ELECTRONIC SUPPLEMENTARY INFORMATION

Host-guest cooperative bridged bicylopolyynic (BBP) open-molecular cages with optical–switching properties

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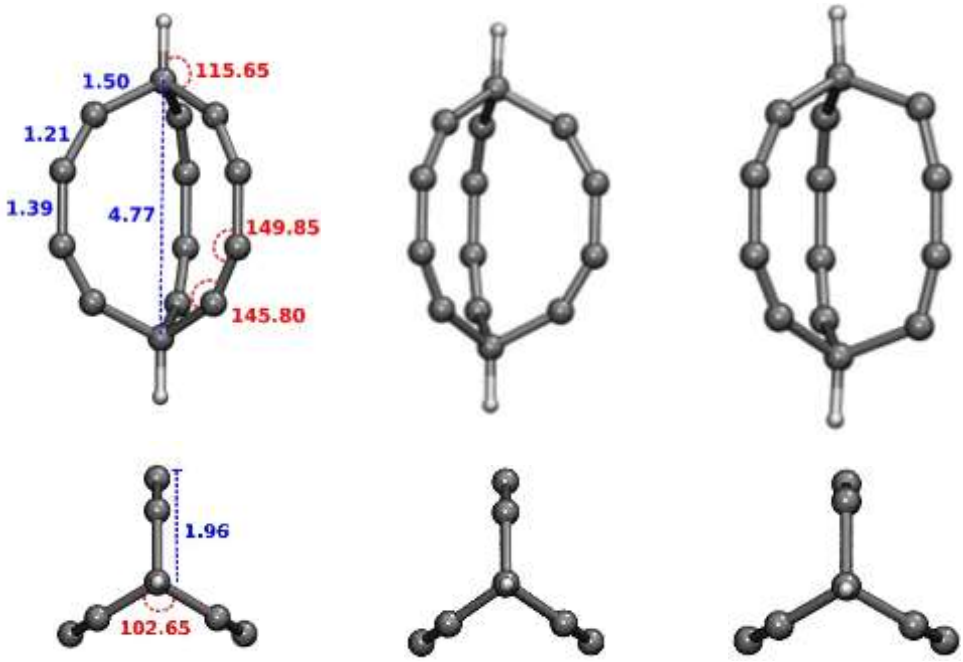
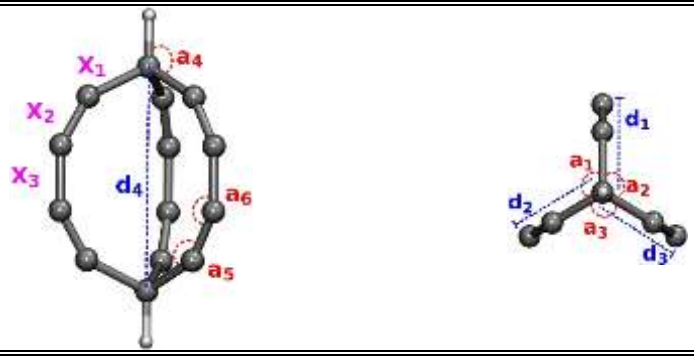
S1. Optimized geometries and important geometrical parameters of the BBP cages in its electronic ground state



BTH (neutral) **BTH (cation)** **BTH (anion)**

Figure S1. Side and top view of the optimized geometries of BTH cage in electronic ground state.

Table S1. Important geometrical parameters and deformation parameter (DP) in the optimized geometries of neutral and charged BTH cages.



Geometrical Parameters of Neutral BTH ($C_{14}H_2$) cage				**Arm1 = Arm2 = Arm3**
Distance	**d_1**	1.958	**x_1**	1.499
	d_2	1.958	**x_2**	1.207
	d_3	1.958	**x_3**	1.386
	d_4	4.771		
Angle	**a_1**	102.648	**a_4**	115.648
	a_2	102.648	**a_5**	145.798

	a_3	102.648		a_6	149.851		

Geometrical Parameters of Cationic BTH ($C_{14}H_2$) cage

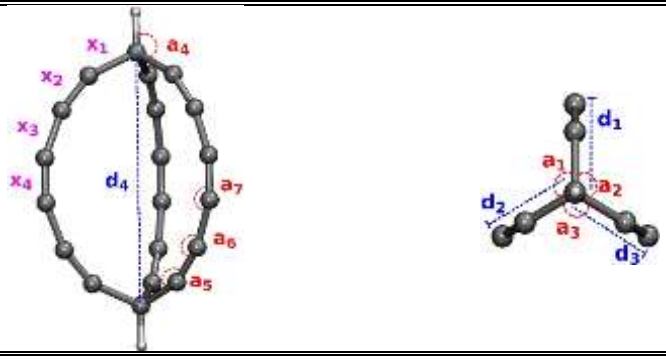
					Arm1		Arm2 = Arm3	
			DP			DP		DP
Distance	d_1	1.963	0.005	x_1	1.492	-0.007	1.492	-0.007
	d_2	1.901	-0.057	x_2	1.207	0.000	1.221	0.014
	d_3	1.901	-0.057	x_3	1.384	-0.002	1.357	-0.029
	d_4	4.861	0.090					
Angle	a_1	103.599	0.951	a_4	118.427	2.779	117.067	1.419
	a_2	103.599	0.951	a_5	145.178	-0.620	148.295	2.497
	a_3	93.334	-9.314	a_6	151.739	1.888	149.636	-0.215

Geometrical Parameters of Anionic BTH ($C_{14}H_2$) cage

					Arm1		Arm2 = Arm3	
			DP			DP		DP
Distance	d_1	1.777	-0.181	x_1	1.555	0.056	1.496	-0.003
	d_2	1.927	-0.031	x_2	1.254	0.047	1.212	0.005
	d_3	1.927	-0.031	x_3	1.335	-0.051	1.381	-0.005
	d_4	4.816	0.045					
Angle	a_1	106.126	3.478	a_4	112.715	-2.933	114.545	-1.103
	a_2	106.126	3.478	a_5	123.551	-22.247	145.142	-0.656
	a_3	101.747	-0.901	a_6	166.110	16.259	150.861	1.010

* All the distances are given in Å and angles are in ° (degree)

Table S2. Important geometrical parameters and deformation parameter (DP) in the optimized geometries of neutral and charged BIN cages.



Geometrical Parameters of Neutral BIN ($C_{20}H_2$) cage

				Arm1 = Arm2 = Arm3
Distance	d_1	2.620	x_1	1.486
	d_2	2.620	x_2	1.206
	d_3	2.620	x_3	1.372
	d_4	6.847	x_4	1.211
Angle	a_1	104.083	a_4	114.435
	a_2	104.083	a_5	154.481
	a_3	104.083	a_6	160.948
			a_7	159.006

Geometrical Parameters of Cationic BIN ($C_{20}H_2$) cage								
					Arm1		Arm2 = Arm3	
			DP			DP		DP
Distance	d_1	2.624	0.004	x_1	1.481	-0.005	1.481	-0.005
	d_2	2.519	-0.101	x_2	1.206	0.000	1.216	0.010
	d_3	2.519	-0.101	x_3	1.371	-0.001	1.348	-0.024
	d_4	6.957	0.110	x_4	1.210	-0.001	1.223	0.012
Angle	a_1	105.047	0.964	a_4	116.737	2.302	115.705	1.270
	a_2	105.047	0.964	a_5	153.070	-1.411	155.633	1.152
	a_3	96.040	-8.043	a_6	162.670	1.722	161.027	0.079
				a_7	159.638	0.632	159.791	0.785

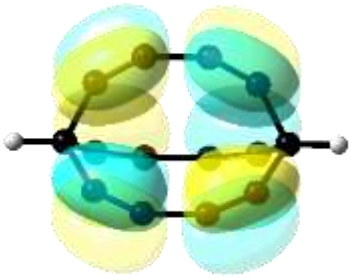
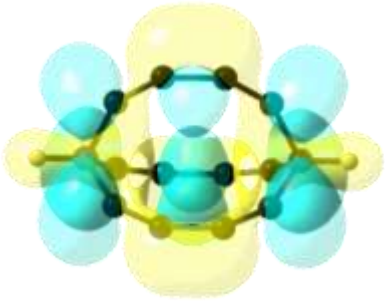
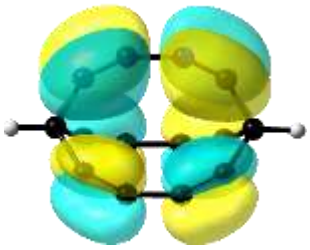
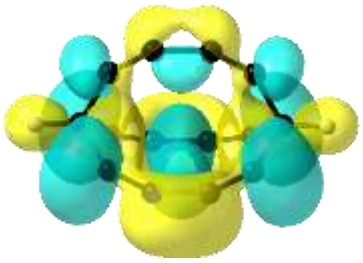
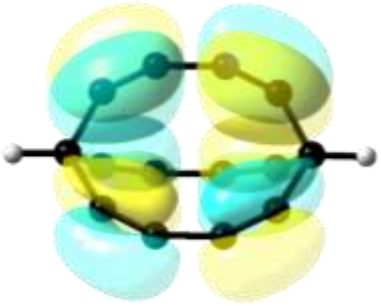
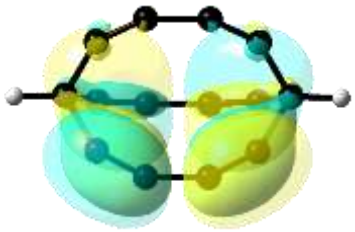
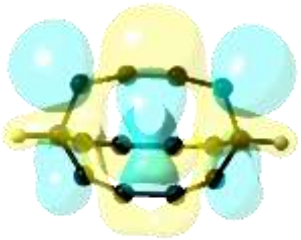
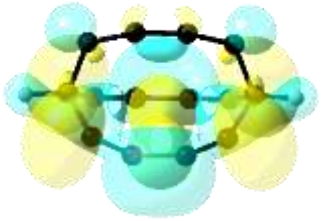
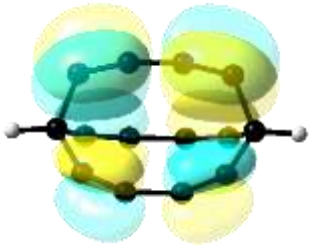
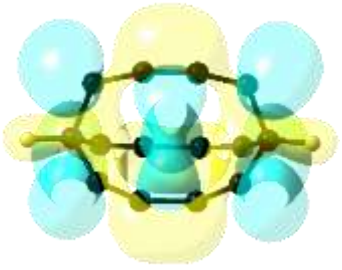
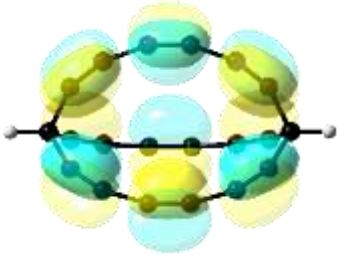
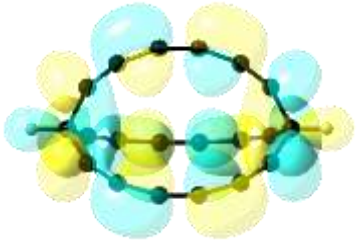
Geometrical Parameters of Anionic BIN ($C_{20}H_2$) cage								
					Arm1		Arm2 = Arm3	
			DP			DP		DP
Distance	d_1	2.232	-0.388	x_1	1.533	0.047	1.481	-0.005
	d_2	2.543	-0.077	x_2	1.25	0.044	1.209	0.003
	d_3	2.543	-0.077	x_3	1.328	-0.044	1.37	-0.002
	d_4	7.015	0.168	x_4	1.246	0.035	1.213	0.002
Angle	a_1	106.605	2.522	a_4	113.053	-1.382	113.51	-0.925
	a_2	106.605	2.522	a_5	126.886	-27.595	155.928	1.447
	a_3	102.725	-1.358	a_6	173.058	12.110	160.694	-0.254
				a_7	166.188	7.182	160.264	1.258

* All the distances are given in Å and angles are in ° (degree)

S2. Frontiers molecular orbitals analysis, dipole moment, point group for the neutral and charged BBP cages

Table S3. The calculated dipole moment, point group, and energy gap values between the HOMO and LUMO in neutral and charged BBP cages.

Systems	Dipole Moment (Debye)	Point Group	Energy gap (eV)	
			α spin state	β spin state
C_{14} (Neutral)	0.000	D_{3h}	6.03	--
C_{14} (Cation)	1.538	C_{2v}	5.90	3.33
C_{14} (Anion)	3.107	C_{2v}	3.98	5.00
C_{20} (Neutral)	0.000	D_{3h}	5.94	--
C_{20} (Cation)	2.185	C_{2v}	5.44	2.59
C_{20} (Anion)	3.843	C_{2v}	3.46	4.88

System	HOMO	LUMO
Neutral BTH		
Cationic BTH (α-spin state)		
Cationic BTH (β-spin state)		
Anionic BTH (α-spin state)		
Anionic BTH (β-spin state)		
Neutral BIN		

