Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A new strategy to generate Super and Hyper Acids with simple organic molecules exploiting σ-hole interaction.

Supporting Information

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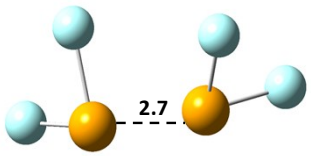


G

Figure S1. The interaction between the two adjacent SeF_2 (G) of cpA of system **3**.

The associative interaction energy can be obtained by single-point calculation (vibrationless) performed at M06-2X/6-311+G(2d,p) level of theory of system 3 (Figure S1 G) and their respective components at infinite separation.

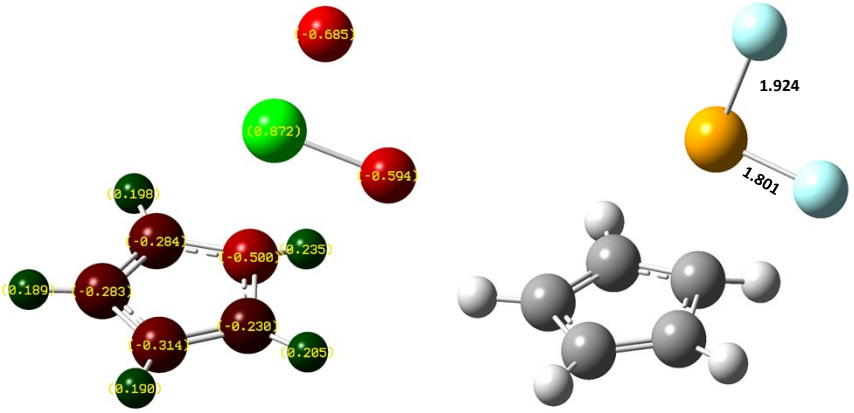
The interaction energy between two adjacent molecules was calculated through the simple equation:

$$\Delta E_{interaction} = 2 * E_{SeF2} - E_{ad} \qquad (5)$$

Where $\Delta E_{interaction}$ is the associative interaction energy among SeF_2 molecules, E_{SeF2} is the energy of individual SeF_2 molecule and E_{ad} is the energy of the interacted unperturbed SeF_2 molecules.

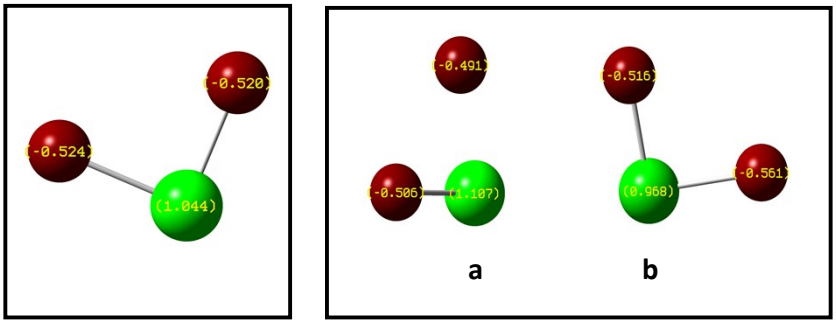
Table S1. Associative interaction energy for two adjacent SeF_2 molecules at M06-2X/6-311+G(2d,p) level of theory.

E_{SeF2} (Hartree)	Number of SeF_2	N* E_{SeF2} (Hartree)	E_{ad} (Hartree)	$\Delta E_{interaction}$ (kcal/mol)
-2601.18737	2	-5202.37474	-5202.34871	16.33



A B

Figure S2: (A) NBO analysis between single SeF_2 molecule and cpA anion (1) showing the charge donation from anion to σ- hole of SeF_2 molecule; (B) elongation of Se-F bond when SeF_2 interacts with negative charge of cpA.



(i) (ii)

Figure S3: NBO analysis for single SeF_2 (i) and two adjacent interacting SeF_2 (ii) of system 3.

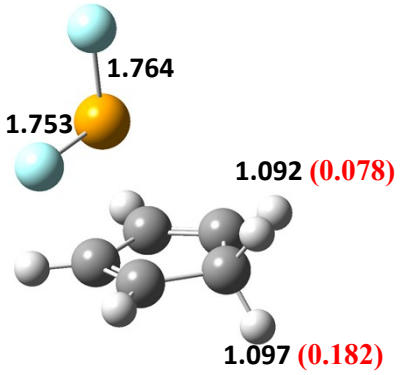
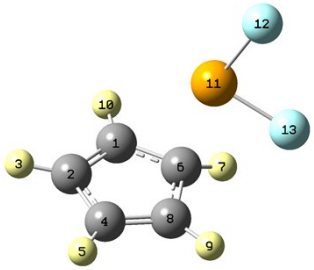


Figure S4. The polarization of –C-H bonds of cyclopentadiene in the presence of single SeF_2 (1) molecule. The mulliken charges on the hydrogens of –C-H bonds are shown in red colour.



Donar	Acceptor	E_2 (kcal/mol)
Lone pair od Se(11)	BD*C 1 - C 2	0.12
Lone pair od Se(11)	BD*C 4 - C 8	0.21
Lone pair od Se(11)	BD*C 1 - C 2	0.06
Lone pair od Se(11)	BD*C 1 - C 2	0.36
Lone pair od Se(11)	BD*C 4 - C 8	0.93
Lone pair od Se(11)	BD* C 6 - H 7	0.59
Lone pair od Se(11)	BD* C 6 - C 8	0.80
Lone pair od Se(11)	BD* C 8 - H 9	0.09

Table S2: Second order perturbation NBO analysis between the lone pair of Se atom and the π^* of cpA.

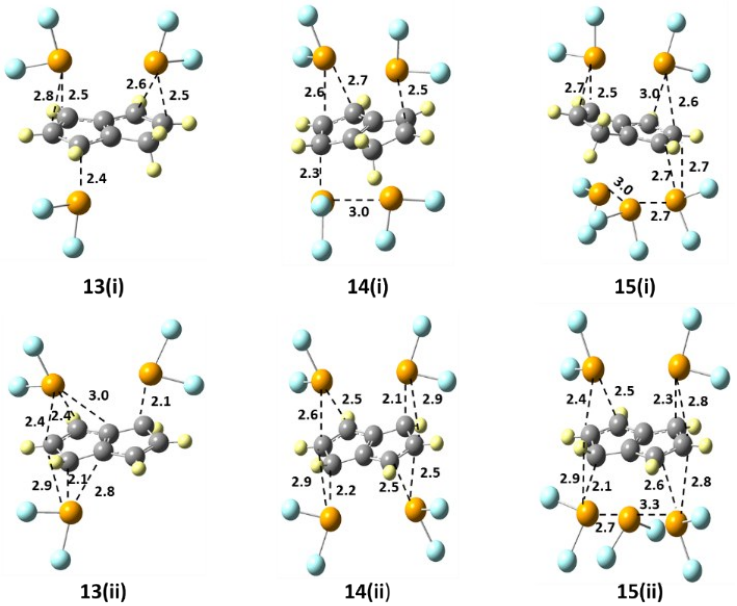


Figure S5. pentalene mono (13i-15i) and dianion (13ii-15ii) systems with an increasing number of SeF_2 molecules. Distances are given in Å

AIM calculations.

