

Electronic Supplementary Information for:

**Electron Confinement Meet Electron Delocalization: Non-Additivity and Finite-Size Effects in the Polarizabilities and Dispersion Coefficients of the Fullerenes**

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**FINITE-FIELD EXPRESSIONS FOR THE STATIC ISOTROPIC (ELECTRONIC) MULTIPOLE POLARIZABILITIES**

Finite-field expressions for the static isotropic (electronic) dipole ( $\alpha_1$ ), quadrupole ( $\alpha_2$ ), and octupole ( $\alpha_3$ ) polarizabilities were computed using the pure Cartesian tensor formalism [1–3]:

$$\alpha_1 = \frac{1}{3}(M_{x,x} + M_{y,y} + M_{z,z}) \quad (\text{S1})$$

$$\alpha_2 = \frac{1}{5}(M_{xxx,xx} + M_{yyy,yy} + M_{zzz,zz} + 3M_{xy,xy} + 3M_{yz,yz} + 3M_{xz,xz} - M_{xx,yy} - M_{xx,zz} - M_{yy,zz}) \quad (\text{S2})$$

$$\begin{aligned} \alpha_3 = & \frac{1}{7}(M_{xxxx,xxx} + M_{yyyy,yyy} + M_{zzz,zzz} + 15M_{xyz,xyz} + 6M_{xxy,xyx} + 6M_{xxz,xxz} + 6M_{xyy,xyy} + 6M_{xzz,xzz} \\ & + 6M_{yyz,yyz} + 6M_{yzz,yzz} - 3M_{xxx,xyy} - 3M_{xxx,xzz} - 3M_{yyy,xyx} - 3M_{yyy,yzz} - 3M_{zzz,xxz} - 3M_{zzz,yyz} \\ & - 3M_{xxy,yzz} - 3M_{xxz,yyz} - 3M_{xyy,xzz}) \end{aligned} \quad (\text{S3})$$

in which  $M_{a,a'}$ ,  $M_{ab,a'b'}$ , and  $M_{abc,a'b'c'}$  are the Cartesian derivatives ( $a, b, c, a', b', c' \in \{x, y, z\}$ ) of the total energy ( $E$ ) or multipole moments ( $\mu$ ,  $\Theta$ ,  $\Omega$ ) with respect to an applied electric field ( $F_a$ ), field gradient ( $F_{ab} \equiv \nabla_a F_b$ ), and field Laplacian ( $F_{abc} \equiv \nabla_a \nabla_b F_c$ ):

$$M_{a,a'} = - \left. \frac{\partial^2 E}{\partial F_a \partial F_{a'}} \right|_{F=0} = - \left. \frac{\partial \mu_a}{\partial F_{a'}} \right|_{F=0} \quad (\text{S4})$$

$$M_{ab,a'b'} = - \left. \frac{\partial^2 E}{\partial F_{ab} \partial F_{a'b'}} \right|_{F=0} = - \left. \frac{\partial \Theta_{ab}}{\partial F_{a'b'}} \right|_{F=0} \quad (\text{S5})$$

$$M_{abc,a'b'c'} = - \left. \frac{\partial^2 E}{\partial F_{abc} \partial F_{a'b'c'}} \right|_{F=0} = - \left. \frac{\partial \Omega_{abc}}{\partial F_{a'b'c'}} \right|_{F=0}. \quad (\text{S6})$$

**IDENTIFYING THE LOWEST ENERGY ISOMERS OF THE C<sub>60</sub>–C<sub>84</sub> FULLERENES**

To identify the most stable (lowest energy) isomers of C<sub>60</sub>, C<sub>70</sub>, C<sub>76</sub>, C<sub>78</sub>, and C<sub>84</sub>, we first sorted each set of isomers by pentagon signature ( $P_1$ ), second moment hexagon signature ( $H_2$ ), volume, and Fowler asymmetry parameter ( $F$ ) following Ref. [4]. After sorting, we used the face-spiral algorithm in the **Fullerene** (v4.4) program to generate initial coordinates for the first 20 isomers of each fullerene [5]. The geometries of these selected isomers were first optimized using the SCAN [6] functional and the “tier-1” numeric atom-centered basis set in **FHI-aims** [7] according to the following convergence criteria:  $10^{-6}$  eV for the total energy and  $10^{-5}$  au for the charge density during self-consistent field (SCF) optimizations;  $3 \times 10^{-5}$  eV/Å for the maximum force during geometry optimizations. All fullerene geometries (initially optimized at the SCAN/tier-1 level in **FHI-aims**) were further optimized at the SCAN0/6-31G(d) level using **Q-Chem** (v5.1) [8] and the following convergence criteria:  $10^{-10}$  au for the DIIS error in conjunction with a  $10^{-14}$  integral threshold value during SCF optimizations;  $3.0 \times 10^{-4}$  Hartree/Bohr for the maximum gradient component and  $10^{-6}$  Hartree for the energy change between successive steps during geometry optimizations. The SG-2 quadrature grid [9] (default for DFT calculations with meta-GGA functionals) was employed during all **Q-Chem** calculations. Following geometry optimizations at the SCAN0/6-31G(d) level in **Q-Chem**, the isomers corresponding to each fullerene were ranked according to their relative SCAN0/6-31G(d) energetics, and the lowest energy isomer in each set was used throughout this work (unless otherwise specified); optimized Cartesian coordinates for the lowest energy isomers of C<sub>60</sub>, C<sub>70</sub>, C<sub>76</sub>, C<sub>78</sub>, and C<sub>84</sub> can be found in Tables S7–S11 at the end of this document. For comparative purposes, the relative energies ( $\Delta E$ ) and polarizability differences ( $\Delta\alpha_\ell$  for  $\ell = 1, 2, 3$ )—computed with

respect to the lowest energy isomers—are provided below in Table S1 for the second lowest energy isomers of  $C_{60}$ – $C_{84}$ . From this table, one can see that the computed  $\alpha_\ell$  values are within  $\pm 2.0\%$  (of the lowest energy isomers) for the fullerenes with more sizable energetic gaps ( $C_{60}$  and  $C_{70}$ ) and within  $\pm 0.4\%$  for fullerenes with significantly smaller energetic separations ( $C_{84}$ ). As such, the inclusion of these higher energy isomers are expected to have a minor impact on the effective  $\alpha_\ell$  (and  $C_n$ ) scaling laws derived in the work.

TABLE S1. Molecular point groups, relative energies ( $\Delta E$  in kcal/mol), and polarizability differences ( $\Delta\alpha_\ell$  for  $\ell = 1, 2, 3$  in %) corresponding to the second lowest energy isomers of  $C_{60}$ – $C_{84}$ . All  $\Delta E$  and  $\Delta\alpha_\ell$  values were computed with respect to the lowest energy isomer at the SCAN0/6-31G(d)//SCAN0/6-31G(d) and SCAN0/aug-pc-1//SCAN0/6-31G(d) levels of theory, respectively.