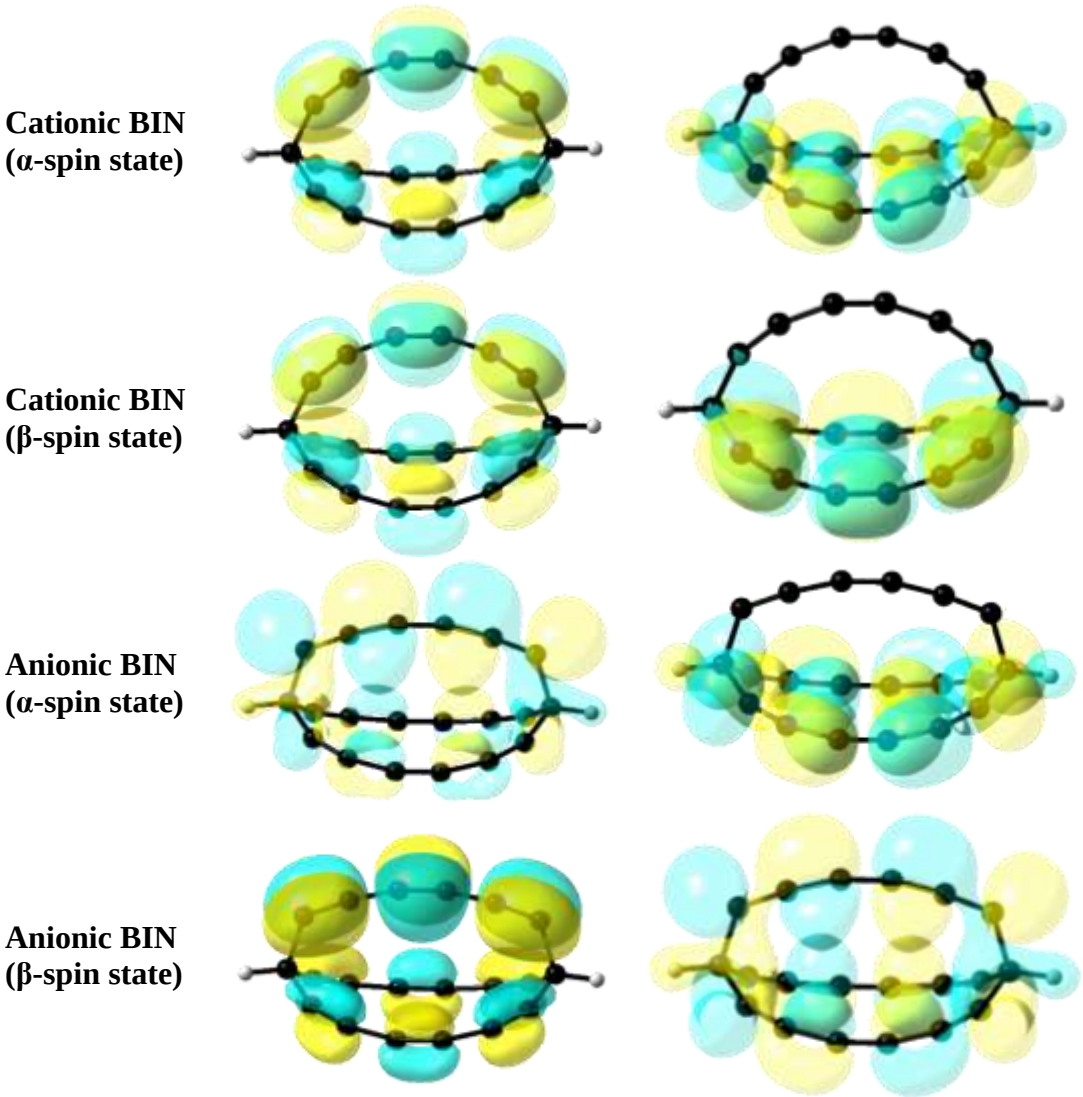


Figure S2. HOMO and LUMO of the neutral and charged BTH and BIN cages

S3. MESP and NPA charges on BTH cage

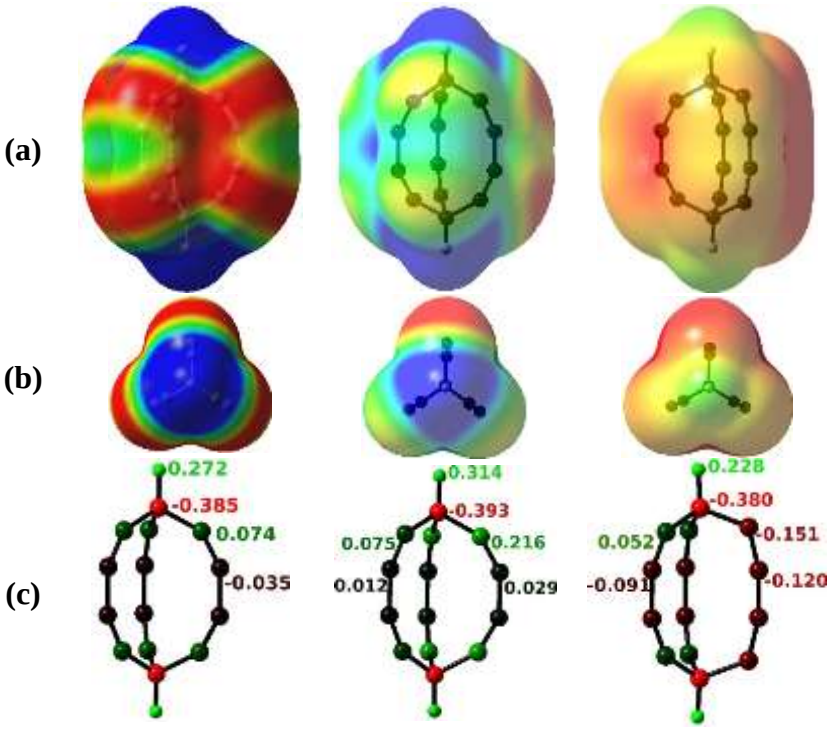


Figure S3. MESP and NPA charges on neutral and charged BTH cage. (a) Side view of the electrostatic potential, (b) Top view of the electrostatic potential, and (c) Atomic charges.

S4. Photophysical properties of neutral and charged BBP cages

Table S4. Oscillatory strength, excitation wavelength and absorption coefficient for the most important optical excitations in the neutral and charged BBP cages.

System	Oscillatory strength (f)	Excitation Wavelength (λ) in nm	Absorption coefficient (ε) in $Lmol^{-1}cm^{-1}$
Neutral BTH	0.027	315.51	939.11
	0.053	251.69	1796.40
Anionic BTH	0.012	733.29	972.01
	0.013	700.44	997.28
	0.078	386.22	3077.34
Cationic BTH	0.022	676.18	1399.84
	0.060	522.16	2342.62
	0.015	385.97	650.20
Neutral BIN	0.018	339.28	600.06
	0.042	256.52	1407.37
Anionic BIN	0.013	717.54	833.25
	0.063	505.69	4532.03
	0.016	454.56	4620.76
	0.075	454.17	4620.76
Cationic BIN	0.044	1010.24	2617.74
	0.051	790.53	2865.76
	0.021	560.62	1636.03
	0.018	526.49	1441.98

S5. Optimized geometries of the complexes of BTH cage with guest (Li^+, Li, Ne, Ar) atom/ion.

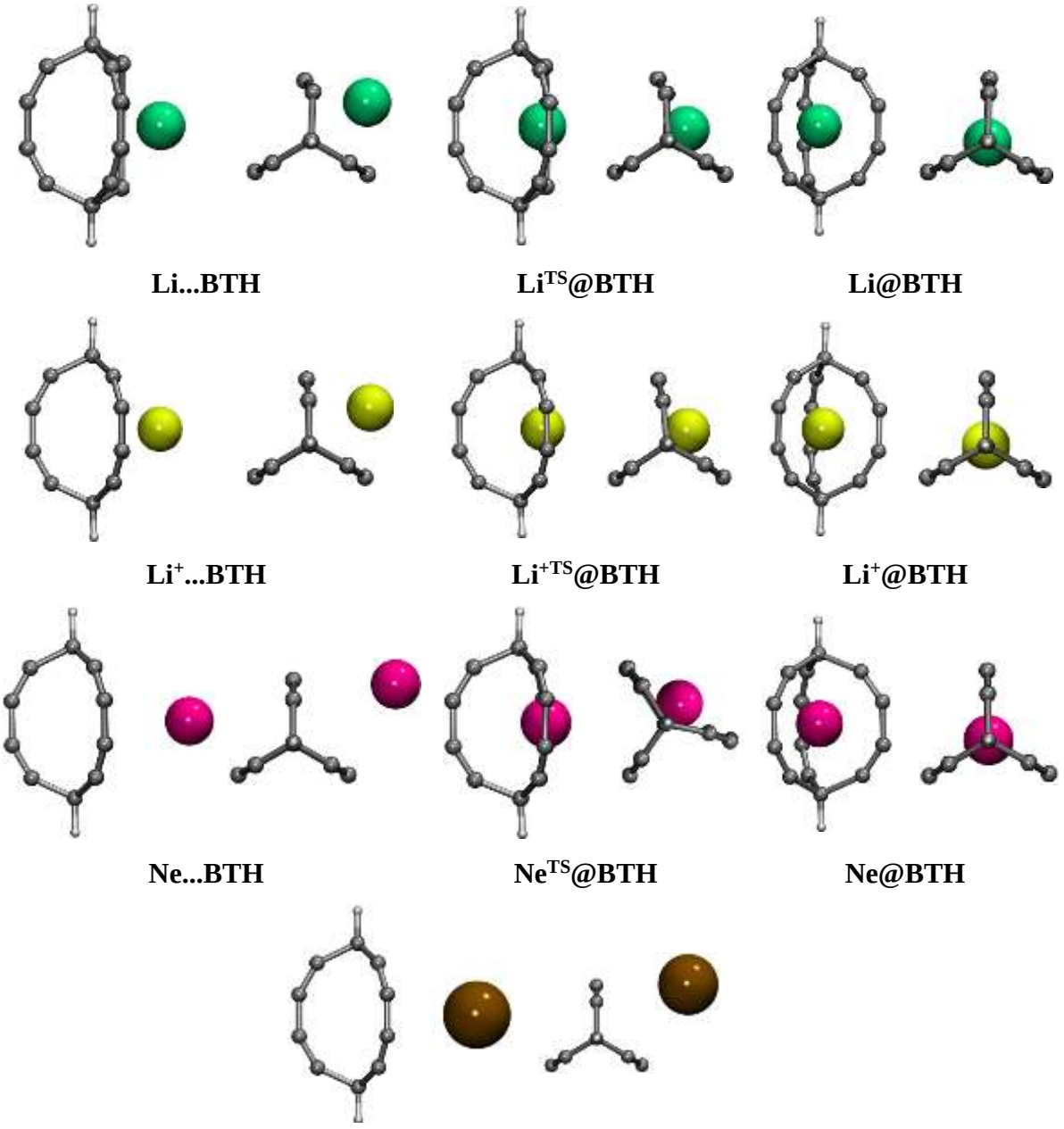


Figure S4. Side and top view of the optimized geometries the complexes of BTH cage with guest (Li+, Li, Ne, Ar) atom/ion in their electronic ground state.

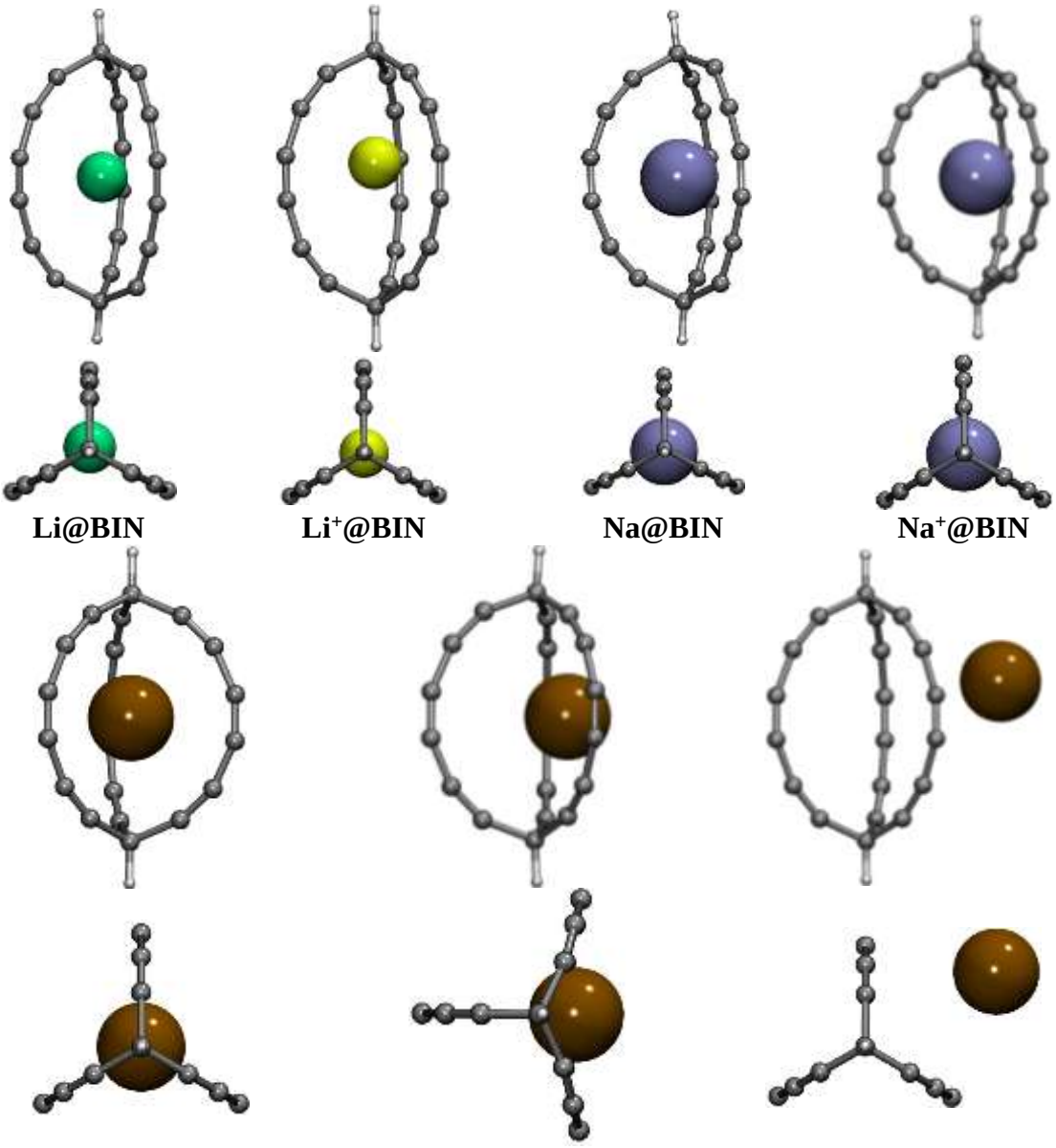


Figure S5. Side and top view of the optimized geometries the complexes of BIN cage with guest (Li, Na, and Ar) atom/ion in their electronic ground state.

Table S5. Geometrical parameters and deformation parameter (DP) in the complexes of BTH cage.

		Endohedral complex of Li with BTH (Li@BTH)						
					Arm1		Arm2 = Arm3	
			DP			DP		DP
C – C								
Distance	**d1**	1.912	-0.046	**X1**	1.560	0.061	1.506	0.007
	d2	1.983	0.025	**X2**	1.249	0.042	1.216	0.009
	d3	1.983	0.025	**X3**	1.349	-0.037	1.391	0.005
	d4	4.786	0.015					
Angle	**a1**	105.650	3.002	**a4**	113.141	-2.507	114.840	-0.808
	a2	105.650	3.002	**a5**	130.537	-15.261	147.973	2.175

	a3	101.532	-1.116	**a6**	159.925	10.074	148.060	-1.791

Li – C Distances: Li – C (Arm1) = 2.028, Li – C (Arm2=Arm3) = 2.101 ; Li – CH = 2.393

TS complex of Li with BTH (Li^{TS}@BTH)

					Arm1		Arm2	
			DP			DP		DP
C – C								
Distance	**d1**	1.954	-0.004	**X1**	1.568	0.069	1.491	-0.008
	d2	2.054	0.096	**X2**	1.253	0.046	1.213	0.006
	d3	1.936	-0.022	**X3**	1.357	-0.029	1.376	-0.010
	d4	4.749	-0.022					
Angle	**a1**	107.085	4.437	**a4**	112.167	-3.481	116.007	0.359
	a2	106.265	3.617	**a5**	132.139	-13.659	143.138	-2.660
	a3	100.595	-2.053	**a6**	154.956	5.105	145.092	-4.759

Li – C Distances: Li – C (Arm1) = 1.985; Li – C (Arm2=Arm3) = 1.930 ; Li – CH = 2.469 ; Li – Center = 0.660

Exohedral complex of Li with BTH (Li...BTH)

					Arm1		Arm2	
			DP			DP		DP
C – C								
Distance	**d1**	1.809	-0.149	**X1**	1.559	0.060	1.495	-0.004
	d2	1.922	-0.036	**X2**	1.259	0.052	1.213	0.006
	d3	1.984	0.026	**X3**	1.336	-0.050	1.393	0.007
	d4	4.800	0.029					
Angle	**a1**	103.084	0.436	**a4**	112.794	-2.854	114.653	-0.995
	a2	107.388	4.740	**a5**	125.075	-20.723	149.723	3.925
	a3	101.560	-1.088	**a6**	160.430	10.579	147.402	-2.449

Li – C Distances: Li – C (Arm1) = 2.093 and Li – C (Arm2) = 2.256 ; Li – CH = 3.149; Li – Centre = 2.038

Endohedral complex of Li^+ with BTH (Li^+@BTH)

					Arm1 = Arm2 = Arm3	
			DP			DP
C – C						
Distance	**d1**	2.006	0.048	**X1**	1.513	0.014
	d2	2.006	0.048	**X2**	1.211	0.004
	d3	2.006	0.048	**X3**	1.399	0.013
	d4	4.775	0.004			
Angle	**a1**	102.224	-0.424	**a4**	116.000	0.352
	a2	102.224	-0.424	**a5**	148.231	2.433
	a3	102.224	-0.424	**a6**	147.769	-2.082

Li+ – C Distances: Li+ – C = 2.124 : Li+ – CH = 2.387

TS complex of Li^+ with BTH (Li^{+TS}@BTH)

					Arm1		Arm2 = Arm3	
			DP			DP		DP
Distance	**d1**	1.959	0.001	**X1**	1.498	-0.001	1.522	0.023
	d2	2.059	0.101	**X2**	1.207	0.000	1.214	0.007

	d3	2.059	0.101	**X3**	1.386	0.000	1.410	0.024
	d4	4.737	-0.034					
Angle	**a1**	101.57	-1.078	**a4**	117.043	1.395	114.908	-0.740
	a2	101.57	-1.078	**a5**	144.533	-1.265	150.425	4.627
	a3	104.935	2.287	**a6**	150.240	0.389	145.176	-4.675