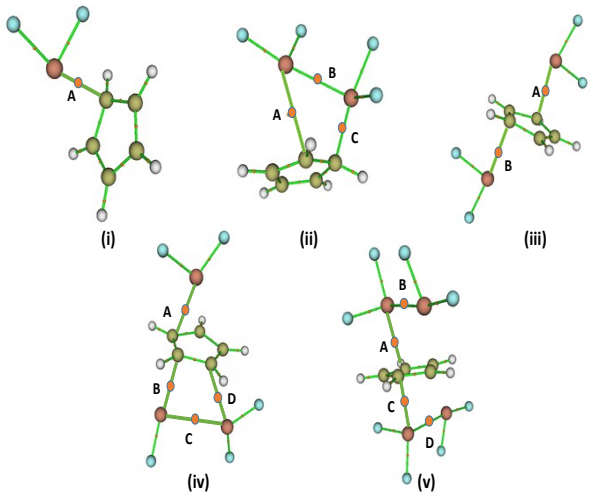


Figure S6. AIM picture showing (3,-1) critical points of cyclopentadienyl ion and SeF_2

Table S3. AIM values for (3,-1) critical points of cyclopentadienyl ion and SeF_2

Structure Number	CP	Potential energy density V(r)	kinetic energy G(r)	Total Energy density H(r)	Laplacian electron density ($\nabla^2 r$)	|V(r)| / G(r)	energy density E(r)
i	A	-0.05661	0.03131	-0.02530	0.02402	1.80816	-0.02530
ii	A	-0.00692	0.00813	0.00121	0.03737	0.85118	0.00121
	B	-0.03400	0.02253	-0.01147	0.04425	1.50908	0.00121
	C	-0.07537	0.03595	-0.03942	-0.01386	2.09636	-0.03942
iii	A	-0.04131	0.02586	-0.01544	0.04168	1.59711	-0.01544
	B	-0.02770	0.02165	-0.00604	0.06243	1.27914	-0.00604
iv	A	-0.01847	0.01837	-9.868E-05	0.07307	1.00537	-0.00010
	B	-0.02086	0.01973	-0.00113	0.07441	1.05716	-0.00113
	C	-0.01808	0.01680	-0.00128	0.06206	1.07645	-0.00128
	D	-0.02102	0.01867	-0.00235	0.06530	1.12564	-0.00235
v	A	-0.03341	0.02322	-0.01019	0.05210	1.43901	-0.01019
	B	-0.03035	0.02128	-0.00907	0.04881	1.42647	-0.00907
	C	-0.03341	0.02322	-0.01019	0.05210	1.43902	-0.01019
	D	-0.03037	0.02128	-0.00908	0.04880	1.42675	-0.00908

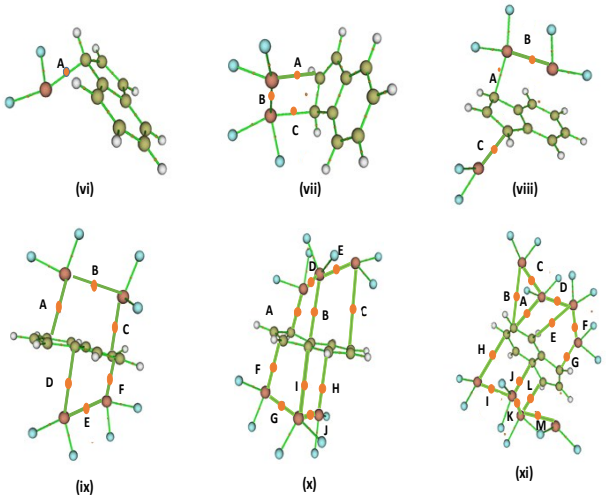


Figure S7. AIM picture showing (3,-1) critical points of iso-indene ion and SeF_2

Table S4. AIM values for (3,-1) critical points of iso-indene ion and SeF_2

Structure Number	CP	Potential energy density V(r)	kinetic energy G(r)	Total Energy density H(r)	Laplacian electron density ($\nabla^2 r$)	|V(r)| / G(r)	energy density E(r)
vi	A	-0.07235	0.03646	-0.03589	0.00228	1.98437	-0.03589
vii	A	-0.00649	0.00781	0.00132	0.03653	0.83080	0.00132
	B	-0.03425	0.02254	-0.01172	0.04329	1.51985	-0.01172
	C	-0.08561	0.03894	-0.04667	-0.03093	2.19856	-0.04667
viii	A	-0.06179	0.03246	-0.02933	0.01254	1.90343	-0.02933
	B	-0.08561	0.03894	-0.04667	-0.03093	2.19856	-0.04667
	C	-0.03071	0.02264	-0.00807	0.05830	1.35628	-0.00807
ix	A	-0.00824	0.00959	0.00136	0.04380	0.85852	0.00136
	B	-0.02327	0.01781	-0.00546	0.04938	1.30679	-0.00546
	C	-0.05390	0.03008	-0.02382	0.02505	1.79179	-0.02382
	D	-0.00824	0.00959	0.00136	0.04380	0.85852	0.00136
	E	-0.01988	0.01648	-0.00340	0.05234	1.20608	-0.00340
	F	-0.02540	0.02016	-0.00524	0.05966	1.26015	-0.00524
x	A	-0.05708	0.03119	-0.02589	0.02120	1.83004	-0.02589
	B	-0.00696	0.00827	0.00131	0.03833	0.84171	0.00131
	C	-0.00285	0.00375	0.00090	0.01858	0.76094	0.00090
	D	-0.02751	0.01946	-0.00806	0.14560	1.41410	-0.00806
	E	-0.02288	0.01779	-0.00508	0.05084	1.28571	-0.00508
	F	-0.02116	0.01777	-0.00339	0.05753	1.19069	-0.00339
	G	-0.02302	0.01787	-0.00515	0.05086	1.28847	-0.00515
	H	-0.00457	0.00562	0.00105	0.02669	0.81335	0.00105
	I	-0.00627	0.00759	0.00132	0.03562	0.82602	0.00132
	J	-0.00756	0.00809	0.00054	0.03451	0.93384	0.00054
xi	A	-0.00620	0.00739	0.00119	0.03432	0.83884	0.00119
	B	-0.00436	0.00560	0.00124	0.02733	0.77893	0.00124
	C	-0.02017	0.01665	-0.00352	0.05251	1.21153	-0.00352
	D	-0.01887	0.01551	-0.00336	-0.00336	1.21687	-0.00336
	E	-0.00519	0.00639	0.00121	0.03040	0.81123	0.00121
	F	-0.02628	0.01911	-0.00717	0.04778	1.37502	-0.00717
	G	-0.02776	0.02046	-0.00730	0.05266	1.35662	-0.00730
	H	-0.00540	0.00659	0.00120	0.03115	0.81859	0.00120
	I	-0.01336	0.01251	-0.00085	0.04660	1.06836	-0.00085
	J	-0.00688	0.00826	0.00138	0.03854	0.83336	0.00138
	K	-0.01977	0.01580	-0.00397	0.04730	1.25148	-0.00397
	L	-0.03054	0.02154	-0.00899	0.05020	1.41746	-0.00899
	M	-0.01056	0.01060	0.00004	0.04258	0.99600	0.00004

