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


# Supporting Information

# for

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

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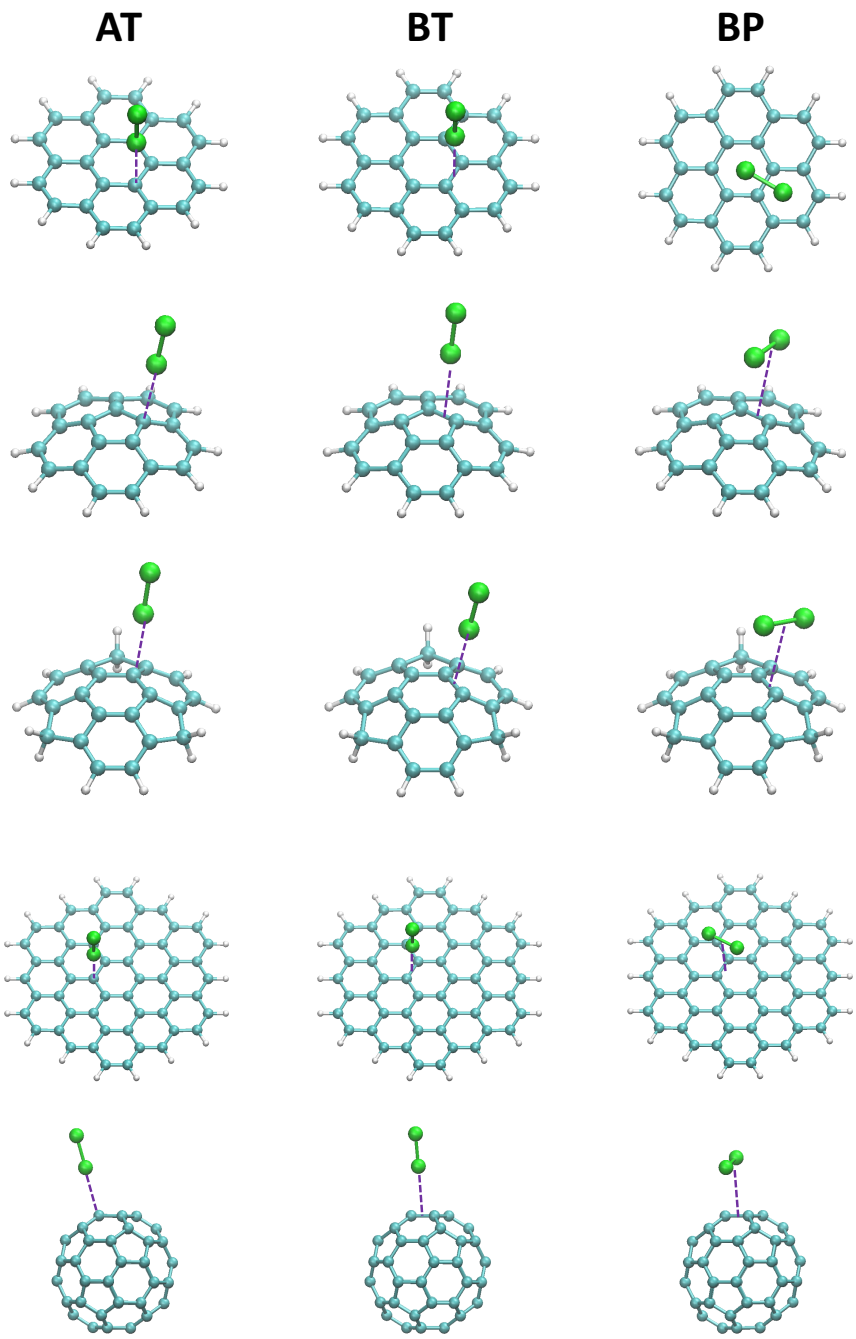


**Figure S1.** Orientations considered for performing the potential energy scans. In curved structures the same lines are also followed by the concave face.

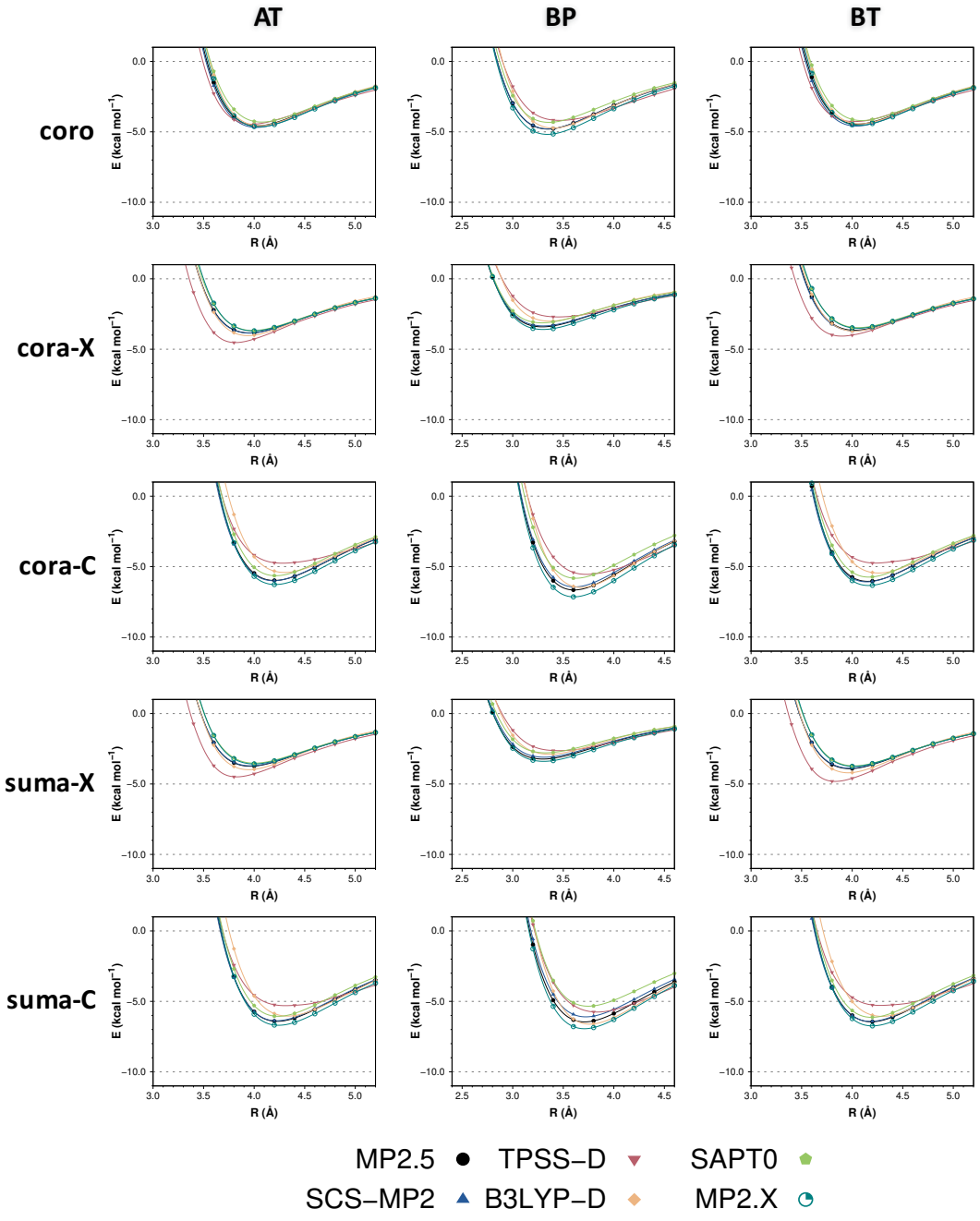


**Figure S2.** Potential energy curves for complexes with $Cl_2$ as obtained with different methods. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex and concave sides of the bowls, respectively.

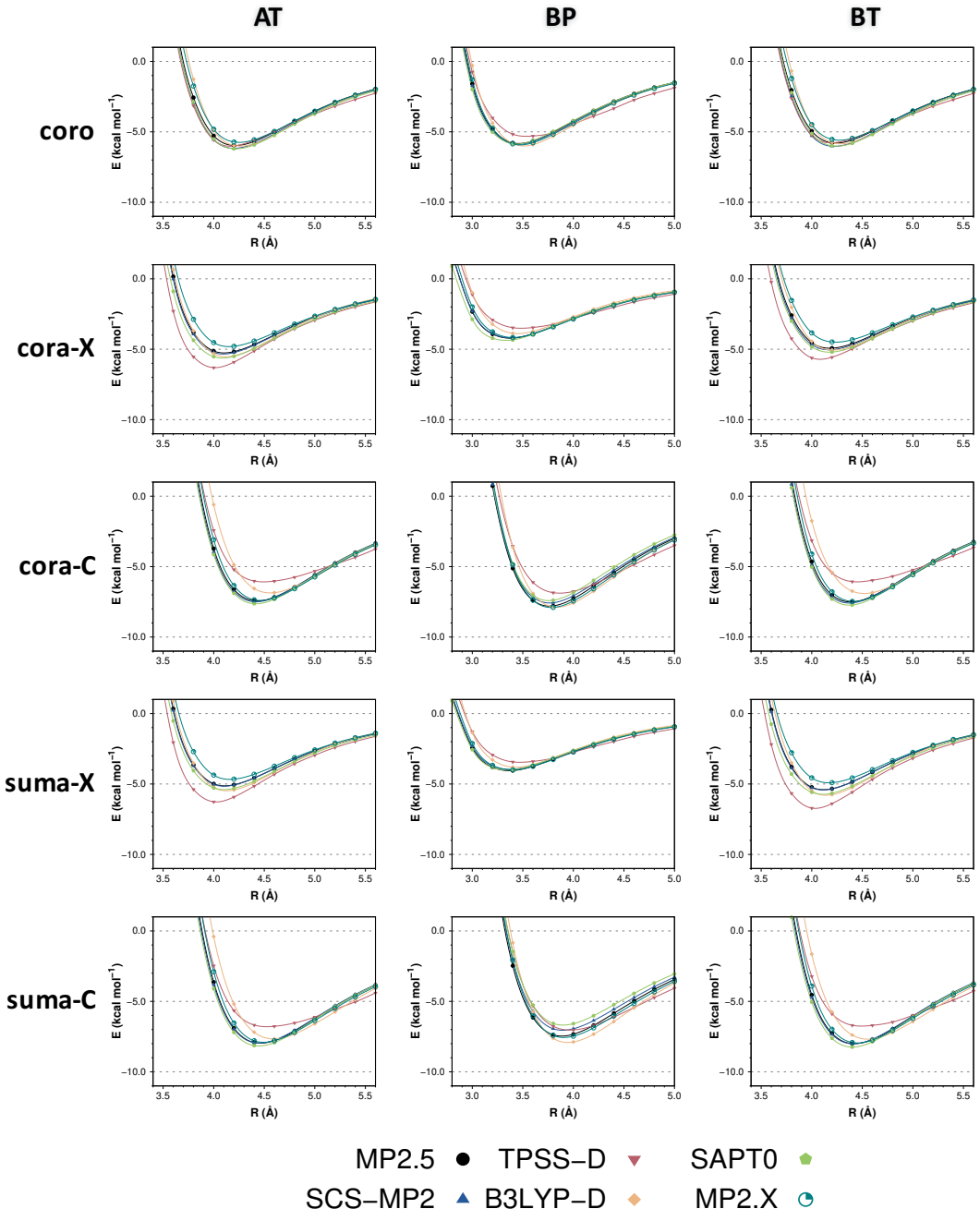


**Figure S3.** Potential energy curves for complexes with $Br_2$ as obtained with different methods. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex and concave sides of the bowls, respectively.

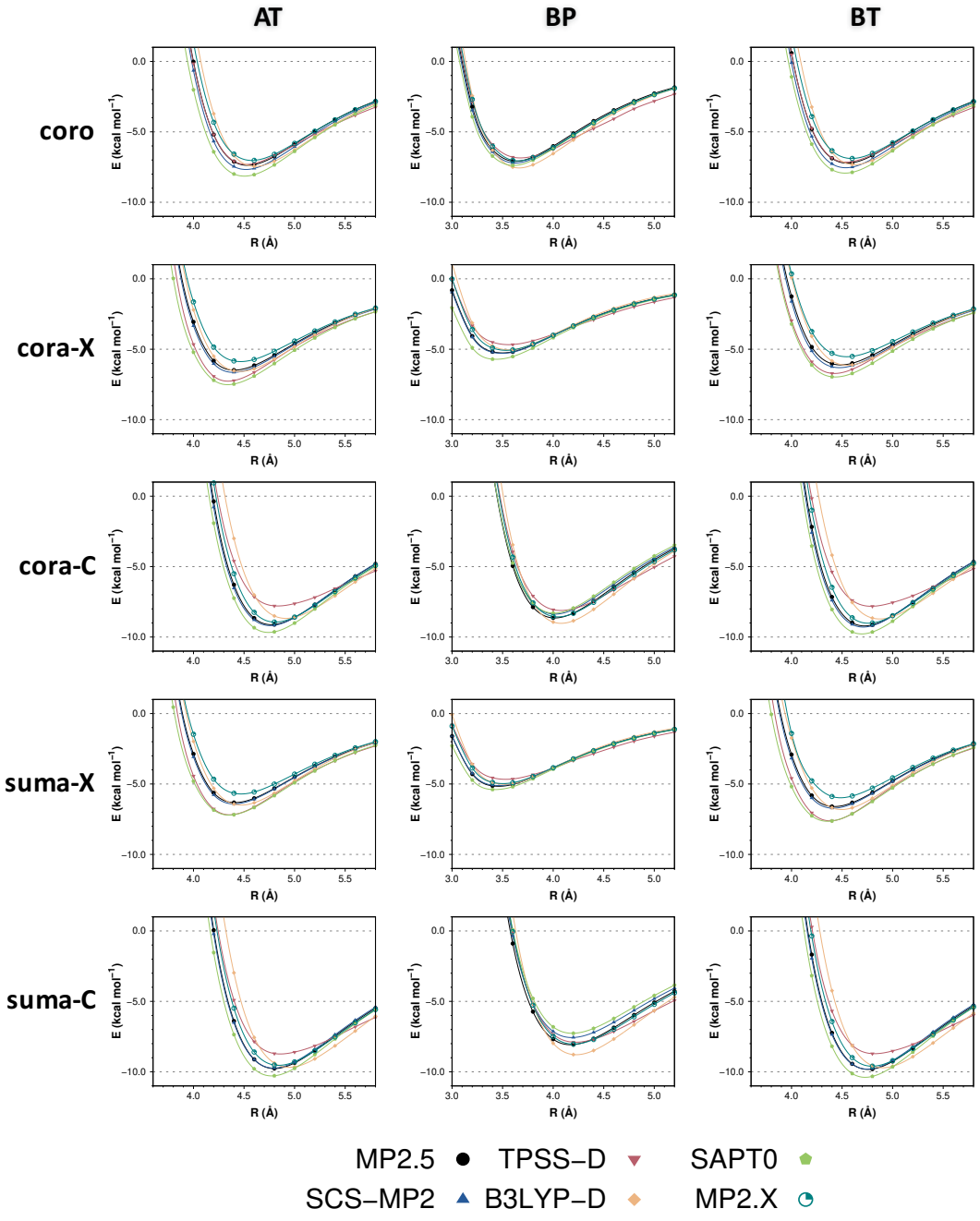


**Figure S4.** Potential energy curves for complexes with $I_2$ as obtained with different methods. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex and concave sides of the bowls, respectively.

