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

Supporting Information

Aromatic Ouroboroi: Heterocycles involving a σ-donor-acceptor bond and 4n+2 π-Electrons

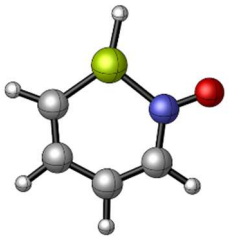
Rodrigo Báez-Grez,[a] Diego Inostroza,[a] Victor García,[a, b] Alejandro Vásquez-Espinal,[a] Kelling J. Donald*[c] and William Tiznado*[a]

a) *Computational and Theoretical Chemistry Group, Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andrés Bello, República 498, Santiago, Chile.*

b) *Departamento Académico de Fisicoquímica, Facultad de Química e Ingeniería Química, Universidad Nacional Mayor de San Marcos, Lima, Perú.*

c) *Department of Chemistry, Gottwald Center for the Sciences, University of Richmond, 28 Westhampton Way, Richmond, VA, 23173, United States.*

Table S1. Cartesian coordinates of the systems studied at the B3LYP/cc-pVTZ level.

3		C	-1.854734438	-0.207240317	-0.000198077
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		H	-2.399569381	1.784246066	-0.001343368
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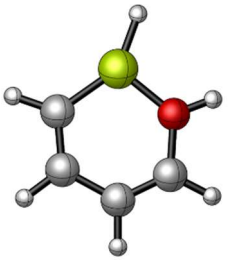
4		C	1.297134000	-0.671187000	0.000000000
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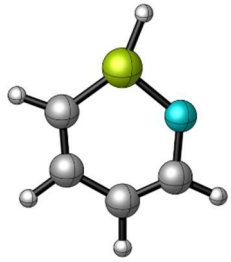
5		C	1.293059000	-0.642972000	0.000000000
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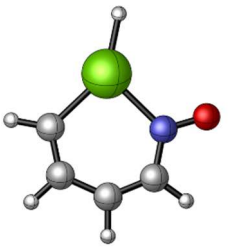
6		C	-1.947334000	0.471909000	-0.000209000
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		H	-2.953241000	0.889639000	-0.000347000
		H	-2.681752000	-1.431289000	-0.000577000
		H	1.044107000	2.336421000	0.000235000
		H	-1.307858000	2.501279000	0.000315000
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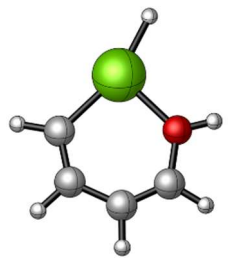
7		C	-1.102807000	1.273662000	-0.000146000
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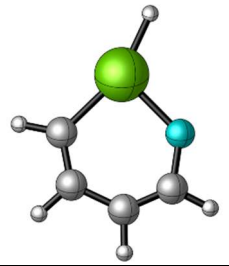
8		C	1.022700000	1.321266000	0.000015000
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		C	1.659155000	0.004229000	-0.000044000
		H	1.748528000	2.133748000	0.000047000
		H	-0.524699000	2.639946000	0.000071000
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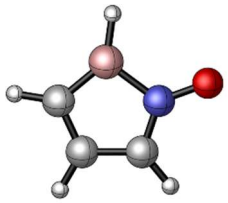
9		C	0.637747116	1.559679661	0.000000000
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		N	0.000000000	-0.791449448	0.000000000
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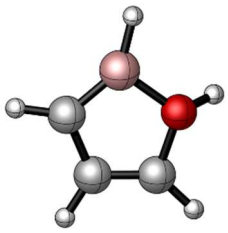
		O	0.106657200	-2.044160023	0.000000000
10		C	1.234643000	0.400517000	0.006481000
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		H	2.293002000	0.601542000	0.011168000
		H	-0.203390000	2.446269000	0.020301000
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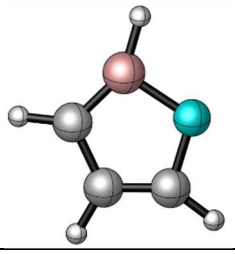
11		C	-1.220001277	-0.407265098	0.000000000
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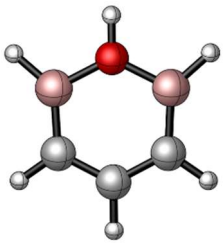
12		C	1.242188000	0.770348000	0.000000000
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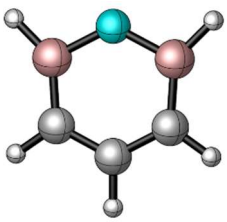
13		C	1.244047000	0.748768000	0.000000000
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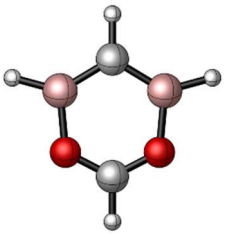
14		O	-1.125354000	-0.712624000	0.000000000
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		H	0.000716000	2.607018000	0.000000000
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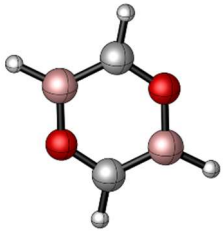
15		O	0.000000000	-1.378636000	0.000000000
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		C	1.172126000	0.762874000	0.000000000
		B	1.236570000	-0.731633000	0.000000000
		H	-2.002332000	-1.459356000	0.000000000
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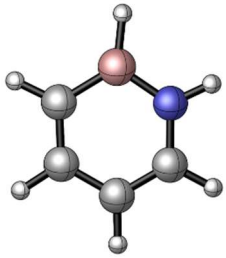
16		C	1.206431000	0.731182000	0.000000000
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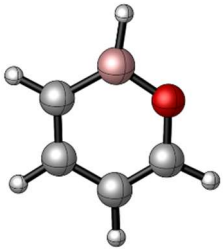
17		C	1.174376000	0.754769000	0.000000000
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		C	1.173652000	-0.672236000	0.000000000
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		H	-0.080579000	-2.421604000	0.000000000
		H	2.097976000	-1.230887000	0.000000000

Table S2. RCS obtained from different integration planes (see Figure S1)

System	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
1	a	12.17	16.99	-4.93	12.17

System	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
2	12.90	17.41	-4.59	12.82	12.90