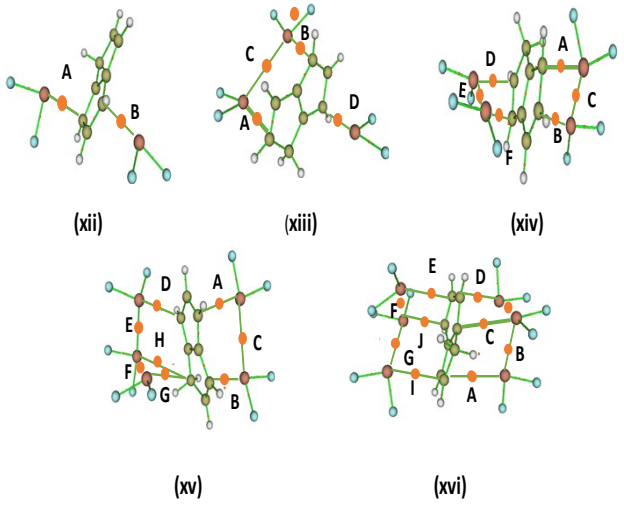


Figure-S8. AIM picture showing (3,-1) critical points of pentalene monoanion and SeF_2

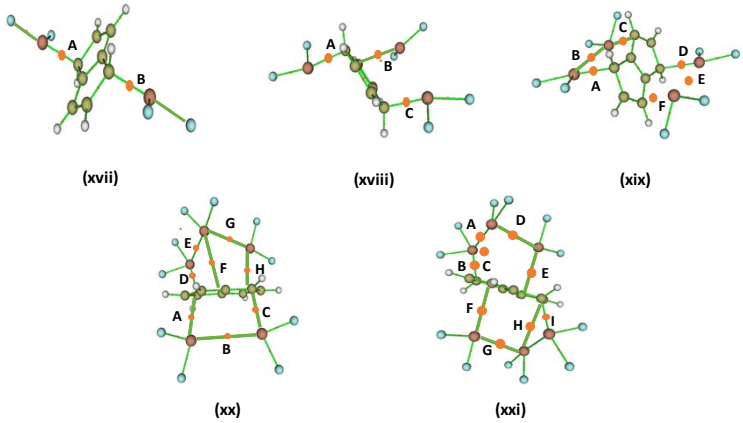


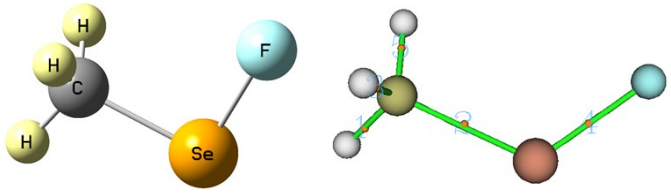
Figure-S9. AIM picture showing (3,-1) critical points of pentalene dianion and SeF_2

Table S5. AIM values for (3,-1) critical points of pentalene monoanion and SeF_2

Structure Number	CP	Potential energy density V(r)	kinetic energy G(r)	Total Energy density H(r)	Laplacian electron density ($\nabla^2 r$)	|V(r)| / G(r)	energy density E(r)
xii	A	-0.04180	0.02663	-0.01517	0.04583	1.56978	-0.01517
	B	-0.03816	0.02536	-0.01280	0.05024	1.50470	-0.01280
xiii	A	-0.03407	0.02437	-0.00970	0.05867	1.39811	-0.00970
	B	-0.03001	0.21976	0.18975	0.05577	0.13656	-0.00803
	C	-0.00291	0.00370	0.00080	0.01801	0.78442	0.00080
	D	-0.03339	0.02316	-0.01023	0.05171	1.44184	-0.01023
xiv	A	-0.05136	0.02888	-0.02248	0.02561	1.77828	-0.02248
	B	-0.00755	0.00885	0.00130	0.04061	0.85275	0.00130
	C	-0.02491	0.01856	-0.00635	0.04882	1.34241	-0.00635
	D	-0.02360	0.01975	-0.00385	0.06361	1.19484	-0.00385
	E	-0.00210	0.00278	0.00067	0.01378	0.75848	0.00067
	F	-0.03392	0.02473	-0.00920	0.06213	1.37187	-0.00920
xv	A	-0.02068	0.01756	-0.00312	0.05779	1.17751	-0.00312
	B	-0.03067	0.02254	-0.00813	0.05764	1.36060	-0.00813
	C	-0.00651	0.00730	0.00079	0.03235	0.89174	0.00079
	D	-0.02296	0.01771	-0.00524	0.04989	1.29589	-0.00524
	E	-0.03250	0.02238	-0.01012	0.04906	1.45203	-0.01012
	F	-0.01012	0.01584	0.00572	0.05135	0.63868	-0.00300
	G	-0.00569	0.00677	0.00108	0.03141	0.840513	0.00108
	H	-0.00852	0.00967	0.00114	0.04323	0.88187	0.00114
xvi	A	-0.00383	0.00481	0.00098	0.02315	0.79636	0.00098
	B	-0.02053	0.01676	-0.00377	0.05194	1.22514	-0.00377
	C	-0.00674	0.00796	0.00122	0.03674	0.84672	0.00122
	D	-0.02396	0.01931	-0.00465	0.05861	0.24095	-0.00465
	E	-0.00648	0.00762	0.00115	0.03509	0.84946	0.00115
	F	-0.02971	0.02076	-0.00896	0.04720	1.43149	-0.00896
	G	-0.00691	0.00753	0.00063	0.03263	0.91686	0.00063
	I	-0.00944	0.01022	0.00078	0.04400	0.92356	0.00078
	J	-0.03981	0.02521	-0.01460	0.04246	1.57899	-0.01460

