Theoretical study of complexes formed between cations and curved aromatic systems: electrostatics does not always control cation-π interaction

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***Supplementary information TOC*:**

Fig. ESI 1. Molecular Electrostatic Potential in the directions normal to the rings of Sumanene and Corannulene (see Fig. 1 in the body of the paper) computed at the riMP2/aVDZ level of calculation

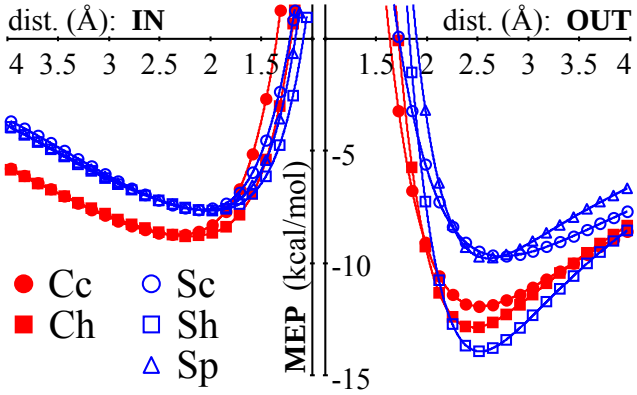

Table ESI 1. Eint (in kcal/mol) in the minima of the Mb···M scans computed at the levels of calculation: *X* = MP2.X; *S* = SCS-MP2/CBS; *M* = M062X/6-31+G*.

			Mb = Corannulene				**Mb** = Sumanene					
	M	**level**	**Cc in**	**Cc out**	**Ch in**	**Ch out**	**Sc in**	**Sc out**	**Sh in**	**Sh out**	**Sp in**	**Sp out**
monoatomic cations	N	*X*	-28.46	-28.37	-27.66	-27.98	-28.95	-27.74	-27.51	-29.79	-26.57	-22.50
		S	-28.30	-28.85	-27.55	-28.17	-28.55	-28.12	-27.06	-29.71	-26.24	-22.68
		M	-31.66	-31.06	-30.97	-30.91	-32.73	-30.94	-30.98	-32.98	-29.84	-24.90
	K	*X*	-27.09	-23.64	-25.00	-22.83	-27.19	-23.10	-24.31	-23.98	-24.40	-18.23
		S	-26.25	-23.49	-24.22	-22.43	-26.11	-23.08	-23.37	-23.47	-23.46	-17.90
		M	-27.37	-24.28	-25.22	-23.35	-27.38	-23.74	-24.52	-24.42	-24.61	-18.43
tetrahedral cations	A1	*X*	-26.72	-22.71		-22.26	-27.07	-21.73		-23.38		-17.88
		S	-25.87	-22.75		-21.97	-26.07	-21.81		-22.96		-17.64
		M	-26.44	-22.66		-22.15	-27.31	-21.96		-23.26		-17.72
	A2	*X*	-28.63	-24.32		-23.75	-28.35	-24.04		-24.69		-17.28
		S	-27.60	-24.08		-23.24	-27.29	-23.88		-24.08		-16.84
		M	-28.57	-24.62		-23.94	-28.62	-24.57		-24.95		-17.13
	A3	*X*	-29.30	-23.43		-21.94	-30.86	-23.81		-23.26		-17.96