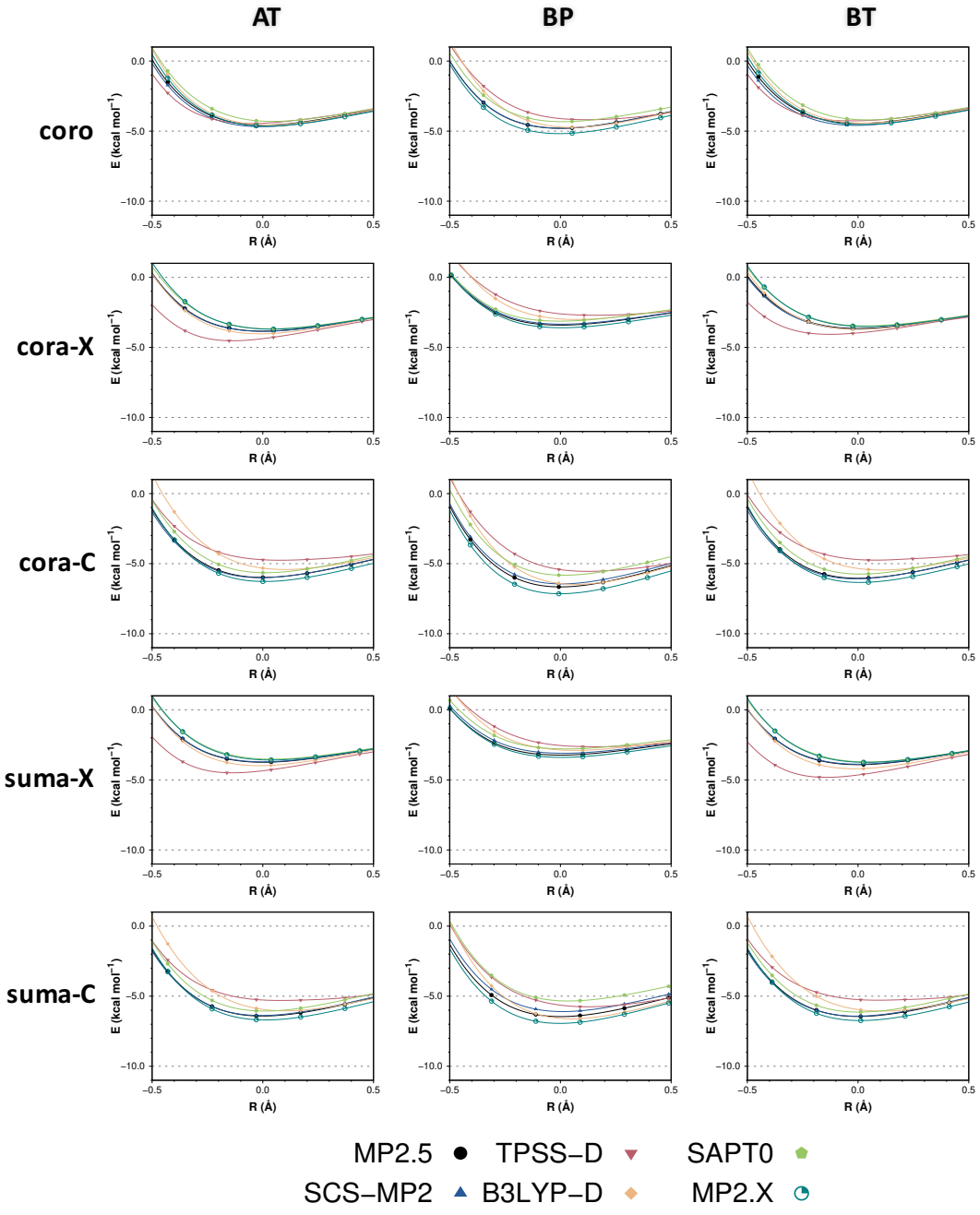


**Figure S5.** Potential energy curves for complexes with $Cl_2$ as obtained with different methods. The origin corresponds to the equilibrium distance as obtained with MP2.5. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex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

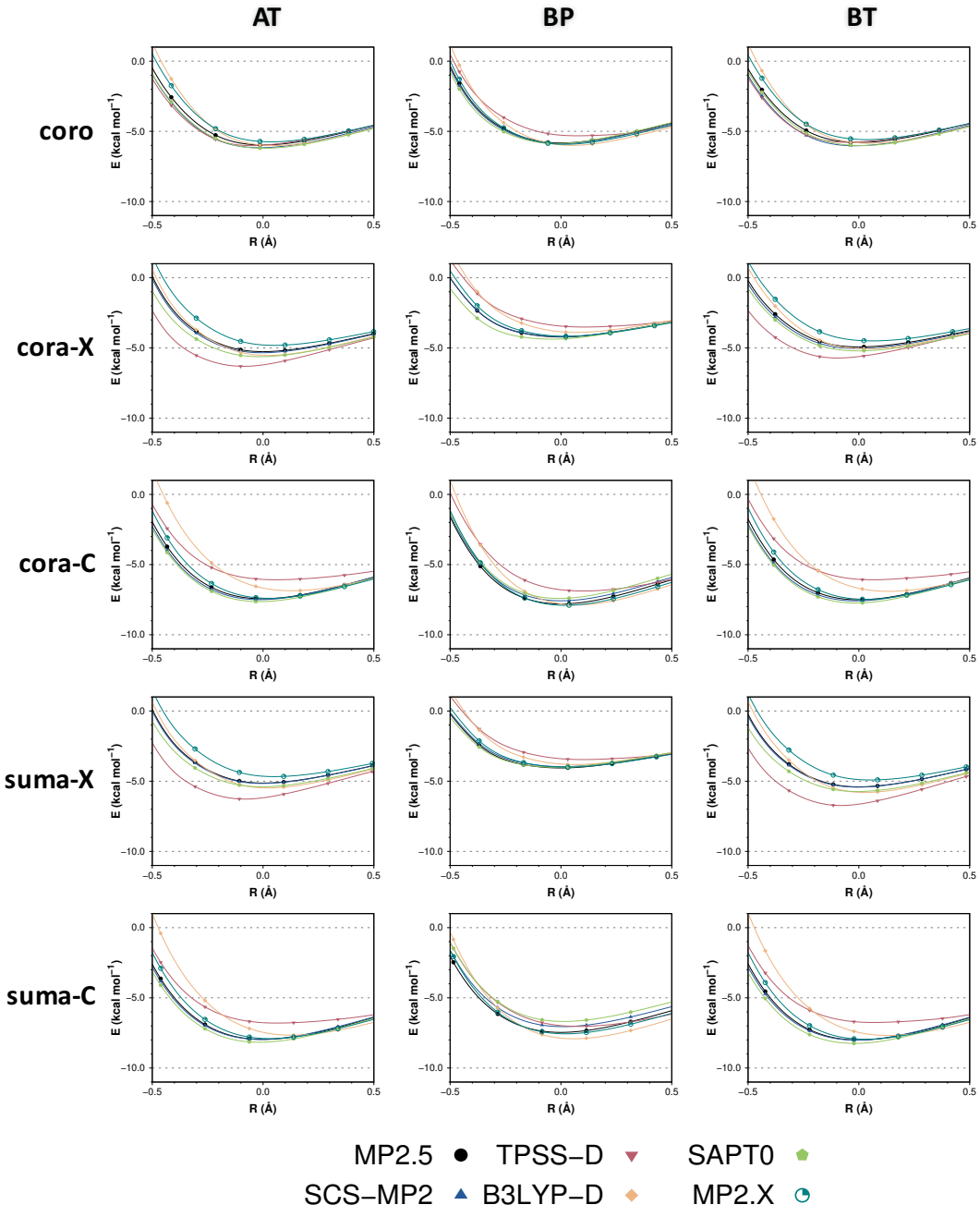


**Figure S6.** Potential energy curves for complexes with $Br_2$ as obtained with different methods. The origin corresponds to the equilibrium distance as obtained with MP2.5. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex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

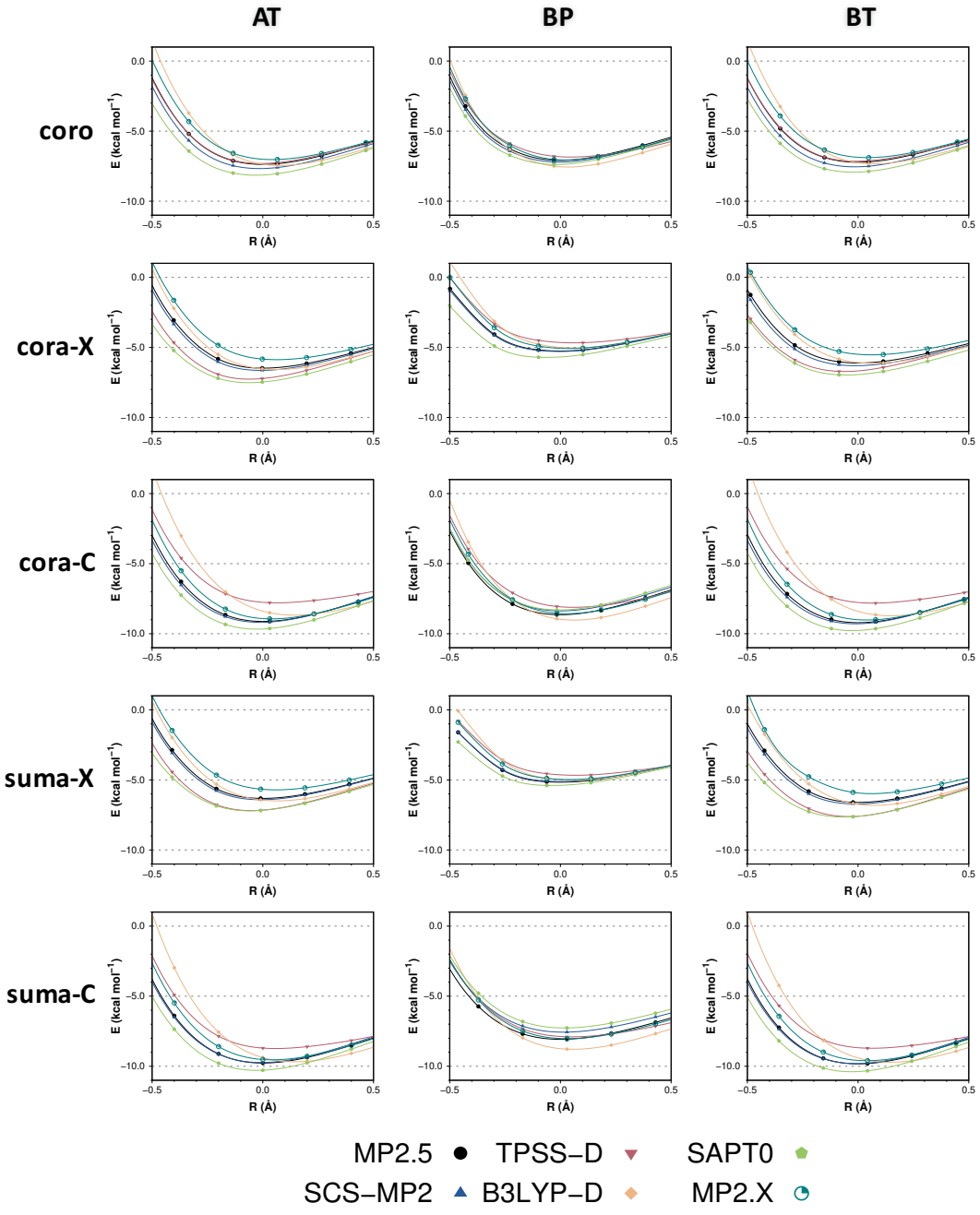


**Figure S7.** Potential energy curves for complexes with $I_2$ as obtained with different methods. The origin corresponds to the equilibrium distance as obtained with MP2.5. D indicates the D3BJ dispersion model. MP2.X: MP3 correction obtained with the cc-pVDZ basis set. X and C indicate the convex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

**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 $I_2$ 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.

| | | AT | | BP | | BT | |
|---|---|---|---|---|---|---|---|
| | | **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 |
| **$I_2$** | **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 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.

| | | AT | | 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 |
| **$I_2$** | **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 $I_2$ 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.

| | | AT | | BP | | BT | |
|---|---|---|---|---|---|---|---|
| | | **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 |
| **$I_2$** | **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 SAPT0/jun-cc-pVDZ potential energy curves. C and X refer to the concave and convex sides of the bowls, respectively.

| | | AT | | BP | | BT | |
|---|---|---|---|---|---|---|---|
| | | **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 |
| **$I_2$** | **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 $I_2$ 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.

| | | AT | | BP | | BT | |
|---|---|---|---|---|---|---|---|
| | | **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 |
| **$I_2$** | **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 |
| **$I_2$** | 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 |

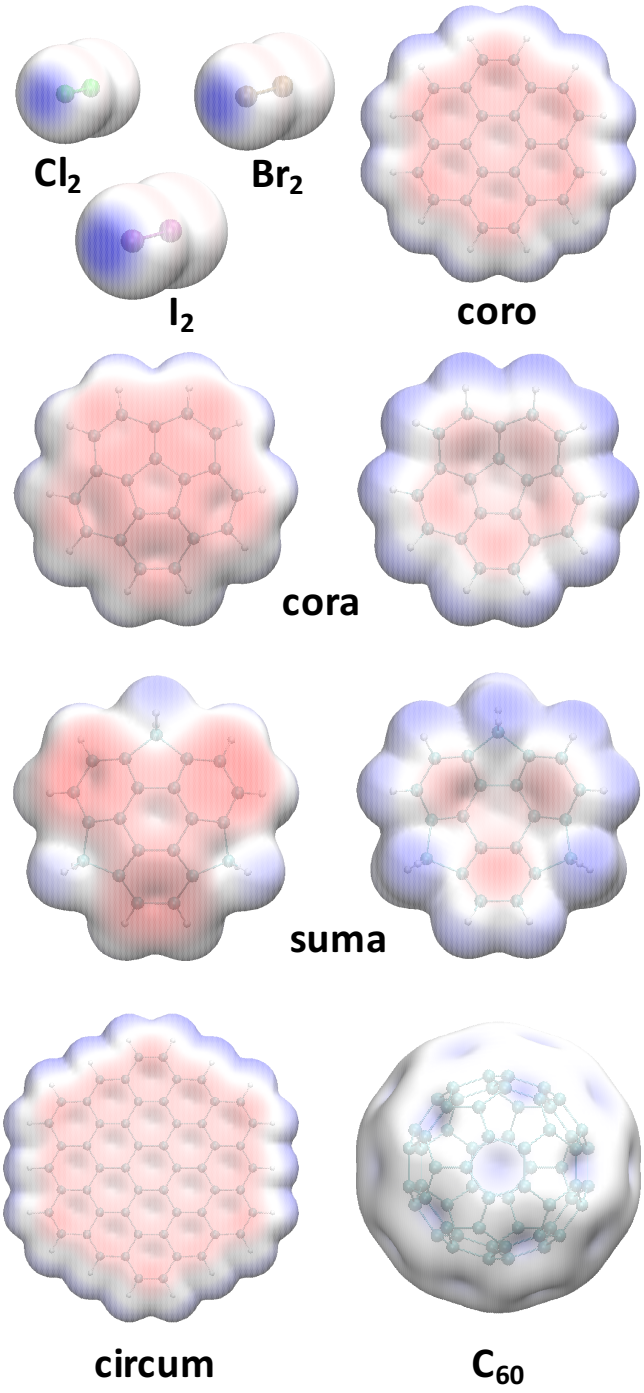


**Figure S8.** Molecular electrostatic potential of the species considered in this work as obtained at the TPSS-D3BJ/def2-TZVP level, mapped onto an isosurface of density 0.001 a.u. The colour scale goes from -0.040 a.u. (red) to 0.040 a.u. (blue). The maximum values for the σ-hole are 25.8 kcal $mol^{-1}$, 29.8 kcal $mol^{-1}$ and 32.3 kcal $mol^{-1}$ for $Cl_2$, $Br_2$ and $I_2$, respectively.

