Supporting Information

for

Size and Curvature Effects upon the Halogen Interaction with Extended π Systems

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Figure S1. Orientations considered for performing the potential energy scans. In curvedstructures the same lines are also followed by the concave face.Page S1

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Figure S3. Potential energy curves for complexes with Br₂ as obtained with different methods. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. C and X refer to the concave and convex sides of the bowls, respectively. **Page S3**

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Figure S1. Orientations considered for performing the potential energy scans. In curved structures the same lines are also followed by the concave face.



Figure S2. Potential energy curves for complexes with Cl_2 as obtained with different methods. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex and concave sides of the bowls, respectively.



Figure S3. Potential energy curves for complexes with Br₂ as obtained with different methods. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex and concave sides of the bowls, respectively.



Figure S4. Potential energy curves for complexes with I_2 as obtained with different methods. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex and concave sides of the bowls, respectively.



Figure S5. Potential energy curves for complexes with Cl_2 as obtained with different methods. The origin corresponds to the equilibrium distance as obtained with MP2.5. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex and concave sides of the bowls, respectively.



Figure S6. Potential energy curves for complexes with Br_2 as obtained with different methods. The origin corresponds to the equilibrium distance as obtained with MP2.5. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex and concave sides of the bowls, respectively.



Figure S7. Potential energy curves for complexes with I_2 as obtained with different methods. The origin corresponds to the equilibrium distance as obtained with MP2.5. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex and concave sides of the bowls, respectively.

			AT	BP		ВТ	
		R	E	R	E	R	E
Cl ₂	coro	4.02	-4.68	3.35	-4.79	4.04	-4.59
	cora-X	3.95	-3.85	3.30	-3.34	4.02	-3.69
	cora-C	4.19	-6.00	3.61	-6.44	4.14	-6.08
	suma-X	3.96	-3.71	3.31	-3.10	3.98	-3.88
	suma-C	4.22	-6.38	3.72	-6.10	4.18	-6.42
Br ₂	coro	4.20	-6.17	3.46	-5.89	4.22	-6.03
	cora-X	4.10	-5.34	3.38	-4.19	4.17	-5.04
	cora-C	4.42	-7.50	3.76	-7.58	4.37	-7.59
	suma-X	4.10	-5.16	3.37	-3.96	4.11	-5.42
	suma-C	4.45	-7.96	3.89	-7.05	4.41	-8.01
l ₂	coro	4.52	-7.67	3.62	-7.21	4.54	-7.55
	cora-X	4.39	-6.64	3.49	-5.29	4.47	-6.31
	cora-C	4.76	-9.19	4.02	-8.37	4.71	-9.29
	suma-X	4.40	-6.41	3.46	-5.11	4.41	-6.72
	suma-C	4.79	-9.73	4.18	-7.57	4.75	-9.81

Table S1. Equilibrium distance (Å, to the centre of the X_2 bond) and interaction energy (kcal mol⁻¹) obtained for the complexes of Cl_2 , Br_2 and l_2 with coronene, corannulene, and sumanene as obtained by interpolation of the SCS-MP2/CBS potential energy curves. C and X refer to the concave and convex sides of the bowls, respectively.

Table S2. Equilibrium distance (Å, to the centre of the X ₂ bond) and interaction energy (kcal mol ⁻¹)
obtained for the complexes of Cl_2 , Br_2 and I_2 with coronene, corannulene, and sumanene as obtained by
interpolation of the TPSS-D3BJ/def2TZVP potential energy curves. C and X refer to the concave and convex
sides of the bowls, respectively.

		ŀ	AT	I	BP	BT	
		R	E	R	E	R	E
Cl ₂	coro	3.98	-4.46	3.47	-4.19	4.02	-4.27
	cora-X	3.82	-4.53	3.45	-2.71	3.90	-4.07
	cora-C	4.28	-4.76	3.73	-5.55	4.23	-4.75
	suma-X	3.83	-4.49	3.46	-2.63	3.83	-4.82
	suma-C	4.31	-5.30	3.83	-5.76	4.28	-5.29
Br ₂	coro	4.16	-6.02	3.53	-5.32	4.19	-5.77
	cora-X	4.01	-6.31	3.48	-3.51	4.08	-5.72
	cora-C	4.49	-6.08	3.86	-6.88	4.45	-6.08
	suma-X	4.02	-6.27	3.47	-3.46	4.04	-6.73
	suma-C	4.53	-6.80	3.97	-7.04	4.49	-6.76
l ₂	coro	4.52	-7.31	3.67	-6.85	4.54	-7.15
	cora-X	4.34	-7.27	3.56	-4.68	4.43	-6.72
	cora-C	4.83	-7.79	4.08	-8.12	4.79	-7.82
	suma-X	4.36	-7.19	3.53	-4.67	4.38	-7.62
	suma-C	4.86	-8.73	4.22	-7.90	4.82	-8.71

Table S3. Equilibrium distance (Å, to the centre of the X_2 bond) and interaction energy (kcal mol⁻¹) obtained for the complexes of Cl_2 , Br_2 and l_2 with coronene, corannulene, and sumanene as obtained by interpolation of the B3LYP-D3BJ/def2TZVP potential energy curves. C and X refer to the concave and convex sides of the bowls, respectively.

		ŀ	AT		BP	ВТ		
		R	E	R	E	R	E	
Cl ₂	coro	4.05	-4.56	3.40	-4.74	4.07	-4.43	
	cora-X	3.94	-4.03	3.37	-3.01	4.02	-3.71	
	cora-C	4.30	-5.42	3.68	-6.48	4.26	-5.45	
	suma-X	3.94	-3.98	3.36	-2.89	3.96	-4.20	
	suma-C	4.33	-6.05	3.76	-6.62	4.29	-6.06	
Br ₂	coro	4.27	-6.01	3.51	-6.00	4.29	-5.85	
	cora-X	4.12	-5.53	3.45	-3.89	4.21	-5.06	
	cora-C	4.56	-6.86	3.84	-7.88	4.52	-6.91	
	suma-X	4.13	-5.48	3.43	-3.81	4.14	-5.80	
	suma-C	4.59	-7.66	3.94	-7.92	4.55	-7.68	
l2	coro	4.61	-7.45	3.66	-7.56	4.63	-7.33	
	cora-X	4.46	-6.58	3.56	-5.04	4.55	-6.14	
	cora-C	4.91	-8.68	4.08	-9.03	4.87	-8.72	
	suma-X	4.47	-6.49	3.52	-5.02	4.49	-6.81	
	suma-C	4.95	-9.68	4.23	-8.79	4.90	-9.71	

Table S4. Equilibrium distance (Å, to the centre of the X ₂ bond) and interaction energy (kcal mol ⁻¹)
obtained for the complexes of Cl ₂ , Br ₂ and I ₂ with coronene, corannulene, and sumanene as obtained by
interpolation of the SAPTO/jun-cc-pVDZ potential energy curves. C and X refer to the concave and convex
sides of the bowls, respectively.