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
3	a	-1.68	5.88	-7.56	-1.85
	b	-1.32	2.03	-3.35	
	c	-1.82	7.39	-9.21	
	d	-2.16	7.50	-9.66	
	e	-2.12	7.15	-9.27	
	f	-1.99	9.61	-11.60	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
4	a	2.45	7.48	-5.03	2.24
	b	2.57	3.79	-1.22	
	c	2.12	8.47	-6.35	
	d	2.00	9.81	-7.81	
	e	2.11	8.92	-6.81	
	f	2.19	11.48	-9.29	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
5	a	1.28	6.63	-5.35	1.11
	b	1.55	2.01	-0.46	
	c	1.06	7.23	-6.18	
	d	0.82	8.87	-8.04	
	e	0.91	8.16	-7.25	
	f	1.02	10.91	-9.89	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
6	a	-0.89	5.37	-6.27	-0.79
	b	0.39	1.11	-0.72	
	c	-0.92	7.63	-8.54	
	d	-1.22	7.86	-9.08	
	e	-1.18	7.49	-8.67	
	f	-0.92	9.92	-10.84	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
7	a	0.85	6.10	-5.24	0.88
	b	1.67	2.25	-0.59	
	c	0.66	7.61	-6.94	
	d	0.44	8.93	-8.49	
	e	0.68	7.97	-7.29	
	f	0.97	10.88	-9.90	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
8	a	0.41	5.85	-5.44	0.41
	b	1.49	2.11	-0.62	
	c	0.25	6.65	-6.40	
	d	-0.04	8.39	-8.42	
	e	0.04	7.59	-7.55	
	f	0.30	10.51	-10.20	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
9	a	-10.42	5.48	-15.91	-9.72
	b	-9.42	4.09	-13.51	
	c	-9.79	6.22	-16.01	
	d	-9.13	6.00	-15.13	
	e	-9.84	6.95	-16.79	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
10	a	6.21	11.33	-5.13	6.66
	b	7.12	9.85	-2.73	
	c	6.80	12.17	-5.36	
	d	6.49	12.10	-5.61	
	e	6.71	12.73	-6.02	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
11	a	4.47	9.78	-5.31	4.87
	b	5.51	7.06	-1.56	
	c	4.99	10.10	-5.11	
	d	4.57	10.53	-5.96	
	e	4.78	11.26	-6.48	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
12	a	4.87	9.51	-4.63	5.04
	b	5.22	10.17	-4.95	
	c	5.02	11.95	-6.93	
	d	5.02	11.95	-6.93	
	e	5.22	10.17	-4.95	
	f	4.87	9.51	-4.63	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
13	a	2.99	7.53	-4.53	3.07
	b	3.24	8.58	-5.33	
	c	2.96	10.64	-7.68	
	d	2.96	10.64	-7.68	
	e	3.24	8.58	-5.33	
	f	2.99	7.53	-4.53	

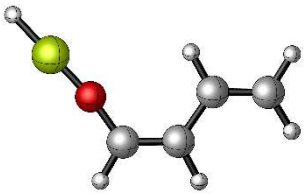
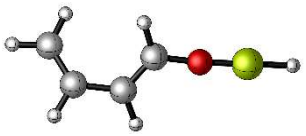
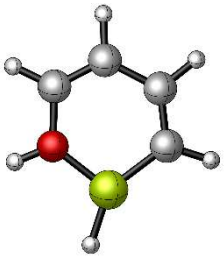
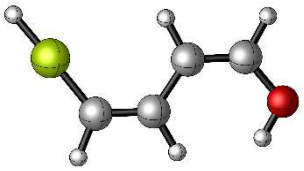
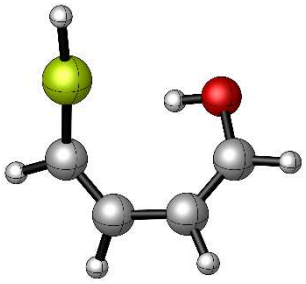
	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
14	a	5.01	10.83	-5.82	4.94
	b	5.06	8.47	-3.41	
	c	4.75	10.84	-6.09	
	d	4.75	10.84	-6.09	
	e	5.06	8.47	-3.41	
	f	5.01	10.83	-5.82	

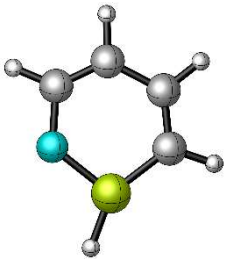
	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
15	a	7.73	11.98	-4.25	7.83
	b	7.81	11.04	-3.23	
	c	7.91	14.45	-6.54	
	d	7.73	11.96	-4.23	
	e	7.85	10.74	-2.89	
	f	7.94	13.76	-5.82	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
16	a	8.65	14.19	-5.54	8.74
	b	8.71	13.20	-4.49	
	c	8.63	14.48	-5.85	
	d	8.79	12.76	-3.97	
	e	8.85	14.16	-5.32	
	f	8.78	15.04	-6.26	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
17	a	7.03	10.87	-3.84	7.02
	b	7.02	11.48	-4.47	
	c	7.01	13.52	-6.51	
	d	6.90	12.51	-5.60	
	e	7.12	12.70	-5.58	
	f	7.04	13.80	-6.77	

Table S3. Structures, relative energies and Cartesian coordinates at the B3LYP/cc-pVTZ level of the isomers obtained from the molecular dynamic simulations of systems **4**, **5**, **10**, **11**, **12**, **13**, **14**, **15**, **16** and **17**.