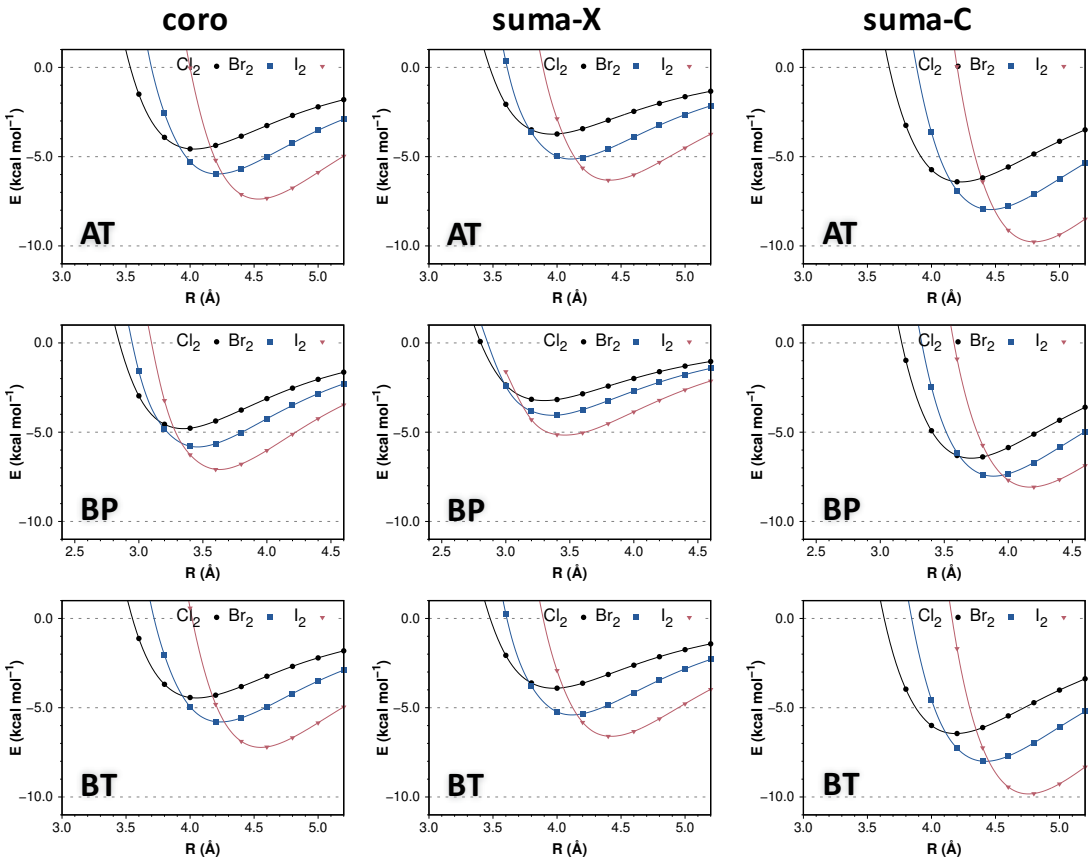


**Figure S9.** Potential energy curves obtained at the MP2.5 level for the different complexes with coronene and sumanene. X and C indicate the convex and concave sides of the bowls, respectively.

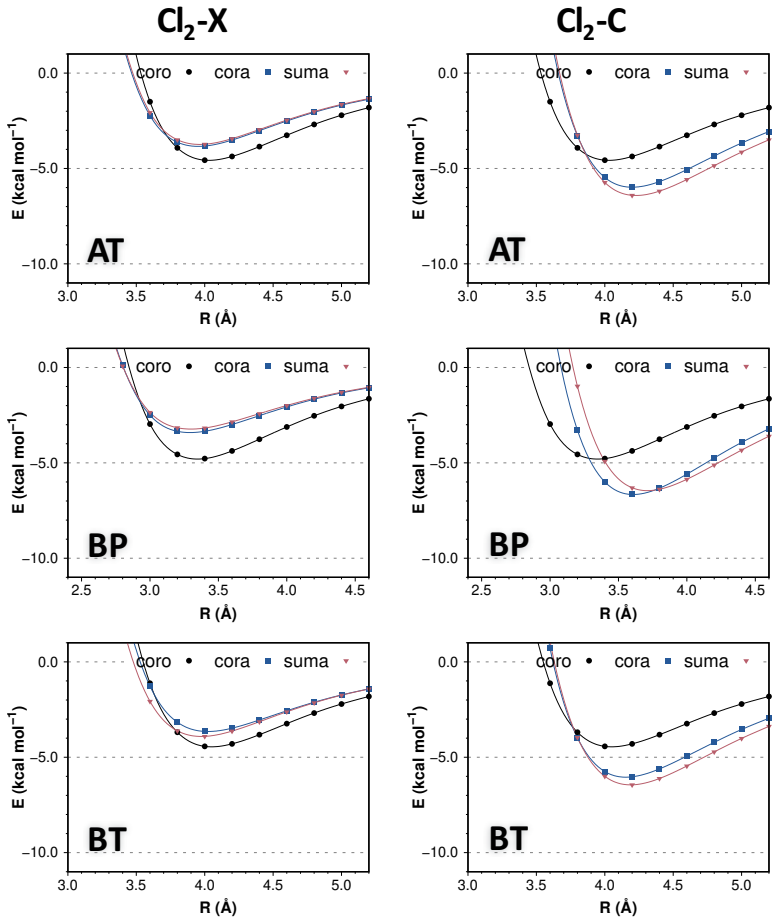


**Figure S10.** Potential energy curves obtained at the MP2.5 level for the different complexes with $Cl_2$. X and C indicate the convex and concave sides of the bowls, respectively.

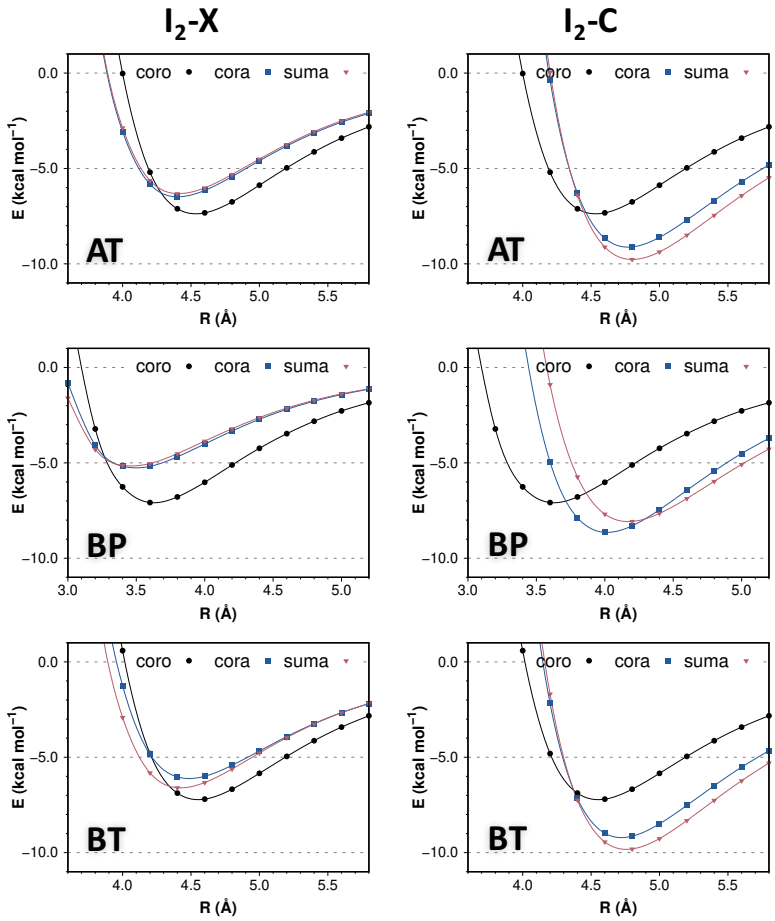


**Figure S11.** Potential energy curves obtained at the MP2.5 level for the different complexes with $I_2$. X and C indicate the convex and concave sides of the bowls, respectively.

**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 SAPT0/jun-cc-pVDZ. **Convex** face of the bowls.

| | Orient. | R (Å) | $E_{ele}$ | $E_{rep}$ | $E_{dis}$ | $E_{ind}$ | $E_{tot}$ |
|---|---|---|---|---|---|---|---|
| **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-$I_2$** | **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-$I_2$** | **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-$I_2$** | **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 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 SAPT0/jun-cc-pVDZ. **Concave** face of the bowls.

| | **Orient.** | **R (Å)** | **$E_{ele}$** | **$E_{rep}$** | **$E_{dis}$** | **$E_{ind}$** | **$E_{tot}$** |
|---|---|---|---|---|---|---|---|
| **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-$Br_2$** | **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-$I_2$** | **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-$I_2$** | **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 |

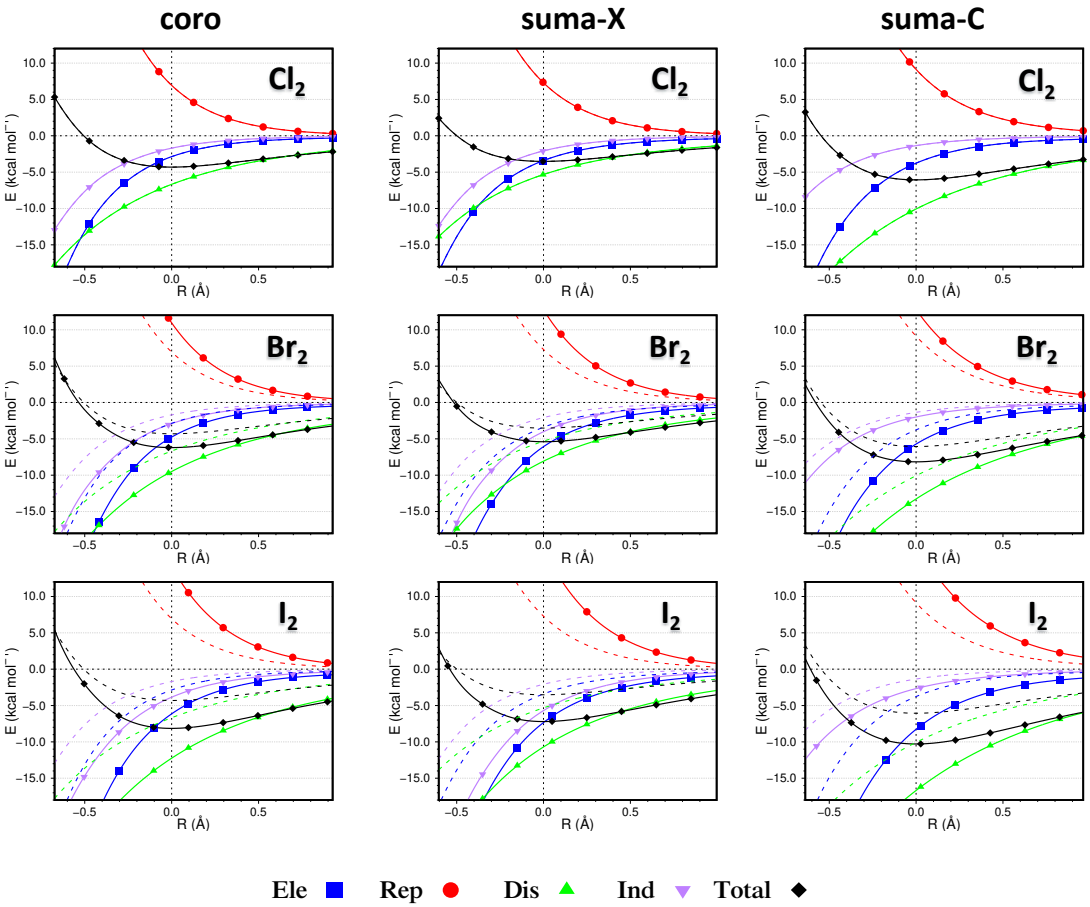


**Figure S12.** SAPT0 contributions for AT complexes formed by halogens with coronene and sumanene. Dotted lines correspond to $Cl_2$ complexes. Origin at the minima. C and X refer to the concave and convex sides of the bowls, respectively.