		ŀ	٩T	E	3P	ВТ	
		R	E	R	E	R	E
Cl ₂	coro	4.07	-4.31	3.36	-4.33	4.09	-4.20
	cora-X	3.99	-3.67	3.29	-3.13	4.06	-3.47
	cora-C	4.21	-5.65	3.62	-5.83	4.16	-5.74
	suma-X	4.00	-3.52	3.32	-2.79	4.02	-3.71
	suma-C	4.24	-6.06	3.75	-5.34	4.19	-6.13
Br ₂	coro	4.22	-6.20	3.44	-5.87	4.25	-6.01
	cora-X	4.09	-5.62	3.34	-4.37	4.17	-5.21
	cora-C	4.42	-7.64	3.75	-7.41	4.37	-7.74
	suma-X	4.10	-5.40	3.35	-4.01	4.11	-5.73
	suma-C	4.45	-8.16	3.90	-6.68	4.40	-8.25
l ₂	coro	4.50	-8.14	3.61	-7.38	4.53	-7.93
	cora-X	4.34	-7.52	3.43	-5.71	4.43	-6.97
	cora-C	4.74	-9.67	4.01	-8.30	4.69	-9.78
	suma-X	4.35	-7.21	3.42	-5.40	4.36	-7.65
	suma-C	4.77	-10.29	4.19	-7.27	4.73	-10.39

Table S5. Equilibrium distance (Å, to the centre of the X_2 bond) and interaction energy (kcal mol⁻¹) obtained for the complexes of Cl_2 , Br_2 and l_2 with coronene, corannulene, and sumanene as obtained by interpolation of the MP2.X (MP3/cc-pVDZ) potential energy curves. C and X refer to the concave and convex sides of the bowls, respectively.

		ŀ	AT.	I	3P	ВТ	
		R	E	R	E	R	E
Cl ₂	coro	4.05	-4.65	3.34	-5.18	4.07	-4.53
	cora-X	3.99	-3.70	3.30	-3.60	4.06	-3.51
	cora-C	4.21	-6.27	3.61	-7.15	4.16	-6.34
	suma-X	4.00	-3.58	3.30	-3.39	4.01	-3.75
	suma-C	4.24	-6.70	3.71	-6.94	4.20	-6.74
Br ₂	coro	4.25	-5.75	3.47	-5.93	4.27	-5.59
	cora-X	4.15	-4.81	3.40	-4.17	4.24	-4.50
	cora-C	4.46	-7.40	3.78	-7.90	4.42	-7.47
	suma-X	4.16	-4.67	3.39	-4.00	4.17	-4.91
	suma-C	4.49	-7.90	3.90	-7.56	4.45	-7.95
I2	coro	4.58	-7.03	3.65	-7.06	4.59	-6.89
	cora-X	4.47	-5.88	3.54	-5.08	4.55	-5.53
	cora-C	4.81	-8.94	4.05	-8.57	4.76	-9.02
	suma-X	4.47	-5.71	3.50	-4.97	4.48	-5.98
	suma-C	4.84	-9.54	4.20	-8.03	4.80	-9.60

Table S6. Mean absolute deviation in equilibrium distances (10^{-3} Å) and energies (kcal mol⁻¹) for the interpolated minima obtained with the different methods, taking MP2.5 as a reference.

	SCS-MP2		TPSS		B3LYP		SAPT0		MP2.X	
	ΔR	ΔE	ΔR	ΔE	ΔR	ΔE	ΔR	ΔE	ΔR	ΔE
Cl ₂	6.4	0.08	108.6	0.77	54.9	0.26	24.8	0.38	16.6	0.24
Br ₂	7.8	0.11	77.8	0.85	69.0	0.29	14.1	0.27	34.5	0.19
l2	9.4	0.16	51.9	0.69	85.2	0.25	36.8	0.64	43.6	0.30
All X ₂	7.9	0.12	79.5	0.77	69.7	0.27	25.2	0.43	31.6	0.24



Figure S8. Molecular electrostatic potential of the species considered in this work as obtained at the TPSS-D3BJ/def2-TZVP level, mapped onto an isosurface of density 0.001 a.u. The colour scale goes from -0.040 a.u. (red) to 0.040 a.u. (blue). The maximum values for the σ -hole are 25.8 kcal mol⁻¹, 29.8 kcal mol⁻¹ and 32.3 kcal mol⁻¹ for Cl₂, Br₂ and I₂, respectively.



Figure S9. Potential energy curves obtained at the MP2.5 level for the different complexes with coronene and sumanene. X and C indicate the convex and concave sides of the bowls, respectively.



Figure S10. Potential energy curves obtained at the MP2.5 level for the different complexes with Cl₂. X and C indicate the convex and concave sides of the bowls, respectively.



Figure S11. Potential energy curves obtained at the MP2.5 level for the different complexes with I₂. X and C indicate the convex and concave sides of the bowls, respectively.

