967070	2.448560
H	0.622740	-1.563290	-2.527490
H	0.639600	-1.790060	2.267900
C	1.191120	-0.302120	0.708950
H	2.245730	-0.296190	1.008330
H	1.536470	3.255050	-2.533440
H	2.464670	-3.376020	-2.730120
H	3.714720	-5.194470	-1.576090
H	3.670080	-5.361790	0.934260
H	2.417140	-3.680770	2.279930
Ag	-3.633320	-0.749690	1.113150
Ag	-2.698120	-5.099980	-1.479680
Ag	1.349380	6.007180	0.199420
Ag	5.390680	-3.668070	-0.122400

Table S32: Cartesian coordinates of [janusene-Ag_4]$^{4+}$ **4h** and **4i**

4h	x	y	z
C	1.183480	-0.269960	-0.902150
C	0.638560	-1.620170	-1.487010
C	0.724310	-1.762360	1.118200
C	0.776580	0.907130	1.326320
C	0.368640	1.020700	-1.247610
C	1.610260	-2.804370	0.433110
C	2.351530	-3.793750	1.060200
C	3.051370	-4.741070	0.261280
C	3.034110	-4.624650	-1.156190
C	2.322800	-3.579290	-1.769990
C	1.583100	-2.707070	-0.978970
C	-0.654350	-2.019880	0.541150
C	-1.786070	-2.437750	1.267920
C	-2.981140	-2.769080	0.586420
C	-3.026560	-2.686710	-0.845630
C	-1.871260	-2.273340	-1.558960
C	-0.696690	-1.961040	-0.865570
C	-0.680840	1.097830	0.966240
C	-1.708270	1.373130	1.862360
C	-3.005800	1.663720	1.363000
C	-3.241910	1.630000	-0.040320
C	-2.184920	1.347040	-0.930210
C	-0.908250	1.113890	-0.427730
C	1.221470	2.177320	-0.729140
C	1.466750	2.099130	0.665080
C	2.140100	3.114930	1.327000
C	2.500130	4.279110	0.611470
C	2.246710	4.363080	-0.787460
C	1.638270	3.275590	-1.463530
H	-1.726460	-2.574490	2.348940
H	-3.820230	-3.208400	1.134700
H	-4.000330	-2.697470	-1.353360
H	-1.923280	-2.149310	-2.641650
H	-1.519090	1.430390	2.934340
H	-3.773420	2.054810	2.034130
H	-4.214410	1.933320	-0.429590
H	-2.366580	1.383690	-2.004090
H	2.308610	3.072920	2.402470
H	2.800690	5.171720	1.166370
H	2.313230	5.329890	-1.296560
H	2.172750	-0.135790	-1.355170
H	0.179350	1.100740	-2.323480
H	0.942300	0.886440	2.408600
H	0.595380	-1.587660	-2.580620
H	0.742680	-1.853140	2.209260
C	1.328750	-0.385120	0.643640
H	2.391340	-0.439040	0.908320
H	1.421900	3.359240	-2.528000
H	2.305460	-3.503650	-2.856870
H	3.479740	-5.407600	-1.772240
H	3.367450	-5.684740	0.723110
H	2.347030	-3.902690	2.144530
Ag	-3.580590	-0.554380	1.127360
Ag	-2.895520	-4.910920	-1.499470
Ag	5.292440	-4.170610	0.162620
Ag	4.598500	4.278780	-0.622840