System		Relative energy (kcal/mol)	Coordinates		
4		0.0	C -1.246217000 -0.425118000 -0.000663000 C -2.577939000 -0.529035000 0.000602000 Be 2.719225000 -0.978101000 0.001099000 O 1.676437000 -0.057920000 -0.000359000 C 0.809029000 0.962977000 0.000060000 C -0.523607000 0.828470000 -0.000248000 H -0.649498000 -1.330105000 -0.002255000 H -3.070047000 -1.491299000 -0.000261000 H 1.273202000 1.942862000 0.000267000 H -1.099544000 1.745547000 0.000372000 H 3.704928000 -1.862042000 -0.000017000 H -3.215039000 0.347034000 0.001863000
		3.3	C -1.800646000 -0.508042000 0.075912000 C -2.500238000 0.608861000 -0.129768000 Be 3.242738000 0.078856000 -0.101240000 O 1.859486000 0.129184000 0.022132000 C 0.539307000 0.281671000 0.184363000 C -0.357942000 -0.673202000 -0.075488000 H -2.340101000 -1.401852000 0.375208000 H -3.566653000 0.640466000 0.045030000 H 0.244431000 1.252793000 0.568093000 H 0.007664000 -1.646364000 -0.384116000 H 4.560833000 0.031790000 -0.217804000 H -2.035896000 1.518540000 -0.488623000
		26.5	C 1.296966000 0.671173000 0.000000000 C 1.451882000 -0.672371000 0.000000000 Be 0.088222000 -1.699026000 0.000000000 O -1.221333000 -0.681422000 0.000000000 C -1.180957000 0.721581000 0.000000000 C 0.000000000 1.335002000 0.000000000 H 2.147797000 1.349084000 0.000000000 H 2.487835000 -1.005243000 0.000000000 H -2.150748000 1.191165000 0.000000000 H -0.033064000 2.416794000 0.000000000 H -0.330746000 -2.989061000 0.000000000 H -2.110644000 -1.047571000 0.000000000
		41.1	C -0.597756000 -0.599471000 -0.000001000 C -1.949931000 -0.652516000 -0.000016000 Be -3.003908000 0.630557000 0.000079000 O 2.421062000 -0.371933000 0.000007000 C 1.545568000 0.660691000 0.000002000 C 0.203303000 0.602452000 -0.000010000 H -0.045812000 -1.541286000 -0.000011000 H -2.355110000 -1.664930000 -0.000049000 H 2.070680000 1.605752000 -0.000035000 H -0.309714000 1.557020000 -0.000004000 H -3.866436000 1.640594000 -0.000140000 H 1.946424000 -1.210847000 0.000013000
		43.5	C -0.761092000 -1.088154000 -0.170636000 C -1.633636000 -0.053363000 -0.235806000 Be -1.609522000 1.395117000 0.587507000 O 1.238343000 1.107561000 -0.456069000 C 1.469425000 -0.056152000 0.196923000 C 0.598145000 -1.064038000 0.354805000 H -1.069138000 -2.062310000 -0.549496000 H -2.572167000 -0.309423000 -0.731740000 H 2.486588000 -0.113247000 0.559714000 H 0.979365000 -1.964937000 0.817706000 H -1.710676000 2.546578000 1.237445000 H 0.380320000 1.032625000 -0.906821000