	Orient.	R (Å)	E _{ele}	Erep	E _{dis}	Eind	E _{tot}
coro-Cl ₂	AT	4.07	-2.87	6.94	-6.68	-1.70	-4.31
	BP	3.36	-2.70	6.60	-7.76	-0.47	-4.33
	BT	4.09	-2.58	6.42	-6.55	-1.49	-4.20
coro-Br ₂	AT	4.22	-4.76	10.95	-9.49	-2.90	-6.20
	BP	3.44	-3.81	9.02	-10.41	-0.66	-5.87
	BT	4.25	-4.21	9.90	-9.20	-2.50	-6.01
coro-l ₂	AT	4.50	-6.14	14.10	-12.25	-3.85	-8.14
	BP	3.61	-4.97	11.51	-13.05	-0.87	-7.38
	BT	4.53	-5.58	12.99	-11.94	-3.40	-7.93
cora-Cl ₂	AT	3.99	-3.47	7.60	-5.62	-2.19	-3.67
	BP	3.29	-2.31	5.64	-6.05	-0.41	-3.13
	BT	4.06	-2.86	6.61	-5.46	-1.76	-3.47
cora-Br ₂	AT	4.09	-6.17	13.19	-8.48	-4.17	-5.62
	BP	3.34	-3.23	7.74	-8.29	-0.59	-4.37
	BT	4.17	-4.97	11.11	-8.08	-3.27	-5.21
cora-l₂	AT	4.34	-7.56	17.23	-11.27	-5.92	-7.52
	BP	3.43	-4.38	10.49	-10.93	-0.89	-5.71
	BT	4.43	-6.23	14.57	-10.65	-4.67	-6.97
suma-Cl ₂	AT	4.00	-3.40	7.29	-5.33	-2.08	-3.52
	BP	3.32	-2.17	5.09	-5.36	-0.35	-2.79
	BT	4.02	-3.94	8.09	-5.55	-2.31	-3.71
suma-Br ₂	AT	4.10	-6.07	12.77	-8.07	-4.02	-5.40
	BP	3.35	-3.09	7.13	-7.54	-0.51	-4.01
	BT	4.11	-7.09	14.41	-8.50	-4.55	-5.73
suma-l ₂	AT	4.35	-7.34	16.53	-10.70	-5.70	-7.21
	BP	3.42	-4.18	9.86	-10.28	-0.80	-5.40
	BT	4.36	-8.46	18.55	-11.30	-6.44	-7.65

Table S7. Equilibrium distance (Å, to the centre of the X_2 bond) and contributions to the interaction energy (kcal mol⁻¹) obtained for the complexes of Cl_2 , Br_2 and I_2 with coronene, corannulene, and sumanene as obtained by interpolation SAPTO/jun-cc-pVDZ. **Convex** face of the bowls.

	Orient.	R (Å)	E _{ele}	Erep	E _{dis}	Eind	E _{tot}
cora-Cl ₂	AT	4.21	-3.23	8.31	-9.40	-1.33	-5.65
	BP	3.62	-4.25	10.01	-10.68	-0.90	-5.83
	BT	4.16	-3.22	8.39	-9.61	-1.31	-5.74
cora-Br₂	AT	4.42	-4.94	11.69	-12.43	-1.96	-7.64
	BP	3.75	-6.26	14.16	-13.93	-1.38	-7.41
	BT	4.37	-4.92	11.74	-12.64	-1.92	-7.74
cora-l ₂	AT	4.74	-7.18	15.67	-15.59	-2.57	-9.67
	BP	4.01	-7.94	17.88	-16.47	-1.77	-8.30
	BT	4.69	-7.25	15.91	-15.87	-2.56	-9.78
suma-Cl ₂	AT	4.24	-3.76	9.12	-10.06	-1.36	-6.06
	BP	3.75	-3.80	10.05	-10.68	-0.92	-5.34
	BT	4.19	-3.82	9.17	-10.17	-1.31	-6.13
suma-Br ₂	AT	4.45	-5.72	12.81	-13.26	-1.99	-8.16
	BP	3.90	-5.51	13.94	-13.78	-1.33	-6.68
	BT	4.40	-5.79	12.85	-13.38	-1.92	-8.25
suma-l ₂	AT	4.77	-8.26	17.33	-16.68	-2.67	-10.29
	BP	4.19	-6.65	17.07	-16.06	-1.63	-7.27
	BT	4.73	-8.42	17.49	-16.85	-2.61	-10.39

Table S8. Equilibrium distance (Å, to the centre of the X_2 bond) and contributions to the interaction energy (kcal mol⁻¹) obtained for the complexes of Cl_2 , Br_2 and I_2 with coronene, corannulene, and sumanene as obtained by interpolation SAPTO/jun-cc-pVDZ. **Concave** face of the bowls.



Figure S12. SAPTO contributions for AT complexes formed by halogens with coronene and sumanene. Dotted lines correspond to Cl₂ complexes. Origin at the minima. C and X refer to the concave and convex sides of the bowls, respectively.



Figure S13. SAPTO contributions for BP complexes formed by halogens with coronene, corannulene and sumanene. Dotted lines correspond to Cl_2 complexes. Origin at the minima. C and X refer to the concave and convex sides of the bowls, respectively.



Figure S14. SAPTO contributions for BT complexes formed by halogens with coronene, corannulene and sumanene. Dotted lines correspond to Cl₂ complexes. Origin at the minima. C and X refer to the concave and convex sides of the bowls, respectively.



Figure S15. SAPTO contributions for complexes formed by Cl_2 and corannulene and sumanene. Dotted lines correspond to the convex face. Origin at the minima.



Figure S16. SAPTO contributions for complexes formed by I_2 and corannulene and sumanene. Dotted lines correspond to the convex face. Origin at the minima.



Figure S17. SAPTO contributions for complexes formed by Cl_2 and the different bowls. Dotted lines correspond to coronene complexes. Origin at the minima.



Figure S18. SAPTO contributions for complexes formed by Br₂ and the different bowls. Dotted lines correspond to coronene complexes. Origin at the minima.



Figure S19. SAPTO contributions for complexes formed by I_2 and the different bowls. Dotted lines correspond to coronene complexes. Origin at the minima.