		S	-28.22	-23.15		-21.54	-29.65	-23.60		-22.68		-17.54
		M	-29.58	-23.96		-22.34	-31.27	-24.53		-23.66		-18.28
	T1	*X*	-16.43	-12.30		-10.98	-16.47	-12.05		-11.11		-9.27
		S	-15.34	-12.03		-10.58	-15.08	-11.78		-10.61		-8.84
		M	-15.89	-11.55		-10.29	-16.22	-11.31		-10.39		-8.65
	T2	*X*	-17.29	-14.26		-12.15	-15.69	-13.73		-12.22		-9.43
		S	-15.97	-13.97		-11.64	-14.09	-13.52		-11.64		-8.97
		M	-16.47	-13.43		-11.14	-14.93	-12.91		-11.39		-8.45
	T3	*X*	-16.99	-15.24		-13.24	-15.71	-14.72		-13.38		-11.89
		S	-15.64	-15.07		-12.83	-14.09	-14.53		-12.78		-11.42
		M	-16.08	-14.13		-12.17	-14.84	-13.62		-12.24		-11.14
flat cations	G1 *T-shap.*	*X*	-19.37	-15.41		-14.48	-18.59	-14.79		-15.06		-10.03
		S	-18.37	-15.19		-14.11	-17.72	-14.83		-14.60		-9.78
		M	-18.70	-15.12		-14.24	-18.21	-14.60		-14.76		-9.39
	G2 *T-shap.*	*X*	-20.04	-19.16		-17.79	-18.77	-18.16		-18.66		-11.12
		S	-19.03	-18.99		-17.38	-17.62	-18.11		-18.10		-10.79
		M	-19.29	-18.12		-16.81	-18.27	-17.31		-17.71		-9.89
	G3 *stacked*	*X*	-19.44	-15.11		-13.04	-15.20	-14.12		-11.96		-11.67
		S	-18.27	-15.08		-12.65	-13.74	-14.13		-11.56		-11.30
		M	-19.99	-15.27		-13.03	-15.18	-13.91		-11.69		-11.84
	I2 *T-shap.*	*X*	-21.35	-17.66	-20.08	-15.80	-20.66	-17.28	-19.62	-16.63	-19.07	-10.41
		S	-21.04	-17.96	-19.87	-15.74	-20.28	-17.67	-19.32	-16.44	-18.76	-10.31
		M	-20.15	-17.06	-19.00	-15.01	-19.84	-16.79	-18.85	-15.99	-18.40	-9.37
	I5 *stacked*	*X*	-20.61	-15.49	-21.83	-13.04	-18.45	-14.85	-20.47	-12.25	-20.90	-11.99
		S	-21.03	-16.31	-22.09	-13.48	-18.44	-15.73	-20.29	-12.60	-20.64	-12.16
		M	-21.36	-14.98	-22.27	-12.50	-18.82	-14.46	-20.60	-11.73	-21.07	-11.45