Li+ – C Distances: Li+ – C = 1.986; Li+ – CH = 2.490 ; Li+ – centre = 0.766

Exohedral complex of Li^+ with BTH (Li^+...BTH)

			Arm1			Arm2 = Arm3		
			DP			**DP**		**DP**
Distance	**d1**	1.938	-0.020	**X1**	1.494	-0.005	1.500	0.001
	d2	1.994	0.036	**X2**	1.206	-0.001	1.210	0.003
	d3	1.994	0.036	**X3**	1.384	-0.002	1.394	0.008
	d4	4.777	0.006					
Angle	**a1**	102.264	-0.384	**a4**	116.972	1.324	115.730	0.082
	a2	102.264	-0.384	**a5**	144.870	-0.928	148.662	2.864
	a3	101.608	-1.040	**a6**	150.691	0.840	147.603	-2.248

Li+ – C Distances: Li+ – C = 2.244; Li+ – CH = 3.227 ; Li1 – centre = 2.170

Endohedral complex of Ne with BTH (Ne@BTH)

			Arm1 = Arm2 = Arm3			
			DP			**DP**
Distance	**d1**	2.126	0.168	**X1**	1.542	0.043
	d2	2.126	0.168	**X2**	1.218	0.011
	d3	2.126	0.168	**X3**	1.419	0.033
	d4	4.600	-0.171			
Angle	**a1**	105.947	3.299	**a4**	112.800	-2.848
	a2	105.947	3.299	**a5**	148.139	2.341
	a3	105.947	3.299	**a6**	144.661	-5.190

Ne – C Distances: Ne – C = 2.241; Ne – CH = 2.300

TS complex of Ne with BTH (Ne^{TS}@BTH)

			Arm1			Arm2 = Arm3		
			DP			**DP**		**DP**
Distance	**d1**	2.029	0.071	**X1**	1.498	-0.001	1.569	0.07
	d2	2.173	0.215	**X2**	1.208	0.001	1.222	0.015
	d3	2.173	0.215	**X3**	1.387	0.001	1.435	0.049
	d4	4.597	-0.174					
Angle	**a1**	100.925	-1.723	**a4**	114.919	-0.729	111.761	-3.887
	a2	100.925	-1.723	**a5**	145.681	-0.117	148.337	2.539
	a3	115.75	13.102	**a6**	147.403	-2.448	143.329	-6.522

Ne – C Distances: Ne – C (Arm2=Arm3) = 2.168; Ne – CH = 2.366; Ne – centre = 0.564

Exohedral complex of Ne with BTH (Ne…BTH)

			Arm1			Arm2 = Arm3		
			DP			**DP**		**DP**
Distance	**d1**	1.958	0.000	**X1**	1.500	0.001	1.500	0.001

	d2	1.958	0.000	**X2**	1.207	0.000	1.207	0.000
	d3	1.958	0.000	**X3**	1.386	0.000	1.386	0.000
	d4	4.771	0.000					
Angle	**a1**	102.651	0.003	**a4**	115.642	-0.006	115.644	-0.004
	a2	102.651	0.003	**a5**	145.836	0.038	145.779	-0.019
	a3	102.662	0.014	**a6**	149.819	-0.032	149.858	0.007
Ne – C Distances: Ne – C = 3.246 : Ne – CH = 4.366 ; Ne – Centre = 3.657								

Exohedral complex of Ar with BTH (Ar…BTH)

					Arm1		**Arm2 = Arm3**	
			DP			**DP**		**DP**
Distance	**d1**	1.958	0.000	**X1**	1.499	0.000	1.499	0.000
	d2	1.958	0.000	**X2**	1.207	0.000	1.207	0.000
	d3	1.958	0.000	**X3**	1.386	0.000	1.386	0.000
	d4	4.771	0.000					
Angle	**a1**	102.645	-0.003	**a4**	115.651	0.003	115.500	-0.148
	a2	102.645	-0.003	**a5**	145.796	-0.002	145.805	0.007
	a3	102.649	0.001	**a6**	149.853	0.002	149.845	-0.006
Ar – C Distances: Ar – C Arm = 3.503 ; Ar – CH = 4.625 ; Ar – Centre = 3.962								

* All the distances are given in Ang and angle are in ° (degree)

Table S6. Geometrical parameters and deformation parameter (DP) in the complexes of BIN cage.

Endohedral complex of Li with BIN (Li@BIN)								
					Arm1		Arm2 = Arm3	
			DP			DP		DP
Distance	**d1**	2.134	-0.486	**X1**	1.521	0.035	1.483	-0.003
	d2	2.456	-0.164	**X2**	1.241	0.035	1.210	0.004
	d3	2.456	-0.164	**X3**	1.336	-0.036	1.369	-0.003
	d4	7.155	0.308	**X4**	1.247	0.036	1.216	0.005
Angle	**a1**	104.894	0.811	**a4**	114.445	0.010	114.876	0.441
	a2	104.894	0.811	**a5**	131.474	-23.007	153.778	-0.703
	a3	101.394	-2.689	**a6**	171.214	10.266	160.029	-0.919
				a7	166.700	7.694	163.562	4.556
Li–C Distances: Li–C (Arm1) = 2.134 ; Li–C (Arm2) = 2.456 ; Li–CH = 3.578								

Endohedral complex of Li^+ with BIN (Li^+@BIN)									
					Arm2 = Arm3		Arm2 = Arm3		
			DP			DP		DP	
Distance	**d1**	2.508	-0.112	**X1**	1.488	0.002	**X1'**	1.486	0.000
	d2	2.508	-0.112	**X2**	1.207	0.001	**X2'**	1.205	-0.001
	d3	2.508	-0.112	**X3**	1.373	0.001	**X3'**	1.371	-0.001
	d4	7.007	0.160	**X4**	1.213	0.002			
Angle	**a1**	102.665	-1.418	**a4**	115.635	1.200	**a4'**	115.656	1.221
	a2	102.665	-1.418	**a5**	153.664	-0.817	**a5'**	154.045	-0.436
	a3	102.665	-1.418	**a6**	160.424	-0.524	**a6'**	158.942	-2.006
				a7	160.451	1.445	**a7'**	163.765	4.759
Li–C Distances: Li+ – C = 2.527 ; Li1 – CH = 3.087 ; Li1 – CH = 3.920									

Endohedral complex of Na with BIN (Na@BIN)								
					Arm1		Arm2 = Arm3	
			DP			DP		DP
Distance	**d1**	2.451	-0.169	**X1**	1.523	0.037	1.481	-0.005

	d2	2.591	-0.029	**X2**	1.244	0.038	1.210	0.004
	d3	2.591	-0.029	**X3**	1.333	-0.039	1.372	0.000
	d4	6.930	0.083	**X4**	1.248	0.037	1.216	0.005
Angle	**a1**	106.104	2.021	**a4**	113.794	-0.641	113.709	-0.726
	a2	106.104	2.021	**a5**	131.941	-22.540	158.867	4.386
	a3	102.416	-1.667	**a6**	172.548	11.600	158.406	-2.542
				a7	162.409	3.403	158.777	-0.229

Na–C Distances: Na–C (Arm1) = 2.529 ; Na–C (Arm2) = 2.661 ; Na–CH = 3.466

Endohedral complex of Na^+ with BIN (Na^+@BIN)

			DP		**Arm1 = Arm2 = Arm3**	
Distance	**d1**	2.658	0.038	**X1**	1.487	0.001
	d2	2.658	0.038	**X2**	1.206	0.000
	d3	2.658	0.038	**X3**	1.375	0.003
	d4	6.819	-0.028	**X4**	1.213	0.002
Angle	**a1**	103.578	-0.505	**a4**	114.866	0.431
	a2	103.578	-0.505	**a5**	156.691	2.210
	a3	103.578	-0.505	**a6**	159.720	-1.228
				a7	158.456	-0.550

Na+–C Distances: Na1 – C = 2.727 ; Na1 – CH = 3.409

Endohedral complex of K with BIN (K@BIN)

			Arm1			**Arm2**		**Arm3**
			DP			**DP**		**DP**
C – C Distance	**d1**	2.698	0.078	**X1**	1.522	0.036	1.485	-0.001	1.486
	d2	2.760	0.140	**X2**	1.242	0.036	1.212	0.006	1.212
	d3	2.762	0.142	**X3**	1.339	-0.033	1.376	0.004	1.376
	d4	6.678	-0.169	**X4**	1.249	0.038	1.217	0.006	1.217
Angle	**a1**	107.281	3.198	**a4**	112.810	-1.625	112.405	-2.030	112.375
	a2	107.189	3.106	**a5**	137.502	-16.979	161.904	7.423	162.036

	a3	104.234	0.151	**a6**	172.664	11.716	157.853	-3.095	157.824
				a7	156.145	-2.861	155.655	-3.351	155.626

K–C Distances: K– C (Arm1) = 2.769; K– C (Arm2) = 2.829; K– C (Arm3) = 2.826; K– CH = 3.339

TS complex of K with BIN (K^{TS}@BIN)

					Arm1		Arm2		Arm3
			DP			DP		DP	
C – C Distance	**d1**	2.717	0.097	**X1**	1.521	0.035	1.494	0.008	1.481
	d2	2.930	0.310	**X2**	1.246	0.040	1.212	0.006	1.210
	d3	2.489	-0.131	**X3**	1.343	-0.029	1.383	0.011	1.364
	d4	6.637	-0.210	**X4**	1.250	0.039	1.217	0.006	1.215
Angle	**a1**	106.897	2.814	**a4**	111.991	-2.444	111.616	-2.819	114.260
	a2	109.176	5.093	**a5**	139.399	-15.082	163.247	8.766	151.733
	a3	102.345	-1.738	**a6**	163.581	2.633	156.959	-3.989	160.488
				a7	154.790	-4.216	154.603	-4.403	158.371

K–C Distances: K–C (Arm1) = 2.681; K–C (Arm2) = 2.749; K– C (Arm3) = 3.642; K–CH = 3.443; K–Centre = 1.103

Exohedral complex of K with BIN (K…BIN)

					Arm1		Arm2		Arm3
			DP			DP		DP	
C – C Distance	**d1**	2.429	-0.191	**X1**	1.526	0.040	1.481	-0.005	1.480
	d2	2.477	-0.143	**X2**	1.249	0.043	1.209	0.003	1.208
	d3	2.718	0.098	**X3**	1.330	-0.042	1.373	0.001	1.368
	d4	6.885	0.038	**X4**	1.249	0.038	1.214	0.003	1.212
Angle	**a1**	107.652	3.569	**a4**	112.925	-1.510	112.928	-1.507	114.461
	a2	105.450	1.367	**a5**	130.901	-23.580	160.612	6.131	153.561
	a3	102.526	-1.557	**a6**	169.531	8.583	158.610	-2.338	161.460
				a7	160.472	1.466	157.966	-1.040	159.476

K–C Distances: K–C (Arm1) = 2.741; K0 – C (Arm2) = 2.874; K–C (Arm3) = 5.066; K–CH = 4.249; K–Centre = 2.598

Endohedral complex of Ne with BIN (Ne@BIN)

					Arm1=Arm2 = Arm3	
			DP			DP
C – C Distance	**d1**	2.739	0.119	**X1**	1.486	0.000
	d2	2.739	0.119	**X2**	1.206	0.000
	d3	2.739	0.119	**X3**	1.374	0.002
	d4	6.675	-0.172	**x4**	1.211	0.000
Angle	**a1**	104.914	0.831	**a4**	113.715	-0.720
	a2	104.914	0.831	**a5**	157.211	2.730
	a3	104.914	0.831	**a6**	160.024	-0.924
				a7	156.479	-2.527

Ne–C Distances: Ne – C = 2.805; Ne – CH = 3.338

TS complex of Ne with BIN (Ne^{TS}@BIN)

					Arm1		Arm2 = Arm3	
			DP			DP		DP
Distance	**d1**	2.721	0.101	**X1**	1.486	0.000	1.488	0.002
	d2	2.798	0.178	**X2**	1.205	-0.001	1.207	0.001
	d3	2.798	0.178	**X3**	1.371	-0.001	1.371	-0.001
	d4	6.620	-0.227	**X4**	1.210	-0.001	1.212	0.001
Angle	**a1**	103.863	-0.220	**a4**	114.021	-0.414	113.269	-1.166
	a2	103.863	-0.220	**a5**	154.349	-0.132	159.107	4.626
	a3	107.668	3.585	**a6**	159.983	-0.965	159.797	-1.151
				a7	157.440	-1.566	154.717	-4.289

Ne–C Distances: Ne – C = 2.629 ; Ne – CH = 3.501 ; Ne – Centre = 1.143

Exohedral complex of Ne with BIN (Ne...BIN)

					Arm2 = Arm3		Arm2 = Arm3		
			DP			DP		DP	
Distance	**d1**	2.508	-0.112	**X1**	1.488	0.002	**X1'**	1.486	0.000
	d2	2.508	-0.112	**X2**	1.207	0.001	**X2'**	1.205	-0.001
	d3	2.508	-0.112	**X3**	1.373	0.001	**X3'**	1.371	-0.001
	d4	7.007	0.160	**X4**	1.213	0.002			

Angle	**a1**	102.665	-1.418	**a4**	115.635	1.200	**a4'**	115.656	1.221
	a2	102.665	-1.418	**a5**	153.664	-0.817	**a5'**	154.045	-0.436
	a3	102.665	-1.418	**a6**	160.424	-0.524	**a6'**	158.942	-2.006
				a7	160.451	1.445	**a7'**	163.765	4.759

Ne–C Distances: Ne – C = 3.292 ; Ne – CH = 4.365 ; Ne – CH = 5.753 ; Ne – Center = 3.790

Endohedral complex of Ar with BIN (Ar@BIN)

					Arm1=Arm2 = Arm3	
			DP			**DP**
C – C Distance	**d1**	2.870	0.250	**X1**	1.493	0.007
	d2	2.870	0.250	**X2**	1.208	0.002
	d3	2.870	0.250	**X3**	1.381	0.009
	d4	6.465	-0.382	**x4**	1.214	0.003
Angle	**a1**	106.462	2.379	**a4**	112.335	-2.100
	a2	106.462	2.379	**a5**	160.140	5.659
	a3	106.462	2.379	**a6**	157.649	-3.299
				a7	154.546	-4.460

Ar–C Distances: Ar – CH = 3.232 ; Ar – C = 2.933

TS complex of Ar with BIN (Ar^{TS}@BIN)

					Arm1		**Arm2 = Arm3**	
			DP			**DP**		**DP**
Distance	**d1**	2.793	0.173	**X1**	1.485	-0.001	1.500	0.014
	d2	2.904	0.284	**X2**	1.205	-0.001	1.210	0.004
	d3	2.904	0.284	**X3**	1.371	-0.001	1.386	0.014
	d4	6.452	-0.395	**x4**	1.210	-0.001	1.216	0.005
Angle	**a1**	103.254	-0.829	**a4**	113.539	-0.896	111.834	-2.601
	a2	103.254	-0.829	**a5**	154.470	-0.011	160.812	6.331
	a3	112.564	8.481	**a6**	159.258	-1.690	156.706	-4.242
				a7	156.234	-2.772	153.535	-5.471

Ar–C Distances: Ar – CH = 3.339 ; Ar – C (Arm1) = 3.704 ; Ar – C (Arm2) = 2.813 ; Ar – Centre = 0.862

Exohedral complex of Ar with BIN (Ar...BIN)

					Arm2 = Arm3		Arm2 = Arm3		
			DP			DP		DP	
Distance	**d1**	2.621	0.001	**X1**	1.486	0.000	**X1'**	1.486	0.000
	d2	2.622	0.002	**X2**	1.206	0.000	**X2'**	1.206	0.000
	d3	2.622	0.002	**X3**	1.371	-0.001	**X3'**	1.371	-0.001
	d4	6.844	-0.003	**X4**	1.211	0.000			
Angle	**a1**	104.072	-0.011	**a4**	114.424	-0.011	**a4'**	114.417	-0.018
	a2	104.072	-0.011	**a5**	154.521	0.040	**a5'**	154.534	0.053
	a3	104.132	0.049	**a6**	160.984	0.036	**a6'**	160.954	0.006
				a7	158.882	-0.124	**a7'**	158.997	-0.009

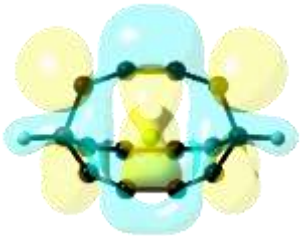
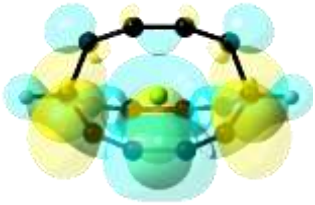
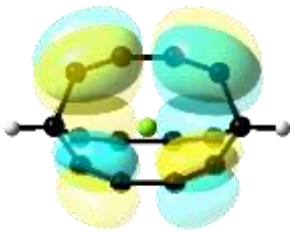
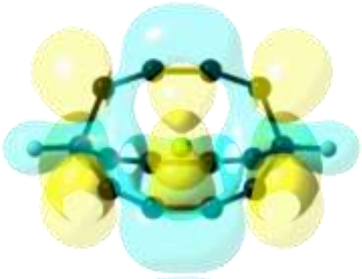
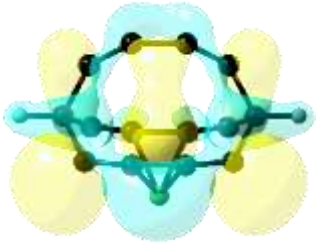
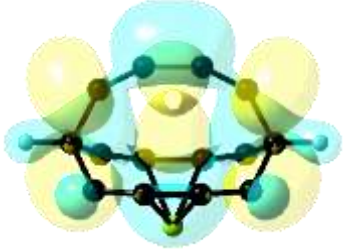
Ar–C Distances: Ar – C = 3.513; Ar – CH = 4.618; Ar – CH = 5.940 ; Ar – Centre = 4.073

* All the distances are given in Ang and angle are in ° (degree)

S6. Frontiers molecular orbitals, energy gap, dipole moment, point group of the studied complexes

Table S7. The calculated dipole moment, point group, and energy gap values between the HOMO and LUMO in various complexes of BTH and BIN cages.