Table S6. AIM values for (3,-1) critical points of pentalene dianion and SeF_2

Structure Number	CP	Potential energy density V(r)	kinetic energy G(r)	Total Energy density H(r)	Laplacian electron density ($\nabla^2 r$)	|V(r)| / G(r)	energy density E(r)
xvii	A	-0.094235	0.04265	-0.05159	-0.03576	2.20963	-0.05159
	B	-0.094175	0.04262	-0.05155	-0.03570	2.20940	-0.05155
xviii	A	-0.081572	0.03917	-0.04240	-0.01291	2.08242	-0.04240
	B	-0.039035	0.02777	-0.01127	0.06601	1.40569	-0.01127
	C	-0.080260	0.03865	-0.04161	-0.01181	2.07637	-0.04161
xix	A	-0.041606	0.03585	-0.00575	0.00474	1.16040	-0.03467
	B	-0.002567	0.00331	0.00074	0.01618	0.77647	0.00074
	C	-0.036180	0.02583	-0.01035	0.06190	1.40086	-0.01035
	D	-0.070511	0.03585	-0.03466	0.00477	1.96672	-0.03466
	E	-0.002581	0.00332	0.00074	0.01625	0.77698	0.00074
	F	-0.036126	0.02581	-0.01032	0.06195	1.39989	-0.01032
xx	A	-0.039846	0.02716	-0.01269	0.05786	1.46731	-0.01269
	B	-0.003023	0.00382	0.00080	0.01849	0.79077	0.00080
	C	-0.049266	0.02899	-0.02028	0.03485	1.69947	-0.02028
	D	-0.087060	0.03910	-0.04796	-0.03544	2.22657	-0.04796
	E	-0.030334	0.02041	-0.00992	0.04197	1.48601	-0.00992
	F	-0.004845	0.00590	0.00106	0.02783	0.82093	0.00106
	G	-0.008486	0.00894	0.00045	0.03754	0.94977	0.00045
	H	-0.021768	0.01790	-0.00387	0.05612	1.21613	-0.00387
xxi	A	-0.036677	0.02313	-0.01354	0.03836	1.58549	-0.01354
	B	-0.084908	0.03820	-0.04671	-0.03405	2.22288	-0.04671
	C	-0.006629	0.00783	0.00120	0.03613	0.84660	0.00120
	D	-0.011782	0.01116	-0.00062	0.04217	1.05557	-0.00062
	E	-0.009864	0.01091	0.00104	0.04780	0.90435	0.00104
	F	-0.008783	0.00996	0.00117	0.04453	0.88201	0.00117
	G	-0.013455	0.01225	-0.00120	0.04421	1.09799	-0.00120
	H	-0.006756	0.00796	0.00120	0.03664	0.84904	0.00120
	I	-0.086480	0.03865	-0.04783	-0.03669	2.23731	-0.04783



H_a H_b

Figure S10. Optimized structure of the model system (H_a, methyl selenium fluoride) at M06-2X/6-311+G(2d,p) level of theory and the AIM generated critical points shown in (H_b).

Table S7. AIM values for model system H_b

Structure Number	Cp	Potential Energy Density V(r)	Kinetic Energy G(r)	Total Energy Density H(r)	Laplacian Electron Density ($\nabla^2 r$)	|V(r)| / G(r)	Energy Density E(r)	DI
H_b	2	-0.13502	0.05195	-0.08306	-0.12444	2.59877	-0.08306	1.2681

Table S8. Delocalization index values for cyclopentadiene and iso-indene with distance.

Structure Number	Distance	Delocalization Index	Structure Number	Distance	Delocalization Index	Structure Number	Distance	Delocalization Index	Number	Distance	Delocalization Index
1	2.3	0.7294	7	2.2	0.0038	10	2.7	0.6975	11	2.9	0.0279
2	2.4	0.6010		2.8	0.0552		2.8	0.1183		3.0	0.4876
	2.5	0.4318		3.2	0.0652		2.9	0.1590		3.0	0.3899
3	2.2	0.8252	8	2.2	0.7408		3.2	0.0216		3.3	0.1223
	2.7	0.8604		2.8	0.7108		2.3	0.0216			
	3.2	0.1199		3.2	0.0494		2.8	0.0651			
4	2.4	0.2027		2.6	0.3417		2.9	0.4768			
	2.6	0.2662		2.5	0.4577		3.4	0.1265			
	2.8	0.4545	9	2.3	0.3892	11	2.9	0.4182			
	3.2	0.0526		2.9	0.0291		2.8	0.6526			
5	2.5	0.4705		3.2	0.1049		2.9	0.5010			
	2.8	0.7932		2.4	0.6866		2.9	0.5545			
	3.4	0.0654		2.9	0.6930		3.2	0.0982			
6	2.2	0.8266		3.2	0.0476		3.2	0.0995			
							2.5	0.0406			

The activation energy for cyclopentadiene with a weak base such as NH_3 was calculated in the presence of SeF_2 and without the presence of SeF_2. To calculate the stability of the salt produced by the conjugate base and conjugate acid the energy differences were calculated.

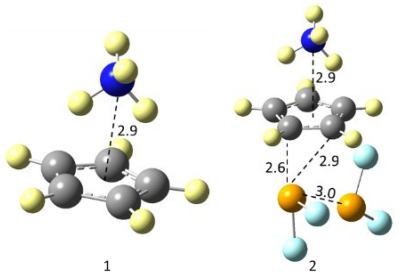


Figure S11. Complex formation of cyclopentadienyl ion and a weak base (NH_3) in the absence of SeF_2 (1) and in the presence of SeF_2 (2).

Table S9. Complexation energy using M06-2X/6-311+G(2d,p) level for cyclopentadienyl ion with a weak base (NH_3) in the absence (1) and in the presence of SeF_2 (2).

	E_{base}	E_{acid}	E_{SeF2}	$E_{complex}$	ΔE $\Delta E = E_{complex} - (E_{acid} + E_{base}$ in kcal/mol
1	-56.5091	-193.9671	-	-250.4457	19.1
2	-56.5091	-193.9671	-2601.1792	-5452.8392	-2.9

Cartesian Co-ordinates of systems.

System 1.

1	6	0	-0.062291	0.183915	-0.241164
2	6	0	-0.551380	-0.711640	-1.157032
3	1	0	-0.134240	-0.908976	-2.135981
4	6	0	-1.732406	-1.327754	-0.614481
5	1	0	-2.363122	-2.036954	-1.132431
6	6	0	-0.972030	0.230732	0.880710
7	1	0	-0.672863	0.521333	1.879203
8	6	0	-1.969603	-0.785435	0.620805
9	1	0	-2.806447	-0.993829	1.271684
10	1	0	0.808512	0.814233	-0.358683

11	34	0	-2.095520	2.110435	0.340206
12	9	0	-3.253954	3.646184	0.301615
13	9	0	-2.914196	1.803740	1.915640

System 2.

1	34	0	-2.276282	-1.471109	4.792897
2	9	0	-3.802179	-1.962270	3.764976
3	9	0	-1.581077	-2.861379	3.905767
4	34	0	-1.666634	0.678143	3.275890
5	9	0	-1.520922	2.186029	2.206197
6	9	0	-3.419924	0.907978	3.216431
7	6	0	-0.296302	-1.474926	5.655054
8	6	0	-0.264288	-0.439201	6.687306
9	1	0	-0.846516	-0.462346	7.598222
10	6	0	0.548764	0.567287	6.274531
11	1	0	0.715389	1.502854	6.790798
12	6	0	0.651692	-1.012968	4.633913
13	1	0	0.870011	-1.556919	3.726074
14	6	0	1.124704	0.209778	4.993845
15	1	0	1.775118	0.841393	4.404115
16	1	0	-0.270702	-2.519719	5.952229

System 3.