Table ESI 2. E_{int} (in kcal/mol) in the minima of the scans performed at the MP2.X level of calculation organized in descending order of stability. Labels for the outer complexes are in **red** color and for the inner complexes in **blue**. As a reference, the values of the molecular electrostatic potential (in kcal/mol) in the minima of Fig. 3 are also included in the first line.

	MEP	Sh o -13.9	Ch o -12.9	Cc o -11.9	Sp o -9.8	Sc o -9.7	Ch i -8.8	Cc i -8.8	Sh i -7.7	Sp i -7.7	Sc i -7.6
monoatomic cations	N	Sh o -29.8	Sc i -29.0	Cc i -28.5	Cc o -28.4	Ch o -28.0	Sc o -27.7	Ch i -27.7	Sh i -27.5	Sp i -26.6	Sp o -22.5
	K	Sc i -27.2	Cc i -27.1	Ch i -25.0	Sp i -24.4	Sh i -24.3	Sh o -24.0	Cc o -23.6	Sc o -23.1	Ch o -22.8	Sp o -18.2
tetrahedral cations	A1				Sc i -27.1	Cc i -26.7	Sh o -23.4	Cc o -22.7	Ch o -22.3	Sc o -21.7	Sp o -17.9
	A2				Cc i -28.6	Sc i -28.3	Sh o -24.7	Cc o -24.3	Sc o -24.0	Ch o -23.8	Sp o -17.3
	A3				Sc i -30.9	Cc i -29.3	Sc o -23.8	Cc o -23.4	Sh o -23.3	Ch o -21.9	Sp o -18.0
	T1				Sc i -16.5	Cc i -16.4	Cc o -12.3	Sc o -12.0	Sh o -11.1	Ch o -11.0	Sp o -9.3
	T2				Cc i -17.3	Sc i -15.7	Cc o -14.3	Sc o -13.7	Sh o -12.2	Ch o -12.2	Sp o -9.4
	T3				Cc i -17.0	Sc i -15.7	Cc o -15.2	Sc o -14.7	Sh o -13.4	Ch o -13.2	Sp o -11.9
flat cations	G1 *T-shap.*				Cc i -19.4	Sc i -18.6	Cc o -15.4	Sh o -15.1	Sc o -14.8	Ch o -14.5	Sp o -10.0
	G2 *T-shap.*				Cc i -20.0	Cc o -19.2	Sc i -18.8	Sh o -18.7	Sc o -18.2	Ch o -17.8	Sp o -11.1
	G3 *stacked*				Cc i -19.4	Sc i -15.2	Cc o -15.1	Sc o -14.1	Ch o -13.0	Sh o -12.0	Sp o -11.7
	I2 *T-shap.*	Cc i -21.4	Sc i -20.7	Ch i -20.1	Sh i -19.6	Sp i -19.1	Cc o -17.7	Sc o -17.3	Sh o -16.6	Ch o -15.8	Sp o -10.4
	I5 *stacked*	Ch i -21.8	Sp i -20.9	Cc i -20.6	Sh i -20.5	Sc i -18.4	Cc o -15.5	Sc o -14.8	Ch o -13.0	Sh o -12.2	Sp o -12.0

Table ESI 3. Ionization potential and HOMO energies (in atomic units) of the fragments of the cation-π complexes studied, computed at the PBE/aVDZ level of calculation. These values are used in the SAPT(DFT) calculations.

	Ioniz. Pot.	HOMO
Corannulene	0.287281	-0.207502
Sumanene	0.262624	-0.190759
Sodium	1.832202	-1.332328
Potassium	1.162489	-0.914581
Ammonium	0.974144	-0.769845
Tetramethylammonium	0.638598	-0.520627
Guanidinium	0.583778	-0.448164
Imidazolium	0.563126	-0.435742

Note on the acronyms used. The positions (ring and side) of the π-system (C = corannulene; S = sumanene) explored in the study are defined in Fig. 1 of the main text. Cations (in general, M) are symbolized by a letter: N = Na^+, K = K^+, A = ammonium, T = tetramethylammonium, G = guanidinium and I = imidazolium. The orientations by which the polyatomic cations (A, T, G and I) face the molecular bowl (in general, Mb) are defined in Fig. 2 of the main text, and are represented by a number. The acronym that identifies a particular cation-π complex is formed combining the position of the Mb with the cation information. *Examples*:

CcNi = complex formed between Corannulene by its central ring with the Na^+ cation by the inner face of the Mb.

ShA3o = complex formed between Sumanene by its lateral hexagonal ring with the Ammonium cation with three (3) hydrogen groups oriented to the Mb and by its outer side.

Table ESI 4. Interaction energies and their contributions (all in kcal/mol) for the **Coranulenne-cation** complexes studied. The SAPT(DFT)/aVDZ calculations were made at the Mb···M distance of the minima found in the MP2.X scans.