Molecule (Symmetry)	$\Delta E$ (kcal/mol)	$\Delta\alpha_1$ (in %)	$\Delta\alpha_2$ (in %)	$\Delta\alpha_3$ (in %)
$C_{60}(C_{2v})$	39.81	+1.54	+1.13	+1.47
$C_{70}(C_s)$	31.39	-0.11	+1.01	+1.91
$C_{76}(C_1)$	20.14	–	–	–
$C_{78}(D_{3h})^a$	5.15	–	–	–
$C_{84}(D_2)$	0.32	+0.34	+0.13	+0.20

<sup>a</sup> $C_{78}$  also has a second  $C_{2v}$  isomer ( $\Delta E = 6.18$  kcal/mol) that is structurally distinct from the lowest energy  $C_{2v}$  isomer considered throughout the main text.

### AB INITIO METHOD CALIBRATION: BENCHMARK MULTIPOLE POLARIZABILITIES FOR THE CAGE ISOMER OF $C_{20}$

Since  $C_{20}$  is the smallest possible cage-like fullerene [10], we used this system as a benchmark when determining an accurate, reliable, and computationally feasible *ab initio* level of theory for computing the static isotropic (electronic) multipole polarizabilities in the larger  $C_{60}$ – $C_{84}$  fullerenes. The corresponding theoretical reference values for the  $\alpha_\ell$  series in  $C_{20}$  were obtained using quantum mechanical calculations that include a sophisticated treatment of electron correlation effects at the complete basis set (CBS) limit. More specifically, we computed  $\alpha_\ell$  with  $\ell = 1, 2, 3$  for  $C_{20}$  at the (orbital-relaxed) CCSD/CBS level of theory *via* finite-field derivatives of the following total energy expression:

$$E^{\text{CCSD/CBS}} = E^{\text{MP2/CBS}} + \left( E^{\text{CCSD/d-aug-cc-pVDZ}} - E^{\text{MP2/d-aug-cc-pVDZ}} \right), \quad (\text{S7})$$

in which  $E^{\text{MP2/CBS}}$  was obtained using the two-point extrapolation procedure of Halkier *et al.* [11] in conjunction with the d-aug-cc-pVDZ and d-aug-cc-pVTZ basis sets [12]. For all calculations performed in this section, we used the  $C_{20}$  fullerene geometry provided in Ref. [13], which was optimized at the CCSD/cc-pVTZ level of theory and translated to the (nuclear) center of charge. Using the CCSD/CBS  $\alpha_\ell$  values as a benchmark, we assessed the performance of a number of different *ab initio* methods and basis sets (see Table S2). Tested exchange-correlation functionals included: B3LYP [14, 15], CAM-B3LYP [16], SCAN [6], and SCAN0 [17]; tested basis sets included: Zm3PolC [18], Sadlej [19], aug-pc-X (with X = 1,2,3) [20–23], aug-cc-pVXZ (with X = D,T) [24], and d-aug-cc-pVXZ (with X = D,T) [12]. Orbital-relaxed  $\alpha_\ell$  values at the HF and DFT (MP2 and CCSD) levels were computed as first (second) derivatives of the corresponding multipole moments (total energies) using the finite-field approach described above (see Eqs. (S1)–(S6)); for a description of the computational methods used to perform all of the polarizability calculations in this section, see the *Computational Details* section directly below. From this table, one can see that the SCAN0/aug-pc-3 and SCAN0/Sadlej values are in excellent agreement with the reference CCSD/CBS level; since the differences in %Error and MAPE between these levels is  $\leq 0.5\%$ , the more computationally efficient SCAN0/Sadlej level of theory (with  $N_{\text{basis}} = 480$ ) was used to compute  $\alpha_\ell$  for the larger  $C_{60}$ – $C_{84}$  fullerenes. Here, we note in passing that SCAN0/aug-pc-1 (which was initially used to compute the  $\Delta\alpha_\ell$  values during the isomer screening protocol, see Table S1) was also replaced in favor of SCAN0/Sadlej, as this level of theory yielded  $\alpha_\ell$  errors that were  $\approx 2.5\times$  smaller for  $C_{20}$  (see Table S2).

### COMPUTATIONAL DETAILS: AB INITIO DETERMINATION OF $\alpha_\ell$ FOR THE $C_{60}$ – $C_{84}$ FULLERENES

Using geometries (corresponding to the lowest energy isomer of each fullerene) optimized at the SCAN0/6-31G(d) level,  $\alpha_\ell$  values with  $\ell = 1, 2, 3$  were computed at the (orbitally-relaxed) SCAN0/Sadlej level of theory *via* finite-field

TABLE S2. Values (in atomic units) for the multipole polarizabilities ( $\alpha_\ell$  with  $\ell = 1, 2, 3$ ) of the cage isomer of  $C_{20}$  computed at various different levels of theory. Also provided are the number of basis functions ( $N_{\text{basis}}$ ), the corresponding percent errors (%Error) with respect to the benchmark CCSD/CBS values, and the mean absolute percent errors (MAPE, averaged over all three  $\alpha_\ell$  values). Multipole polarizabilities computed using SCAN0/aug-pc-3 and SCAN0/Sadlej show very high fidelity to the reference CCSD/CBS values, and are highlighted in bold green font.