Systems	Dipole Moment (Debye)	Point Group	Energy gap (eV)	
			α-spin state	β-spin state
Li@BTH	2.799	C_{2v}	3.74	5.44
Li...BTH	3.763	C_s	4.37	5.24
Li^+@BTH	0.000	D_{3h}	6.32	--
Li^+...BTH	5.270	C_{2v}	6.14	--
Ne@BTH	0.000	D_{3h}	6.34	--
Ne...BTH	0.028	C_{2v}	6.03	--
Ar...BTH	0.019	C_{2v}	6.03	--
Li@BIN	3.070	C_{2v}	3.39	4.91
Li^+@BIN	0.543	C_{3v}	5.83	--
Na@BIN	3.940	C_{2v}	3.28	5.11
Na^+@BIN	0.000	D_{3h}	6.08	--
K@BIN	4.128	C_s	3.05	5.33
K...BIN	6.483	C_1	3.51	5.07
Ne@BIN	0.000	D_{3h}	6.10	--
Ne...BIN	0.024	C_s	5.94	--
Ar@BIN	0.000	D_{3h}	6.30	--
Ar...BIN	0.024	C_s	5.94	--

System	HOMO	LUMO
Li@BTH (α-spin state)		
Li@BTH (β-spin state)		
Li…BTH (α-spin state)		

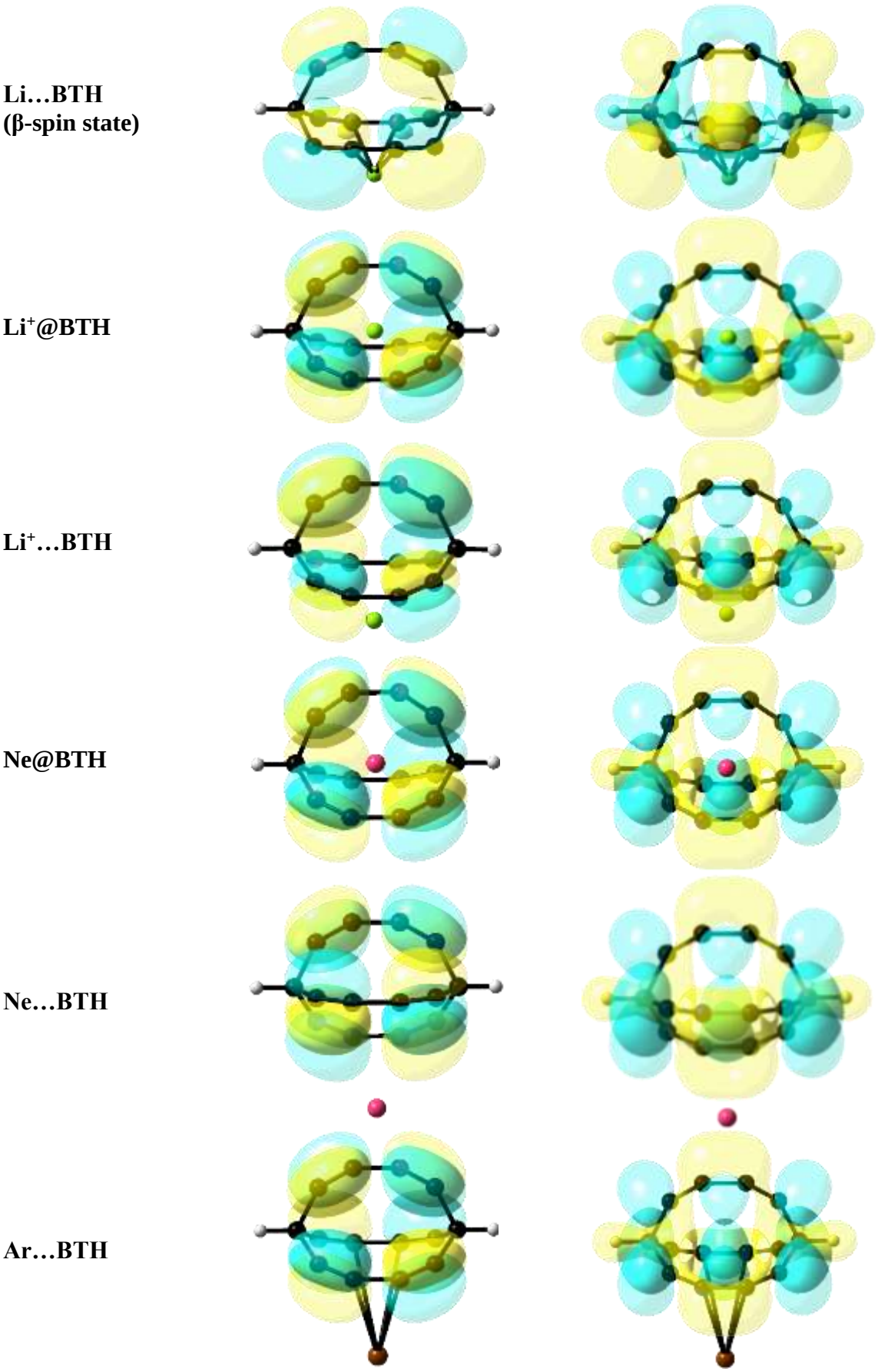
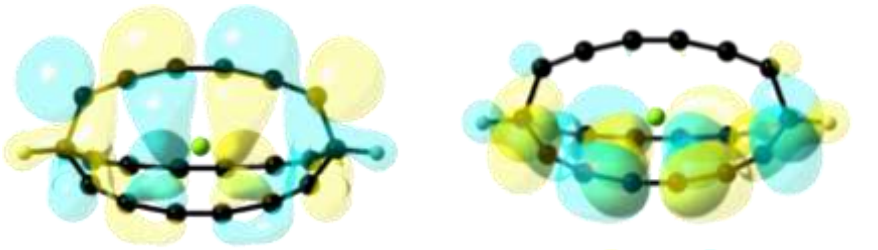
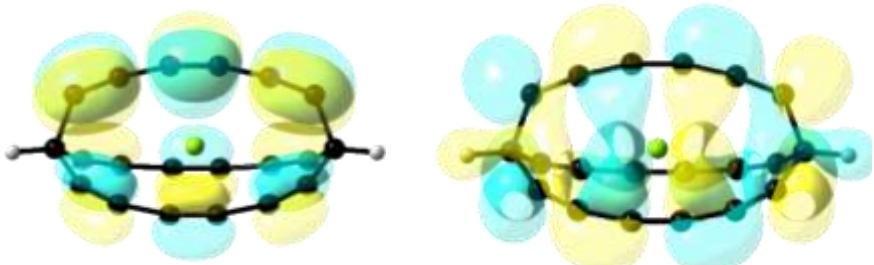


Figure S6. Frontier's molecular orbitals of the complexes of BTH cage

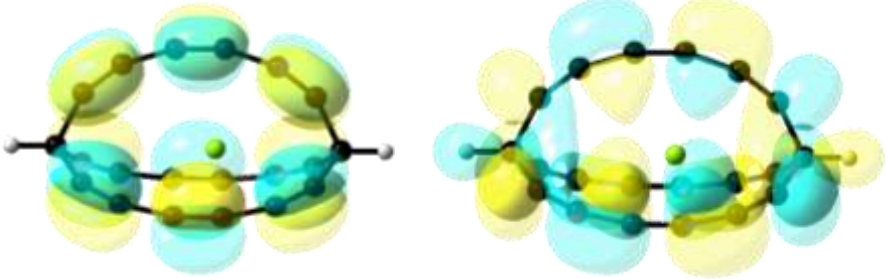
Li@BIN
(α-spin state)



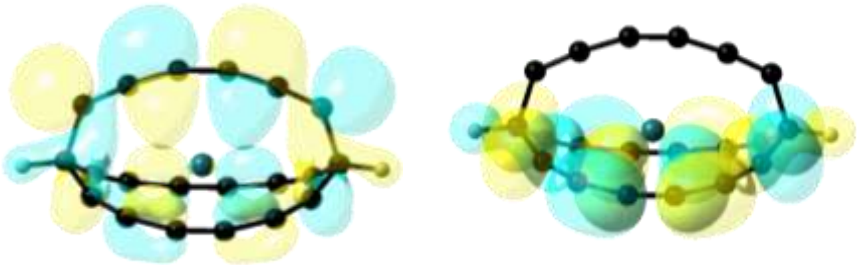
Li@BIN
(β-spin state)



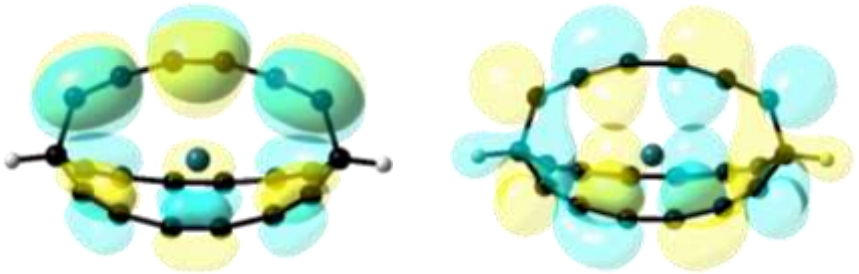
Li^{+}@BTH



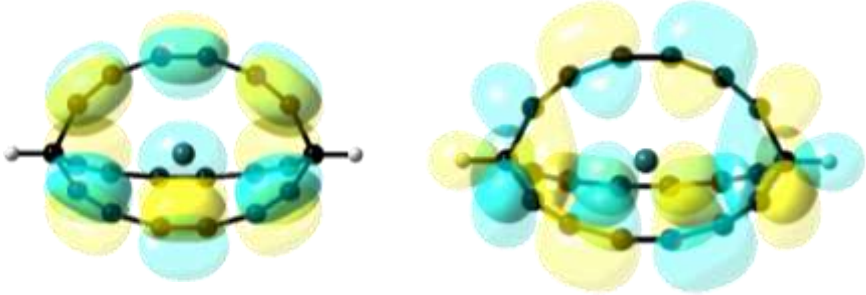
Na@BIN
(α-spin state)



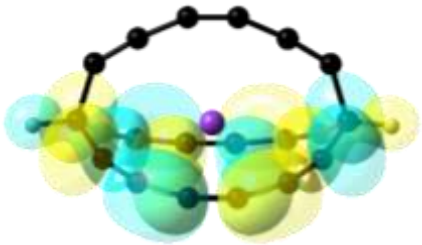
Na@BIN
(β-spin state)



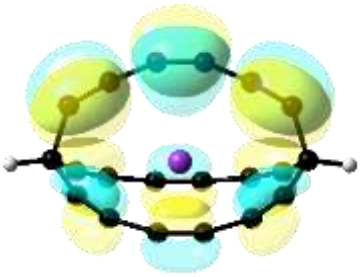
Na^{+}@BIN



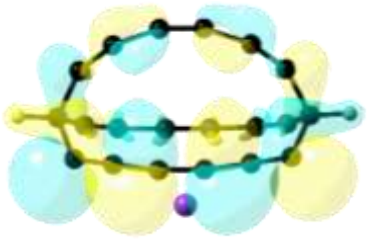
K@BIN
(α-spin state)

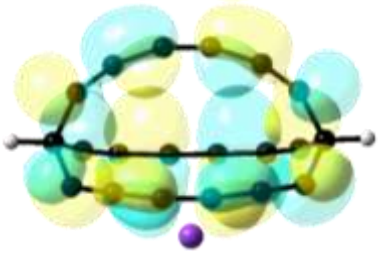


K@BIN
(β-spin state)

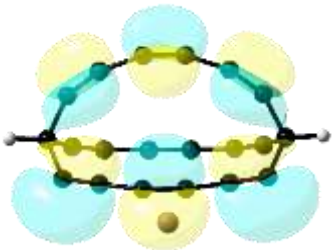


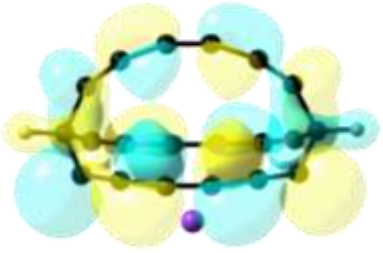
K…BIN
(α-spin state)



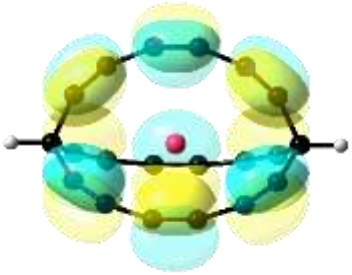


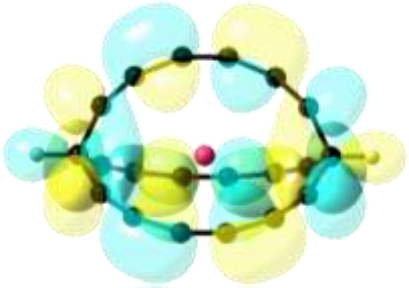
K…BIN
(β-spin state)