	Orient.	R (Å)	E _{ele}	E _{rep}	E _{dis}	Eind	E _{tot}
circum-Cl ₂	AT	4.03	-3.11	7.97	-8.22	-1.89	-5.25
	BP	3.31	-3.21	7.64	-9.78	-0.51	-5.85
	BT	4.03	-3.07	7.85	-8.20	-1.82	-5.23
circum-Br₂	AT	4.18	-5.07	12.28	-11.51	-3.16	-7.46
	BP	3.36	-5.00	11.43	-13.72	-0.77	-8.07
	BT	4.19	-4.94	11.98	-11.43	-3.02	-7.41
circum-l ₂	AT	4.45	-6.76	16.54	-15.21	-4.37	-9.81
	BP	3.53	-6.43	14.24	-17.37	-0.98	-10.55
	BT	4.46	-6.58	16.04	-15.05	-4.16	-9.74
C ₆₀ -Cl ₂	AT	4.03	-2.52	6.36	-5.17	-1.72	-3.05
	BP	3.31	-2.05	4.92	-5.62	-0.36	-3.11
	BT	4.10	-2.02	5.66	-5.16	-1.41	-2.93
C ₆₀ -Br ₂	AT	4.13	-4.48	10.93	-7.72	-3.31	-4.57
	BP	3.33	-2.99	7.03	-7.92	-0.55	-4.43
	BT	4.23	-3.38	9.06	-7.42	-2.54	-4.28
C ₆₀ -I ₂	AT	4.40	-4.98	13.46	-9.99	-4.51	-6.02
	BP	3.39	-4.21	10.08	-10.98	-0.89	-6.00
	BT	4.49	-4.08	11.93	-9.78	-3.69	-5.63

Table S9. Equilibrium distance (Å, to the centre of the X_2 bond) and contributions to the interaction energy (kcal mol⁻¹) obtained for the complexes of Cl_2 , Br_2 and I_2 with circumcoronene and C_{60} as obtained by interpolation SAPTO/jun-cc-pVDZ.





Figure S20. SAPTO contributions for complexes formed by circumcoronene in BT orientation. Dotted lines correspond to complexes with coronene. The origin corresponds to the equilibrium distance of the circumcoronene complexes.



Figure S21. SAPTO contributions for complexes formed by circumcoronene. Dotted lines correspond to complexes with coronene.

		AT		E	3P	BT		
	Radius (Å)	R (Å)	E	R (Å)	E	R (Å)	E	
Cl₂	5.0	4.01	-4.59	3.32	-4.65	4.06	-4.43	
	7.5	4.01	-4.79	3.29	-5.06	4.04	-4.71	
	10.0	4.02	-4.90	3.28	-5.27	4.04	-4.85	
	15.0	4.02	-5.03	3.29	-5.48	4.03	-4.99	
	20.0	4.02	-5.09	3.29	-5.57	4.03	-5.06	
	30.0	4.03	-5.14	3.30	-5.66	4.03	-5.12	
	40.0	4.03	-5.17	3.30	-5.71	4.03	-5.15	
	∞	4.03	-5.25	3.31	-5.85	4.03	-5.23	
	-40.0	4.04	-5.38	3.33	-6.06	4.04	-5.36	
	-30.0	4.04	-5.44	3.33	-6.15	4.04	-5.42	
	-20.0	4.04	-5.57	3.35	-6.34	4.04	-5.54	
	-15.0	4.04	-5.73	3.36	-6.57	4.04	-5.70	
	-10.0	4.04	-6.12	3.36	-7.15	4.05	-6.06	
	-7.5	4.05	-6.63	3.41	-7.88	4.06	-6.55	
	-5.0	4.06	-8.28	3.57	-10.06	4.09	-8.18	
Br ₂	5.0	4.14	-6.66	3.36	-6.51	4.20	-6.42	
	7.5	4.15	-6.91	3.34	-7.03	4.18	-6.78	
	10.0	4.16	-7.04	3.35	-7.29	4.18	-6.95	
	15.0	4.16	-7.19	3.35	-7.55	4.18	-7.12	
	20.0	4.17	-7.25	3.36	-7.67	4.18	-7.20	
	30.0	4.17	-7.32	3.37	-7.79	4.18	-7.27	
	40.0	4.18	-7.35	3.37	-7.85	4.19	-7.31	
	8	4.18	-7.46	3.36	-8.07	4.19	-7.41	
	-40.0	4.19	-7.63	3.38	-8.33	4.20	-7.58	
	-30.0	4.19	-7.70	3.38	-8.45	4.20	-7.65	
	-20.0	4.20	-7.87	3.40	-8.69	4.20	-7.81	
	-15.0	4.20	-8.07	3.43	-9.00	4.21	-8.00	
	-10.0	4.21	-8.57	3.48	-9.76	4.22	-8.47	
	-7.5	4.22	-9.22	3.53	-10.79	4.23	-9.10	
	-5.0	4.25	-11.36	3.70	-13.53	4.28	-11.21	
I ₂	5.0	4.40	-8.83	3.45	-8.81	4.46	-8.50	
	7.5	4.42	-9.17	3.45	-9.41	4.44	-8.98	
	10.0	4.43	-9.33	3.46	-9.70	4.44	-9.20	
	15.0	4.44	-9.50	3.48	-9.98	4.44	-9.41	
	20.0	4.44	-9.58	3.49	-10.10	4.45	-9.49	
	30.0	4.44	-9.64	3.50	-10.24	4.45	-9.57	
	40.0	4.44	-9.68	3.51	-10.31	4.45	-9.61	
	8	4.45	-9.81	3.53	-10.55	4.46	-9.74	
	-40.0	4.46	-10.03	3.56	-10.94	4.47	-9.96	
	-30.0	4.47	-10.13	3.56	-11.11	4.47	-10.05	
	-20.0	4.47	-10.35	3.58	-11.48	4.48	-10.26	
	-15.0	4.48	-10.62	3.57	-11.93	4.49	-10.52	
	-10.0	4.49	-11.28	3.63	-12.98	4.51	-11.15	
	-7.5	4.50	-12.15	3.70	-14.33	4.53	-11.99	
	-5.0	4.55	-14.94	3.95	-17.03	4.58	-14.79	

Table S10. Interaction energies as the circumcoronene is curved. SAPTO/jun-cc-pVDZ. Negative radius correspond to complexes by the concave face.



Figure S22. SAPTO contributions to changes on the interaction energy as the circumcoronene molecule is curved. BT complexes. Negative values correspond to the concave face.



Figure S23. SAPTO contributions to changes on the interaction energy as the circumcoronene molecule is curved. R fixed at the minimum of the planar species. Negative values correspond to the concave face.

