Supporting information for "Freezing out Structural Effects: Strong Dye-dye Couplings in Gaseous Rhodamine Dimers at Cryogenic Temperatures"

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Contents

Mass scans

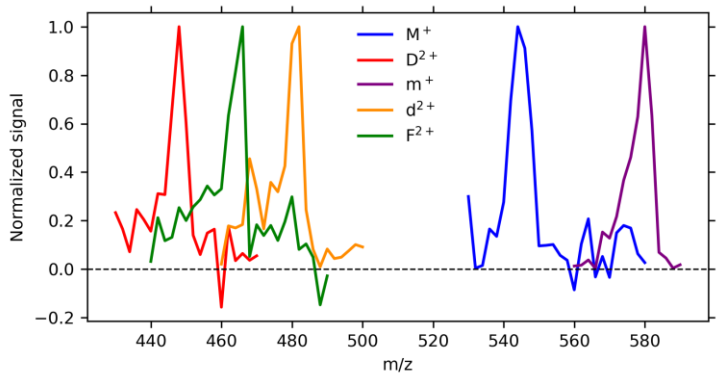

Figure S1: Mass scans of ions studied in this work

Lifetime measurements

Excited-state lifetimes were measured by collecting the time-response signal from the photomultiplier tube (PMT), then fitting the time-trace with an exponentially modified Gaussian to extract the excited-state lifetime. Experimental parameters, namely the excitation wavelength and long-pass filters used, are enumerated in Table S1.

Table S1: Experimental parameters for lifetime experiments

Species	Long-pass filter (nm)	Excitation wavelength (nm)	Fitted lifetime (ns)
M^+	500	495	5 ± 1
m^+	550	535	6 ± 1
D^{2+}	500	488	5 ± 1
d^{2+}	600	564	7 ± 1
F^{2+}	500	498	5 ± 1

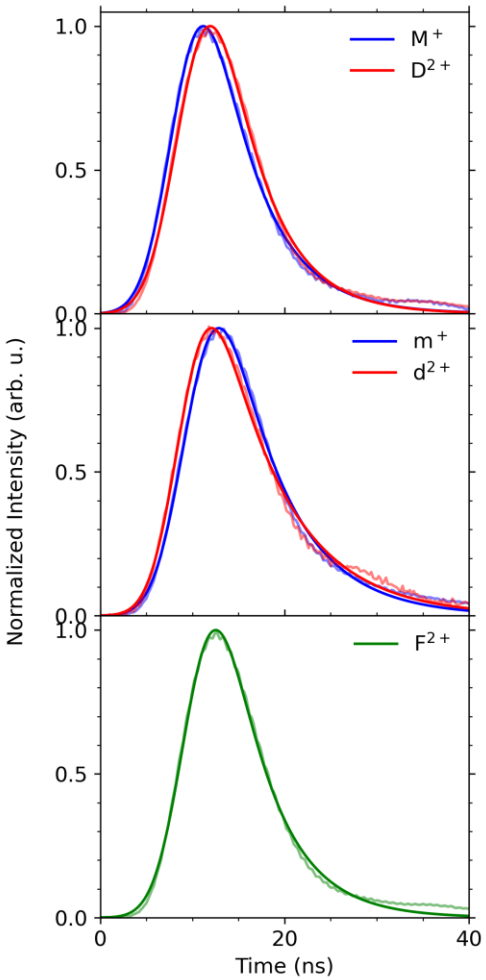

Figure S2: Fluorescence decay (PMT signal) and fits for all species studied. The darker, solid line represents the fit.

Calculated ground-state energies

For all results below, structure **I** is the lowest-energy ground-state geometry, while structure **II** is the next-highest in energy in the ground state, at the ωB97XD/def2-SVP level of theory. Inter-dye separation is calculated as the distance between the centres of the xanthene moieties of the rhodamine dyes in the dimers.

Table S2: Ground-state computational data for systems studied

	Structure I (lowest-energy geometry)	Structure II (next-highest energy geometry)	
System	Inter-dye separation (Å)	Energy relative to lowest-energy geometry (meV)	Inter-dye separation (Å)
M^{+} (R575^{+} monomer)	—	27	—
m^{+} (RB^{+} monomer)	—	157	—
D^{2+} (R575^{+} homodimer)	4.8	31	6.0
d^{2+} (RB^{+} homodimer)	4.2	130	7.8
F^{2+} (heterodimer)	7.9	37	7.7

Ground-state geometries

Below are the structures of the calculated geometries of all systems studied.