compl.	Eint	Rep	Elec	Pol	Disp
CcNi	-25.11	6.59	-8.01	-22.97	-0.72
ChNi	-24.75	7.60	-9.11	-22.57	-0.68
CcNo	-27.27	7.18	-11.80	-22.08	-0.57
ChNo	-26.66	7.76	-11.78	-22.08	-0.58
CcKi	-23.22	11.28	-9.49	-19.48	-5.53
ChKi	-21.82	10.64	-9.68	-18.02	-4.76
CcKo	-22.35	9.52	-12.06	-16.38	-3.43
ChKo	-21.54	9.80	-11.48	-16.41	-3.44
CcA1i	-22.31	15.67	-9.01	-20.42	-8.55
CcA1o	-21.09	10.82	-10.35	-16.60	-4.96
ChA1o	-20.49	11.35	-9.90	-16.80	-5.14
CcA2i	-23.61	16.68	-9.94	-21.12	-9.22
CcA2o	-22.34	13.56	-12.49	-17.67	-5.74
ChA2o	-21.79	14.59	-12.11	-18.43	-5.84
CcA3i	-24.22	15.68	-10.28	-20.36	-9.27
CcA3o	-21.59	11.35	-12.35	-15.32	-5.28
ChA3o	-20.21	11.11	-11.04	-15.11	-5.16
CcT1i	-12.48	14.76	-7.58	-7.07	-12.59
CcT1o	-10.94	7.21	-7.73	-4.71	-5.71
ChT1o	-9.75	6.77	-6.45	-4.68	-5.38
CcT2i	-13.31	17.28	-9.22	-7.80	-13.57
CcT2o	-12.81	8.25	-8.89	-5.20	-6.96
ChT2o	-10.87	8.02	-7.29	-5.19	-6.41
CcT3i	-13.06	18.28	-9.27	-7.98	-14.09
CcT3o	-13.84	10.28	-9.60	-6.58	-7.94
ChT3o	-11.93	8.64	-7.45	-6.13	-7.00
CcG1i	-14.72	14.59	-7.74	-10.80	-10.78
CcG1o	-13.45	9.59	-9.13	-8.10	-5.81
ChG1o	-12.76	9.30	-8.26	-8.25	-5.54
CcG2i	-14.79	20.93	-9.28	-13.13	-13.30
CcG2o	-17.12	12.92	-10.61	-11.98	-7.45
ChG2o	-15.85	11.56	-9.55	-11.25	-6.61
CcG3i	-15.40	19.51	-11.84	-8.70	-14.37
CcG3o	-13.79	8.39	-10.01	-4.88	-7.29
ChG3o	-11.78	7.95	-7.89	-5.05	-6.78
CcI2i	-16.85	17.81	-9.00	-13.29	-12.36
ChI2i	-16.12	14.53	-7.70	-11.86	-11.08
CcI2o	-16.02	10.39	-10.02	-9.80	-6.59
ChI2o	-14.25	9.51	-8.66	-9.27	-5.83
CcI5i	-16.36	22.36	-12.28	-9.50	-16.93
ChI5i	-17.52	20.66	-11.66	-10.75	-15.76
CcI5o	-14.34	8.61	-10.00	-5.22	-7.73
ChI5o	-12.10	7.14	-7.71	-4.93	-6.60

Table ESI 5. Interaction energies and their contributions (all in kcal/mol) for the **Sumanene-cation** complexes studied. The SAPT(DFT)/aVDZ calculations were made at the Mb···M distance of the minima found in the MP2.X scans.