Level of Theory	$N_{\text{basis}}$	$\alpha_1$	%Error	$\alpha_2$	%Error	$\alpha_3$	%Error	MAPE
SCAN0/Zm3PolC <sup>a</sup>	360	182.1	-2.6%	6056.4	-2.2%	224178.1	-4.4%	3.1%
B3LYP/Sadlej <sup>a</sup>	480	186.4	-0.3%	6381.1	+3.0%	242796.7	+3.5%	2.3%
CAM-B3LYP/Sadlej <sup>a</sup>	480	186.9	0.0%	6283.3	+1.4%	239585.6	+2.1%	1.2%
<b>SCAN0/Sadlej<sup>a</sup></b>	480	184.8	<b>-1.1%</b>	6218.1	<b>+0.4%</b>	231550.7	<b>-1.3%</b>	<b>0.9%</b>
SCAN/aug-pc-1 <sup>a</sup>	460	181.7	-2.8%	6124.8	-1.1%	226900.3	-3.3%	2.4%
SCAN0/aug-pc-1 <sup>a</sup>	460	183.4	-1.9%	6147.4	-0.8%	229736.1	-2.1%	1.6%
SCAN0/aug-pc-2 <sup>a</sup>	920	184.2	-1.5%	6192.5	0.0%	230640.4	-1.7%	1.1%
<b>SCAN0/aug-pc-3<sup>a</sup></b>	1780	185.8	<b>-0.6%</b>	6204.2	<b>+0.2%</b>	231159.6	<b>-1.5%</b>	<b>0.7%</b>
HF/Sadlej <sup>a</sup>	480	198.8	+6.3%	6672.5	+7.7%	265735.1	+13.3%	9.1%
HF/d-aug-cc-pVDZ <sup>a</sup>	640	201.8	+7.9%	6704.4	+8.2%	268938.1	+14.7%	10.3%
HF/d-aug-cc-pVTZ <sup>a</sup>	1240	201.3	+7.7%	6681.5	+7.9%	268204.2	+14.3%	10.0%
MP2/d-aug-cc-pVDZ <sup>a</sup>	640	178.5	-4.5%	6495.4	+4.9%	235291.9	+0.3%	3.2%
MP2/d-aug-cc-pVTZ <sup>a</sup>	1240	176.5	-5.6%	6382.2	+3.0%	227925.8	-2.8%	3.8%
MP2/CBS <sup>a</sup>	–	175.9	-5.9%	6344.3	+2.4%	225133.4	-4.0%	4.1%
CCSD/Zm3PolC <sup>a</sup>	360	184.7	-1.2%	6221.7	+0.4%	237668.5	+1.3%	1.0%
CCSD/aug-cc-pVDZ <sup>a</sup>	460	189.8	+1.5%	6344.6	+2.4%	244029.8	+4.0%	2.7%
CCSD/d-aug-cc-pVDZ <sup>a</sup>	640	189.5	+1.4%	6345.6	+2.4%	244724.8	+4.3%	2.7%
LR-CCSD/cc-pVTZ <sup>b</sup>	600	176.6	-5.5%	–	–	–	–	–
<b>CCSD/CBS<sup>a</sup></b>	–	<b>186.9</b>	–	<b>6194.5</b>	–	<b>234566.3</b>	–	–

<sup>a</sup>This work; orbital-relaxed finite-field calculation. <sup>b</sup>Ref. [25].

first derivatives of the corresponding multipole moments ( $\boldsymbol{\mu}, \boldsymbol{\Theta}, \boldsymbol{\Omega}$ ) via Eqs. (S4)–(S6) for the  $C_{60}(I_h)$ ,  $C_{70}(D_{5h})$ ,  $C_{76}(D_2)$ ,  $C_{78}(C_{2v})$ , and  $C_{84}(D_{2d})$  fullerenes (see Table S3). All  $\alpha_\ell$  calculations were performed using Q-Chem (v5.1) [8] according to the following convergence criteria:  $10^{-10}$  au for the DIIS error in conjunction with a  $10^{-14}$  integral threshold value during SCF optimizations; the SG-2 grid [9] (default for DFT calculations with meta-GGA functionals) was used for numerical quadrature during all calculations. With each molecule translated to the (nuclear) center of charge, finite (electric) dipole fields, quadrupole fields (field gradients), and octupole fields (field Laplacians) were applied in Q-Chem to compute  $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$ , respectively. Standard central-difference formulae were used in conjunction with a finite-field step size of  $\delta = -1.8897261250 \times 10^{-5}$  au.

TABLE S3. Values (in atomic units) for the multipole polarizabilities ( $\alpha_\ell$  with  $\ell = 1, 2, 3$ ) of the  $C_{60}$ – $C_{84}$  fullerenes computed at the SCAN0/Sadlej//SCAN0/6-31G(d) level of theory.

Molecule	$\alpha_1$	$\alpha_2$	$\alpha_3$
$C_{60}(I_h)$	536.81	42808.37	3318595.48
$C_{70}(D_{5h})$	663.83	57995.33	5149960.46
$C_{76}(D_2)$	724.76	68712.75	6539186.36
$C_{78}(C_{2v})$	754.16	72172.65	6909503.65
$C_{84}(D_{2d})$	808.60	83006.18	8336174.90

**AB INITIO + HS/MSFA FREQUENCY-DEPENDENT POLARIZABILITIES AND DISPERSION COEFFICIENTS**

Frequency-dependent polarizabilities  $\alpha_\ell(iu)$  (in the imaginary frequency domain) were obtained by inputting the static *ab initio*  $\alpha_\ell$  values into the hollow sphere (HS) model of Tao and Perdew [26] and invoking the modified single-frequency approximation (MSFA) of Tao *et al.* [27], *i.e.*,

$$\alpha_\ell^{\text{MSFA}}(iu) = \alpha_\ell \left[ \left( \frac{\omega_\ell^2}{\omega_\ell^2 + u^2} \right) \frac{1 - \rho_\ell}{1 - \beta_\ell \rho_\ell} \right]. \quad (\text{S8})$$

In this expression, the fullerene is assumed to be metallic ( $\omega_g \rightarrow 0$ ) and  $\rho_\ell = (1 - t_\ell/R_\ell)^{2\ell+1}$  defines the shell shape in terms of  $R_\ell = \alpha_\ell^{1/(2\ell+1)}$  (the  $\ell$ -dependent fullerene radius) and  $t_\ell = t = 3.4$  Bohr (the fullerene shell thickness [28, 29]; taken to be  $\ell$ -independent [30]). The  $\beta_\ell = \omega_\ell^2 \tilde{\omega}_\ell^2 / [(\omega_\ell^2 + u^2)(\tilde{\omega}_\ell^2 + u^2)]$  term accounts for coupling between the sphere and cavity plasmon oscillations, and is given in terms of  $\omega_\ell = \omega_p \sqrt{\ell/(2\ell+1)}$  (the generalized local sphere plasmon frequency) and  $\tilde{\omega}_\ell = \omega_p \sqrt{(\ell+1)/(2\ell+1)}$  (local cavity frequency), both of which depend on  $\omega_p = \sqrt{4\pi\rho_\ell}$  (the local plasmon frequency of the extended electron gas). In the MSFA, the  $\ell$ -dependent electron density is approximated as  $\rho_\ell = \bar{N}/V_\ell$ , in which  $\bar{N}$  is the number of valence electrons in the outermost sub-shell and  $V_\ell = \frac{4\pi}{3} [R_\ell^3 - (R_\ell - t_\ell)^3] = \frac{4\pi}{3} [R_\ell^3 - (R_\ell - t)^3]$ .