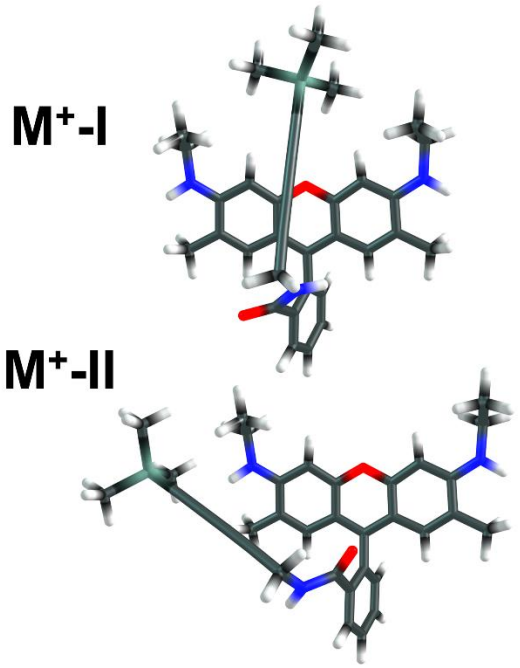

Figure S3: Ground-state geometries of **M**$^{+}$**-I** and **M**$^{+}$**-II**

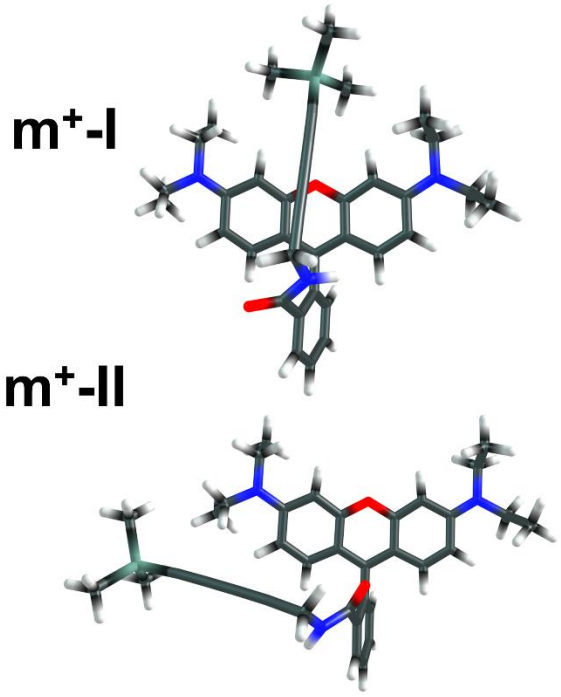

Figure S4: Ground-state geometries of **m⁺-I** and **m⁺-II**

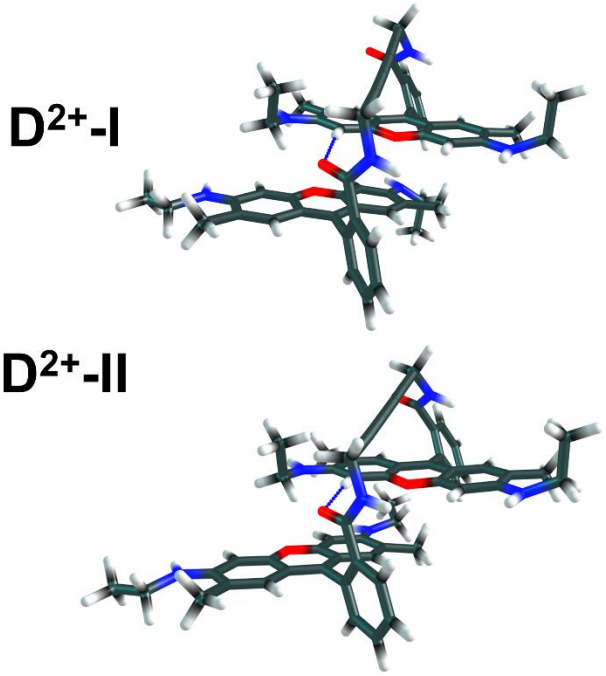

Figure S5: Ground-state geometries of **D²⁺-I** and **D²⁺-II**

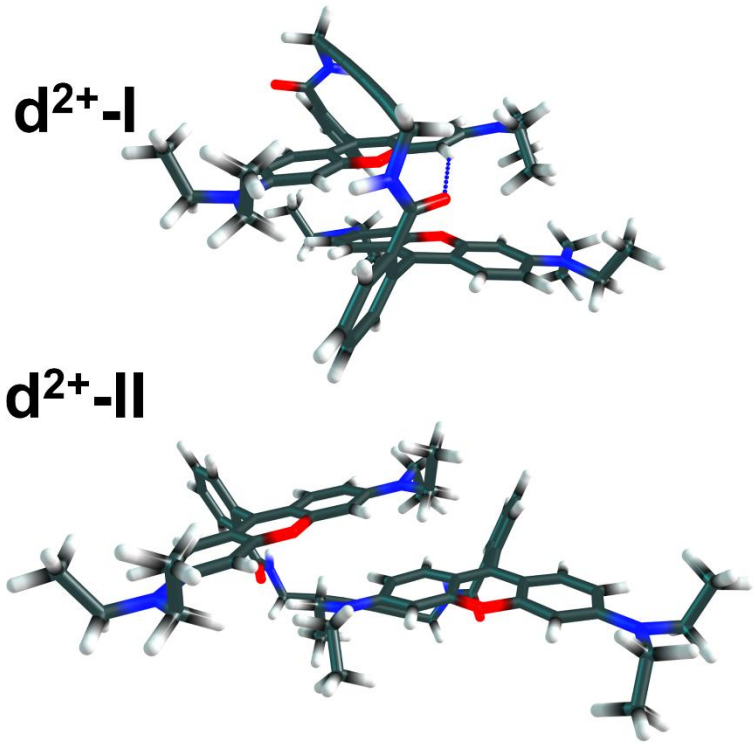

Figure S6: Ground-state geometries of **d^{2+}-I** and **d^{2+}-II**

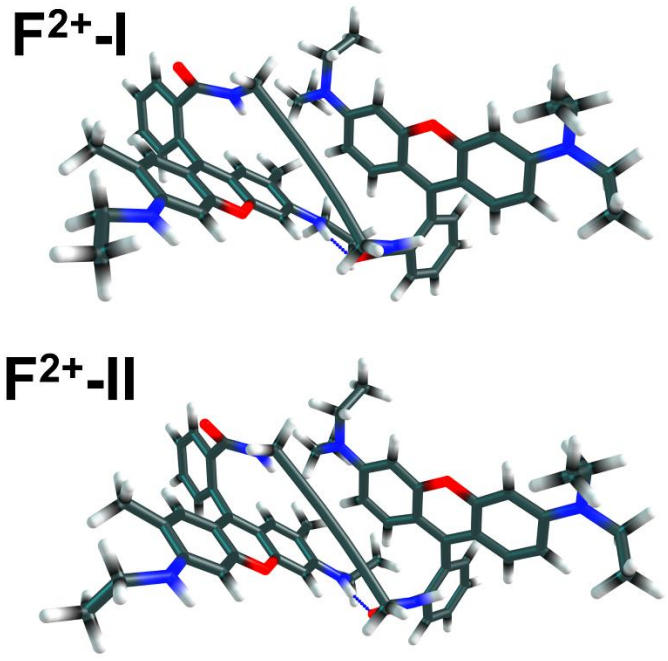

Figure S7: Ground-state geometries of **F^{2+}-I** and **F^{2+}-II**

Excited-state results

Below are the excited-state results for the first eight excited states at ωB97XD/def2-SVP.

Table S3: Excited-state results for bare R575+ and RB+

	$R575^+$			**RB^+**		
Transition ($S_0 \rightarrow S_n$)	Energy (eV)	Wavelength (nm)	Oscillator strength	Energy (eV)	Wavelength (nm)	Oscillator strength
1	3.16	393	0.90	3.01	411	1.01
2	3.75	330	0.00	3.72	333	0.00
3	4.53	274	0.21	4.40	281	0.15
4	4.60	270	0.00	4.61	269	0.00
5	4.68	265	0.00	4.72	263	0.00
6	4.96	250	0.27	4.85	256	0.34
7	5.01	247	0.00	4.95	250	0.01
8	5.08	244	0.08	4.99	249	0.05

Table S4: Excited-state results for **M^+** ($R575^+$ monomer)

	M^+-I			**M^+-II**		
Transition ($S_0 \rightarrow S_n$)	Energy (eV)	Wavelength (nm)	Oscillator strength	Energy (eV)	Wavelength (nm)	Oscillator strength
1	3.06	405	0.71	3.07	404	0.86
2	3.61	344	0.00	3.69	336	0.00
3	4.13	300	0.00	4.37	284	0.16
4	4.23	293	0.15	4.40	282	0.04
5	4.25	292	0.00	4.43	280	0.00
6	4.44	279	0.02	4.56	272	0.00
7	4.48	277	0.00	4.70	264	0.00
8	4.51	275	0.01	4.76	260	0.00

Table S5: Excited-state results for **m^+** (RB^+ monomer)

	m^+-I			**m^+-II**		
Transition ($S_0 \rightarrow S_n$)	Energy (eV)	Wavelength (nm)	Oscillator strength	Energy (eV)	Wavelength (nm)	Oscillator strength
1	2.94	422	0.84	2.97	417	0.97
2	3.58	346	0.00	3.67	338	0.00
3	4.07	305	0.00	4.26	291	0.18
4	4.15	299	0.13	4.35	285	0.04
5	4.19	296	0.01	4.48	277	0.00
6	4.39	282	0.02	4.64	267	0.00
7	4.47	277	0.00	4.71	263	0.00
8	4.51	275	0.01	4.74	262	0.01

Table S6: Excited-state results for **D^{2+}** ($R575^{+}$ homodimer)

	D^{2+}-I			**D^{2+}-II**		
Transition ($S_0 \rightarrow S_n$)	Energy (eV)	Wavelength (nm)	Oscillator strength	Energy (eV)	Wavelength (nm)	Oscillator strength
1	2.89	428	0.11	2.94	421	1.12
2	3.05	407	1.33	2.99	414	0.47
3	3.24	383	0.00	3.45	360	0.00
4	3.53	351	0.00	3.53	351	0.01
5	3.56	348	0.03	3.60	344	0.01
6	3.59	346	0.00	3.69	336	0.00
7	4.05	306	0.08	4.06	305	0.02
8	4.09	303	0.04	4.09	303	0.13

Table S7: Excited-state results for **d^{2+}** (RB^{+} homodimer)

	d^{2+}-I			**d^{2+}-II**		
Transition ($S_0 \rightarrow S_n$)	Energy (eV)	Wavelength (nm)	Oscillator strength	Energy (eV)	Wavelength (nm)	Oscillator strength
1	2.84	437	0.42	2.90	427	1.21
2	2.99	415	1.09	2.97	418	0.66
3	3.45	360	0.02	3.59	345	0.00
4	3.50	354	0.02	3.66	339	0.01
5	3.58	346	0.00	3.79	327	0.01
6	3.78	328	0.01	3.99	310	0.00
7	3.98	311	0.18	4.23	293	0.27
8	4.07	305	0.02	4.33	287	0.13

Table S8: Excited-state results for **F^{2+}** (heterodimer)

	F^{2+}-I			**F^{2+}-II**		
Transition ($S_0 \rightarrow S_n$)	Energy (eV)	Wavelength (nm)	Oscillator strength	Energy (eV)	Wavelength (nm)	Oscillator strength
1	2.85	435	1.08	2.85	434	1.00
2	2.93	423	0.71	2.96	419	0.81
3	3.45	359	0.01	3.50	354	0.00
4	3.54	350	0.00	3.56	348	0.00
5	3.59	346	0.00	3.59	345	0.00
6	4.06	305	0.15	4.10	303	0.14
7	4.23	293	0.08	4.19	296	0.16
8	4.24	293	0.06	4.34	286	0.01

Coordinates

Coordinates for all calculated structures in this report.