1	6	0	-0.579174	-0.325236	1.407845
2	6	0	-0.958547	-1.194291	0.341596
3	1	0	-0.499085	-1.194088	-0.635782
4	6	0	-2.323719	-1.561779	0.593064

5	1	0	-2.912511	-2.195709	-0.054025
6	6	0	-1.625001	-0.288259	2.339709
7	1	0	-1.577593	0.157324	3.322616
8	6	0	-2.712917	-1.053039	1.811709
9	1	0	-3.657236	-1.223135	2.306745
10	1	0	0.383196	0.150973	1.523985
11	34	0	0.127762	-3.144582	1.142578
12	9	0	-0.501060	-3.803402	-0.391728
13	9	0	0.841806	-4.851000	1.400760
14	34	0	-2.160595	1.800783	0.983686
15	9	0	-0.683493	2.566250	1.618001
16	9	0	-2.582214	3.410677	0.227502

System 4.

1	6	0	-1.200174	2.216983	3.874800
2	6	0	-1.310962	1.186910	2.982944
3	1	0	-1.153447	1.242167	1.915364
4	6	0	-1.699759	0.003607	3.707364
5	1	0	-1.947561	-0.951346	3.267519
6	6	0	-1.600526	1.758365	5.197883
7	1	0	-1.126505	2.159041	6.085479
8	6	0	-1.811932	0.332538	5.048579
9	1	0	-2.108776	-0.342387	5.838395
10	1	0	-0.928065	3.238005	3.648698
11	34	0	-4.239962	2.469958	2.899614
12	9	0	-4.889238	2.388292	1.184670
13	9	0	-5.894014	2.736151	3.454015

14	34	0	0.671380	-0.495946	4.596109
15	9	0	0.006434	-1.910641	5.433202
16	9	0	2.332349	-1.101737	4.996071
17	34	0	-3.611061	2.680331	5.571821
18	9	0	-2.580317	4.128227	5.631655
19	9	0	-4.952051	3.916148	5.977093

System 5.

1	6	0	-1.586535	1.858853	3.945393
2	6	0	-2.191567	0.880489	3.092126
3	1	0	-2.453301	1.023387	2.053982
4	6	0	-2.422314	-0.263182	3.832199
5	1	0	-2.929484	-1.150060	3.481308
6	6	0	-1.350058	1.235053	5.192673
7	1	0	-0.878323	1.693768	6.048609
8	6	0	-1.838400	-0.090867	5.128214
9	1	0	-1.959068	-0.754062	5.972237
10	1	0	-1.173547	2.806437	3.631944
11	34	0	-4.031866	3.583937	2.389322
12	9	0	-4.433381	4.325743	0.779476
13	9	0	-5.244695	4.624627	3.117940
14	34	0	0.444931	-0.684277	4.390429
15	9	0	0.839426	-0.580743	6.106999
16	9	0	2.137651	-1.226999	4.119927
17	34	0	-3.723017	2.594534	4.942469
18	9	0	-2.730651	3.820053	5.734704
19	9	0	-5.153726	3.395409	5.683544

20	34	0	-0.772577	-3.147702	4.178580
21	9	0	0.867535	-3.775066	4.224526
22	9	0	-1.364448	-4.855497	3.985561

System 6.

1	6	0	-0.145683	-0.720107	-1.067138
2	6	0	-0.085356	0.549451	-1.695415
3	6	0	-1.214099	1.069706	-2.326593
4	6	0	-2.387117	0.326525	-2.336971
5	6	0	-2.447746	-0.921016	-1.710045
6	6	0	-1.332835	-1.444252	-1.065313
7	6	0	1.141137	-0.982727	-0.422809
8	6	0	1.976855	0.151713	-0.814946
9	6	0	1.260609	1.062811	-1.522131
10	1	0	-1.179267	2.042956	-2.805032
11	1	0	-3.269387	0.719777	-2.829419
12	1	0	-3.375834	-1.480661	-1.721037
13	1	0	-1.383905	-2.403159	-0.561273
14	1	0	1.558939	-1.983430	-0.429360
15	1	0	3.006069	0.256402	-0.500019
16	1	0	1.604759	2.030899	-1.859326
17	34	0	0.691705	-0.769570	1.697372
18	9	0	0.807107	-0.754882	3.633979
19	9	0	2.447058	-1.162745	1.855860

System 7.

1	6	0	-1.294891	-0.049806	-0.711089
2	6	0	-2.022025	0.613114	0.308851
3	6	0	-3.244994	0.104191	0.735557

4	6	0	-3.750952	-1.037438	0.123977
5	6	0	-3.047860	-1.671494	-0.900626
6	6	0	-1.813208	-1.187461	-1.319292
7	6	0	0.027855	0.580950	-0.815514
8	6	0	-0.044362	1.725151	0.101135
9	6	0	-1.219810	1.732182	0.771148
10	1	0	-3.789846	0.581691	1.542166
11	1	0	-4.698916	-1.446119	0.452835
12	1	0	-3.459331	-2.562962	-1.358399
13	1	0	-1.254849	-1.699938	-2.094921
14	1	0	0.482370	0.723080	-1.791207
15	1	0	0.780974	2.404409	0.258338
16	1	0	-1.498441	2.400876	1.573441
17	34	0	1.284908	-0.996886	-0.017880
18	9	0	2.741546	-1.993462	0.665086
19	9	0	2.493637	0.324133	0.081674
20	34	0	-0.349652	-1.325025	2.237185
21	9	0	-1.293100	-1.753726	3.754917
22	9	0	1.085836	-1.969154	3.020339

System 8.

1	6	0	1.439005	1.506173	0.541633
2	6	0	2.179283	0.883007	-0.491403
3	6	0	3.146075	-0.072342	-0.191011
4	6	0	3.378897	-0.391279	1.139446
5	6	0	2.665561	0.240336	2.162103
6	6	0	1.692235	1.185904	1.874897
7	6	0	0.372393	2.301298	-0.067408

8	6	0	0.629418	2.241232	-1.490197
9	6	0	1.681512	1.384092	-1.761088
10	1	0	3.693914	-0.569900	-0.982902
11	1	0	4.118166	-1.142157	1.388998
12	1	0	2.864819	-0.027526	3.192647
13	1	0	1.125293	1.655312	2.670610
14	1	0	0.013447	3.217443	0.384983
15	1	0	0.017751	2.726249	-2.236540
16	1	0	1.952308	1.001635	-2.733995
17	34	0	-1.359236	0.964421	0.386776
18	9	0	-3.036383	0.166583	0.500294
19	9	0	-2.178736	1.984202	-0.829042
20	34	0	-0.025607	-1.381568	-0.532437
21	9	0	0.650730	-3.021559	-0.937933
22	9	0	-1.643225	-2.009487	-0.795530
23	34	0	2.903341	3.571028	-1.901394
24	9	0	2.171256	3.618242	-3.513026
25	9	0	3.922130	4.986438	-2.410776

System 9.