Cartesian coordinates (Å) for the optimised structures of the species considered in this work at the TPSS-D3BJ/def2-TZVP level.

		Coronene	
С	0.686551	3.681472	-0.000003
С	0.686551	-3.681472	-0.000002
С	0.712378	1.233848	-0.000001
С	0.712378	-1.233848	0.000001
Ċ	1.423652	2,465709	-0.000003
c	1 423652	-2 465709	0.000000
c	1.423032	-0.000000	0.000000
c	2 845004	2 125212	0.000001
c	2.845094	2.455515	-0.000004
c	2.845094	-2.435313	0.000004
C	2.84/22/	-0.000000	0.000002
C	3.531660	1.246173	-0.000000
C	3.531660	-1.246173	0.000005
С	-0.686551	3.681472	-0.000001
С	-0.686551	-3.681472	-0.000003
С	-0.712378	1.233848	0.000000
С	-0.712378	-1.233848	-0.000000
С	-1.423652	2.465709	0.000001
С	-1.423652	-2.465709	-0.000002
С	-1.424774	0.000000	0.000001
С	-2.845094	2.435313	0.000003
С	-2.845094	-2.435313	-0.000003
C	-2.847227	-0.000000	0.000003
c	-3 531660	1 246173	0.000004
ĉ	-3 531660	-1 246173	-0.000000
ц	1 222512	4 621225	-0.000000
н Ц	1.233312	4.021225	-0.000004
	2.205.455	-4.021225	-0.000002
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н	3.385455	-3.3/8882	0.000005
н	4.619007	1.242297	0.000000
н	4.619007	-1.242297	0.000006
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Н	-1.233512	-4.621225	-0.000004
Н	-3.385455	3.378882	0.000004
Н	-3.385455	-3.378882	-0.000005
Н	-4.619007	1.242297	0.000005C
Н	-4.619007	-1.242297	-0.000001
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c	0.975652	0.708852	0.000051
c	0.975055	-0.708852	0.000031
C	-0.372654	1.146943	0.000017
C	-0.372654	-1.146943	0.000017
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С	2.010261	1.460510	0.536318
С	2.010261	-1.460510	0.536318
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С	-0.767884	-2.363172	0.536269
С	-2.484860	0.000000	0.535928
С	0.322579	3.240792	0.894435
С	0.322579	-3.240792	0.894435
С	1.643956	2.811494	0.894432
С	1.643956	-2.811494	0.894432
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c	3.182105	-0.694697	0.893892
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r	-2.166008	-2.432293	0.894127
r r	-2 082620	1 208261	0.802076
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L LI	-2.382050	-1.3U8284	0.0939/5
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н	4.065385	1.210002	1.264393