compl.	Eint	Rep	Elec	Pol	Disp
ScNi	-25.23	8.27	-7.41	-25.22	-0.87
ShNi	-24.25	8.89	-8.91	-23.48	-0.75
SpNi	-23.57	7.83	-7.03	-23.61	-0.76
ScNo	-26.81	7.68	-10.30	-23.50	-0.69
ShNo	-28.26	9.10	-14.35	-22.37	-0.64
SpNo	-21.41	7.87	-5.87	-22.80	-0.60
ScKi	-23.01	13.92	-9.06	-21.48	-6.39
ShKi	-21.09	11.35	-8.73	-18.65	-5.06
SpKi	-21.03	11.50	-8.09	-19.16	-5.29
ScKo	-22.14	9.65	-10.97	-17.12	-3.71
ShKo	-22.74	10.27	-13.08	-16.40	-3.53
SpKo	-17.00	8.95	-6.43	-16.22	-3.30
ScA1i	-22.49	17.00	-8.69	-21.38	-9.41
ScA1o	-20.36	9.92	-9.09	-16.15	-5.04
ShA1o	-21.60	11.75	-11.33	-16.77	-5.25
SpA1o	-16.36	10.35	-5.62	-16.23	-4.86
ScA2i	-23.33	18.11	-9.01	-22.40	-10.02
ScA2o	-22.31	13.17	-11.33	-18.22	-5.93
ShA2o	-22.74	14.82	-13.35	-18.28	-5.93
SpA2o	-15.60	11.17	-5.19	-16.62	-4.97
ScA3i	-25.22	19.49	-11.01	-22.96	-10.75
ScA3o	-22.08	12.19	-11.82	-16.74	-5.71
ShA3o	-21.48	12.34	-12.87	-15.56	-5.40
SpA3o	-16.35	10.41	-6.90	-14.86	-5.00
ScT1i	-12.05	19.03	-7.90	-8.17	-15.00
ScT1o	-10.80	7.37	-7.29	-4.97	-5.90
ShT1o	-9.87	7.40	-6.89	-4.87	-5.51
SpT1o	-8.06	6.40	-4.71	-4.54	-5.21
ScT2i	-11.78	20.41	-8.37	-8.76	-15.06
ScT2o	-12.45	8.87	-8.54	-5.57	-7.20
ShT2o	-10.98	8.30	-7.50	-5.30	-6.47
SpT2o	-8.22	6.27	-4.62	-4.59	-5.27
ScT3i	-11.86	21.68	-9.67	-8.68	-15.18
ScT3o	-13.47	10.47	-9.30	-6.77	-7.87
ShT3o	-12.07	10.25	-8.35	-6.59	-7.37
SpT3o	-10.45	10.14	-6.44	-6.46	-7.69
ScG1i	-14.21	16.84	-6.99	-11.87	-12.19
ScG1o	-13.39	8.83	-8.22	-8.18	-5.82
ShG1o	-13.32	9.62	-8.99	-8.31	-5.64
SpG1o	-8.77	6.54	-3.51	-7.24	-4.56
ScG2i	-14.30	18.75	-7.52	-12.52	-13.01
ScG2o	-16.37	12.60	-9.71	-11.80	-7.45
ShG2o	-16.59	14.24	-11.17	-12.26	-7.39
SpG2o	-9.74	7.23	-3.49	-8.68	-4.80
ScG3i	-11.74	20.72	-9.14	-8.93	-14.39
ScG3o	-13.14	7.60	-8.97	-4.91	-6.86
ShG3o	-10.99	7.18	-7.08	-4.84	-6.26
SpG3o	-10.41	7.91	-6.26	-5.28	-6.78
ScI2i	-16.09	19.49	-8.09	-13.90	-13.60
ShI2i	-15.53	16.47	-6.85	-12.49	-12.66
SpI2i	-14.82	15.98	-5.71	-12.33	-12.76
ScI2o	-15.77	10.84	-9.44	-10.30	-6.87
ShI2o	-15.00	10.63	-9.70	-9.70	-6.23
SpI2o	-9.28	6.09	-3.58	-7.51	-4.28
ScI5i	-14.08	25.64	-10.78	-10.81	-18.13
ShI5i	-16.02	22.66	-9.74	-12.32	-16.62
SpI5i	-16.11	25.93	-11.40	-12.86	-17.77
ScI5o	-13.85	8.71	-9.39	-5.38	-7.80
ShI5o	-11.46	6.99	-7.05	-4.95	-6.45
SpI5o	-10.91	7.68	-6.93	-5.17	-6.50