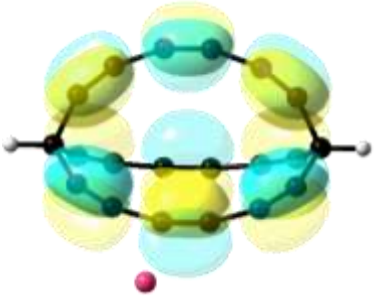


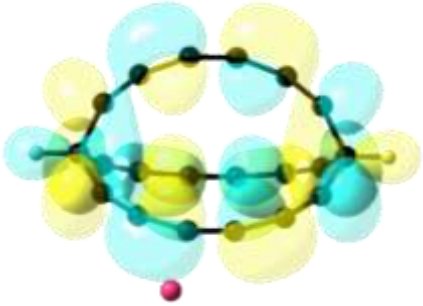
Ne@BTH





Ne…BTH





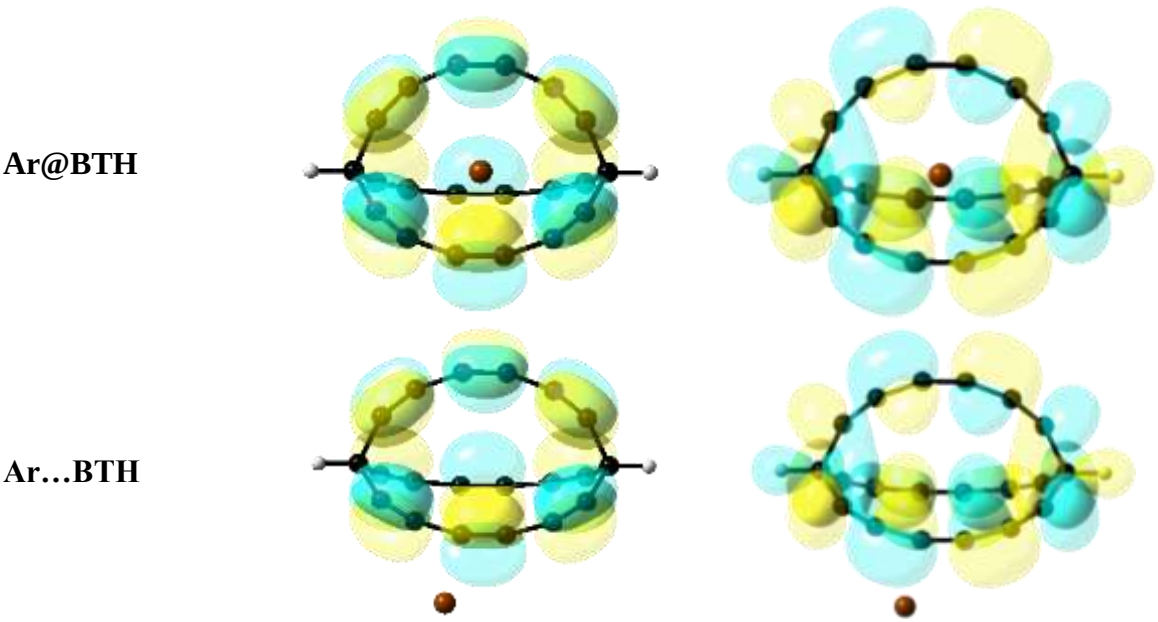
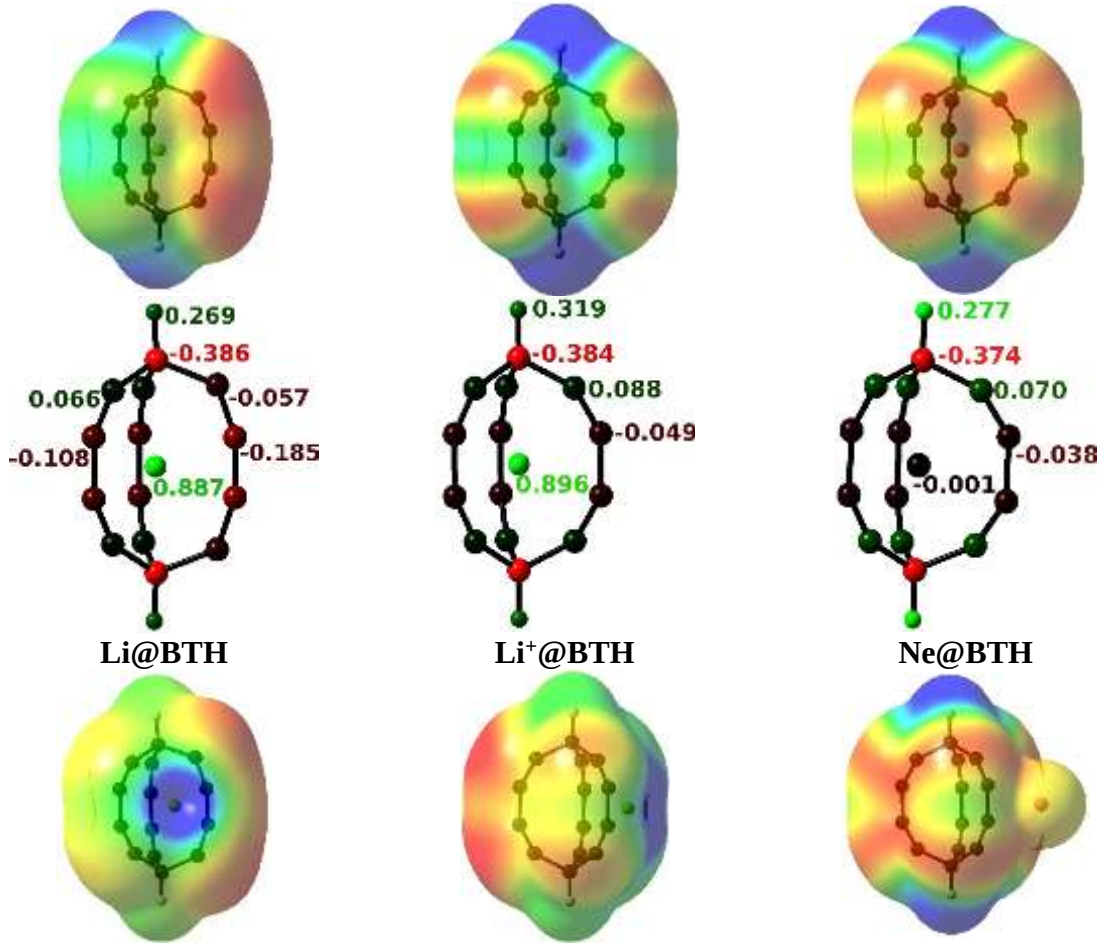


Figure S7. Frontier's molecular orbitals of the complexes of BIN cage

S7. MESP and NPA Charges on complexes



Li@BTH **Li^{+}@BTH** **Ne@BTH**

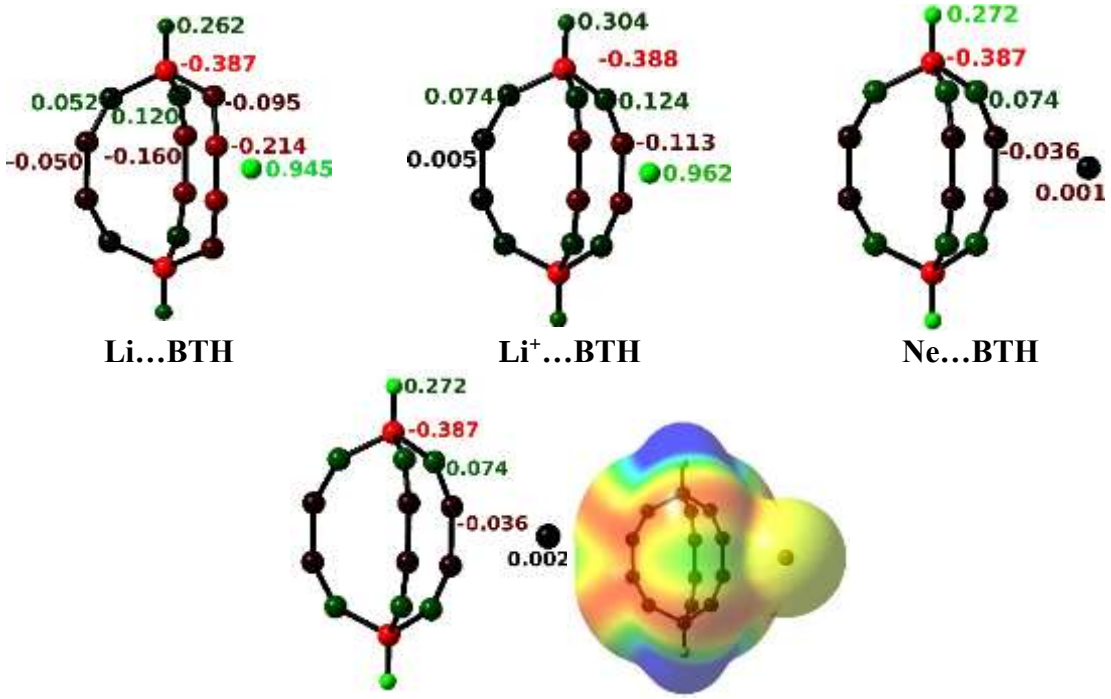
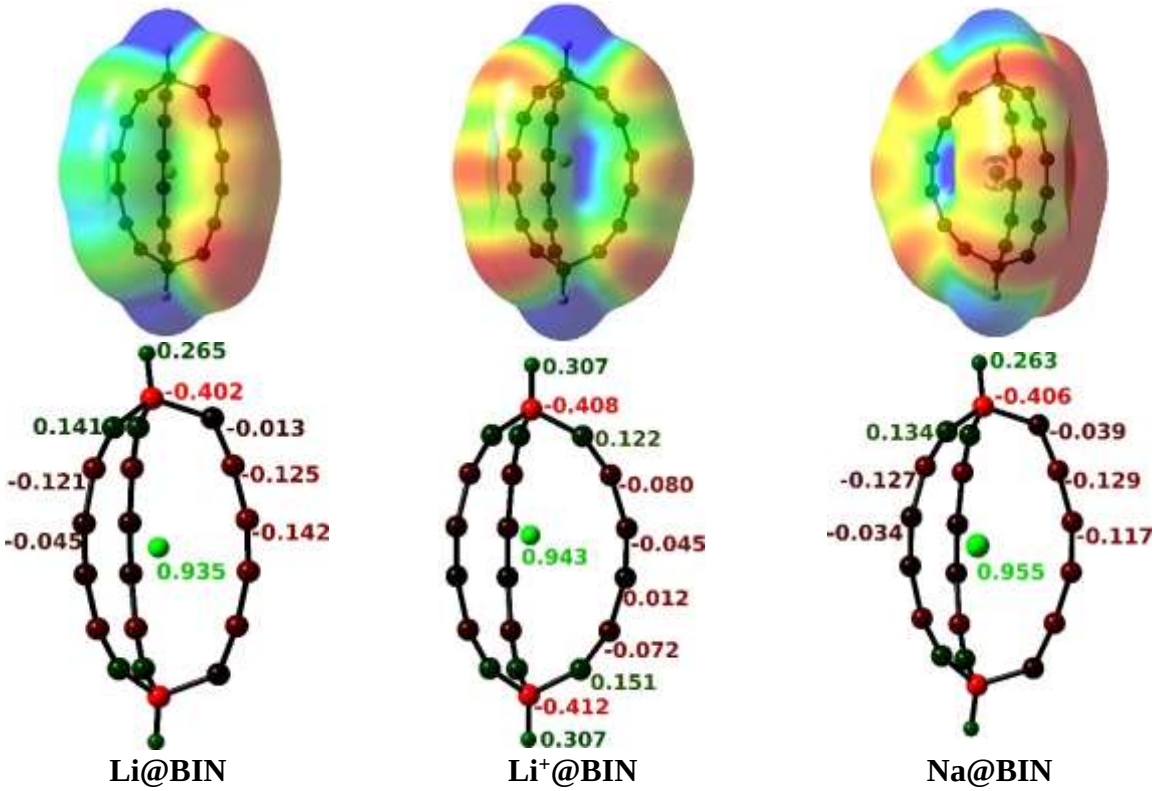


Figure S8. Molecular electrostatic potential and atomic charges on the BTH complexes.



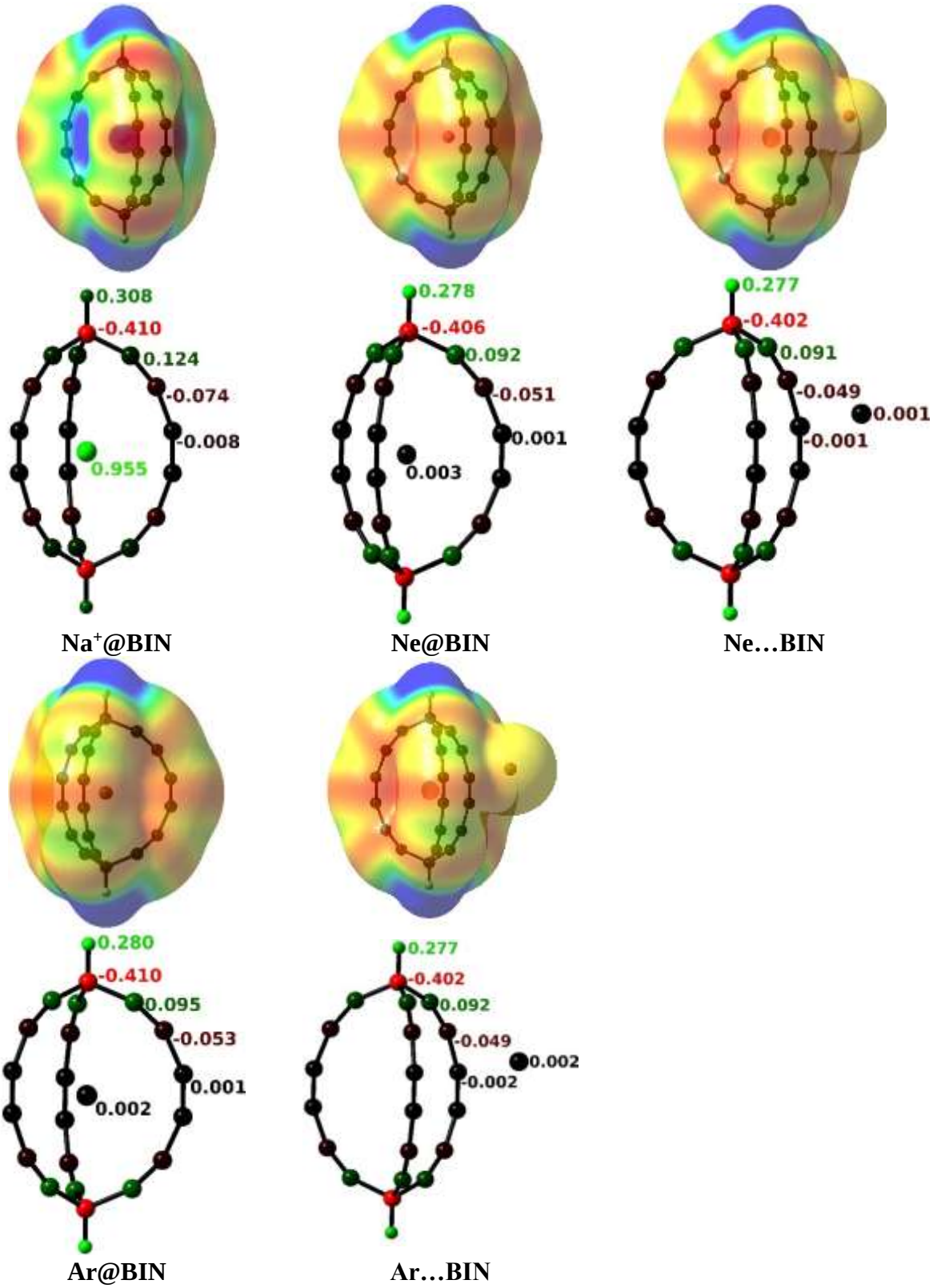


Figure S9. Molecular electrostatic potential and atomic charges on the BIN complexes.

S8. IRC for the TS of the complex of Li with BTH cage

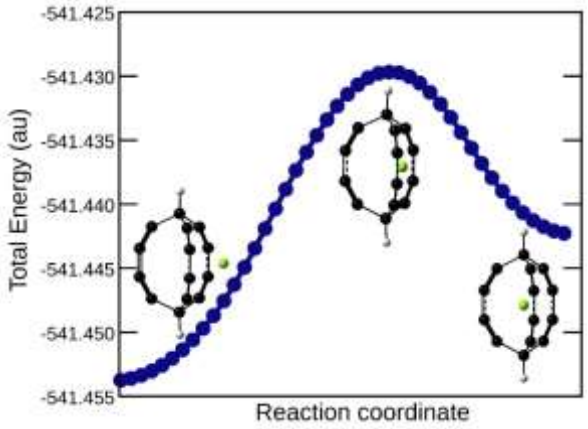
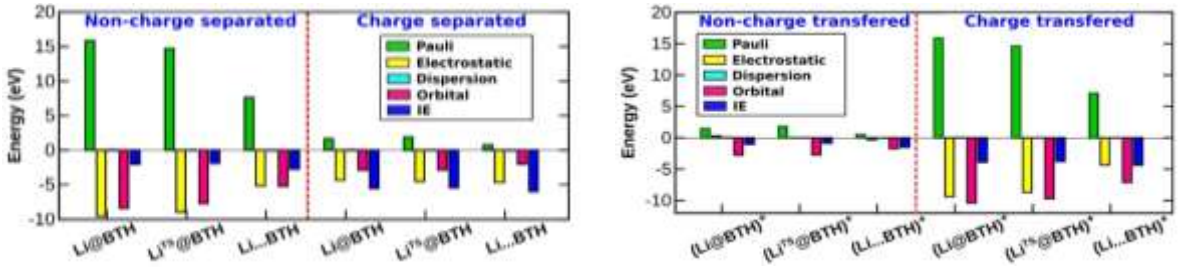


Figure S10. Intrinsic reaction coordinate (IRC) obtained from the TS of the complex of Li with the BTH cage.