4i	x	y	z
C	1.269310	-0.285360	-0.894520
C	0.645890	-1.615750	-1.441410
C	0.852400	-1.750210	1.156900
C	0.757620	0.911970	1.304550
C	0.540700	1.043670	-1.292990
C	1.692970	-2.800080	0.436790
C	2.444840	-3.797570	1.038870
C	3.039500	-4.794500	0.229860
C	2.925790	-4.721950	-1.188950
C	2.218840	-3.651310	-1.787720
C	1.580980	-2.726510	-0.975290
C	-0.559150	-1.986810	0.657180
C	-1.655430	-2.319490	1.440260
C	-2.903510	-2.549640	0.821880
C	-3.017100	-2.479810	-0.598060
C	-1.879190	-2.176870	-1.381870
C	-0.671020	-1.915080	-0.752840
C	-0.671880	1.094340	0.834350
C	-1.783450	1.258850	1.648150
C	-3.050620	1.460800	1.057270
C	-3.169630	1.532170	-0.362130
C	-2.018800	1.401410	-1.173070
C	-0.789440	1.165920	-0.575320
C	1.393000	2.164950	-0.709120
C	1.510390	2.094830	0.701660
C	2.179690	3.085010	1.403490
C	2.696060	4.205000	0.695700
C	2.579770	4.264290	-0.722440
C	1.957470	3.214710	-1.423150
H	-1.572850	-2.378000	2.525180
H	-3.801840	-2.639300	1.437360
H	-4.004350	-2.493770	-1.067760
H	-1.971140	-2.123120	-2.466310
H	-1.697360	1.206160	2.733090
H	-3.948290	1.411040	1.678550
H	-4.158560	1.527850	-0.827940
H	-2.114930	1.457970	-2.256980
H	2.244810	3.060280	2.491030
H	2.942020	5.113630	1.257840
H	2.857010	5.176620	-1.254360
H	2.269300	-0.221090	-1.339890
H	0.436890	1.129370	-2.379930
H	0.836650	0.886080	2.396680
H	0.549340	-1.588960	-2.532050
H	0.928570	-1.838120	2.245970
C	1.395360	-0.366270	0.659000
H	2.454780	-0.344270	0.941340
H	1.859220	3.273580	-2.506650
H	2.119340	-3.612790	-2.872070
H	3.206960	-5.581980	-1.803720
H	3.415770	-5.706750	0.701260
H	2.519070	-3.871020	2.123420
Ag	-3.129230	-4.794990	-0.066550
Ag	-3.442780	3.760330	0.456370
Ag	5.207180	-4.290900	-0.663450
Ag	4.951700	3.956770	0.246050

Table S33: Cartesian coordinates of [janusene-Ag_5]$^{5+}$ **5**

5	x	y	z
C	1.260262	-0.278881	-0.868493
C	0.518778	-1.566795	-1.397742
C	0.998192	-1.815277	1.157491
C	0.587771	0.846217	1.310037
C	0.699914	1.124978	-1.284113
C	1.809704	-2.788829	0.298105
C	2.685918	-3.757186	0.773562
C	3.210732	-4.704456	-0.125870
C	2.906643	-4.620050	-1.509664
C	2.074136	-3.573636	-1.993036
C	1.515178	-2.689338	-1.083467
C	-0.434713	-2.121991	0.798191
C	-1.403680	-2.628015	1.666643
C	-2.685785	-2.952406	1.170839
C	-2.984866	-2.740676	-0.212024
C	-1.984895	-2.226420	-1.078255
C	-0.708939	-1.930029	-0.575222
C	-0.765620	1.093275	0.659812
C	-1.984134	1.280343	1.330463
C	-3.133223	1.696378	0.605692
C	-3.039028	1.926802	-0.801252
C	-1.812534	1.717172	-1.464114
C	-0.695012	1.302004	-0.736100
C	1.526749	2.173535	-0.531983
C	1.428249	2.051971	0.876796
C	2.024862	2.978319	1.718160
C	2.676040	4.099042	1.148780
C	2.787725	4.216109	-0.262718
C	2.235686	3.219170	-1.104246
H	-1.183996	-2.752341	2.727602
H	-3.496169	-3.198902	1.873995
H	-3.931788	-3.091685	-0.633195
H	-2.201642	-2.132142	-2.143080
H	-2.047310	1.178899	2.414749
H	-4.041779	1.967999	1.151670
H	-3.953534	2.104194	-1.388377
H	-1.745356	1.860716	-2.542975
H	1.937360	2.900194	2.801463
H	2.921995	4.949573	1.792289
H	3.119219	5.158258	-0.710684
H	2.262782	-0.329988	-1.308316
H	0.746643	1.263800	-2.369172
H	0.517029	0.761436	2.399560
H	0.296505	-1.497307	-2.467838
H	1.200955	-1.941218	2.226024
C	1.368091	-0.369758	0.677793
H	2.411135	-0.225221	0.981484
H	2.308141	3.329550	-2.185954
H	1.827407	-3.528338	-3.053585
H	3.084602	-5.486786	-2.160302
H	3.751496	-5.569304	0.264688
H	2.914687	-3.838542	1.835910
Ag	-2.955386	-5.609962	1.517703
Ag	-3.766270	4.582721	-1.143478
Ag	5.209735	-4.249508	-1.812559
Ag	5.045576	3.936821	0.598950
Ag	-3.665096	-0.557080	0.274113