Table S9: Coordinates of **M$^+$-I** (R575$^+$ monomer with linker)

Element	X	Y	Z
Si	-4.87558	-0.48037	0.041437
C	-5.09636	-2.22271	-0.61891
H	-6.02116	-2.29561	-1.21277
H	-4.25605	-2.51341	-1.26897
H	-5.16339	-2.94952	0.20465
C	-6.2736	0.010519	1.183498
H	-7.23297	0.008498	0.642326
H	-6.35896	-0.68777	2.029791
H	-6.11461	1.020167	1.592123
C	-4.69355	0.742515	-1.37413
H	-4.5969	1.77067	-0.99241
H	-3.8107	0.510142	-1.9897
H	-5.58009	0.712334	-2.02698
C	-3.28427	-0.44698	0.998211
C	-2.20539	-0.43673	1.571803
C	-0.95841	-0.41967	2.157946
C	0.155649	-0.41091	2.641949
C	1.508813	-0.35341	3.201983
H	1.872142	-1.36578	3.435335
H	1.494893	0.213803	4.146813
N	2.45031	0.223294	2.266811
H	2.269664	1.15721	1.92075
C	3.46174	-0.507	1.715836
O	3.764906	-1.62093	2.089013
C	4.182085	0.17254	0.579811
C	5.571966	0.291365	0.641406
C	3.493916	0.620479	-0.56161
C	6.275489	0.886967	-0.4013
H	6.095974	-0.08863	1.520515
C	4.210607	1.213558	-1.60821
C	5.59348	1.350629	-1.52576
H	7.360817	0.984679	-0.33951
H	3.678203	1.549193	-2.50109
H	6.141809	1.810598	-2.34991
C	2.026328	0.41919	-0.71228
C	1.146585	1.523667	-0.69855
C	1.492925	-0.87383	-0.84475
C	1.543259	2.873151	-0.45786
C	-0.2424	1.292197	-0.86018
C	0.086076	-1.02302	-0.98949

C	2.260244	-2.07927	-0.80237
C	0.646662	3.904181	-0.36849
H	2.607494	3.083985	-0.33175
C	-1.17905	2.305512	-0.78992
C	-0.52976	-2.256	-1.03698
H	3.344924	-2.00375	-0.71826
C	1.687666	-3.31878	-0.82818
C	-0.7644	3.621165	-0.52698
H	-2.22687	2.037524	-0.89866
C	0.245435	-3.42397	-0.92184
H	-1.61484	-2.28285	-1.10608
O	-0.70801	0.053585	-1.07112
C	2.519257	-4.56615	-0.73111
H	2.374586	-5.22177	-1.60564
H	3.58616	-4.3199	-0.67045
H	2.269809	-5.14381	0.174671
N	-0.32294	-4.64197	-0.90441
C	1.094888	5.313962	-0.10254
H	2.187254	5.371157	-0.0185
H	0.790663	5.993611	-0.91567
H	0.671899	5.703974	0.838527
N	-1.65475	4.626739	-0.41867
H	-1.29759	5.541512	-0.18123
H	0.290567	-5.43454	-0.77223
C	-3.09873	4.475444	-0.47425
H	-3.35829	3.856921	-1.34877
H	-3.51789	5.470921	-0.67652
C	-3.71061	3.896566	0.798632
H	-4.80341	3.830346	0.693715
H	-3.32735	2.887807	1.015715
H	-3.49147	4.536723	1.665378
C	-1.75231	-4.90475	-0.88181
H	-2.23881	-4.30321	-1.66623
H	-1.88865	-5.95347	-1.18048
C	-2.40144	-4.65344	0.475689
H	-1.93306	-5.27387	1.253404
H	-2.31639	-3.59945	0.780638
H	-3.46963	-4.909	0.432411

Table S10: Coordinates of **M^+-II** ($R575^+$ monomer with linker)

Element	X	Y	Z
C	1.581203	0.510746	-1.4094
C	0.342673	1.073025	-1.28679
C	-0.82489	0.311753	-0.97957
C	-0.66293	-1.09251	-0.87427
C	0.575914	-1.69898	-0.9666

C	1.723602	-0.91321	-1.1806
C	-2.09161	0.86776	-0.73327
C	-2.95906	-1.38604	-0.47583
C	-3.18292	0.013502	-0.49676
C	-4.50945	0.456837	-0.22262
H	-4.69733	1.531494	-0.194
C	-5.54392	-0.40656	0.00944
C	-5.28497	-1.8306	-0.01238
C	-3.97789	-2.29357	-0.24711
H	0.23019	2.146969	-1.44707
H	0.633351	-2.77723	-0.83237
H	-3.72977	-3.35289	-0.23447
O	-1.72356	-1.88557	-0.65019
N	2.955917	-1.45171	-1.21064
N	-6.31038	-2.68075	0.192166
C	-2.24738	2.346113	-0.69214
C	-1.67465	3.080788	0.362949
C	-2.91663	3.017106	-1.71714
C	-1.79345	4.471549	0.376111
C	-3.0275	4.407235	-1.69525
H	-3.3449	2.445548	-2.54361
C	-2.4698	5.134441	-0.64731
H	-1.37774	5.042198	1.209957
H	-3.55299	4.921468	-2.50198
H	-2.56557	6.221341	-0.62087
C	-0.99639	2.33008	1.479222
O	-1.47185	1.312074	1.942005
N	0.17984	2.865756	1.911611
H	0.592562	3.63091	1.393457
C	0.98931	2.188522	2.903821
H	0.344452	1.433641	3.37757
H	1.303335	2.89681	3.687029
C	2.175325	1.539133	2.335997
C	3.177229	1.026928	1.87905
C	4.317468	0.465155	1.344494
C	5.319272	-0.01942	0.837578
Si	6.850647	-0.71075	0.034093
C	8.297949	0.367554	0.523033
H	9.225338	-0.00261	0.058027
H	8.145887	1.408589	0.200379
H	8.440173	0.365669	1.614278
C	7.074494	-2.47738	0.616947
H	7.98777	-2.90737	0.175854
H	7.175267	-2.52186	1.712042
H	6.227415	-3.11755	0.328108
C	6.561298	-0.64467	-1.82398

H	6.342932	0.382069	-2.15665
H	7.465258	-0.98126	-2.35617
H	5.735434	-1.29708	-2.14963
C	3.27776	-2.82826	-0.87947
H	4.289552	-3.01907	-1.2667
H	2.611299	-3.49553	-1.44805
C	3.220821	-3.13865	0.61326
H	3.485086	-4.19121	0.790359
H	3.924676	-2.50406	1.169859
H	2.215677	-2.96513	1.024201
C	-6.20971	-4.12739	0.268951
H	-5.56411	-4.48229	-0.5497
H	-7.21	-4.53138	0.05779
C	-5.70982	-4.63788	1.616516
H	-4.70672	-4.25036	1.847682
H	-6.38648	-4.33096	2.42718
H	-5.65912	-5.736	1.611614
H	-7.20889	-2.2738	0.411544
H	3.731405	-0.80026	-1.19676
C	-6.93373	0.090808	0.292884
H	-7.65506	-0.27157	-0.45847
H	-7.28608	-0.23554	1.285708
H	-6.96838	1.18717	0.279153
C	2.780672	1.328811	-1.79631
H	3.547425	1.339818	-1.00567
H	3.250579	0.93071	-2.71045
H	2.494823	2.369582	-1.99381

Table S11: Coordinates of **m^+-I** (RB^+ monomer with linker)

Element	X	Y	Z
C	2.157109	-3.23177	-0.86073
C	0.794181	-3.14871	-0.82801
C	0.117888	-1.89523	-0.84135
C	0.943306	-0.74187	-0.91178
C	2.32108	-0.80311	-0.9568
C	2.981606	-2.05183	-0.91785
C	-1.27713	-1.73201	-0.70855
C	-0.91381	0.678073	-0.70032
C	-1.80198	-0.43272	-0.62039
C	-3.18243	-0.11801	-0.43553
H	-3.90981	-0.92901	-0.38774
C	-3.61134	1.167596	-0.29612
C	-2.69121	2.27752	-0.318
C	-1.32809	1.984736	-0.56293
H	2.615065	-4.21761	-0.82373
H	0.203127	-4.06514	-0.7749