	4.005205	1 210002	1 264202
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н	-4.000007	-1.410499	1,264839
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		Sumanene	
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ĉ	0.012710	1.410093	-0.000004
C	0.012/10	-1.410094	-0.000064
С	1.214797	0.716031	-0.000066
С	1.214797	-0.716030	-0.000066
С	-1.227482	0.694023	0.000131
С	-1.227482	-0.694023	0.000131
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C	2.361381	-1.210913	0.631776
С	-0.132011	2.650546	0.631647
С	-0.132011	-2.650546	0.631647
С	-2.229320	1.439549	0.632024
Ċ	-2 229321	-1 439549	0 632024
ĉ	2.223321	0.00000	0.052024
C	5.297590	0.000000	0.887045
C	-1.648/36	2.855/6/	0.886625
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С	1.034055	3.221162	1.151567
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ĉ	2 272474	2 506055	1 151685
ç	2.272474	2.500055	1.151005
C	2.2/24/4	-2.506055	1.151685
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С	-3.306463	-0.715039	1.152123
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	-2.080241	-3.602889	0.206377
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н	1.002536	-4.167703	1.686148
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н	3,107912	-2.952002	1.686365
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Ċ	-1 422734	2 464136	0 000014
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С	1.422734	-2.464136	0.000017
С	1.422734	2.464136	0.000021
С	-2.842971	-2.462623	0.000012
C	2 842971	-2 462623	0 000005
ĉ	2.012371	2.102023	0.000014
C	2.642971	2.402025	0.000014
C	-2.842971	2.462623	0.000003
С	-3.554261	1.230696	-0.000001
С	3.554261	-1.230696	0.000002
С	-3.554261	-1.230696	0.000005
Ċ	3 554261	1,230696	0.000007
ĉ	0.711.270	2,200000	0.000045
C	-0./112/0	3.093308	0.000015
C	0.711270	-3.693308	0.000017
С	-0.711270	-3.693308	0.000020
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С	-1.431432	4.929422	0.000006
r	1 421/22	-4 020/22	0 000000
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C	4.984845	-1.225130	-0.000013
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c	-2.832569	-4.905984	0.000011
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С	4.986327	3.666801	-0.000002
C	4.986327	-3.666801	-0.000022
C	-4.986327	3.666801	-0.000022
C	-5.008819	2.484/32	-0.000025
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c	0.682470	-6.151495	0.000006
С	-0.682470	-6.151495	0.000011
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н	3.376680	5.848436	0.000006
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н	6.756130	-2.480037	-0.000038
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н	-0.730130	7 090807	0.000015
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H H H	1.230124 5.525952 -5.525952	4.610755 -4.610755	-0.000001 -0.000007 -0.000005
H H H	1.230124 5.525952 -5.525952 5.525952	4.610755 -4.610755 -4.610755	-0.000001 -0.000007 -0.000005 -0.000032
н Н Н Н	1.230124 5.525952 -5.525952 5.525952 -5.525952	4.610755 -4.610755 -4.610755 4.610755	-0.000001 -0.000007 -0.000005 -0.000032 -0.000030
H H H H	1.230124 5.525952 -5.525952 5.525952 -5.525952	4.610755 -4.610755 -4.610755 4.610755	-0.000001 -0.000007 -0.000005 -0.000032 -0.000030
H H H H	1.230124 5.525952 -5.525952 5.525952 -5.525952	4.610755 -4.610755 -4.610755 4.610755	-0.000001 -0.000007 -0.000005 -0.000032 -0.000030
н Н Н Н С	1.230124 5.525952 -5.525952 -5.525952 -5.525952	4.610755 -4.610755 -4.610755 4.610755 C ₆₀ 1.174657	-0.000001 -0.000007 -0.000005 -0.000032 -0.000030
н н н н с с	1.230124 5.525952 -5.525952 -5.525952 -5.525952 0.381640 0.381640	4.610755 -4.610755 -4.610755 4.610755 C ₆₀ 1.174657 -1.174657	-0.000001 -0.000007 -0.000005 -0.000032 -0.000030 -3.325695 -3.325695
н н н н н с с с	1.230124 5.525952 -5.525952 -5.525952 -5.525952 0.381640 0.381640 1.235043	4.610755 -4.610755 -4.610755 4.610755 C ₆₀ 1.174657 -1.174657 0.000000	-0.000001 -0.000007 -0.000005 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614
H H H H C C C C C	1.230124 5.525952 -5.525952 -5.525952 -5.525952 0.381640 0.381640 1.235043 -0.999346	4.610755 -4.610755 -4.610755 4.610755 4.610755 C ₆₀ 1.174657 -1.174657 0.000000 0.726015	-0.000001 -0.000007 -0.000005 -0.000032 -0.000030 -3.325695 -3.325695 -3.325696 -3.325614 -3.325827
H H H H C C C C C C C	1.230124 5.525952 -5.525952 -5.525952 -5.525952 0.381640 0.381640 1.235043 -0.999346 -0.999346	4.610755 -4.610755 -4.610755 4.610755 4.610755 C ₆₀ 1.174657 -1.174657 0.000000 0.726015 -0.726015	-0.000001 -0.000007 -0.000005 -0.000032 -0.000030 -3.325695 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827
H H H H H C C C C C C C C C	1.230124 5.525952 -5.525952 -5.525952 -5.525952 0.381640 0.381640 1.235043 -0.999346 -0.999346 0.748517	 4.610755 -4.610755 -4.610755 -4.610755 4.610755 1.174657 1.174657 -1.174657 0.000000 0.726015 -0.726015 2.303656 	-0.000001 -0.000007 -0.0000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -3.325827 -2.592017
H H H H H H C C C C C C C C C C C	1.230124 5.525952 -5.525952 -5.525952 -5.525952 0.381640 0.381640 1.235043 -0.999346 -0.999346 0.748517 0.748517	4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -3.325827 -2.592017 -2.592017
H H H H C C C C C C C C C C C C C C C C	1.230124 5.525952 5.525952 5.525952 -5.525952 0.381640 0.381640 1.235043 -0.999346 0.748517 0.748517 2.422225	4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656 -0.000000	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -3.325827 -2.592017 -2.592017
нннн сссссссс	1.230124 5.525952 5.525952 5.525952 -5.525952 0.381640 0.381640 1.235043 -0.999346 -0.999346 0.748517 0.748517 2.422225 -1.959806	4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656 -2.303656 -0.000000 1.423849 4.623429	-0.000001 -0.000007 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592015 -2.592229
н н н н н н н н н н н н н н н н н н н	1.230124 5.525952 5.525952 5.525952 -5.525952 -5.525952 0.381640 0.381640 1.235043 -0.999346 0.748517 0.748517 2.422225 -1.959806 -1.959805	4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656 -2.303656 -0.000000 1.423849 -1.423849 -1.423849 -2.02670	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592015 -2.592229 -2.592229 -2.592229 -2.592229
нннн сссссссссс	1.230124 5.525952 5.525952 5.525952 -5.525952 -5.525952 -5.525952 -3.325952 -3.325952 -3.35040 1.235043 -0.999346 -0.999346 -0.999346 -0.748517 2.42225 -1.959806 -1.959805 1.983645	4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656 -2.303656 -0.000000 1.423849 -1.423849 2.303679 -2.303679 -2.303679	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592015 -2.592229 -1.828671 -1.828671 -1.828671
нннн ссссссссссс	1.230124 5.525952 5.525952 5.525952 -5.525952 -5.525952 -5.525952 -3.525952 -3.525952 -3.525952 -3.525952 -3.99346 0.381640 1.235043 -0.999346 0.748517 2.42225 -1.959806 -1.959805 1.983645 2.803934	4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656 -2.303656 -0.000000 1.423849 2.303679 -2.303679 1.174675	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592015 -2.592229 -1.828671 -1.828671 -1.828671 -1.828671
нннн сссссссссссс	1.230124 5.525952 5.525952 5.525952 -5.525952 -5.525952 -5.525952 -0.381640 1.235043 -0.999346 -0.999346 -0.999346 0.748517 2.42225 -1.959806 -1.959805 1.983645 2.803934 2.803934	4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656 -2.303656 -0.000000 1.423849 2.303679 -1.174675 -1.174675	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592015 -2.592229 -1.828671 -1.828685 -1.828685
нннн сссссссссссссс	1.230124 5.525952 5.525952 5.525952 -5.525952 -5.525952 -5.525952 -0.381640 0.381640 1.235043 -0.999346 -0.999346 -0.999346 -1.959805 1.983645 2.803934 2.803934 -0.250763	4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656 -2.303656 -2.303679 -1.174675 -1.174675 -1.174675 -1.174675	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592017 -2.59229 -1.828671 -1.828671 -1.828685 -1.828705
нннн ссссссссссссссс	1.230124 5.525952 5.525952 5.525952 -5.525952 -5.525952 -5.525952 - 0.381640 0.381640 1.235043 -0.999346 -0.999346 0.748517 2.42225 -1.959806 -1.959805 1.983645 2.803934 2.803934 -0.250763 -0.250763	 4.610755 -4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 1.174657 0.000000 0.726015 2.303656 -2.303656 -0.000000 1.423849 -1.423849 2.303679 -2.303679 1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -3.029651 -3.029651 	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592219 -1.828671 -1.828671 -1.828685 -1.828705 -1.828705 -1.828705
нннн сссссссссссссссс	1.230124 5.525952 5.525952 5.525952 -5.525952 -5.525952 -5.525952 - 0.381640 0.381640 1.235043 -0.999346 -0.999346 0.748517 2.42225 -1.959806 -1.959805 1.983645 2.803934 2.803934 -0.250763 -0.250763 -1.578045	 4.610755 -4.610755 -4.610755 -4.610755 -4.610755 -4.610755 -4.610755 -1.174657 -1.174657 -0.726015 -0.726051 -0.7	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592017 -2.59229 -1.828671 -1.828671 -1.828685 -1.828705 -1.828705 -1.828705 -1.828741
нннн ссссссссссссссссс	1.230124 5.525952 5.525952 5.525952 -5.525952 -5.525952 - 0.381640 0.381640 1.235043 -0.999346 -0.999346 0.748517 2.42225 -1.959806 -1.959805 1.983645 2.803934 2.803934 -0.250763 -0.250763 -1.578045 -1.578045	 4.610755 -4.610755 -4.610755 -4.610755 4.610755 4.610755 4.610755 1.174657 1.174657 0.000000 0.726015 2.303656 -2.303656 -2.303679 1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -1.29651 -3.029651 -3.029651 -3.98460 -2.598460 	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592219 -1.828671 -1.828671 -1.828685 -1.828705 -1.828705 -1.828741 -1.828740
нннн ссссссссссссссссс	1.230124 5.525952 5.525952 5.525952 -5.525952 -5.525952 -5.525952 - 0.381640 0.381640 1.235043 -0.999346 -0.999346 -0.999346 0.748517 2.42225 -1.959806 -1.959805 1.983645 2.803934 -0.250763 -0.250763 -1.578045 -1.578045 -1.578045 -2.959100	4.610755 -4.610755 -4.610755 4.610755 4.610755 4.610755 1.174657 -1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656 -2.303656 -2.303679 1.174675 3.029651 -3.029651 2.598460 -2.598460 0.697804	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592017 -2.592017 -2.592017 -2.59229 -1.828671 -1.828685 -1.828685 -1.828705 -1.828740 -1.828740 -1.82884
нннн сссссссссссссссссс	1.230124 5.525952 -5.525952 -5.525952 -5.525952 -5.525952 -5.525952 -0.381640 1.235043 -0.999346 -0.999346 -0.999346 -0.999346 -0.748517 2.42225 -1.959805 1.983645 1.983645 1.983645 2.803934 -0.250763 -0.250763 -1.578045 -1.578045 -1.578045 -2.959100 -2.959100	4.610755 -4.610755 -4.610755 4.610755 4.610755 4.610755 1.174657 -1.174657 -1.174657 0.000000 0.726015 2.303656 -2.303656 -2.303656 -2.303679 -1.174675 3.029651 -3.029651 2.598460 -2.598460 0.697804 -0.697804	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592017 -2.592017 -2.59229 -1.828671 -1.828671 -1.828685 -1.828685 -1.828745 -1.828740 -1.828740 -1.828894 -1.828894 -1.828894
ннннн сссссссссссссссссссс	1.230124 5.525952 -5.525952 5.525952 -5.525952 -5.525952 -5.525952 -0.381640 1.235043 -0.999346 -0.999346 -0.999346 -0.999346 -0.748517 2.42225 -1.959805 1.983645 1.983645 1.983645 2.803934 -0.250763 -0.250763 -1.578045 -1.578045 -2.959100 -2.959100 0.366842	 A.610755 -4.610755 -4.610755 -4.610755 -4.610755 -4.610755 -4.610755 -4.610755 -4.610755 -1.174657 -0.000000 0.726015 -0.726015 2.303656 -2.303656 -2.303656 -2.303679 -1.174675 -1.029651 -3.029651 -3.0296	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592017 -2.592017 -2.59229 -1.828671 -1.828671 -1.828685 -1.828685 -1.828685 -1.828745 -1.828740 -1.828740 -1.828894 -0.593560
ннннн ссссссссссссссссссссссс	1.230124 5.525952 -5.525952 -5.525952 -5.525952 -5.525952 -5.525952 -0.381640 1.235043 -0.999346 -0.999346 -0.999346 -0.999346 -0.999346 -1.959805 1.983645 1.983645 1.983645 1.983645 2.803934 -0.250763 -0.250763 -1.578045 -1.578045 -1.578045 -2.959100 -2.959100 0.366842 0.366842 0.366842	4.610755 -4.610755 -4.610755 4.610755 4.610755 4.610755 1.174657 -1.174657 -1.174657 -0.000000 0.726015 2.303656 -2.303656 -2.303656 -2.303679 -1.174675 -1.174675 3.029651 -3.029651 2.598460 -2.598460 0.697804 3.478379 -3.478379 -3.478379 -3.478379 -3.2755 -1.17875 -3.02651 -3.029656 -3.029656 -3.0	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325696 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592017 -2.592017 -2.592017 -2.592017 -2.59229 -1.828671 -1.828671 -1.828685 -1.828745 -1.828745 -1.828740 -1.828740 -1.828894 -0.593560 -0.593560 -0.593560
ннннн сосососососососососососососос	1.230124 5.525952 -5.525952 -5.525952 -5.525952 -5.525952 -5.525952 -0.381640 1.235043 -0.999346 -0.999346 -0.999346 -0.999346 -0.748517 2.42225 -1.959805 1.983645 1.983645 1.983645 1.983645 2.803934 -0.250763 -0.250763 -1.578045 -1.578045 -1.578045 -2.959100 0.366842 0.366842 1.747767	4.610755 -4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 -1.174657 0.000000 0.726015 -0.726015 2.303656 -2.303656 -2.303656 -2.303679 -1.174675 -1.174675 3.029651 2.598460 0.697804 3.478379 -3.478379 -3.478379 -3.478379 -3.29642	-0.000001 -0.000007 -0.000032 -0.000032 -0.000030 -3.325695 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.59229 -1.828671 -1.828671 -1.828685 -1.828671 -1.828685 -1.828675 -1.828745 -1.828745 -1.828740 -1.82875 -1.82875 -1.82870 -1.8287
ннннн сосососососососососососососос	1.230124 5.525952 -5.525952 -5.525952 -5.525952 -5.525952 -5.525952 -0.381640 1.235043 -0.999346 -0.999346 -0.999346 -0.999346 -0.999346 -1.959805 1.983645 1.983645 1.983645 1.983645 2.803934 -0.250763 -0.250763 -1.578045 -1.578045 -1.578045 -2.959100 0.366842 0.366842 1.747767 1.747767	4.610755 -4.610755 -4.610755 -4.610755 4.610755 4.610755 1.174657 -1.174657 -1.174657 -0.000000 0.726015 2.303656 -2.303656 -2.303656 -2.303679 -1.174675 -1.174675 -1.174675 -1.174675 -1.174675 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -2.303679 -3.029651 -3.029651 -3.029642 -3.029642 -3.029642 -3.029642	-0.000001 -0.000007 -0.000005 -0.000032 -0.000032 -0.000030 -3.325696 -3.325696 -3.325614 -3.325827 -3.325827 -2.592017 -2.592017 -2.592017 -2.592017 -2.592017 -2.59229 -1.828671 -1.828671 -1.828671 -1.828685 -1.828745 -1.828745 -1.828740 -1.828740 -1.828740 -1.828740 -1.828894 -0.593560 -0.593529 -0.593529 -0.593529 -0.593529