5		0.0	C	1.293252000	0.643256000	0.000000000
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			C	-1.190378000	0.744667000	0.000000000
			C	0.000000000	1.319548000	0.000000000
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			H	-2.179997000	1.163503000	0.000000000
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	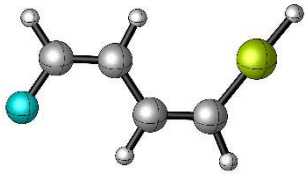	4.3	C	0.579042000	-0.613868000	0.000053000
			C	1.929172000	-0.653120000	0.000078000
			Be	2.980546000	0.636020000	-0.000249000
			F	-2.308581000	-0.450599000	-0.000208000
			C	-1.542289000	0.655361000	0.000191000
			C	-0.212596000	0.600609000	0.000116000
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			H	2.340904000	-1.663296000	0.000192000
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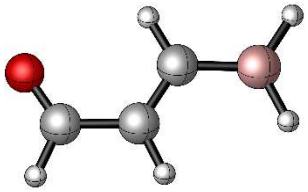
10		0.0	C	-0.965026000	-0.374282000	-0.000023000
			B	-2.487594000	-0.114610000	0.000010000
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			H	-3.268975000	-1.011161000	0.000159000
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	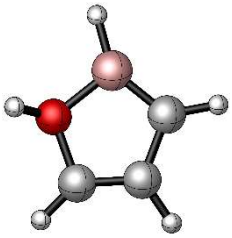	6.2	C	1.234643000	0.400516000	0.006481000
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	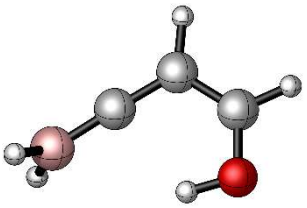	26.2	C	-1.018890000	0.346284000	0.014815000
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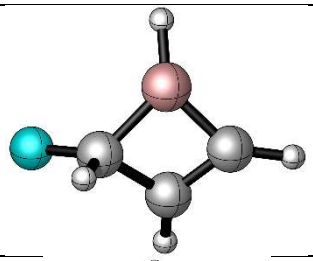
11		0.0	C	1.633414000	-0.026389000	0.025197000
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			F	-1.747371000	-0.021113000	-0.238029000
			C	-0.536832000	0.031789000	0.447970000
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	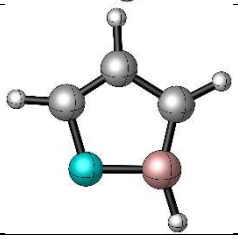	10.9	C	1.219807000	0.407021000	0.000000000
			B	0.905209000	-0.988445000	0.000000000
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	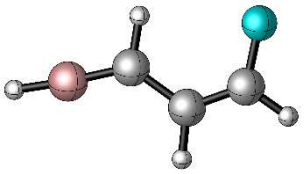	14.4	C	-1.125206000	-0.268399000	0.000152000
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			H	-0.764401000	-1.300575000	0.000325000
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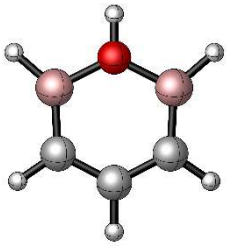
12		0.0	C	1.242188000	-0.770348000	0.000000000
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	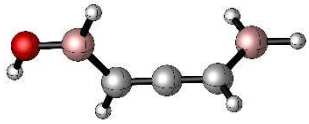	17.6	C	1.989657000	-0.351497000	0.380771000
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			B	-1.617332000	0.351565000	0.346174000
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			H	2.511387000	1.351014000	-1.166835000
			H	4.069817000	0.713882000	0.023087000
			H	-1.341602000	1.119306000	1.211960000
			H	-0.764675000	-1.224262000	-1.125591000
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	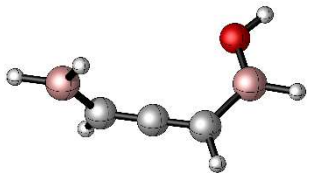	17.9	C	-1.711871000	-0.039935000	-0.544593000
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			B	1.909740000	-0.260843000	0.201927000
			O	1.899419000	1.054530000	-0.134307000
			B	-2.613493000	0.570201000	0.529658000
			H	-3.661686000	1.048735000	0.229054000
			H	-2.267256000	0.562886000	1.667375000
			H	2.924937000	-0.790482000	0.546240000
			H	0.604055000	-2.133023000	0.397444000
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	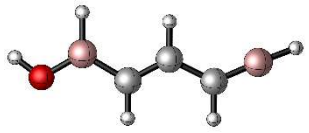	29.3	C	2.056372000	-0.355726000	-0.000364000
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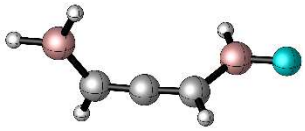
13		0.0	C	-1.964714000	-0.376282000	-0.364853000
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			C	0.538152000	-0.518635000	0.382035000
			B	1.604488000	0.316096000	-0.350695000
			F	2.868125000	0.242092000	0.054183000
			B	-2.876646000	0.689149000	0.255108000
			H	-4.011160000	0.775403000	-0.092217000
			H	-2.444890000	1.425936000	1.081595000
			H	1.350878000	1.029701000	-1.268834000
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	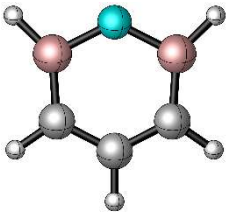	0.2	C	1.244047000	-0.748768000	-0.000000000
			C	-0.000399000	-1.391443000	0.000000000
			C	-1.244393000	-0.748250000	0.000000000
			B	-1.338294000	0.701965000	0.000000000
			F	-0.000000000	1.384804000	-0.000000000
			B	1.339345000	0.701034000	-0.000000000
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			H	-2.178535000	1.528410000	0.000000000
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	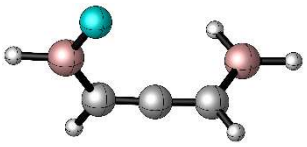	1.1	C	1.671923000	0.070533000	-0.546214000
			C	0.515897000	0.589434000	-0.214032000
			C	-0.646123000	1.064069000	0.146746000
			B	-1.915290000	0.186846000	0.197939000
			F	-1.856318000	-1.097763000	-0.132919000
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			H	2.235668000	-0.526907000	1.666685000
			H	-2.973274000	0.623739000	0.529108000
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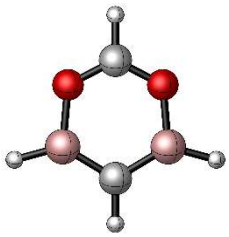
14		0.0	O	1.125354000	0.712624000	0.000000000
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	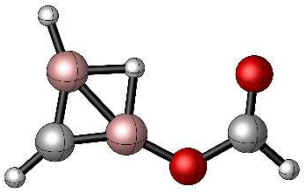	24.5	O	-1.833528000	0.918056000	0.000459000
			C	-1.701935000	-0.269161000	-0.000095000
			O	-0.518235000	-0.931993000	-0.000291000
			B	0.713667000	-0.287540000	-0.000151000
			C	2.134040000	-0.444167000	0.000409000
			B	1.883141000	0.970736000	-0.000319000
			H	-2.524707000	-0.991939000	-0.000524000
			H	2.938205000	-1.151485000	0.001232000
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	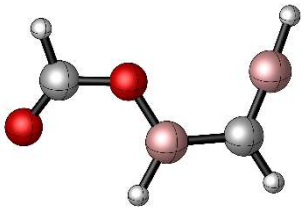	32.7	O	-2.335211000	-0.408933000	-0.212599000
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			H	-1.977924000	1.512463000	0.323846000
			H	2.591686000	-1.494648000	0.021468000
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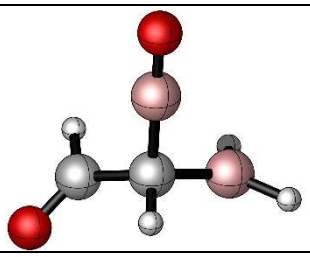
15		0.0	O	2.179992000	0.731223000	-0.170955000
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			O	-2.310363000	0.887700000	0.103555000