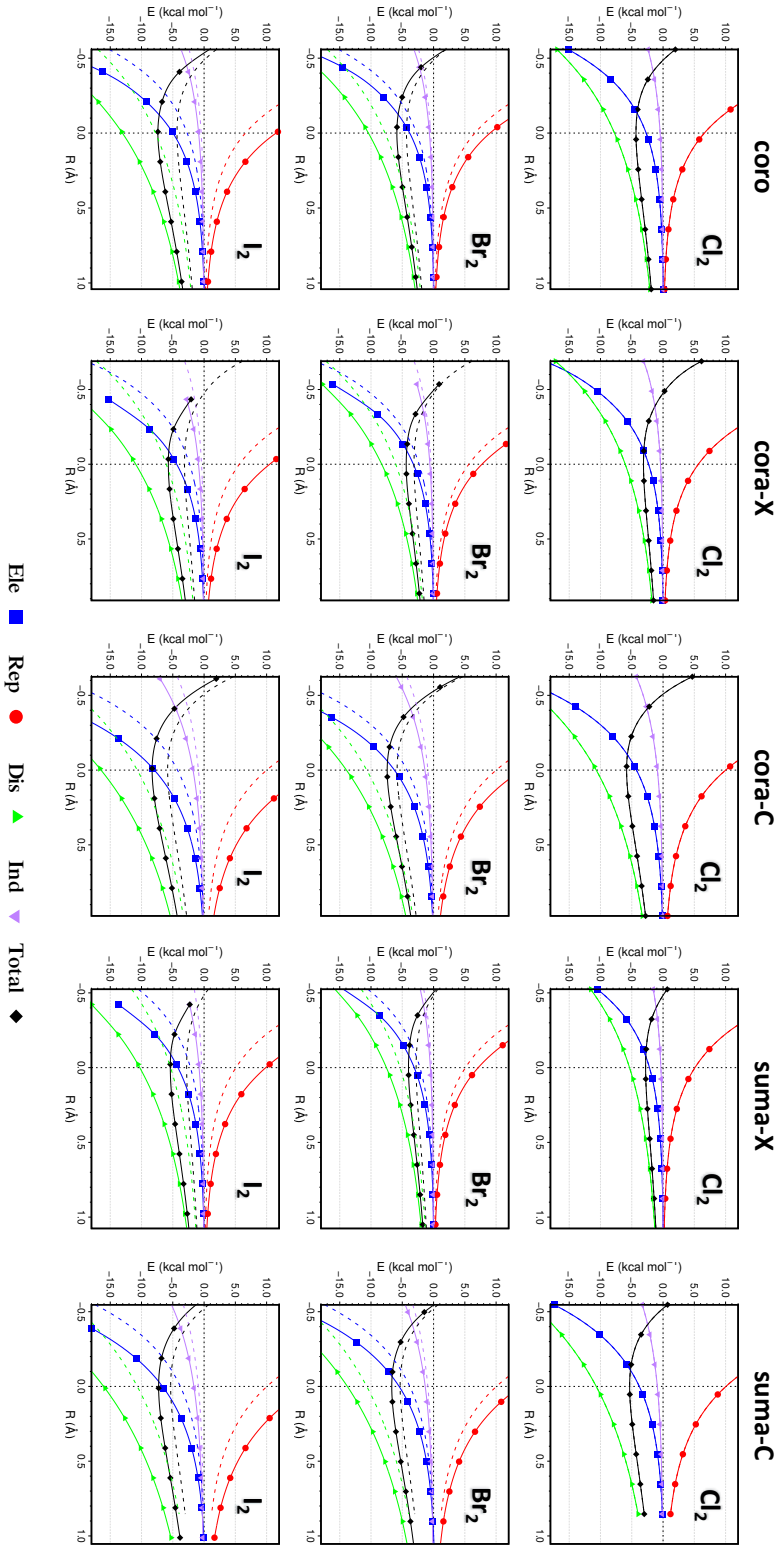


**Figure S13.** SAPT0 contributions for BP complexes formed by halogens with coronene, corannulene and sumanene. Dotted lines correspond to $Cl_2$ complexes. Origin at the minima. C and X refer to the concave and convex sides of the bowls, respectively.

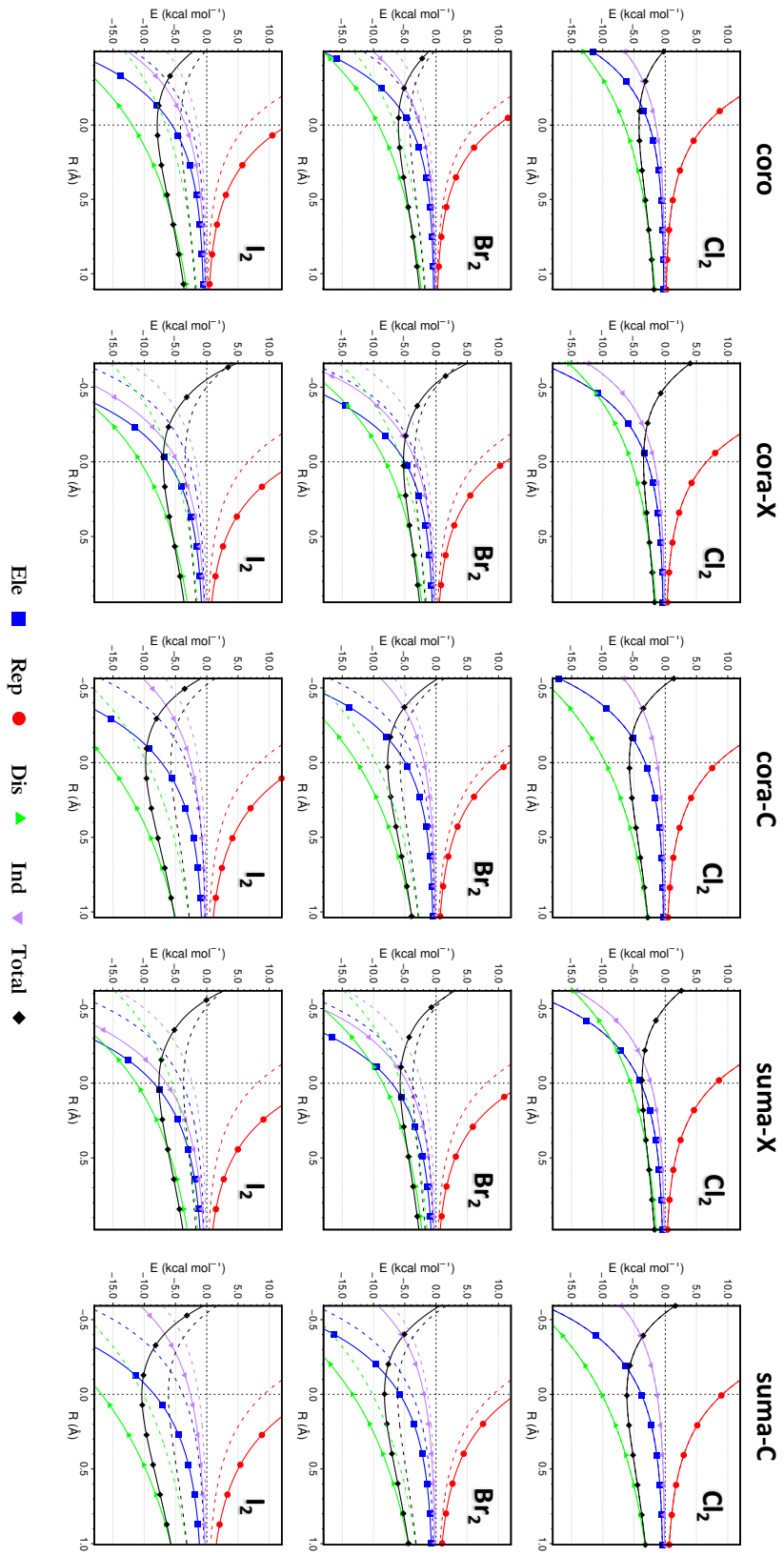


**Figure S14.** SAPT0 contributions for BT complexes formed by halogens with coronene, corannulene and sumanene. Dotted lines correspond to $Cl_2$ complexes. Origin at the minima. C and X refer to the concave and convex sides of the bowls, respectively.

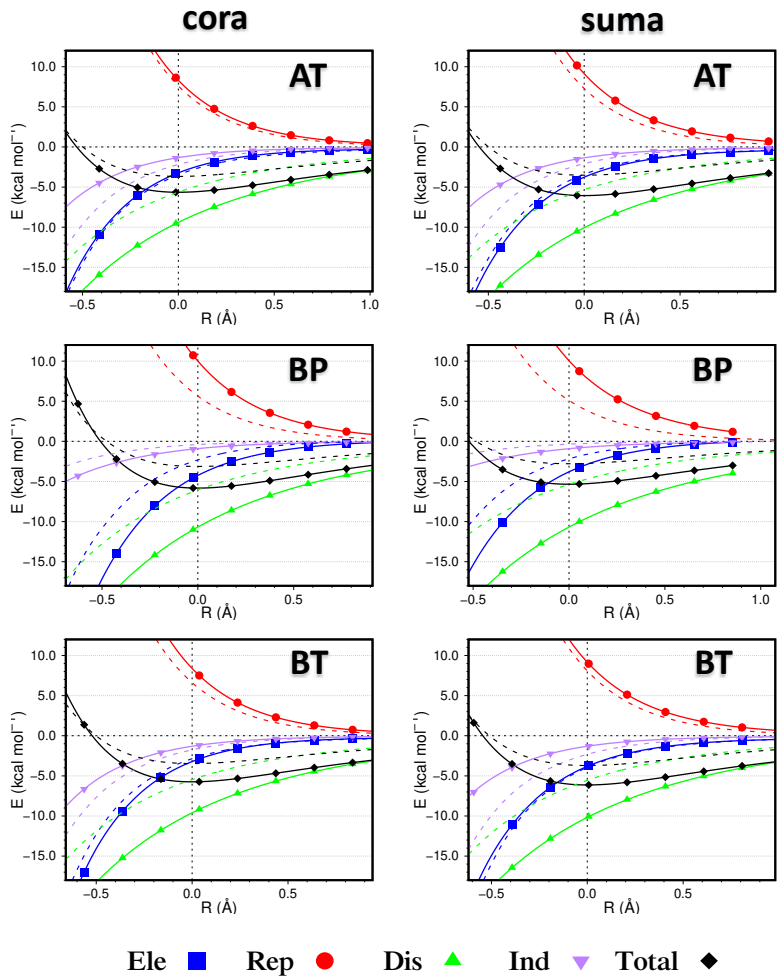


**Figure S15.** SAPT0 contributions for complexes formed by $Cl_2$ and corannulene and sumanene. Dotted lines correspond to the convex face. Origin at the minima.

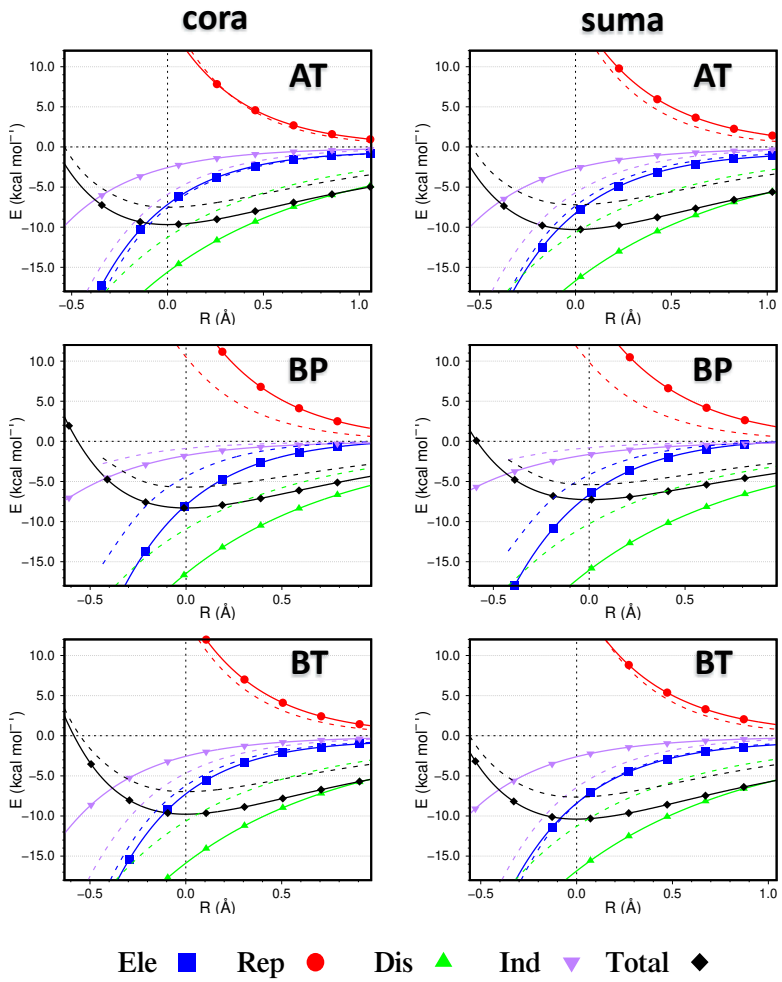


**Figure S16.** SAPT0 contributions for complexes formed by $I_2$ and corannulene and sumanene. Dotted lines correspond to the convex face. Origin at the minima.

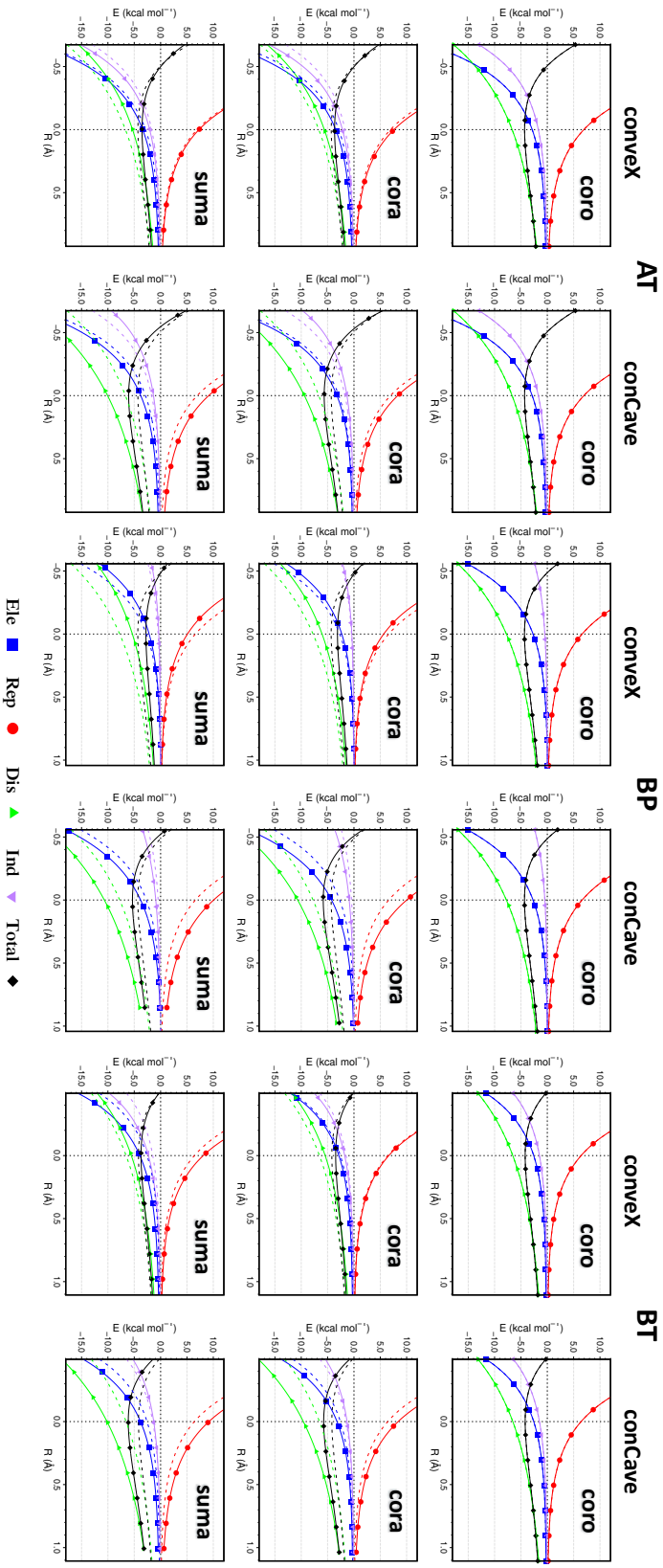


**Figure S17.** SAPT0 contributions for complexes formed by $Cl_2$ and the different bowls. Dotted lines correspond to coronene complexes. Origin at the minima.