With *ab initio* + HS/MSFA  $\alpha_\ell(iu)$  values in hand, the corresponding homo-/hetero- molecular dispersion coefficients ( $C_n$  with  $n = 6, 8, 10$ ) between molecules A and B were computed *via* the Casimir-Polder relationship [31]:

$$C_n^{\text{AB}} = \frac{(n-2)!}{2\pi} \sum_{\ell=1}^{\frac{n}{2}-2} \frac{1}{(2\ell)!(2\ell')!} \int_0^\infty du \alpha_\ell^{\text{A}}(iu) \alpha_{\ell'}^{\text{B}}(iu), \quad (\text{S9})$$

in which  $\ell' = \frac{n}{2} - \ell - 1$ . Three-body homo-/hetero- molecular  $C_9$  coefficients (between molecules A, B, and C) were computed *via* :

$$C_9^{\text{ABC}} = \frac{\pi}{3} \int_0^\infty du \alpha_1^{\text{A}}(iu) \alpha_1^{\text{B}}(iu) \alpha_1^{\text{C}}(iu). \quad (\text{S10})$$

All integrals in Eqs. (S9) and (S10) were performed analytically using **Mathematica** (v11), and the final values for the dispersion coefficients are provided in Tables S4 and S5.

TABLE S4. Homo-/hetero- molecular  $C_6, C_8, C_{10}$  dispersion coefficients (in atomic units) for the  $C_{60}$ – $C_{84}$  fullerenes. All dispersion coefficients were computed by inputting the *ab initio*  $\alpha_\ell$  values (computed at the SCAN0/Sadlej//SCAN0/6-31G(d) level of theory) into the HS/MSFA model (for the frequency dependence) followed by analytical evaluation of the Casimir-Polder integral (see Eqs. (S8) and (S9)).

A–B	$C_6$	$C_8$	$C_{10}$
$C_{60}$ – $C_{60}$	98967	42070750	14620311062
$C_{70}$ – $C_{70}$	146241	68911039	26963338127
$C_{76}$ – $C_{76}$	173454	88605067	37417198227
$C_{78}$ – $C_{78}$	186335	96385618	41138189628
$C_{84}$ – $C_{84}$	214304	118721424	53826704958
$C_{60}$ – $C_{70}$	120288	53916469	19917119452
$C_{60}$ – $C_{76}$	130998	61315555	23584490317
$C_{60}$ – $C_{78}$	135764	63990191	24751610151
$C_{60}$ – $C_{84}$	145599	71300987	28481234711
$C_{70}$ – $C_{76}$	159267	78203933	31802566469
$C_{70}$ – $C_{78}$	165073	81588114	33358360980
$C_{70}$ – $C_{84}$	177029	90748145	38268930320
$C_{76}$ – $C_{78}$	179778	92415405	39234522424
$C_{76}$ – $C_{84}$	192799	102648842	44924002421
$C_{78}$ – $C_{84}$	199831	107034920	47091516175

TABLE S5. Homo-/hetero- molecular  $C_9$  dispersion coefficients (in atomic units) for the  $C_{60}$ – $C_{84}$  fullerenes. All dispersion coefficients were computed by inputting the *ab initio*  $\alpha_\ell$  values (computed at the SCAN0/Sadlej//SCAN0/6-31G(d) level of theory) into the HS/MSFA model (for the frequency dependence) followed by analytical evaluation of the Casimir-Polder integral (see Eqs. (S8) and (S10)).

A–B–C	$C_9$	A–B–C	$C_9$
$C_{60}$ – $C_{60}$ – $C_{60}$	39636451	–	–
$C_{70}$ – $C_{70}$ – $C_{70}$	72377616	–	–
$C_{76}$ – $C_{76}$ – $C_{76}$	93698712	–	–
$C_{78}$ – $C_{78}$ – $C_{78}$	104726882	–	–
$C_{84}$ – $C_{84}$ – $C_{84}$	129113297	–	–
$C_{60}$ – $C_{60}$ – $C_{70}$	48439100	$C_{70}$ – $C_{70}$ – $C_{78}$	81861428
$C_{60}$ – $C_{60}$ – $C_{76}$	52789964	$C_{70}$ – $C_{70}$ – $C_{84}$	87777714
$C_{60}$ – $C_{60}$ – $C_{78}$	54779706	$C_{70}$ – $C_{76}$ – $C_{76}$	85971747
$C_{60}$ – $C_{60}$ – $C_{84}$	58739013	$C_{70}$ – $C_{76}$ – $C_{78}$	89219141
$C_{60}$ – $C_{70}$ – $C_{70}$	59206074	$C_{70}$ – $C_{76}$ – $C_{84}$	95667154
$C_{60}$ – $C_{70}$ – $C_{76}$	64525518	$C_{70}$ – $C_{78}$ – $C_{78}$	92589975
$C_{60}$ – $C_{70}$ – $C_{78}$	66960054	$C_{70}$ – $C_{78}$ – $C_{84}$	99281552
$C_{60}$ – $C_{70}$ – $C_{84}$	71799552	$C_{70}$ – $C_{84}$ – $C_{84}$	106456744
$C_{60}$ – $C_{76}$ – $C_{76}$	70323127	$C_{76}$ – $C_{76}$ – $C_{78}$	97238483
$C_{60}$ – $C_{76}$ – $C_{78}$	72976794	$C_{76}$ – $C_{76}$ – $C_{84}$	104266036
$C_{60}$ – $C_{76}$ – $C_{84}$	78251124	$C_{76}$ – $C_{78}$ – $C_{78}$	100912825
$C_{60}$ – $C_{78}$ – $C_{78}$	75731243	$C_{76}$ – $C_{78}$ – $C_{84}$	108205872
$C_{60}$ – $C_{78}$ – $C_{84}$	81204605	$C_{76}$ – $C_{84}$ – $C_{84}$	116025999
$C_{60}$ – $C_{84}$ – $C_{84}$	87073551	$C_{78}$ – $C_{78}$ – $C_{84}$	112295516
$C_{70}$ – $C_{70}$ – $C_{76}$	78882252	$C_{78}$ – $C_{84}$ – $C_{84}$	120411144

### COMPARISON TO AVAILABLE THEORETICAL DATA FOR $\alpha_1$ AND $C_6$ IN THE $C_{60}$ – $C_{84}$ FULLERENES

A comparison between our  $\alpha_1$  and  $C_6$  values for the  $C_{60}$ ,  $C_{70}$ ,  $C_{78}$ , and  $C_{84}$  fullerenes and those from previous work is provided in Table S6.

TABLE S6. Summary of *ab initio*  $\alpha_1$  and  $C_6$  values (in atomic units) for the  $C_{60}$ ,  $C_{70}$ ,  $C_{78}$ , and  $C_{84}$  fullerenes.