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			B	-0.200721000	-1.853607000	0.113323000
			H	1.084384000	0.327634000	1.471422000
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	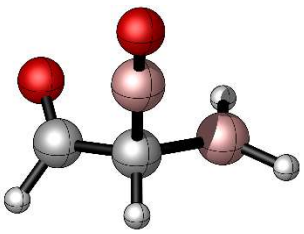	1.5	O	1.641766000	-0.918419000	-0.564872000
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			O	-2.219117000	-0.778051000	-0.184675000
			C	0.075252000	0.535316000	0.551727000
			B	0.101152000	1.779483000	-0.415143000
			H	1.849344000	-0.507169000	1.392376000
			H	-0.577010000	2.717603000	-0.153878000
			H	-0.099179000	0.850375000	1.586223000
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	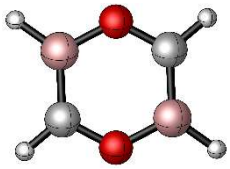	7.1	O	-0.000000000	1.378636000	0.000000000
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			B	1.236461000	-0.731673000	0.000000000
			O	0.000001000	-1.378679000	0.000000000
			C	-1.172126000	-0.762874000	0.000000000
			B	-1.236570000	0.731633000	0.000000000
			H	2.002332000	1.459356000	0.000000000
			H	2.206018000	-1.410792000	0.000000000
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	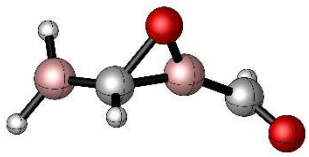	44.1	O	2.445878000	-0.228666000	0.404986000
			C	1.566476000	-0.335047000	-0.422351000
			B	0.110454000	0.176525000	-0.108728000
			O	-0.666656000	1.220706000	-0.259992000
			C	-1.303008000	0.057474000	0.543602000
			B	-2.300882000	-0.840213000	-0.143927000
			H	1.779161000	-0.807520000	-1.405703000
			H	-2.517200000	-0.732108000	-1.308295000
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	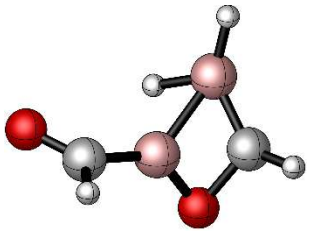	47.5	O	-2.321179000	0.256978000	-0.217208000
			C	-1.413602000	-0.258887000	0.396913000
			B	0.094539000	-0.138650000	-0.054558000
			O	1.024065000	-1.075046000	-0.397414000
			C	1.730397000	-0.001891000	0.254491000
			B	1.158515000	1.296681000	-0.107046000
			H	-1.628915000	-0.850435000	1.315030000
			H	0.324576000	1.119295000	-1.022357000
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	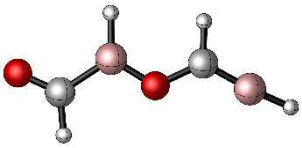	62.3	O	-2.920435000	0.094301000	0.000876000
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			B	-0.479197000	0.464739000	-0.000437000
			O	0.673757000	-0.234820000	-0.000688000
			C	1.926707000	0.345501000	-0.000164000
			B	3.148561000	-0.322830000	0.000851000
			H	-1.720995000	-1.517657000	-0.001372000
			H	-0.489540000	1.656303000	-0.000112000
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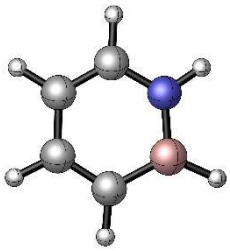
16		0.0	C	-1.206431000	-0.731182000	0.000000000
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			N	1.182671000	0.680745000	0.000000000
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			H	0.049143000	2.437883000	0.000000000
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	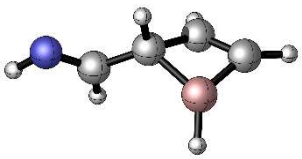	74.0	B	1.113065000	1.025723000	0.065724000
			C	2.179600000	-0.013493000	-0.110679000
			H	3.225562000	-0.211377000	0.054026000
			C	1.100959000	-0.817725000	0.087881000
			H	1.033116000	-1.754691000	0.638519000
			C	-0.068800000	0.018517000	-0.386398000
			H	-0.219596000	-0.038612000	-1.460281000
			C	-1.354247000	-0.038562000	0.347580000
			H	-1.274125000	-0.111455000	1.441281000
			N	-2.470271000	0.014758000	-0.253836000
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	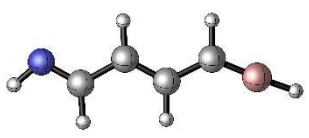	82.6	B	3.268795000	-0.187954000	0.000581000
			C	1.986615000	0.342431000	-0.000327000
			H	1.981266000	1.436138000	-0.000564000
			C	0.694786000	-0.298371000	-0.000385000
			H	0.684716000	-1.384084000	-0.000584000
			C	-0.491283000	0.340132000	-0.000217000
			H	-0.543665000	1.422915000	0.000000000
			C	-1.755977000	-0.364495000	-0.000054000
			H	-1.683004000	-1.459460000	-0.000635000
			N	-2.872539000	0.255079000	0.000451000
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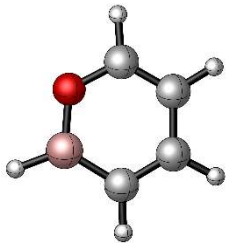
17		0.0	C	1.174376000	-0.754769000	0.000000000
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			O	-1.183356000	0.720787000	-0.000000000
			C	0.000000000	1.343283000	0.000000000
			C	1.173652000	0.672236000	0.000000000
			H	2.134520000	-1.260033000	0.000000000
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	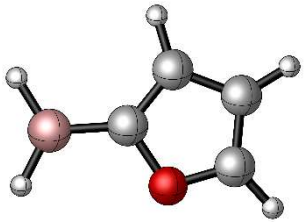	37.9	C	-0.112227000	1.148068000	0.000109000
			C	0.754688000	0.073751000	0.000300000
			B	2.257783000	-0.020933000	-0.000260000
			O	-0.024291000	-1.082680000	0.000168000
			C	-1.307537000	-0.710723000	-0.000024000
			C	-1.433096000	0.650245000	-0.000259000
			H	0.193722000	2.180741000	0.000214000
			H	2.886019000	0.989274000	0.000267000
			H	2.804601000	-1.075741000	-0.000875000
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	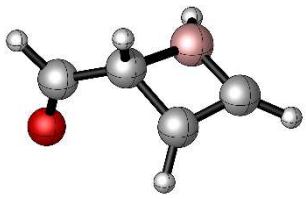	60.3	C	0.850601000	-0.745094000	0.338679000
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			B	1.036028000	0.872114000	-0.533111000
			O	-1.918155000	-0.539799000	-0.520792000
			C	-1.485568000	0.315644000	0.217374000
			C	-0.056388000	0.434543000	0.588988000
			H	0.525616000	-1.781928000	0.329988000
			H	2.936631000	-0.653647000	-0.380443000
			H	0.871460000	1.467872000	-1.543574000
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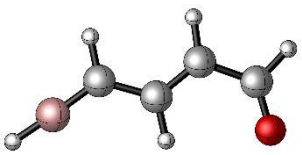
		71.5	C	-0.509244000	-0.078541000	-0.000058000
			C	-1.894441000	0.303735000	-0.000104000
			B	-3.018410000	-0.514409000	0.000108000
			O	2.255059000	-0.885598000	-0.000022000
			C	1.919910000	0.282684000	0.000036000
			C	0.540670000	0.769059000	0.000093000
			H	-0.272591000	-1.137046000	-0.000280000
			H	-2.111206000	1.374180000	-0.000445000
			H	-3.989572000	-1.163179000	0.000310000
			H	2.691516000	1.078386000	0.000030000
			H	0.392067000	1.842869000	0.000224000