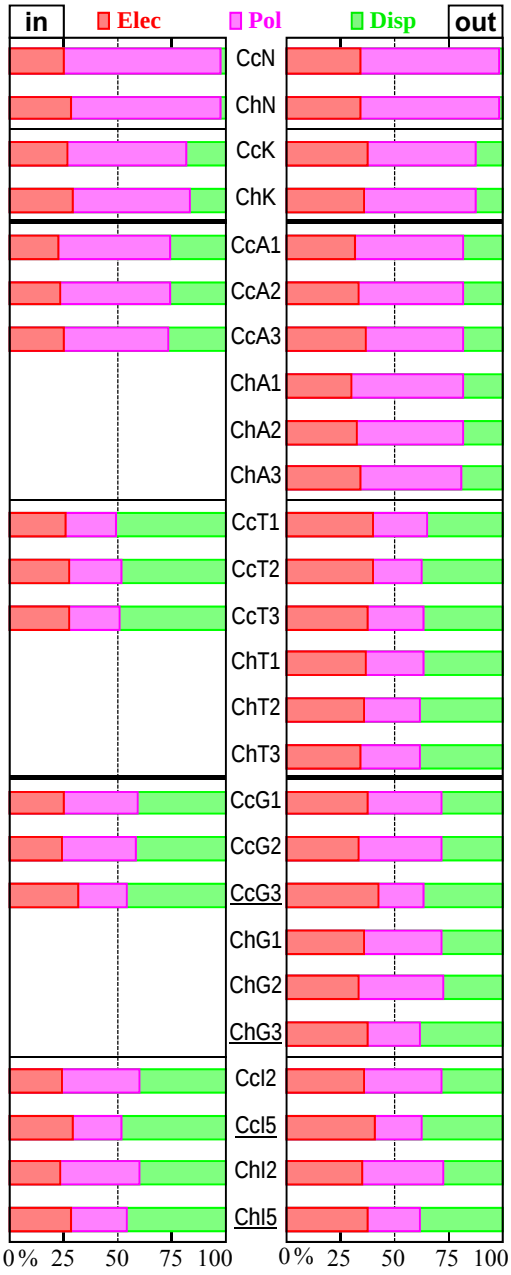

Fig. ESI 2. Relative contributions (expressed in %) of Electrostatic, Polarization and Dispersion to the stabilization of the **Corannulene-cation** complexes studied. Labels of the complexes in stacked configuration appear underlined.

The values of relative contributions to the stability of one complex are calculated using the data of Tables ESI 4 and ESI 5:

$$\%\mathrm{Elec} = \frac{\mathrm{Elec}\cdot 100\%}{\mathrm{Elec} + \mathrm{Pol} + \mathrm{Disp}}$$

and similar with %Pol and %Disp.