H	2.856173	0.141666	-0.98021
H	-4.67482	1.340953	-0.15119
H	-0.56371	2.754454	-0.62075
O	0.396283	0.483753	-0.92031
N	4.330843	-2.13469	-0.92881
N	-3.11312	3.539662	-0.09695
C	5.022699	-3.42157	-0.87617
H	4.500981	-4.13717	-1.52761
H	6.009302	-3.27539	-1.33709
C	5.184571	-3.98743	0.530562
H	4.211071	-4.12377	1.02444
H	5.686582	-4.96464	0.488983
H	5.792934	-3.32296	1.160017
C	-4.53007	3.853201	0.094003
H	-4.57575	4.810898	0.629596
H	-4.9739	3.113682	0.77628
C	-5.32916	3.944519	-1.20152
H	-6.38281	4.164246	-0.97769
H	-4.94736	4.744909	-1.8504
H	-5.291	3.002693	-1.76833
C	-2.17464	-2.91745	-0.63571
C	-2.85674	-3.24295	0.549634
C	-2.3889	-3.68461	-1.78705
C	-3.76642	-4.30209	0.556064
C	-3.27867	-4.75512	-1.76298
H	-1.86831	-3.42405	-2.71139
C	-3.97054	-5.06226	-0.59187
H	-4.31173	-4.52493	1.475192
H	-3.44118	-5.34416	-2.66744
H	-4.67601	-5.89491	-0.57458
C	-2.67957	-2.42615	1.803925
O	-3.61677	-1.89063	2.356718
N	-1.39145	-2.3362	2.244511
H	-0.6635	-2.83362	1.747528
C	-0.99941	-1.41783	3.291553
H	-0.49698	-1.95147	4.114505
H	-1.92605	-0.9867	3.700177
C	-0.12495	-0.35674	2.783581
C	0.610801	0.499655	2.335505
C	1.412226	1.477183	1.786976
C	2.090267	2.333406	1.239407
Si	3.022076	3.644395	0.313378
C	4.386456	4.306383	1.408114
H	3.977021	4.749503	2.328521
H	5.083148	3.505427	1.699232
H	4.961669	5.084368	0.881772

C	3.71585	2.847852	-1.24052
H	4.235424	3.596341	-1.85932
H	4.443289	2.061362	-0.98851
H	2.913064	2.403864	-1.84964
C	1.783636	4.979489	-0.14612
H	2.28626	5.813011	-0.66186
H	1.013788	4.583569	-0.82716
H	1.285069	5.384628	0.747941
C	5.152573	-0.92702	-0.86198
H	4.792918	-0.2066	-1.61384
H	6.163456	-1.21017	-1.18394
C	5.214472	-0.27853	0.518947
H	5.873654	0.601551	0.485967
H	4.224951	0.053509	0.867205
H	5.621898	-0.97374	1.265816
C	-2.1749	4.660788	-0.12581
H	-1.25737	4.370905	0.408036
H	-2.62061	5.469326	0.469183
C	-1.84611	5.169381	-1.52558
H	-1.41156	4.377572	-2.15353
H	-2.74347	5.548472	-2.03398
H	-1.11996	5.992569	-1.463

Table S12: Coordinates of **m$^+$-II** (RB$^+$ monomer with linker)

C	1.699397	-0.47274	-0.71216
C	0.668993	0.407413	-0.86623
C	-0.69054	0.017511	-0.68984
C	-0.91121	-1.34923	-0.37321
C	0.114929	-2.26186	-0.23049
C	1.461952	-1.85376	-0.37495
C	-1.79419	0.885972	-0.7665
C	-3.23776	-1.01651	-0.27835
C	-3.08563	0.366566	-0.55969
C	-4.28093	1.140863	-0.56187
H	-4.21043	2.215698	-0.73285
C	-5.50401	0.578516	-0.34098
C	-5.65011	-0.83297	-0.09525
C	-4.46697	-1.60769	-0.0578
H	2.716232	-0.10913	-0.84464
H	0.890845	1.443425	-1.12689
H	-0.16308	-3.28692	-0.00049
H	-6.37737	1.226314	-0.34136
H	-4.47243	-2.67242	0.159913
O	-2.16072	-1.81785	-0.20297
N	2.486067	-2.71674	-0.19945
N	-6.86982	-1.38803	0.086768

C	3.875042	-2.30988	-0.40996
H	4.048382	-1.33564	0.067926
H	4.502192	-3.01947	0.146707
C	4.302657	-2.27611	-1.87321
H	3.683642	-1.58205	-2.46043
H	5.347292	-1.94116	-1.9485
H	4.232221	-3.26911	-2.33854
C	-8.08498	-0.57447	0.11406
H	-8.92318	-1.24364	-0.12322
H	-8.04965	0.153367	-0.70985
C	-8.34219	0.12657	1.444065
H	-9.25521	0.735488	1.377674
H	-8.47906	-0.59921	2.257536
H	-7.50923	0.789515	1.720561
C	-1.61947	2.326406	-1.09957
C	-1.03012	3.226538	-0.19451
C	-2.04775	2.788351	-2.3477
C	-0.90631	4.57308	-0.54594
C	-1.90917	4.131289	-2.69245
H	-2.49159	2.085004	-3.05581
C	-1.34674	5.02737	-1.78704
H	-0.48551	5.282817	0.17027
H	-2.24834	4.477437	-3.67043
H	-1.25397	6.08399	-2.04413
C	-0.56035	2.702349	1.135989
O	-1.17777	1.849032	1.742642
N	0.62102	3.223751	1.568573
H	1.142995	3.824621	0.942965
C	1.34018	2.643695	2.686627
H	0.666065	1.911048	3.154888
H	1.571657	3.411037	3.442797
C	2.578247	2.000453	2.239861
C	3.609684	1.527911	1.806542
C	4.785057	1.007986	1.307247
C	5.830959	0.562832	0.857167
Si	7.484033	-0.02933	0.233624
C	7.576825	-1.88741	0.48558
H	8.580215	-2.25175	0.213258
H	7.394861	-2.15474	1.537715
H	6.848037	-2.42533	-0.13883
C	7.599033	0.414937	-1.58504
H	8.558915	0.07002	-2.00125
H	6.790406	-0.0465	-2.17206
H	7.54104	1.504832	-1.7273
C	8.803033	0.845524	1.233094
H	9.805403	0.535945	0.896968

H	8.727456	1.937494	1.119368
H	8.713581	0.606711	2.303669
C	2.238809	-4.12444	0.103234
H	1.443962	-4.19248	0.861009
H	3.143332	-4.51324	0.590245
C	1.898715	-4.97779	-1.11492
H	1.693291	-6.01213	-0.80389
H	1.011477	-4.59733	-1.64174
H	2.732472	-5.00008	-1.83026
C	-7.00966	-2.81201	0.383536
H	-6.34083	-3.38069	-0.27996
H	-8.02858	-3.10371	0.094548
C	-6.76035	-3.17781	1.843682
H	-5.75743	-2.87025	2.17375
H	-7.49488	-2.69849	2.505429
H	-6.84519	-4.26575	1.977769

Table S13: Coordinates of **D^{2+}-I** ($R575^{+}$ homodimer)

Element	X	Y	Z
C	4.897291	1.848322	0.122895
C	4.521993	0.533094	0.274094
C	3.21214	0.0457	0.015518
C	2.267645	0.997836	-0.43425
C	2.60788	2.322001	-0.62688
C	3.915144	2.78582	-0.37693
C	2.812226	-1.30697	0.149846
C	0.603122	-0.63806	-0.63567
C	1.488462	-1.64799	-0.15977
C	0.948538	-2.9692	-0.06048
H	1.589258	-3.76415	0.322787
C	-0.31936	-3.28094	-0.45761
C	-1.15971	-2.23252	-1.00017
C	-0.68472	-0.90854	-1.04253
H	5.266697	-0.17647	0.639166
H	1.844528	2.995011	-1.02054
H	-1.29291	-0.08949	-1.42487
O	1.006345	0.639691	-0.71616
N	4.155459	4.1077	-0.5839
H	3.335892	4.609466	-0.90301
N	-2.39132	-2.54246	-1.43802
H	-2.63378	-3.52381	-1.46193
C	5.401304	4.765051	-0.97694
H	5.180442	5.841416	-0.99131
H	6.164254	4.635201	-0.20187
C	5.919795	4.318813	-2.3382
H	5.182958	4.520739	-3.1297

H	6.844077	4.858416	-2.589
H	6.141583	3.240706	-2.35102
C	-3.29865	-1.62464	-2.1127
H	-3.33797	-0.67976	-1.55239
H	-4.30238	-2.06987	-2.04933
C	-2.92331	-1.34834	-3.56363
H	-3.65686	-0.66294	-4.01101
H	-1.9329	-0.87514	-3.63486
H	-2.90983	-2.27347	-4.15812
C	3.787061	-2.35024	0.571654
C	4.150196	-3.39129	-0.30166
C	4.321869	-2.32682	1.865875
C	4.996992	-4.4085	0.142826
C	5.186037	-3.33134	2.29222
H	4.031724	-1.52069	2.540898
C	5.52002	-4.3772	1.432345
H	5.248173	-5.22419	-0.538
H	5.59652	-3.30243	3.303454
H	6.190927	-5.17032	1.767093
C	3.601058	-3.46187	-1.70376
O	2.937236	-4.40198	-2.08592
N	3.903054	-2.38256	-2.48005
H	4.493553	-1.65203	-2.10308
C	3.314312	-2.19131	-3.78703
H	2.822345	-3.13771	-4.05835
H	4.094151	-1.99871	-4.54067
C	2.335891	-1.09861	-3.79655
C	1.53482	-0.18667	-3.80004
C	0.595363	0.822868	-3.80059
C	-0.25345	1.689232	-3.77944
C	-1.3189	2.695597	-3.78961
H	-1.0892	3.47516	-4.53057
H	-2.25406	2.209821	-4.10906
N	-1.54875	3.337812	-2.50748
C	-2.25828	2.714408	-1.53501
H	-1.14092	4.246498	-2.33616
O	-2.64345	1.562463	-1.66623
C	-2.57984	3.523367	-0.30995
C	-2.7688	4.908362	-0.40322
C	-2.76225	2.893148	0.936022
C	-3.11351	5.66744	0.710894
H	-2.6846	5.403548	-1.37304
C	-3.09566	3.666942	2.053139
C	-3.27216	5.044145	1.945284
H	-3.26931	6.742868	0.610873
H	-3.22605	3.177209	3.02081