Molecule →	$C_{60}$		$C_{70}$		$C_{78}$		$C_{84}$	
Method [Ref] ↓	$\alpha_1$	$C_6/10^3$	$\alpha_1$	$C_6/10^3$	$\alpha_1$	$C_6/10^3$	$\alpha_1$	$C_6/10^3$
TD-HF/Sadlej [32]	539.5	101.0	–	–	–	–	–	–
TD-B3LYP/Sadlej [32]	557.2	101.8	–	–	–	–	–	–
TD-HF/Sadlej [33]	536.6	100.1	659.1	141.6	748.3	178.2	806.1	207.7
TD-B3LYP/Sadlej [33]	554.5	100.8	685.3	143.0	778.7	180.0	837.4	209.8
TD-CAM-B3LYP/Sadlej [33]	542.1	98.8	666.5	139.8	757.0	176.1	815.5	205.4
MP2/aug-cc-pVTZ [34]	559.6	–	–	–	–	–	–	–
LR-CC2/aug-cc-pVDZ [35]	623.7	–	–	–	–	–	–	–
LR-CCSD/Zm3PolC [36]	555.3	–	–	–	–	–	–	–
SCAN0/Sadlej (This work)	536.8	99.0	663.8	146.2	754.2	186.3	808.6	214.3

### COMPUTATIONAL DETAILS: *AB INITIO* DETERMINATION OF $\alpha^{\text{zpvC}}$ FOR THE $C_{60}$ AND $C_{70}$ FULLERENES

Zero-point vibrational contributions (zpvC) to  $\alpha_1$  for the  $C_{60}$  and  $C_{70}$  fullerenes were computed at the SCAN/tier-1//SCAN/tier-1 level in FHI-aims [7]. As described above, the geometries of the  $C_{60}$  (1812Ih) and  $C_{70}$  (8149D5h)

isomers were optimized using the SCAN [6] functional and the “tier-1” numeric atom-centered basis set in FHI-aims [7]. Following geometry optimization, numerical evaluation of the corresponding Hessian (assembled at the SCAN/tier-1 level of theory using a finite-difference step size of  $\delta = 0.0025$  Å) was performed using an in-house Numpy/Scipy script to obtain the (harmonic) vibrational frequencies ( $\{\omega_i\}$ ) and normal modes ( $\{\mathbf{q}_i\}$ ). All calculations in FHI-aims used the following more stringent convergence criteria:  $10^{-8}$  eV for the total energy and  $10^{-7}$  au for the charge density during SCF optimizations;  $3 \times 10^{-7}$  eV/Å for the maximum force during geometry optimizations. Displaced geometries for each fullerene were then generated by perturbing the optimized structure along each normal mode in both the positive and negative directions with a finite-difference step size of  $\Delta q = 0.130683$  [37, 38], followed by single-point energy evaluations at the SCAN/tier-1 level. Displacements included: four single displacements,  $\{\pm\Delta q_i\}$  and  $\{\pm 2\Delta q_i\}$ , along each normal mode  $\mathbf{q}_i$ ; four double displacements,  $\{\pm\Delta q_i, \pm\Delta q_j\}$  along combinations of two normal modes  $\mathbf{q}_i$  and  $\mathbf{q}_j$  (with  $i \neq j$ ). With 174 and 204 normal modes for  $C_{60}$  and  $C_{70}$  (*i.e.*,  $3N-6$  normal modes), the total number of displaced geometries (or single-point energy evaluations) required to compute  $\alpha^{\text{zpv}}c$  was  $4 \times 174 + 4 \times \frac{(174 \cdot 173)}{2} = 60,900$  for  $C_{60}$  and  $4 \times 204 + 4 \times \frac{(204 \cdot 203)}{2} = 83,640$  for  $C_{70}$ , for a total of 144,540 DFT calculations. For  $C_{70}$ ,  $\alpha^{\text{zpv}}c = 9.6$  au at the SCAN/tier-1//SCAN/tier-1 level, and the contribution from each mode is plotted in Fig. S1. Similar to  $C_{60}$ , the higher-frequency (bond-stretching) modes contribute more to  $\alpha^{\text{zpv}}c$ . While all mode contributions were positive in  $C_{60}$ , the contribution from a single mode ( $\omega \approx 900$   $\text{cm}^{-1}$ ) is slightly negative in  $C_{70}$ .

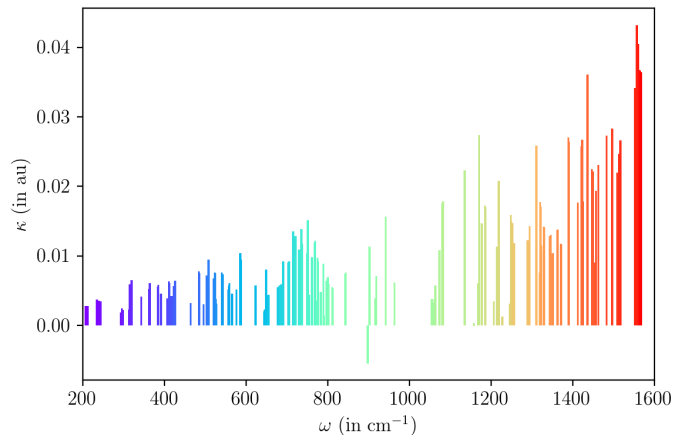


FIG. S1. Individual mode contributions ( $\kappa$  in au) as a function of frequency ( $\omega$  in  $\text{cm}^{-1}$ ) to the zero-point vibrational contribution ( $\alpha_1^{\text{zpv}c}$ ) in  $C_{70}$  computed at the SCAN/tier-1//SCAN/tier-1 level of theory.

## OPTIMIZED CARTESIAN COORDINATES FOR THE $C_{60}$ – $C_{84}$ FULLERENES

Optimized Cartesian coordinates for the  $C_{60}$ – $C_{84}$  fullerenes at the SCAN0/6-31G(d) level of theory can be found below in Tables S7–S11.

TABLE S7: Optimized Cartesian coordinates for the  $C_{60}(I_h)$  fullerene at the SCAN0/6-31G(d) level of theory.