S9. Energy decomposition analysis (EDA)



(a) **(b)**

Figure S11. *IE* and its various components. (a) Endohedral, exohedral, and interlinking TS complexes of Li with BTH in non-charge separated and charge separated state. (b) Endohedral, exohedral, and interlinking TS complexes of Li^+ with BTH in non-charge separated and charge separated state.

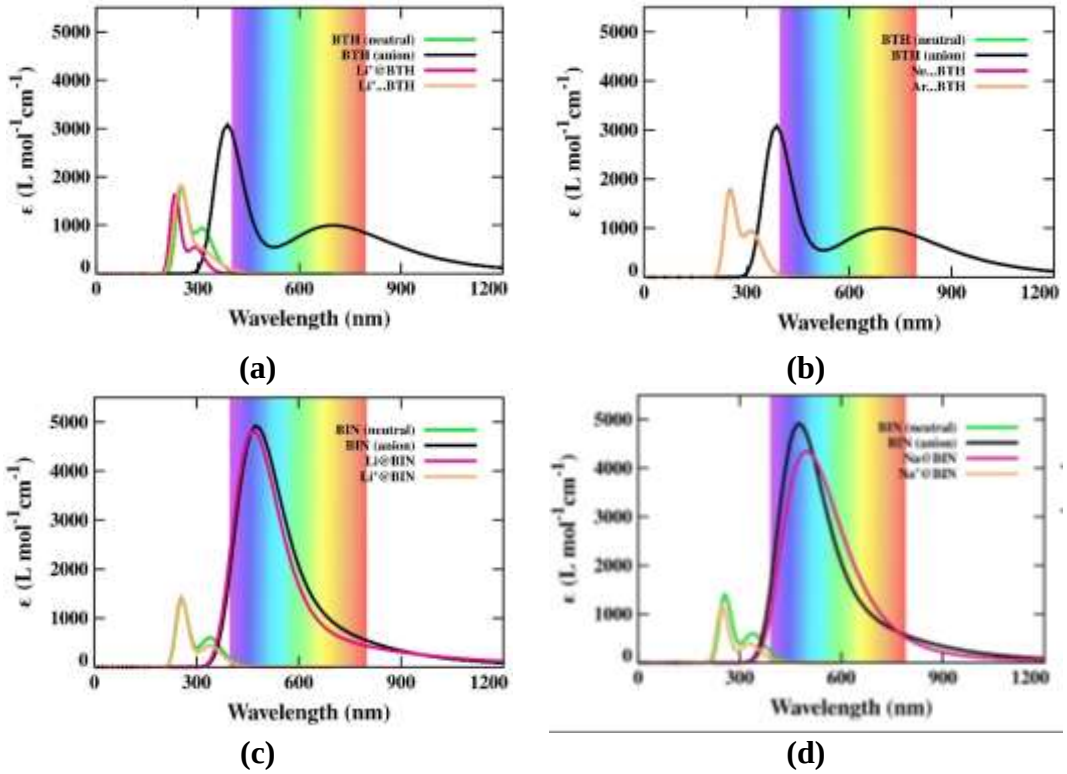
Table S8. *IE* values and its various energy components for the studied complexes

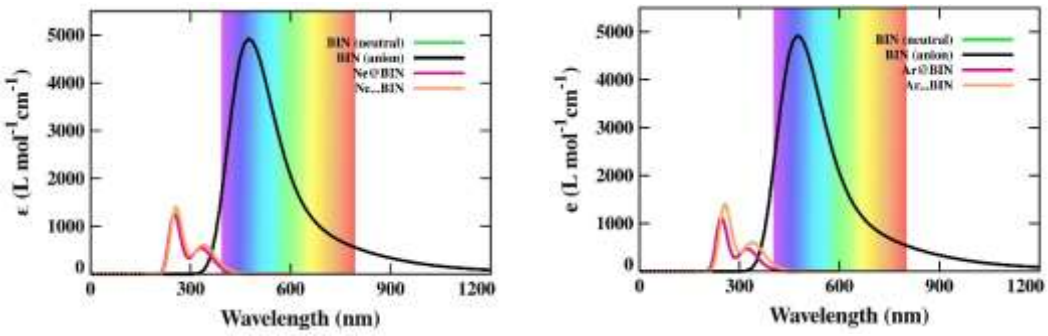
Guest atom/ion	Configuration	Pauli	Electrostatic	Steric	Dispersion	Orbital	*IE*
			BTH complexes				
Li (Non-CS)	Endo	15.88	-9.52	6.36	0.04	-8.41	-2.02
	Exo	7.62	-5.13	2.49	-0.03	-5.19	-2.73
	TS	14.71	-8.93	5.78	0.02	-7.70	-1.90
Li (CS)	Endo	1.67	-4.34	-2.68	0.04	-2.89	-5.53
	Exo	0.76	-4.68	-3.92	-0.03	-2.02	-5.96
	TS	1.92	-4.50	-2.59	0.02	-2.85	-5.42
Li^+	Endo	1.46	0.26	1.72	0.04	-2.76	-1.00
	Exo	0.52	-0.30	0.23	-0.03	-1.73	-1.53
	TS	1.80	0.03	1.84	0.02	-2.72	-0.87
Ne	Endo	6.79	-2.42	4.37	-0.08	-0.52	3.77
	Exo	0.06	-0.03	0.03	-0.05	-0.01	-0.02
	TS	6.48	-2.33	4.16	-0.11	-0.49	3.56
Ar	Exo	0.14	-0.06	0.08	-0.12	-0.02	-0.05
			BIN complexes				

Li (Non-CS)	Endo	8.61	-5.57	3.04	-0.07	-5.64	-2.67
Li (CS)	Endo	0.48	-4.25	-3.77	-0.07	-2.07	-5.90
Li^+	Endo	0.25	-0.22	0.03	-0.07	-1.78	-1.82
Na (Non-CS)	Endo	8.14	-5.33	2.81	-0.10	-4.73	-2.02
Na (CS)	Endo	0.76	-4.29	-3.53	-0.10	-1.50	-5.13
Na^+	Endo	0.49	-0.33	0.16	-0.10	-1.37	-1.31
K (Non-CS)	Endo	10.43	-6.83	3.60	-0.08	-5.24	-1.72
	Exo	4.82	-3.36	1.45	-0.18	-3.57	-2.29
	TS	9.16	-6.05	3.11	-0.18	-4.76	-1.83
K (CS)	Endo	2.19	-4.64	-2.44	-0.08	-1.58	-4.10
	Exo	0.88	-4.03	-3.15	-0.18	-1.04	-4.37
	TS	2.12	-4.63	-2.51	-0.18	-1.48	-4.16
Ne	Endo	0.66	-0.27	0.39	-0.23	-0.04	0.13
	Exo	0.05	-0.02	0.03	-0.05	0.00	-0.03
	TS	0.82	-0.33	0.49	-0.18	-0.04	0.27
Ar	Endo	2.77	-1.12	1.66	-0.39	-0.25	1.02
	Exo	0.13	-0.05	0.08	-0.13	-0.01	-0.06
	TS	2.82	-1.12	1.70	-0.32	-0.26	1.12

*All the energy values are given in eV

S10. Photophysical properties of the complexes





(e) **(f)**

Figure S12. Optical absorption spectra of the complexes. (a) Complexes of Li with BTH, (b) Complexes of noble gases with BTH, (c) Complexes of Li and Li^+ with BIN, (d) Complexes of Na and Na^+ with BIN, (e) Complexes of Ne with BIN, and (f) Complexes of Ar with BIN.

Table S9. Spectral data for most important electronic excitations in the complexes.

System	Oscillatory strength (f)	Excitation Wavelength (λ) in nm	Absorption coefficient (ε) in $Lmol^{-1}cm^{-1}$
Li@BTH	0.01	868.31	435.01
	0.04	448.87	4124.24
	0.08	424.93	4478.70
	0.03	380.29	2902.78
Li...BTH	0.01	667.47	613.22
	0.01	361.09	1609.70
	0.02	354.44	1565.41
Li^+@BTH	0.02	293.16	547.26
	0.05	232.52	1640.50
Li^+...BTH	0.02	259.95	1618.18
	0.03	243.51	1768.17
Ne...BTH	0.03	315.55	939.42
	0.05	251.78	1786.35
Ar...BTH	0.03	315.63	931.13
	0.05	251.85	1779.11
Li@BIN	0.06	498.14	4390.06
	0.02	448.56	4657.02
	0.07	444.13	4485.18
Li^+@BIN	0.01	339.04	440.91
	0.04	255.23	1431.92
Na@BIN	0.06	549.69	3801.14
	0.01	486.10	4300.88
	0.07	462.49	3965.18
Na^+@BIN	0.01	329.92	389.25
	0.03	248.32	1165.34
K@BIN	0.07	636.52	3059.29
	0.01	553.99	3501.68
	0.07	470.60	3489.31
	0.02	435.44	2716.56

K...BIN	0.01	680.73	629.62
	0.03	500.70	3252.67
	0.03	465.58	3675.67
	0.02	459.78	3669.57
	0.04	417.98	2780.99
Ne@BIN	0.02	332.42	539.10
	0.04	251.28	1270.19
Ne...BIN	0.02	339.26	610.14
	0.04	256.52	1397.22
Ar@BIN	0.01	323.80	470.63
	0.03	245.93	1131.76
Ar...BIN	0.02	339.31	606.79
	0.04	256.59	1393.79

S11. AIMD Simulations

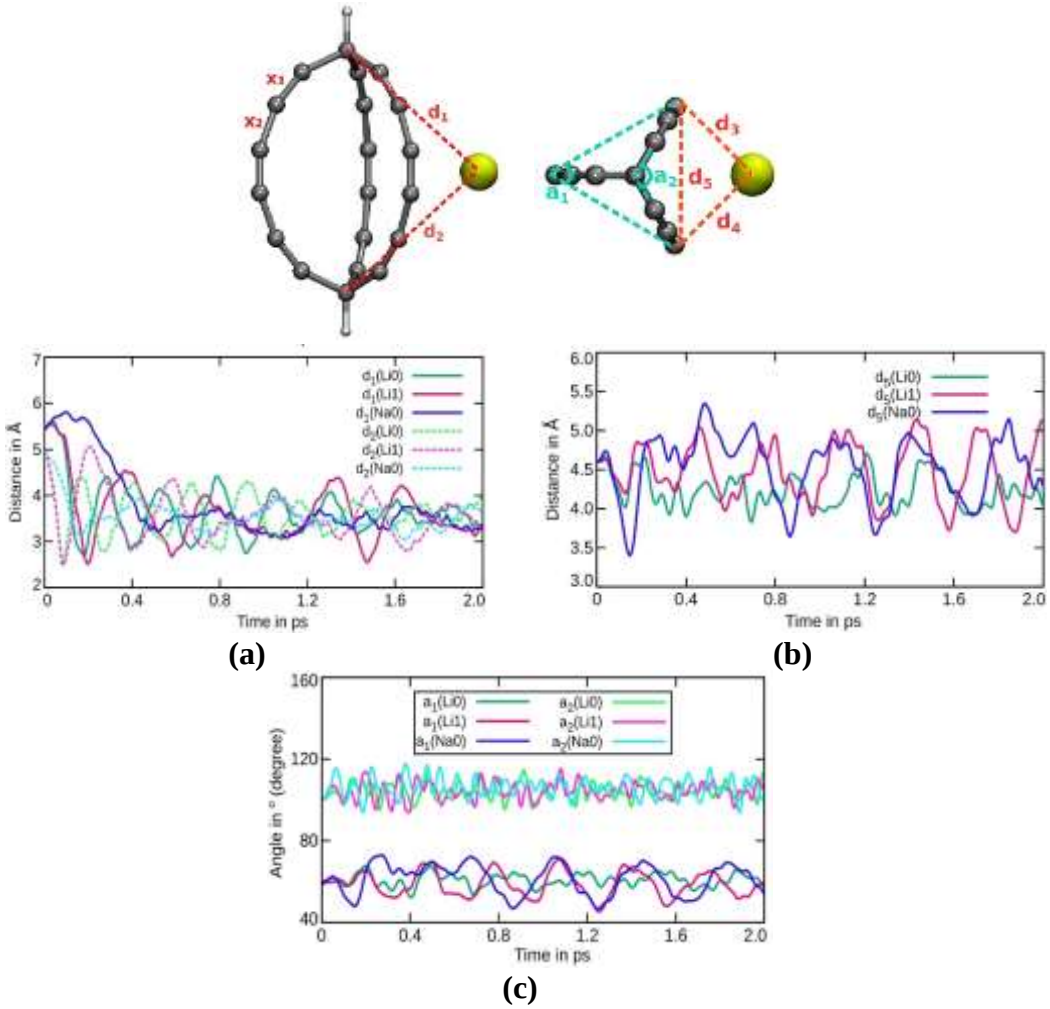


Figure S13. Variation in geometrical parameters during the AIMD simulations. (a) Variation in distance between metal and methanetriyl group (d_1 and d_2), (b) variation in distance between two arms of the cage (d_5), and (c) variation in angle a_1 and a_2 (the notations used for geometrical parameters are illustrated in scheme).

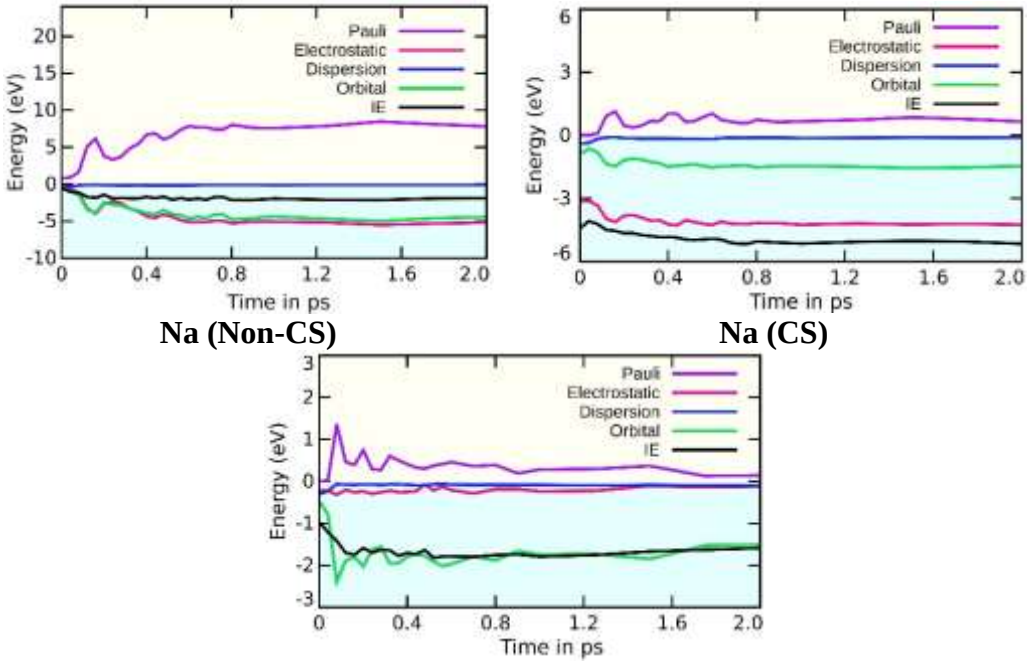


Figure S14. Variation in *IE* and its various energy components during the AIMD simulations complexes of Na and Li^+ with BIN cage.