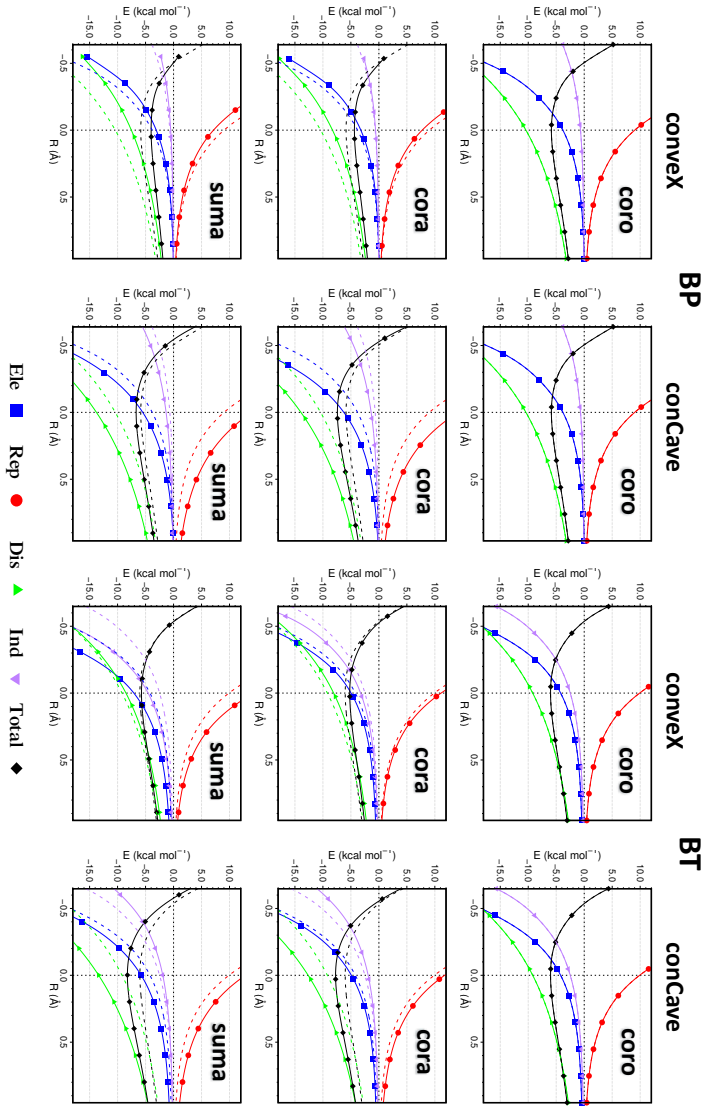


**Figure S18**. SAPT0 contributions for complexes formed by $Br_2$ and the different bowls. Dotted lines correspond to coronene complexes. Origin at the minima.

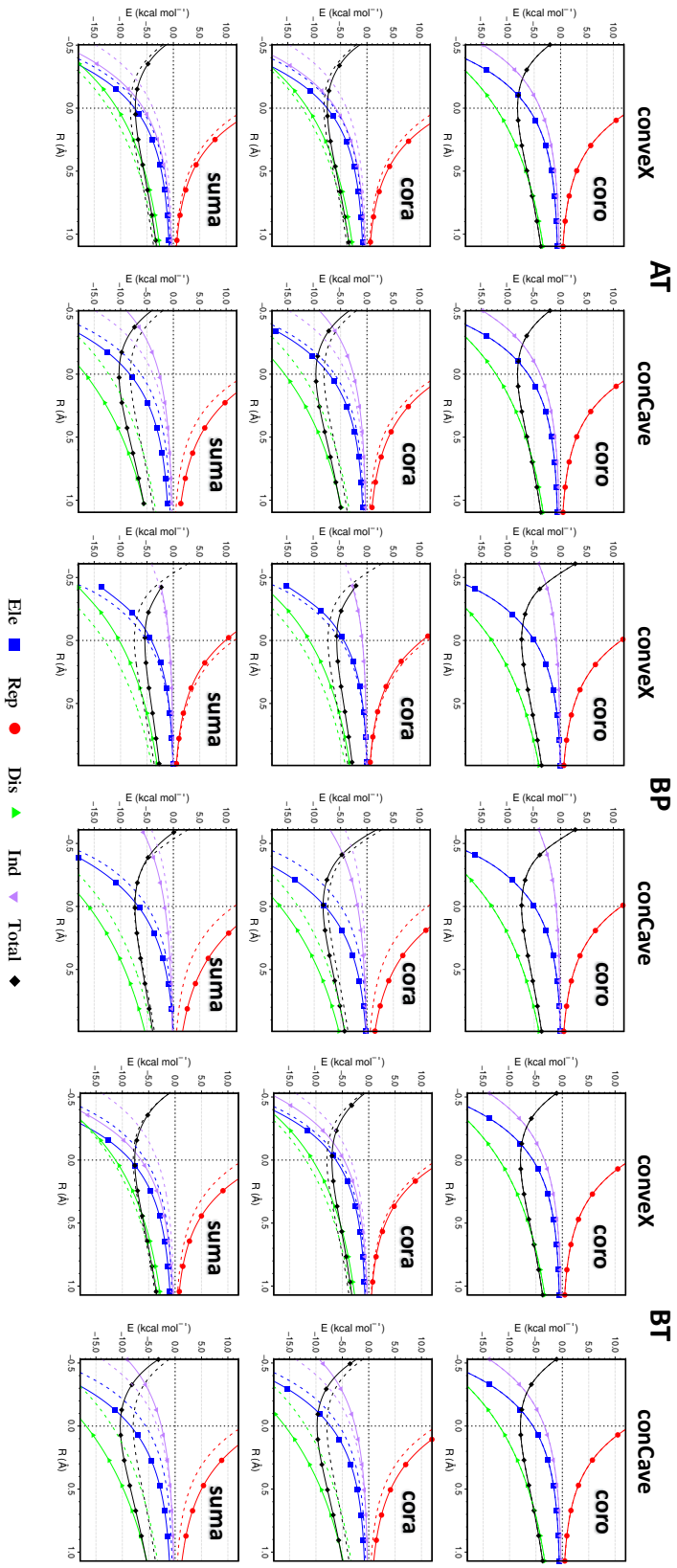


**Figure S19.** SAPT0 contributions for complexes formed by $I_2$ and the different bowls. Dotted lines correspond to coronene complexes. Origin at the minima.

**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 SAPT0/jun-cc-pVDZ.

| | Orient. | R (Å) | $E_{ele}$ | $E_{rep}$ | $E_{dis}$ | $E_{ind}$ | $E_{tot}$ |
|---|---|---|---|---|---|---|---|
| **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-$Br_2$** | **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-$I_2$** | **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 |

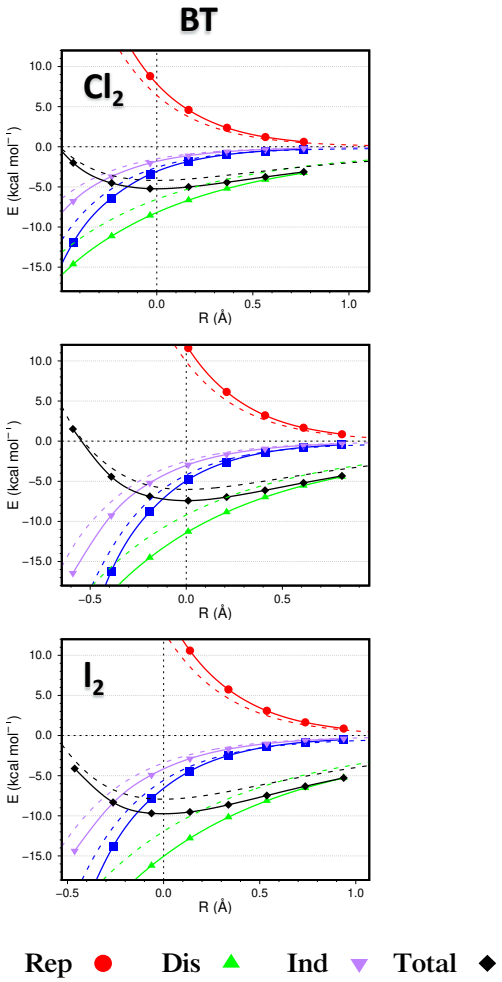


**Figure S20.** SAPT0 contributions for complexes formed by circumcoronene in BT orientation. Dotted lines correspond to complexes with coronene. The origin corresponds to the equilibrium distance of the circumcoronene complexes.

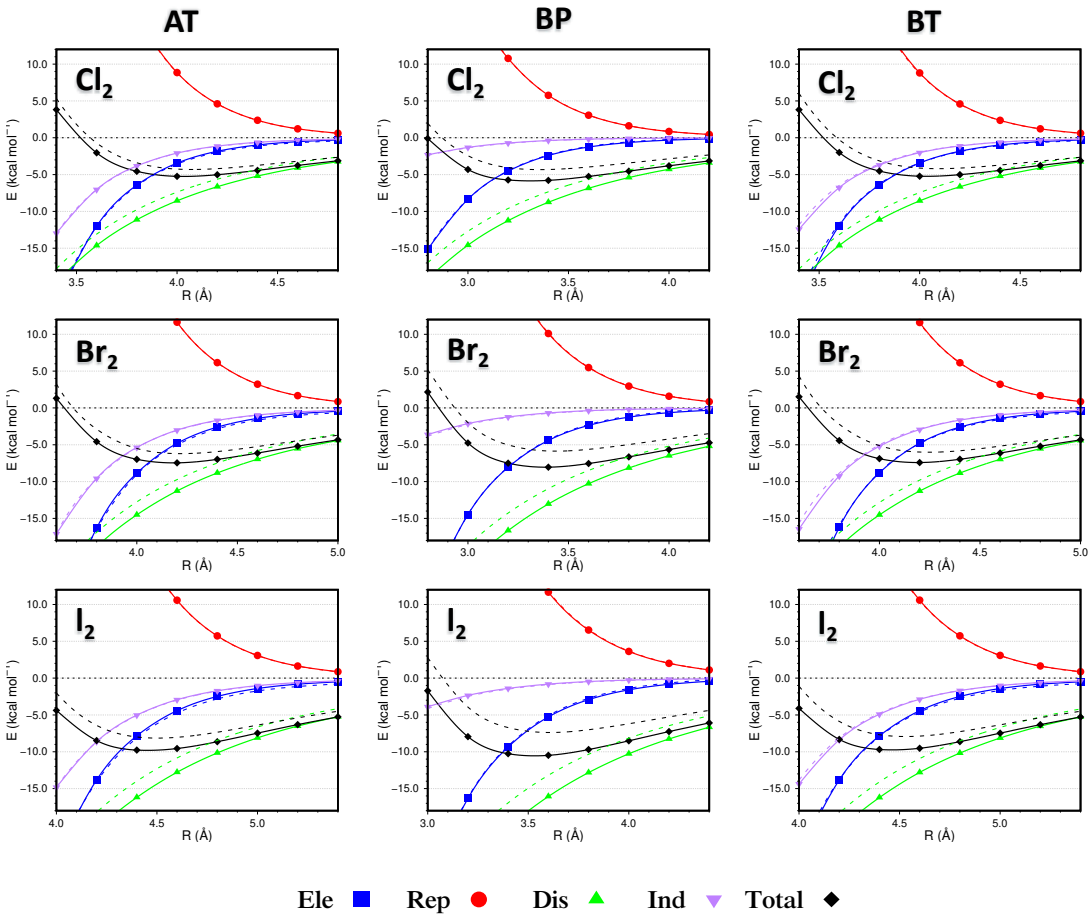


**Figure S21.** SAPT0 contributions for complexes formed by circumcoronene. Dotted lines correspond to complexes with coronene.

**Table S10**. Interaction energies as the circumcoronene is curved. SAPT0/jun-cc-pVDZ. Negative radius correspond to complexes by the concave face.

| | | AT | | BP | | BT | |
|---|---|---|---|---|---|---|---|
| | **Radius (Å)** | **R (Å)** | **E** | **R (Å)** | **E** | **R (Å)** | **E** |
| **$Cl_2$** | 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 |
| | ∞ | 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 |
| | ∞ | 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 |

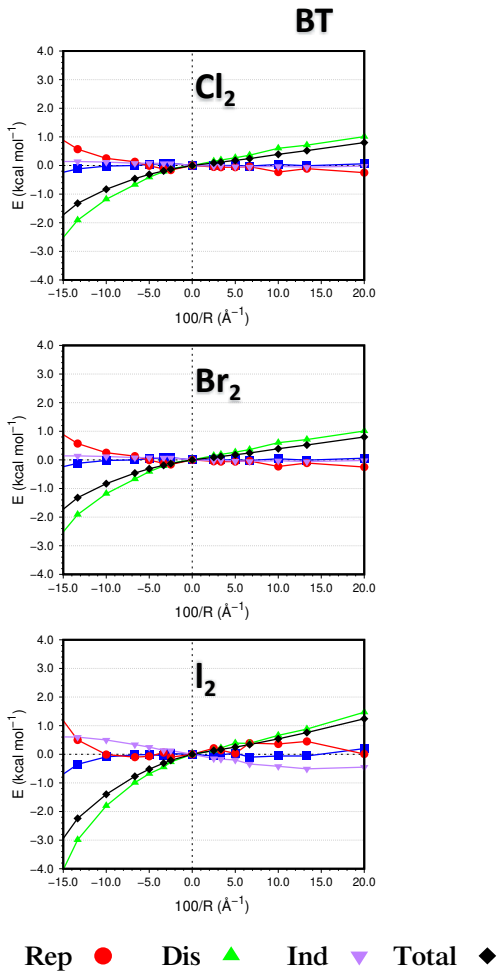


**Figure S22.** SAPT0 contributions to changes on the interaction energy as the circumcoronene molecule is curved. BT complexes. Negative values correspond to the concave face.