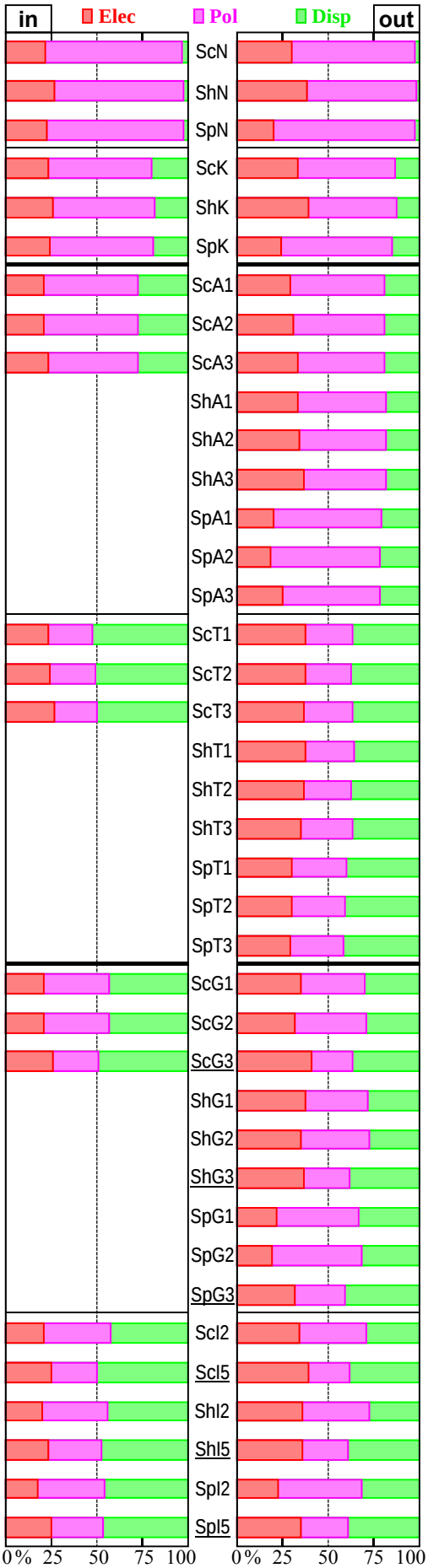

Fig. ESI 3. The same as Fig. ESI 2, here for the **Sumanene-cation** complexes.

Table ESI 6. Interaction energies of selected complexes, computed in the minima of the MP2.X scans. Molecular Bowl: sumanene, central ring.

Cation/orientation	*Level*[*]	in	out
N	*X*	-28.95	-27.74
	M	-32.51	-30.70
	P	-28.50	-29.90
K	*X*	-27.19	-23.10
	M	-27.40	-23.73
	P	-20.48	-21.49
A3	*X*	-30.86	-23.81
	M	-31.20	-24.47
	P	-22.89	-21.81
T3	*X*	-15.71	-14.72
	M	-14.79	-13.56
	P	-5.23	-10.76
G1	*X*	-18.59	-14.79
	M	-18.14	-14.62
	P	-9.73	-12.23
G3	*X*	-15.20	-14.12
	M	-15.10	-13.80
	P	-5.15	-9.74
I2	*X*	-20.66	-17.28
	M	-19.84	-16.79
	P	-10.96	-14.29
I5	*X*	-18.45	-14.85
	M	-18.75	-14.44
	P	-5.94	-9.81

*Level of calculation: ***X*** = MP2.X; ***M*** = M062X/6-31+G*; ***P*** = PBE/6-31+G*

Cartesian coordinates of the polyatomic fragments used in the study
optimization + frequencies computed at the level of calculation: M06-2X/6-31+G*

$C_{20}H_{10}$ = **Corannulene**, C5v

C	-1.14681132	-0.37262104	0.63005922
C	0.00000030	-1.20582856	0.63005925
C	1.14681102	-0.37262180	0.63005925
C	0.70876786	0.97553614	0.63005922
C	-0.70876852	0.97553617	0.63005921
C	-1.45670056	2.00497631	0.09801119
C	-2.81097051	1.64060583	-0.25948582
C	-3.23844597	0.32496873	-0.25948581
C	-2.35699113	-0.76583262	0.09801122
C	-2.42894668	-2.16641682	-0.25948576
C	-1.30979850	-2.97952484	-0.25948574
C	0.00000026	-2.47828642	0.09801127
C	1.30979922	-2.97952496	-0.25948571
C	2.42894641	-2.16641693	-0.25948571
C	2.35699037	-0.76583287	0.09801127
C	3.23844651	0.32496858	-0.25948574
C	2.81097064	1.64060595	-0.25948576
C	1.45670042	2.00497648	0.09801122
C	0.69167121	3.18036601	-0.25948581
C	-0.69167121	3.18036690	-0.25948582
H	-1.21035420	4.06266083	-0.62729684
H	-3.48980004	2.40654649	-0.62729684
H	-4.23784051	0.10431530	-0.62729681
H	-3.36716918	-2.57533327	-0.62729677
H	-1.40877467	-3.99819039	-0.62729673
H	1.40877526	-3.99819002	-0.62729670
H	3.36716917	-2.57533356	-0.62729670
H	4.23784034	0.10431556	-0.62729673
H	3.48979998	2.40654644	-0.62729677
H	1.21035499	4.06266103	-0.62729681

NH_4^+ = **Ammonium cation**, Td

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.02829432
H	0.96948518	0.00000000	-0.34276477
H	-0.48474260	0.83959879	-0.34276477
H	-0.48474259	-0.83959880	-0.34276477