1	6	0	1.327317	1.595733	0.707216
2	6	0	2.205940	1.002039	-0.234325
3	6	0	3.147348	0.052971	0.173185
4	6	0	3.246815	-0.247815	1.524151
5	6	0	2.416763	0.379231	2.459158
6	6	0	1.447910	1.288011	2.062986
7	6	0	0.310515	2.341799	-0.025382
8	6	0	0.717813	2.289540	-1.406564

9	6	0	1.851342	1.502526	-1.546944
10	1	0	3.778112	-0.446167	-0.553676
11	1	0	3.974063	-0.976440	1.858500
12	1	0	2.519439	0.130268	3.508001
13	1	0	0.785095	1.741285	2.790910
14	1	0	-0.188529	3.211753	0.381444
15	1	0	0.162160	2.732999	-2.220216
16	1	0	2.282087	1.171754	-2.480845
17	34	0	-1.414401	0.868869	0.224913
18	9	0	-3.014096	-0.041027	0.151989
19	9	0	-2.115752	1.816064	-1.112014
20	34	0	0.188136	-1.388733	-0.504188
21	9	0	1.021984	-2.967948	-0.820066
22	9	0	-1.339936	-2.126450	-0.949784
23	34	0	2.776792	3.938549	-1.428247
24	9	0	2.789563	3.687961	-3.169569
25	9	0	3.696108	5.453286	-1.700192
26	34	0	4.991792	2.460909	-0.180552
27	9	0	5.963677	3.846810	-0.657883
28	9	0	6.391873	1.734495	0.665781

System 10.

1	6	0	1.299003	1.677622	0.755720
2	6	0	2.253161	1.093630	-0.116726
3	6	0	3.162613	0.144668	0.366123
4	6	0	3.128588	-0.193397	1.710885
5	6	0	2.215649	0.414089	2.578750
6	6	0	1.302917	1.351699	2.117244

7	6	0	0.315713	2.386785	-0.053664
8	6	0	0.803216	2.306180	-1.407875
9	6	0	1.958771	1.549800	-1.463168
10	1	0	3.849021	-0.355430	-0.310109
11	1	0	3.807946	-0.943649	2.093250
12	1	0	2.205436	0.127601	3.622378
13	1	0	0.580560	1.794649	2.793176
14	1	0	-0.227949	3.253800	0.299696
15	1	0	0.299850	2.735950	-2.262432
16	1	0	2.456900	1.213169	-2.361569
17	34	0	-1.327540	0.848538	0.258335
18	9	0	-2.821211	-0.254483	0.298520
19	9	0	-2.099152	1.581322	-1.157520
20	34	0	0.264961	-1.361121	-0.435702
21	9	0	1.019311	-2.959946	-0.789891
22	9	0	-1.214368	-1.942215	-1.157310
23	34	0	2.942748	4.019974	-1.309936
24	9	0	2.803174	3.916539	-3.057979
25	9	0	3.837418	5.542194	-1.483858
26	34	0	5.217152	2.384947	-0.619759
27	9	0	6.131066	3.768928	-1.161987
28	9	0	6.718924	1.568640	-0.114895
29	34	0	3.971266	3.392198	1.970208
30	34	0	-0.910401	-2.018596	2.150466
31	9	0	5.375543	4.440986	1.977614
32	9	0	3.324894	4.138156	3.441515
33	9	0	-1.543875	-2.585491	3.724732

34	9	0	0.738567	-2.342295	2.673102

System 11.

1	6	0	1.015867	1.780491	0.815803
2	6	0	2.050369	1.293934	-0.039395
3	6	0	3.063047	0.471547	0.479185
4	6	0	3.083095	0.210473	1.840490
5	6	0	2.130260	0.789154	2.700573
6	6	0	1.092399	1.558863	2.197786
7	6	0	0.006123	2.390957	-0.012185
8	6	0	0.491967	2.355091	-1.335023
9	6	0	1.752199	1.732758	-1.379133
10	1	0	3.800187	0.017160	-0.176656
11	1	0	3.826425	-0.464526	2.247180
12	1	0	2.204226	0.611217	3.766737
13	1	0	0.348322	1.979550	2.865445
14	1	0	-0.761798	3.064864	0.338358
15	1	0	-0.021560	2.767224	-2.192669
16	1	0	2.286079	1.434997	-2.269947
17	34	0	-1.550535	0.439362	0.072133
18	9	0	-2.798949	-0.837686	-0.050607
19	9	0	-2.127924	1.063195	-1.469237
20	34	0	0.402692	-0.853498	-3.259587
21	9	0	0.682205	-2.577140	-3.222126
22	9	0	0.112738	-0.826020	-4.996008
23	34	0	2.651711	4.100206	-1.124096
24	9	0	2.459140	4.097295	-2.868518
25	9	0	3.390833	5.713194	-1.253900

26	34	0	5.088505	2.718083	-0.764755
27	9	0	5.757527	4.245315	-1.261598
28	9	0	6.738459	2.095035	-0.516269
29	34	0	4.203151	3.244961	2.022287
30	34	0	-0.265003	-1.416969	2.818763
31	9	0	5.206848	4.649675	1.804900
32	9	0	3.790668	3.755524	3.666944
33	9	0	-0.974416	-1.402865	4.439017
34	9	0	-0.980574	-2.955069	2.406944
35	34	0	6.175647	1.235592	2.832377
36	34	0	0.629231	-1.534151	-0.154536
37	9	0	-0.663681	-2.639807	-0.504292
38	9	0	1.806107	-2.863213	-0.116831
39	9	0	7.527247	0.236985	3.416292
40	9	0	7.168363	2.674588	2.877039

System 12(i).

1	6	0	2.110434	-1.085107	-0.199153
2	6	0	2.748940	0.269206	0.035067
3	6	0	1.809324	1.224829	0.144735
4	6	0	0.492926	0.608193	0.002226
5	6	0	0.651574	-0.749110	-0.164655
6	6	0	-0.910592	0.917996	0.048422
7	6	0	-1.578151	-0.303498	-0.204039
8	6	0	-0.631427	-1.352927	-0.375686
9	1	0	2.402194	-1.497258	-1.173499
10	1	0	2.413239	-1.814664	0.558453
11	1	0	3.817681	0.420821	0.099405

12	1	0	1.998907	2.276581	0.312230
13	1	0	-1.363008	1.895230	-0.021109
14	1	0	-2.649630	-0.424103	-0.264625
15	1	0	-0.869477	-2.403462	-0.306436
16	34	0	-1.194457	0.509869	2.407587
17	34	0	-0.699504	-1.139057	-2.737845
18	9	0	-2.876679	1.027523	2.114668
19	9	0	-1.670833	0.410231	4.190907
20	9	0	-2.246097	-2.018093	-2.562527
21	9	0	-0.997628	-1.291037	-4.563269

System 13(i).