С	3.421562	-0.725985	-0.593550
С	-2.341410	2.598414	-0.593597
С	-2.341410	-2.598414	-0.593597
С	-3.194882	1.423738	-0.593632
С	-3.194882	-1.423738	-0.593632
С	2.341410	2.598414	0.593597
С	2.341410	-2.598414	0.593597
С	3.194881	1.423738	0.593632
С	3.194882	-1.423738	0.593632
С	-0.366842	3.478379	0.593560
С	-0.366842	-3.478379	0.593560
С	-1.747767	3.029642	0.593529
С	-1.747767	-3.029642	0.593529
С	-3.421562	0.725984	0.593550
С	-3.421562	-0.725985	0.593550
С	0.250763	3.029651	1.828705
С	0.250763	-3.029651	1.828705
С	1.578044	2.598460	1.828740
С	1.578045	-2.598460	1.828740
C	2.959100	0.697804	1.828894
C	2.959100	-0.697804	1.828894
C	-1.983645	2.303679	1.8286/1
C	-1.983645	-2.303679	1.828671
C	-2.803934	1.1/46/5	1.828685
C	-2.803934	-1.1/46/5	1.828685
c	1.959806	1.423849	2.592229
C	1.959806	-1.423849	2.592229
c	-0.748517	2.303050	2.592017
c	-0./4851/	-2.303050	2.592017
c	-2.422225	-0.000000	2.392013
c	0.999540	0.726015	2 2 2 2 5 9 2 7
c	0.333340	1 174657	2 2 2 5 6 0 6
c	-0.381040	1.174057	2 225606
c	-0.381040	-0.000000	3 325614
C	-1.233043	-0.000000	5.525014
		Ch	
CI	0.000000	0.000000	-1.006146
CL	0.000000	0.000000	1.006146
	1.0000000	5.000000	1.000110
		Br ₂	
Br	0.000000	0.000000	-1.154857
Br	0.000000	0.000000	1.154857