Figure S1. Integration planes considered to average the RCS.

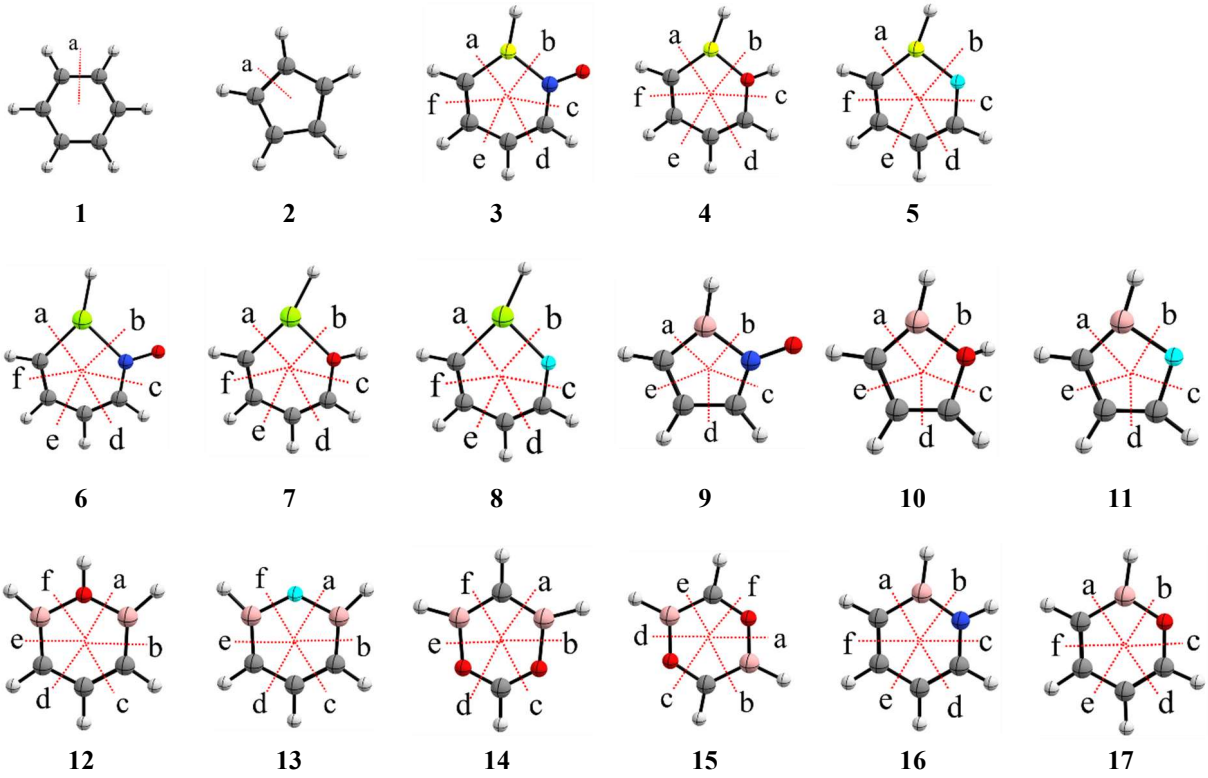


Figure S2. Plot of normalized $NICS_{zz}$ vs normalized RCS computations.

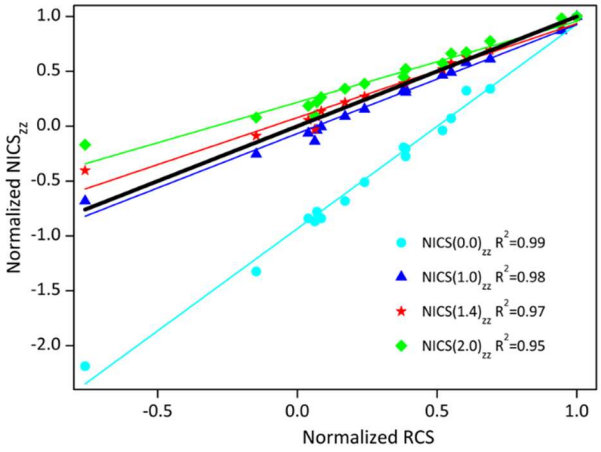


Figure S3. Vector plot visualization of the current density at two different planes for all the systems studied.