1	6	0	2.034891	-1.442079	-0.240410
2	6	0	2.782728	-0.258056	0.339849
3	6	0	1.912866	0.779189	0.588466
4	6	0	0.564343	0.326771	0.330618
5	6	0	0.610507	-1.001500	-0.081267
6	6	0	-0.803139	0.753965	0.385571
7	6	0	-1.560966	-0.339009	-0.069028
8	6	0	-0.702698	-1.429315	-0.404517
9	1	0	2.277528	-1.534649	-1.309070
10	1	0	2.289793	-2.389666	0.234657
11	1	0	3.859656	-0.177307	0.358572
12	1	0	2.211542	1.771670	0.897174
13	1	0	-1.166518	1.762559	0.503743
14	1	0	-2.635565	-0.345924	-0.174936
15	1	0	-1.031277	-2.440576	-0.588551
16	34	0	-1.323452	0.046773	2.729509

17	34	0	-0.508076	-0.722672	-2.752181
18	9	0	-2.994866	0.490520	2.323429
19	9	0	-1.896638	-0.252152	4.429870
20	9	0	-2.080711	-1.536989	-2.893182
21	9	0	-0.608542	-0.416523	-4.553969
22	34	0	2.387010	-0.530588	2.770421
23	9	0	3.966598	0.290424	2.812865
24	9	0	2.716531	-1.031337	4.476768

System 14(1).

1	6	0	1.924607	-1.630685	-0.219635
2	6	0	2.844623	-0.557101	0.321434
3	6	0	2.149799	0.605797	0.550501
4	6	0	0.745155	0.356259	0.282480
5	6	0	0.591298	-0.949974	-0.144420
6	6	0	-0.534536	1.008206	0.265390
7	6	0	-1.455657	0.066287	-0.175029
8	6	0	-0.775847	-1.167498	-0.536932
9	1	0	2.178859	-1.853748	-1.262052
10	1	0	1.983968	-2.568749	0.334833
11	1	0	3.920400	-0.646077	0.353834
12	1	0	2.596837	1.550781	0.825826
13	1	0	-0.736574	2.050184	0.462714
14	1	0	-2.510605	0.251102	-0.318523
15	1	0	-1.265285	-2.129976	-0.472036
16	34	0	-1.436921	0.032386	2.522125
17	34	0	-0.690483	-1.120125	-2.826048

18	9	0	-2.952306	0.876537	2.168101
19	9	0	-2.056363	-0.313781	4.173255
20	9	0	0.159106	-2.648449	-2.502326
21	9	0	-0.425381	-1.589973	-4.592711
22	34	0	2.427771	-0.615643	2.794829
23	9	0	4.067455	0.060465	2.780019
24	9	0	2.702211	-1.018012	4.531145
25	34	0	1.392226	0.800582	-2.763048
26	9	0	2.710121	2.039048	-2.933635
27	9	0	1.133969	0.857547	-4.500412

System 15(i) :

1	6	0	0.211601	1.168470	-0.489980
2	6	0	1.339287	1.224151	0.396931
3	6	0	1.488000	2.528332	0.893981
4	6	0	0.416075	3.287843	0.340753
5	6	0	-0.358972	2.465885	-0.486877
6	6	0	-0.255670	4.566242	0.487329
7	6	0	-1.430742	4.533715	-0.216700
8	6	0	-1.570018	3.225533	-0.971454
9	1	0	1.945580	0.375809	0.679663
10	1	0	2.319349	2.894380	1.476296
11	1	0	-2.073197	5.386202	-0.383418
12	1	0	-2.518694	2.723270	-0.773164
13	1	0	0.113865	5.426639	1.028815
14	1	0	-0.251384	0.258445	-0.841903
15	34	0	0.181049	1.818172	3.092909
16	34	0	0.125837	1.815254	-3.596332

17	9	0	-0.571928	1.323208	4.639965
18	9	0	1.440096	0.597093	3.312283
19	9	0	1.087601	1.433939	-5.007948
20	9	0	-1.066351	2.632019	-4.679049
21	34	0	-2.292170	3.946173	2.070568
22	9	0	-2.471448	5.705476	2.134620
23	9	0	-3.416986	3.853017	3.470287
24	34	0	2.206200	0.781996	-2.153852
25	9	0	1.774058	-0.863876	-1.708064
26	9	0	3.166445	0.095915	-3.503220
27	34	0	1.542779	4.140214	-2.386712
28	9	0	2.476694	5.514471	-1.739731
29	9	0	2.021107	4.525481	-4.036374
30	1	0	-1.547600	3.452810	-2.045209

System 16(i).

1	6	0	0.126314	0.912869	-0.531119
2	6	0	1.155006	0.857058	0.430729
3	6	0	1.346969	2.155213	1.006072
4	6	0	0.421838	3.014277	0.316986
5	6	0	-0.335553	2.265379	-0.570779
6	6	0	-0.193276	4.331969	0.468314
7	6	0	-1.325650	4.365997	-0.267909
8	6	0	-1.545525	3.055909	-0.991884
9	1	0	1.701269	-0.031404	0.713909
10	1	0	2.275387	2.463302	1.466420
11	1	0	-1.967719	5.227367	-0.390111
12	1	0	-2.466251	2.568241	-0.650965

13	1	0	0.188654	5.149839	1.064613
14	1	0	-0.319339	0.057200	-1.020141
15	34	0	0.275744	1.967686	3.133881
16	34	0	0.267237	1.783742	-3.687040
17	9	0	-0.224107	1.621501	4.848171
18	9	0	1.472448	0.688339	3.347634
19	9	0	1.429028	1.476676	-4.951853
20	9	0	-0.892444	2.377126	-4.920763
21	34	0	-2.412678	4.034768	2.522661
22	9	0	-2.132645	5.765237	2.361608
23	9	0	-3.273052	4.263559	4.033995
24	34	0	2.330086	1.084821	-1.955713
25	9	0	2.299231	-0.667842	-1.827477
26	9	0	3.606185	0.928884	-3.183358
27	34	0	1.301292	4.342628	-2.687864
28	9	0	2.020062	5.923613	-2.280464
29	9	0	1.595296	4.606055	-4.396790
30	1	0	-1.654199	3.228303	-2.068339
31	34	0	-1.821269	0.544593	2.029065
32	9	0	-3.388129	-0.249166	1.581504
33	9	0	-2.711885	1.456094	3.270297

System 12(ii).