C	1.22725208	0.00000000	−3.30272818
C	0.37924175	−1.16718608	−3.30272818
C	2.40625954	0.00000000	−2.57504102
C	0.74357509	−2.28848881	−2.57504102
C	−0.24935847	−3.00964905	−1.81627209
C	−0.99286779	−0.72136067	−3.30272818
C	−1.94670486	−1.41436387	−2.57504102
C	−1.56729208	−2.58142646	−1.81627209
C	1.97076257	2.28828799	−1.81627209
C	0.74357509	2.28848881	−2.57504102
C	2.78529033	1.16718671	−1.81627209

*Continued on next page*

TABLE S7 – *Continued from previous page*

C	0.37924175.	1.16718608	-3.30272818
C	-0.99286779	0.72136067	-3.30272818
C	-0.24935847	3.00964905	-1.81627209
C	-1.56729208	2.58142646	-1.81627209
C	-1.94670486	1.41436387	-2.57504102
C	3.17439815	1.41433032	0.58938493
C	2.32605104	2.58197994	0.58938493
C	3.39946455	0.72164715	-0.58938493
C	1.73681954	3.01008168	-0.58938493
C	0.36416509	3.45608415	-0.58938493
C	1.56729208	2.58142646	1.81627209
C	0.24935847	3.00964905	1.81627209
C	-0.36416509	3.45608415	0.58938493
C	3.17439815	-1.41433032	0.58938493
C	2.93940235	-0.69287870	1.81627209
C	3.39946455	-0.72164715	-0.58938493
C	2.93940235	0.69287870	1.81627209
C	1.94670486	1.41436387	2.57504102
C	1.94670486	-1.41436387	2.57504102
C	0.99286779	-0.72136067	3.30272818
C	0.99286779	0.72136067	3.30272818
C	1.97076257	-2.28828799	-1.81627209
C	1.73681954	-3.01008168	-0.58938493
C	2.78529033	-1.16718671	-1.81627209
C	2.32605104	-2.58197994	0.58938493
C	1.56729208	-2.58142646	1.81627209
C	0.36416509	-3.45608415	-0.58938493
C	-0.36416509	-3.45608415	0.58938493
C	0.24935847	-3.00964905	1.81627209
C	-1.22725208	0.00000000	3.30272818
C	-0.37924175	-1.16718608	3.30272818
C	-0.74357509	-2.28848881	2.57504102
C	-2.40625954	0.00000000	2.57504102
C	-1.97076257	2.28828799	1.81627209
C	-0.74357509	2.28848881	2.57504102
C	-0.37924175	1.16718608	3.30272818
C	-2.78529033	1.16718671	1.81627209
C	-3.17439815	1.41433032	-0.58938493
C	-2.32605104	2.58197994	-0.58938493
C	-1.73681954	3.01008168	0.58938493
C	-3.39946455	0.72164715	0.58938493
C	-3.17439815	-1.41433032	-0.58938493
C	-2.93940235	-0.69287870	-1.81627209
C	-2.93940235	0.69287870	-1.81627209
C	-3.39946455	-0.72164715	0.58938493
C	-1.97076257	-2.28828799	1.81627209
C	-1.73681954	-3.01008168	0.58938493
C	-2.32605104	-2.58197994	-0.58938493
C	-2.78529033	-1.16718671	1.81627209

TABLE S8: Optimized Cartesian coordinates for the  $C_{70}(D_{5h})$  fullerene at the SCAN0/6-31G(d) level of theory.

C	2.39747577	-0.00000000	3.19938261
C	2.76290826	-1.15500181	2.42517580
C	1.22591526	-0.00000000	3.94146362
C	1.95225760	-2.27076672	2.42517580
C	1.71837578	-2.98463573	1.19768792
C	2.37164242	-2.62518617	-0.00000000
C	1.71837578	-2.98463573	-1.19768792

*Continued on next page*



TABLE S8 – *Continued from previous page*


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C	0.74086076	2.28013496	3.19938261
C	1.95225760	2.27076672	2.42517580
C	0.37882865	1.16591469	3.94146362
C	2.76290826	1.15500181	2.42517580
C	3.36956458	0.71196932	1.19768792
C	3.22957822	1.44433883	-0.00000000
C	3.36956458	0.71196932	-1.19768792
C	3.22957822	-1.44433883	-0.00000000
C	3.36956458	-0.71196932	1.19768792
C	3.36956458	-0.71196932	-1.19768792
C	-1.93959864	1.40920090	3.19938261
C	-1.55634671	2.55841282	2.42517580
C	-0.99178628	0.72057491	3.94146362
C	-0.24468639	2.98459709	2.42517580
C	0.36412966	3.42465697	1.19768792
C	-0.37565330	3.51783666	-0.00000000
C	0.36412966	3.42465697	-1.19768792
C	2.37164242	2.62518617	-0.00000000
C	1.71837578	2.98463573	1.19768792
C	1.71837578	2.98463573	-1.19768792
C	-1.93959864	-1.40920090	3.19938261
C	-2.91413277	-0.68958064	2.42517580
C	-0.99178628	-0.72057491	3.94146362
C	-2.91413277	0.68958064	2.42517580
C	-3.14452007	1.40458509	1.19768792
C	-3.46174473	0.72980379	-0.00000000
C	-3.14452007	1.40458509	-1.19768792
C	-1.76382260	3.06679311	-0.00000000
C	-2.30754994	2.55657565	1.19768792
C	-2.30754994	2.55657565	-1.19768792
C	0.74086076	-2.28013496	3.19938261
C	-0.24468639	-2.98459709	2.42517580
C	0.37882865	-1.16591469	3.94146362
C	-1.55634671	-2.55841282	2.42517580
C	-2.30754994	-2.55657565	1.19768792
C	-1.76382260	-3.06679311	-0.00000000
C	-2.30754994	-2.55657565	-1.19768792
C	-3.46174473	-0.72980379	-0.00000000
C	-3.14452007	-1.40458509	1.19768792
C	-3.14452007	-1.40458509	-1.19768792
C	-0.37565330	-3.51783666	-0.00000000
C	0.36412966	-3.42465697	1.19768792
C	0.36412966	-3.42465697	-1.19768792
C	-1.93959864	-1.40920090	-3.19938261
C	-1.55634671	-2.55841282	-2.42517580
C	-0.24468639	-2.98459709	-2.42517580
C	-0.99178628	-0.72057491	-3.94146362
C	-1.93959864	1.40920090	-3.19938261
C	-2.91413277	0.68958064	-2.42517580
C	-2.91413277	-0.68958064	-2.42517580
C	-0.99178628	0.72057491	-3.94146362
C	0.74086076	2.28013496	-3.19938261
C	-0.24468639	2.98459709	-2.42517580
C	-1.55634671	2.55841282	-2.42517580
C	0.37882865	1.16591469	-3.94146362
C	2.39747577	-0.00000000	-3.19938261
C	2.76290826	1.15500181	-2.42517580
C	1.95225760	2.27076672	-2.42517580
C	1.22591526	-0.00000000	-3.94146362
C	0.74086076	-2.28013496	-3.19938261
C	1.95225760	-2.27076672	-2.42517580
C	2.76290826	-1.15500181	-2.42517580
C	0.37882865	-1.16591469	-3.94146362

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TABLE S9: Optimized Cartesian coordinates for the  $C_{76}(D_2)$  fullerene at the SCAN0/6-31G(d) level of theory.