S12. CARTESIAN COORDINATES

Neutral BTH

C	0.00000000	1.35173900	1.73658400
C	0.00000000	1.95788800	0.69299000
C	0.00000000	1.95788800	-0.69299000
C	0.00000000	1.35173900	-1.73658400
C	-1.17064000	-0.67586900	1.73658400
C	0.00000000	0.00000000	2.38563200
C	0.00000000	0.00000000	-2.38563200
C	-1.17064000	-0.67586900	-1.73658400
C	-1.69558100	-0.97894400	-0.69299000
C	-1.69558100	-0.97894400	0.69299000
C	1.17064000	-0.67586900	1.73658400
C	1.17064000	-0.67586900	-1.73658400
C	1.69558100	-0.97894400	-0.69299000
C	1.69558100	-0.97894400	0.69299000
H	0.00000000	0.00000000	3.47186000
H	0.00000000	0.00000000	-3.47186000

Anionic BTH

C	-1.16065200	1.74956300	-0.67561600
C	-1.69035300	0.69065200	-0.93620300
C	-1.69035300	-0.69065200	-0.93620300
C	-1.16065200	-1.74956300	-0.67561600
C	0.00000000	1.88479300	1.46555800
C	0.00000000	2.40806800	0.00095200
C	0.00000000	-2.40806800	0.00095200
C	0.00000000	-1.88479300	1.46555800
C	0.00000000	-0.66735800	1.76661300
C	0.00000000	0.66735800	1.76661300
C	1.16065200	1.74956300	-0.67561600
C	1.16065200	-1.74956300	-0.67561600
C	1.69035300	-0.69065200	-0.93620300
C	1.69035300	0.69065200	-0.93620300
H	0.00000000	3.49229300	-0.05690700
H	0.00000000	-3.49229300	-0.05690700

Cationic BTH

C	0.00000000	1.75473300	1.39583900
C	0.00000000	0.69197800	1.96714400
C	0.00000000	-0.69197800	1.96714400
C	0.00000000	-1.75473300	1.39583900
C	1.08504600	1.73159400	-0.68301700
C	0.00000000	2.43034000	0.06509300
C	0.00000000	-2.43034000	0.06509300
C	1.08504600	-1.73159400	-0.68301700
C	1.59240400	-0.67847900	-1.03405900
C	1.59240400	0.67847900	-1.03405900
C	-1.08504600	1.73159400	-0.68301700
C	-1.08504600	-1.73159400	-0.68301700
C	-1.59240400	-0.67847900	-1.03405900
C	-1.59240400	0.67847900	-1.03405900
H	0.00000000	3.51643400	0.03645000
H	0.00000000	-3.51643400	0.03645000

Neutral BIN

C	0.00000000	2.61988300	0.60530700
C	0.00000000	2.61988300	-0.60530700
C	-1.84335000	-1.06425800	1.88578500
C	-1.17156600	-0.67640400	2.80874600
C	0.00000000	2.12851700	1.88578500
C	0.00000000	0.00000000	3.42341200
C	0.00000000	1.35280800	2.80874600
C	0.00000000	2.12851700	-1.88578500
C	0.00000000	1.35280800	-2.80874600

C	0.00000000	0.00000000	-3.42341200
C	-1.17156600	-0.67640400	-2.80874600
C	-1.84335000	-1.06425800	-1.88578500
C	-2.26888500	-1.30994200	-0.60530700
C	-2.26888500	-1.30994200	0.60530700
C	1.84335000	-1.06425800	1.88578500
C	2.26888500	-1.30994200	0.60530700
C	1.17156600	-0.67640400	2.80874600
C	2.26888500	-1.30994200	-0.60530700
C	1.84335000	-1.06425800	-1.88578500
C	1.17156600	-0.67640400	-2.80874600
H	0.00000000	0.00000000	-4.51219700
H	0.00000000	0.00000000	4.51219700

Cationic BIN

C	0.00000000	0.60512900	2.62802700
C	0.00000000	-0.60512900	2.62802700
C	1.72988200	1.87603600	-1.10345900
C	1.10058700	2.81884900	-0.66248600
C	0.00000000	1.89002900	2.15114000
C	0.00000000	3.47870700	0.07591300
C	0.00000000	2.84396900	1.41405100
C	0.00000000	-1.89002900	2.15114000
C	0.00000000	-2.84396900	1.41405100
C	0.00000000	-3.47870700	0.07591300
C	1.10058700	-2.81884900	-0.66248600
C	1.72988200	-1.87603600	-1.10345900
C	2.10956900	-0.61139800	-1.37279300
C	2.10956900	0.61139800	-1.37279300
C	-1.72988200	1.87603600	-1.10345900
C	-2.10956900	0.61139800	-1.37279300
C	-1.10058700	2.81884900	-0.66248600
C	-2.10956900	-0.61139800	-1.37279300
C	-1.72988200	-1.87603600	-1.10345900
C	-1.10058700	-2.81884900	-0.66248600
H	0.00000000	-4.56694200	0.05008000
H	0.00000000	4.56694200	0.05008000

Anionic BIN

C	2.25503500	0.60659400	-1.17964800
C	2.25503500	-0.60659400	-1.17964800
C	-1.84204800	1.89599800	-0.97126800
C	-1.15678000	2.83508000	-0.63927300
C	1.84204800	1.89599800	-0.97126800
C	0.00000000	3.50726600	-0.00428100
C	1.15678000	2.83508000	-0.63927300
C	1.84204800	-1.89599800	-0.97126800
C	1.15678000	-2.83508000	-0.63927300

C	0.00000000	-3.50726600	-0.00428100
C	-1.15678000	-2.83508000	-0.63927300
C	-1.84204800	-1.89599800	-0.97126800
C	-2.25503500	-0.60659400	-1.17964800
C	-2.25503500	0.60659400	-1.17964800
C	0.00000000	1.91226200	1.91109000
C	0.00000000	0.62287700	2.22807400
C	0.00000000	3.08139200	1.46806300
C	0.00000000	-0.62287700	2.22807400
C	0.00000000	-1.91226200	1.91109000
C	0.00000000	-3.08139200	1.46806300
H	0.00000000	-4.58740000	-0.13539500
H	0.00000000	4.58740000	-0.13539500

Endohedral complex of Li^+ with BTH (Li^+@BTH)

C	0.00000000	1.36004500	1.72391600
C	0.00000000	2.00592400	0.69948700
C	0.00000000	2.00592400	-0.69948700
C	0.00000000	1.36004500	-1.72391600
C	-1.17783300	-0.68002200	1.72391600
C	0.00000000	0.00000000	2.38727500
C	0.00000000	0.00000000	-2.38727500
C	-1.17783300	-0.68002200	-1.72391600
C	-1.73718100	-1.00296200	-0.69948700
C	-1.73718100	-1.00296200	0.69948700
C	1.17783300	-0.68002200	1.72391600
C	1.17783300	-0.68002200	-1.72391600
C	1.73718100	-1.00296200	-0.69948700
C	1.73718100	-1.00296200	0.69948700
H	0.00000000	0.00000000	3.47448600
H	0.00000000	0.00000000	-3.47448600
Li	0.00000000	0.00000000	0.00000000

TS complex of Li^+ with BTH (Li^{+TS}@BTH)

C	1.20707400	1.70162100	0.64892300
C	1.85215900	0.70480500	0.90330900
C	1.85215900	-0.70480500	0.90330900
C	1.20707400	-1.70162100	0.64892300
C	-1.20707400	1.70162100	0.64892300
C	0.00000000	2.36872900	0.00481000
C	0.00000000	-2.36872900	0.00481000
C	-1.20707400	-1.70162100	0.64892300
C	-1.85215900	-0.70480500	0.90330900
C	-1.85215900	0.70480500	0.90330900
C	0.00000000	1.74100400	-1.35538600
C	0.00000000	-1.74100400	-1.35538600
C	0.00000000	-0.69303200	-1.95459100

C	0.00000000	0.69303200	-1.95459100
H	0.00000000	3.45523200	0.04787500
H	0.00000000	-3.45523200	0.04787500
Li	0.00000000	0.00000000	0.77090100

Exohedral complex of Li^+ with BTH (Li^+…BTH)

C	-1.16630900	1.71857100	0.60527000
C	-1.75177200	0.69702400	0.88349900
C	-1.75177200	-0.69702400	0.88349900
C	-1.16630900	-1.71857100	0.60527000
C	0.00000000	1.74372600	-1.41760200
C	0.00000000	2.38863500	-0.06970000
C	0.00000000	-2.38863500	-0.06970000
C	0.00000000	-1.74372600	-1.41760200
C	0.00000000	-0.69199500	-2.00802900
C	0.00000000	0.69199500	-2.00802900
C	1.16630900	1.71857100	0.60527000
C	1.16630900	-1.71857100	0.60527000
C	1.75177200	-0.69702400	0.88349900
C	1.75177200	0.69702400	0.88349900
H	0.00000000	3.47519500	-0.04308800
H	0.00000000	-3.47519500	-0.04308800
Li	0.00000000	0.00000000	2.09989700

Endohedral complex of Li with BTH (Li@BTH)

C	1.16642400	1.72802900	0.68925800
C	1.74711000	0.69573700	0.96666100
C	1.74711000	-0.69573700	0.96666100
C	1.16642400	-1.72802900	0.68925800
C	-1.16642400	1.72802900	0.68925800
C	0.00000000	2.39314600	0.00749800
C	0.00000000	-2.39314600	0.00749800
C	-1.16642400	-1.72802900	0.68925800
C	-1.74711000	-0.69573700	0.96666100
C	-1.74711000	0.69573700	0.96666100
C	0.00000000	1.84789300	-1.45378300
C	0.00000000	-1.84789300	-1.45378300
C	0.00000000	-0.67440600	-1.88263500
C	0.00000000	0.67440600	-1.88263500
H	0.00000000	3.47643100	0.05817300
H	0.00000000	-3.47643100	0.05817300
Li	0.00000000	0.00000000	0.02954400

TS complex of Li with BTH (Li^{TS}@BTH)

C	-1.70896900	-1.28616900	0.47637100
C	-0.70977900	-1.95749600	0.66691300
C	0.69513400	-1.96280600	0.65299400

C	1.69512900	-1.29786400	0.44495800
C	-1.75111200	0.16619900	-1.33200800
C	-2.37477100	-0.00522000	0.01241500
C	2.37425700	-0.01765900	0.01005600
C	1.75300000	0.18034100	-1.33116900
C	0.68874300	0.31875800	-1.89717700
C	-0.68736100	0.31009700	-1.89767400
C	-1.80858700	1.15914300	0.89629700
C	1.82016700	1.13332400	0.92617100
C	0.68668500	1.66076600	1.02138700
C	-0.67002200	1.66971500	1.00784900
H	-3.45843700	-0.04443600	0.03245100
H	3.45746700	-0.06748100	0.03060900
Li	-0.00470400	-0.10495200	0.66421200

Exohedral complex of Li with BTH (Li…BTH)

C	-0.17006400	1.41186200	1.85457600
C	0.04163800	1.77670200	0.66803000
C	0.04163800	1.77670200	-0.66803000
C	-0.17006400	1.41186200	-1.85457600
C	1.27112000	-0.57402200	1.74892900
C	0.04727100	-0.03212000	2.40001900
C	0.04727100	-0.03212000	-2.40001900
C	1.27112000	-0.57402200	-1.74892900
C	1.82053100	-0.77441600	-0.68969700
C	1.82053100	-0.77441600	0.68969700
C	-1.02740700	-0.81679400	1.71819500
C	-1.02740700	-0.81679400	-1.71819500
C	-1.54934300	-1.20961600	-0.69667600
C	-1.54934300	-1.20961600	0.69667600
H	0.02432800	-0.07998800	3.48360200
H	0.02432800	-0.07998800	-3.48360200
Li	-1.75120000	0.92694900	0.00000000

Endohedral complex of Ne with BTH (Ne@BTH)

C	0.00000000	1.42154700	1.70252100
C	0.00000000	2.12581800	0.70929000
C	0.00000000	2.12581800	-0.70929000
C	0.00000000	1.42154700	-1.70252100
C	1.23109600	-0.71077300	1.70252100
C	0.00000000	0.00000000	2.30008800
C	0.00000000	0.00000000	-2.30008800
C	1.23109600	-0.71077300	-1.70252100
C	1.84101300	-1.06290900	-0.70929000
C	1.84101300	-1.06290900	0.70929000
C	-1.23109600	-0.71077300	1.70252100
C	-1.23109600	-0.71077300	-1.70252100
C	-1.84101300	-1.06290900	-0.70929000

C	-1.84101300	-1.06290900	0.70929000
H	0.00000000	0.00000000	3.38570400
H	0.00000000	0.00000000	-3.38570400
Ne	0.00000000	0.00000000	0.00000000

TS complex of Ne with BTH (Ne^{TS}@BTH)

C	0.00000000	1.71100900	-1.34552400
C	0.00000000	0.69335300	-1.99625700
C	0.00000000	-0.69335300	-1.99625700
C	0.00000000	-1.71100900	-1.34552400
C	1.32893500	1.69772000	0.61178600
C	0.00000000	2.29834100	0.03252400
C	0.00000000	-2.29834100	0.03252400
C	1.32893500	-1.69772000	0.61178600
C	2.03709700	-0.71739100	0.78880700
C	2.03709700	0.71739100	0.78880700
C	-1.32893500	1.69772000	0.61178600
C	-1.32893500	-1.69772000	0.61178600
C	-2.03709700	-0.71739100	0.78880700
C	-2.03709700	0.71739100	0.78880700
H	0.00000000	3.38323000	0.06728300
H	0.00000000	-3.38323000	0.06728300
Ne	0.00000000	0.00000000	0.59622900

Exohedral complex of Ne with BTH (Ne…BTH)

C	0.00000000	1.73628000	-1.73188100
C	0.00000000	0.69296900	-2.33864600
C	0.00000000	-0.69296900	-2.33864600
C	0.00000000	-1.73628000	-1.73188100
C	1.17056100	1.73665000	0.29528400
C	0.00000000	2.38532900	-0.38053300
C	0.00000000	-2.38532900	-0.38053300
C	1.17056100	-1.73665000	0.29528400
C	1.69625200	-0.69290400	0.59688100
C	1.69625200	0.69290400	0.59688100
C	-1.17056100	1.73665000	0.29528400
C	-1.17056100	-1.73665000	0.29528400
C	-1.69625200	-0.69290400	0.59688100
C	-1.69625200	0.69290400	0.59688100
H	0.00000000	3.47171100	-0.38078200
H	0.00000000	-3.47171100	-0.38078200
Ne	0.00000000	0.00000000	3.27623300

Exohedral complex of Ar with BTH (Ar…BTH)

C	-1.17043800	1.73660500	-0.00959100
C	-1.69680800	0.69295400	0.29132900
C	-1.69680800	-0.69295400	0.29132900

C	-1.17043800	-1.73660500	-0.00959100
C	0.00000000	1.73666000	-2.03674100
C	0.00000000	2.38559300	-0.68527300
C	0.00000000	-2.38559300	-0.68527300
C	0.00000000	-1.73666000	-2.03674100
C	0.00000000	-0.69295000	-2.64290400
C	0.00000000	0.69295000	-2.64290400
C	1.17043800	1.73660500	-0.00959100
C	1.17043800	-1.73660500	-0.00959100
C	1.69680800	-0.69295400	0.29132900
C	1.69680800	0.69295400	0.29132900
H	0.00000000	3.47195600	-0.68523200
H	0.00000000	-3.47195600	-0.68523200
Ar	0.00000000	0.00000000	3.27709800

Endohedral complex of Li^+ with BIN (Li^+@BIN)