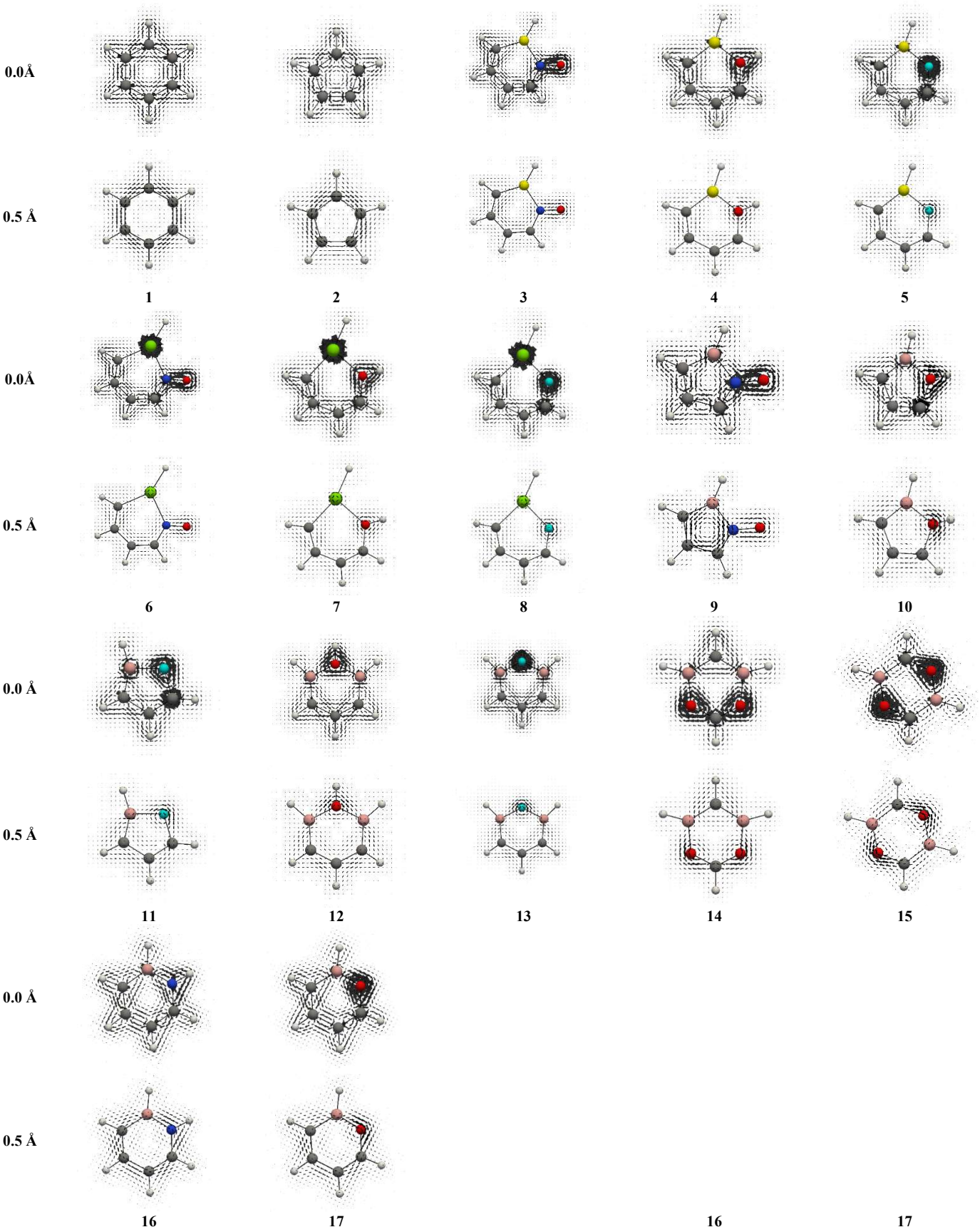
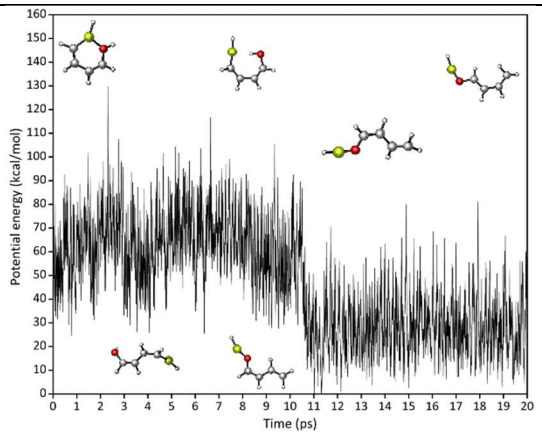
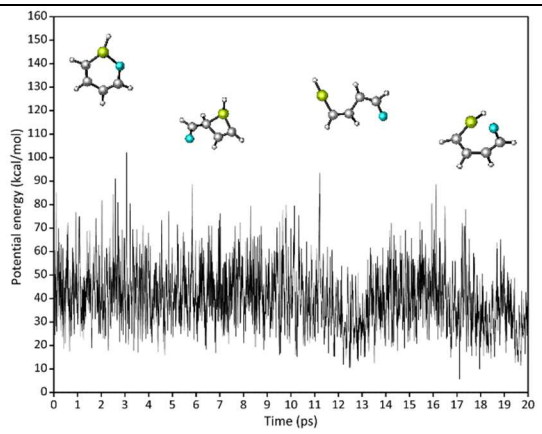


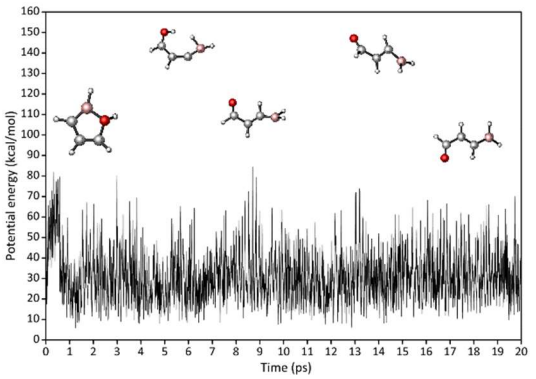
Figure S4. Energy profiles showing molecular structural changes along the BOMD simulations.