C	0.15448551	2.47317142	2.70668710
C	1.48223938	2.03935522	2.62932986
C	2.29970506	2.71391695	1.69180271
C	3.47059232	2.08047210	1.15545509
C	3.82798555	0.83353518	1.60334424
C	0.69104875	-0.23335106	3.33782782
C	1.78934713	0.67715904	3.02683257
C	3.01134824	0.14147468	2.57842825
C	0.90846413	-1.60304811	3.15507012
C	2.12703783	-2.11112253	2.62704698
C	3.17094994	-1.25539398	2.34330627
C	-0.69104875	0.23335106	3.33782782
C	-1.78934713	-0.67715904	3.02683257
C	-0.90846413	1.60304811	3.15507012
C	-3.01134824	-0.14147468	2.57842825
C	3.95152877	1.44065397	-1.14656833
C	4.34935899	0.14269191	-0.67977516
C	3.56977755	2.41403884	-0.23816067
C	4.34935899	-0.14269191	0.67977516
C	3.95152877	-1.44065397	1.14656833
C	3.82798555	-0.83353518	-1.60334424
C	3.47059232	-2.08047210	-1.15545509
C	3.56977755	-2.41403884	0.23816067
C	1.80373203	3.18909581	-1.73146361
C	2.12703783	2.11112253	-2.62704698
C	2.47671590	3.29954936	-0.53548372
C	3.17094994	1.25539398	-2.34330627
C	3.01134824	-0.14147468	-2.57842825
C	0.90846413	1.60304811	-3.15507012
C	0.69104875	0.23335106	-3.33782782
C	1.78934713	-0.67715904	-3.02683257
C	1.48223938	-2.03935522	-2.62932986
C	0.15448551	-2.47317142	-2.70668710
C	2.29970506	-2.71391695	-1.69180271
C	-1.72348647	3.52496376	-0.67473161
C	-0.34392174	3.79493486	-0.64205838
C	0.38832313	3.40499920	-1.78584590
C	-0.15448551	2.47317142	-2.70668710
C	-1.48223938	2.03935522	-2.62932986
C	-2.29970506	2.71391695	-1.69180271
C	-3.82798555	0.83353518	-1.60334424
C	-3.47059232	2.08047210	-1.15545509
C	-0.90846413	-1.60304811	-3.15507012
C	-0.69104875	-0.23335106	-3.33782782
C	-1.78934713	0.67715904	-3.02683257
C	-3.01134824	0.14147468	-2.57842825
C	0.34392174	3.79493486	0.64205838
C	1.72348647	3.52496376	0.67473161
C	-2.47671590	3.29954936	0.53548372
C	-1.80373203	3.18909581	1.73146361
C	-0.38832313	3.40499920	1.78584590
C	-3.56977755	2.41403884	0.23816067
C	-2.12703783	2.11112253	2.62704698
C	-3.17094994	1.25539398	2.34330627
C	-3.95152877	1.44065397	1.14656833
C	-3.95152877	-1.44065397	-1.14656833
C	-4.34935899	-0.14269191	-0.67977516
C	-4.34935899	0.14269191	0.67977516
C	-3.56977755	-2.41403884	-0.23816067

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TABLE S9 – *Continued from previous page*

C	-1.80373203	-3.18909581	-1.73146361
C	-2.12703783	-2.11112253	-2.62704698
C	-3.17094994	-1.25539398	-2.34330627
C	-2.47671590	-3.29954936	-0.53548372
C	1.72348647	-3.52496376	-0.67473161
C	0.34392174	-3.79493486	-0.64205838
C	-0.38832313	-3.40499920	-1.78584590
C	0.38832313	-3.40499920	1.78584590
C	1.80373203	-3.18909581	1.73146361
C	2.47671590	-3.29954936	0.53548372
C	-1.72348647	-3.52496376	0.67473161
C	-0.34392174	-3.79493486	0.64205838
C	-3.82798555	-0.83353518	1.60334424
C	-3.47059232	-2.08047210	1.15545509
C	-2.29970506	-2.71391695	1.69180271
C	-1.48223938	-2.03935522	2.62932986
C	-0.15448551	-2.47317142	2.70668710

TABLE S10: Optimized Cartesian coordinates for the  $C_{78}(C_{2v})$  fullerene at the SCAN0/6-31G(d) level of theory.

C	4.18634767	-0.69534461	-1.16981510
C	3.39235376	-1.40335178	-2.13414214
C	4.18634767	0.69534461	-1.16981510
C	2.69630693	-0.72084514	-3.10180975
C	0.72578511	-3.58745012	-0.84764418
C	2.76069866	-2.51950258	-1.48701946
C	1.45685398	-2.93650592	-1.85466501
C	0.73069474	-2.23611346	-2.90459425
C	-0.73069474	-2.23611346	-2.90459425
C	1.39765375	-1.16750212	-3.52545401
C	-1.39765375	-1.16750212	-3.52545401
C	4.03460849	0.71843639	1.25641860
C	4.03460849	-0.71843639	1.25641860
C	4.08159485	1.40959227	0.06512165
C	4.08159485	-1.40959227	0.06512165
C	3.20111726	-2.54066087	-0.13019437
C	2.36487020	-2.99869968	0.90159381
C	1.17574828	-3.64498622	0.48507065
C	1.17700007	2.33432898	2.96867641
C	2.36421698	2.30063981	2.18236198
C	3.17626699	1.16231113	2.32131911
C	2.70088263	0.00000000	3.00745292
C	0.72806178	-1.21416679	3.68381545
C	1.45146551	0.00000000	3.66500779
C	0.72806178	1.21416679	3.68381545
C	2.36421698	-2.30063981	2.18236198
C	3.17626699	-1.16231113	2.32131911
C	1.17700007	-2.33432898	2.96867641
C	2.36487020	2.99869968	0.90159381
C	3.20111726	2.54066087	-0.13019437
C	0.00000000	3.03593919	2.52343477
C	0.00000000	3.66203557	1.31405773
C	1.17574828	3.64498622	0.48507065
C	-1.17700007	2.33432898	2.96867641
C	-2.36421698	2.30063981	2.18236198
C	-3.17626699	1.16231113	2.32131911
C	-0.72806178	-1.21416679	3.68381545
C	-1.45146551	0.00000000	3.66500779
C	-0.72806178	1.21416679	3.68381545

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TABLE S10 – *Continued from previous page*