H	-3.54337	5.627032	2.827304
C	-2.61445	1.425779	1.17294
C	-3.68143	0.545847	0.963325
C	-1.42669	0.924755	1.75437
C	-3.53537	-0.82207	1.31794
C	-4.92431	0.920904	0.375025
C	-1.35868	-0.44723	2.096747
C	-0.27709	1.708516	2.038289
C	-4.55691	-1.72629	1.13615
C	-5.95871	0.052358	0.151939
H	-5.03417	1.958466	0.056341
C	-0.24588	-0.98357	2.713197
C	0.853186	1.212275	2.645518
H	-0.29184	2.758687	1.740215
C	-5.79307	-1.32888	0.574754
H	-4.40116	-2.75813	1.454213
H	-0.26169	-2.04015	2.984177
C	0.861785	-0.178	3.032351
O	-2.39286	-1.2723	1.861891
N	-6.73522	-2.28394	0.448325
H	-6.44605	-3.19577	0.783831
N	1.915767	-0.78274	3.656104
H	1.75841	-1.77385	3.798558
C	-8.17192	-2.19625	0.184649
C	-8.8153	-3.55418	0.408626
H	-8.3531	-1.86927	-0.84811
H	-8.62791	-1.45445	0.857246
H	-8.68652	-3.89267	1.447971
H	-9.8932	-3.49487	0.209426
H	-8.39252	-4.31293	-0.26731
C	2.779236	-0.20937	4.690575
C	2.020428	0.30416	5.907148
H	3.416648	0.575041	4.265171
H	3.463074	-1.01705	4.98915
H	2.722621	0.698394	6.655274
H	1.324409	1.112367	5.635514
H	1.437152	-0.50014	6.379007
C	-7.1828	0.556547	-0.56977
H	-7.031	1.600317	-0.87149
H	-7.37845	-0.02195	-1.48343
H	-8.08756	0.525099	0.050969
C	2.04497	2.115272	2.825763
H	1.891008	3.055209	2.280859
H	2.22285	2.372664	3.880275
H	2.960651	1.650883	2.430142
C	6.283646	2.254746	0.551504

H	6.24816	3.069812	1.289203
H	6.794521	1.405838	1.023306
H	6.911119	2.585681	-0.28811
C	-0.83962	-4.68755	-0.38078
H	-0.09484	-5.35792	0.064754
H	-1.75731	-4.74942	0.227345
H	-1.06673	-5.08481	-1.3842

Table S14: Coordinates of **D^{2+}-II** ($R575^{+}$ homodimer)

Element	X	Y	Z
C	-4.96255	2.685342	-0.78336
C	-4.82797	1.322681	-0.66366
C	-3.61473	0.669342	-0.31112
C	-2.49649	1.506087	-0.07461
C	-2.58792	2.878741	-0.17376
C	-3.80665	3.511786	-0.503
C	-3.46563	-0.72933	-0.16842
C	-1.15288	-0.33065	0.496868
C	-2.22164	-1.23693	0.240131
C	-1.93746	-2.62371	0.440929
H	-2.72309	-3.35068	0.235378
C	-0.73447	-3.07356	0.90071
C	0.305677	-2.11011	1.196132
C	0.074056	-0.74191	0.964872
H	-5.70008	0.699476	-0.87027
H	-1.70073	3.470386	0.056902
H	0.837354	0.009555	1.158746
O	-1.30829	0.986288	0.27369
N	-3.79902	4.866282	-0.56742
H	-2.88964	5.266825	-0.37357
N	1.486853	-2.54456	1.665275
H	1.563187	-3.52891	1.883141
C	-4.89076	5.816451	-0.3626
H	-4.47622	6.805689	-0.60155
H	-5.68645	5.649263	-1.09606
C	-5.44106	5.808945	1.058104
H	-4.65663	6.054043	1.789367
H	-6.2436	6.55337	1.158753
H	-5.85491	4.824469	1.324578
C	2.584591	-1.68934	2.090504
H	2.729409	-0.89319	1.347286
H	3.495111	-2.30537	2.074867
C	2.37867	-1.06723	3.466153
H	3.243562	-0.43867	3.720562
H	1.480834	-0.43175	3.482477
H	2.271587	-1.83858	4.242676

C	-4.59963	-1.64668	-0.46599
C	-5.15974	-2.4686	0.527927
C	-5.07476	-1.74306	-1.78122
C	-6.14031	-3.40196	0.186416
C	-6.0709	-2.65884	-2.10813
H	-4.64598	-1.10427	-2.55743
C	-6.60007	-3.49422	-1.12436
H	-6.54522	-4.05258	0.964009
H	-6.43203	-2.72379	-3.13626
H	-7.3766	-4.21772	-1.37893
C	-4.67463	-2.40745	1.953824
O	-4.23178	-3.38505	2.518912
N	-4.75529	-1.17292	2.525884
H	-5.17657	-0.41339	2.006219
C	-4.13835	-0.87647	3.800391
H	-3.84001	-1.83828	4.244335
H	-4.86387	-0.41018	4.485498
C	-2.96623	-0.00648	3.652531
C	-2.00504	0.723126	3.519941
C	-0.8926	1.524975	3.371538
C	0.10112	2.204348	3.220526
C	1.327718	2.992682	3.066938
H	1.272691	3.894221	3.694756
H	2.178118	2.394933	3.428537
N	1.60571	3.399262	1.701188
C	2.222378	2.557541	0.837527
H	1.273354	4.301077	1.392767
O	2.514337	1.416812	1.167915
C	2.55204	3.076472	-0.53443
C	2.467465	4.436107	-0.86182
C	3.001865	2.171186	-1.51518
C	2.788951	4.89591	-2.1345
H	2.176225	5.172099	-0.1098
C	3.318909	2.640915	-2.79407
C	3.209817	3.992904	-3.10721
H	2.722651	5.961069	-2.36201
H	3.664617	1.933094	-3.55074
H	3.467168	4.341153	-4.1091
C	3.194522	0.708666	-1.28288
C	4.427812	0.216032	-0.83188
C	2.193226	-0.21071	-1.65879
C	4.613429	-1.18561	-0.71753
C	5.518085	1.035141	-0.42415
C	2.455522	-1.59751	-1.53913
C	0.930802	0.150088	-2.20148
C	5.797365	-1.7212	-0.26396

C	6.712869	0.549733	0.040758
H	5.380353	2.117093	-0.47251
C	1.519699	-2.54194	-1.90159
C	-0.02517	-0.75655	-2.59016
H	0.724754	1.213862	-2.33624
C	6.884754	-0.89149	0.103072
H	5.895666	-2.80718	-0.22363
H	1.770785	-3.59588	-1.77361
C	0.259103	-2.16531	-2.41225
O	3.631565	-2.04054	-1.05995
N	8.010663	-1.51439	0.501219
H	7.946052	-2.52584	0.503514
N	-0.59088	-3.1682	-2.72887
H	-0.19316	-4.09582	-2.64452
C	9.366221	-1.01916	0.734462
C	10.30253	-2.19119	0.975677
H	9.385581	-0.34847	1.604337
H	9.709351	-0.44635	-0.13992
H	10.33548	-2.8634	0.104807
H	11.32231	-1.8255	1.152899
H	9.997053	-2.77062	1.860113
C	-2.02683	-3.15924	-2.96817
C	-2.61501	-4.52879	-2.67487
H	-2.25399	-2.87272	-4.00747
H	-2.49562	-2.42026	-2.30872
H	-3.70402	-4.50778	-2.81731
H	-2.20427	-5.29744	-3.34731
H	-2.4154	-4.83151	-1.63586
C	7.759862	1.531944	0.503166
H	7.36737	2.554019	0.430533
H	8.038476	1.363261	1.552502
H	8.675568	1.492181	-0.10086
C	-1.28362	-0.23875	-3.24188
H	-1.18236	0.83483	-3.44643
H	-1.47964	-0.73748	-4.20065
H	-2.17276	-0.36598	-2.60897
C	-6.27817	3.236325	-1.27015
H	-6.1432	3.845349	-2.17597
H	-6.95578	2.412773	-1.52836
H	-6.78892	3.853624	-0.51787
C	-0.48149	-4.53776	1.11596
H	-1.36777	-5.13103	0.858989
H	0.36199	-4.89983	0.503956
H	-0.2491	-4.75626	2.171418