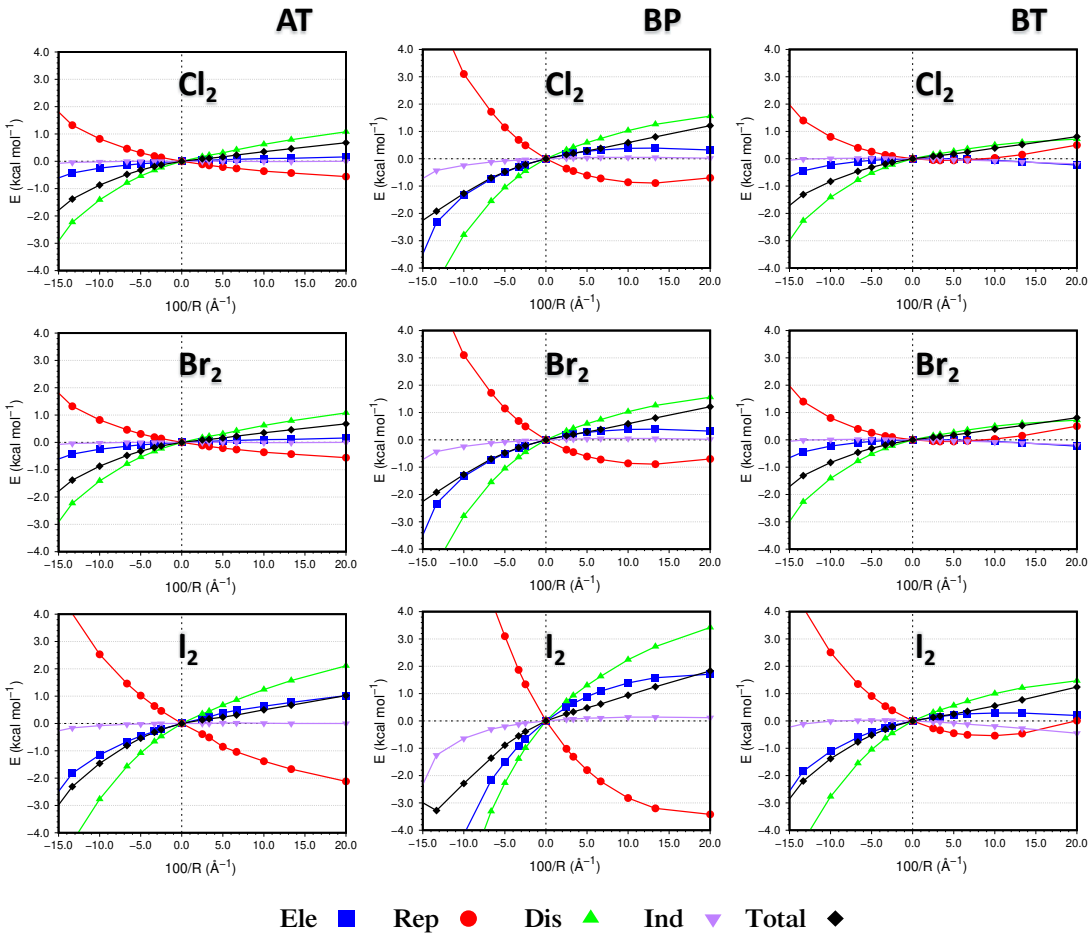


**Figure S23.** SAPT0 contributions to changes on the interaction energy as the circumcoronene molecule is curved. R fixed at the minimum of the planar species. Negative values correspond to the concave face.

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

**Coronene**

| | | | |
|---|---|---|---|
| C | 0.686551 | 3.681472 | -0.000003 |
| C | 0.686551 | -3.681472 | -0.000002 |
| C | 0.712378 | 1.233848 | -0.000001 |
| C | 0.712378 | -1.233848 | 0.000001 |
| C | 1.423652 | 2.465709 | -0.000003 |
| C | 1.423652 | -2.465709 | 0.000000 |
| C | 1.424774 | -0.000000 | 0.000001 |
| C | 2.845094 | 2.435313 | -0.000004 |
| C | 2.845094 | -2.435313 | 0.000004 |
| C | 2.847227 | -0.000000 | 0.000002 |
| C | 3.531660 | 1.246173 | -0.000000 |
| C | 3.531660 | -1.246173 | 0.000005 |
| C | -0.686551 | 3.681472 | -0.000001 |
| C | -0.686551 | -3.681472 | -0.000003 |
| C | -0.712378 | 1.233848 | 0.000000 |
| C | -0.712378 | -1.233848 | -0.000000 |
| C | -1.423652 | 2.465709 | 0.000001 |
| C | -1.423652 | -2.465709 | -0.000002 |
| C | -1.424774 | 0.000000 | 0.000001 |
| C | -2.845094 | 2.435313 | 0.000003 |
| C | -2.845094 | -2.435313 | -0.000003 |
| C | -2.847227 | -0.000000 | 0.000003 |
| C | -3.531660 | 1.246173 | 0.000004 |
| C | -3.531660 | -1.246173 | -0.000000 |
| H | 1.233512 | 4.621225 | -0.000004 |
| H | 1.233512 | -4.621225 | -0.000002 |
| H | 3.385455 | 3.378882 | -0.000005 |
| H | 3.385455 | -3.378882 | 0.000005 |
| H | 4.619007 | 1.242297 | 0.000000 |
| H | 4.619007 | -1.242297 | 0.000006 |
| H | -1.233512 | 4.621225 | -0.000000 |
| H | -1.233512 | -4.621225 | -0.000004 |
| H | -3.385455 | 3.378882 | 0.000004 |
| H | -3.385455 | -3.378882 | -0.000005 |
| H | -4.619007 | 1.242297 | 0.000005C |
| H | -4.619007 | -1.242297 | -0.000001 |

**Corannulene**

| | | | |
|---|---|---|---|
| C | 0.975653 | 0.708852 | 0.000051 |
| C | 0.975653 | -0.708852 | 0.000051 |
| C | -0.372654 | 1.146943 | 0.000017 |
| C | -0.372654 | -1.146943 | 0.000017 |
| C | -1.205939 | -0.000000 | -0.000138 |
| C | 2.010261 | 1.460510 | 0.536318 |
| C | 2.010261 | -1.460510 | 0.536318 |
| C | -0.767884 | 2.363172 | 0.536269 |
| C | -0.767884 | -2.363172 | 0.536269 |
| C | -2.484860 | 0.000000 | 0.535928 |
| C | 0.322579 | 3.240792 | 0.894435 |
| C | 0.322579 | -3.240792 | 0.894435 |
| C | 1.643956 | 2.811494 | 0.894432 |
| C | 1.643956 | -2.811494 | 0.894432 |
| C | 3.182105 | 0.694697 | 0.893892 |
| C | 3.182105 | -0.694697 | 0.893892 |
| C | -2.166008 | 2.432293 | 0.894127 |
| C | -2.166008 | -2.432293 | 0.894127 |
| C | -2.982650 | 1.308284 | 0.893976 |
| C | -2.982650 | -1.308284 | 0.893975 |
| H | 0.105450 | 4.239897 | 1.265423 |
| H | 0.105450 | -4.239897 | 1.265423 |
| H | 2.406848 | 3.492191 | 1.265414 |
| H | 2.406848 | -3.492191 | 1.265414 |
| H | 4.065385 | 1.210002 | 1.264393 |
| H | 4.065385 | -1.210002 | 1.264393 |
| H | -2.577636 | 3.368217 | 1.265064 |
| H | -2.577637 | -3.368217 | 1.265064 |
| H | -4.000007 | 1.410499 | 1.264839 |
| H | -4.000007 | -1.410499 | 1.264839 |

**Sumanene**

| | | | |
|---|---|---|---|
| C | 0.012710 | 1.410093 | -0.000064 |
| C | 0.012710 | -1.410094 | -0.000064 |
| C | 1.214797 | 0.716031 | -0.000066 |
| C | 1.214797 | -0.716030 | -0.000066 |
| C | -1.227482 | 0.694023 | 0.000131 |
| C | -1.227482 | -0.694023 | 0.000131 |
| C | 2.361381 | 1.210913 | 0.631776 |
| C | 2.361381 | -1.210913 | 0.631776 |
| C | -0.132011 | 2.650546 | 0.631647 |
| C | -0.132011 | -2.650546 | 0.631647 |
| C | -2.229320 | 1.439549 | 0.632024 |
| C | -2.229321 | -1.439549 | 0.632024 |
| C | 3.297390 | 0.000000 | 0.887045 |
| C | -1.648736 | 2.855767 | 0.886625 |
| C | -1.648736 | -2.855767 | 0.886625 |
| C | 1.034055 | 3.221162 | 1.151567 |
| C | 1.034055 | -3.221162 | 1.151567 |
| C | 2.272474 | 2.506055 | 1.151685 |
| C | 2.272474 | -2.506055 | 1.151685 |
| C | -3.306463 | 0.715039 | 1.152123 |
| C | -3.306463 | -0.715039 | 1.152123 |
| H | 4.160554 | -0.000000 | 0.207295 |
| H | -2.080241 | 3.602889 | 0.206377 |
| H | -2.080241 | -3.602889 | 0.206377 |
| H | 1.002536 | 4.167703 | 1.686148 |
| H | 1.002536 | -4.167703 | 1.686148 |
| H | 3.107912 | 2.952002 | 1.686365 |
| H | 3.107912 | -2.952002 | 1.686365 |
| H | -4.110405 | 1.215639 | 1.686708 |
| H | -4.110405 | -1.215639 | 1.686708 |
| H | 3.690143 | 0.000000 | 1.908686 |
| H | -1.845251 | 3.196484 | 1.908044 |
| H | -1.845251 | -3.196484 | 1.908044 |

**Circumcoronene**

| | | | |
|---|---|---|---|
| C | -1.419577 | 0.000000 | 0.000018 |
| C | 1.419577 | 0.000000 | 0.000021 |
| C | -0.709774 | 1.229338 | 0.000020 |
| C | -0.709774 | -1.229338 | 0.000022 |
| C | 0.709774 | -1.229338 | 0.000022 |
| C | 0.709774 | 1.229338 | 0.000023 |
| C | -2.845432 | 0.000000 | 0.000008 |
| C | 2.845432 | -0.000000 | 0.000011 |
| C | -1.422734 | 2.464136 | 0.000014 |
| C | -1.422734 | -2.464136 | 0.000019 |
| C | 1.422734 | -2.464136 | 0.000017 |
| C | 1.422734 | 2.464136 | 0.000021 |
| C | -2.842971 | -2.462623 | 0.000012 |
| C | 2.842971 | -2.462623 | 0.000005 |
| C | 2.842971 | 2.462623 | 0.000014 |
| C | -2.842971 | 2.462623 | 0.000003 |
| C | -3.554261 | 1.230696 | -0.000001 |
| C | 3.554261 | -1.230696 | 0.000002 |
| C | -3.554261 | -1.230696 | 0.000005 |
| C | 3.554261 | 1.230696 | 0.000007 |
| C | -0.711270 | 3.693308 | 0.000015 |
| C | 0.711270 | -3.693308 | 0.000017 |
| C | -0.711270 | -3.693308 | 0.000020 |
| C | 0.711270 | 3.693308 | 0.000019 |
| C | -1.431432 | 4.929422 | 0.000006 |
| C | 1.431432 | -4.929422 | 0.000008 |
| C | -1.431432 | -4.929422 | 0.000016 |
| C | 1.431432 | 4.929422 | 0.000015 |
| C | -3.553485 | -3.704312 | 0.000008 |

| | | | |
|---|---|---|---|
| C | 3.553485 | 3.704312 | 0.000009 |
| C | 3.553485 | -3.704312 | -0.000006 |
| C | -3.553485 | 3.704312 | -0.000007 |
| C | -4.984845 | 1.225130 | -0.000014 |
| C | 4.984845 | -1.225130 | -0.000013 |
| C | -4.984845 | -1.225130 | -0.000007 |
| C | 4.984845 | 1.225130 | -0.000006 |
| C | -2.832569 | 4.905984 | -0.000005 |
| C | -2.832569 | -4.905984 | 0.000011 |
| C | 2.832569 | -4.905984 | -0.000004 |
| C | 2.832569 | 4.905984 | 0.000011 |
| C | -5.665131 | -0.000000 | -0.000017 |
| C | 5.665131 | -0.000000 | -0.000017 |
| C | -4.986327 | -3.666801 | -0.000002 |
| C | 4.986327 | 3.666801 | -0.000002 |
| C | 4.986327 | -3.666801 | -0.000022 |
| C | -4.986327 | 3.666801 | -0.000022 |
| C | -5.668819 | 2.484732 | -0.000025 |
| C | 5.668819 | -2.484732 | -0.000025 |
| C | -5.668819 | -2.484732 | -0.000010 |
| C | 5.668819 | 2.484732 | -0.000010 |
| C | -0.682470 | 6.151495 | 0.000007 |
| C | 0.682470 | -6.151495 | 0.000006 |
| C | -0.682470 | -6.151495 | 0.000011 |
| C | 0.682470 | 6.151495 | 0.000011 |
| H | 3.376680 | 5.848436 | 0.000006 |
| H | -3.376680 | 5.848436 | -0.000012 |
| H | -3.376680 | -5.848436 | 0.000006 |
| H | 3.376680 | -5.848436 | -0.000013 |
| H | 6.753395 | -0.000000 | -0.000029 |
| H | -6.753395 | -0.000000 | -0.000027 |
| H | 6.756130 | -2.480037 | -0.000038 |
| H | -6.756130 | 2.480037 | -0.000036 |
| H | 6.756130 | 2.480037 | -0.000020 |
| H | -6.756130 | -2.480037 | -0.000019 |
| H | -1.230124 | 7.090807 | 0.000001 |
| H | 1.230124 | 7.090807 | 0.000008 |
| H | -1.230124 | -7.090807 | 0.000007 |
| H | 1.230124 | -7.090807 | -0.000001 |
| H | 5.525952 | 4.610755 | -0.000007 |
| H | -5.525952 | -4.610755 | -0.000005 |
| H | 5.525952 | -4.610755 | -0.000032 |
| H | -5.525952 | 4.610755 | -0.000030 |

**$C_{60}$**

| | | | |
|---|---|---|---|
| C | 0.381640 | 1.174657 | -3.325695 |
| C | 0.381640 | -1.174657 | -3.325696 |
| C | 1.235043 | 0.000000 | -3.325614 |
| C | -0.999346 | 0.726015 | -3.325827 |
| C | -0.999346 | -0.726015 | -3.325827 |
| C | 0.748517 | 2.303656 | -2.592017 |
| C | 0.748517 | -2.303656 | -2.592017 |
| C | 2.422225 | -0.000000 | -2.592015 |
| C | -1.959806 | 1.423849 | -2.592229 |
| C | -1.959805 | -1.423849 | -2.592229 |
| C | 1.983645 | 2.303679 | -1.828671 |
| C | 1.983645 | -2.303679 | -1.828671 |
| C | 2.803934 | 1.174675 | -1.828685 |
| C | 2.803934 | -1.174675 | -1.828685 |
| C | -0.250763 | 3.029651 | -1.828705 |
| C | -0.250763 | -3.029651 | -1.828705 |
| C | -1.578045 | 2.598460 | -1.828741 |
| C | -1.578045 | -2.598460 | -1.828740 |
| C | -2.959100 | 0.697804 | -1.828894 |
| C | -2.959100 | -0.697804 | -1.828894 |
| C | 0.366842 | 3.478379 | -0.593560 |
| C | 0.366842 | -3.478379 | -0.593560 |
| C | 1.747767 | 3.029642 | -0.593529 |
| C | 1.747767 | -3.029642 | -0.593529 |
| C | 3.421562 | 0.725985 | -0.593550 |
| C | 3.421562 | -0.725985 | -0.593550 |
| C | -2.341410 | 2.598414 | -0.593597 |
| C | -2.341410 | -2.598414 | -0.593597 |
| C | -3.194882 | 1.423738 | -0.593632 |
| C | -3.194882 | -1.423738 | -0.593632 |
| C | 2.341410 | 2.598414 | 0.593597 |
| C | 2.341410 | -2.598414 | 0.593597 |
| C | 3.194881 | 1.423738 | 0.593632 |
| C | 3.194882 | -1.423738 | 0.593632 |
| C | -0.366842 | 3.478379 | 0.593560 |
| C | -0.366842 | -3.478379 | 0.593560 |
| C | -1.747767 | 3.029642 | 0.593529 |
| C | -1.747767 | -3.029642 | 0.593529 |
| C | -3.421562 | 0.725984 | 0.593550 |
| C | -3.421562 | -0.725985 | 0.593550 |
| C | 0.250763 | 3.029651 | 1.828705 |
| C | 0.250763 | -3.029651 | 1.828705 |
| C | 1.578044 | 2.598460 | 1.828740 |
| C | 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 | 1.828671 |
| C | -1.983645 | -2.303679 | 1.828671 |
| C | -2.803934 | 1.174675 | 1.828685 |
| C | -2.803934 | -1.174675 | 1.828685 |
| C | 1.959806 | 1.423849 | 2.592229 |
| C | 1.959806 | -1.423849 | 2.592229 |
| C | -0.748517 | 2.303656 | 2.592017 |
| C | -0.748517 | -2.303656 | 2.592017 |
| C | -2.422225 | -0.000000 | 2.592015 |
| C | 0.999346 | 0.726015 | 3.325827 |
| C | 0.999346 | -0.726015 | 3.325827 |
| C | -0.381640 | 1.174657 | 3.325696 |
| C | -0.381640 | -1.174657 | 3.325696 |
| C | -1.235043 | -0.000000 | 3.325614 |