C	-2.70088263	0.00000000	3.00745292
C	0.72578511	3.58745012	-0.84764418
C	1.45685398	2.93650592	-1.85466501
C	2.76069866	2.51950258	-1.48701946
C	3.39235376	1.40335178	-2.13414214
C	2.69630693	0.72084514	-3.10180975
C	-0.73069474	2.23611346	-2.90459425
C	0.73069474	2.23611346	-2.90459425
C	1.39765375	1.16750212	-3.52545401
C	-1.39765375	1.16750212	-3.52545401
C	-0.68206600	0.00000000	-3.92803194
C	0.68206600	0.00000000	-3.92803194
C	-0.72578511	3.58745012	-0.84764418
C	-2.76069866	2.51950258	-1.48701946
C	-1.45685398	2.93650592	-1.85466501
C	-2.36487020	2.99869968	0.90159381
C	-1.17574828	3.64498622	0.48507065
C	-3.20111726	2.54066087	-0.13019437
C	-4.18634767	0.69534461	-1.16981510
C	-3.39235376	1.40335178	-2.13414214
C	-2.69630693	0.72084514	-3.10180975
C	-4.18634767	-0.69534461	-1.16981510
C	-4.03460849	-0.71843639	1.25641860
C	-4.03460849	0.71843639	1.25641860
C	-4.08159485	1.40959227	0.06512165
C	-4.08159485	-1.40959227	0.06512165
C	-1.17700007	-2.33432898	2.96867641
C	-2.36421698	-2.30063981	2.18236198
C	-3.17626699	-1.16231113	2.32131911
C	-1.17574828	-3.64498622	0.48507065
C	0.00000000	-3.66203557	1.31405773
C	0.00000000	-3.03593919	2.52343477
C	-3.20111726	-2.54066087	-0.13019437
C	-2.36487020	-2.99869968	0.90159381
C	-2.69630693	-0.72084514	-3.10180975
C	-3.39235376	-1.40335178	-2.13414214
C	-2.76069866	-2.51950258	-1.48701946
C	-1.45685398	-2.93650592	-1.85466501
C	-0.72578511	-3.58745012	-0.84764418

TABLE S11: Optimized Cartesian coordinates for the  $C_{84}(D_{2d})$  fullerene at the SCAN0/6-31G(d) level of theory.

C	-2.34681285	0.72969839	3.36820633
C	-1.17292014	1.40733292	3.76625677
C	-3.94989250	-0.68362702	1.47719467
C	-3.94989250	0.68362702	1.47719467
C	-3.15431927	1.41173840	2.44168945
C	-3.95864732	-1.38571161	0.24172869
C	-3.95864732	1.38571161	0.24172869
C	-3.84011201	0.72570106	-0.99537632
C	-3.84011201	-0.72570106	-0.99537632
C	-2.57708540	-0.72535308	-3.11475767
C	-3.17209194	-1.44925528	-2.06935099
C	-2.61053299	-2.72556699	-1.82001821
C	-2.72556699	2.61053299	1.82001821
C	-1.44925528	3.17209194	2.06935099
C	-0.72535308	2.57708540	3.11475767
C	0.72535308	2.57708540	3.11475767

*Continued on next page*

TABLE S11 – *Continued from previous page*

C	1.44925528	3.17209194	2.06935099
C	2.72556699	2.61053299	1.82001821
C	-3.28571990	2.63078259	0.49659764
C	-0.72570106	3.84011201	0.99537632
C	0.72570106	3.84011201	0.99537632
C	-2.63078259	3.28571990	-0.49659764
C	-1.38571161	3.95864732	-0.24172869
C	-2.61053299	2.72556699	-1.82001821
C	-2.57708540	0.72535308	-3.11475767
C	-3.17209194	1.44925528	-2.06935099
C	1.17292014	1.40733292	3.76625677
C	3.15431927	1.41173840	2.44168945
C	2.34681285	0.72969839	3.36820633
C	3.94989250	0.68362702	1.47719467
C	3.94989250	-0.68362702	1.47719467
C	2.63078259	3.28571990	-0.49659764
C	3.28571990	2.63078259	0.49659764
C	3.95864732	1.38571161	0.24172869
C	1.38571161	3.95864732	-0.24172869
C	-0.00000000	0.68162807	4.17798961
C	3.15431927	-1.41173840	2.44168945
C	2.34681285	-0.72969839	3.36820633
C	1.17292014	-1.40733292	3.76625677
C	-0.00000000	-0.68162807	4.17798961
C	3.28571990	-2.63078259	0.49659764
C	2.72556699	-2.61053299	1.82001821
C	1.44925528	-3.17209194	2.06935099
C	0.72535308	-2.57708540	3.11475767
C	2.63078259	-3.28571990	-0.49659764
C	3.95864732	-1.38571161	0.24172869
C	3.84011201	-0.72570106	-0.99537632
C	3.84011201	0.72570106	-0.99537632
C	-3.15431927	-1.41173840	2.44168945
C	-2.34681285	-0.72969839	3.36820633
C	-1.17292014	-1.40733292	3.76625677
C	-0.72535308	-2.57708540	3.11475767
C	-1.44925528	-3.17209194	2.06935099
C	-2.72556699	-2.61053299	1.82001821
C	-2.63078259	-3.28571990	-0.49659764
C	-3.28571990	-2.63078259	0.49659764
C	1.38571161	-3.95864732	-0.24172869
C	0.72570106	-3.84011201	0.99537632
C	-0.72570106	-3.84011201	0.99537632
C	-1.38571161	-3.95864732	-0.24172869
C	1.41173840	-3.15431927	-2.44168945
C	0.68362702	-3.94989250	-1.47719467
C	-0.68362702	-3.94989250	-1.47719467
C	1.40733292	-1.17292014	-3.76625677
C	0.72969839	-2.34681285	-3.36820633
C	2.61053299	2.72556699	-1.82001821
C	3.17209194	1.44925528	-2.06935099
C	2.57708540	0.72535308	-3.11475767
C	2.57708540	-0.72535308	-3.11475767
C	3.17209194	-1.44925528	-2.06935099
C	2.61053299	-2.72556699	-1.82001821
C	-0.68362702	3.94989250	-1.47719467
C	0.68362702	3.94989250	-1.47719467
C	0.72969839	2.34681285	-3.36820633
C	1.41173840	3.15431927	-2.44168945
C	1.40733292	1.17292014	-3.76625677
C	-0.68162807	-0.00000000	-4.17798961
C	-1.40733292	1.17292014	-3.76625677
C	-0.72969839	2.34681285	-3.36820633

*Continued on next page*

TABLE S11 – *Continued from previous page*

C	-1.41173840	3.15431927	-2.44168945
C	0.68162807	-0.00000000	-4.17798961
C	-1.41173840	-3.15431927	-2.44168945
C	-0.72969839	-2.34681285	-3.36820633
C	-1.40733292	-1.17292014	-3.76625677

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