Table S15: Coordinates of **d^{2+}-I** (RB^{+} homodimer)

Element	X	Y	Z
C	0.9589	-2.78137	-2.44779
C	-0.2823	-2.80297	-1.88031
C	-0.89059	-1.62608	-1.34994
C	-0.11086	-0.43937	-1.4371
C	1.141158	-0.38944	-2.01138
C	1.705079	-1.5551	-2.57743
C	-2.18915	-1.55907	-0.80401
C	-1.82259	0.823681	-0.45052
C	-2.67431	-0.30934	-0.36591
C	-3.96059	-0.06965	0.203603
H	-4.67091	-0.89149	0.286803
C	-4.34757	1.16918	0.625918
C	-3.46751	2.304722	0.535193
C	-2.18851	2.080104	-0.01772
H	1.361124	-3.71125	-2.8442
H	-0.83286	-3.74419	-1.84751
H	1.64651	0.574333	-1.9998
H	-5.35142	1.283366	1.028559
H	-1.45965	2.872408	-0.15029
O	-0.58264	0.715557	-0.94326
N	2.87704	-1.51399	-3.24612
N	-3.83675	3.525728	0.979048
C	3.567783	-2.73512	-3.65719
H	2.864233	-3.40527	-4.17383
H	4.307072	-2.44674	-4.41565
C	4.261561	-3.45753	-2.50778
H	3.546424	-3.756	-1.7265
H	4.764478	-4.36348	-2.87464
H	5.018005	-2.80772	-2.04554
C	-2.90786	4.650177	0.908834
H	-1.91736	4.314476	1.257395
H	-3.24217	5.393908	1.644646
C	-2.80177	5.30241	-0.46802
H	-2.50526	4.58062	-1.24494
H	-3.75978	5.74211	-0.77734
H	-2.06458	6.120241	-0.43856
C	-3.00955	-2.79135	-0.65835
C	-4.25902	-2.94334	-1.28566
C	-2.53769	-3.81347	0.174702
C	-5.03254	-4.07677	-1.02723
C	-3.29813	-4.95654	0.398346
H	-1.56648	-3.69025	0.656554
C	-4.5534	-5.08494	-0.19523
H	-6.01301	-4.16635	-1.49898
H	-2.91321	-5.74879	1.043563

H	-5.15846	-5.97537	-0.01549
C	-4.81204	-1.8859	-2.2067
O	-5.86944	-1.33506	-1.98288
N	-4.02118	-1.60216	-3.27804
H	-3.16697	-2.12755	-3.41581
C	-4.27597	-0.46616	-4.13912
H	-5.27191	-0.07916	-3.87623
H	-4.31203	-0.77495	-5.19574
C	-3.25703	0.570861	-3.95597
C	-2.37115	1.379928	-3.77265
C	-1.35952	2.280588	-3.51935
C	-0.44926	3.031325	-3.23822
C	0.628672	3.9209	-2.80076
H	1.603189	3.495646	-3.08038
H	0.541815	4.897588	-3.30045
N	0.627464	4.118908	-1.36343
C	1.360235	3.331667	-0.53094
H	-0.06705	4.745947	-0.97887
O	2.086505	2.445462	-0.94742
C	1.231474	3.657918	0.935476
C	1.003464	4.986269	1.324065
C	1.358455	2.670581	1.935075
C	0.880296	5.344709	2.662483
H	0.95988	5.770474	0.565464
C	1.219567	3.044299	3.279111
C	0.982418	4.365521	3.645806
H	0.72026	6.389275	2.935069
H	1.314497	2.27936	4.052937
H	0.892531	4.62849	4.701257
C	1.658861	1.224689	1.70174
C	0.684137	0.247896	2.007478
C	2.952825	0.800905	1.367767
C	1.037668	-1.12638	1.9371
C	-0.63439	0.525598	2.472536
C	3.227252	-0.59197	1.267794
C	4.061272	1.67523	1.161256
C	0.194225	-2.14319	2.345725
C	-1.48465	-0.46192	2.878318
H	-0.97026	1.56181	2.511015
C	4.477521	-1.09218	0.968789
C	5.306559	1.203876	0.880985
H	3.898513	2.750824	1.229485
C	-1.07883	-1.84365	2.888154
H	0.587822	-3.15614	2.308077
H	-2.48247	-0.18287	3.209481
H	4.591037	-2.17297	0.944125

C	5.568012	-0.20999	0.765541
H	6.109246	1.920681	0.724701
O	2.25627	-1.4943	1.503837
N	-1.87376	-2.80119	3.40946
N	6.800581	-0.66386	0.473721
C	-3.14749	-2.49064	4.060132
C	-4.32425	-2.45746	3.095736
H	-3.05771	-1.54344	4.61029
H	-3.31064	-3.2583	4.829851
H	-4.18565	-1.67814	2.333757
H	-4.43815	-3.41893	2.574398
H	-5.25686	-2.24855	3.638598
C	7.955761	0.226082	0.339832
C	8.118235	0.786167	-1.06702
H	8.843808	-0.35775	0.620676
H	7.88964	1.030339	1.085164
H	8.226357	-0.02403	-1.8034
H	7.251161	1.397016	-1.35837
H	9.016954	1.416047	-1.12449
C	-5.20934	3.801622	1.412124
H	-5.53591	3.010253	2.10315
H	-5.17614	4.720086	2.013192
C	-6.2012	3.963077	0.265725
H	-7.20733	4.153694	0.664984
H	-5.92928	4.809105	-0.38061
H	-6.25009	3.059839	-0.35998
C	-1.44958	-4.19648	3.492202
H	-2.36192	-4.81052	3.496435
H	-0.91148	-4.476	2.575354
C	-0.60315	-4.49377	4.724057
H	-1.15564	-4.2644	5.646753
H	-0.32979	-5.55792	4.750607
H	0.32268	-3.90021	4.725822
C	7.07771	-2.08907	0.30739
H	6.228137	-2.5658	-0.20131
H	7.925526	-2.1746	-0.38779
C	7.397594	-2.79677	1.618295
H	6.55502	-2.73845	2.322687
H	7.619946	-3.85706	1.433368
H	8.276189	-2.34778	2.103803
C	3.534402	-0.23863	-3.52967
H	4.116757	-0.3767	-4.45128
H	2.760761	0.505368	-3.76993
C	4.431436	0.27602	-2.41237
H	4.894722	1.22596	-2.71534

Table S16: Coordinates of **d^{2+}-II** (RB^{+} homodimer)

Element	X	Y	Z
C	-0.60802	-0.71685	-0.80474
C	-1.83693	-1.15204	-0.40051
C	-2.94932	-0.27358	-0.26408
C	-2.69538	1.08901	-0.55936
C	-1.44244	1.564776	-0.90448
C	-0.35312	0.676753	-1.05695
C	-4.25792	-0.65666	0.112459
C	-4.95498	1.656955	-0.23696
C	-5.27536	0.309778	0.095178
C	-6.65671	0.038239	0.339144
H	-6.95994	-0.98413	0.566918
C	-7.60577	1.012228	0.271665
C	-7.26375	2.377627	-0.04603
C	-5.89683	2.661919	-0.29549
H	0.18723	-1.4494	-0.92433
H	-1.96706	-2.21273	-0.19023
H	-1.36083	2.628767	-1.11054
H	-8.6411	0.741552	0.466347
H	-5.5518	3.654844	-0.57272
O	-3.68253	2.0018	-0.50322
N	0.878629	1.115794	-1.40158
N	-8.20749	3.333166	-0.10525
C	1.136814	2.539479	-1.59045
H	0.637187	3.095277	-0.78178
H	2.214059	2.690355	-1.43411
C	0.734826	3.094754	-2.95419
H	-0.32537	2.907248	-3.17697
H	0.900313	4.181641	-2.98004
H	1.331292	2.645844	-3.75969
C	-9.63345	3.042738	0.056975
H	-9.86891	2.081818	-0.42066
H	-10.1806	3.797992	-0.52519
C	-10.0899	3.066789	1.509903
H	-9.89172	4.04606	1.969761
H	-11.1707	2.877406	1.570994
C	-4.5602	-2.01822	0.637631
C	-4.47986	-3.18618	-0.13983
C	-4.93363	-2.12213	1.984054
C	-4.79583	-4.42067	0.435021
C	-5.23113	-3.35864	2.552086
H	-4.99971	-1.21609	2.591236
C	-5.17077	-4.51144	1.773211
H	-4.78204	-5.32376	-0.17967
H	-5.52624	-3.41751	3.601343