1	6	0	-0.243473	0.651530	-0.124057
2	6	0	0.700775	0.626248	0.853709
3	6	0	1.054583	2.005923	1.273474
4	6	0	0.258565	2.840499	0.352819
5	6	0	-0.531528	2.037850	-0.432798

6	6	0	-0.029474	4.226835	0.044356
7	6	0	-0.973694	4.252258	-0.933399
8	6	0	-1.327225	2.872548	-1.353608
9	1	0	1.104052	-0.252062	1.338430
10	1	0	2.116064	2.219662	1.380175
11	1	0	-1.377001	5.130529	-1.418148
12	1	0	-2.388556	2.658715	-1.461386
13	1	0	0.451833	5.088934	0.487133
14	1	0	-0.724730	-0.210687	-0.566663
15	34	0	0.308038	2.373342	3.186646
16	34	0	-0.579056	2.506995	-3.266715
17	9	0	0.016557	2.408493	5.224954
18	9	0	1.573542	1.180253	3.707254
19	9	0	-0.287214	2.474128	-5.304799
20	9	0	-1.844773	3.700312	-3.786622

System 13(ii).

1	6	0	-0.230657	0.635756	-0.062362
2	6	0	0.787146	0.672420	0.845309
3	6	0	1.018770	2.043855	1.327975
4	6	0	0.079662	2.835478	0.525018
5	6	0	-0.683511	1.989891	-0.262227
6	6	0	-0.350759	4.188186	0.295398
7	6	0	-1.381347	4.145854	-0.653073
8	6	0	-1.552789	2.772324	-1.149323
9	1	0	1.322198	-0.178873	1.242761
10	1	0	2.047047	2.375906	1.431869
11	1	0	-1.834314	5.010672	-1.113976

12	1	0	-2.551179	2.434183	-1.400277
13	1	0	0.114169	5.090489	0.664944
14	1	0	-0.651081	-0.249910	-0.517301
15	34	0	0.384874	2.075500	3.371794
16	34	0	-0.505963	2.709050	-3.013298
17	9	0	0.311154	1.767640	5.336110
18	9	0	1.813840	0.974830	3.560592
19	9	0	0.034367	2.881246	-4.919866
20	9	0	-1.907070	3.684547	-3.612938
21	34	0	-2.449922	4.241602	1.552834
22	9	0	-2.568950	5.970520	1.071643
23	9	0	-3.834867	4.670213	2.721467

System 14(ii).

1	6	0	0.184241	0.802235	-0.311622
2	6	0	1.235298	0.990023	0.594046
3	6	0	1.237640	2.355480	1.104110
4	6	0	0.190190	3.008923	0.316887
5	6	0	-0.473639	2.077558	-0.463757
6	6	0	-0.467861	4.284216	0.164707
7	6	0	-1.518863	4.096370	-0.741148
8	6	0	-1.521194	2.730850	-1.250951
9	1	0	1.866870	0.206998	0.986063
10	1	0	2.182478	2.842043	1.309650
11	1	0	-2.150056	4.879368	-1.133840
12	1	0	-2.465863	2.244127	-1.456830
13	1	0	-0.120757	5.240080	0.527588
14	1	0	-0.162669	-0.153500	-0.675031

15	34	0	0.465872	2.072562	3.131157
16	34	0	-0.748490	3.013494	-3.277759
17	9	0	0.323447	1.604653	5.013345
18	9	0	2.063283	1.248920	3.333315
19	9	0	-0.604643	3.481601	-5.159796
20	9	0	-2.345818	3.837143	-3.480994
21	34	0	-2.446904	4.046380	1.605195
22	9	0	-2.679966	5.770250	1.186277
23	9	0	-3.789572	4.331302	2.839439
24	34	0	2.163412	1.042611	-1.752651
25	9	0	2.398825	-0.681295	-1.335169
26	9	0	3.505802	0.760849	-2.987431

System 15(ii).

1	6	0	0.235686	0.791093	-0.235610
2	6	0	1.237213	0.897569	0.738519
3	6	0	1.330236	2.245855	1.220659
4	6	0	0.374559	2.985066	0.426160
5	6	0	-0.310488	2.102491	-0.406122
6	6	0	-0.216578	4.294330	0.291886
7	6	0	-1.260988	4.202155	-0.624399
8	6	0	-1.316155	2.838467	-1.207544
9	1	0	1.829589	0.077580	1.116654
10	1	0	2.229865	2.656589	1.654713
11	1	0	-1.787876	5.044343	-1.045864
12	1	0	-2.308769	2.408553	-1.308454
13	1	0	0.149049	5.218010	0.717015
14	1	0	-0.157501	-0.132278	-0.633867

15	34	0	0.182497	1.869415	3.187743
16	34	0	-0.655286	2.854991	-3.219214
17	9	0	-0.360619	1.377747	4.933232
18	9	0	1.669675	0.953133	3.602409
19	9	0	-0.500383	3.254184	-5.096447
20	9	0	-1.949091	4.089281	-3.386568
21	34	0	-2.361050	4.092006	1.532953
22	9	0	-2.515052	5.841128	1.190048
23	9	0	-3.723329	4.389357	2.743649
24	34	0	2.294224	0.761912	-1.885203
25	9	0	2.417465	-0.932354	-1.329369
26	9	0	3.609147	0.407285	-3.076489
27	34	0	1.742106	3.983681	-2.497032
28	9	0	3.411872	4.737515	-2.271077
29	9	0	1.759609	4.668568	-4.114797

System 16(ii).

1	6	0	-0.249329	0.672226	-0.248189
2	6	0	0.648445	0.530169	0.769822
3	6	0	1.025519	1.856704	1.326137
4	6	0	0.302300	2.792356	0.445037
5	6	0	-0.464293	2.089837	-0.456733
6	6	0	0.081796	4.209136	0.240974
7	6	0	-0.814559	4.350501	-0.778062
8	6	0	-1.182753	3.024838	-1.340033
9	1	0	1.021658	-0.402184	1.168468
10	1	0	2.094765	2.017272	1.444264
11	1	0	-1.190129	5.282120	-1.176040

12	1	0	-2.248359	2.859005	-1.478257
13	1	0	0.549483	5.015199	0.789518
14	1	0	-0.720482	-0.134061	-0.793579
15	34	0	0.445338	2.040630	3.352714
16	34	0	-0.566606	2.866998	-3.364267
17	9	0	0.364694	1.758596	5.256345
18	9	0	1.708287	0.784147	3.537912
19	9	0	-0.461451	3.170707	-5.263142
20	9	0	-1.829678	4.122899	-3.550397
21	34	0	-2.496300	3.535316	1.754100
22	9	0	-3.116622	5.197440	1.497593
23	9	0	-3.891868	3.175310	2.768336
24	34	0	2.266879	1.250933	-1.785292
25	9	0	2.716157	-0.473468	-1.640083
26	9	0	3.667677	1.543029	-2.814858
27	34	0	1.671329	4.199852	-2.771876
28	9	0	3.331058	5.004319	-2.584356
29	9	0	2.236529	3.639464	-4.338032
30	34	0	-1.791585	0.699843	2.802203
31	9	0	-3.446371	-0.116615	2.637295
32	9	0	-2.333221	1.238440	4.382797