**$Cl_2$**

| | | | |
|---|---|---|---|
| Cl | 0.000000 | 0.000000 | -1.006146 |
| Cl | 0.000000 | 0.000000 | 1.006146 |

**$Br_2$**

| | | | |
|---|---|---|---|
| Br | 0.000000 | 0.000000 | -1.154857 |
| Br | 0.000000 | 0.000000 | 1.154857 |

**$I_2$**

| | | | |
|---|---|---|---|
| I | 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 |
| C | -2.682885 | -4.844566 | 0.735204 |
| C | -2.682885 | 4.844566 | 0.735204 |
| C | 4.525225 | -0.000000 | 3.005608 |
| C | -4.525225 | -0.000000 | 3.005608 |
| C | 4.184182 | -3.616306 | 2.293254 |
| C | -4.184182 | 3.616306 | 2.293254 |
| C | -4.184182 | -3.616306 | 2.293254 |
| C | 4.184182 | 3.616306 | 2.293254 |
| C | 4.526805 | 2.451675 | 3.009732 |
| C | -4.526805 | -2.451675 | 3.009732 |
| C | 4.526805 | -2.451675 | 3.009732 |
| C | -4.526805 | 2.451675 | 3.009732 |
| C | 0.681235 | 6.091446 | -0.004628 |
| C | -0.681235 | -6.091446 | -0.004628 |
| C | 0.681235 | -6.091446 | -0.004628 |
| C | -0.681235 | 6.091446 | -0.004628 |
| H | -3.139104 | 5.775642 | 1.068979 |
| H | 3.139104 | 5.775642 | 1.068979 |
| H | 3.139104 | -5.775642 | 1.068979 |
| H | -3.139104 | -5.775642 | 1.068979 |
| H | -4.768854 | -0.000000 | 4.059869 |
| H | 4.768854 | -0.000000 | 4.059869 |
| H | -4.769506 | -2.448012 | 4.063912 |
| H | 4.769506 | 2.448012 | 4.063912 |
| H | -4.769506 | 2.448012 | 4.063912 |
| H | 4.769506 | -2.448012 | 4.063912 |
| H | 1.220585 | 7.029796 | 0.100009 |
| H | -1.220585 | 7.029796 | 0.100009 |
| H | 1.220585 | -7.029796 | 0.100009 |
| H | -1.220585 | -7.029796 | 0.100009 |
| H | -4.456042 | 4.521857 | 2.837445 |
| H | 4.456042 | -4.521857 | 2.837445 |
| H | -4.456042 | -4.521857 | 2.837445 |
| H | 4.456042 | 4.521857 | 2.837445 |

**Circumcoronene R=7.0Å**

| | | | |
|---|---|---|---|
| C | 1.411060 | -0.000000 | 0.100199 |
| C | -1.411060 | -0.000000 | 0.100199 |
| C | 0.710766 | 1.222474 | -0.000000 |
| C | 0.710766 | -1.222474 | -0.000000 |
| C | -0.710766 | -1.222474 | -0.000000 |
| C | -0.710766 | 1.222473 | 0.000000 |
| C | 2.781025 | 0.000000 | 0.502506 |
| C | -2.781025 | -0.000000 | 0.502506 |
| C | 1.414027 | 2.450149 | 0.100775 |
| C | 1.414027 | -2.450149 | 0.100775 |
| C | -1.414027 | -2.450149 | 0.100775 |
| C | -1.414027 | 2.450149 | 0.100775 |
| C | 2.778830 | -2.448648 | 0.501632 |
| C | -2.778830 | -2.448648 | 0.501632 |
| C | -2.778830 | 2.448648 | 0.501632 |
| C | 2.778830 | 2.448648 | 0.501632 |
| C | 3.436618 | 1.223821 | 0.803236 |
| C | -3.436618 | -1.223821 | 0.803236 |
| C | 3.436618 | -1.223821 | 0.803236 |
| C | -3.436618 | 1.223821 | 0.803236 |
| C | 0.712945 | 3.671017 | 0.000241 |
| C | -0.712945 | -3.671017 | 0.000241 |
| C | 0.712945 | -3.671017 | 0.000241 |
| C | -0.712945 | 3.671017 | 0.000241 |
| C | 1.425575 | 4.904018 | 0.102854 |
| C | -1.425575 | -4.904018 | 0.102854 |
| C | 1.425575 | -4.904018 | 0.102854 |
| C | -1.425575 | 4.904018 | 0.102854 |
| C | 3.435368 | -3.682157 | 0.802621 |
| C | -3.435368 | 3.682157 | 0.802621 |
| C | -3.435368 | -3.682157 | 0.802621 |
| C | 3.435368 | 3.682158 | 0.802621 |
| C | 4.629791 | 1.218502 | 1.581545 |
| C | -4.629791 | -1.218502 | 1.581545 |
| C | 4.629791 | -1.218502 | 1.581545 |
| C | -4.629791 | 1.218502 | 1.581545 |
| C | 2.766301 | 4.880856 | 0.496460 |
| C | 2.766301 | -4.880856 | 0.496460 |
| C | -2.766301 | -4.880856 | 0.496460 |
| C | -2.766301 | 4.880856 | 0.496460 |
| C | 5.170873 | -0.000000 | 2.061934 |
| C | -5.170873 | -0.000000 | 2.061934 |
| C | 4.631439 | -3.646277 | 1.582908 |
| C | -4.631439 | 3.646277 | 1.582908 |
| C | -4.631439 | -3.646277 | 1.582908 |
| C | 4.631439 | 3.646278 | 1.582908 |
| C | 5.173760 | 2.471418 | 2.064755 |
| C | -5.173760 | -2.471418 | 2.064755 |
| C | 5.173760 | -2.471418 | 2.064755 |
| C | -5.173760 | 2.471418 | 2.064755 |
| C | 0.681957 | 6.126884 | -0.002763 |
| C | -0.681957 | -6.126883 | -0.002763 |
| C | 0.681957 | -6.126883 | -0.002763 |
| C | -0.681957 | 6.126883 | -0.002763 |
| H | -3.272098 | 5.818473 | 0.720539 |
| H | 3.272098 | 5.818473 | 0.720539 |
| H | 3.272098 | -5.818473 | 0.720539 |
| H | -3.272098 | -5.818473 | 0.720539 |
| H | -5.883768 | -0.000000 | 2.880523 |
| H | 5.883768 | -0.000000 | 2.880523 |
| H | -5.885825 | -2.467152 | 2.883167 |

| | | | |
|---|---|---|---|
| H | 5.885825 | 2.467152 | 2.883167 |
| H | -5.885825 | 2.467152 | 2.883167 |
| H | 5.885825 | -2.467152 | 2.883167 |
| H | 1.225928 | 7.065770 | 0.067035 |
| H | -1.225928 | 7.065770 | 0.067035 |
| H | 1.225928 | -7.065770 | 0.067035 |
| H | -1.225928 | -7.065770 | 0.067035 |
| H | -5.059219 | 4.575533 | 1.955198 |
| H | 5.059219 | -4.575533 | 1.955199 |
| H | -5.059219 | -4.575533 | 1.955199 |
| H | 5.059219 | 4.575533 | 1.955199 |

**Circumcoronene R=10.0Å**

| | | | |
|---|---|---|---|
| C | 1.414842 | 0.000000 | 0.075340 |
| C | -1.414842 | 0.000000 | 0.075340 |
| C | 0.710328 | 1.225588 | -0.000000 |
| C | 0.710328 | -1.225588 | -0.000000 |
| C | -0.710328 | -1.225588 | -0.000000 |
| C | -0.710328 | 1.225588 | 0.000000 |
| C | 2.809311 | 0.000000 | 0.378097 |
| C | -2.809311 | -0.000000 | 0.378097 |
| C | 1.417907 | 2.456518 | 0.075782 |
| C | 1.417907 | -2.456518 | 0.075782 |
| C | -1.417907 | -2.456518 | 0.075782 |
| C | -1.417907 | 2.456518 | 0.075782 |
| C | 2.806988 | -2.455012 | 0.377418 |
| C | -2.806988 | -2.455012 | 0.377418 |
| C | -2.806988 | 2.455012 | 0.377418 |
| C | 2.806988 | 2.455012 | 0.377418 |
| C | 3.488432 | 1.226941 | 0.604220 |
| C | -3.488432 | -1.226941 | 0.604220 |
| C | 3.488432 | -1.226941 | 0.604220 |
| C | -3.488432 | 1.226941 | 0.604220 |
| C | 0.712208 | 3.681160 | 0.000148 |
| C | -0.712208 | -3.681160 | 0.000148 |
| C | 0.712208 | -3.681160 | 0.000148 |
| C | -0.712208 | 3.681160 | 0.000148 |
| C | 1.428145 | 4.915544 | 0.077195 |
| C | -1.428145 | -4.915544 | 0.077194 |
| C | 1.428145 | -4.915544 | 0.077195 |
| C | -1.428145 | 4.915544 | 0.077195 |
| C | 3.487370 | -3.692223 | 0.603837 |
| C | -3.487370 | 3.692222 | 0.603837 |
| C | -3.487370 | -3.692222 | 0.603837 |
| C | 3.487370 | 3.692223 | 0.603837 |
| C | 4.785407 | 1.221513 | 1.199919 |
| C | -4.785407 | -1.221513 | 1.199919 |
| C | 4.785407 | -1.221513 | 1.199919 |
| C | -4.785407 | 1.221513 | 1.199919 |
| C | 2.795383 | 4.892260 | 0.373960 |
| C | 2.795383 | -4.892260 | 0.373960 |
| C | -2.795383 | -4.892260 | 0.373960 |
| C | -2.795383 | 4.892260 | 0.373960 |
| C | 5.389201 | -0.000000 | 1.561101 |
| C | -5.389201 | -0.000000 | 1.561101 |
| C | 4.787029 | -3.655621 | 1.200826 |
| C | -4.787029 | 3.655620 | 1.200826 |
| C | -4.787029 | -3.655621 | 1.200827 |
| C | 4.787029 | 3.655621 | 1.200827 |
| C | 5.392470 | 2.477500 | 1.563215 |
| C | -5.392470 | -2.477500 | 1.563215 |
| C | 5.392470 | -2.477500 | 1.563215 |
| C | -5.392470 | 2.477500 | 1.563215 |
| C | 0.682195 | 6.138045 | -0.001995 |
| C | -0.682195 | -6.138045 | -0.001995 |
| C | 0.682195 | -6.138045 | -0.001995 |
| C | -0.682195 | 6.138045 | -0.001995 |
| H | -3.318086 | 5.832038 | 0.542407 |
| H | 3.318086 | 5.832038 | 0.542407 |
| H | 3.318086 | -5.832038 | 0.542407 |
| H | -3.318086 | -5.832038 | 0.542406 |
| H | -6.266236 | -0.000000 | 2.202750 |
| H | 6.266236 | -0.000000 | 2.202750 |
| H | -6.268649 | -2.473042 | 2.204692 |
| H | 6.268649 | 2.473042 | 2.204692 |
| H | -6.268649 | 2.473042 | 2.204692 |
| H | 6.268649 | -2.473042 | 2.204692 |
| H | 1.227778 | 7.077116 | 0.050364 |
| H | -1.227778 | 7.077116 | 0.050364 |
| H | 1.227778 | -7.077116 | 0.050364 |
| H | -1.227778 | -7.077116 | 0.050364 |
| H | -5.264965 | 4.591675 | 1.482088 |
| H | 5.264965 | -4.591675 | 1.482088 |
| H | -5.264965 | -4.591675 | 1.482088 |
| H | 5.264965 | 4.591675 | 1.482088 |

**Circumcoronene R=15.0Å**

| | | | |
|---|---|---|---|
| C | 1.417494 | 0.000000 | 0.050314 |
| C | -1.417494 | 0.000000 | 0.050314 |
| C | 0.710024 | 1.227706 | 0.000000 |
| C | 0.710024 | -1.227706 | -0.000000 |
| C | -0.710024 | -1.227706 | -0.000000 |
| C | -0.710024 | 1.227706 | 0.000000 |
| C | 2.829427 | 0.000000 | 0.252638 |
| C | -2.829427 | 0.000000 | 0.252638 |
| C | 1.420620 | 2.460836 | 0.050611 |
| C | 1.420620 | -2.460836 | 0.050611 |
| C | -1.420620 | -2.460836 | 0.050611 |
| C | -1.420620 | 2.460836 | 0.050611 |
| C | 2.827018 | -2.459326 | 0.252176 |
| C | -2.827018 | -2.459326 | 0.252176 |
| C | -2.827018 | 2.459326 | 0.252176 |
| C | 2.827018 | 2.459326 | 0.252176 |
| C | 3.525127 | 1.229062 | 0.403648 |
| C | -3.525127 | -1.229062 | 0.403648 |
| C | 3.525127 | -1.229062 | 0.403648 |
| C | -3.525127 | 1.229062 | 0.403648 |
| C | 0.711695 | 3.688038 | 0.000084 |
| C | -0.711695 | -3.688038 | 0.000084 |
| C | 0.711695 | -3.688038 | 0.000084 |
| C | -0.711695 | 3.688038 | 0.000084 |
| C | 1.429972 | 4.923370 | 0.051487 |
| C | -1.429972 | -4.923370 | 0.051487 |
| C | 1.429972 | -4.923370 | 0.051487 |
| C | -1.429972 | 4.923370 | 0.051487 |
| C | 3.524212 | -3.699062 | 0.403430 |
| C | -3.524212 | 3.699062 | 0.403430 |
| C | -3.524212 | -3.699062 | 0.403430 |
| C | 3.524212 | 3.699062 | 0.403430 |
| C | 4.896306 | 1.223557 | 0.806397 |
| C | -4.896306 | -1.223557 | 0.806397 |
| C | 4.896306 | -1.223557 | 0.806397 |
| C | -4.896306 | 1.223557 | 0.806397 |
| C | 2.816091 | 4.900000 | 0.250063 |
| C | 2.816091 | -4.900000 | 0.250063 |
| C | -2.816091 | -4.900000 | 0.250063 |
| C | -2.816091 | 4.900000 | 0.250063 |
| C | 5.543131 | -0.000000 | 1.047588 |
| C | -5.543131 | -0.000000 | 1.047588 |
| C | 4.897869 | -3.661952 | 0.806943 |
| C | -4.897870 | 3.661952 | 0.806943 |
| C | -4.897870 | -3.661952 | 0.806943 |
| C | 4.897870 | 3.661952 | 0.806943 |
| C | 5.546648 | 2.481606 | 1.048992 |
| C | -5.546648 | -2.481606 | 1.048992 |
| C | 5.546648 | -2.481606 | 1.048992 |
| C | -5.546648 | 2.481606 | 1.048992 |
| C | 0.682357 | 6.145618 | -0.001295 |
| C | -0.682357 | -6.145618 | -0.001295 |
| C | 0.682357 | -6.145618 | -0.001295 |
| C | -0.682357 | 6.145618 | -0.001295 |
| H | -3.350730 | 5.841272 | 0.362540 |
| H | 3.350730 | 5.841272 | 0.362540 |
| H | 3.350730 | -5.841272 | 0.362540 |

| | | | |
|---|---|---|---|
| H | -3.350729 | -5.841272 | 0.362540 |
| H | -6.537476 | 0.000000 | 1.488106 |
| H | 6.537475 | -0.000000 | 1.488106 |
| H | -6.540094 | -2.477015 | 1.489373 |
| H | 6.540094 | 2.477016 | 1.489373 |
| H | -6.540094 | 2.477015 | 1.489373 |
| H | 6.540094 | -2.477016 | 1.489373 |
| H | 1.229090 | 7.084820 | 0.033616 |
| H | -1.229090 | 7.084820 | 0.033616 |
| H | 1.229090 | -7.084820 | 0.033616 |
| H | -1.229090 | -7.084820 | 0.033616 |
| H | -5.410446 | 4.602505 | 0.995352 |
| H | 5.410446 | -4.602505 | 0.995352 |
| H | -5.410446 | -4.602505 | 0.995352 |
| H | 5.410446 | 4.602505 | 0.995352 |