H	-5.42826	-5.48124	2.202448
C	-4.06974	-3.06225	-1.58214
O	-4.39107	-2.10471	-2.25639
N	-3.26979	-4.06743	-2.03379
H	-2.95627	-4.77687	-1.38385
C	-2.60425	-3.99186	-3.31826
H	-2.99838	-3.1023	-3.83207
H	-2.85097	-4.86773	-3.93983
C	-1.14961	-3.89518	-3.16649
C	0.056081	-3.86353	-3.02792
C	1.432187	-3.82609	-2.9327
C	2.644575	-3.78332	-2.90476
C	4.106771	-3.71784	-3.00906
H	4.466214	-4.59819	-3.56289
H	4.37371	-2.83139	-3.60509
N	4.81761	-3.64317	-1.75043
C	5.040875	-2.45494	-1.13325
H	5.087352	-4.50498	-1.29551
O	4.574873	-1.40586	-1.54676
C	5.922244	-2.49605	0.083336
C	6.938856	-3.4476	0.221359
C	5.771708	-1.50779	1.0715
C	7.781531	-3.44028	1.329538
H	7.104358	-4.18699	-0.5651
C	6.618724	-1.50845	2.183664
C	7.617017	-2.47138	2.315614
H	8.574428	-4.18508	1.41546
H	6.491783	-0.74525	2.954742
H	8.27203	-2.4572	3.188547
C	4.718346	-0.45526	1.015327
C	5.04018	0.858927	0.64918
C	3.407931	-0.73842	1.448267
C	4.043704	1.867793	0.733885
C	6.313773	1.266592	0.156767
C	2.458353	0.31372	1.517092
C	2.952773	-2.02678	1.841894
C	4.281557	3.183631	0.390644
C	6.566964	2.55715	-0.19889
H	7.099285	0.516037	0.057028
C	1.160602	0.123202	1.950354
C	1.672217	-2.23903	2.264346
H	3.650681	-2.86483	1.803504
C	5.554407	3.57915	-0.09536
H	3.466711	3.890043	0.52582
H	7.559109	2.807713	-0.56643
H	0.513431	0.995773	1.988155

C	0.723471	-1.16121	2.350264
H	1.378743	-3.24918	2.54078
O	2.804094	1.567411	1.167742
N	5.80862	4.850834	-0.46294
N	-0.5332	-1.3788	2.797122
C	7.141288	5.272336	-0.90526
C	8.128255	5.518563	0.230358
H	7.006064	6.192212	-1.48941
H	7.535918	4.530751	-1.61481
H	7.785286	6.327376	0.89002
H	8.273931	4.61846	0.845442
H	9.104815	5.810933	-0.18077
C	-0.9496	-2.67006	3.340455
C	-1.45132	-3.65028	2.287231
H	-1.74695	-2.471	4.071166
H	-0.12509	-3.10535	3.922872
H	-0.68775	-3.84251	1.518276
H	-1.7148	-4.60868	2.756912
H	-2.35251	-3.26351	1.79156
C	-7.87081	4.734542	-0.35159
H	-6.93333	4.978543	0.168042
H	-8.64528	5.342351	0.138075
C	-7.78903	5.08109	-1.83325
H	-7.00899	4.496231	-2.34217
H	-8.74516	4.879895	-2.33799
H	-7.55828	6.148064	-1.96079
C	1.948185	0.19199	-1.78316
H	1.994005	-0.64393	-1.07139
H	2.901726	0.723746	-1.66046
C	1.829459	-0.33563	-3.20598
H	2.680253	-0.99753	-3.40859
H	0.902045	-0.91065	-3.34689
H	1.842886	0.48086	-3.94066
C	4.791189	5.892267	-0.32351
H	3.827827	5.497253	-0.68071
H	5.05622	6.69736	-1.02173
C	4.657622	6.453605	1.088508
H	5.586605	6.943166	1.410936
H	3.854945	7.204117	1.118959
H	4.419036	5.667097	1.819252
C	-1.51781	-0.30504	2.863983
H	-1.39217	0.354053	1.994058
H	-2.50711	-0.76905	2.737088
C	-1.46229	0.487823	4.163922
H	-0.48403	0.973113	4.294332
H	-2.23525	1.269622	4.167501

H	-1.6343	-0.16234	5.034304
H	-9.57288	2.301282	2.107175

Table S17: Coordinates of **F^{2+}-I** (heterodimer)

Element	X	Y	Z
C	-0.81207	-2.02964	1.133976
C	-1.91355	-1.98024	0.331281
C	-2.98034	-1.06857	0.57366
C	-2.81905	-0.20258	1.690397
C	-1.7232	-0.25272	2.52679
C	-0.68404	-1.18181	2.288981
C	-4.16624	-0.99289	-0.18237
C	-4.90158	0.818733	1.282724
C	-5.1357	-0.03511	0.165528
C	-6.35918	0.181114	-0.5406
H	-6.57899	-0.43266	-1.41574
C	-7.25596	1.131639	-0.15509
C	-7.02414	1.965651	1.001044
C	-5.79689	1.784284	1.690554
H	-1.9727	-2.6599	-0.51889
H	-1.70711	0.437963	3.365653
H	-5.52059	2.385024	2.553173
O	-3.76644	0.703918	1.994143
N	0.384251	-1.27351	3.112722
N	-7.93881	2.864517	1.405917
C	1.457621	-2.2326	2.863837
H	1.689393	-2.23411	1.787844
H	2.354708	-1.8449	3.368064
C	1.171837	-3.64841	3.352915
H	0.26344	-4.06038	2.889213
H	2.014632	-4.3094	3.105224
H	1.035698	-3.67517	4.442729
C	-9.18798	3.080819	0.668636
H	-9.90332	3.518088	1.377364
H	-9.61336	2.106551	0.38821
C	-9.04464	3.985935	-0.54958
H	-8.70947	4.992117	-0.26287
H	-8.3232	3.581659	-1.27502
H	-10.0152	4.086368	-1.05555
C	-4.4242	-1.92607	-1.31531
C	-3.70206	-1.87383	-2.52054
C	-5.41489	-2.90394	-1.15691
C	-3.98517	-2.78695	-3.54032
C	-5.6935	-3.80468	-2.18118
H	-5.96544	-2.96068	-0.21527

C	-4.98421	-3.74073	-3.37972
H	-3.40863	-2.73912	-4.46602
H	-6.46888	-4.55993	-2.0407
H	-5.20511	-4.44073	-4.1873
C	-2.57151	-0.91419	-2.74591
O	-1.48611	-1.30619	-3.15508
N	-2.81304	0.388914	-2.48136
H	-3.73408	0.673992	-2.17387
C	-1.7566	1.379667	-2.54439
H	-2.21555	2.37212	-2.65992
H	-1.15263	1.193449	-3.44618
C	-0.86949	1.372749	-1.37586
C	-0.08629	1.372175	-0.44892
C	0.849736	1.37707	0.563832
C	1.705832	1.405262	1.424736
C	2.742705	1.417587	2.456266
H	3.280376	2.379447	2.452507
H	2.275436	1.333337	3.451442
N	3.72448	0.377503	2.235782
C	5.065394	0.64301	2.287908
H	3.408163	-0.50092	1.846522
O	5.51165	1.680274	2.728239
C	5.95317	-0.44343	1.741013
C	7.031125	-0.87807	2.514768
C	5.76814	-0.96475	0.446827
C	7.899557	-1.8519	2.029688
H	7.182498	-0.44061	3.503486
C	6.651198	-1.93779	-0.0355
C	7.708092	-2.38268	0.754659
H	8.734771	-2.19133	2.644819
H	6.520613	-2.32902	-1.04699
H	8.394237	-3.13714	0.365563
C	4.689267	-0.44852	-0.43849
C	3.593315	-1.26715	-0.79194
C	4.724871	0.871323	-0.9125
C	2.557737	-0.72409	-1.59454
C	3.412257	-2.60663	-0.35213
C	3.652732	1.34664	-1.71815
C	5.765714	1.804673	-0.62797
C	1.448629	-1.46026	-1.94315
C	2.320909	-3.37945	-0.67457
H	4.182478	-3.0377	0.291039
C	3.634213	2.633597	-2.20225
C	5.779781	3.099907	-1.0737
H	6.590556	1.470693	0.002494
C	1.29897	-2.7997	-1.52158