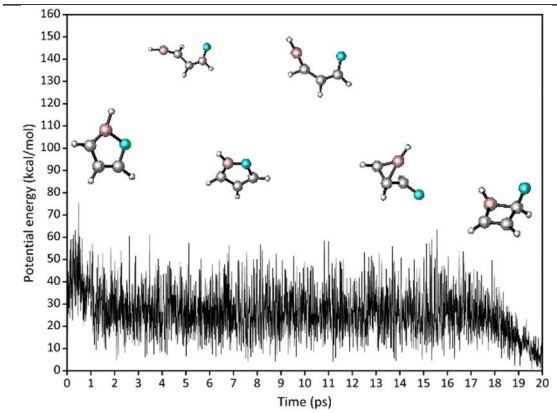
System 4



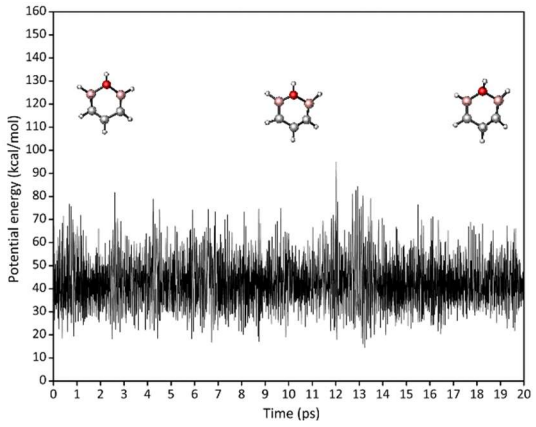
System 5



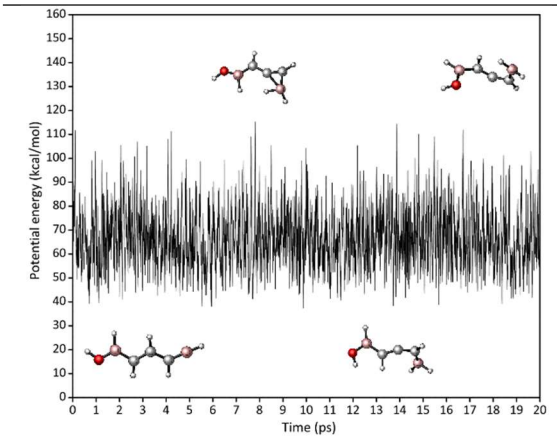
System 10



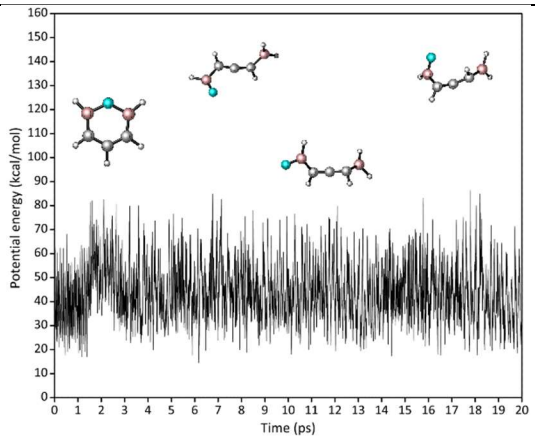
System 11



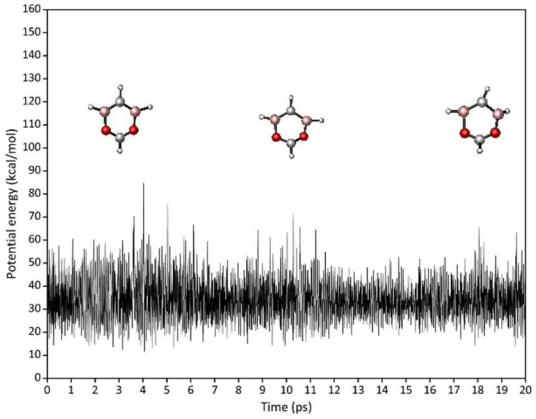
System 12



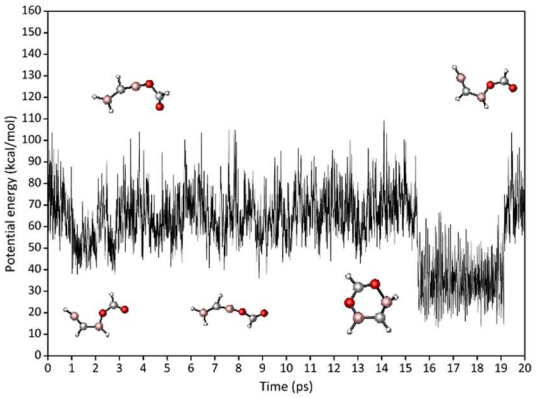
Linear system 12



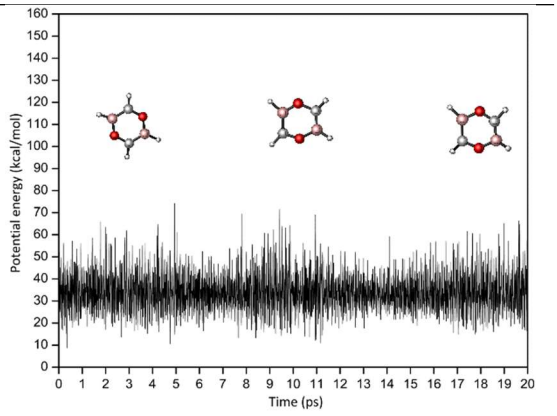
System 13



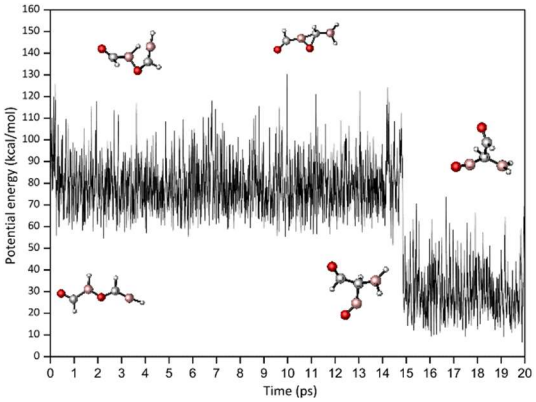
System 14



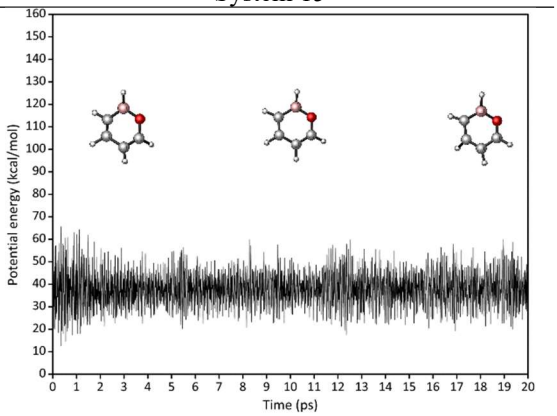
Linear system 14



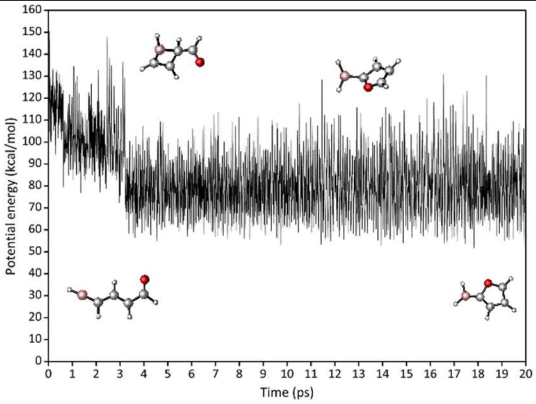
System 15



Linear system 15



System 17



Linear system 17