$C_4H_{12}N^+$ = **Tetramethylammonium cation**, Td

N	0.00000000	0.00000000	0.00000000
C	1.49852706	0.00000000	0.00000000
C	-0.49950902	-1.22354222	0.70641243
C	-0.49950902	-0.00000000	-1.41282486
C	-0.49950902	1.22354222	0.70641243
H	1.95971433	0.00000000	0.98901930
H	1.95971433	-0.85651584	-0.49450965
H	1.95971433	0.85651584	-0.49450965
H	-0.18700994	-1.31459477	1.74800095
H	-1.58569445	-1.31459477	0.75898165
H	-0.18700994	-2.17111061	0.26447200
H	-1.58569445	-0.00000000	-1.51796329
H	-0.18700994	0.85651584	-2.01247294
H	-0.18700994	-0.85651584	-2.01247294
H	-0.18700994	2.17111061	0.26447199
H	-1.58569445	1.31459477	0.75898165
H	-0.18700994	1.31459477	1.74800095

$C_{21}H_{12}$ = **Sumanene**, C3v

C	0.69117819	-1.22833915	-0.69998887
C	-0.69117746	-1.22833925	-0.69998889
C	-1.40936173	0.01559176	-0.69998889
C	-0.71818436	1.21274712	-0.69998887
C	0.71818436	1.21274785	-0.69998884
C	1.40936262	0.01559260	-0.69998884
C	2.64539924	-0.13212532	-0.06831382
C	2.85085915	-1.64594370	0.18489616
C	1.43712444	-2.22491944	-0.06831387
C	0.71411463	-3.30021949	0.45185711
C	-0.71411310	-3.30022080	0.45185708
C	-1.43712375	-2.22492018	-0.06831392
C	-2.85085917	-1.64594515	0.18489606
C	-2.64539921	-0.13212676	-0.06831392
C	-3.21513206	1.03166889	0.45185708
C	-2.50101760	2.26855004	0.45185711
C	-1.20827558	2.35704545	-0.06831387
C	-0.00000095	3.29188830	0.18489616
C	1.20827469	2.35704614	-0.06831382
C	2.50101682	2.26855140	0.45185720
C	3.21513109	1.03166983	0.45185720
H	4.16042959	0.99672100	0.98847121
H	3.18882078	-1.84106632	1.20671417
H	3.59682417	-2.07662667	-0.49568583
H	1.21703102	-4.10139783	0.98847111
H	-1.21702966	-4.10139761	0.98847107
H	-3.18882036	-1.84106724	1.20671406
H	-3.59682303	-2.07662781	-0.49568595
H	-4.16042979	0.99671836	0.98847107
H	-2.94340058	3.10467739	0.98847111
H	-0.00000144	3.68213296	1.20671417
H	-0.00000121	4.15325444	-0.49568583
H	2.94339912	3.10467852	0.98847121

$CH_6N_3^+$ = **Guanidinium cation**, C3

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33259541
N	1.15406206	0.00000000	-0.66629598
N	-1.15405782	-0.00312600	-0.66629598
H	-1.19021509	-0.20083352	-1.65782873
H	-2.03221182	0.19342044	-0.20395746
H	-0.84034614	-0.19760886	1.86013720
H	0.83920536	0.19892436	1.86146692
H	2.03136541	-0.19533190	-0.20184417
H	1.19220876	0.19665048	-1.65796901

$C_3H_5N_2^+$ = **Imidazolium cation**, C2v

C	0.00598162	0.76338267	2.76894399
N	-1.07470959	0.09187609	3.15925224
C	-0.70160801	-1.05633494	3.82664158
C	0.65842025	-1.07167526	3.83555810
N	1.06604223	0.06772966	3.17328730
H	0.02006885	1.69692224	2.22633090
H	-2.02876475	0.38938239	2.98632881
H	-1.42100895	-1.75100181	4.23041160
H	1.35661468	-1.78233179	4.24862208
H	2.02874995	0.34361599	3.01293043