H	0.674282	-1.00067	-2.55729
H	2.794753	2.940264	-2.82781
C	4.6866	3.539391	-1.92223
O	2.625496	0.543745	-2.04007
N	0.163045	-3.42751	-1.90864
H	-0.44435	-2.84383	-2.48799
N	4.585703	4.766846	-2.46663
H	3.744269	4.911032	-3.01246
C	-0.15079	-4.85014	-1.95872
C	-1.5102	-5.05291	-2.60467
H	-0.1688	-5.28301	-0.9497
H	0.617829	-5.39188	-2.53498
H	-1.74142	-6.12449	-2.66891
H	-2.308	-4.57002	-2.01933
H	-1.53366	-4.63902	-3.62374
C	5.548919	5.860244	-2.57855
C	4.998342	6.932443	-3.50354
H	6.499113	5.478962	-2.97978
H	5.753151	6.295555	-1.59057
H	5.717148	7.757664	-3.59011
H	4.82049	6.536131	-4.51482
H	4.056773	7.349691	-3.11487
C	6.895942	4.003151	-0.61237
H	7.524917	3.470092	0.111101
H	7.544501	4.334691	-1.43387
H	6.506651	4.89504	-0.10295
C	2.225126	-4.76301	-0.08088
H	1.323582	-4.88107	0.539306
H	2.208629	-5.5528	-0.8433
H	3.092298	-4.95405	0.564583
C	-7.68378	3.734343	2.556602
C	-6.81668	4.948466	2.240995
H	-7.23984	3.133179	3.363868
H	-8.66109	4.0608	2.935424
H	-6.64856	5.533632	3.156114
H	-5.83576	4.655672	1.838701
H	-7.3025	5.605529	1.506775
C	0.418692	-0.54131	4.378806
C	-0.46727	-1.12932	5.472486
H	0.154808	0.511134	4.189649
H	1.464649	-0.53304	4.715783
H	-1.52145	-1.17244	5.163632
H	-0.15006	-2.14684	5.738014
H	-0.40368	-0.50901	6.377622
H	-8.16381	1.251882	-0.7415
H	-0.03525	-2.75015	0.891311

Table S18: Coordinates of **F^{2+}-II** (heterodimer)

Element	X	Y	Z
C	-0.6247	-1.74929	1.195849
C	-1.7376	-1.78951	0.409729
C	-2.82704	-0.89511	0.605843
C	-2.66709	0.069175	1.63911
C	-1.55397	0.117242	2.453786
C	-0.5004	-0.81007	2.277905
C	-4.03809	-0.93675	-0.10974
C	-4.79645	0.976942	1.204074
C	-5.03464	0.010223	0.18339
C	-6.29106	0.106067	-0.49026
H	-6.51678	-0.60402	-1.28805
C	-7.2106	1.058108	-0.16719
C	-6.96975	2.014951	0.887914
C	-5.7144	1.945976	1.547293
H	-1.79071	-2.52875	-0.3883
H	-1.54532	0.868394	3.239221
H	-5.43472	2.637763	2.337582
O	-3.63704	0.968923	1.886042
N	0.585175	-0.82209	3.084704
N	-7.90224	2.920198	1.232459
C	1.578955	-1.89318	3.001459
H	1.886373	-2.01794	1.951216
H	2.470354	-1.54065	3.538065
C	1.128093	-3.23193	3.576565
H	0.236274	-3.61784	3.062035
H	1.932199	-3.97384	3.467585
H	0.891391	-3.14876	4.645701
C	-9.18529	3.013962	0.527994
H	-9.89133	3.495567	1.217037
H	-9.58102	2.001204	0.365584
C	-9.12264	3.793297	-0.78058
H	-8.81873	4.835369	-0.61126
H	-8.41183	3.343144	-1.48934
H	-10.114	3.805268	-1.25505
C	-4.29342	-1.99814	-1.12638
C	-3.65054	-2.03103	-2.37643
C	-5.18595	-3.02484	-0.79255
C	-3.90444	-3.0849	-3.26055
C	-5.44442	-4.06059	-1.68633
H	-5.67427	-3.0127	0.184393
C	-4.80658	-4.08908	-2.92583
H	-3.38756	-3.10124	-4.22212

H	-6.14497	-4.85068	-1.41006
H	-5.00931	-4.89766	-3.63018
C	-2.63336	-1.01232	-2.79674
O	-1.56911	-1.3576	-3.29554
N	-2.9458	0.287958	-2.60587
H	-3.84694	0.536188	-2.21803
C	-1.96314	1.33323	-2.81724
H	-2.48995	2.284594	-2.97906
H	-1.40367	1.108744	-3.73804
C	-1.01818	1.466859	-1.70285
C	-0.21119	1.571418	-0.80272
C	0.738323	1.703042	0.188453
C	1.598714	1.84155	1.033574
C	2.649875	1.975131	2.03873
H	3.319361	2.814236	1.785975
H	2.206203	2.227554	3.016274
N	3.449008	0.766993	2.105233
C	4.80082	0.838309	2.29091
H	3.043478	-0.08183	1.733538
O	5.347845	1.844102	2.689893
C	5.579518	-0.40327	1.941544
C	6.541701	-0.84881	2.85061
C	5.442224	-1.0517	0.697585
C	7.341574	-1.94821	2.553346
H	6.660967	-0.31393	3.794812
C	6.26282	-2.14789	0.403157
C	7.203208	-2.59626	1.326807
H	8.085306	-2.29168	3.274495
H	6.178363	-2.63531	-0.57073
H	7.841069	-3.44687	1.079849
C	4.481373	-0.56185	-0.32803
C	3.384212	-1.35735	-0.72373
C	4.625939	0.715723	-0.89797
C	2.44135	-0.82685	-1.64498
C	3.111926	-2.66688	-0.23709
C	3.63805	1.183864	-1.80648
C	5.689909	1.616506	-0.60247
C	1.341094	-1.54423	-2.05135
C	2.035914	-3.42793	-0.62727
H	3.798005	-3.08579	0.501619
C	3.717654	2.434866	-2.37357
C	5.794727	2.880934	-1.12321
H	6.453994	1.290691	0.103933
C	1.109782	-2.86212	-1.59103
H	0.640821	-1.08794	-2.75075
H	2.941612	2.732583	-3.08019

C	4.791222	3.30852	-2.07945
O	2.594212	0.410395	-2.14878
N	-0.00574	-3.46519	-2.05577
H	-0.58494	-2.85465	-2.63847
N	4.784162	4.509794	-2.69838
H	3.992466	4.63608	-3.31766
C	-0.41881	-4.86096	-2.06412
C	-1.55476	-5.17526	-1.09806
H	0.443011	-5.51005	-1.88294
H	-0.74548	-5.08701	-3.09125
H	-1.27002	-4.97808	-0.05354
H	-2.44707	-4.57353	-1.32756
H	-1.8393	-6.23426	-1.17775
C	5.884473	5.42806	-2.98428
C	6.876953	4.879532	-4.00188
H	6.388256	5.719237	-2.05708
H	5.417809	6.345787	-3.36835
H	7.669967	5.616514	-4.19253
H	7.351297	3.953771	-3.64261
H	6.382413	4.656934	-4.95884
C	6.894711	3.773175	-0.60856
H	6.485037	4.705707	-0.19408
H	7.428391	3.267998	0.205856
H	7.633461	4.034803	-1.37914
C	1.853105	-4.77897	0.018683
H	2.522076	-4.87303	0.884145
H	0.826139	-4.93374	0.378258
H	2.09651	-5.60754	-0.6624
C	-7.63755	3.917883	2.272166
C	-6.81992	5.11356	1.795325
H	-7.14946	3.421815	3.124192
H	-8.61197	4.256774	2.647311
H	-5.84312	4.806247	1.393927
H	-7.34931	5.671101	1.010697
H	-6.64217	5.800961	2.634351
C	0.696452	0.102373	4.212348
C	-0.04606	-0.34048	5.468183
H	0.346997	1.092754	3.88652
H	1.768648	0.219139	4.425945
H	-1.1152	-0.5031	5.268289
H	0.370917	-1.27286	5.872876
H	0.042821	0.430259	6.246743
H	-8.14375	1.084808	-0.72492
H	0.175883	-2.4553	0.992133