**Circumcoronene R=20.0Å**

| | | | |
|---|---|---|---|
| C | 1.418238 | -0.000000 | 0.037741 |
| C | -1.418238 | -0.000000 | 0.037741 |
| C | 0.709836 | -1.228341 | 0.000000 |
| C | 0.709836 | 1.228341 | 0.000000 |
| C | -0.709836 | 1.228341 | -0.000000 |
| C | -0.709836 | -1.228341 | 0.000000 |
| C | 2.836168 | -0.000000 | 0.189557 |
| C | -2.836168 | -0.000000 | 0.189557 |
| C | 1.421407 | -2.462181 | 0.037967 |
| C | 1.421407 | 2.462181 | 0.037967 |
| C | -1.421407 | 2.462181 | 0.037967 |
| C | -1.421407 | -2.462181 | 0.037967 |
| C | 2.833874 | 2.460701 | 0.189228 |
| C | -2.833874 | 2.460701 | 0.189228 |
| C | -2.833874 | -2.460701 | 0.189228 |
| C | 2.833874 | -2.460701 | 0.189228 |
| C | 3.537659 | -1.229829 | 0.302855 |
| C | -3.537659 | 1.229829 | 0.302855 |
| C | 3.537659 | 1.229829 | 0.302855 |
| C | -3.537659 | -1.229829 | 0.302855 |
| C | 0.711467 | -3.690235 | 0.000061 |
| C | -0.711467 | 3.690235 | 0.000061 |
| C | 0.711467 | 3.690235 | 0.000061 |
| C | -0.711467 | -3.690235 | 0.000061 |
| C | 1.430453 | -4.925959 | 0.038607 |
| C | -1.430453 | 4.925959 | 0.038607 |
| C | 1.430453 | 4.925959 | 0.038607 |
| C | -1.430453 | -4.925959 | 0.038607 |
| C | 3.536937 | 3.701290 | 0.302728 |
| C | -3.536937 | -3.701290 | 0.302728 |
| C | -3.536937 | 3.701290 | 0.302728 |
| C | 3.536937 | -3.701290 | 0.302728 |
| C | 4.934794 | -1.224368 | 0.606303 |
| C | -4.934794 | 1.224368 | 0.606303 |
| C | 4.934794 | 1.224368 | 0.606303 |
| C | -4.934794 | -1.224368 | 0.606303 |
| C | 2.823225 | -4.902490 | 0.187699 |
| C | 2.823225 | 4.902490 | 0.187699 |
| C | -2.823225 | 4.902490 | 0.187699 |
| C | -2.823225 | -4.902490 | 0.187699 |
| C | 5.596335 | -0.000000 | 0.787252 |
| C | -5.596335 | -0.000000 | 0.787252 |
| C | 4.936620 | 3.664340 | 0.606772 |
| C | -4.936620 | -3.664340 | 0.606772 |
| C | -4.936620 | 3.664340 | 0.606772 |
| C | 4.936620 | -3.664340 | 0.606772 |
| C | 5.600294 | -2.483123 | 0.788408 |
| C | -5.600294 | 2.483123 | 0.788408 |
| C | 5.600294 | 2.483123 | 0.788408 |
| C | -5.600294 | -2.483123 | 0.788408 |
| C | 0.682515 | -6.148488 | -0.000955 |
| C | -0.682515 | 6.148488 | -0.000955 |
| C | 0.682515 | 6.148488 | -0.000955 |
| C | -0.682515 | -6.148488 | -0.000955 |
| H | -3.362029 | -5.844276 | 0.272084 |
| H | 3.362029 | -5.844276 | 0.272084 |
| H | 3.362029 | 5.844276 | 0.272084 |
| H | -3.362029 | 5.844276 | 0.272084 |
| H | -6.631779 | -0.000000 | 1.120845 |
| H | 6.631779 | -0.000000 | 1.120845 |
| H | -6.634804 | 2.478230 | 1.121912 |
| H | 6.634804 | -2.478230 | 1.121912 |
| H | -6.634804 | -2.478230 | 1.121912 |
| H | 6.634804 | 2.478230 | 1.121912 |
| H | 1.229927 | -7.087563 | 0.025242 |
| H | -1.229927 | -7.087563 | 0.025242 |
| H | 1.229927 | 7.087563 | 0.025242 |
| H | -1.229927 | 7.087563 | 0.025242 |
| H | -5.460847 | -4.606550 | 0.748206 |
| H | 5.460847 | 4.606550 | 0.748206 |
| H | -5.460847 | 4.606550 | 0.748206 |
| H | 5.460847 | -4.606550 | 0.748206 |

**Circumcoronene R=30.0Å**

| | | | |
|---|---|---|---|
| C | 1.419054 | 0.000000 | 0.025182 |
| C | -1.419054 | 0.000000 | 0.025182 |
| C | 0.709836 | 1.228927 | -0.000000 |
| C | 0.709836 | -1.228927 | -0.000000 |
| C | -0.709836 | -1.228927 | -0.000000 |
| C | -0.709836 | 1.228927 | 0.000000 |
| C | 2.841449 | 0.000000 | 0.126490 |
| C | -2.841449 | -0.000000 | 0.126490 |
| C | 1.422213 | 2.463322 | 0.025332 |
| C | 1.422213 | -2.463322 | 0.025332 |
| C | -1.422213 | -2.463322 | 0.025332 |
| C | -1.422213 | 2.463322 | 0.025332 |
| C | 2.838992 | -2.461810 | 0.126256 |
| C | -2.838992 | -2.461810 | 0.126256 |
| C | -2.838992 | 2.461810 | 0.126256 |
| C | 2.838992 | 2.461810 | 0.126256 |
| C | 3.547003 | 1.230284 | 0.202070 |
| C | -3.547003 | -1.230284 | 0.202070 |
| C | 3.547003 | -1.230284 | 0.202070 |
| C | -3.547003 | 1.230284 | 0.202070 |
| C | 0.711382 | 3.692004 | 0.000037 |
| C | -0.711382 | -3.692004 | 0.000037 |
| C | 0.711382 | -3.692004 | 0.000037 |
| C | -0.711382 | 3.692004 | 0.000037 |
| C | 1.431064 | 4.927909 | 0.025751 |
| C | -1.431064 | -4.927908 | 0.025751 |
| C | 1.431064 | -4.927909 | 0.025751 |
| C | -1.431064 | 4.927909 | 0.025751 |
| C | 3.546184 | -3.703012 | 0.201973 |
| C | -3.546184 | 3.703012 | 0.201973 |
| C | -3.546184 | -3.703012 | 0.201973 |
| C | 3.546185 | 3.703012 | 0.201973 |
| C | 4.962744 | 1.224733 | 0.405116 |
| C | -4.962744 | -1.224733 | 0.405116 |
| C | 4.962744 | -1.224733 | 0.405116 |
| C | -4.962744 | 1.224733 | 0.405116 |
| C | 2.828465 | 4.904487 | 0.125255 |
| C | 2.828465 | -4.904487 | 0.125255 |
| C | -2.828465 | -4.904487 | 0.125255 |
| C | -2.828465 | 4.904487 | 0.125255 |
| C | 5.634737 | -0.000000 | 0.525827 |
| C | -5.634737 | -0.000000 | 0.525827 |
| C | 4.964255 | -3.665601 | 0.405370 |
| C | -4.964255 | 3.665601 | 0.405370 |
| C | -4.964255 | -3.665601 | 0.405370 |
| C | 4.964255 | 3.665601 | 0.405370 |
| C | 5.638393 | 2.483962 | 0.526527 |
| C | -5.638393 | -2.483962 | 0.526527 |
| C | 5.638393 | -2.483962 | 0.526527 |
| C | -5.638393 | 2.483961 | 0.526527 |
| C | 0.682445 | 6.150016 | -0.000637 |
| C | -0.682445 | -6.150016 | -0.000637 |
| C | 0.682445 | -6.150016 | -0.000637 |

| | | | |
|---|---|---|---|
| C | -0.682445 | 6.150016 | -0.000637 |
| H | -3.370211 | 5.846639 | 0.181546 |
| H | 3.370211 | 5.846638 | 0.181546 |
| H | 3.370211 | -5.846638 | 0.181546 |
| H | -3.370211 | -5.846638 | 0.181546 |
| H | -6.699477 | -0.000000 | 0.749826 |
| H | 6.699477 | -0.000000 | 0.749826 |
| H | -6.702202 | -2.479293 | 0.750450 |
| H | 6.702202 | 2.479293 | 0.750450 |
| H | -6.702202 | 2.479293 | 0.750450 |
| H | 6.702202 | -2.479293 | 0.750450 |
| H | 1.229867 | 7.089298 | 0.016820 |
| H | -1.229867 | 7.089298 | 0.016820 |
| H | 1.229867 | -7.089298 | 0.016820 |
| H | -1.229867 | -7.089298 | 0.016820 |
| H | -5.497169 | 4.608716 | 0.499831 |
| H | 5.497169 | -4.608716 | 0.499831 |
| H | -5.497169 | -4.608716 | 0.499831 |
| H | 5.497169 | 4.608716 | 0.499831 |

**Circumcoronene R=40.0Å**

| | | | |
|---|---|---|---|
| C | 1.419281 | 0.000000 | 0.018889 |
| C | -1.419281 | 0.000000 | 0.018889 |
| C | 0.709807 | 1.229107 | 0.000000 |
| C | 0.709807 | -1.229107 | 0.000000 |
| C | -0.709807 | -1.229107 | 0.000000 |
| C | -0.709807 | 1.229107 | 0.000000 |
| C | 2.843195 | 0.000000 | 0.094886 |
| C | -2.843195 | -0.000000 | 0.094886 |
| C | 1.422443 | 2.463684 | 0.019002 |
| C | 1.422443 | -2.463684 | 0.019002 |
| C | -1.422443 | -2.463684 | 0.019002 |
| C | -1.422443 | 2.463684 | 0.019002 |
| C | 2.840732 | -2.462172 | 0.094710 |
| C | -2.840732 | -2.462172 | 0.094710 |
| C | -2.840732 | 2.462172 | 0.094710 |
| C | 2.840732 | 2.462172 | 0.094710 |
| C | 3.550182 | 1.230464 | 0.151579 |
| C | -3.550182 | -1.230464 | 0.151579 |
| C | 3.550182 | -1.230464 | 0.151579 |
| C | -3.550182 | 1.230464 | 0.151579 |
| C | 0.711335 | 3.692580 | 0.000027 |
| C | -0.711335 | -3.692580 | 0.000027 |
| C | 0.711335 | -3.692580 | 0.000027 |
| C | -0.711335 | 3.692580 | 0.000027 |
| C | 1.431226 | 4.928575 | 0.019314 |
| C | -1.431226 | -4.928575 | 0.019314 |
| C | 1.431226 | -4.928575 | 0.019314 |
| C | -1.431226 | 4.928575 | 0.019314 |
| C | 3.549378 | -3.703586 | 0.151507 |
| C | -3.549378 | 3.703586 | 0.151507 |
| C | -3.549378 | -3.703586 | 0.151507 |
| C | 3.549378 | 3.703586 | 0.151507 |
| C | 4.972419 | 1.224906 | 0.304045 |
| C | -4.972419 | -1.224906 | 0.304045 |
| C | 4.972419 | -1.224906 | 0.304045 |
| C | -4.972419 | 1.224906 | 0.304045 |
| C | 2.830260 | 4.905147 | 0.093965 |
| C | 2.830260 | -4.905147 | 0.093965 |
| C | -2.830260 | -4.905146 | 0.093965 |
| C | -2.830260 | 4.905146 | 0.093965 |
| C | 5.648046 | -0.000000 | 0.394591 |
| C | -5.648046 | -0.000000 | 0.394591 |
| C | 4.973921 | -3.666131 | 0.304234 |
| C | -4.973921 | 3.666131 | 0.304234 |
| C | -4.973921 | -3.666131 | 0.304234 |
| C | 4.973921 | 3.666131 | 0.304234 |
| C | 5.651720 | 2.484305 | 0.395116 |
| C | -5.651720 | -2.484305 | 0.395116 |
| C | 5.651720 | -2.484305 | 0.395116 |
| C | -5.651720 | 2.484305 | 0.395116 |
| C | 0.682455 | 6.150672 | -0.000477 |
| C | -0.682455 | -6.150672 | -0.000477 |
| C | 0.682455 | -6.150672 | -0.000477 |
| C | -0.682455 | 6.150672 | -0.000477 |
| H | -3.373038 | 5.847425 | 0.136189 |
| H | 3.373038 | 5.847425 | 0.136189 |
| H | 3.373038 | -5.847425 | 0.136189 |
| H | -3.373038 | -5.847425 | 0.136189 |
| H | -6.723069 | -0.000000 | 0.562998 |
| H | 6.723069 | -0.000000 | 0.562998 |
| H | -6.725805 | -2.479625 | 0.563464 |
| H | 6.725805 | 2.479625 | 0.563464 |
| H | -6.725805 | 2.479625 | 0.563464 |
| H | 6.725805 | -2.479625 | 0.563464 |
| H | 1.229977 | 7.089964 | 0.012616 |
| H | -1.229977 | 7.089964 | 0.012616 |
| H | 1.229977 | -7.089964 | 0.012616 |
| H | -1.229977 | -7.089964 | 0.012616 |
| H | -5.509775 | 4.609612 | 0.375107 |
| H | 5.509775 | -4.609613 | 0.375107 |
| H | -5.509775 | -4.609613 | 0.375107 |
| H | 5.509775 | 4.609613 | 0.375107 |