C	0.00000000	2.51953200	-0.59752400
C	0.00000000	2.49632000	0.61553100
C	1.80550700	-1.04241000	-1.90028400
C	1.16164200	-0.67067400	-2.85089800
C	0.00000000	2.08482000	-1.90028400
C	0.00000000	0.00000000	-3.49456600
C	0.00000000	1.34134900	-2.85089800
C	0.00000000	2.08776800	1.92475700
C	0.00000000	1.33940300	2.86932000
C	0.00000000	0.00000000	3.51265200
C	1.15995700	-0.66970200	2.86932000
C	1.80806000	-1.04388400	1.92475700
C	2.16187700	-1.24816000	0.61553100
C	2.18197900	-1.25976600	-0.59752400
C	-1.80550700	-1.04241000	-1.90028400
C	-2.18197900	-1.25976600	-0.59752400
C	-1.16164200	-0.67067400	-2.85089800
C	-2.16187700	-1.24816000	0.61553100
C	-1.80806000	-1.04388400	1.92475700
C	-1.15995700	-0.66970200	2.86932000
H	0.00000000	0.00000000	4.60145200
H	0.00000000	0.00000000	-4.58324100
Li	0.00000000	0.00000000	-0.40766400

Endohedral complex of Li with BIN (Li@BIN)

C	2.13289700	0.60814700	-1.14736400
C	2.13289700	-0.60814700	-1.14736400
C	-1.78783500	1.92141700	-0.97115300
C	-1.14721500	2.89451400	-0.64770500
C	1.78783500	1.92141700	-0.97115300
C	0.00000000	3.57763500	-0.00332300
C	1.14721500	2.89451400	-0.64770500

C	1.78783500	-1.92141700	-0.97115300
C	1.14721500	-2.89451400	-0.64770500
C	0.00000000	-3.57763500	-0.00332300
C	-1.14721500	-2.89451400	-0.64770500
C	-1.78783500	-1.92141700	-0.97115300
C	-2.13289700	-0.60814700	-1.14736400
C	-2.13289700	0.60814700	-1.14736400
C	0.00000000	1.92304300	1.89794200
C	0.00000000	0.62335600	2.20516900
C	0.00000000	3.07272100	1.43143600
C	0.00000000	-0.62335600	2.20516900
C	0.00000000	-1.92304300	1.89794200
C	0.00000000	-3.07272100	1.43143600
H	0.00000000	-4.65987700	-0.09909900
H	0.00000000	4.65987700	-0.09909900
Li	0.00000000	0.00000000	0.07095000

Endohedral complex of Na^+ with BIN (Na^+@BIN)

C	0.00000000	2.65846200	0.60633400
C	0.00000000	2.65846200	-0.60633400
C	-1.86507800	-1.07680300	1.88507600
C	-1.16845500	-0.67460800	2.78397300
C	0.00000000	2.15360600	1.88507600
C	0.00000000	0.00000000	3.40929700
C	0.00000000	1.34921600	2.78397300
C	0.00000000	2.15360600	-1.88507600
C	0.00000000	1.34921600	-2.78397300
C	0.00000000	0.00000000	-3.40929700
C	-1.16845500	-0.67460800	-2.78397300
C	-1.86507800	-1.07680300	-1.88507600
C	-2.30229600	-1.32923100	-0.60633400
C	-2.30229600	-1.32923100	0.60633400
C	1.86507800	-1.07680300	1.88507600
C	2.30229600	-1.32923100	0.60633400
C	1.16845500	-0.67460800	2.78397300
C	2.30229600	-1.32923100	-0.60633400
C	1.86507800	-1.07680300	-1.88507600
C	1.16845500	-0.67460800	-2.78397300
H	0.00000000	0.00000000	-4.49895500
H	0.00000000	0.00000000	4.49895500
Na	0.00000000	0.00000000	0.00000000

Endohedral complex of Na with BIN (Na@BIN)

C	0.00000000	0.62406700	-2.37844600
C	0.00000000	-0.62406700	-2.37844600
C	-1.88065600	1.88686000	0.99422800
C	-1.15428200	2.78852300	0.64351800

C	0.00000000	1.89520300	-1.97544300
C	0.00000000	3.46510200	0.00865600
C	0.00000000	3.02232600	-1.44883500
C	0.00000000	-1.89520300	-1.97544300
C	0.00000000	-3.02232600	-1.44883500
C	0.00000000	-3.46510200	0.00865600
C	-1.15428200	-2.78852300	0.64351800
C	-1.88065600	-1.88686000	0.99422800
C	-2.32596100	-0.60777300	1.21431000
C	-2.32596100	0.60777300	1.21431000
C	1.88065600	1.88686000	0.99422800
C	2.32596100	0.60777300	1.21431000
C	1.15428200	2.78852300	0.64351800
C	2.32596100	-0.60777300	1.21431000
C	1.88065600	-1.88686000	0.99422800
C	1.15428200	-2.78852300	0.64351800
H	0.00000000	-4.54514400	0.13926300
H	0.00000000	4.54514400	0.13926300
Na	0.00000000	0.00000000	0.07281400

Endohedral complex of K with BIN (K@BIN)

C	2.45020700	-1.33656300	0.60850000
C	2.45020700	-1.33656300	-0.60850000
C	0.04464400	2.08503500	1.84896700
C	0.02886400	1.44202400	2.91144200
C	1.94430800	-1.08027300	1.86186700
C	-0.00165700	-0.01797300	3.33879900
C	1.15798700	-0.68785100	2.69606200
C	1.94430800	-1.08027300	-1.86186700
C	1.15798700	-0.68785100	-2.69606200
C	-0.00165700	-0.01797300	-3.33879900
C	0.02886400	1.44202400	-2.91144200
C	0.04464400	2.08503500	-1.84896700
C	0.05951700	2.62635900	-0.62431700
C	0.05951700	2.62635900	0.62431700
C	-1.98660600	-1.00735100	1.86179400
C	-2.50180700	-1.24611300	0.60851300
C	-1.18659000	-0.64157400	2.69511300
C	-2.50180700	-1.24611300	-0.60851300
C	-1.98660600	-1.00735100	-1.86179400
C	-1.18659000	-0.64157400	-2.69511300
H	-0.00482200	-0.14124600	-4.42139400
H	-0.00482200	-0.14124600	4.42139400
K	-0.00509300	-0.07084900	0.00000000

TS complex of K with BIN (K^{TS}@BIN)

C	0.62479500	-2.31614500	-1.33289300
C	-0.62479100	-2.31614300	-1.33290500
C	1.85800800	2.26757600	-0.27852900
C	2.66276600	1.36148600	-0.24723700
C	1.84011900	-1.77023600	-1.16161000
C	3.31867800	0.03757400	-0.02501000
C	2.78096900	-0.96274200	-1.03741300
C	-1.84011100	-1.77023300	-1.16161300
C	-2.78096000	-0.96274200	-1.03741800
C	-3.31867800	0.03757200	-0.02501900
C	-2.66276500	1.36148400	-0.24724100
C	-1.85800700	2.26757200	-0.27853700
C	-0.60853200	2.86077500	-0.27726000
C	0.60853000	2.86077700	-0.27725900
C	1.87531800	-0.67360500	2.03048200
C	0.60745400	-0.87004300	2.49324600
C	2.78688300	-0.36106000	1.29801600
C	-0.60746800	-0.87004300	2.49324700
C	-1.87533100	-0.67360400	2.03048200
C	-2.78689100	-0.36105800	1.29801100
H	-4.40434300	0.11573000	-0.06593300
H	4.40434400	0.11573200	-0.06591500
K	0.00000500	0.25713500	-0.91628300

Exohedral complex of K with BIN (K…BIN)

C	0.62433600	0.09969600	2.29806000
C	-0.62451200	0.10029000	2.29789100
C	1.88051200	-1.20773900	-1.69435200
C	2.75972100	-0.67512500	-1.05763500
C	1.87748300	-0.00031100	1.86484800
C	3.44290600	0.22966500	-0.10481000
C	2.96214300	-0.19850300	1.27809500
C	-1.87767800	0.00090200	1.86465100
C	-2.96230100	-0.19724900	1.27769800
C	-3.44235200	0.23127100	-0.10544100
C	-2.75944700	-0.67396300	-1.05805000
C	-1.88032900	-1.20695000	-1.69459200
C	-0.60719400	-1.51552200	-2.10717300
C	0.60725700	-1.51570100	-2.10698700
C	1.88814900	2.29204600	-0.53145400
C	0.60723900	2.76544800	-0.61117200
C	2.82614500	1.54042500	-0.40831100
C	-0.60526600	2.76562800	-0.61130100
C	-1.88643400	2.29288400	-0.53183900
C	-2.82472900	1.54161800	-0.40882700
H	-4.52580000	0.21039500	-0.20332300

H	4.52636900	0.20813800	-0.20238700
K	-0.00181400	-2.12796800	0.70052200

Endohedral complex of Ne with BIN (Ne@BIN)

C	0.00000000	2.73905700	0.60558700
C	0.00000000	2.73905700	-0.60558700
C	-1.89731700	-1.09541700	1.86516400
C	-1.17853600	-0.68042800	2.73988900
C	0.00000000	2.19083300	1.86516400
C	0.00000000	0.00000000	3.33768800
C	0.00000000	1.36085600	2.73988900
C	0.00000000	2.19083300	-1.86516400
C	0.00000000	1.36085600	-2.73988900
C	0.00000000	0.00000000	-3.33768800
C	-1.17853600	-0.68042800	-2.73988900
C	-1.89731700	-1.09541700	-1.86516400
C	-2.37209300	-1.36952900	-0.60558700
C	-2.37209300	-1.36952900	0.60558700
C	1.89731700	-1.09541700	1.86516400
C	2.37209300	-1.36952900	0.60558700
C	1.17853600	-0.68042800	2.73988900
C	2.37209300	-1.36952900	-0.60558700
C	1.89731700	-1.09541700	-1.86516400
C	1.17853600	-0.68042800	-2.73988900
H	0.00000000	0.00000000	-4.42745900
H	0.00000000	0.00000000	4.42745900
Ne	0.00000000	0.00000000	0.00000000

TS complex of Ne with BIN (Ne^{TS}@BIN)

C	0.00000000	0.60518800	-2.72704600
C	0.00000000	-0.60518800	-2.72704600
C	-2.00333700	1.85065500	0.93250100
C	-1.20106200	2.69688000	0.62266600
C	0.00000000	1.87113100	-2.20112800
C	0.00000000	3.30975700	-0.00597500
C	0.00000000	2.75869400	-1.38564700
C	0.00000000	-1.87113100	-2.20112800
C	0.00000000	-2.75869400	-1.38564700
C	0.00000000	-3.30975700	-0.00597500
C	-1.20106200	-2.69688000	0.62266600
C	-2.00333700	-1.85065500	0.93250100
C	-2.55777700	-0.60593700	1.12804500
C	-2.55777700	0.60593700	1.12804500
C	2.00333700	1.85065500	0.93250100
C	2.55777700	0.60593700	1.12804500
C	1.20106200	2.69688000	0.62266600
C	2.55777700	-0.60593700	1.12804500

C	2.00333700	-1.85065500	0.93250100
C	1.20106200	-2.69688000	0.62266600
H	0.00000000	-4.39888900	0.03679300
H	0.00000000	4.39888900	0.03679300
Ne	0.00000000	0.00000000	1.13668900

Exohedral complex of Ne with BIN (Ne...BIN)

C	0.95225300	-0.65754800	2.27279800
C	1.11417600	0.54216800	2.27148300
C	-2.62153700	-1.47795500	0.00000000
C	-1.97285600	-2.49421900	0.00000000
C	0.54214100	-1.89436100	1.84519000
C	-0.71166300	-3.27956800	0.00000000
C	0.03893900	-2.75847900	1.17162300
C	1.03909200	1.84321900	1.84438600
C	0.77625300	2.80862500	1.17170700
C	0.18590100	3.50589500	0.00000000
C	-1.23553500	3.07332500	0.00000000
C	-2.12548000	2.25994800	0.00000000
C	-2.78151400	1.05564300	0.00000000
C	-2.94144000	-0.14434200	0.00000000
C	0.54214100	-1.89436100	-1.84519000
C	0.95225300	-0.65754800	-2.27279800
C	0.03893900	-2.75847900	-1.17162300
C	1.11417600	0.54216800	-2.27148300
C	1.03909200	1.84321900	-1.84438600
C	0.77625300	2.80862500	-1.17170700
H	0.32784300	4.58544500	0.00000000
H	-0.85317200	-4.35916200	0.00000000
Ne	3.21958300	-1.38221300	0.00000000

Endohedral complex of Ar with BIN (Ar@BIN)

C	0.00000000	2.86970900	0.60690200
C	0.00000000	2.86970900	-0.60690200
C	-1.97137200	-1.13817200	1.85351300
C	-1.19632500	-0.69069800	2.66485900
C	0.00000000	2.27634400	1.85351300
C	0.00000000	0.00000000	3.23240100
C	0.00000000	1.38139700	2.66485900
C	0.00000000	2.27634400	-1.85351300
C	0.00000000	1.38139700	-2.66485900
C	0.00000000	0.00000000	-3.23240100
C	-1.19632500	-0.69069800	-2.66485900
C	-1.97137200	-1.13817200	-1.85351300
C	-2.48524100	-1.43485500	-0.60690200
C	-2.48524100	-1.43485500	0.60690200

C	1.97137200	-1.13817200	1.85351300
C	2.48524100	-1.43485500	0.60690200
C	1.19632500	-0.69069800	2.66485900
C	2.48524100	-1.43485500	-0.60690200
C	1.97137200	-1.13817200	-1.85351300
C	1.19632500	-0.69069800	-2.66485900
H	0.00000000	0.00000000	-4.32343400
H	0.00000000	0.00000000	4.32343400
Ar	0.00000000	0.00000000	0.00000000

TS complex of Ar with BIN (Ar^{TS}@BIN)

C	0.00000000	0.60519900	-2.75425200
C	0.00000000	-0.60519900	-2.75425200
C	-2.14326600	1.84865400	0.84680500
C	-1.24757500	2.63069400	0.62086700
C	0.00000000	1.85951900	-2.20193200
C	0.00000000	3.22599400	0.03876800
C	0.00000000	2.71895900	-1.35715100
C	0.00000000	-1.85951900	-2.20193200
C	0.00000000	-2.71895900	-1.35715100
C	0.00000000	-3.22599400	0.03876800
C	-1.24757500	-2.63069400	0.62086700
C	-2.14326600	-1.84865400	0.84680500
C	-2.74511400	-0.60806200	0.98540100
C	-2.74511400	0.60806200	0.98540100
C	2.14326600	1.84865400	0.84680500
C	2.74511400	0.60806200	0.98540100
C	1.24757500	2.63069400	0.62086700
C	2.74511400	-0.60806200	0.98540100
C	2.14326600	-1.84865400	0.84680500
C	1.24757500	-2.63069400	0.62086700
H	0.00000000	-4.31461000	0.10681200
H	0.00000000	4.31461000	0.10681200
Ar	0.00000000	0.00000000	0.90041200

Exohedral complex of Ar with BIN (Ar^{TS}@BIN)

C	0.57391500	-0.72770800	2.27706900
C	1.00804600	0.40238100	2.27517900
C	-3.08565400	-0.69685700	0.00000000
C	-2.69129800	-1.83619500	0.00000000
C	-0.10948100	-1.83636500	1.84737400
C	-1.64729400	-2.89340700	0.00000000
C	-0.79659200	-2.56099800	1.17179600
C	1.23982900	1.68408100	1.84609200
C	1.20977500	2.68319300	1.17193200
C	0.79887800	3.49875500	0.00000000
C	-0.68434100	3.40963700	0.00000000

C	-1.73881600	2.82510000	0.00000000
C	-2.65598200	1.80546800	0.00000000
C	-3.08791200	0.67453800	0.00000000
C	-0.10948100	-1.83636500	-1.84737400
C	0.57391500	-0.72770800	-2.27706900
C	-0.79659200	-2.56099800	-1.17179600
C	1.00804600	0.40238100	-2.27517900
C	1.23982900	1.68408100	-1.84609200
C	1.20977500	2.68319300	-1.17193200
H	1.18903000	4.51529200	0.00000000
H	-2.03616900	-3.91041100	0.00000000
Ar	2.89420900	-2.05900700	0.00000000