		12	
L	0.000000	0.000000	-1.341621
I	0.000000	0.000000	1.341621

Cartesian coordinates (Å) for the optimised structures of circumcoronene with different curvatures at the TPSS-D3BJ/def2-TZVP level.

Circumcoronene R=5.0Å			
C 1.399818	0.000000	0.149073	
C -1.399818	0.000000	0.149073	
C 0.712145	1.212511	-0.000000	
C 0.712145	-1.212511	-0.000000	
C -0.712145	-1.212511	-0.000000	
C -0.712145	1.212511	0.000000	
C 2.699670	0.000000	0.746737	
C -2.699670	0.000000	0.746737	
C 1.402404	2.429645	0.149864	
C 1.402404	-2.429645	0.149864	
C -1.402404	-2.429645	0.149864	
C -1.402404	2.429645	0.149864	
C 2.697893	-2.428157	0.745620	
C -2.697893	-2.428157	0.745620	
C -2.697893	2.428157	0.745620	
C 2.697893	2.428157	0.745620	
C 3.285896	1.213828	1.194149	
C -3.285897	-1.213828	1.194149	
C 3.285896	-1.213828	1.194149	
C -3.285897	1.213828	1.194149	
C 0.715169	3.638487	0.000549	
C -0.715169	-3.638487	0.000549	
C 0.715169	-3.638487	0.000549	
C -0.715169	3.638487	0.000549	
C 1.418254	4.867369	0.153955	
C -1.418254	-4.867369	0.153955	
C 1.418254	-4.867369	0.153955	
C -1.418254	4.867369	0.153955	
C 3.284291	-3.650039	1.192848	
C-3.284291	3.650039	1.192848	
C -3.284291	-3.650039	1.192848	
C 3.284291	3.650040	1.192848	
C 4.182831	1.208831	2.290744	
C -4.182831	-1.208831	2.290744	
C 4.182830	-1.208831	2.290744	
C -4.182831	1.208831	2.290744	
C 2.682885	4.844566	0.735204	
C 2.682885	-4.844566	0.735204	
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H 4.769506	2.448012	4.063912	
н -4.769506	2.448012	4.063912	
п 4.769506	-2.448012	4.063912	

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	H -4.456042	4.521857	2.837445
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c c	-0 710766	-1 222474	-0.000000
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ĉ	1 425575	4 904018	0 102854
ĉ	-1 425575	-4 904018	0 102854
c c	1 425575	-/ 90/018	0.102054
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ĉ	-0 681957	-6 126882	-0 002763
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c c	-0 710328	-1 225588	-0.000000
c c	-0 710328	1 225588	0.000000
c c	2 809311	0.000000	0.378097
c c	2.809311	0.000000	0.378097
c c	1 417007	2 466619	0.378037
c	1.417907	2.450516	0.075782
C C	1.417907	-2.450518	0.075782
C	-1.41/90/	-2.456518	0.075782
C	-1.41/90/	2.456518	0.075782
C	2.806988	-2.455012	0.377418
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С	-2.806988	2.455012	0.377418
С	2.806988	2.455012	0.377418
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c	4 024704	1 224260	0.302720
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